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Using Instrumented Three-Mass Vehicle for Identifying Bridge Damping Ratio

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The vehicle scanning method has been applied to identify the modal parameters of a bridge since 2004. Among these modal parameters, the bridge frequency has attracted lots of attention in comparison with the bridge damping ratio in structural health monitoring. As the information of bridge damping ratio can be used in conjunction with the information of bridge frequencies under some situations for bridge health monitoring, while the identification approaches to the bridge damping ratio remain limited, this study focuses on the approach to the identification of bridge damping ratio. As an example, Figure 1 shows an instrumented three-mass vehicle with six sensors equally spaced by d_0. The projected locations of sensors on the bridge are the scanning point (SPs); Δy_i denotes the *i*th vertical distance between the sensor and the SP. The theoretical derivation of the amplitude ratio leads to the following formula for identifying the bridge damping ratio ξ_n:

$$\xi_n = \frac{\ln\left[\dfrac{A\left[Y_{i+M}\left(t+M\Delta t_1\right)\right]}{A\left[Y_i\left(t\right)\right]}\right]}{-\omega_{bn} M \Delta t_1} \tag{1}$$

where $A\left[Y_i\left(t\right)\right]$ denotes the *i*th amplitude of an analytical signal; $M\Delta t_1$ denotes the time interval behind the *i*th sensor; ω_{bn} is the bridge frequency. Based on Eq. (1), further investigation can be conducted to shown the liability of the proposed approach by considering various practical factors.

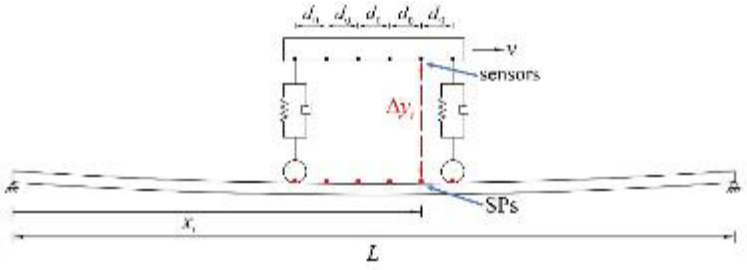

Figure 1.

Keywords: vehicle scanning method, bridge damping ratio, three-mass vehicle

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A phase field model to simulate concrete fracture behaviour under elevated temperatures

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Phase field method has become a popular approach to model fracture behaviour of different materials. Its attraction stems from the ability to simulate crack initiation, propagation, and branching without the need for ad-hoc criteria. In addition, cracks are tracked automatically by the propagation of a smooth crack field on a fixed mesh.

In the present study, a phase field method is applied to simulate concrete fracture behaviour under elevated temperatures at the laboratory sample scale. This necessitates explicit description of the bi-phasic aggregate-mortar meso-structure of concrete. Moreover, the interfacial transition zone is modelled simply as a weak layer of elements around the aggregates. The governing problem is essentially a coupled Multiphysics problem for three fields, the displacement, the phase field, and the temperature field. A globally iterative staggered approach is developed to solve the governing equations for the three fields. The method is demonstrated in 2D numerical examples where thermally pre-treated concrete sample is subjected to uniaxial tension. An example is shown in Figure 1, where a concrete sample is slowly heated up to about 200 °C.

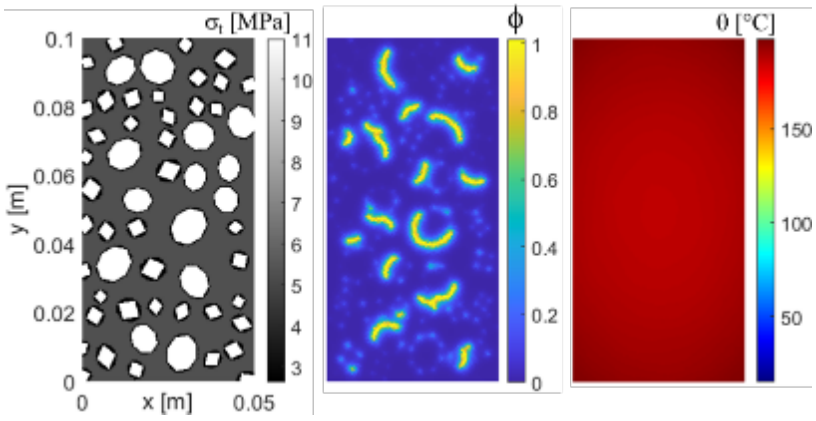

Figure 1.

The concrete mesostructure is shown on the left in terms of the tensile strength distribution of the phases. The element type used here is linear 3-node triangle. The phase field variable representing the fractured state of the material at the end of heating is shown in the middle. It can be noticed that most of the fracturing occurs at the weak transition zone around the aggregates where the tensile strength is 50 % of that of the mortar.

Keywords: Phase field method, concrete fracture, meso-structure, thermal weakening, staggered approach

Tensor-represented Model for the MPH method and its Extensions

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The tensor-represented model for the Moving Particle Hydrodynamics (MPH) method [1-3] is developed and tested with some constitutive equations. For applying various constitutive equations, the tensors, e.g., stress, strain and strain rate tensors, are to be directly expressed in the discretised formulations. However, the viscosity models in the particle methods often do not include such tensors explicitly. In this study, the discretised approximation for the velocity gradient and the stress divergence are derived

$$(\nabla \mathbf{u})_i \approx \left(\sum_j \mathbf{u}_{ij} \otimes \mathbf{r}_{ij} \frac{w_{ij}'}{|\mathbf{r}_{ij}|} \right) \mathbf{A}_i^{-1}, \qquad \mathbf{A}_i = \sum_j \mathbf{r}_{ij} \otimes \mathbf{r}_{ij} \frac{w_{ij}'}{|\mathbf{r}_{ij}|}$$

and

$$\nabla \cdot \mathbf{T} \approx \sum_j (\mathbf{T}_i \mathbf{A}_i^{-1} \mathbf{r}_{ij} + \mathbf{T}_j \mathbf{A}_j^{-1} \mathbf{r}_{ij}) \frac{w_{ij}'}{|\mathbf{r}_{ij}|}$$

respectively. This derivation is based on the dissipative function with respect to the viscosity term. With using the tensor-based model, the test calculations are conducted with some constitutive laws represented by these tensors, e.g., anisotropy and viscoelasticity.

Keywords: Particle Methods, SPH, MPS, MPH, Tensor-representation, Constitutive laws

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Phase-field modeling of creep crack propagation using isogeometric analysis

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The significant impact of creep fracture on the structural integrity and service life of materials under high-temperature conditions is a major concern in engineering and material science. Over extended periods, materials subjected to sustained stress and elevated temperatures experience time-dependent deformation known as creep, which can lead to the initiation and propagation of cracks. Understanding the mechanisms and behavior of creep crack growth is essential for predicting the lifespan of these components and ensuring their safe operation. This work introduces a novel multi-patch isogeometric creep phase-field model, which is designed to predict creep crack propagation in elastoplastic materials. The main contributions of this work include the following: (1) A phase-field framework is developed to effectively simulate creep fracture in elastoplastic metallic materials, which incorporates an asymptotic creep degradation function shown in Figure 1 to accurately simulate the accumulation of material damage due to creep. It successfully captures the characteristic behavior of creep crack propagation, marked by a slow progression in the initial stages and then a rapid acceleration as the damage advances. (2) Building on the creep phase-field theory, a multi-patch isogeometric analysis framework based on LR NURBS is further developed to address creep crack simulation. By partitioning the computational domain into multiple patches, this framework achieves multi-patch modeling and coupled solving for geometrically complex models, enhancing the entire creep phase-field framework's ability to accurately capture creep behavior in complex structural components. In addition, LR NURBS enable local mesh refinement near cracks to reduce computational time. To avoid computational errors due to discontinuities in variables at coupling boundaries, the overall governing equations are derived based on Nitsche's method. The accuracy of this approach is validated through comparisons with experimental and numerical results.

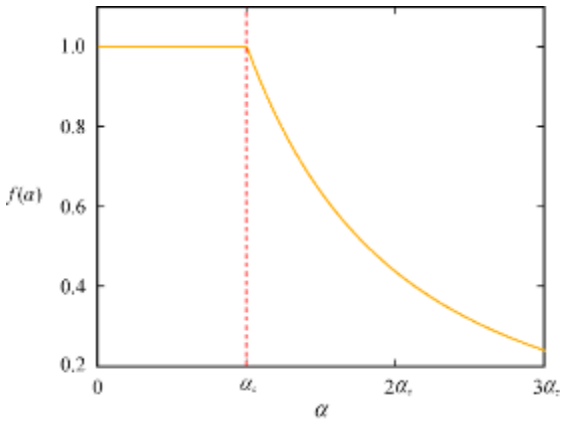

Figure 1.

Keywords: Creep crack growth, Isogeometric phase-field model, Asymptotic degradation function, Multi-patch modelling, Nitsche's method, LR NURBS

A Topological Metamaterial for Polarization-dependent Elastic Wave Demultiplexing

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Abstract

The manipulation of elastic waves through topological metamaterials has garnered significant research attention due to its promising industrial applications. However, the complexity introduced by intense wave polarization poses challenges, particularly in the realm of mono-polarized waves, thereby hindering the advancement of topological elastic metamaterials. In response to this limitation, we introduce a novel frame structure configured as a hexagonal lattice, which exhibits independent control over in-plane and out-of-plane polarized bandgaps through the utilization of accidental Dirac cones. Our in-depth investigations reveal that these accidental Dirac cones stratify the parametric space into four distinct regions, each characterized by unique valley Chern numbers. By integrating unit cells from these diverse regions, we achieve polarization-dependent topological protected interface modes, enabling scenarios where only in-plane or out-of-plane modes are supported, as well as those accommodating both. Leveraging this unique property, our study demonstrates polarization-dependent waveguiding and wave separation. To validate our theoretical findings, we fabricated one of the designed models using 3D printing and conducted experimental verification of polarization-dependent waveguiding. Further analysis confirms the independence of in-plane and out-of-plane waveguiding, even in the presence of intersections in their pathways. This discovery paves the way for the design of innovative elastic devices capable of carrying and encrypting information, as exemplified by several prototypes presented in this paper. Our work not only broadens the application scope of topological elastic metamaterials from mono-polarized to dual-polarized waves but also holds immense potential for the exploration and development of more advanced elastic devices for wave manipulation.

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Learning Non-Ideal Single Vortex Flows Using the Differentiable Vortex **Particle Method**

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Vortex flows represent a fundamental class of ubiquitous fluid phenomena, manifesting in various forms such as turbulent structures, swirling water patterns, turbomachinery flows, and atmospheric systems like hurricanes. Despite their prevalence and significance, a comprehensive understanding of the underlying vortex dynamics remains an open challenge in contemporary scientific research.

Machine learning methods have recently been increasingly introduced to fluid mechanics, achieving remarkable success. Among these, a deep learning-enhanced vortex particle method, differentiable vortex particle method, has been proposed. This method leverages the differentiable characteristics of neural networks to learn and predict vortex flows. However, the initial version of differentiable vortex particle method is limited in its applicability, as it only addresses highly idealized vortex flow scenarios, restricting its relevance to general vortex flows. This approach is grounded in the vorticity transport equation:

$$\frac{D\boldsymbol{\omega}}{Dt} = \frac{\partial \boldsymbol{\omega}}{\partial t} + \boldsymbol{u}\cdot\nabla\boldsymbol{\omega} = \boldsymbol{\omega}\cdot\nabla\boldsymbol{u} + \nu\nabla^2\boldsymbol{\omega} + \nabla\times\boldsymbol{b}, \tag{1}$$

where $\boldsymbol{\omega}$ represents the vorticity vector, t signifies time, $\boldsymbol{u}$ denotes the velocity, $\boldsymbol{b}$ corresponds to the non-conservative body force, and ν refers to the kinematic viscosity. The initial version of the differentiable vortex particle method is confined to $D\boldsymbol{\omega}/Dt = 0$, which assumes two-dimensional flow, inviscid conditions, and the absence of non-conservative body forces. Furthermore, part of the training dataset for the original differentiable vortex particle method was generated by the traditional vortex particle method, which are often considered insufficiently accurate to serve as ground truth data from the perspective of fluid mechanics researchers.

In this work, we extend the applicability of the differentiable vortex particle method to more general, non-ideal conditions and introduce viscous single vortex flow, specifically the Lamb-Oseen vortex, as a benchmark. The Lamb-Oseen vortex, with its exact solution derived from the Navier-Stokes equations, serves as ground truth data for training. We rigorously evaluate the performance of the differentiable vortex particle method on the Lamb-Oseen vortex across different Reynolds numbers, demonstrating superior accuracy compared to convolutional neural network-based and physics-informed neural network-based methods, shown in Figure 1.

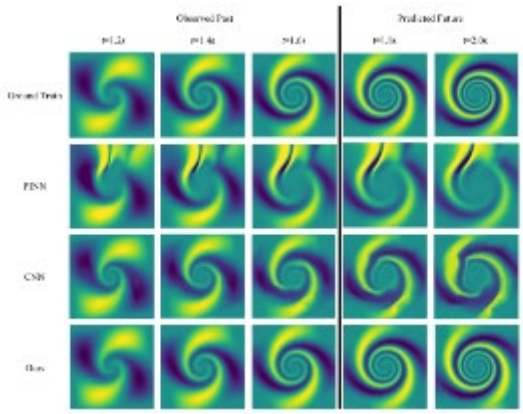

Figure 1.

Keywords: vortex dynamics, vortex particle method, deep learning, Lamb-Oseen vortex

Electrodeposition Coating Simulation Based on Lab Experiments and Manufacturing Line Monitoring for Automotive Design

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Electrodeposition (ED) coating simulation is an indispensable technology for recent automotive design. In the cationic ED coating, the coating objects (cathodes) are dipped in a paint pool with electrodes (anodes), and direct current is applied from the anodes to the cathodes (Fig. 1). To ensure the corrosion-resistant performance of automobiles, a minimum coating film must be applied to the entire undercarriage area during the ED process. In particular, the position and size of ED holes (small holes on the undercarriage to pass electric current from the outside to the inside area) are important factors in determining the inner film thickness; thus, automotive ED simulations must be highly accurate.

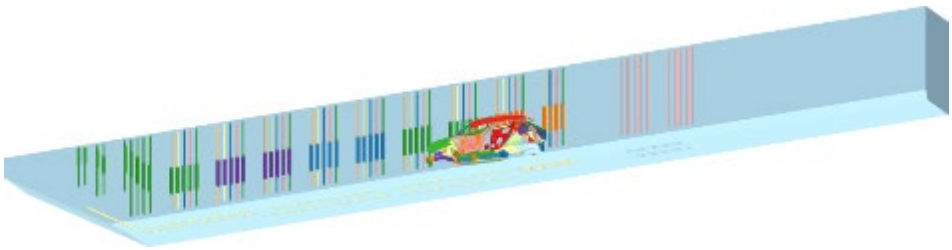

Figure 1.

Our group has been conducting lab experiments and manufacturing line monitoring for ED coating with our original devices. Besides, an ED coating simulator, "EDESFEM" [1], has been developed for large-scale actual ED line simulations. Adopting the next-gen finite element method using 4-node tetrahedral meshes called ES-FEM-T4 [2], the simulator can efficiently analyze the complex geometry of a carbody with many ED holes. An accurate numerical ED model can be constructed through the lab experiments, full-scale ED simulations can be done with the simulator, and the analysis results can be validated with the line monitoring results. Our ED modeling / simulation / validation suite enables us to pioneer the automotive evidence-based design that balances between corrosion resistance and strength/stiffness preservation.

Keywords: Automotive electrodeposition (ED), ED holes, Film thickness, Complex geometry, Tetrahedral mesh, Smoothed finite element method.

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Robust Framework for Long-Duration Dynamic Analysis of Linear and Nonlinear Systems: The AT-PINN-HC Approach

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Structural dynamic analysis plays a crucial role in the fields of civil, mechanical, aerospace, and vehicle engineering. The dynamic behaviour of structures can be investigated by solving the following equation:

$$m\frac{\partial^2 w(x,t)}{\partial t^2} + c\frac{\partial w(x,t)}{\partial t} + \mathfrak{D}[w(\boldsymbol{x},t)] = f(\boldsymbol{x},t)$$

where $w(\boldsymbol{x},t)$ is the vibration displacement; m is the mass property; c denotes the damping coefficient; $\mathfrak{D}[w(\boldsymbol{x},t)]$ is the elastic restoring force that can be either linear or nonlinear; and $f(\boldsymbol{x},t)$ is the external excitation. The physics-informed neural network (PINN) [1], an innovative deep learning technique, offers a new avenue to tackling the governing equations of physical problems, making it a promising option for dynamic analysis. However, existing PINNs encounter considerable inaccuracies when conducting 'long-duration' dynamic predictions. To address this issue, we have developed an advanced time-marching physics-informed neural network that incorporates effective hard-constraint strategies (AT-PINN-HC) [2]. Numerical experiments have shown that the present approach significantly enhances both accuracy and efficiency compared to traditional PINNs. It is capable of providing accurate solutions for long-duration dynamic analyses in both linear and nonlinear systems, such as a panel subjected to multi-physics loads and a nonlinear arch structure exerted by in-plane forces.

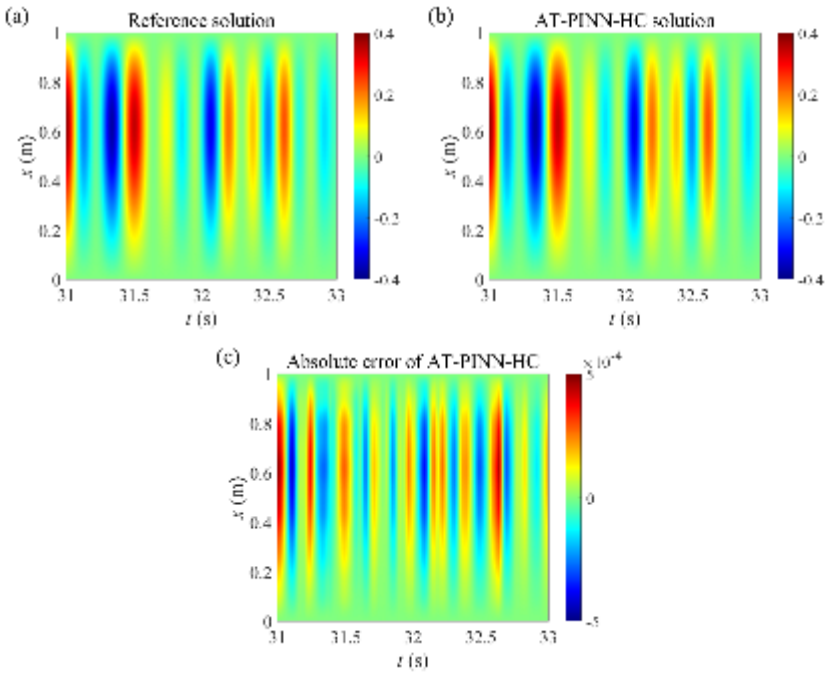

Figure 1.

Keywords: Physics-informed neural network; dynamic analysis; nonlinear vibration; deep learning; hard constraints.

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Planar Fault Transformation and Unfaulting of interstitial Dislocation Loops in Irradiated Intermetallic Alloys

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The present study has systematically investigated unfaulting mechanism of single-layer interstitial dislocation Loops (IDLs) in irradiated FCC-(Ni,Al), $L1_2$-(Ni_3Al,Ni_3Fe) to extend the existing unfaulting theory from pristine FCC lattice to the $L1_2$ ordered lattice, employing atomistic simulations combining continuum theory. Two types of variants for the IDLs have been determined with different superlattice planar faults enclosed in the Frank loop. The unfaulting routes of IDLs by Shockley partial loops have been unveiled through examining the energy barriers of superlattice planar fault transformation. The symmetry breaking occurring in the unfaulting processes were further elucidated and summarized. A continuum model has been formulated to enable quantitative theoretical analysis of the energetics of IDLs and prediction of the unfaulting threshold. These findings clarify the effects of complex faults and symmetry breaking on unfaulting behaviours of IDLs in irradiated $L1_2$-(Ni_3Al, Ni_3Fe), and could be transferable to other $L1_2$ systems, and more generally, other chemically complex intermetallic alloys [1-5].

Keywords: Dislocation loop, superlattice planar fault, irradiation, intermetallic alloys

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Studying debris and flood flow in complex topographies and mitigating structures using the VOF method

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Extreme floods can trigger debris flows, where water mixes with soil, rocks, and vegetation to form fast-moving, destructive torrents. These flows clog drainage, destabilize roads, and increase risks to property and the environment, necessitating resilient infrastructure. Addressing these challenges requires the development of resilient infrastructures. The outcomes of this study aimed to strengthen the Hobart region's structural capabilities, reducing the risk of future flooding and debris flow disasters while protecting the local community and environment.

Flow simulations were conducted using FLOW-3D with the volume of fluid (VOF) approach [1]. The governing equations included continuity and momentum equations, with an implicit GMRES solver for pressure-velocity coupling. Both laminar and LES turbulent conditions were analyzed for Newtonian and viscoplastic fluids, considering the Reynolds and Bingham numbers.

The study focused on the Hobart Rivulet, using a dam-break scenario with boulders and trees to simulate debris dynamics. Various mitigation structures, including arranged barriers, porous and gabion structures, non-linear weirs, debris breakers, energy dissipators, and steep stepped designs were evaluated using recent available geotechnical data and studies [2,3]. The numerical method was validated against previous studies [4,5,6,7,8] and results demonstrated its accuracy. Figure 1 presents velocity contours for a porous barrier with 0.5 porosity against a dam break study at time 0 (s), 1(s), and 8(s) from the left to right.

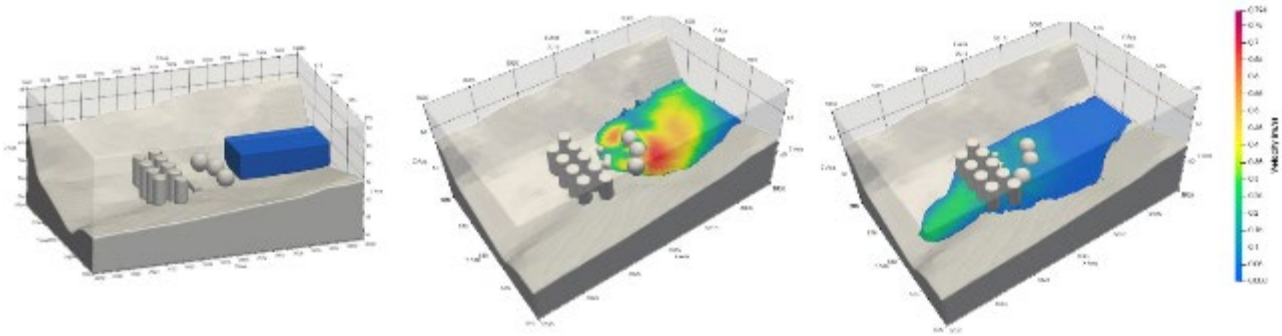

Figure 1.

Keywords: Flood and debris flows, VOF method, viscoplastic fluid, porous structures

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Numerical Analysis of Lamella Clarifiers in Sugar Mills

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This paper uses numerical simulations to examine the effect of Lamella clarifier plate spacing on the operational dynamics of these clarifier units, specifically within the framework of sugar mill clarification processes, aiming to improve their efficiency and performance.

ANSYS Fluent 2024 R1 was used for the two-dimensional numerical simulations and the results were analysed in terms of cross-sectional analysis, particle entrainment, fluid velocities, pressure distributions, and settling efficiency to understand the behaviour of the multi-phase fluid mixture inside the device. The numerical simulations were carried out for 9 plate spacings with dimensions from 50 mm to 250 mm in increments of 25 mm in Lamella clarifiers, with each clarifier has three plates inside. For each plate spacing, numerical simulations were carried out at three inlet velocities of 0.03 m/s, 0.06 m/s, and 0.08 m/s.

The obtained particle velocity and sugar juice contours at the inlet velocity of 0.06 m/s are presented in Figure 1, as an example.

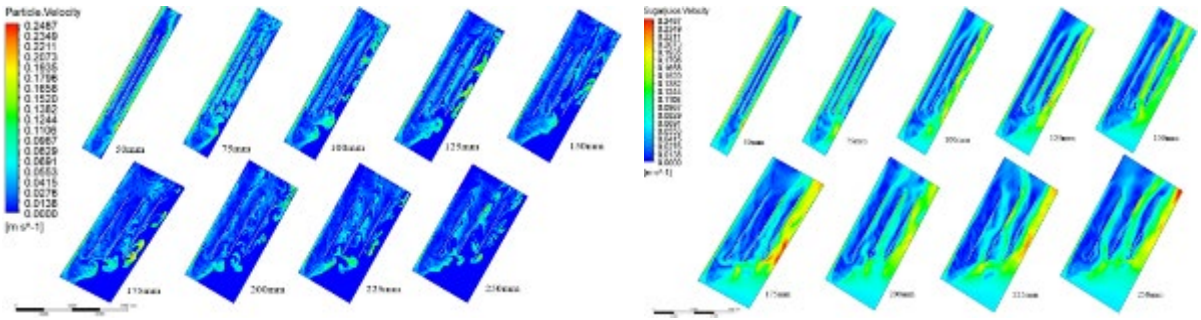

Figure 1. The particle velocity and sugar juice contours at the inlet velocity of 0.06 m/s for the 9 plate spacings.

The results show that as the plate spacings were increased, the settling efficiency was improved, due to the reduced hydraulic resistance and better flow distribution. Nevertheless, beyond a specific plate spacing, the efficiency began to decline. The reason is that once the channel widths exceeded a critical size, it enabled the opportunity for particles to bypass the plates without settling. This indicates that the relationship between the settling efficiency and plate spacing is non-linear and is significantly affected by the interactions of particles, fluid flow, turbulence and particle settling dynamics.

The numerical results showed the highest average calculated settling efficiency was achieved at 175mm plate spacing, indicating this was the optimum spacing to maximise settling efficiency. It was also found that an appropriate selection of the inlet velocity is essential when aiming to achieve the desired separation performance.

Keywords: Lamella clarifier, plate spacing, sugar mill, settling efficiency, numerical simulation

Optimal Design of Bionic Centrifugal Fans in Use of Taguchi Method and Analysis of Variance

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This study aims at improving the performance of centrifugal fans employed in totally-enclosed-fan-cooled (TEFC) motors by introducing leading-edge serrations, mimicking the leading-edge comb on owl wings, and suction-side ridges, imitating the soft down coat on the owl wing surface. A numerical wind tunnel is established according to the experimental standards of the Air Movement and Control Association (AMCA) 210. The influences and optimal values of four geometric dimensions related to the bionic structures are studied in use of Taguchi method and analysis of variance (ANOVA) at low, medium, and high flow rates.

The investigation shows that among the four geometric dimensions, the suction-side ridge height has the most significant impact and that most bionic fans possess higher total pressure and total pressure efficiency. A detailed examination on the flow fields indicates that the leading-edge serrations break down large vortices at the leading edge into smaller ones, thereby reducing their impact on the downstream. On the other hand, the suction-side ridges guide fluid flow toward the trailing edge and induce streamwise vortices on the suction side, which suppress flow separation and improve the fluid flow in the fan blade region. Consequently, the bionic fan effectively reduces the overall turbulent kinetic energy and produces a stronger, more uniform flow field behind the fan, thereby enhancing the fan's aerodynamic performance.

Keywords: Bionic blades, Leading-edge serrations, Suction-side ridges, Taguchi method, Analysis of variance (ANOVA)

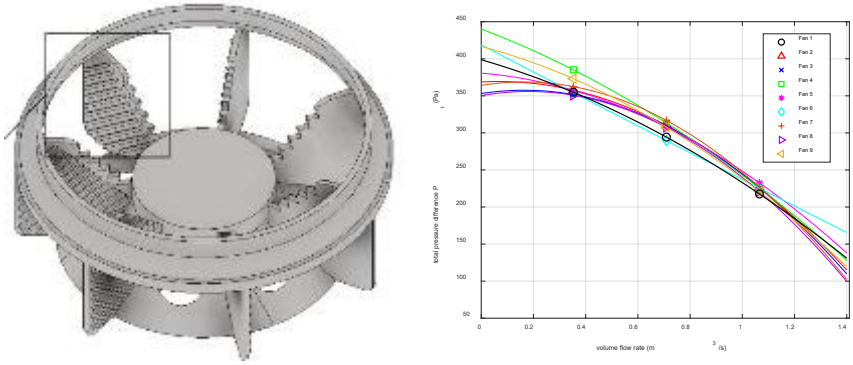

Figure 1.

Keywords: Bionic blade optimization, Leading-edge serrations, Suction-side ridges, Taguchi method, Analysis of variance

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Topology optimization of thermomechanical problems considering eigenvalue effects

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In electric-powered mobility, designing efficient structures that enhance heat dissipation and suppress battery vibrations is a critical challenge. While previous studies have applied topology optimization based on transient analysis [1], modeling thermal and vibration response times using thermal eigenvalues [2] and incorporating eigenvalue analysis with thermal stress considerations [3] can streamline the process and significantly reduce computational costs. This study proposes a level-set topology optimization method [4] that optimizes thermal and vibration performance under transient conditions by leveraging thermal and vibration eigenvalues. A weighted sum method is employed to handle multiple objectives. However, focusing solely on transient response may lead to localized heat concentration. To address this issue, steady-state heat transfer results are incorporated as constraints. Sensitivity analysis is performed using the adjoint variable method, demonstrating that eigenvalue calculations are computationally more efficient than conventional time-stepped transient analysis. Numerical examples confirm improvements in response speed and illustrate the effects of weighting and constraints, highlighting the effectiveness of this approach for designing thermomechanical structures.

Keywords: Optimal design, Topology optimization, Level-set method, Eigenvalue problem, Thermomechanical problem

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Bio-Inspired Flight for Martian Exploration

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Recently, bio-inspired flight mechanisms (such as flapping wings) have been identified as a candidate for Martian aircraft design due to their high lift and efficiency in low Reynolds number environments [1]. The low atmospheric density on Mars leads to low Reynolds numbers and moderate-high Mach number (due to the operational speeds required to achieve sufficient lift). While natural flyers fit the low Reynolds number criteria, they also travel at low speeds corresponding to an incompressible flow regime. This research aims to identify the effects of compressibility on the aerodynamic force and acoustic profiles of flapping wing vehicles and their corresponding unsteady flow structures to inform future Martian UAV design.

This study is conducted numerically utilising an in-house FSI solver consisting of three distinct components: the finite difference method for laminar aerodynamics, the finite element method for the structure dynamics and the feedback immersed boundary method for FSI coupling. Details of the solver and validation studies applied to bio-inspired flapping wings and highly compressible flows can be found in our previous works [2,3]. This study considers a dual wing bumblebee-inspired configuration with rigid flapping wings in the hovering flight condition. The wings undergo symmetrical flapping motion in the horizontal stroke plane and pitching motion occurs about the wing's leading edges. The stroke and pitch angle amplitudes are fixed at $A_\phi = 100^o$ and $\alpha = 45^o$. A Reynolds number of $Re = 200$ is considered in this study and the average leading edge Mach number is incrementally increased over the range $Ma = 0.4 - 1.4$.

The average lift coefficient was observed to decrease with increasing Mach number and the temporal force behaviour was repeated periodically (inclusive of forward and backstroke) rather than every half period as has been observed for single wings [2]. This was due to the pressure distribution over the body and its asymmetry through the vertical plane. The decrease in lift coefficient was attributed to the unsteady vortex decay with increasing Mach number. The presence of a shock wave resulted in an increase of leading-edge vortex average pressure and a reduction in its size. The acoustic profile was observed to very significantly with Mach number variations in both amplitude and directionality. In particular, the secondary fundamental frequency was observed to increase from a 4-pole to 6-pole sound source with increasing Mach number.

Keywords: Bio-inspired, rarefied flow, compressibility, computational fluid mechanics, immersed boundary method

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Super-simulations of Floating Offshore Wind Turbine on Fugaku

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ABSTRACT

A floating offshore wind farm (FOWF) consisting of tens of large-scale floating offshore wind turbines (FOWT) is expected to play a key role of achieving a Carbon Neutrality society by 2050. To promote such FOWFs in an East Asia region including Japan, we need to realize long-term safe and robust operations under severe weather and ocean conditions caused due to typhoons as well as significant cost reduction. To do so, we need to drastically increase accuracy and efficiency of design and analysis tools for FOWF / FOWT. For those purposes, we have been developing multiscale and multiphysics integrated simulations for FOWF / FOWT on an Exascale supercomputer Fugaku. We briefly call them Super-simulations. The simulations consist of the following four software components.

(a) LBM (Lattice Boltzmann Method)-based large-scale LES (Large Eddy Simulation) simulator of a whole wind farm, named FFX, in which an actuator line model is employed,

(b) FEM-based large-scale LES simulator of one to a few FOWTs to evaluate an effect of wake into power generation as well as flow loading, named FFB, in which a high-fidelity rotating rotor model is employed,

(c) Flow-induced vibration and dynamic responses of FOWT using FEM-based parallel structure solver named ADVENTURE_Solid and a fatigue analysis tool named ADVENTURE_Fatigue, and

(d) A parallel coupling tool to deal with Fluid-Structure Interaction (FSI), named REVOCAP_Coupler.

In this presentation, we describe Fugaku-based super-simulations of an NREL 5MW FOWT with both WT and Floator, focusing on its fatigue damage and ultimate strength under various air flow and floating conditions.

A Hybrid CFD and Machine Learning Approach for Modeling Aerosol Dispersion in Indoor Environments

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Indoor aerosol pollution from cough droplets poses significant risks to both air quality and public health. The dispersion of these droplets is influenced by factors such as airflow, temperature, and humidity. This makes accurate prediction computationally expensive. This study proposes a hybrid approach that combines Computational Fluid Dynamics and Machine Learning to model aerosol dispersion efficiently in indoor environments. CFD simulations provide data on airflow and droplet movement. This data is used to construct a high-fidelity Gaussian distribution model for pollutant spread. The Adaptive Polynomial Feature Random Forest algorithm is applied to predict key parameters and enhance computational efficiency. Compared to traditional CFD simulations, the hybrid approach reduces computational time by 76.4%. It also maintains high accuracy with Mean Absolute Error below 0.07 and Mean Squared Error below 0.014. This method offers an effective solution for predicting indoor aerosol dispersion and provides insights for air quality management and pollutant control in enclosed spaces.

Keywords: Cough droplets, droplets distribution, Gaussian Models, Machine Learning

A Simplified Model Established by Morphometric Parameters for Urban Ventilation Potential

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Ventilation potential and urban morphology are interconnected factors that significantly influence the air quality, thermal comfort, and energy efficiency in cities. Urban morphology, including the arrangement and density of buildings, plays a crucial role in determining the effectiveness of urban ventilation. Urban design strategies that consider building form, density, and street orientation can optimize the ventilation potential. For instance, configurations with lower cooling loads and higher ventilation potentials have been identified, suggesting that thoughtful urban planning can improve the energy performance and air quality. In view of the fact that the current urban wind corridor assessment mainly takes the roughness height or sky view factor (SVF) as the basic index, it is difficult to reflect the actual ventilation status of the plot near the surface. Therefore, in this study, the urban ventilation potential (V_P) is redefined and expressed as the flow decay condition in the urban atmospheric boundary layer, which is defined as follows:

$$V_P = \frac{q_i}{q_{inlet}} \tag{1}$$

where q_{inlet} denotes the incoming flow and q_i denotes the flow after blowing through a specific urban region. This study analyses the ventilation potential of the Taipei area in three steps. First, a Weather Research and Forecasting Model (WRF) simulation is conducted to obtain the prevailing summer wind speed and direction for 47 zones of 2 km × 2 km, as shown in Figure 1(a). These data are then used as the inflow condition for the CFD simulation, the flow field in the area is simulated, and the horizontal (x-y plane) wind field data distributed uniformly as a 10m grid are taken out, as shown in Figure 1(b).

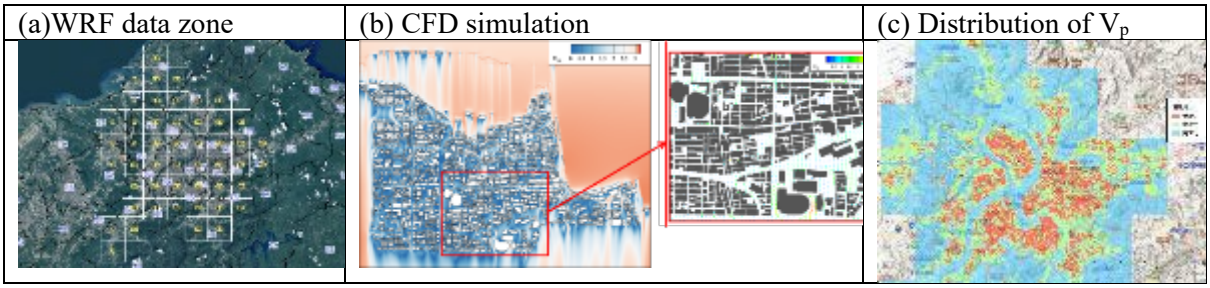

Figure 1.

The objective of this study is to develop a simplified model that correlates five parameters of urban morphometrics: average building height (H_{ave}), plan area index (λ_p), frontal area index (λ_f), standard deviation of building height (σ_H), and maximum building height (H_{max}), with reference to the logarithmic law determination method of Kanda [1]. A simplified ventilation potential prediction model is developed utilizing two methodologies: a general regression model and a neural network.

Keywords: urban boundary layer, morphometric parameters, ventilation potential

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Bio-Inspired Spider Web Helmet for Cyclist Head Injury Mitigation: A Study on Mechanical Protective Performance

Abstract: To mitigate the risk of head injuries for riders during collisions and further enhance the protective performance of helmets, this study integrated a spider web structure into the helmet liner and compared its protective performance with that of traditional expanded polystyrene (EPS) foam liners. Initially, a finite element coupling model of the helmet and head was developed, and a simulated drop test was conducted according to the ECE R22.05 standards. The head's center-of-mass acceleration was used as a primary metric to validate the consistency between the simulation and actual experimental results. Subsequently, two innovative liner structures were designed based on the unique mechanical properties of the spider web structure. Finally, the new liner structure was applied in helmet collision scenarios to obtain the kinematics and biomechanical parameters of the human head model. The risks of skull fracture and craniocerebral injury were used as key criteria to comprehensively evaluate the protective performance of the new helmet. The results indicate that, compared to helmets with either EPS foam liners or spider web structure liners alone, helmets with EPS + spider web structure liners exhibit significantly improved protective performance. In flat anvil collision tests, the head's center-of-mass acceleration was reduced by 6g, the HIC15 value by 1352, and the probability of skull fracture decreased by 14%, although the probability of mild brain injury increased slightly by 2%. In ball anvil collision tests, the EPS + spider web structure liner reduced the head's center-of-mass acceleration by 44g, the HIC15 value by 1176, the probability of skull fracture by 9%, and the probability of mild brain injury by 5%. The novel liner structure effectively absorbs and dissipates collision energy, significantly mitigating the impact on the rider's head. The research findings not only provide a scientific basis for understanding the biomechanical mechanisms of head injuries but also open new avenues for the development of related safety protective equipment.

Keywords : vehicle engineering; head collision injury; biomechanical parameters; helmet design; spider web liner

Temperature-Dependent SWRC Model for Expansive Soils Considering Bound Water Dehydration

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Expansive soils are widespread and known for their significant volume changes in response to variations in moisture content. In addition to moisture fluctuations, temperature changes—especially cyclic heating and cooling—can significantly influence the mechanical and hydraulic properties of expansive soils, further complicating their behaviour in engineering applications. Previous studies have shown that cyclic temperature variations can lead to alterations in the soil's water retention characteristics, which in turn affect its volume change, strength, and stress-strain behavior. However, the impact of cyclic heating-cooling on the soil-water retention curve (SWRC) of expansive soils remains insufficiently explored.

This study introduces a novel Soil Water Retention Curve (SWRC) model for expansive soils that incorporates the effects of cyclic temperature changes on water retention behaviour, with a particular focus on the dynamics of bound water dehydration and hydration. The proposed model integrates bound water dehydration processes within the framework of SWRC, which distinguishes between free water and bound water retention. The void ratio is divided into two components: the free water void ratio and the bound water void ratio. During cyclic thermal loading, bound water undergoes dehydration and rehydration, which directly influences the soil's water retention characteristics. The model includes a temperature-dependent equation for bound water content, capturing the temperature-driven shifts in the water retention behaviour of expansive soils. The anticipated results from this study will provide valuable insights for improving the prediction of expansive soil behaviour, particularly in regions where temperature fluctuations are significant.

Keywords: Expansive soils, Soil Water Retention Curve (SWRC), temperature fluctuations, bound water dehydration, cyclic heating-cooling

A Localizing Gradient Damage Model for the Dynamic Fracture of Quasi-Brittle Materials

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This presentation focuses on the dynamic fracture of quasi-brittle materials such as concrete and ceramics under different loading rates. With a view towards an ease of implementation, a simple form of damage model is considered with the necessary constitutive relations, to adequately capture the dynamic fracture responses under mixed mode loading condition [1].

Specifically, an energetic split into tensile and compressive components enabled the imposition of damage descriptors only on the former, to avoid spurious compression induced damage in mixed mode dynamic fracture phenomenon. Moreover, a history-dependent dynamic increase factor is introduced to capture the rate dependent behavior accurately, without inducing numerical instabilities. The numerical solutions are regularized via the localizing gradient enhancement to give sharp damage profiles resembling the development of macroscopic cracks.

Finally, to facilitate an ease of implementation in the commercial software ABAQUS, the class of built-in thermal-mechanical elements is utilized, together with the VUMAT-VUMATHT subroutines. Validation of the model's capabilities is demonstrated through the Compact Tension Test and the Kalthoff-Winkler Test, underscoring its potential to accurately model the rate-dependent effect in dynamic mixed mode fracture.

Keywords: Dynamic fracture, localizing gradient damage.

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Damage Detection for Building Using AI-Enabled Strategies

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Buildings may suffer from natural hazards such as earthquakes, typhoons, and landslides. In the past, numerous studies have applied machine learning to establish complex relationships between various inputs and outputs, enabling the prediction of tasks that are challenging to measure by advanced instruments. In practical applications, accelerometers are often used to measure structural responses, and through double integral, displacement-related information can be obtained. However, the derived displacements may encounter accumulated errors due to the constant term and result in substantial distortions to be obtained. Moreover, stiffness is also considered a crucial indicator for detecting structural conditions. While design codes and past studies have highlighted the significance of inter-story drift and structural stiffness as crucial damage indicators, only limited studies considered both story drift and structural stiffness within a single neural network.

This study introduces three multi-target neural networks designed to estimate story drifts and remaining stiffness using acceleration responses, as illustrated in Figure 1. All three networks share the same architectural modules and undergo parallel training for drift and stiffness estimation. The key distinction among them lies in their choice of loss functions and optimization strategies. The first model utilizes the mean squared error (MSE) loss function for training. The second model replaces MSE with a physics-guided loss function. The third model applies loss-conditional training [1], enabling a more practical approach to optimizing the weighting of losses. Additionally, the study assesses the performance of these neural networks using a three-story numerical building and validates the experimental results with a six-story full-scale structure. The findings demonstrate that all three neural networks can accurately estimate story drift and residual stiffness ratios, thereby improving overall structural damage detection. Notably, the physics-guided neural network incorporating loss-conditional training enhances model convergence speed and improves overall performance.

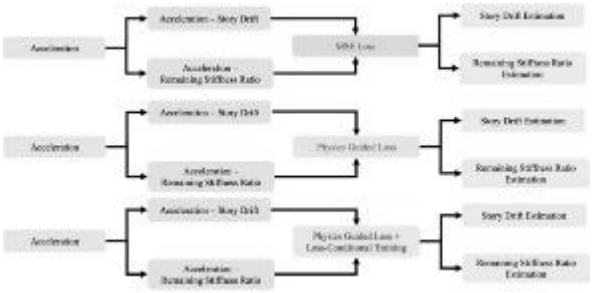

Figure 1. Three multi-target damage detection strategies.

Keywords: Damage detection, multi-target neural network, physics-guided loss function, loss-conditional training, story drift estimation, remaining stiffness ratio

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Immersed-Boundary Meshfree Methods with Consistent Weight-Learning Numerical Integration

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Meshfree methods based upon nodal discretizations provide a robust way to construct arbitrary order smooth approximants. Nonetheless, the very popular Galerkin meshfree methods still necessitate background integration cells to implement the numerical integration of weak form, although the meshfree discretization and shape function construction do not need orderly connected elements [1, 2]. Similar to the finite element mesh generation, the generation of background integration cells is still tedious and time-consuming, which severely reduces the efficiency of Galerkin meshfree methods. Therefore, the development of an efficient Galerkin meshfree formulation that completely eliminate the background integration cells is highly desirable. In the meantime, the rapid advancement of machine learning techniques enables the efficiency improvement of meshfree numerical integration through a careful design of loss functions and a proper construction of learning models.

In this talk, we present an efficient immersed-boundary meshfree framework with machine learning-assisted numerical integration [3]. In particular, an immersed-boundary is employed to realize a uniform nodal discretization and periodic arrangement of Gauss integration points in the embedded domain for Galerkin meshfree methods, which are then trimmed by the meshfree discretized boundary of the physical domain to obtain the discrete model for meshfree computation. This methodology completely avoids the construction of explicit background integration cells and significantly upgrades the efficiency of pre-processing. Furthermore, the use of integer support sizes facilitates a natural alignment between the influence domains of meshfree shape functions and the virtual integration cells for interior regions, and thus the basis degree correspondent normal order Gauss integration would give satisfactory integration accuracy. For the near boundary regions, a loss function in accordance with the integration consistency [2] is devised to optimize the corresponding integration weights and ensure the overall integration accuracy from a global point of view. Consequently, an efficient immersed-boundary Galerkin meshfree method with learned weight learning is rationally established. The efficiency and accuracy of the proposed framework are validated through several typical examples.

Keywords: Meshfree method, numerical integration, integration consistency, immersed boundary discretization, machine learning

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Computational Advances in Material Design, Simulation, and Additive Manufacturing

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Computational tools play a crucial role in materials design, optimization, modeling, and manufacturing processes, enabling the development of advanced materials with tailored properties. This presentation will explore various computational modeling approaches, including multi-scale physics-based simulations and machine learning-driven design, to demonstrate their impact across these domains. Several case studies will be discussed, including high-energy absorption materials for impact resistance, metamaterials engineered for noise and vibration control, and bionic helical carbon fiber tow structures. Additionally, the integration of topology optimization with additive manufacturing constraints will be examined to showcase how computational techniques enhance material performance while ensuring manufacturability. These innovations pave the way for next-generation materials with optimized structural, mechanical, and functional properties, driving advancements in aerospace, automotive, and defense applications.

Keywords: materials design, metamaterials, topology optimization, machine learning, additive manufacturing

Numerical analysis of crack growth in mud wall's structure using phase field fracture model

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In buildings with mud walls, changes in environmental conditions such as temperature and humidity induce deformation, which leads to the occurrence and progression of cracks. In this study, we created a simple model of expansion and contraction due to temperature rise and drying, and used a phase field-based numerical simulation to examine the effects of reinforcement on the structure of an actual building. In this study, we took a horizontal cross-section of a wall at the height of an opening in an actual building with double-layered earthen walls, assumed that the columns would not deform, and constructed a computational mesh based on the actual dimensional ratio for one of the three walls (Figure 1). It is assumed that the temperature of both the inside and outside of the exterior wall increases over time and shrinks at the same thermal drying shrinkage rate, the elastic energy of the entire system increases over time and is eventually broken and released. Since the drying thermal shrinkage is set to occur from the wall surface in proportion to time, the time until destruction corresponds to the magnitude of the strain due to shrinkage. If there is no backing plate on the interior wall, cracks begin to occur relatively quickly due to stress concentration at the corners of the interior columns (Figure 2), but if the wall is fixed with a backing plate as in an actual building, the stress concentration is relatively alleviated and cracks are less likely to occur (Figure 3). From these results, it is expected that applying a backing plate to the interior wall will make cracks less likely to occur.

Figure 1.

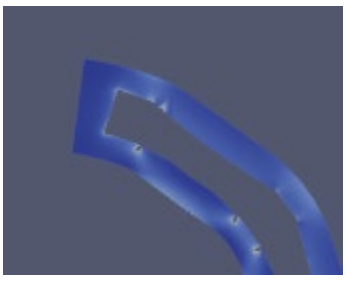

Figure 2.

Figure 3.

Keywords: Fracture, drying, shrinkage, phase field model, FEM, earth wall

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Development of a machine-learning based surrogate model to efficiently conduct total system performance assessments

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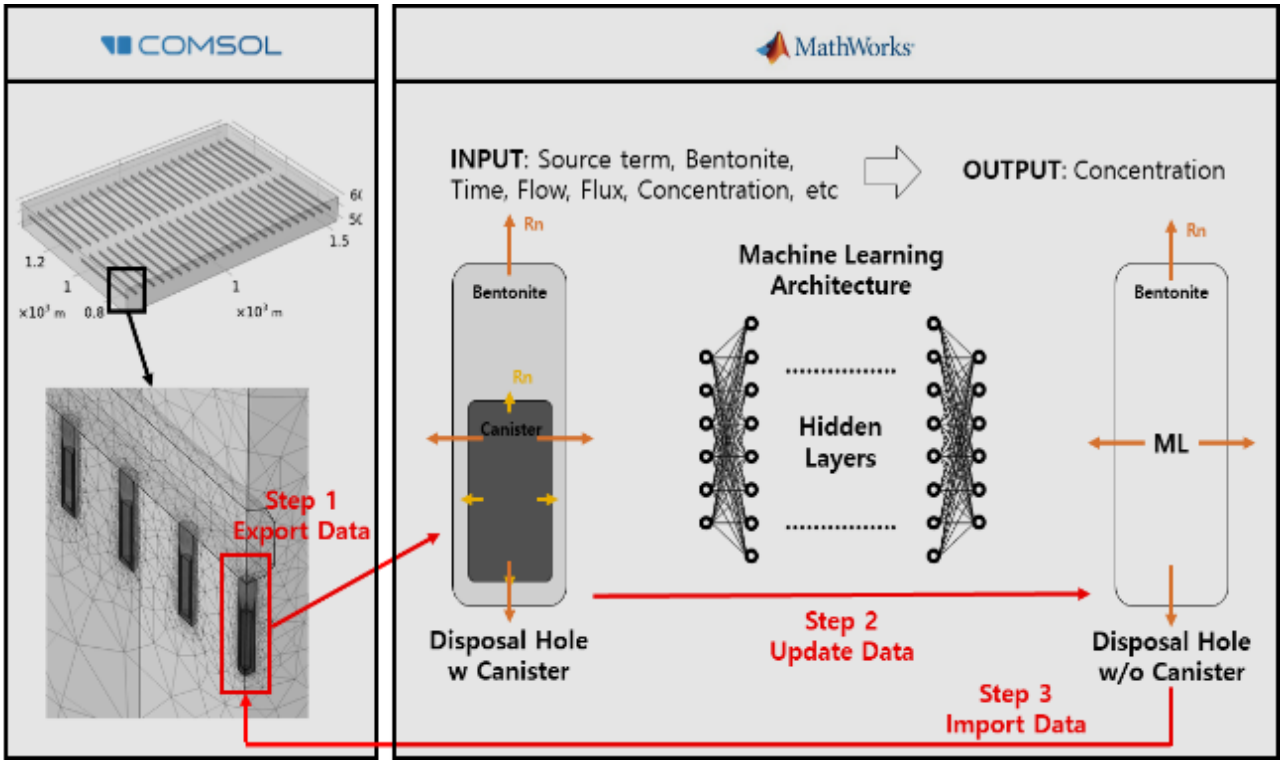
The Total System Performance Assessment (TSPA) for a deep geological repository of spent nuclear fuel is an extremely challenging task, as it requires evaluating thousands of disposal holes and the surrounding geological environment over a period of more than 100,000 years. This process demands a significant amount of computational resources. In particular, most of the computational cost is concentrated on the disposal holes, requiring a comprehensive approach that accounts for various multi-physics phenomena, including thermal, hydraulic, mechanical, and chemical processes. In this study, we propose a method to reduce the computational burden by replacing the physical phenomena occurring in the disposal holes with a machine learning-based surrogate model. The core concept is to eliminate the internal region of the disposal hole from the TSPA analysis while using a machine learning-based surrogate model to predict and replace the physical phenomena occurring inside the hole. This enables the development of a simplified model that maintains accuracy while significantly improving computational efficiency. As a result, this study demonstrates that the proposed approach can drastically reduce the computational resources required for TSPA while maintaining the reliability of the analysis.

Figure 1. Schematic description for machine-learning based surrogate model



Keywords: Spent nuclear fuel, Disposal, Total system performance assessment, Machine-learning

High Performance Cooling Solution for IGBT Power Modules via Graphite TIM and Two-layered Micro-Channel Heat Sink

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The IGBT power module is a key component in the inverter units of electric vehicles, wind turbines, and solar cells. However, its compact design results in high internal heat generation with limited surface area. Micro-channel heat sinks are an effective cooling solution due to their compactness and ability to handle high heat densities. These heat sinks are thermally coupled to the power module using thermal interface materials, typically thermal grease. The thermal grease interface contributes significantly to the total thermal resistance due to having relatively lower thermal conductivity (<5 W/m·K) compared to other parts of the assembly. This highlights the need for higher thermal conductivity thermal interface for enhancing the cooling performance which is the main aim of this research.

This study explores the use of graphite sheet thermal interface material, a flexible material with enormous thermal conductivity (>100 W/m·K), offering lower thermal resistance and longer lifespan compared to conventional thermal grease. Furthermore, the graphite sheet will be integrated into novel designs for micro-channel heat sink to improve cooling of the IGBT power modules. The proposed internal designs feature pin-fin geometries with various cross-sections, while considering a two-layered top cover and employing highly conductive material for the lid. The analysis is conducted through numerical simulations of conjugate fluid flow and heat transfer in a heat sink, which is coupled thermally to the power module. Having validated the numerical simulation, the results of the proposed designs with new graphite thermal interface material are compared with a baseline case featuring a simple rectangular-channel microchannel heat sink and thermal grease interface.

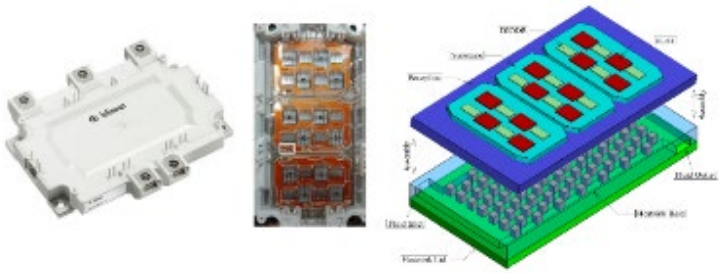

Figure 1.

The findings of this study demonstrate that using a graphite sheet as the TIM significantly decreases the total thermal resistance, resulting in lower maximum temperature in the power module. Also significant improvements in the cooling performance of the heat sink when utilizing all three pin-fin designs with the graphite sheet will be outcome. Among them, the diamond-shaped pin-fin provides the highest cooling efficiency. However, considering the need for an economical design with lower pumping power

requirements, the circular pin-fin design is identified as the most practical choice. Finally, incorporating a second row of microchannels in the top cover proves beneficial, as it substantially reduces pumping power while maintaining nearly the same thermal performance. All these modifications enhance the heat sink's cooling capacity, ultimately improving the power module's maximum power load and reliability.

Keywords: IGBT power module, Micro-channel heat sink, heat transfer, Graphite TIM, two-layered

A Face-Scaling Scaled Boundary Finite Element Method for Plate and Shell Member Simulation

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A scaled boundary finite element method (SBFEM) based on the Hamiltonian system is developed for the numerical simulation of plates and shells. Unlike the conventional SBFEM which employs a single point as the scaling centre, the proposed method utilizes a circumferential boundary face as the transformation centre for plates and shells as illustrated in Figure 1.

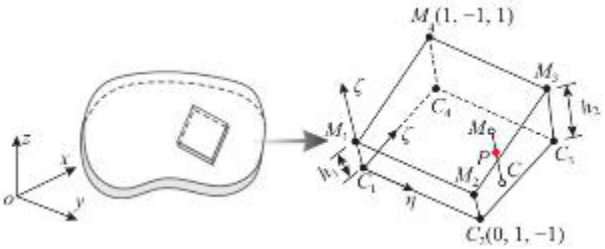

Figure 1.

In this novel SBFEM, the structural surface is discretised using two-dimensional spectral elements. The transformation relationship between the boundary face and the scaling face is established, as shown in equations 1~3.

$$\hat{x} = \boldsymbol{N}(\eta,\zeta)[\boldsymbol{x}_d + \xi(\boldsymbol{x}_u - \boldsymbol{x}_d)] \tag{1}$$

$$\hat{y} = \boldsymbol{N}(\eta,\zeta)[\boldsymbol{y}_d + \xi(\boldsymbol{y}_u - \boldsymbol{y}_d)] \tag{2}$$

$$\hat{z} = \boldsymbol{N}(\eta,\zeta)[\boldsymbol{z}_d + \xi(\boldsymbol{z}_u - \boldsymbol{z}_d)] \tag{3}$$

In which $(\hat{x},\hat{y},\hat{z})$ are the coordinates of an arbitrary point P in the global coordinate system, $(\boldsymbol{x_d},\boldsymbol{y_d},\boldsymbol{z_d})$ and $(\boldsymbol{x_u},\boldsymbol{y_u},\boldsymbol{z_u})$ are the column vector composed of the element nodal coordinates at the bottom & top scaling face, $\boldsymbol{N}$ is the row vector composed of the shape functions of the element nodal displacement field. The governing equations in terms of the scaling face are derived within the Hamiltonian framework. To determine the Hamiltonian coefficient matrix of the governing equation, a quadratic polynomial fitting approach is employed based on the coefficient matrix with the local radial parameter as a variable.

This process yields the stiffness matrix and the nodal displacement function of the structures. The proposed SBFEM, formulated and solved within the framework of 3D solid theory, effectively mitigates the locking issues commonly encountered in traditional finite element methods for plates and shells. Furthermore, the method is applicable to structures with arbitrary shapes and varying thicknesses. The accuracy and reliability of the proposed model are validated through benchmark numerical examples.

Keywords: Scaled boundary finite element method; Plate and shell members; Face-scaling element; Hamilton system; Spectral element; Model verification.

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Recent Progress on AI-based Damage Assessment of Composite Laminates

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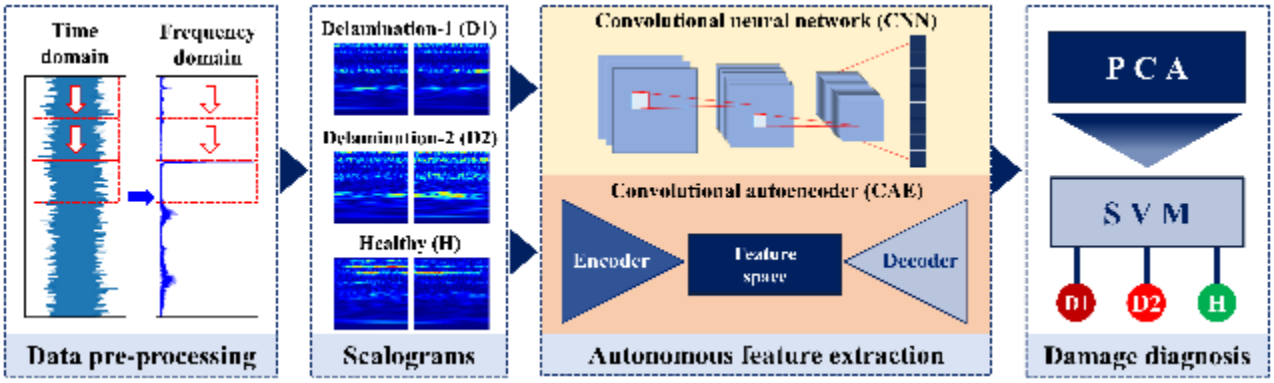
Laminated composites are extensively employed across aerospace, automotive, and marine sectors, primarily due to their superior strength-to-weight ratios and high stiffness. The orthotropic nature of these materials enables the customization of mechanical properties. However, it also introduces complex failure mechanisms that challenge damage assessment processes. Conventional non-destructive evaluation (NDE) techniques and structural health monitoring (SHM) approaches, including surface acoustic wave (SAW) methodologies, face considerable obstacles in the real-time detection of damage within composite structures. While real-time vibration data from these composites can be readily obtained, the inherent global response characteristics often impede the precise localization of damage. Recent advancements in artificial intelligence (AI)-based damage detection methodologies have significantly improved capabilities in inferring local damage states from global sensor data [1]. This paper presents recent progress of AI-based damage assessment of composite laminates using global structural vibration data.



Keywords: Laminated composites, vibration, damage, machine learning, deep learning

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Modelling Requirements for Resolving Physiological Functions of Respiratory Airflow

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The respiratory system is a remarkable structure with complex physiological functions that sustain life autonomously by delivering oxygen to the body and expelling carbon dioxide. On average, a person takes about 20,000 to 25,000 breaths per day, equating to approximately 10,000 to 12,500 litres of air. Hidden within this system are evolutionary anatomical features that serve as defence mechanisms, protecting us from airborne pollutants and viruses. Recent advancements in radiology have enabled multiphase flow simulations within computational fluid dynamics (CFD) for respiratory models. New simulation techniques can be applied to help reveal the intricate and evolutionary adaptations of the airways that serve to protect us. This includes scale resolving simulations, particle tracking, multiphase flows, heat and mass transfer models, and dynamic wall motions. Applying these new techniques opens up the ability to explore how the airway anatomy functions, and its impact on physiology. This can be leveraged to enhance drug delivery, while offering new strategies to combat systemic diseases and inhalation exposure risk. Continued work in this field will aim to enable instant diagnosis directly from a visit to the radiology centre.

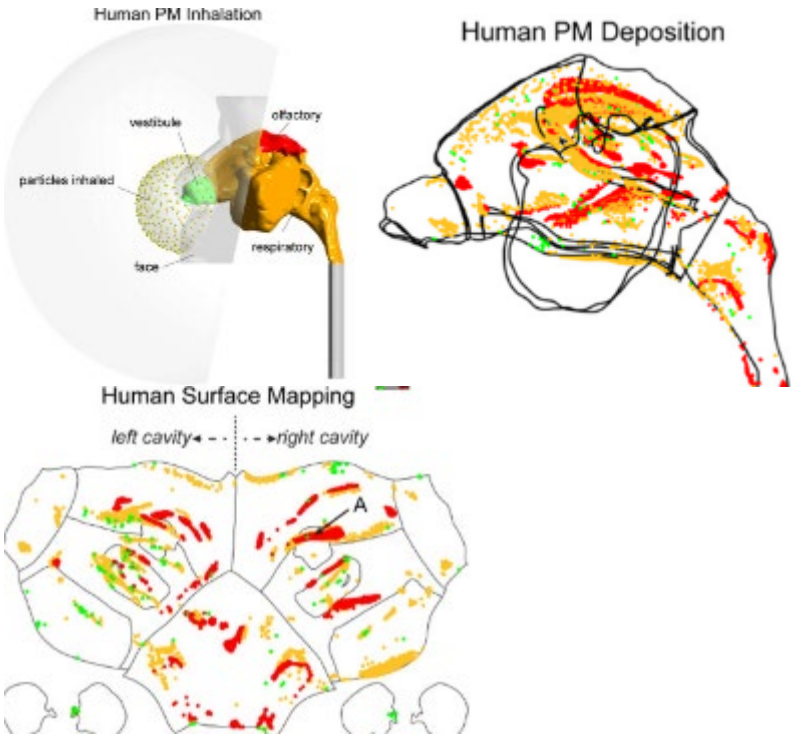

Figure 1. Combined anatomy with multiphase and multi-physics computational modelling requirements for understanding inhalation risk.

Keywords: respiratory airway, inhalation, Computational Fluid Dynamics, particle deposition, nasal airway

Innovative Design and Structural Performance Analysis of Topological Interlocking Bricks for Tubular Structures

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Topological interlocking is an innovative design approach where individual bricks interlock through precise geometric shapes and arrangements, forming stable, binder-free structures that rely on global peripheral constraints for stability. This approach offers numerous advantages, including enhanced bending flexibility, robust fracture resistance, resilience to missing blocks, and exceptional energy absorption capacity. Over the years, various approaches have been explored for designing topological interlocking bricks, including polyhedral shapes and assemblies formed from Platonic solids. Efforts to enhance load-bearing capacity led to the development of osteomorphic bricks, which feature curved surfaces for improved interface contact. More recent designs aim to increase stability and resistance to out-of-plane movement. Despite these advancements, the morphology of interlocking bricks has a significant impact on the structural performance of assemblies, making it essential to explore and optimise their design. However, existing literature primarily focuses on a limited range of topological interlocking designs, many of which lack explicit descriptions of brick profiles and interlocking effects, leaving a substantial gap in design methodologies for topological interlocking bricks, particularly those with curved interfaces. Moreover, most studies have concentrated on the quasi-static behaviour of planar structures, with limited focus on the impact performance of these assemblies, particularly in tubular structures with non-planar surfaces.

This study introduces an innovative methodology for designing non-planar topological interlocking bricks with curved interfaces for assembling tubular structures. The proposed design method focuses on developing key curved interfaces, which are assembled to create interlocking bricks. For non-planar topological interlocking bricks, the approach begins with a 3D base pattern featuring polygonal top and bottom surfaces. The design process involves generating rotated curved interfaces in the circumferential direction using a rotation matrix and creating trapezoidal curved interfaces in the longitudinal direction by applying surface curvature functions through control points. The developed non-planar bricks can be assembled into rings, which can then be combined to form tubular structures. Numerical examples demonstrate the effectiveness of the proposed approach in designing interlocking bricks. Furthermore, finite element analysis (FEA) is conducted to compare the impact performance of interlocking structures against conventional monolithic designs. Results indicate that the interlocking assemblies exhibit improved impact resistance and localised failure, highlighting their potential for applications in resilient infrastructure.

Keywords: Topological interlocking, non-planar brick, curved interface, impact resistance, numerical simulation, structural performance

Construction of a C^1 polygonal element based on the scaled boundary coordinates

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We construct a new polygonal C^1 spline element based on the scaled boundary coordinates to address the plate bending problems in the Kirchhoff-love formulation. The Bernstein interpolations are utilized in both radial and circumferential directions in the scaled boundary coordinates. At the beginning of construction, the C^1 continuity conditions inside an S-domain and normal derivatives constraining conditions are imposed by a simple linear system on the S-net coefficients. Then the corresponding unisolvency theorem is proved by studying the dimension of the spline space $S_{4,3}^{1,*}(\mathcal{T}_S)$. To satisfy the C^1 connection between different polygonal elements, we construct the Hermite interpolation by equivalently transforming part of the S-net coefficients to proper boundary degrees of freedom, namely, three degrees of freedom at each vertex and a normal derivative at the midpoint of each edge. Moreover, we discuss the convergence analysis of the proposed element over convex meshes by finding the necessary and sufficient geometric conditions. Then the proposed spline element bases have explicit expressions and the computation of the stiffness matrix can be greatly simplified by using the S-net coefficients. Some numerical tests verify the cubic polynomial completeness, the optimal 4-th order convergence rate, and the continuity of the derivatives. It also shows other good properties like superconvergence in the square mesh and insensitivity to the mesh distortion.

Keywords: Polygonal element, Plate bending problems, Scaled boundary finite element method, Spline finite element method, S-net method

Surface electromyography (sEMG) based approach to terrain recognition for assisting control of transfemoral prosthesis

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Introduction

Different types of prostheses are commonly in use for transfemoral amputees [1]. A recent trend in active prostheses is to read brain generated signal and bring locomotion as per the user's intent i.e. volitional control. This surface electromyographic (sEMG) signal is employed in machine learning control, which can serve for various purposes like recognizing different gait phases, ambulation modes, surfaces, joint kinematics, and transition between ambulation modes [2]. In this research hypothesized Hybrid Multilayer Perceptron (MLP) - Support Vector Machine (SVM) model is successfully employed to anticipate five different surfaces (level ground, ramp ascend, ramp descend, stair ascend and stair descend).

Methods and Materials

Twenty healthy participants with no previous record of lower limb injuries, disabilities and any neurological disorders are hired to walk over five terrains for two minutes each. sEMG signals are collected from seven lower limb muscles, involved in knee movements and used for surface prediction[3,4]. This sEMG signal data is employed as input in hybrid MLP–SVM model to classify five different surfaces.

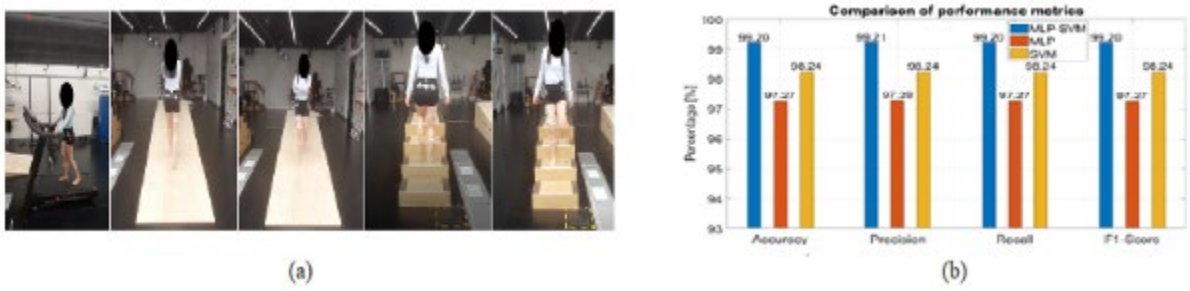

Figure 1. (a) Participant walking on five terrains (b) Performance metrics comparison of Hybrid MLP-SVM, MLP and SVM algorithms

Results and Discussion

This hybrid model provides novel features along with improved accuracy. The hybrid model is compared with MLP and SVM for evaluating performance metrics including accuracy, precision, recall

and F1-score. Among three models, hybrid MLP-SVM model shows a higher accuracy of 99.42% for surface prediction among five terrains, as shown in figure 1(b).

Keywords: Terrain estimation, surface prediction, MLP-SVM, transfemoral prosthesis control, ambulation with prosthesis.

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Wrist Finite Element Model for Wrist Biomechanics Analysis and Pathology Treatment

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This study presents a comprehensive wrist finite element model [1] constructed from a CT scan of a 68-year-old male (type I wrist) and application for wrist pathology treatment. This model intricately captures the bone and soft tissue geometries to study the biomechanics of wrist axial loading through tendon-driven simulations and grasping biomechanics using metacarpal loads. Validation is carried out by assessing the radial and ulnar axial loading distribution, radiocarpal articulation contact patterns, and other standard finite element metrics [2-5]. This study also investigates the effects of Scaphotrapeziotrapezoid (STT) fusion on wrist biomechanics based on the validated wrist model. We simulated STT arthrodesis by creating a unified bone complex comprising the scaphoid, trapezium, and trapezoid, including filled articular spaces. The model was analyzed under physiological grasping loads, examining both radial and ulnar axial load distributions and articular contact pressures at the radioscaphoid and radiolunate interfaces. The fused STT complex becomes a major load-bearing structure, while radiocarpal contact pressures at both the radioscaphoid and radiolunate interfaces show reductions compared to the healthy model. This altered load distribution pattern suggests significant biomechanical adaptations following the procedure. The comparative analyses between healthy and fused models provide valuable insights into post-surgical wrist mechanics, potentially aiding surgical planning. Our findings contribute to the understanding of post-arthrodesis carpal load transfer mechanisms and their clinical implications.

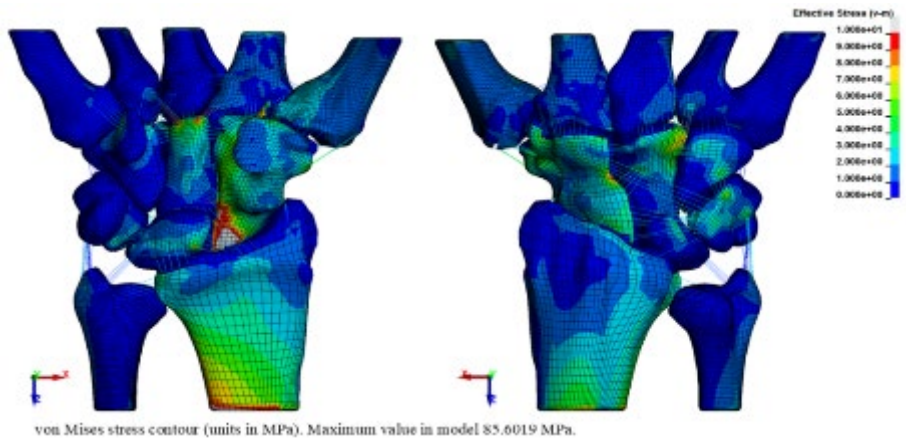

Fig. 1. STT fusion model stress contours for metacarpal-based grasping. Volar (left) and dorsal (right) views.

Keywords: Wrist finite element model, wrist biomechanics, STT arthrodesis, wrist pathology,

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On the automated model discovery with Constitutive Artificial Neural Networks

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Constitutive modeling underpins both computational and structural mechanics. In finite element analysis, it is implemented through a material subroutine—a function that translates local strain data into corresponding stresses. This subroutine is repeatedly called across all finite elements, at every integration point, within each time step, and during every Newton iteration. Although modern finite element software provides a wide array of available material models, selecting an appropriate model often depends on subjective user input.

In this work, we aim to reduce this dependency and automate material modeling. We capitalize on recent progress in constitutive neural networks, machine learning, and artificial intelligence [1] to systematically discover optimal constitutive relationships. Our approach screens thousands of configurations assembled from a handful of functional building blocks [2] and merges them into a single universal material subroutine containing over 60,000 possible models, each built from 16 unique terms [3].

Results indicate that data-driven constitutive neural networks can reliably identify diverse arterial models and plug them directly into a finite element simulation, yielding stress and strain predictions that align well with established constitutive approaches. By consolidating numerous individualized subroutines into one universal model—populated via fully automated discovery—finite element analyses become more straightforward, robust, and less prone to human error. This represents a transformative step in how we simulate materials and structures, eliminating many of the traditional challenges associated with manual model selection.

Keywords: Constitutive Artificial Neural Networks, Finite Element Analysis, Constitutive Modeling

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Data-driven algorithm based on the scaled boundary finite element method and deep learning for crack detection in large-scale structures

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Structural defect identification is a vital aspect of structural health monitoring used to assess the safety of engineering structures. However, quantitatively determining the dimensions of structural defects is often difficult. Therefore, this study presents an innovative data-driven algorithm that combines the scaled boundary finite element method (SBFEM) and a deep learning framework based on a dilated causal convolutional neural network (CNN) to identify crack-like defects in large-scale structures. The SBFEM is used to simulate different crack-like defects. Mesh generation is significantly simplified by a simple procedure that requires only changing the scale centre at the crack tip and the positions of the nodes at the crack opening. This minimises remeshing and enables simple generation of sufficient data to train the neural network. In addition, an absorbing boundary model based on Rayleigh damping is used to avoid computing the entire model when simulating wave propagation in large-scale structures. To ensure that sequential data remain ordered and to obtain a large receptive field without increasing the complexity of the neural network, a dilated causal CNN is employed in the deep learning framework. Therefore, more historical information is captured, and the complex mapping relationship between the echo signal and the crack information is efficiently learnt. The proposed model can accurately identify the number, location, and depth of cracks in large-scale structures. Moreover, it is robust to noise, which is demonstrated via numerical examples. Therefore, the proposed algorithm provides valuable insight into the detection and diagnosis of structural defects, which can ultimately improve the safety of engineering structures.

Keywords: scaled boundary finite element method; dilated causal convolutional neural network; boundary absorbing layer; large-scale structures; crack detection

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Advanced Topology Optimisation for Porous Hip Implants: Bridging in Silico Models and In Vitro Tests

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Total joint replacement is a cost-effective surgical operation performed in orthopaedics in which a damaged joint is replaced with a medical implant. This can relieve pain, improve motion, and allow patients to return to normal daily activities. However, there are a lot of issues regarding the conventional solid implantation, such as high potential risk of stress shielding, customised design for different purposes or patients, specific anisotropic and heterogeneous microstructures to restore biological functions. A Floating Projection Topology Optimisation (FPTO) algorithm with ersatz material model and multiple constraints is used in this research for implants design [1]. The algorithm develops with a global volume constraint to control total volume fraction, a local porous infill volume constraint to generate porous infill and the objective of maximising stiffness constrained by lower volume fraction for reducing stress shielding effect. The proposed FPTO-finite-element-musculoskeletal modelling and analysing approach allows weight factors for considering multiple loading cases in accordance with varieties of postures in gait cycle. Validations and simulation-predicted testing are conduct by finite element analysis (FEA) under varieties of loading cases to investigate the performance of the porous implant design. As results, FPTO is feasible in designing medical implants with lower stiffness for reducing stress shielding effect. Smooth boundary of implants by FPTO can be obtained directly without post-processing, and multiple constraints are allowable. Compared with conventional design, the proposed implant can approximate natural bone structure and load transmission path. Finite-element-based FPTO design provides tailored anisotropic and heterogeneous topology based on host bone and muscle conditions for better biomechanical performance and durable serviceability whilst being lightweight. With FPTO technique, it is expected to shed new light on design of porous implant considering tailored biomechanical environment.

Keywords: Customised Hip Implant; Floating Projection Topology Optimisation; Stress Shielding; Anisotropic and Heterogeneous Microstructures; Finite Element Musculoskeletal Modelling

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Shear wall layout optimisation with a gradient-based method

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Design of the lateral force resisting system is one of the earliest stages of design of a multistorey building and has a great impact on the overall efficiency of the building. A conventional approach to design of the lateral force resisting system involves locating shear walls throughout the building to control the lateral displacement. This process is typically done by engineers relying on experience to choose locations and lengths for each shear wall. This requires tedious manual work and does not significantly explore all the design possibilities. Moreover, in practice, it is desirable to find the layout of shear walls with the lowest total volume as this will minimise material usage and hence cost. Shear wall layout optimisation can alleviate both these issues by automating the search for efficient shear wall layouts. With this, the optimisation problem for shear wall layout optimisation is defined as:

$$\begin{aligned} &\text{minimise} \quad f(\boldsymbol{x}) = \sum_{i=1}^{N_{SW}} L_i t_i h_i \\ &\text{such that} \quad g_i(\boldsymbol{x}) \leq 0 \qquad\qquad i = 1, \dots, m \end{aligned} \tag{1}$$

where $\boldsymbol{x}$ is the vector of design variables, f is the objective function (total volume of shear walls), N_{SW} is the number of shear walls, L_i, t_i, and h_i are the length, thickness, and height of the i-th shear wall, g_i is the i-th constraint and m is the number of constraints. The constraints are used to ensure the adequacy of the lateral force resisting system and typically include criteria such as storey drift, period ratio, or base moments, among others.

Existing research on shear wall layout optimisation is mainly focused on the following formulation. All possible shear wall locations are defined, and they are discretised into segments of a chosen length, e.g. 1 m. The design variables are then 0 or 1 for each segment to represent its absence or presence in the structure, so design vector $\boldsymbol{x}$ is a vector of 0's and 1's. This formulation has some significant downsides. The number of segments and hence design variables is very large, in the hundreds for a typical building. This increases the time needed to converge. The design variables are also discrete, so gradient-based methods cannot be used, and metaheuristic methods must be used instead. This also increases the time needed to converge. The formulation also only allows for shear walls with a length of a multiple of the discretisation length. This limits the ability of the formulation to represent all possible shear wall layouts.

In this paper, we formulate the shear walls with a continuous length and position, so $\boldsymbol{x}$ is a design vector of continuous values that control the shear wall's lengths and positions. We use a thickness interpolation method to represent any length of shear wall on the fixed and discretised finite element mesh. We then show how the gradient of the objective function and each constraint can be efficiently calculated, enabling gradient-based optimisation. We use the nonlinear optimisation library Ipopt to solve the optimisation problem and show that this formulation enables significantly faster convergence than what presently exists in the literature.

Keywords: Structural optimisation, shear wall layout optimisation, gradient-based optimisation, lateral force resisting system

A Fully Eulerian Approach for Transient Fluid-Structure Interaction Topology Optimization

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Fluid-structure interaction (FSI) problems, involving the interaction between fluid flows and structural deformations, play a crucial role in engineering fields such as biomechanics, aerospace, and civil engineering. These interactions are often characterized by complex geometries, large deformations, and transient behaviors, making accurate and efficient computational modeling essential. While topology optimization has been applied to stationary FSI problems [1][2], existing methods frequently rely on linear elasticity assumptions, limiting their ability to handle large deformations.

To address above issue, we propose a novel topology optimization framework for transient FSI problems using a fully Eulerian approach [3][4]. The proposed method formulates the optimization problem through unified governing equations and derives sensitivities using the continuous adjoint method. A cell-centered finite volume discretization ensures numerical robustness and scalability, avoiding common issues of conventional Lagrangian-based methods such as mesh distortion. This approach enables efficient computation for complex multi-physics interactions and provides a stable numerical framework of large-deformation FSI systems. In the presentation, several numerical examples will be presented to demonstrate the effectiveness of the method in optimizing FSI systems under dynamic fluid forces.

Keywords: Topology optimization, Fluid-structure interaction, Eulerian method, Transient state, Finite volume method

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Accelerating PINNs with combined Chebyshev Spectral Approximation and Separation Strategy for Seepage Consolidation Analysis

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The finite element method (FEM), a standard numerical technique for solving partial differential equations (PDEs), inherently suffers from mesh-dependent limitations. In seepage-consolidation coupling problems, for instance, temporal and spatial step sizes must simultaneously satisfy the respective Courant-Friedrichs-Lewy (CFL) conditions of both solid and fluid phases. Physics-informed neural networks (PINNs), which eliminate meshing by encoding physical laws via automatic differentiation, have emerged as a promising alternative. However, within existing frameworks, the computational efficiency of PINNs remains suboptimal compared to FEM for general applications, primarily due to the number of required training points and exponentially growing computational costs when computing seepage-consolidation coupling functions by automatic differentiation. To address this limitation, we propose a hybrid architecture integrating separable network decomposition and Chebyshev spectral approximation techniques (Fig. 1). Our method combines dimension-wise function decoupling via low-rank tensor representations with localized Chebyshev spectral differentiation, achieving $\mathcal{O}(Nd)$ computational complexity for d-dimensional PDEs while using Chebyshev spectral approximation to compute the higher-order derivatives in PDE residual at a low cost. The numerical experiments demonstrate up to 4× faster convergence compared to baseline PINN on a 2-d Poisson benchmark problem, maintaining accuracy. The proposed method was successfully extended to diverse seepage consolidation problems, demonstrating comparable effectiveness. This work establishes a new paradigm with higher performance for solving seepage-consolidation coupling problem with machine learning architectures.

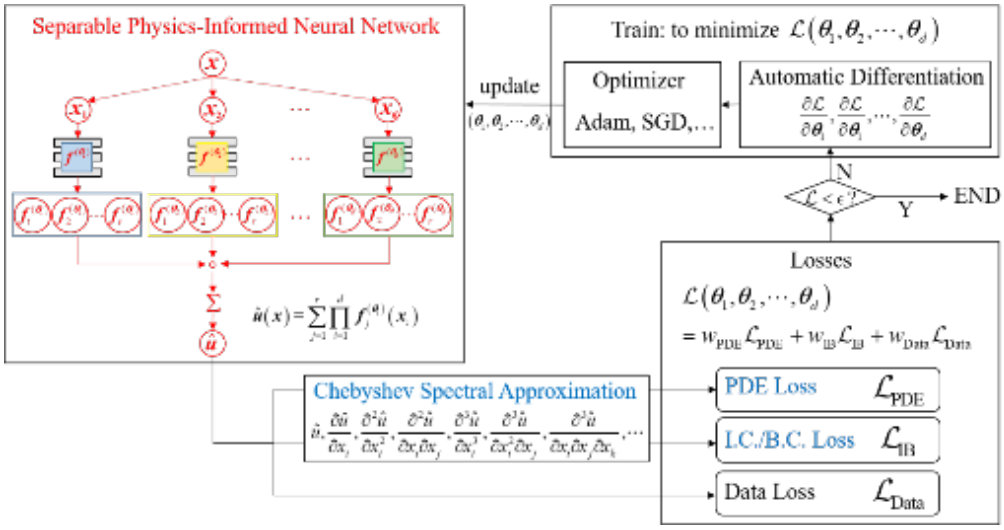

Figure 1.

Keywords: Physics-informed neural network, Low-rank tensor representations, Chebyshev spectral approximation, Higher-order nonlinear differential equation, Seepage-consolidation coupling

Coarse-Mesh Fracture Analysis Using the Quadrature Element Method Integrated with the Phase-Field Model

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Predicting crack propagation contributes to structural risk mitigation in civil engineering. Traditional models rely on explicit crack path tracking and predefined failure criteria, failing to handle complex branching scenarios. While the phase-field method overcomes this through diffuse fracture, it demands prohibitively fine meshes. To address these limitations, we integrate the quadrature element method [1] with the Phase-field method to enable coarse-mesh fracture analysis. Unlike traditional methods [2], quadrature element method constructs high-order elements through differential quadrature rules, eliminating the need for mesh refinement while accurately resolving sharp crack gradients. Through the computation of benchmark examples, including the single-edge cracked plate under tension and notched concrete beam under three-point bending, we demonstrate the effectiveness of the proposed method. The phase-field governing equations is discretized as:

$$\begin{cases} \sum_{i=1}^{N_\xi}\sum_{j=1}^{N_\eta} W_i W_j \left[\left(1-I_{ij}d\right)^2 + k \right] B_{ij}^T D_{ij}^T E D_{ij} B_{ij} \left|J\right|_{ij} c = F^c \\ \sum_{i=1}^{N_\xi}\sum_{j=1}^{N_\eta} W_i W_j \left[I_{ij}^T \left(\frac{g_c}{l_0} + 2H_{ij} \right) I_{ij} + g_c l_0 \bar{B}_{ij}^T \bar{D}_{ij}^T \bar{D}_{ij} \bar{B}_{ij} \right] |J|_{ij} d = F^d \end{cases}, \quad (1)$$

Where N_ξ and N_η are the numbers of integration points in the ξ and η directions, W_i and W_j are the weighting coefficients, D_{ij} and $\bar{D}_{ij}$ are differential operators from Gauss-Lobatto quadrature, B_{ij} is the strain matrix, $\bar{B}_{ij}$ is the phase field gradient matrix and *c* is the nodal displacement vector, *d* is the nodal phase field vector, k is a very small dimensionless parameter to avoid numerical singularity, *E* is the elastic stiffness matrix, g_c is the critical energy release rate, H_{ij} is the history field variable, l_0 is the length scale parameter, *J* is the Jacobian matrix, I_{ij} is a row vector representing that its element corresponding to d_{ij} is 1 and the others are 0, F^c is the nodal force vector, F^d is the nodal force vector for phase field residual equation.

The proposed method attains development in two cases: For the single-edge cracked plate under tension, it reduces degrees of freedom by 77% compared to conventional methods; In the three-point bending test, the method achieves comparable accuracy with 0.4-mm elements (traditional method: 0.0008 mm), slashing computational costs.

Keywords: phase field model, fracture, quadrature element method, energy minimization, coarse-mesh analysis

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Numerical Study on Aerodynamic Characteristics of a Square Cylinder under Unsteady Accelerating Flows

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Unsteady accelerating flows exhibit pronounced time-varying characteristics, making it difficult to apply traditional steady aerodynamic methods to accurately assess their effects [1][2]. This study employs computational fluid dynamics (CFD) simulations to investigate aerodynamic responses of a square cylinder under accelerating flows, focusing specifically on transient changes in aerodynamic force and vortex shedding characteristics.

$$F_x(t) = \frac{1}{2}\rho b U_w^2 \overline{C_D} + \rho \overline{C_m} b d a_w \quad (1)$$

The investigated case involves a uniform, low-turbulence flow field with the wind speed accelerating from 4 m/s to 14 m/s. The time-varying lift and drag forces were obtained from integrating the instantaneous surface pressure distributions. Furthermore, using the Morison equation (Eq. 1), these aerodynamic forces were decomposed into steady and unsteady components to discuss the inertial force effects induced by fluid acceleration.

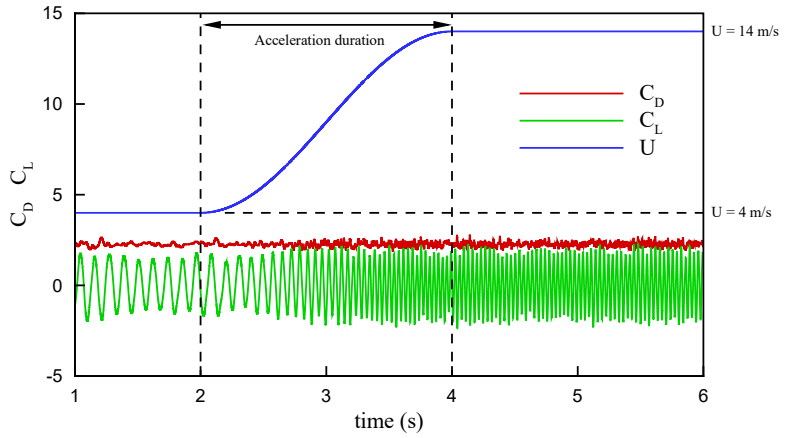

Figure 1.

Moreover, the study examines the impact of acceleration timing by initiating flow acceleration at different phases of the vortex-shedding cycle. The results suggest that the timing of flow acceleration relative to vortex formation or shedding can slightly influence vortex dynamics, wake structures, and transient aerodynamic loads.

Keywords: Accelerating flow, computational fluid dynamics, vortex shedding.

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Linear and nonlinear anisotropic enhancements of fiber-reinforced hyperelastic materials

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In this study, we investigate linear and nonlinear anisotropic enhancements of fiber-reinforced hyperelastic materials by using an additional term with a negative exponent on I_4, i.e., $I_4^{-M} - 1$ ($M > 0$), where I_4 is the pseudo-invariant of the right Cauchy-Green tensor, defined as the square of the stretch in a fiber direction. Although the quadratic energy $(I_4 - 1)^2$ is standard, its use leads to instability, e.g., under uniaxial compression in the fiber direction, the corresponding stress behaves nonmonotonically and the instantaneous stiffness changes negatively in the region [1,2]. It is found that the use of the specific linear combination of $(I_4 - 1) + (I_4^{-M} - 1)/M$, is unconditionally free from the instability under the uniaxial loading as well as equibiaxial and plane strain loadings. The instantaneous stiffness is enhanced linearly regardless of the tension or compression side of the applied stretch, unlike the use of $(I_4 - 1)^2$.

Keywords: Anisotropy, Hyperelasticity, Fiber-reinforced materials, Strain energy functions

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Measuring Brain Strain in Head Impact with Wearable Sensor and Deep Learning Brain Model

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Timely intervention and treatment for traumatic brain injury (TBI) can significantly alleviate symptoms and improve recovery. However, current clinical diagnostic methods are not real-time, as cognitive tests, serum biomarker tests, and MRI scans all require hours before providing results. Given that the "Golden Therapeutic Time Window" for TBI is within a few hours post-injury, there is a critical need for a rapid, real-time detection method. Although initial neurological injuries are often too mild to detect directly, the mechanical loading that triggers them can be measured. To achieve this, we developed an instrumented mouthguard embedded with an inertia sensor unit to measure head kinematics with high accuracy. With the head acceleration collected by the mouthguard, finite element (FE) brain models can calculate brain strain and predict TBI [1]. However, FE models require long computational times, making them difficult to deploy with the instrumented mouthguard for real-time TBI monitoring.

To accelerate brain strain calculation, we developed a deep-learning brain model (DLBM) capable of real-time brain strain prediction. The brain strain predicted by DLBM and the FE models are compared in Fig.1. Unlike FE models, which require hours for computation, DLBM provides rapid predictions, making it suitable for TBI monitoring. In practice, we found that head impact scenarios influence the computational accuracy of deep learning models. To address this, we developed a scenario recognition-adaptive modeling algorithm, enabling high-precision brain strain calculations across various head impact scenarios. By implementing this approach with the Stanford Football team, we successfully detected a player with a high risk of TBI before clinical diagnosis. This combination of precise head acceleration measurement and real-time brain strain computation offers a powerful tool for early TBI risk assessment, enabling timely intervention within the critical therapeutic window.

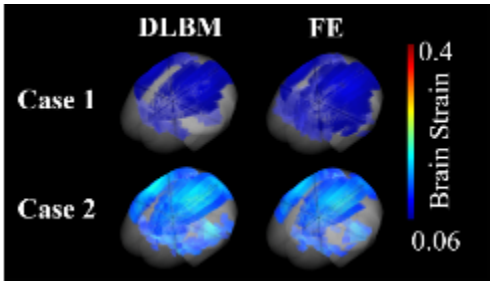

Figure 1. Brain strain given by the deep learning brain model (DLBM) and the finite element (FE) brain model in two cases.

Keywords: traumatic brain injury, deep learning brain model

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Phase Field Fracture Models for Inelastic Mechanical Properties of Additive Manufactured Metallic Materials

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Phase field fracture models have gained extensive attention because of its excellent capability for predicting complicated fracture phenomena such as crack nucleation, propagation, branching and merging [1]. However, their study on additive manufactured metallic materials remains understudied. Due to scanning strategy, the constitutive relations of 3D printed metals can exhibit different behaviour compared with traditionally fabricated materials. In this regard, a phase field model is incorporated with stress state dependent fracture initiation criteria such that fracture behaviour of specimens covering a wide range of stress states can be properly captured [2]. Second, this model is applied to 3D printed 316L steel. It is found that scanning strategy induced anisotropy should be considered [3]. Subsequently, explicit phase field models are developed for crushing simulation and dynamic loading. Deformation modes, crack evolution, force-displacement curves of 3D printed tubal and triply periodic minimal surface structures can be well predicted [4, 5]. More importantly, fracture mechanisms under crushing behaviour are analysed. Lastly, phase field model has been proposed for dynamic ductile fracture, considering strain rate, temperature, stress state, and orientation dependency [6]. It has been calibrated by 3D printed material specimens and validated by crack propagation samples and TPMS structures.

Keywords: Phase field fracture model, additive manufacturing, stress state, strain rate, crushing behaviour, triply periodic minimal surface structures

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On the formulation of finite strain multi-material topology optimization

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The study aims to present a formulation of finite strain multi-material topology optimization [1] by enhancing the single-material topology optimization framework [2,3]. The primal problem describes multi-material responses in which both elastic and inelastic deformation are considered. The continuous adjoint problem is performed to derive the governing equations of the adjoint problem and sensitivity. Notably, the employed formulation does not rely on either spatial discretization or temporal discretization, and thus, the derived equations can be implemented in arbitrary computational frameworks. Numerical example in Figure 1 demonstrates the ability of the proposed method, in which the displacement magnitude-dependent optimal designs are realized.

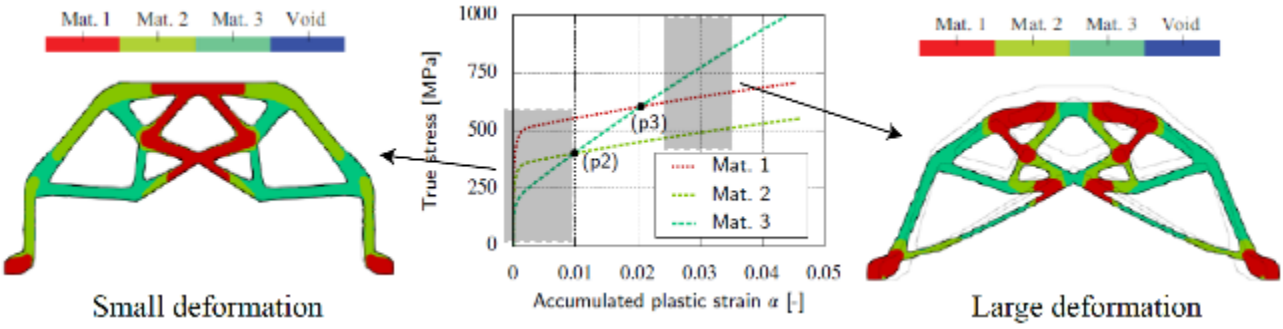

Figure 1. Multi-material topology optimization for small and large deformations

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Keywords: Topology optimization, Finite strain, Multi-material, Adjoint method

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Traffic Simulation in Case of Vehicle Platoon Merging to Main Lane Traffic Flow

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For solving traffic problem, Intelligent Transport Systems (ITS) using inter-vehicle communication technology have been studied. Vehicle platoon is a method in which vehicles travel in a row over a short distance between vehicles, which can help alleviate traffic congestion and improve fuel efficiency. Since multiple vehicles travel over a short distance, traffic capacity in the entire road can be increased. In real life, a mix traffic situation of the communication vehicles that carry out inter-vehicle communications and non-communication vehicles that do not communicate between vehicles is considered. In this study, we will consider speed control of vehicles in the platoon when the platoon of the communication vehicles merges to the traffic flow of non-communicated vehicles.

It is assumed that a two-lane road will be one lane in this study. The platoon of three communication vehicles, X0, X1, and X2, changes lanes from the branch lane to the main lane to avoid colliding with non-communication vehicles NC1, NC2 and NC3, which travel on the main line at the meeting point of the main and branch roads. In addition, the speed control of vehicles is performed using the Helly model [1], which is given as follows.

$$\ddot{x}_n(t+\Delta t) = \alpha\left(\dot{x}_{n-1}(t) - \dot{x}_n(t)\right) + \beta(x_{n-1}(t) - x_n(t) - D) \quad (1)$$

where $x_n(t)$ and $x_{n-1}(t)$ denote the positions of the vehicle n and its nearest frontal vehicle $n-1$, respectively. D is the ideal vehicle distance. α and β are the model parameters which are determined by minimizing the estimation function.

Figure 1 shows the traffic flow after the platoon merges to the main lane traffic flow. Figure 2 is plotted with the time as horizontal and the vehicle position as the vertical axis, respectively. The results show that the vehicles in platoon can merge to the main lane traffic flow without car collisions.

Keywords: Traffic congestion, Helly model, Vehicle Platoon, Merging

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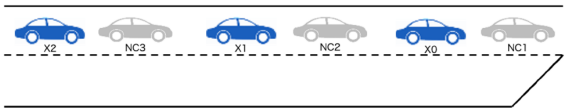

Figure 1: Traffic flow after platoon merges to the main lane. Blue vehicles and grey vehicles are communication and non-communication vehicles, respectively

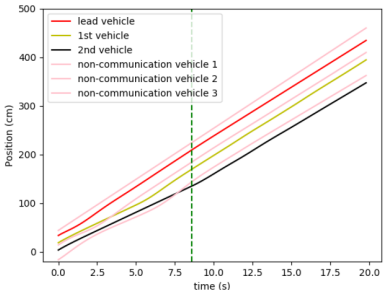

Figure 2: Vehicle positions

Differentiable Material Point Method for 3D Concrete Printing

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In recent years, 3D concrete printing (3DCP) has rapidly developed in the construction industry, offering a highly automated process that significantly reduces material, labor, and time costs. However, the extrusion-flow behavior of fresh concrete during printing process and resulting layer deformations often cause deviations from the original design. This discrepancy, which largely stems from the lack of understanding of the influence of key process parameters, severely affects the final product quality and hinders the wider adoption of 3DCP.

To gain insight into the impact of the extrusion-flow process on layer deformation, we established a numerical model for 3DCP process using the material point method. A differentiable material point method solver, based on the moving least-squares material point method (MLS-MPM) formulation, was developed. The solver's ability to simulate flow dynamics was first validated through three classical CFD benchmarks: Poiseuille flow, the dam break test for free-surface behavior, and the fresh concrete slump test. These benchmarks cover a range of scenarios from 2D Newtonian case to 3D non-Newtonian flow. Then, the simulation framework for the extrusion-flow process was established with weakly compressible Bingham fluid assumption. Several numerical printing cases with various printable materials, process parameters and number of layers were conducted. The strong agreement between numerical and experimental cross-section shapes confirms the accuracy of the material point method. With the reliable forward simulation model, automatic differentiation was executed to compute parameter gradients—such as printing velocity and nozzle height—in relation to the final cross-section shape. This quantitative analysis provides deeper insights into the process mechanics and offers a pathway for optimizing product quality in 3D concrete printing.

Dimension liftings for quantum Computation of partial differential equations and related problems

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Quantum computers have the potential to gain algebraic and even up to exponential speed up compared with its classical counterparts, and can lead to technology revolution in the 21st century. Since quantum computers are designed based on quantum mechanics principle, they are most suitable to solve the Schrodinger equation, and linear PDEs (and ODEs) evolved by unitary operators. The most efficient quantum PDE solver is quantum simulation based on solving the Schrodinger equation. It will be interesting to explore what other problems in scientific computing, such as ODEs, PDEs, and linear algebra that arise in both classical and quantum systems, can be handled by quantum simulation.

We will present a systematic way to develop quantum simulation algorithms for general differential equations. Our basic framework is dimension lifting, that transfers nonlinear PDEs to linear ones, and linear ones to Schrodinger type PDEs. For non-autonomous PDEs and ODEs, or Hamiltonian systems with time-dependent Hamiltonians, we also add an extra dimension to transform them into autonomous PDEs that have only time-independent coefficients, thus quantum simulations can be done without using the cumbersome Dyson's series and time-ordering operators. Our formulation allows both qubit and qumode (continuous-variable) formulations, and their hybridizations, and provides the foundation for analog quantum computing.

Vehicle Scanning Method for Non-Destructive Bridge Inspection: From Theory to Experimental Validation

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Abstract

The Vehicle Scanning Method (VSM) offers a novel, non-destructive approach to bridge health monitoring by using vehicle-bridge interaction (VBI) dynamics. This study advances the VSM framework originally proposed by Y.B. Yang et al. (JSV, 2004), which utilizes an instrumented test vehicle as a mobile sensor to extract bridge dynamic properties, such as frequencies and vibration modes, from its response while traversing a bridge. We present the theoretical foundation of VSM, rooted in VBI, where the bridge's response excites the vehicle, embedding structural information within its dynamic signature. A key innovation is the design of a single degree of freedom (SDF) test vehicle, featuring tunable frequencies, elastic steel wheels, and a lightweight 30 kg frame, enhancing mobility and measurement precision. Experimental validation was conducted at the Institute of Theoretical and Applied Mechanics (ITAM) laboratory using an acrylic test beam simulating a simply supported bridge. Frequency measurements from the SDF vehicle demonstrated alignment with theoretical predictions, confirming VSM's efficacy. Applied to tied-arch bridges, this method addresses the challenges of conventional fixed-sensor systems—cost, time, and traffic disruption—offering a cost-effective, repeatable, and sustainable solution for structural health monitoring, with potential for broader implementation.

Title: Hydrodynamics and coherent structures of the sheared convective boundary layer

Abstract: A linear stability analysis is conducted for inviscid sheared convective boundary layer flow, in which the sheared instability with stable stratification coexists with and caps over the thermal instability with unstable stratification. Two shear-thermal hybrid instabilities, the hybrid shear stratified (HSS) and hybrid Rayleigh-Benard (HRB) modes, are obtained by solving the eigenvalue problems based on the Taylor-Goldstein equation. A map of the unique critical boundary, which separates the effective regions of the HSS and HRB modes, is constructed and found to be dependent on stable/unstable stratification factors J_s and J_b as well as wavenumber of perturbation. The examinations of the subordinate eigenfunctions indicate that the shear instability is well developed in the HSS mode, in which the large vortex structures may prevail and suppress the formation of convective rolls; the shear instability in the HRB mode is either "partly developed" when $J_b < J_{b;cr}$ or "undeveloped" when $J_b > J_{b,cr}$, thus only plays a secondary role to modify the dominant convective rolls, and as J_b increases, the eigenfunctions of the HSS mode exhibit different transitional behaviors in the two regions, signifying the "shear enhancement" and "shear sheltering" of the entrainment of buoyancy flux. The direct numerical simulations (DNS) verify the HSS mode, in which the Kelvin-Helmholtz (KH) eddies developed in stable stratified layer prevent plume from merging into large scale thermal circulation, therefore corresponding to "shear sheltering" of the entrainment of buoyancy flux. For the flow structures pertaining to the HRB mode, the relatively weakened KH eddies still modify the development of thermal circulation, leading to both the "shear enhancement" and "shear sheltering" of the entrainment of buoyancy flux.

Ellipsoidal Particle model for the Moving Particle Hydrodynamics method

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The ellipsoidal particle model of the Moving Particle Hydrodynamics (MPH) method [1] is presented for thin computational geometries. Calculations including thin layers (e.g. tsunami, fluid lubrication) require high resolution to fit the thin layer, making the computational cost expensive. In meshfree methods, several ellipsoidal particle models [2-3] have been developed that change the aspect ratio of particles to reduce the number of particles required and thus reduce the computational cost. However, these methods are not consistent with the analytical mechanics framework and require empirical stabilization techniques. In this study, we present an ellipsoidal particle method that is consistent with the analytical mechanics by extending the MPH method. The discretised equations are obtained from the Lagrangian and the dissipation function corresponding to ellipsoidal particles. Several simulations were performed, and the computational time was reduced.

Keywords: Computational fluid dynamics, Mesh-free methods, Particle methods, Moving Particle Hydrodynamics, Ellipsoidal particles

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Life Cycle Assessment of Reinforced Concrete Panel Considering Multi-Ion Corrosion: A Coupled Chemical and Electrochemical Model

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Reinforced concrete has been widely used in bridges and building structures. Given the complex service environment, the life span of RC structures are continuously affected by destructive corrosion resulting from the penetration of different ions, eventually leading to premature cracking and delamination. Though some studies focus on the effects of chloride ion corrosion or carbonation on the service life of reinforced structures, in-depth investigation on multiple ions corrosion have yet been carried out.

In this study, a coupled chemo-electro-mechanical model is developed to investigate the service life of reinforced concrete panels under coastal and marine environment. The model incorporates the diffusion-reaction behaviour of corrosive ions, the theory of porous media, Fick's second law and Hill function with updated factors. Reaction products like rust on rebar surface are attributed to concrete cracking and further delamination.

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (D_i \nabla c_i) = R_i \,, \tag{1}$$

$$D_{eff}^0 = D_0 \phi_{ini}^{por} \tau = D_0 \frac{2\phi_{ini}^{por}}{3-\phi_{ini}^{por}}, \tag{2}$$

$$\boldsymbol{\frac{\partial c_i}{\partial t} + \nabla \cdot J_i + u \cdot \nabla c_i = R_i}, \tag{3}$$

The criteria of failure take into account both debonding caused by increasing internal stress as well as the reduction in rebar diameter due to electrochemical reactions. Results show that the combined effect of multiple corrosive ions can significantly impair the service life of the RC panel. Both a small variation in chloride ion concentration and cover depth can significantly affect the service life, while surface treatment is effective regarding prolonging the service life of reinforced concrete.

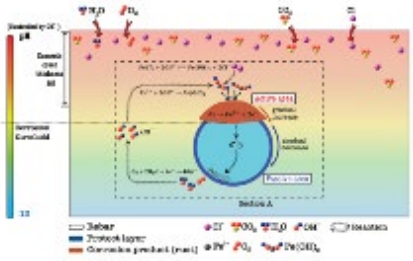

Figure 1.

Keywords: Reinforced concrete; multiple-ion attack; concrete and rebar corrosion; delamination; life cycle

Compression After Impact test analyses of CFRTP laminates by the eXtended Finite Element Method

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Due to high specific strength and stiffness, carbon fiber-reinforced plastics (CFRPs) have been widely used in aviation industries in recent years. However, CFRP laminate is susceptible to out-of-plane load, leading to complex damage such as delamination, matrix crack, and fiber breakage. Because the damage may cause a decrease in compressive strength, CAI (Compression After Impact) strength is important in designing CFRP laminate structures. Recently, carbon-fiber-reinforced thermoplastics (CFRTPs) have emerged as an alternative to thermoset CFRPs. CFRTPs offer higher fracture toughness and superior damage tolerance, enabling rapid mass production with shorter manufacturing cycles than thermoset CFRPs. This study applies the extended finite element method (XFEM) to damage propagation analyses of both CFRP and CFRTP laminates. In XFEM, the approximated displacement fields are expressed as follows:

$$\mathbf{u}^h = \sum_{I=1}^{m} N_I(r_1, r_2\ r_3)\mathbf{u}_I + \sum_{J} N_J(r_1, r_2\ r_3)\mathbf{a}_J\left(F(\mathbf{x}) - F(\mathbf{x}_J)\right) \tag{1}$$

where N_I is a finite element interpolation function for the m-node element; r_1, r_2, and r_3 are the natural coordinate of an element; $\boldsymbol{u}_I$ is a nodal degree of freedom for normal node I; $F(\boldsymbol{x})$ is an enrichment function; and $\boldsymbol{a}_J$ is nodal degree of freedom for enrichment node J.

An eight-node quadrilateral interface element and an eight-node element enriched with only the Heaviside function are used to model delamination and matrix cracks, respectively. In addition, the zig-zag cohesive zone model is employed for delamination, and matrix cracks are used to perform the implicit analysis successfully. This presentation shows damage propagation analyses for CAI tests performed by XFEM using eight-node solid or continuum-based shell elements. It discusses the results and compares them with those of the experiments for validation [1][2].

Keywords: XFEM, Cohesive zone model, Damage propagation, CFRTP, CAI

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A Concurrent Multiscale Method for Mechanical Characteristics of Additively Manufactured Part: Finite Cell - Crystal Plasticity Self-consistent Clustering Analysis

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Abstract

Metal additive manufacturing (AM) is an advanced technology capable of producing complex structures. However, accurately and efficiently predicting the mechanical behaviors of additive manufactured components is challenging due to inevitable process-induced defects and spatially varying microstructures. In this study, a finite cell method– crystal plasticity self-consistent clustering analysis (FCM-CPSCA) concurrent multiscale algorithm is proposed to predict the mechanical behaviors of as-built components. The finite cell method is used to solve macroscopic problems, directly combined with computed tomography scan data to avoid the complex 3D geometric reconstruction process, while capturing the real geometric morphology. The self-consistent clustering analysis is used to solve the microscale volume element considering the as-built material microstructure, significantly reducing the computational cost of microscale solutions. The advantages of the proposed method in terms of accuracy and efficiency are demonstrated through several numerical examples. The computational efficiency of the proposed FCM-CPSCA concurrent multiscale algorithm is improved by 75 times while maintaining an error within 5% in the tensile simulation of a dog-bone specimen compared to the traditional numerical method. The utility of the method is demonstrated by conducting a concurrent multiscale simulation of the compression of an octet lattice unit cell in laser powder bed fusion, achieving good agreement with experimental results and a 12% improvement in prediction accuracy compared to the traditional numerical method. This method could be a useful tool for evaluating the performance of AM parts as well as for structural optimization

Assessing the Structural Reliability of Cladding Panels Under Hail Impact

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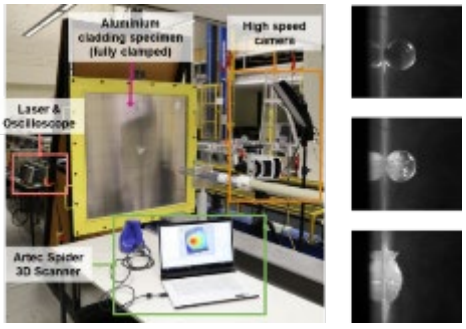
Over the past three decades, severe weather patterns have increased substantially, posing hazards to property and occupant safety worldwide. This includes cities across North America, Europe, and Oceania. In Australia, hailstorms have caused widespread destruction of building cladding, leading to billions of dollars in damage and displacing thousands of residents. This work addresses the urgent need for advancements in understanding the fundamental mechanisms behind hailstorm damage on cladding panels, aiming to facilitate future technology development for risk control.

In order to assess the life-cycle performance of cladding panels in resisting hailstorm attack, we present a structural reliability-based approach to estimating the probability of intervention (PoI) required after a hailstorm event, as shown in Eq. (1).

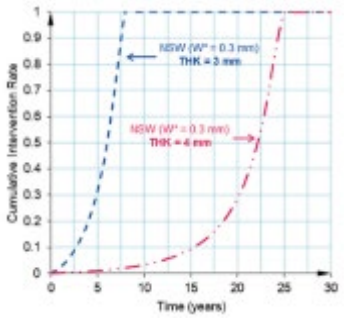
$$PoI(t) = \left(\int_{R(t,n)}^{\infty} g_n(w)\, dw\right) h_T(t), \tag{1}$$

where, $R(t,n)$ is the remaining capacity at the time instance t; $g_n(w)$ is the distribution function of indentation (w) distribution on the surface of the cladding; and $h_T(t)$ is the hazard function.

The prediction results were validated using gas gun dynamic testing, as shown in Figure 1(a). Figure 1(b) shows that an aluminium panel with a 3 mm thickness, installed in New South Wales, would require intervention in approximately seven years. Increasing the panel thickness by 1 mm would significantly enhance its resistance to hailstorms, but also substantially increase costs.



(a)



(b)

Figure 1. (a) Experimental setup of dynamic testing [1]; (b) Intervention rate for aluminium alloy panels exposed to hail hazard in New South Wales [1].

Keywords: Building cladding, energy absorption, structural reliability, impact actions, plate structure

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Mechanistic data-driven modeling and computational mechanics for viscoelastic materials

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This work combines numerical experiments, big data and artificial intelligence to establish a data-driven constitutive model of viscoelastic materials and develop the corresponding computational methods. By incorporating prior knowledge of microscopic deformation mechanisms and viscoelastic theory into a deep learning framework, a Memory Decay Network (MDN) was constructed. The network training process integrates the memory decay effect of viscoelasticity and the second law of thermodynamics as mechanical constraints, and the data-driven constitutive model of viscoelastic materials under framework of small deformation and finite deformation is built with only a small amount of data. The corresponding computational method is proposed for numerical implementation through finite element method. The prediction of the data-driven computational method is compared with the test data set to verify the capability of the proposed data-driven computational method to characterize the mechanical response of viscoelastic materials with microstructures.

Keywords: data-driven computational mechanics, viscoelastic materials, memory decay network

References

CFD-Based Investigation of Optimized Ventilation Strategies for Building Morphological Improvement

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This study examines the effects of building morphological modifications on wind speed at Banqiao Station in New Taipei City, Taiwan, using Computational Fluid Dynamics (CFD)numerical simulations. The study area is situated on the southwest side of the main road behind the central hub of Banqiao Station. Prior studies have demonstrated the significance of architectural modifications in improving ventilation. Huang et al. [1] highlighted that the introduction of openings can enhance street-level airflow and influence pollutant dispersion, while Juan et al. [2] suggested that rounded building corners can increase wind energy density and mitigate turbulence effects.

Figure 1 shows the building model at Banqiao Station in New Taipei City, Taiwan. The CFD software ANSYS Fluent® is utilized in the analysis. The simulation is based on the steady-state, incompressible turbulent airflows over the buildings to probe the environmental velocity and pressure field. The computational model is based on the following governing equations as follows:

$$\frac{\partial u_i}{\partial x_i} = 0 \qquad (1)$$

$$\frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[(\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \rho_{ref} g_i \qquad (2)$$

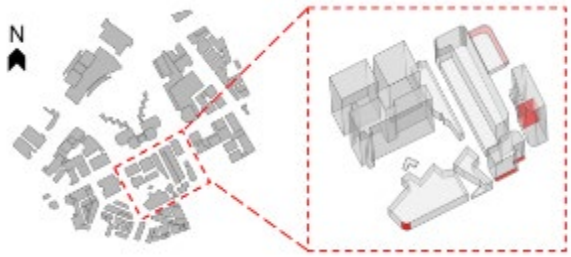

Figure1. Building model in CFD simulations

The simulation results in Fig.2 reveal a 38% increase in wind speed at the pedestrian level (i.e. z=2 m) and a 22% increase in wind speed variation at a height of 32 m at the designated monitoring point. These findings underscore the effectiveness of morphological modifications in enhancing airflow dynamics and optimizing urban wind environments to improve pedestrian comfort.

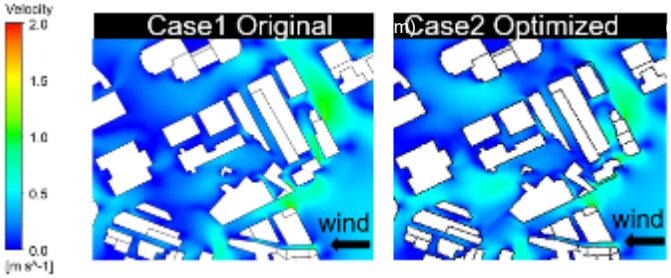

Figure2. Predicted contours of mean velocity at 2m height for different building models

Keywords: CFD, Pedestrian Comfort Layer, Building Morphology

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Topology Optimisation of Self-Sensing Soft Robotic Grippers

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Soft robotic grippers are widely regarded as the standard solution for handling complex, delicate, and deformable objects [1]. To be incorporated into an effective control system, feedback on a gripper's internal state – the stress and strain fields – during operation is invaluable, ensuring effective grips and preventing structural failure [2]. We consider the possibility of obtaining such information by utilizing a soft piezoresistive material for the gripper and exploiting the piezoresistive effect.

In this work, we perform topology optimisation of these so-called self-sensing grippers. Topology optimisation approaches for compliant mechanisms generally focus on balancing the objectives of compliance around objects and overall stiffness. This work introduces, for the first time, an objective term for recoverability into the topology optimisation formulation for compliant mechanisms. Recoverability measures how effectively a geometry leverages the piezoresistive effect in recovering information about the structure's internal state.

We consider a coupled structural and electrical multiphysics model and adopt a level-set topology optimisation approach that is particularly well-suited to the given problem by exploiting bespoke machinery developed in the Julia software package GridapTopOpt [3]. Our work advances the development of self-sensing grippers for next-generation robotic systems. Future direction for this work involves prototyping optimized geometries by using recent developments in additive manufacturing for piezoresistive materials.

Keywords: Compliant grippers, multiphysics, topology optimisation, sensing, piezoresistivity

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A Scaled Boundary Finite Element Formulation Based on Isoparametric Mapping

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An isoparametric mapping technique applicable to a family of polygonal parent elements with an arbitrary number of sides in physical space using the scaled boundary finite element method is presented. The shape functions of the parent elements are constructed from the solution of Laplace's equation formulated in scaled boundary coordinates in the parent element space. An isoparametric concept is applied. The same set of shape functions in the parent element space is used to interpolate both the nodal coordinates and the field variable of an element in physical space. A Jacobian transformation relates the domain transformation between the physical space and the parent elements. The resulting formulation satisfies linear completeness and guarantees convergence in the limit of mesh refinement. Numerical integration is used to integrate the stiffness matrix and load/residual load vectors. Standard finite element procedures adopted for nonlinear engineering problems can be applied directly. Applications of the formulation to various problems in engineering including elasticity, finite strain (Figure 1 (a)) and elasto-plasticity with phase field damage (Figure 1 (b)) will be demonstrated.

(a) (b)

Figure 1: Application of scaled boundary finite element formulation with isoparametric mapping; (a) finite strain elasticity; (b) phase field elastoplasticity.

Keywords: Isoparametric mapping; Polygon elements; Parent elements; Scaled boundary finite element

Semi-analytical shell elements with functionally graded elastic materials

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Functionally graded shells are general thin-walled structures with continuously varying material properties along the thickness direction and widely used in engineering. However, the existing shell modeling techniques typically adopt assumed distribution patters for the displacement field through the thickness and exhibit low accuracy/efficiency when dealing with functionally graded shells. In this study, functionally graded elastic shell elements with analytical displacements through the thickness are developed using the scaled boundary finite element method. The middle surface of the shell element is approximated with a quadrilateral spectral element which is scaled along the normal direction to represent the three-dimensional geometry of the shell. Both the power-law and exponential-law material gradations are considered. The assumed natural strain method is applied to alleviate shear and membrane locking. The principle of virtual work is utilized to derive the scaled boundary finite element equation in the thickness coordinate, which is directly solved via the differential quadrature method with five displacement sampling points. The performance of the presented approach is demonstrated through numerical examples covering static and free vibration analyses of thin and thick functionally graded shells with various geometric shapes.

Keywords: scaled boundary finite element method, semi-analytical shell element, functionally graded elastic material

MD Simulation of Effect of Physical Cross-linkages on Mechanical Properties of Polymer Chains' Network

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Soft materials such as rubber and elastomer are mostly used in the cross-linked state of polymer chains. To improve the toughness strength of soft materials, it is usually to add lots of chemical cross-linkages or fillers and as a result, the entangled structures of polymer chains are constructed completely. On the other hand, there are two types of entangled points in the entangled structure of polymer chains: one is the chemical type which is due to the existence of chemical cross-linkages or fillers and obeys the affine deformation; the other one is the physical type, i.e. physical cross-linkages, which is due to the physical interaction between polymer chains and obeys the nonaffine deformation, as shown in Figure 1.

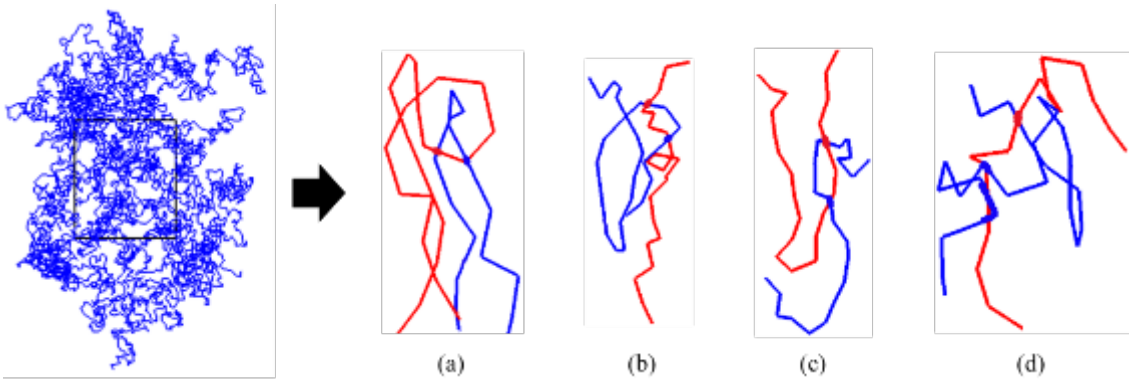

Figure 1.

To enhance the benefit of the addition of chemical cross-linkages or fillers, the fraction of physical cross-linkages in the entangled structure is expected to be clarified quantitatively. However, the count of physical cross-linkages in the entangled structure is not so much easy as the count of chemical cross-linkages or fillers and as a result, the identification of physical cross-linkages has been a pressing issue by now. Therefore, in this paper, I at first construct a polymer chains' network with molecular dynamics method. Then, the relative positional relationship between the central points of the adjacent polymer chains are taken into consideration to identify the existence of physical cross-linkages. Finally, a series computational models of the polymer chains' networks with different densities of monomers are employed to investigate the effect of physical cross-linkages on the mechanical properties of polymer chains' network, for example, the elastic modulus.

Keywords: MD simulation, physical cross-linkage, polymer chains' network, mechanical property

Template for APCOM-ACCM 2025 Abstract Submission

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The Linear Variable Differential Transformer (LVDT) plays a critical role in measuring relative displacement in seismic attenuation systems, where its performance directly impacts the accuracy of vibration measurements. This study introduces an effective non-contact eddy current field model for analyzing the electromagnetic behavior of LVDTs. Utilizing the face-smoothed finite element method (FS-FEM) with a parsimonious linear tetrahedral mesh, the approach applies smoothing operations to the magnetic vector potential, magnetic flux density, and electric scalar potential gradient, ensuring precise solutions. The magnetic flux density is used to evaluate the LVDT's linearity under specified conditions. Validation against standard finite element method (FEM) solutions using dense meshes demonstrates that FS-FEM achieves higher accuracy and computational efficiency. Further validation compares numerical predictions of the LVDT's differential voltage with experimental results, showing that FS-FEM reduces prediction errors to 78.1% of those observed with FEM. The results highlight FS-FEM as a reliable and efficient tool for accurately predicting the linear performance of LVDTs under practical conditions.

The control discrete equations can be written in the following matrix form

$$\begin{bmatrix} \int_{\Omega}\left[\begin{matrix} v\nabla\times N_i\cdot\nabla\times(\ )+v\nabla\cdot N_i\nabla\cdot(\ ) \\ +j\omega\sigma N_i\cdot(\ ) \end{matrix}\right]d\Omega & \int_{\Omega} j\omega\sigma N_i\cdot\nabla(\ )d\Omega \\ \int_{\Omega_l} j\omega\sigma\nabla N_i\cdot(\ )d\Omega & \int_{\Omega_l} j\omega\sigma\nabla N_i\cdot\nabla(\ )d\Omega \end{bmatrix}\begin{bmatrix}\dot{A}\\ \dot{\varphi}\end{bmatrix} = \begin{bmatrix}\int_{\Omega} N_i\cdot\dot{J}_S d\Omega \\ 0\end{bmatrix} \tag{1}$$

Where Ω represents the eddy problem domain, N_i is the shape function of the element at node i, A_i and ϕ_i are the the vector magnetic potential and the scalar potential at node i, v is the magnetoresistance, ω is the sinusoidally varying angular frequency, $\dot{J}_S$ is the coil current density, and the dots above the field variables indicate that they are complex values.

Keywords: LVDT, Eddy, FEM, Gradient smoothing, FS-FEM, Linear relationship, Prediction

Particle-laden natural convection adjacent to vertical thermal wall

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Particle-laden natural convection is widely present in the atmosphere and water bodies. For instance, particles are transported vertically by natural convection on sunlit building walls, affecting the urban atmosphere. Under the Boussinesq approximation, the governing equations for the particle-laden natural convection are as follows:

$$\nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\frac{1}{\rho}\frac{\partial p}{\partial x} + \nu \nabla^2 \mathbf{u} + \mathbf{g}\beta(T - T_0) + \mathbf{S}_{pM}, \tag{2}$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla)T = \nu \nabla^2 T + S_{pT}, \tag{3}$$

$$\frac{d\mathbf{u}_{P,i}}{dt} = \frac{3\nu C_D \mathrm{Re}_P}{4d_P^2}\frac{\rho}{\rho_P}(\mathbf{u} - \mathbf{u}_{p,i}) + \frac{(\rho_P - \rho)}{\rho_P}(1 - \frac{\rho}{\rho_P})\mathbf{g}. \tag{4}$$

Here, $\mathbf{u}$ and ρ are the velocity and density of the fluid, $\mathbf{u}_{\mathrm{P,i}}$ and ρ_P are the velocity and density of i-th particles. p the pressure, $\mathbf{g}$ the gravitational acceleration, d_P the diameter of particle. $\mathrm{Re_p}$ is the Reynolds number of particle, C_D is the force coefficient, which is a piecewise function depending on $\mathrm{Re_p}$. $\mathbf{S}_{pM}$ and S_{pT} are source terms describing the impact of particles on the flow and temperature fields, respectively.

The transport of particles by the thermal plume adjacent to isoflux-heated walls was investigated numerically. Complex interactions between particles and thermal plumes have been observed, which leads to nonuniform distribution of particles, as shown in Figure 1. Due to the unique flow and temperature profiles of near-wall thermal plumes, these interactions differ from those in the channel turbulence or free turbulence. In this presentation, we will explore the large-scale structures of the plume, particle patterns, and their interactions.

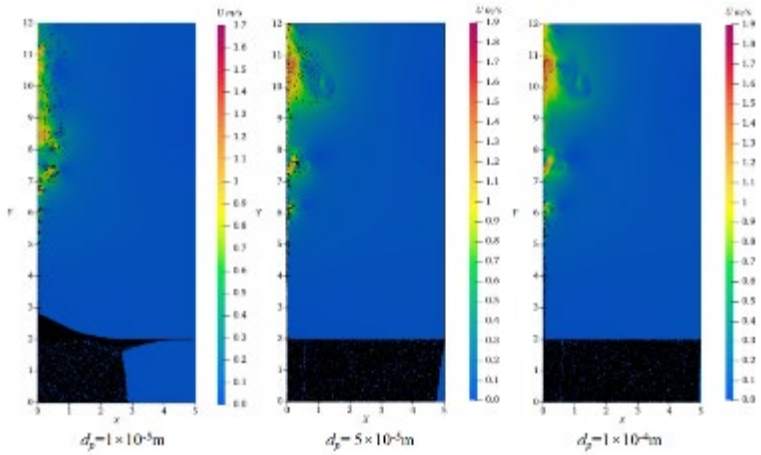

Figure 1. Particles of different size transported by the thermal plume adjacent to isoflux walls. $Ra_q = 3.18\times10^{15}$, $Pr = 0.7$, $\rho_P/\rho = 2250$.

Keywords: boundary-layer flows, thermal plume, clustering, vortex

Stress Distribution and Frequency History of a Shell-Type SRF Cavity Under Frequency Tuning Process

Ming-Chyuan Lin [1*], Yung-Chieh Hsu[2], Meng-Kao Yeh[2] and Chih-Hung Lo[1]

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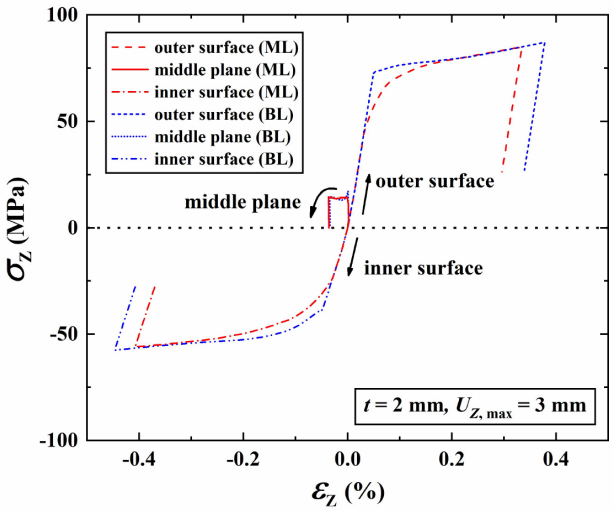
A two-cell superconducting radio-frequency (SRF) cavity is under development in the National Synchrotron Radiation Research Center, Taiwan. This SRF cavity is made of niobium sheet with a target electromagnetic (EM) resonance frequency of 1.5 GHz at its operation temperature of 4.2 K. Due to the machining tolerance, the received SRF cavity has to be tuned to a proper EM resonance frequency at room temperature by longitudinally stretching or compressing the cavity structure to plastic range. The elastoplastic behaviour of the niobium is taken into consideration on the computation model by incremental displacement assignments and kinematic hardening. A multi-physics computation process as consisting of structure deformation and high-frequency EM field computations under the commercial code ANSYS is used to simulate the tuning process. The niobium's stress-strain curve is approached by bilinear and multilinear fittings in the computational model, respectively. The predicted tuning curve with multilinear fitting shows great agreement with the practical one, whereas the bilinear fitting results in a fast computation but with a frequency difference within 50 kHz and higher residual stress. The stress history on the top, middle, and button plane of the shell structure at the iris of the cavity model are examined to show the stress mainly comes from the bending moment, not the longitudinal deformation.



Keywords: Elastoplastic, superconducting RF cavity, stress,

References

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Combining distance field-based boundary condition enforcement and adaptive weight tuning for robust and stable inverse analysis using physics-informed neural networks

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Physics-informed neural networks offer flexible solutions for inverse problems, but boundary conditions and limited data pose challenges. Boundary conditions can be directly encoded into the trial solution, or weights can be tuned to effectively integrate data into the training process. To this end, we modify the loss function used in the literature:

$$\mathcal{L} = \mathcal{L}_{\mathrm{PDE}} + \mathcal{L}_{\mathrm{BC}} + \mathcal{L}_{\mathrm{Data}}, \tag{1}$$

where $\mathcal{L}_{\mathrm{PDE}}$, $\mathcal{L}_{\mathrm{BC}}$, and $\mathcal{L}_{\mathrm{Data}}$ denote residuals of the governing equations, boundary conditions, and observation data, respectively, to the following form:

$$\mathcal{L} = \mathcal{L}_{\mathrm{PDE}} + \lambda_{\mathrm{Data}}\mathcal{L}_{\mathrm{Data}}, \tag{2}$$

where $\mathcal{L}_{\mathrm{BC}}$ is removed by directly encoding the boundary condition into the trial solution. Boundary conditions can be enforced using an implicit distance field [1] and the weight λ_{Data} is tuned adaptively during optimization to avoid tedious and expensive manual tuning [2]. The method is applied to an incompressible flow around a heart-shaped obstacle, which is non-convex geometry. Results shown in Figures 1 and 2 demonstrate the effectiveness of the presented method. We envision that the method can be extended to a wide range of inverse problems.

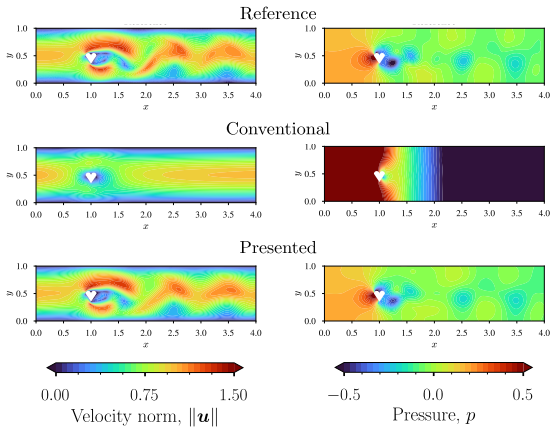

Figure 1.

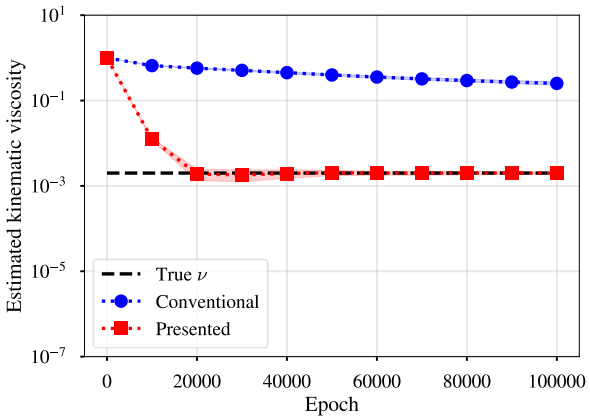

Figure 2.

Keywords: scientific machine learning, physics-informed neural network, inverse analysis

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Automatic differentiation of finite element mesh using a configuration mapping technique

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Differentiable simulation utilizes the automatic differentiation technique to compute derivatives associated with the simulation processes (e.g., finite element (FE) analysis) without manual derivation. In FE-based differentiable simulation, the derivative with respect to the nodal coordinates of an FE mesh is highly desirable and practically useful, yet this issue has received rather limited attention. In this work, we will present a method using the configuration mapping technique that enables the computation of mesh derivatives with automatic differentiation. The implementation of this method is based on the JAX-FEM package [1]. Four applications will be given to demonstrate the strong potential of this strategy. The first application is to optimize a coarse FE mesh to obtain a more accurate solution by considering the mesh derivative of the difference between a manufactured theoretical solution and the numerical solution. The relations between various load cases and the mesh parameters can be obtained using amortized optimization. The second application is about structural shape optimization by directly moving mesh nodal points based on mesh derivative. The third application is to infer the undeformed configuration of a deformed structure by computing the structural displacement in each iterative step with the mesh derivative. The last application is to calculate the energy release rate of a fracturing structure automatically using the mesh derivative.

Keywords: finite element analysis, mesh derivative, automatic differentiation

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Sustainable intralaminar-hybridised natural fibre-reinforced polymer composites – an experimental study for flexural properties under high loading rate

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With the rapid advancement of fibre-reinforced polymer composites (FRPC), the limited research on the high-speed dynamic flexural response on sustainable material combinations suitable for high-performance structures hinders their further applications. In this paper, sustainable composites made from intralaminar-hybridised basalt and flax fabrics, along with their hybrids incorporating carbon fabrics, were fabricated using vacuum assisted resin transfer moulding technique. A modified two-bar Split-Hopkinson Pressure Bar was employed to conduct high-speed three-point bending tests (Figure 1a), while the quasi-static flexural behaviour was assessed with an Instron 5966 electromechanical universal testing machine. Deformation patterns in the dynamic bending tests were captured by using high-speed camera. The damage characteristics (Figure 2), strain rate effects, and energy absorption capability of the different types of FRPCs were then analysed. The results showed that the dynamic flexural properties of the novel basalt, flax, and carbon fibre hybrid composite material outperformed those of the carbon and basalt fibre hybrids, with the ultimate flexural strength reaching over 2,000 MPa at an impact speed of 30.5 m/s, which was 21% higher than its pure carbon fibre reinforced composite counterpart (Figure 1b). It indicates a significant potential for the new materials in resisting high-velocity impacts, making them promising in industrial applications as spacecraft panels, bumpers of racing cars, substitutable bullet proof vessel panels, and so on.

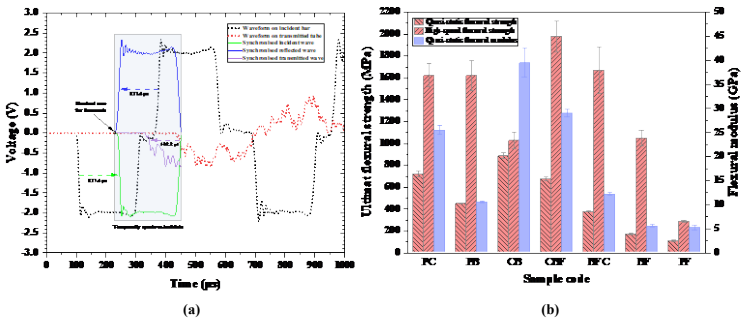

Figure 1. (a) Data process for high-speed flexural test; (b) specific energy absorption for all specimen groups.

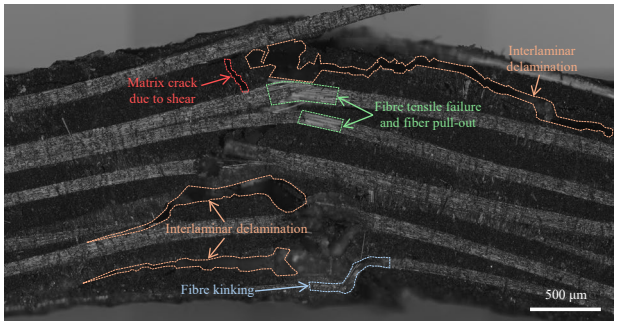

Figure 2. Microscope image of the quasi-static tested carbon fibre specimen.

Keywords: Fibre-reinforced polymer composite, Intralaminar fibre hybridisation, High speed three-point bending test, Split Hopkinson Pressure Bar, Failure mechanism

Image-Based Identification of Finite Element Input Parameters to Simulate Progressive Damage in Composite Materials: Transfer Learning and Interpretability

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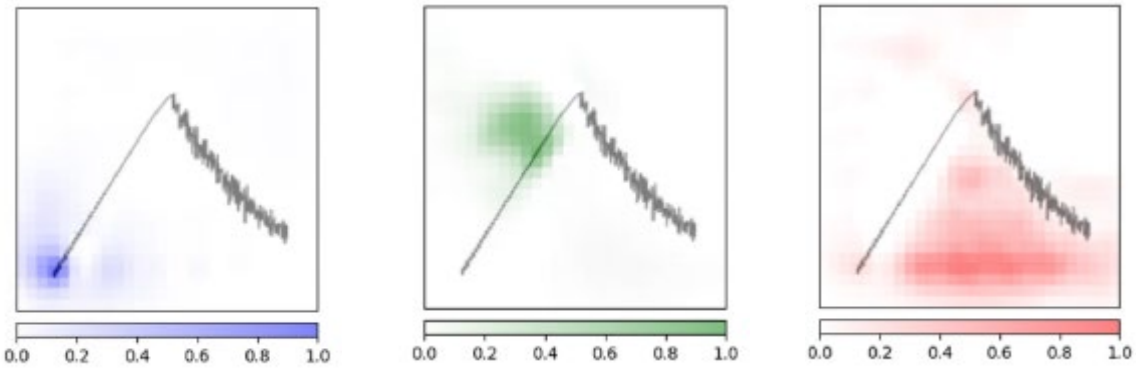
The finite element simulation of progressive damage in fibre reinforced composites is challenging due to the presence of non-linearities across various length scales. Besides the technical challenges, it is important to establish a transparent calibration procedure to determine required input parameters.

This study presents a computational framework based on convolutional neural networks to find suitable input parameters for the simulation of progressive damage by means of continuum damage mechanics. Images of load vs displacement graphs obtained from thousands of simulated compact tension tests on carbon fibre composites are used to apply transfer learning to the pre-trained ResNet-18 model [1]. After training and validation, the neural network is applied to experimental measurements to estimate corresponding simulation input parameters.

In addition, a perturbation-based attribution method using Captum [2] enables the understanding and interpretation of the obtained results. Figure 1 shows the attribution heatmaps where a region with attribution values close to 1.0 indicates that the neural network used the information of this region to estimate a specific input parameter. For example, Figure 1(b) shows that the strength-related simulation input is calibrated based on force values close to the peak of this curve. Most of these results are physically meaningful, and they can provide a visual explanation about the decision process within the convolutional neural networks.



(a) elastic modulus (b) strength (c) energy

Figure 1. Illustration of information used by the convolutional neural network to estimate finite element input parameters.

Keywords: Composites materials, progressive damage, machine learning, parameter identification, interpretability

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Hybrid Torque Control Strategy with Gaussian Process Feedforward for a Novel MRF Dual-Clutch of an Electric Vehicle Transmission

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As a critical component responsible for power transmission, the clutch directly influences the overall vehicle performance, in terms of dynamics, efficiency, safety, and comfort. For EV transmissions based on MRF clutches, clutch engagement and disengagement are managed by adjusting the input current to the clutches, allowing for connecting different gears and altering the transmission ratios [1]. However, MRF clutches exhibit pronounced nonlinear and rate-dependent hysteresis between the input current and output torque , significantly affecting the accuracy of the MRF clutch's torque output [2], especially when precise control is requested quickly, such as dynamic torque tracking and clutch-shifting. Therefore, developing a precise torque control strategy that can address the nonlinear rate-dependent hysteresis issues associated with MRF clutches is crucial.

This study focuses on developing a precise torque control strategy for a novel MRFDC of an EV transmission, considering its inherent hysteresis on the current control input as well as its changing rate. The strategy is a hybrid control strategy combining a pure PI feedback control and a GP-based hysteresis inverse model compensator. The pure PI controller is employed to mitigate the effects of model errors, uncertainties, and disturbances. Meanwhile, a GP-based hysteresis inverse model, with the required torque and its change rate serving as the input, is proposed as a feedforward compensator to obtain compensation current commands considering the rate-dependent hysteresis. The effectiveness of the proposed hybrid control strategy is validated through a series of dynamic tracking and clutch-shifting experiments performed on a prototype MRFDC EV transmission platform. Figure 1 provides the experimental setup and the proposed hybrid controller.

(a) (b)

Figure 1: Block diagram of (a) experimental setup and (b) the hybrid controller.

Keywords: Magnetorheological Fluid Clutch, Electric vehicle transmission, Nonlinear and rate-dependent hysteresis, Hysteresis compensation, Gaussian process

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Level-set topology optimisation with distributed unfitted finite elements and automatic shape differentiation

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Unfitted finite element methods enable integration over a sharp boundary without introducing additional degrees of freedom into a numerical discretisation [1]. These methods are of particular interest in fluid dynamics and, more recently, topology optimisation as they are able to overcome two main challenges in existing methods: (1) Boundary smoothing in conventional level-set methods where integration is relaxed over the whole computational domain can lead to undesirable computational artifacts, particularly in the case of non-linear behaviour or fluid-structure interactions; and (2) Differentiation in a smoothed-boundary regime is unable to fully capture the derivative of a functional under a perturbation of the boundary [2].

In this talk, we extend the shape calculus results developed by Berggren [3] to cases where the interface and background domain boundary intersect and link these theoretical results to automatic shape differentiation for unfitted discretisations. We implement the analytic shape derivatives and unfitted automatic shape differentiation in the Julia package GridapTopOpt [2] and show that the analytic shape derivatives derived by Berggren [3] can be recovered to machine precision regardless of the mesh size. We demonstrate the applicability of the unfitted automatic shape differentiation framework and our implementation by considering the three-dimensional minimum compliance topology optimisation of a linear elastic wheel and a linear elastic structure in a fluid-structure interaction problem with Stokes flow.

The software is open source and available at https://github.com/zjwegert/GridapTopOpt.jl.

Keywords: Shape calculus, automatic differentiation, unfitted finite element methods, CutFEM, memory-distributed computing

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AI-Accelerated Reactive Molecular Dynamics Simulation for Optimizing Epoxy Crosslinking in Fibre Reinforced Polymers

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Fiber reinforced polymers are advancing civil engineering with lightweight, corrosion-resistant solutions for bridge retrofitting, seismic reinforcement, and sustainable construction. In fibre reinforced polymers, the crosslinking reaction of the resin matrix dictates the material's mechanical properties, durability, and thermal stability. Reactive molecular dynamics simulations serve as a powerful tool for investigating the microscopic mechanisms of epoxy resin crosslinking. However, these simulations are highly computationally intensive, particularly for complex crosslinking systems, often resulting in multi-month runtimes and substantial computational resource consumption.

Reactive forcefields can simulate the formation and breaking of chemical bonds during crosslinking reactions, making them particularly well-suited for studying the crosslinking behaviour of polymers such as epoxy resins. In fibre reinforced polymers, these crosslinking reactions govern the resin's network structure, directly impacting its mechanical strength and adhesion to reinforcing fibres. By leveraging reactive forcefields, the molecular behaviour of the resin during the curing process can be captured in detail, enabling predictions of crosslinking degree, network structure, and material properties. In reactive molecular dynamics simulations, the system's energy is decomposed into various contributions and computed using the following equation:

$$E = E_{bond} + E_{over} + E_{under} + E_{lp} + E_{val} + E_{tor} + E_{van\ der\ Waals} + E_{Coulomb} \quad (1)$$

In the equation, E_{bond} (bond energy), E_{over} (over-coordination penalty energy), E_{under} (under-coordination penalty energy), E_{lp} (lone pair energy), E_{val} (valence angle energy), E_{tor} (torsion angle energy) are bond-order dependent terms. $E_{\text{van der Waals}}$ (van der Waals energy) and E_{Coulomb} (Coulomb energy) are non-bonded terms.

We developed an AI-accelerated hybrid molecular dynamics framework that integrates reactive and consistent-valence forcefields, significantly reducing computational costs and accelerating simulation speed. Our machine learning model, trained on 50,000 atomic environments, enables real-time charge prediction during crosslinking molecular dynamics simulations. By strategically replacing reactive forcefield relaxation phases with AI-optimized consistent-valence forcefield simulations, our approach accelerates dynamics while maintaining chemical accuracy. A Python-based integration synchronizes AI-driven charge predictions, reactive forcefield-based crosslinking reaction steps, and consistent-valence forcefield molecular dynamics equilibrium phases into an automated workflow. This approach drastically reduces computational costs by minimizing reactive forcefield usage while preserving mechanistic insights into bond formation and network evolution. Our case study demonstrates that the developed framework achieves orders-of-magnitude speedup in modelling epoxy crosslinking

processes. Specifically, we simulate an epoxy resin crosslinking system using molecular dynamics simulations. The model includes epoxy monomers (DGEBA) and curing agents (DETA), with the crosslinking reaction following an amine-epoxide reaction mechanism. This advanced computational methodology provides an efficient approach for optimizing the interfacial properties of fibre-reinforced polymers.

Keywords: Fibre reinforced polymers, Epoxy crosslinking, Molecular dynamics simulation, Reactive forcefield, Machine learning

Active learning assisted stochastic multi-physical free vibration analysis of sandwich magneto-electro-elastic composites

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Sandwich magneto-electro-elastic composites, as one of the most crucial types of smart materials, have significantly innovated the modern intellectual community [1]. They exhibit muti-physical coupling between magnetic, elastic, and electric fields, possessing unique features such as self-sensing, self-healing, self-actuating capabilities, and exceptional energy conversion properties. Today, sandwich magneto-electro-elastic structures are widely used in renewable energy, automotive, aerospace, robotics, and biomedical engineering disciplines, including applications like sensors for health and usage monitoring systems, energy harvesting materials, and vibration dampers.

The investigation of vibrations in sandwich magneto-electro-elastic composites is one of the most critical tasks in the overall dynamic system of smart materials, as it allows undesirable dynamic behaviour to be minimized to the greatest extent possible. Additionally, multifaceted physically inspired uncertainties inherently exist in the real engineering applications. However, existing research on the multi-physical responses of sandwich composites primarily focuses on deterministic behaviour, where a deterministic model, neglecting intrinsic randomness, serves only as an approximation of realistic structural responses.

Therefore, this research performs a stochastic multi-physical free vibration analysis of sandwich magneto-electro-elastic composites, considering multi-dimensional uncertainties with various distributions. An active learning strategy, specifically the sequential design of experiment enhanced adaptive Kriging [2], is introduced to describe the intricate relationship between intrinsic uncertainties and the multi-physical vibration response. Comprehensive statistical information regarding the dynamic behaviour of smart composites, including the mean, standard deviation, probability density function, and cumulative distribution function, is provided for safety assessment and serviceability limit state design. In numerical experiments, the presented strategy demonstrates greater accuracy and efficiency compared to existing machine learning workhorses. Besides, the developed technique is competent to furnish accurate multi-physical vibration response forecasts under quickly changing conditions, enabling real-time dynamic behaviour surveillance in practical engineering implementation.

Keywords: Sandwich magneto-electro-elastic composites, multi-physical free vibration investigation, stochastic analysis, physically inspired multi-dimensional uncertainties, active learning.

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Operational Safety Assessment of High-Speed Trains in Canyon Wind Environments

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When high-speed trains cross bridge-tunnel transitions in canyons, sudden terrain-induced airflow compression causes sharp aerodynamic load variations on the train surface, critically affecting stability and safety. This study develops a CFD/MBD coupled framework integrating a 3D canyon wind field model for simulations. Comparative analysis between uniform and canyon wind fields reveals transient load distributions and flow dynamics, confirming the necessity of terrain-specific wind modeling. A quantitative model linking train speed, wind velocity, and aerodynamic forces is established.

The computational domain is divided into five subdomains to simulate the complete bridge-tunnel transition in canyons: 1) train startup zone, 2) pre-canyon tunnel, 3) central bridge section with canyon wind effects, 4) post-canyon tunnel, and 5) external zone. The characteristic length is defined as the vertical profile height (H=3.55m) from the train floor to roof, which is shown in figure.1.

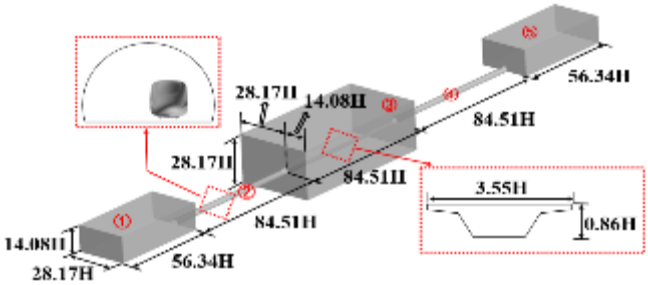

Figure 1. Schematic diagram of the computational domain

The canyon wind model and system dynamics equations are formulated in Equations (1) and (2), respectively.

$$\begin{cases} U = U_u \times \left(\dfrac{x-380}{30}\right)^{0.3}, & 380 \le x \le 350 \\ U = U_u, & 350 < x \le 650 \\ U = U_u \times \left(\dfrac{680-x}{30}\right)^{0.3}, & 650 < x \le 680 \end{cases} \tag{1}$$

$$\mathbf{M}(q)\ddot{\mathbf{q}} = \mathbf{f}(q,\ddot{q},\lambda,t) - \mathbf{G}^{\mathrm{T}}(q)\lambda \tag{2}$$

where U denotes the canyon wind velocity, U_u represents the uniform wind speed,xdefines the tunnel exit position, q is the generalized coordinate vector, M(q) signifies the configuration-dependent symmetric mass matrix, $G^T\lambda$ encapsulates constraint forces, and fincorporates applied forces.

Keywords: High-speed train, canyon wind model, vehicle dynamics, safety analysis.

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Dynamic Numerical Simulation Analysis of Coupled Airflow and Thermal Fields in Zinc Rotary Kiln

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Reducing carbon emissions in zinc metallurgy necessitates advanced modeling tools for optimizing rotary kiln operations [1]. This study establishes a COMSOL-based digital twin framework that accurately predicts coupled flow-thermal behavior in rotary kilns, offering a transformative tool for industrial optimization. The proposed framework achieves simultaneous resolution of fluid dynamics and heat transfer by rigorously accounting for the interactions between gas flow, material heating, and kiln rotation dynamics.

A 3D geometric model of the kiln was constructed, incorporating rotational dynamics and material transport. The simulation integrates turbulent flow via the standard k−ε model and non-isothermal heat transfer, with boundary conditions calibrated to industrial data. The simulation features multi-physics coupling, resolving fluid dynamics and heat transfer simultaneously to capture interactions between airflow, material heating, and kiln rotation. Additionally, temperature-dependent material properties are incorporated, defining the zinc-carbon mixture and air with variable thermal conductivity and density to reflect real-world behavior.

The simulation reveals critical insights into airflow patterns, thermal distribution, and process optimization. Inlet gas forms vortices near the feed zone (Figure 1) before stratifying into upper high-temperature and lower high-velocity layers along the kiln axis, with velocity decreasing at the outlet due to thermal expansion and friction. Temperature peaks higher in the central and upper regions due to radiative heating from the kiln lining, while the lower zone remains cooler. Optimized boundary conditions reduced temperature prediction errors by 18% compared to initial models. Additionally, the model identifies inefficient heat transfer zones, enabling targeted adjustments to airflow and material feed rates, which could potentially reduce energy consumption by 12% in industrial trials.

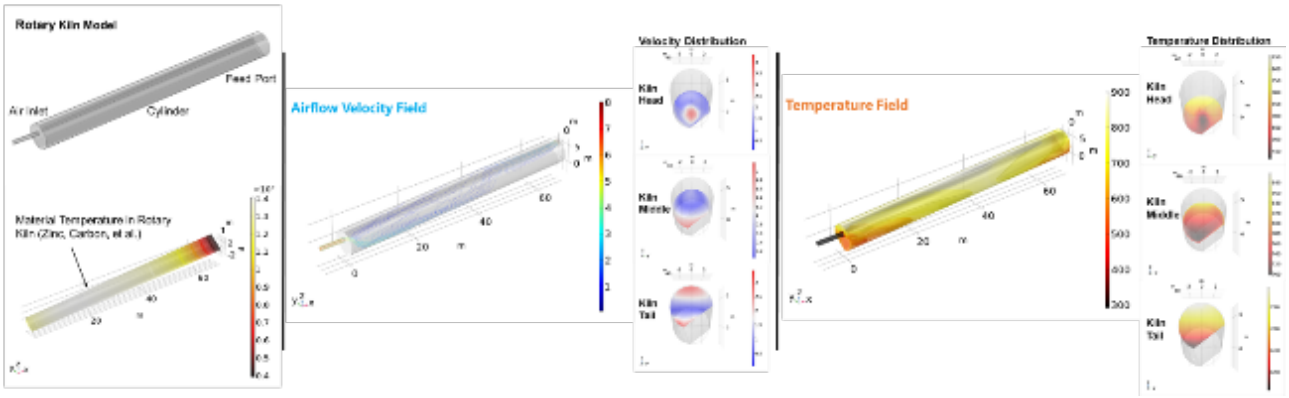

Figure 1.

Keywords: Rotary kiln, digital twin, multi-physics simulation, coupled fields analysis

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Synthetic Data-Driven Fault Diagnosis Approach to Overcome Data Scarcity in the Design Phase of Engineered Systems

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The dearth of data for training artificial intelligence models becomes a major obstacle to the seamless development of health diagnostic models for mission-critical and safety-related engineered systems. To solve this problem, diagnostic models are commonly developed using transfer learning and simulation models. However, it is difficult to ensure the reliability of the diagnostic models when the target and source distributions are misaligned or when the generated data is insufficient [1]. This study proposes a sub-label-guided transfer networks for the health diagnostics of rotating machines. Low-fidelity data is generated by incorporating domain knowledge while high-fidelity data are generated through a simulation model. A sub-label-guided transfer network was developed to maximize the effective use of the generated multi-fidelity data. The validation results using experimental data shows the effectiveness of the proposed method.

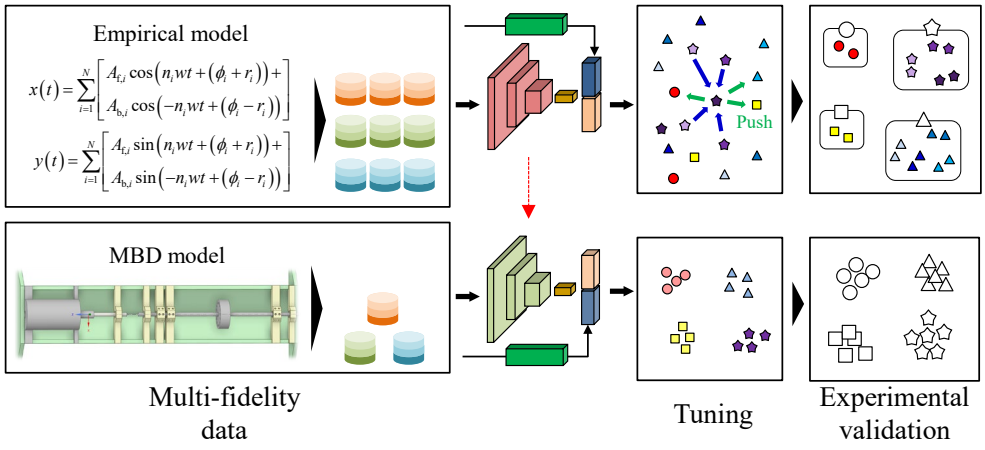

Figure 1. Proposed Sub-label-guided transfer networks [2]

Keywords: Artificial-intelligence-based fault diagnosis, transfer learning, multi-fidelity, data augmentation

Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. RS-2025-00517566).

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Eulerian Elastoplastic Simulation of Structures with Micro-Voids

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Micro-voids commonly found in materials such as concrete, porous ceramics, and polymer foams arise during construction or manufacturing processes and have a profound impact on their mechanical behavior. These voids influence not only the local stress distribution but also amplify stress concentrations and accelerate the progression of plastic deformation, thereby posing significant challenges for conventional Lagrangian finite element methods. Specifically, accurately modeling voids with complex and irregular geometries is hindered by the difficulties associated with generating conforming meshes. Furthermore, large deformation simulation using Lagrangian methods are prone to severe element distortion, often leading to numerical instabilities, reduced accuracy, and in some cases, premature simulation failure.

To address these limitations, we introduce an Eulerian elastoplastic simulation framework that employs spatially fixed orthogonal meshes, effectively decoupling the computational grid from material deformation. By eliminating the need for frequent remeshing, this approach facilitates robust and efficient modeling of materials with intricate internal void structures, even under large deformation conditions. Numerical simulations validate the proposed method, demonstrating its capability to quantitatively assess the effects of voids on stress concentration, localized plastic deformation, and overall material behavior. Key findings emphasize the critical role of void characteristics, such as size, shape, and spatial distribution, in determining the overall structural performance of the material under various loading conditions.

This study establishes a novel and versatile computational framework for analyzing the mechanical behavior of materials containing internal voids. The results provide valuable tools and insights for advancing material design, enabling more accurate structural performance evaluation, and supporting the development of lightweight, high-strength materials for practical applications.

Keywords: Eulerian Structural Simulation, Void, Structural Analysis, Supercomputing

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A Scalable Boundary Finite Element Method Coupled with ABAQUS for Dynamic Analysis of Large-Scale Complex Systems with Interacting Dynamics

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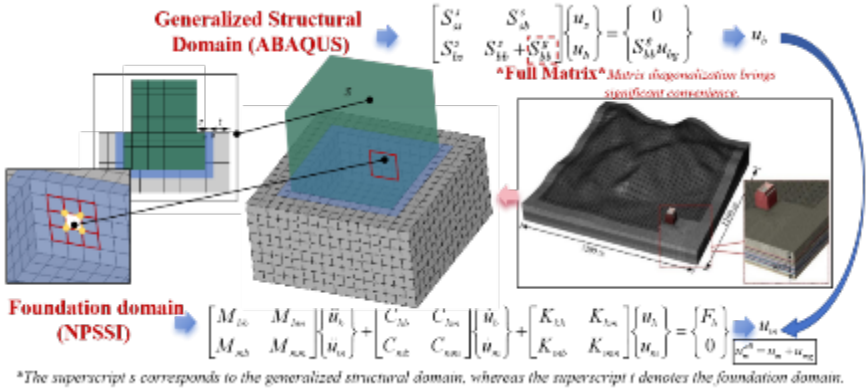
To conduct a reasonable and effective analysis of the dynamic effects of soil-structure interaction (SSI) on the seismic response of complex structures, it is crucial to accurately simulate the radiation conditions of the infinite domain. In this context, the Scaled Boundary Finite Element Method (SBFEM) exhibits significant advantages. The complexity of the interaction system is primarily reflected in three aspects: the intricate structural configurations, diverse element types, and special constraint conditions such as rigid regions or coupling; the presence of various nonlinear mechanical properties within the generalized structural body; and the substantial differences in stiffness and scale among elements in the overall mechanical matrix.

Based on the dynamic infinite-domain model of SBFEM, this study proposes two approaches for developing efficient numerical solution techniques: one fully relying on the ABAQUS platform and the other partially coupled with it, designed for ultra-large-scale interaction analyses. Specifically, a frequency-domain harmonic response technique is employed to develop a block-wise decomposition strategy for the dynamic impedance matrix of the foundation, effectively diagonalizing the foundation's stiffness contributions to the structure. To address the time-domain stability challenges posed by bidirectional seismic excitation in the foundation domain, a substructure mode-based input method is proposed, where the total field motion in the foundation is decomposed into the sum of the input free-field motion and the scattered interaction field. The proposed strategy ensures the computational integrity of the structural side within the ABAQUS platform while eliminating the need for ABAQUS to explicitly provide the dynamic matrix formulation. Finally, numerical experiments are conducted to validate the feasibility of the two proposed implementation strategies. The results demonstrate that the proposed method significantly enhances the computational capacity for solving complex soil-structure interaction problems and provides a viable technical approach for the dynamic response analysis of ultra-large-scale structural systems.



*The superscript s corresponds to the generalized structural domain, whereas the superscript t denotes the foundation domain.

Figure 1.Numerical model of Coupling system and large-scale reactor building-mountain system (the degree of freedom is 11,320,212).

Keywords: Scaled Boundary Finite Element Method; Soil-Structure Dynamic Interaction; Large-Scale Engineering Numerical Analysis; Dynamic Response of Complex Structures; ABAQUS Coupling Programming.

Background Grid-Based Coarsening Technique for Computational Acceleration of the Stabilized LSMPS Method

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Particle methods have gained attention as a computational technique for complex moving boundary problems like free surface flows. However, their uniform spatial resolution across entire domains leads to high computational costs for problems with large scale gaps. To address this challenge, we developed a novel variable resolution method.

Our method uses background grids to generate multi-level coarse particles where high resolution is unnecessary. Fine particles are placed throughout the domain, with larger coarse particles superimposed in low-resolution regions identified by boundary distance (Fig. 1). These coarse particles compute representative values for underlying fine particles. Background grids with spacing twice the fine particle size enable systematic coarse particle placement. Multi-level coarsening is achieved recursively, with particle size doubling at each level, as shown in Fig. 2 (two-dimensional dam break).

The computational procedure involves: (1) generate coarse particles based on boundary distance, (2)

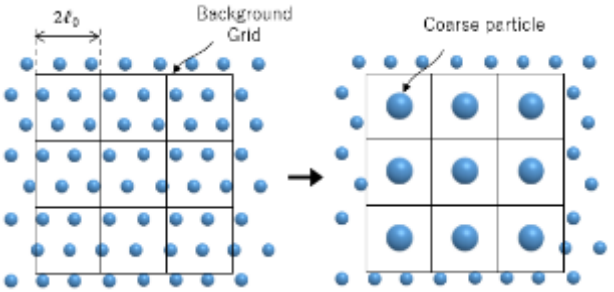

Figure 1.

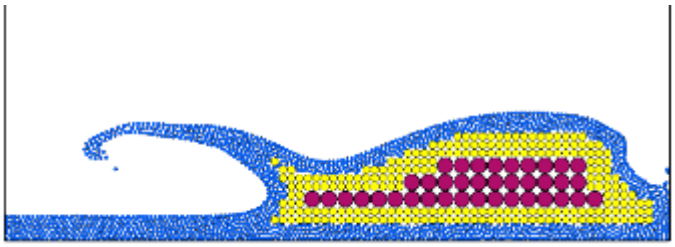

Figure 2.

map velocities from fine to coarse particles, (3) calculate velocities and pressures of representative particles, which are non-coarsened fine particles and particles that will not be further coarsened, using the stabilized LSMPS method [1], (4) update positions of fine particles, and (5) map velocities from coarse to fine particles. The accuracy of this method is maintained by using the least-squares moving particle semi-implicit (LSMPS) scheme for interpolation and mapping operations [2].

Verification using a two-dimensional cavity flow confirmed that this method reduced the number of particles from 1600 to 721, resulting in decreased computational time while approximately preserving accuracy. The proposed method has been extended to more complex problems including free surface flows and three-dimensional analyses. These results will be presented at the conference.

Keywords: computational fluid dynamics, particle method, multi resolution, least squares method

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Extension of Weighted Equation Physics-Informed Neural Networks to Shallow Water Problems

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The shallow water equations (SWEs) are extensively employed in flood analysis; however, their discontinuity characteristics pose significant challenges to the analysis process. Physics-informed neural network (PINN) [1], is a promising method for solving SWE. However, while PINN efficiently handles continuous solutions, it struggles with discontinuities due to the inability to compute the derivatives by automatic differentiation. This work employs a "retreat to advance" [2] strategy to redirect the model's focus from the discontinuity to the smooth area. This approach formalizes the loss function as follows:

$$\mathcal{L} = \omega_{\text{PDE}}\mathcal{L}_{\text{PDE}} + \omega_{\text{RH}}\mathcal{L}_{\text{RH}} + \omega_{\text{IC}}\mathcal{L}_{\text{IC}} + \omega_{\text{BC}}\mathcal{L}_{\text{BC}}; \quad \mathcal{L}_{\text{PDE}} = \frac{1}{N_{\text{PDE}}}\sum_{i=1}^{N_{\text{PDE}}}\left(\lambda_1 \widehat{\text{G}}(\boldsymbol{x};\boldsymbol{\theta})\right)^2 \tag{1}$$

$\mathcal{L}$ is the overall loss, the term $\mathcal{L}_i$ presents the loss of governing equations (PDE), Rankine-Hugoniot (RH) relation, initial conditions, and boundary condition, respectively. ω_i are the coefficients used to balance the loss function terms. $\widehat{\text{G}}$ is the residual of governing equations, with $\boldsymbol{x}$ is the vector of the input value, and $\boldsymbol{\theta}$ is the training parameters vector. λ_1 is the physics-informed pointwise weights used to redirect the model focus. N_{PDE} is the number of PDE's residual points.

By using this strategy, the model will pay less attention to the discontinuity, naturally inducing strong discontinuity solutions without directly modeling the shock. On the other hand, PINN-WE integrates the RH derived from the weak formulation of conservation laws as localized constraints near shock regions to ensure the conservation law within the shock. The results in Figures 1 demonstrate that PINN-WE outperforms standard PINN in capturing shock dynamics without artificial dissipation, highlighting its potential for complex flow simulations and higher-dimensional applications.

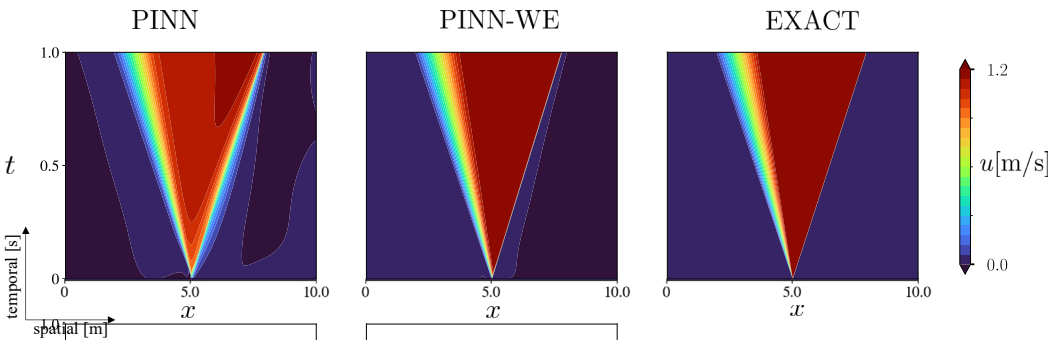

Figure 1.

Keywords: shallow water problems, physics-informed neural network, discontinuity treatment.

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Efficient Topology Optimization with CutFEM and Moving Morphable Component Method for Complex Geometries and Boundary Conditions

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Topology optimization has become a crucial approach in engineering design by allocating materials effectively to optimize structural performance. However, current methods still struggle with issues such as limited geometric complexity, a large number of design variables, strong mesh dependence, and ambiguous boundary treatments, which restrict their applicability in complex scenarios. In this work, we introduce an innovative method that combines the Cut Finite Element Method (CutFEM) and the Moving Morphable Component (MMC) method, enhanced by Nitsche's method, to effectively address these challenges. Our approach not only improves computational efficiency by avoiding the repeated regeneration of the background grid, but also significantly enhances geometric accuracy through high-precision processing of interfaces. To demonstrate the effectiveness of our method, we conducted numerical experiments on a series of benchmark problems including cantilever beams, minimum compliance under uncertain boundary constraints, and multi-material topology optimization. The results indicate that our method outperforms traditional topology optimization techniques in terms of computational efficiency and accuracy. Overall, this study provides a robust and efficient strategy for addressing complex structural design challenges, particularly in multi material and multi physics topology optimization.

Keywords: CutFEM, MMC, topology optimization, Nitsche's method, multi-material, complex geometries, boundary conditions

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Boundary-enhanced physics-informed neural network technique for solving partial differential equations

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In deep learning, solving PDEs using physics-informed neural networks (PINNs) [1] has gained significant popularity. Boundary conditions serve as crucial physical information in PINNs, greatly affecting the predictive performance. We introduce a Boundary enhanced Physics-Informed Neural Network (BG-PINN), a novel framework designed to improve the accuracy of PDE solutions, particularly at domain boundaries. Building upon the foundation of PINNs and g-PINNs [2], BG-PINN incorporates soft boundary constraints by embedding derivative information of boundary conditions into the loss function. The derivative constraints are derived through two primary mechanisms: (1) Explicit Gradient Constraints: direct computation of directional derivatives along boundary tangents by differentiating PDE-prescribed boundary conditions; (2) Implicit Gradient Constraints: inference of hidden gradient terms through physical and geometric properties in free boundary problems, where PDEs lack explicit boundary specifications.

The effectiveness of BG-PINN is demonstrated through real-world case studies, including the Poisson equation, Elasticity equations, Burgers' equation, and Navier-Stokes equations. Comparative numerical experiments show that BG-PINN achieves significantly higher accuracy than traditional PINNs, underscoring its potential for solving complex problems particularly in the accuracy in boundary regions, and free boundary problems governed by partially known physical laws.

$$\frac{\partial \sigma_x}{\partial x}+\frac{\partial \tau_{xy}}{\partial y}+f_x=0,\quad \frac{\partial \sigma_y}{\partial y}+\frac{\partial \tau_{xy}}{\partial x}+f_y=0 \tag{1}$$

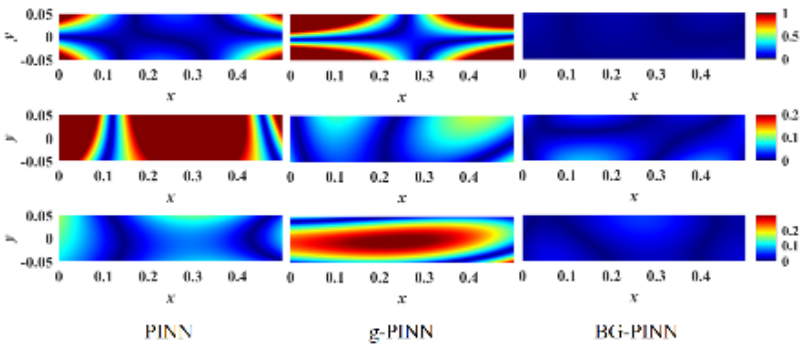

Figure 1. Absolute error contours of stress fields of the pure bending beam problem.

Keywords: Machine learning, boundary-enhanced, physics-informed neural network, explicit gradient constraints, implicit gradient constraints.

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Two-dimensional Failure Envelopes of Conical Footings on Clay

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The stability of shallow foundations on soft clay is a critical concern in offshore geotechnical engineering. Conical footings, owing to their geometric advantages, offer a promising alternative to conventional flat foundations. This study investigates the bearing capacity of conical footings under combined loading, with the objective of establishing two-dimensional failure envelopes that define their ultimate limit states. While previous research has primarily focused on the bearing capacity of strip and circular footings, studies addressing conical footings remain limited. Failure envelopes for flat foundations have been well-documented through plasticity-based solutions, finite element analyses, and physical testing. However, the effects of conical angle on failure mechanisms and load interaction are not yet fully understood. This study systematically investigates how critical factors affect the shape and size of the failure envelopes. Finite element limit analysis is employed to model the response of conical footings on undrained clay, with the soil idealised as a perfectly plastic material following the Tresca yield criterion.

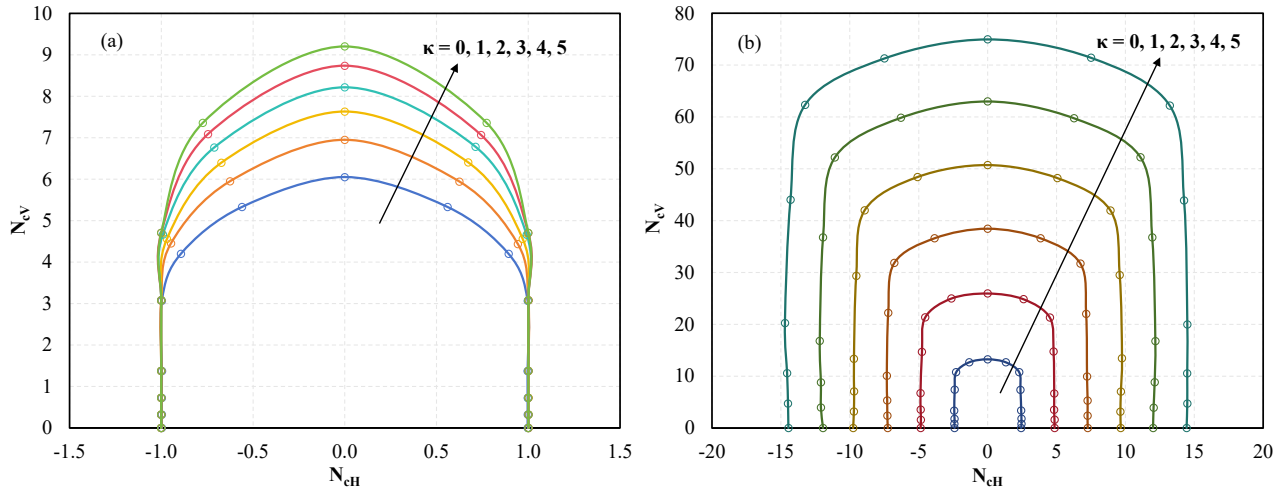

Figure 1 Effect of anisotropy parameter κ on the combined failure envelopes: (a) d/D = 0; (b) d/D = 1

Figure 1 illustrates the failure envelopes of a footing (conical angle β = 180° and roughness coefficient α = 1) under combined vertical and horizontal loading in clay soils. The analysis considers varying embedment ratios (d/D = 0 and 1, where d is the embedment depth and D is the foundation diameter) and strength anisotropy parameter κ ranging from 0 to 5. The results show that increasing the strength anisotropy parameter κ significantly enlarges the failure envelope, particularly for the case of d/D = 1, demonstrating the beneficial effect of strength enhancement with depth. When d/D = 0, the strength anisotropy has little influence on N_{ch} due to the lack of confinement and mobilised side resistance. The embedment ratio d/D notably improves the footing performance by enlarging the failure envelope in both horizontal and vertical directions, primarily due to increased confinement and overburden pressure.

Through a systematic study on the critical influencing factors, some valuable insights into the evaluation of bearing capacity for conical footings in clay soils are obtained.

Keywords: Conical footing, failure envelope, clay, limit analysis, offshore foundation

Toward Quantum Speedup in Simulating Real-time Dynamics of Coupled Dissipative Classical Oscillators

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Real-time dynamics of coupled classical oscillators systems with dissipations have important applications in engineering science, with power systems as a prominent example [1]. Quantum computers offer great potential to speed up these simulations as compared to their classical counterparts. Recently, an exponential speedup has been established for simulating the real-time dynamics of coupled classical oscillators on a quantum computer [2]. However, whether such a quantum speedup will be maintained for important cases of dissipative dynamics of coupled oscillators is unclear. We consider the following dissipative classical oscillator dynamics equation

$$\ddot{\boldsymbol{I}}(t) + A\dot{\boldsymbol{I}}(t) + B = 0 \tag{1}$$

for $\boldsymbol{I}(t)$ being a vector of system variables of length N that one would like to solve as a function of time t. A, B are given matrices of $N \times N$ that govern the underlying dynamics. A dilation technique is proposed to recast the dissipative dynamics in (1) into unitary dynamics at an enlarged space governed by the Schrodinger's equation

$$i\hbar|\dot{\Psi}(t)\rangle = H|\Psi(t)\rangle \tag{2}$$

where the original unknown $\boldsymbol{I}(t)$ is mapped to a wave function $|\Psi(t)\rangle$ with $O(n)$ qubits for $n = log_2(N)$ to be solved. The Hamiltonian H can be constructed in terms of A and B. An efficient fully coherent quantum signal processing (QSP) algorithm combined with the qubitization technique [3] is constructed to solve (2) on a quantum computer by performing a polynomial transformation on a block-encoded H, which in turn gives the solution to the original system dynamics $\boldsymbol{I}(t)$. It is established that to achieve error of ϵ on the simulation, the quantum circuit depth scales as $O\left(\alpha\, t + log\left(\frac{1}{\epsilon}\right)\right)$. The constant α depends on the norm of the Hamiltonian H.

We apply the developed quantum algorithm to a minimal transmission line model with realistic parameters on resistance R, conductance L, and capacitance C as a demonstration. Results from noiseless and noisy emulation with execution on a quantum hardware will be presented. Complexity and resource analysis will be presented for extended models of transmission lines. We will also discuss quantum simulation complexity for generic power systems.

Keywords: quantum algorithms, classical oscillator, dissipative dynamics, quantum signal processing, speedup, quantum linear algebra

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Multiscale modelling of recycled PET and PETG using fused granulate fabrication

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The adoption of fused granulate fabrication (FGF) for large-scale 3D printing using recycled polyethylene terephthalate (rPET) and recycled polyethylene terephthalate glycol (rPETG) presents a promising pathway for sustainable manufacturing [1]. However, the mechanical performance of FGF-printed materials is significantly influenced by printing parameters and interlayer bonding, leading to variability in tensile properties. While experimental studies provide valuable insights, a robust numerical framework is required to accurately predict mechanical behaviours across different printing parameters for optimisation.

This study develops a finite element-based multiscale modelling and analysis approach to evaluate the effects of printing parameters and interlayer bonding on the tensile properties of FGF-printed rPET and rPETG components. The rule of mixtures is utilised as a core mathematical model to estimate the effective mechanical properties at mesoscale. By integrating material characterisation data with finite element modelling and simulations, the multiscale model extracts both upper and lower bounds of tensile strength, effectively capturing the experimental variability observed in printed parts. The results demonstrate that the developed multiscale modelling and analysis approach successfully encompasses most experimental data within a satisfactory range, validating its effectiveness in predicting tensile performance. It offers a reliable tool for optimising FGF printing conditions, reducing the need for extensive experimental trials. Furthermore, the established optimisation and simulation methodology can be extended to other recycled polymer systems, advancing the development of sustainable additive manufacturing solutions.

Keywords: 3D printing, fused granulate fabrication (FGF), printing parameters, numerical analysis, sustainability, tensile properties

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A Data-driven Model for Predicting Railway In-train Forces

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Railway in-train forces are critical for ensuring safe and efficient train operations. However, real-time monitoring of these forces across multiple couplers in various trains remains challenge due to variations in train configurations and coupler locations. We propose In-trainNet, a two-step data-driven framework that leverages automatic train operation system to enhance in-train forces monitoring. In the first step, a specially designed multi-task model is pre-trained to simultaneously estimate multiple in-train forces on multiple couplers for a specific train configuration. In the second step, a transfer learning scheme transfers and adapts the pre-trained model to different train configurations, significantly reducing the need for extensive training data and computational resources. Comparative experiments demonstrate the superior performance of the pre-trained model, which achieves higher accuracy and efficiency compared to single-task models. The integration of transfer learning further enhances the framework's adaptability, enabling robust and accurate monitoring across diverse train configurations. The proposed approach offers a promising solution for real-time, in-situ monitoring of railway in-train forces, with potential applications in both research and industrial applications.

Mechanical analysis of opto-electro-thermo-elastic perovskite structures

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Metal-halide perovskites are emerging photostrictive, electrostrictive, and piezoelectric smart and energy materials, which are promising candidates for next-generation solar cells and photoelectric technologies. However, their static and dynamic structural behaviours considering opto-electro-thermo-mechanical properties in multi-physics fields have not yet been fully understood, thus limiting their engineering applications.

This work proposes a new opto-electro-thermo-elastic constitutive model (Eq 1) taking into account photostriction, photothermal effect, electrostriction, and piezoelectricity for lead halide perovskites and investigates their static and dynamic opto-electro-thermo-mechanical behaviours.

$$\{\sigma_i\}=\left[Q_{ij}\right]\left(\{\varepsilon_j\}-\{\beta_j\}I_L-\{\alpha_j\}\Delta T_L-\{\eta_j\}E_Z^2-\{d_{3j}\}E_Z\right) \tag{1}$$

where $\{\sigma_i\}$ is total stress vector; $[Q_{ij}]$ represents the stiffness matrix of perovskite structures; $\{\varepsilon_j\}$ denotes mechanical strain vector; $\{\beta_j\}$, $\{\alpha_j\}$, $\{\eta_j\}$, and $\{d_{3j}\}$ are photostrictive coefficient vector, thermal expansion coefficient vector, electrostrictive coefficient vector, and piezoelectric coefficient vector, respectively.

The governing equations (Eq 2) of perovskite plates are derived within the theoretical framework of first-order shear deformation theory and numerically solved by using the differential quadrature method.

$$\left(\left[\mathbf{K_L}\right]+\left[\mathbf{K_{NL}}\right]-p\left[\mathbf{K_p}\right]-I_L\left[\mathbf{K_I}\right]-\Delta T_L\left[\mathbf{K_T}\right]-E_Z^2\left[\mathbf{K_E}\right]-E_Z\left[\mathbf{K_{PE}}\right]\right)\mathbf{d}+\left[\mathbf{M}\right]\ddot{\mathbf{d}}=f\left[\mathbf{V}\right] \tag{2}$$

where $[\mathbf{K_L}]$ and $[\mathbf{K_{NL}}]$ are the linear and nonlinear elastic stiffness matrices, respectively; $[\mathbf{K_p}]$, $[\mathbf{K_I}]$, $[\mathbf{K_T}]$, $[\mathbf{K_E}]$, and $[\mathbf{K_{PE}}]$ are the geometric stiffness matrix; $[\mathbf{M}]$ represents the mass matrix; $[\mathbf{V}]$ is the geometric stiffness vector with respect to transverse distributed force.

Comprehensive parametric studies are carried out to examine the effects of multi-physics fields on the linear and nonlinear critical light intensity, critical electric field, static bending, elastic buckling, free vibration, as well as dynamic responses of perovskite plates. Numerical results show that light illumination, photoinduced temperature rise, and applied electric field play an important role in structural properties hence need to be taken into consideration for the design of perovskite-based photoelectric devices.

Keywords: Perovskite plates, Photoinduced deformation, Electrostriction, Static and dynamic analysis, Opto-electro-thermo-mechanical behaviour

A 3D Generative Framework Integrating Time-Series Data from Eulerian Structural Analysis

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Current 3D shape generation models struggle to incorporate mechanical parameters derived from nonlinear phenomena, such as buckling, into the design process. To address this, we propose a novel framework that integrates Eulerian structural analysis and DeepSDF (Signed Distance Function) to enable precise shape generation while maintaining mechanical accuracy and computational efficiency.

The Eulerian method, with its fixed Cartesian meshes, efficiently captures time-series data of velocity fields and spatial coordinates. Unlike traditional Lagrangian methods, it remains stable and computationally efficient, making it ideal for large-scale parallel computations. This approach accurately models dynamic nonlinear behaviors, such as large deformations and buckling, ensuring that generated shapes adhere to specified mechanical constraints.

DeepSDF encodes shapes as signed distance functions, leveraging latent vectors to generate complex geometries with smooth surfaces. By incorporating positional encoding, it captures a wide range of frequency components, enabling precise representation of both macroscopic and microscopic geometric variations essential for nonlinear mechanical performance.

By integrating Eulerian analysis with DeepSDF, our framework establishes a direct link between mechanical response and shape generation, overcoming limitations of conventional data-driven models that lack a physical performance basis. Furthermore, by leveraging time-series data, our approach enables the prediction of nonlinear deformations, allowing for iterative shape refinement based on mechanical behavior over time.

Keywords: Eulerian method, Elastoplastic analysis, 3D generative Madel

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A Parallel distributed processing approach to PINN for solving axisymmetric magnetostatic problems

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Physics-Informed Neural Networks (PINN) is a method of training neural networks by constructing a loss function based on residuals in a boundary value problem for partial differential equations [1]. Furthermore, there is research on the application of PINN to electromagnetic field analysis [2]. In here, the electromagnetic field equations derived from Maxwell's equations deal with vector fields, and the interface conditions of electromagnetic fields inside the analysis domain should be satisfied. However, it is difficult for conventional PINN to inference that satisfy those conditions.

In conventional numerical methods, it is known that the interface conditions of electromagnetic fields can be satisfied naturally by using Nedelec's edge element in FEM and Yee's grid in the FDTD method. However, PINN, which does not use connectivity between training points, cannot be expected to satisfy naturally. To solve this issue, authors have proposed DDM-PINN [3][4]. DDM-PINN is based on the non-overlapping domain decomposition method, such as the Neumann-Neumann algorithm and the Dirichlet-Dirichlet algorithm, and a framework for distributed-memory parallel computation. In this study, DDM-PINN is applied to the analysis of magnetostatic problems, and numerical results are presented using parallel computations.

Keywords: Physics-informed neural networks, domain decomposition method, magnetostatic analysis, parallel computing

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Molecular Dynamics Investigation on Thermal Properties of Graphene Origami/Polymer Nanocomposites.

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ABSTRACT

Graphene/paraffin nanocomposites are promising thermal interface materials (TIMs) to dissipate heat in electronic devices due to the high thermal conductivity (TC) of graphene and easy processing of paraffin. Recent research on graphene-based polymer nanocomposites mainly focuses on the TC improvement via interface engineering. Our previous studies have proved that origami-inspired structural modification not only improves the flexibility of graphene, but also the interfacial strength in the polymer nanocomposites. Here we report the first study of the heat transfer performance of graphene origami (GOri) in polymer matrix. Molecular dynamics (MD) simulations reveal that GOri enhances the TC at the GOri/polymer interface by nearly 300% compared to the pristine graphene fillers. This significant TC improvement is attributed to GOri morphology. From the in-depth analysis of radial distribution function (RDF), mean squared displacement (MSD) and vibrational density of states (VDOS), we confirm that GOri fillers with rough surfaces and hydrogeneration contribute to strong interfacial interactions and phonon coupling at the filler-matrix interfaces. Consequently, However, the presence of creases and sp^3 bonds formed by hydrogenation in GOri give rise to more phonon scattering and thus lead to a reduction in the in-plane TC of GOri/polymer composites. Our findings indicate that GOri is an effective TC filler for improving thermal performance of polymer composites and may offer new design strategies for advanced TIMs.

Deformation-controlled Design through Simultaneous Shape and Multi-material Topology Optimization

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Topology optimization [1] is a computational simulation technique that derives structures maximizing mechanical performance, such as stiffness and strength, across a wealth of physics problems. Among structural optimization methods, topology optimization offers the highest degree of design freedom. Especially, density-based methods are widely adopted across industries due to their simplicity. However, topology optimization inherently generates boundaries within a predefined fixed design domain, making the optimal design highly dependent on this domain.

Recent studies have proposed simultaneous optimization methods that integrate nonparametric shape optimization with topology optimization to overcome this limitation [2,3]. Nonparametric shape optimization is a design methodology that updates structural boundaries based on shape derivatives. By incorporating this approach into topology optimization algorithms, the design boundaries can be dynamically adjusted, effectively expanding the design domain and enhancing optimization potential.

Meanwhile, in structural design, multi-material structures are increasingly explored to enhance multiple structural performances that often exhibit trade-offs. Integrating multi-material design into optimization frameworks enables not only the pursuit of stiffness but also the achievement of complex objectives such as deformation control, significantly broadening the design domain.

Motivated by this background, this study extends the simultaneous optimization of shape and topology to multi-material models. This extension enhances the design domain, enabling the discovery of superior optimal solutions.

In the presentation, numerical examples will be provided to validate the feasibility and effectiveness of the proposed method.

Keywords: Simultaneous optimization, Shape optimization, Topology optimization, Multi-material, Nonparametric

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Finite element modelling of unbound granular pavements considering realistic moving loads

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Unpaved unbound granular pavements are commonly built in low-traffic areas where budget constraints prevent the construction of paved roads. These unpaved pavements typically consist of a base layer constructed using unbound granular materials, overlying the subgrade soil. The performance and maintenance needs of these pavements are governed by the behaviour of constituent materials, which undergo deformation under traffic-induced loads, resulting in a deterioration in pavement geometry. Despite the low traffic volume, heavy vehicles often use these roads, which accelerate the deterioration and pose safety risks to road users. Consequently, these roads require frequent maintenance to sustain a satisfactory level of service. One key reason for this poor performance of unpaved pavements is the reliance on empirical and overly simplified CBR based design method, which often overlooks the complex behaviour of unbound granular materials and subgrade soil under moving loads. Therefore, a comprehensive evaluation of the behaviour of these pavements under realistic moving loads is essential for proper design. With this objective, the behaviour of unbound granular pavements under moving loads, with due consideration for moving tyres with translational and rotational motion effects, is investigated using three-dimensional finite element simulations. The finite element model of the pavement is employed to gain insights into the distribution of stresses, strains and displacements in the pavement substructure. A parametric study is conducted to examine the influence of material properties, tyre movement (translation and rotation) and loading characteristics on pavement performance, emphasising variations in tyre-pavement contact pressure, stresses, strains and pavement deflection. It was found that the consideration of both translation and rotation of tyre leads to more accurate prediction of stress distribution in the pavement layers compared to when only translation is considered. The results also show that stresses, strains and pavement deflection increase with a rise in axle load and inflation pressure, with axle load being more influential. For instance, the peak vertical deflection at the pavement top increases by 49% when the axle load increases from 80 kN to 120 kN (see **Figure 1**) while it rises by only 4% when inflation pressure increases from 500 to 1200 kPa. The predictions are also compared with results from multilayer elastic analysis, a method commonly used in routine engineering practice in Australia. The findings from this study underscore the importance of incorporating realistic tyre movement for accurate prediction of pavement response.

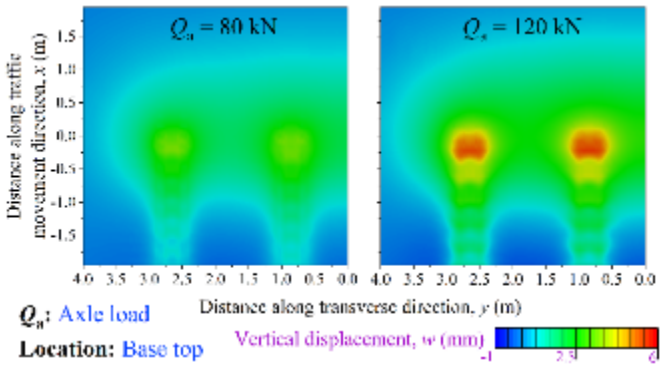

Figure 1.

Keywords: Finite element modelling, material plasticity, moving loads, unbound granular pavements

Vertical coordinate transformations for SPH to improve computational efficiency

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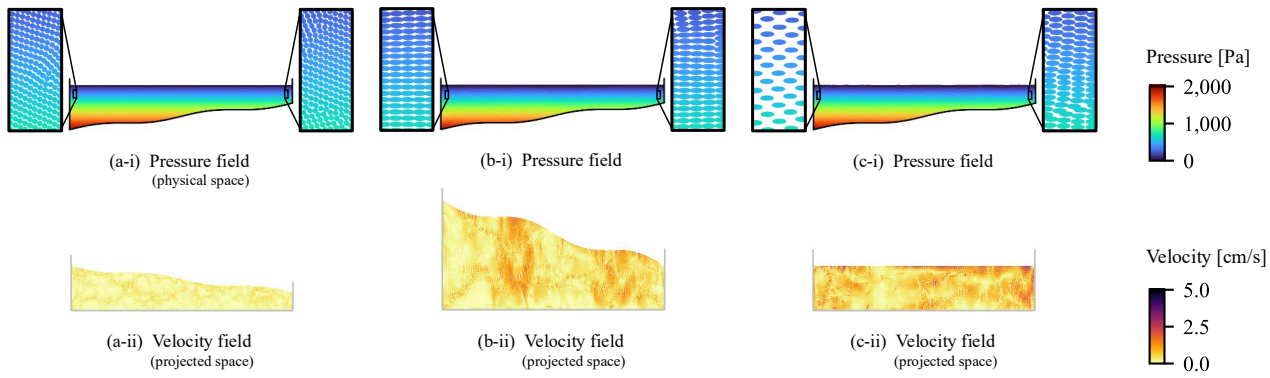
The recent improvements in the accuracy of the Smoothed Particle Hydrodynamics (SPH) method have expanded its applicability. However, the computational cost remains an issue in practical applications. In this study, we aim to improve the computational efficiency of the SPH method by applying vertical coordinate transformations, including the σ-coordinate system [1]. The vertical coordinate transformations are defined as follows:

$$\boldsymbol{r} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \overset{\text{transformation pair}}{\longleftrightarrow} \hat{\boldsymbol{r}} = \begin{bmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{bmatrix} = \begin{bmatrix} x \\ y \\ \alpha(x,y)[z + \beta(x,y)] \end{bmatrix} \tag{1}$$

where $\boldsymbol{r}$ and $\hat{\boldsymbol{r}}$ are the position vectors in physical and projected spaces, respectively. α and β are arbitrary variables. α defines vertical scale ($\alpha > 0$) and β denotes vertical shift.

In this study, we apply three coordinate transformations, namely, bottom boundary-fitted SPH (BF-SPH), bottom boundary-fitted ellipsoidal SPH (BFE-SPH), and σ-SPH using the σ-coordinate system proposed in [2]. The results shown in **Figure 1** indicate that the three methods achieve approximately the same level of accuracy. Additionally, the computation times for BFE-SPH and σ-SPH are about 1/3 and 1/5 of that of BF-SPH, respectively.



(a) BF-SPH (b) BFE-SPH (c) σ-SPH

Figure 1.

Keywords: particle method, Smoothed Particle Hydrodynamics, SPH(2), coordinate transformation, σ-coordinate system

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Machine learning of effective elastic tensor of materials with microstructure

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Architected materials are materials with microstructure, and their mechanical properties may be unconventional, such as effective Poisson's ratio approaching theoretical limits, i.e. -1 and 0.5 for 3D materials, or -1 and 1 for 2D materials. In this work, we use the finite element method to numerically study all components of the effective elastic tensor of architected materials via the homogenization of their unit cells with or without periodic boundary conditions. By varying the geometrical parameters of the star-shaped microstructure, we obtain a dataset that contains information about the correlation between microstructural geometries and their corresponding effective elastic tensor. Then, we conduct machine learning on the dataset with the deep neural network procedure. The data can be successfully trained and validated. Furthermore, our trained neural networks are used to generate desired microstructures when effective properties are specified. The computational cost to use high-fidelity finite element calculations can therefore be largely reduced by using the trained neural networks to design architected materials.

Keywords: Deep neural network, machine learning, microstructure, elastic tensor, negative Poisson's ratio

APCOM-ACCM 2025
Brisbane, Australia
7-10 December 2025

Investigating bubble injection, detachment, and rise behaviour using the phase-field lattice Boltzmann method

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Cost-effective and low-emission hydrogen production is crucial for the decarbonisation of fuels and chemicals. Currently, most produced hydrogen comes from steam methane reformation which emits approximately 10kg equivalence of CO_2 per 1kg of hydrogen. Methane pyrolysis provides an alternative technology in which natural gas is thermally decomposed to form hydrogen gas and solid carbon rather than gaseous carbon products. One technique to facilitate this is a bubble column reactor, where natural gas is injected into a high-temperature liquid column. However, certain limitations are observed in these reactors such as poor H_2 selectivity and difficulties in removal of produced solid carbon. The build-up of carbon in the reactor can lead to clogging, making the process challenging for industrial-scale H_2 production. For molten media bubble column reactors (MMBCRs), experimental observations of the bubble dynamics in molten media are limited due to the challenges posed by the high-temperature molten media restricting conventional measurement techniques. To address this issue, this research seeks to use computational fluid dynamics to resolve the complicated bubble-particle interactions inside molten-media bubble column reactors, as the bubble dynamics strongly affect the conversion efficiency and understanding the particle dynamics is the first step to developing effective removal strategies.

This presentation focuses on the injection dynamics of bubbles into a liquid column. In particular, it presents a detailed validation study for the phase-field lattice Boltzmann method [1] in comparison to experimental work recently published in the literature [2]. The simulation results are compared to the experimental data, analysing the impact of injected gas flow rates, nozzle diameters, and viscosity ratios on the resultant bubble dynamics. The bubble rising time, necking behaviour (see Figure 1), and bubble diameters are thoroughly compared to validate the accuracy of the model. Future development of the model will focus on incorporating the bubble interface behaviour with particle interaction to address the effect of produced solid carbon during methane pyrolysis on the process efficiency.

(a) (b)

Figure 1. Necking behaviour of an injected bubble as (a) observed experimentally in the work of Rabbani and Ray [2], and (b) simulated using the phase-field lattice Boltzmann method.

Keywords: Phase-field, Multiphase flows, Computational fluid dynamics, Methane pyrolysis, Bubble column

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Stabilized velocity-pressure monolithic SPH for incompressible fluid using Variational Multiscale Method

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In incompressible fluids, the monolithic approach is known for its excellence in boundary treatment. However, to our knowledge, implementation in the Smoothed Particle Hydrodynamics (SPH) method has not yet been achieved due to numerical instability issue. Therefore, in this study, we aimed to stabilize it by introducing the Variational Multiscale Method [1]. By decomposing the velocity field into resolvable and subscale components with reference to Chandra et al. [2], time-discretized Navier-Stokes equation and continuity equation can be rewritten as follows:

$$\begin{bmatrix} \left\{1-\left(1-\frac{\tau\rho}{\Delta t}\right)\Delta t\nu\nabla^2\right\}\boldsymbol{I} & \frac{\Delta t}{\rho}\nabla \\ \left(1-\frac{\tau\rho}{\Delta t}\right)\rho\nabla^{\top} & -\tau\rho\nabla^2 \end{bmatrix} \begin{Bmatrix} \bar{\mathbf{v}}_{n+1} \\ p_{n+1} \end{Bmatrix} = \begin{Bmatrix} \bar{\mathbf{v}}_n + \tau\rho\nu\nabla^2\bar{\mathbf{v}}_n + \Delta t\mathbf{g} \\ -\frac{\tau\rho^2}{\Delta t}\nabla\cdot\bar{\mathbf{v}}_n \end{Bmatrix}, \tag{1}$$

where $\rho, \nu, \mathbf{g}, \bar{\mathbf{v}}, p, \Delta t, \tau$ represent density, dynamic viscosity, gravity, resolvable component of velocity, pressure, time increment and stabilization parameter, respectively. This formulation satisfies the numerical stability condition, enabling the solution of velocity and pressure fields to satisfy both Navier-Stokes equation and continuity equation.

Figure 1. and Figure 2. show comparisons between computational results of dam break problem using the proposed method and experimental results. It is confirmed that the proposed method can be applied to complex problems involving free surfaces and walls.

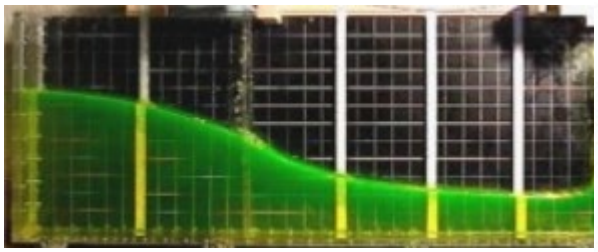

Figure 1.

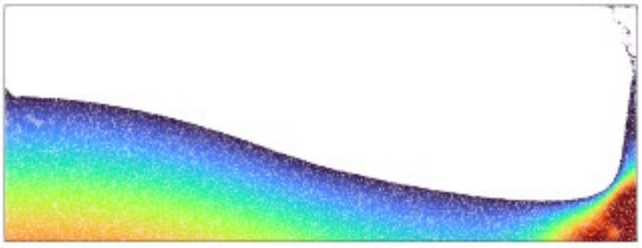

Figure 2.

Keywords: Smoothed Particle Hydrodynamics, Monolithic approach, Variational Multiscale Method, Boundary condition

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Nonlinear Buckling Analysis of Functionally Graded Shells Based on Isogeometric Reissner-Mindlin Theory

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Functionally graded materials (FGMs), characterized by spatially varying mechanical properties, have garnered significant attention in aerospace, marine, and nuclear engineering due to their superior thermal resistance and stress distribution capabilities. However, the nonlinear buckling behavior of FGM shells under complex loading remains a critical challenge, particularly when accounting for geometric nonlinearity and shear deformation effects. An isogeometric Reissner-Mindlin shell theory is utilized, capable of handling nonlinear buckling analysis of FGM shells [1]. Leveraging the seamless integration of geometric modeling and analysis in isogeometric analysis (IGA), Non-Uniform Rational B-Splines (NURBS) is employed to discretize both the shell geometry and the displacement field. The material gradation, governed by a power-law distribution through the thickness, is explicitly incorporated into the constitutive model. The nonlinear governing equations are solved via the Arc-length method to trace equilibrium paths through snap-through and snap-back instabilities. Several numerical examples investigate the influence of gradient indices, boundary conditions, and aspect ratios, exhibiting the accuracy and efficiency of the proposed approach.

$$G(\mathbf{v},\delta\mathbf{v}) = \int_{\Omega_0} \delta\boldsymbol{\varepsilon}^T \boldsymbol{\sigma} \mathrm{d}A - \int_{\Omega_0} \delta\mathbf{v}^T \bar{\mathbf{p}}_0 \mathrm{d}A - \int_{\Gamma_0^N} \delta\mathbf{v}^T \bar{\mathbf{t}}_0 \mathrm{d}s = 0 \tag{1}$$

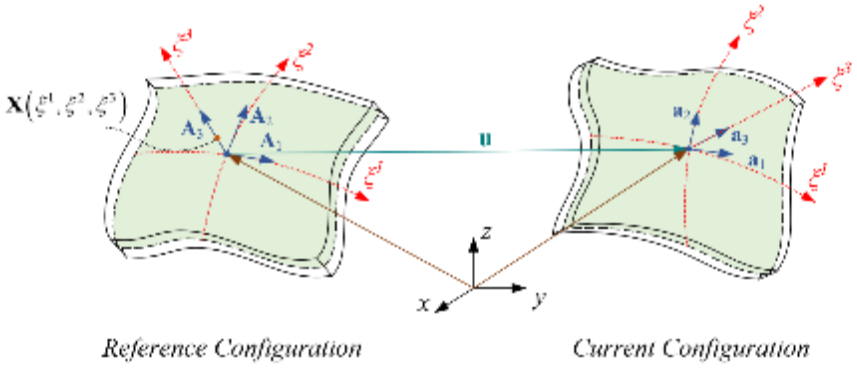

Figure 1. Geometry definition for the shell structure

Keywords: Isogeometric analysis, shell structures, geometric nonlinearity, buckling analysis, arc-length method

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Phase field fracture modelling for elastoplastic shell incorporated with stress-state-based fracture initiation

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Although phase-field models have been extended to simulate shell fracture propagation, most existing models are validated primarily through benchmark numerical examples rather than experimental data. In the few cases where comparisons are made, the focus is typically only on quantitative analysis, limiting their potential for practical industrial applications. To address this gap, this paper introduces a shell phase-field model with five layers of phase-field variables to accurately predict fracture propagation through the thickness, corresponding directly to the five Simpson stress integration points, as shown in **Figure 1**.

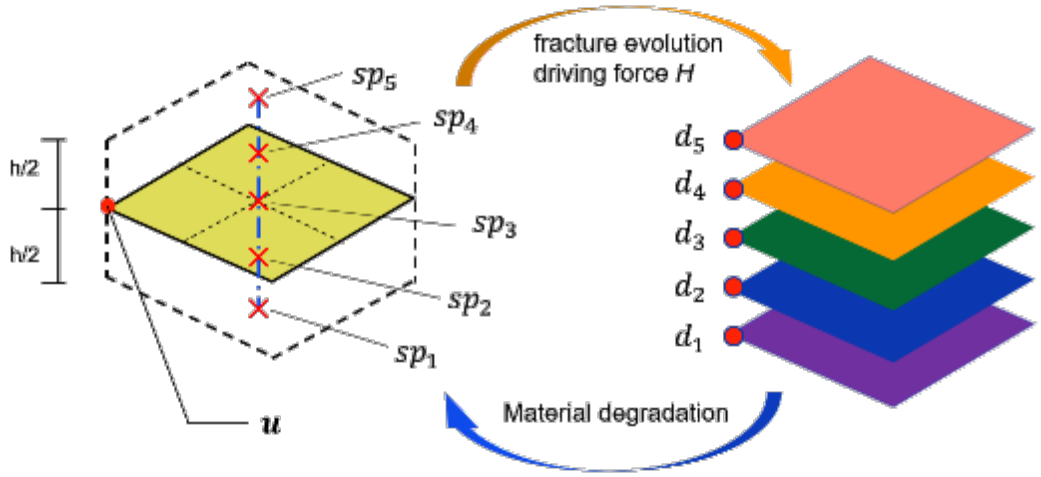

Figure 1. The coupling displacement and phase field evolution for shell element with five Simpson material points adopted along shell thickness.

Additionally, to accurately capture fracture initiation in real structures, a stress-state-dependent fracture strain formulation was employed in each layer, utilizing the MMC criterion for 316L steel and the Bao-Wierzbicki criterion for Ti-6Al-4V. The proposed model was validated both quantitatively through benchmark numerical examples and qualitatively using experimental data. The simulation of a notched cylinder under axial tension demonstrated that fracture strain significantly affects the load-carrying capacity. The typical "flapping" phenomenon in a cracked cylinder under internal pressure was successfully reproduced. In the three-point bending test of a square tube, the model captured five distinct stages of deformation—elastic deformation, local indentation, side-surface buckling, bulge strap growth, and global bending—all of which closely matched experimental observations. Despite a slight delay in the densification of the Gyroid TPMS structure under axial compression, the two characteristic deformation modes were accurately captured, and the global force-displacement curve aligned well with experimental results.

Keywords: phase field; fracture initiation; shell element; Modified Mohr-Column fracture initiation.

Comparative study of locking-free finite elements on bending dominated and incompressible deformation

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The contribution of this study is to compare the performance between three types of locking-free finite elements under bending dominated and incompressible conditions. To avoid shear and volumetric locking in large deformation problem, the conventional finite element method has been developed into Enhanced Assumed Strain method (EAS method) [1, 2], one-point integration finite element and F-bar projection method [3]. In the EAS method, the displacement gradient is enhanced by adding incompatible modes corresponding to discontinuity between finite elements into the conventional compatible mode based on the Hu-Washizu variational principle. Several types of incompatible modes have been developed from H1E9 [1] that was introduced in the original paper of the EAS and into CG9 [4] and TSCG12 [5] that modified the instability of the H1E9. Also, the one-point integration finite element has been proposed to control the hourglass modes which arise by applying one-point Gauss quadrature to isoparametric elements. Moreover, one-point integration finite element combined with EAS has been developed by using a Taylor expansion of the shape function and the stress at the centre of finite elements. In the F-bar method, the deformation gradient is modified by replacing the volumetric component with that evaluated at the centre of finite elements. Moreover, in F-bar projection method, the modified deformation gradient was developed by employment with not only the constitutive law but also the potential energy to modify the unsymmetric tangent matrix of the F-bar method into the symmetric one. Through several numerical examples, the performance of three types of EAS methods, the one-point integration finite elements combined with and without EAS and F-bar projection method are evaluated by comparing their capability to avoid shear and volumetric locking, as well as their computational efficiency.

Keywords: Enhanced Assumed Strain method, one-point integration finite element, F-bar projection method

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Distribution of stress intensity factors around a sharp 3D jointed corner between dissimilar materials under combined loads

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In recent years, piezoelectric materials have been increasingly integrated into various electronic devices. These devices often incorporate stacked layers of different materials to achieve multifunctionality and miniaturization. However, stress concentrations can arise in these stacked regions due to differences in material constants between the joined materials.

In this study, we applied the H-integral method within finite element analysis (FEA) to investigate the coupled singular stress and electric displacement fields around a sharp three-dimensional corner in jointed heterogeneous materials, including piezoelectric materials. We determined singularity eigenvalues and scalar parameters and further computed the stress intensity factor distribution around the jointed corner. This approach is expected to predict both the direction and critical conditions for delamination originating from the sharp three-dimensional corner.

We propose an extended formulation of stress intensity factors (SIFs) for a sharp three-dimensional corner in jointed dissimilar materials, including piezoelectric materials, as

$$\begin{Bmatrix} K_{\mathrm{II}} \\ K_{\mathrm{I}} \\ K_{\mathrm{III}} \\ K_{\mathrm{IV}} \end{Bmatrix} = \lim_{\substack{r\to 0 \\ \theta\to\theta_0 \\ \phi\to\phi_0}} \sqrt{2\pi r}\, l_k^{0.5-\mathrm{Re}[\lambda_1]} \mathbf{\Lambda}(\theta,\phi) \left\langle (r/l_k)^{0.5-\lambda_m} \right\rangle \mathbf{\Lambda}^{-1}(\theta,\phi) \begin{bmatrix} \sigma_{r\theta} \\ \sigma_{\theta\theta} \\ \sigma_{\phi\theta} \\ D_{\theta} \end{bmatrix}. \tag{1}$$

where K_{II}, K_{I}, K_{III} and K_{IV} represent the stress intensity factors, r denotes the distance from the corner, l_k is an arbitrary length, λ_m represents the eigenvalues, $\mathbf{\Lambda}$ is a matrix composed of eigne functions. We computed the distribution of SIFs around the singular point of PZT-4 embedded in resin under combined loading conditions, including a 10 MPa applied stress, a 100˚C temperature change, and a 0.1 C/m² electric field as shown in Fig. 1. Fig. 2 illustrates the distribution of K_{I} and the square root of K_{II} and K_{III}, which are the possible SIF components responsible for delamination. The possible delamination directions are along both sides of face β.

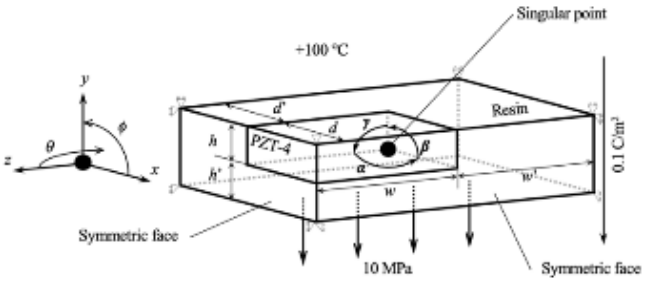

Fig. 1 Sharp corner of embedded PZT-4 in resin.

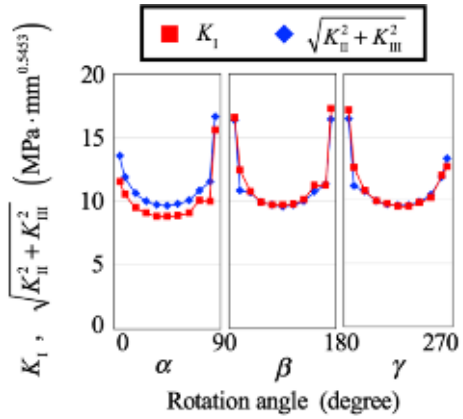

Fig. 2 Distribution of SIF around the corner.

Keywords: Sharp Jointed Corner, Stress Intensity Factor, H-integral, Combined Loads, Piezoelectric Material, Delamination

Physics-informed neural networks with state boundary correction and numerical expansion-regression for multi-contact point stick-slip vibration

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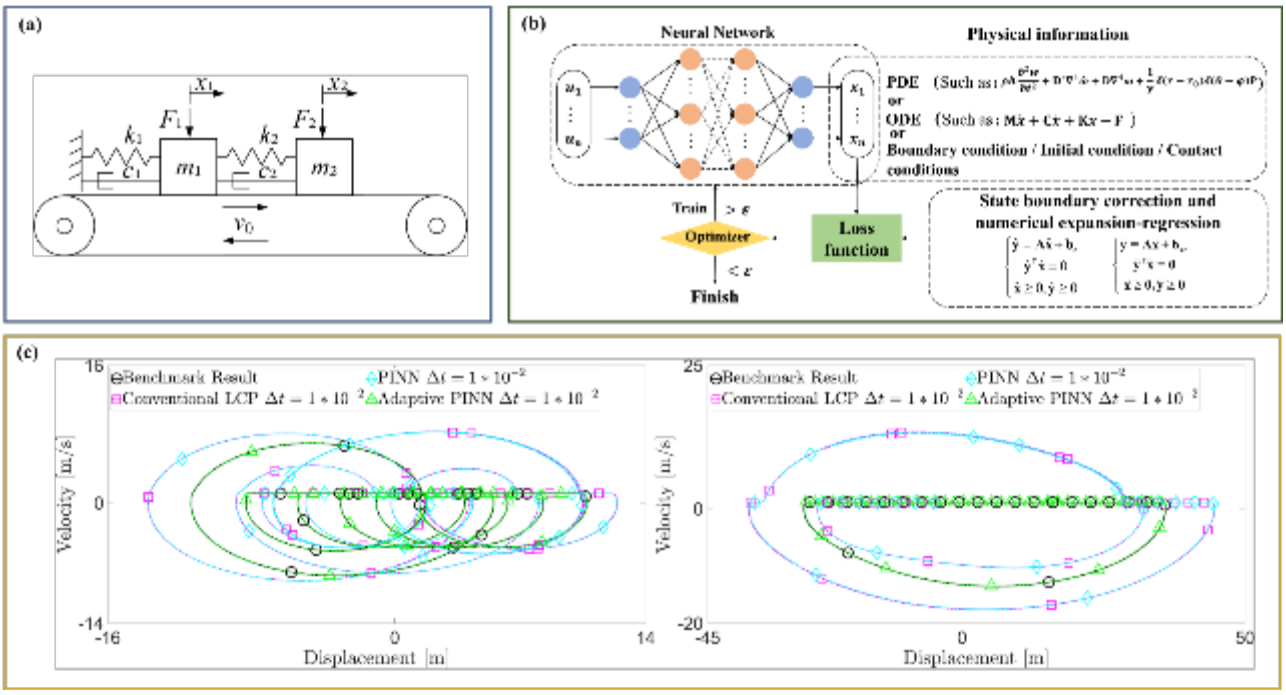
Abstract: Friction-induced vibration (FIV) is a prevalent issue in mechanical systems with frictional contact, leading to complex dynamic behaviors that impact performance and safety in manufacturing, transportation, and aerospace. Despite its significance in reliability and maintenance, FIV remains insufficiently understood. Simulating the non-smooth dynamics of multi-contact friction systems is challenging, as existing methods struggle to accurately and efficiently capture stick-slip vibrations and multi-contact interactions.

To overcome these challenges, previous research proposed a Physics-Informed Neural Network (PINN) framework for simulating friction-induced vibrations, achieving higher accuracy than traditional time-stepping methods. Building on this foundation, the present study develops an Adaptive Physics-Informed Neural Network (Adaptive PINN) framework, which incorporates state transition boundary correction and numerical expansion-regression mechanisms to further enhance solution accuracy and stability. Specifically, the proposed approach enhances the PINN framework by: (1) Implementing a state transition boundary correction method to ensure accurate dynamic transitions even with larger time steps; (2) Applying numerical expansion and result regression to linear complementarity constraint matrices to preserve solution accuracy under high-dimensional constraints. The effectiveness of the Adaptive PINN framework is demonstrated through its application to a 2-degree-of-freedom friction system. The Adaptive PINN methods allow for a large time step with high accuracy compared to conventional methods.



Keywords: Physics-informed neural network, Nonsmooth dynamics, Friction-induced vibration, Stick-slip vibration

LEDDS: A C++-based Portable and Efficient CFD-DEM Solver for Particle-Fluid Simulations

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The Discrete Element Method (DEM) is a powerful tool for simulating particle-based systems and is often coupled with Computational Fluid Dynamics (CFD) to capture fluid-particle interactions. However, CFD-DEM simulations are computationally demanding because they involve resolving both the discrete motion of a large number of particles and the continuous evolution of the surrounding fluid. As a result, they require dedicated parallelization strategies to run efficiently on modern hardware. In this work, we present **LEDDS** (LBM-Enhanced Device-independent DEM Solver), an open-source CFD-DEM solver designed for high performance fluid-particle simulations on both multi-core CPUs and GPUs [1].

LEDDS relies on **parallel algorithms available in the standard library of C++**, which ensures its portability across different hardware architectures without relying on vendor-specific programming models. Its DEM formulation is based on LIGGGHTS but has been rewritten using parallel algorithms for improved efficiency and portability. The solver couples DEM with the open-source fluid solver STLBM. It is based on the Lattice Boltzmann Method, which was here chosen for its high parallel efficiency, accuracy in weakly compressible flows, and natural compatibility with the uniform Cartesian grid used for DEM particle collision detection. A two-way penalization-like coupling enables efficient solver interaction between the fluid and particle phases, while ensuring good performance on GPUs.

To validate LEDDS, we perform benchmark tests covering both particle-particle and fluid-particle interactions, including elastic collisions, wall-particle interactions, many-particle systems, single-particle settling, and particle-laden shear flow. In addition to its good accuracy and robustness properties, performance analysis demonstrate that LEDDS achieves substantial speedups on GPUs, confirming the efficiency of our parallelization strategy. These results highlight the potential of standard C++ for hardware-independent CFD-DEM simulations, establishing LEDDS as a portable and efficient tool for modeling complex particle-fluid systems.

Keywords: Lattice Boltzmann Method, Discrete Element Method, GPU, C++

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Physics-Informed Deep Energy Approach with Phase-Field Modeling for Coupled Thermo-Mechanical and Hydro-Mechanical Fracture

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Fracture modeling is essential for accurately predicting material behavior and failure under complex coupled conditions involving thermal, mechanical, and hydraulic interactions. Conventional numerical methods frequently face challenges in effectively capturing discontinuities, complex interactions, and multi-branched fracture interface tracking encountered during fracture propagation. The phase-field method addresses these challenges by representing fractures as diffuse transition zones rather than sharp interfaces, enabling precise modeling of intricate fracture patterns, including multi-branched cracks.

In this study, we propose a novel computational framework based on the Deep Energy Method (DEM) [1], integrating Physics-Informed Neural Networks (PINNs) with the phase-field method. This approach embeds governing physical principles directly into the neural network training process, ensuring computed solutions rigorously adhere to underlying physical laws. Previous studies have successfully applied DEM combined with Physics-Informed Deep Operator Networks (PI-DeepONets) for predicting crack nucleation and propagation in purely elastic brittle materials [2]; however, extending these techniques to coupled thermo-mechanical and hydro-mechanical scenarios remains unexplored and promising.

To further enhance our methodology, we incorporate Isogeometric Analysis (IGA), which enables precise geometric representation, efficient boundary condition descriptions, and seamless integration with Computer-Aided Design (CAD) tools. This integration significantly improves simulation accuracy and efficiency for complex geometries. Recent research has demonstrated the effectiveness of IGA in adaptive fourth-order phase-field analyses for purely elastic fracture problems using deep energy minimization [3]. Additionally, advanced neural network architectures and neural operators offer considerable potential for efficiently learning complex mappings between function spaces, highlighting exciting directions for future research.

We demonstrate the effectiveness and accuracy of our proposed approach through several benchmark problems involving coupled thermo-mechanical and hydro-mechanical fracture scenarios using PINNs integrated with the phase-field method.

Keywords: Fracture modelling, phase-field method, multiphysics coupling, physics-informed machine learning, isogeometric analysis

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Bound states in the continuum induced by topology optimisation

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Achieving high-quality (high-Q) acoustic resonances is a fundamental challenge in acoustic device design due to energy dissipation and material losses. Bound states in the continuum (BICs) offer a unique solution by enabling lossless wave confinement despite existing within the radiation spectrum [1]. This study introduces a topology optimization approach to designing high-Q resonances based on BICs, effectively minimizing energy leakage and enhancing acoustic wave confinement [2].

Our method explores new topology classes by optimizing a single unit cell within a periodic array, leading to the emergence of quasi-BIC modes. Experimental validation demonstrates sharp pressure field enhancements, offering a robust technique for precise resonance frequency tuning and improved resilience against external perturbations—challenges often encountered in conventional parameter-tuning approaches. These findings hold significant potential for advancing wave-confining applications such as energy harvesting and acoustic filtering, pushing the performance boundaries of acoustic devices.

To account for energy dissipation due to thermal and viscous losses, as well as radiation to outgoing boundaries, the eigenfrequencies of a finite structure are computed as complex values, $\omega_k = \mathrm{Re}(\omega_k) + i\mathrm{Im}(\omega_k)$. The positive imaginary part corresponds to a time dependence factor of $\exp(i\omega t)$ in numerical analysis. The quality factor of each eigenmode is then estimated as $Q_\omega = \mathrm{Re}(\omega_k)/2\mathrm{Im}(\omega_k)$, which serves as the objective function in our proposed topology optimization framework.

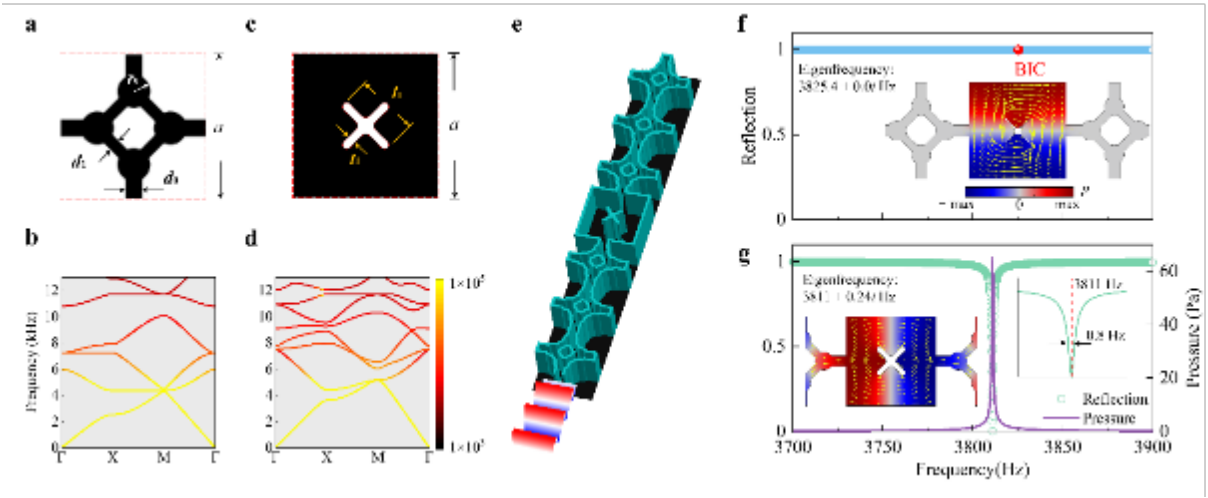

Figure 1.

Keywords: bound states in the continuum, topology optimisation, acoustic metamaterials, high-Q resonance, wave localization.

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Bayesian Data Assimilation Framework for Accurate Phase-Field Simulation of Ostwald Ripening

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Coarsening of dispersed particles or phases through Ostwald ripening is universally observed across diverse materials and aggregation states, including metals, ice, polymers, bubbles, and emulsion droplets. Since microstructural evolution through this phenomenon significantly affects material properties, numerous analytical studies have been conducted to predict Ostwald ripening, most notably through the Lifshitz-Slyozov-Wagner (LSW) theory. Recently, phase-field (PF) method, which excels in analyzing moving boundary problems, has enabled Ostwald ripening simulations that explicitly consider the dynamics of individual particles or phases [1, 2]. However, existing PF models for Ostwald ripening include numerous model parameters and material properties that are difficult to measure experimentally, such as (anisotropic) interfacial energy, mobility, and diffusion coefficients. To achieve highly accurate numerical prediction of Ostwald ripening, developing methods to accurately identify these parameters and material properties is essential.

Data assimilation has recently emerged as a powerful tool for enhancing the accuracy of numerical simulations [3]. This method integrates observational data obtained from experiments or atomistic calculations into simulations based on Bayesian inference. By calibrating various parameters within PF models to align simulation results closely with observational data, data assimilation offers a promising inverse problem approach for identifying model parameters and material properties that are otherwise difficult to measure.

This study aims to develop a comprehensive material property evaluation framework capable of simultaneously identify multiple parameters and material properties from observational data of Ostwald ripening. In this presentation, we propose a framework that directly estimates multiple property values—including interfacial properties, diffusion coefficients, and capillary length—by integrating Ostwald ripening observational data into PF simulations through data assimilation. Furthermore, we validate the proposed method via numerical experiments using synthetic observational data and application to actual observational data obtained from diffusion-time-scale atomistic calculations.

Keywords: Ostwald ripening, coarsening, phase-field model, data assimilation

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DBF-Net: A Generalized DL Framework for Predicting Dynamic Boundary Flow Fields in Aero-Structure Interaction

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Fluid-structure interaction (FSI) problems, particularly those in aerodynamic systems, pose significant challenges due to high nonlinearity, dynamic boundary conditions, and the considerable computational cost required for accurate simulations. In this work, we introduce **DBF-Net**-a generalized deep learning framework for predicting dynamic boundary flow fields in aerodynamic-structure interaction applications. DBF-Net employs a point-based encoder-decoder architecture to handle unstructured point clouds, extracting local geometric and flow-related features to accommodate complex surface motions and deformations, without relying on fixed grid resolution or topological constraints. Additionally, a DynamicFusionUnit captures temporal dependencies by processing current and previous latent representations. To enable real-time or accelerated simulations, we couple DBF-Net with a Python-based FSI framework that integrates a native structural solver, drastically reducing reliance on high-fidelity CFD simulations. We validate the method on three representative transonic FSI test cases: (1) a forced-motion simulation of a two-degree-of-freedom Isogai airfoil, (2) dynamic aeroelasticity of the same airfoil at varying speed indices, and (3) fluid-structure interaction of a flexible 3D AGARD445.6 wing. In all cases, DBF-Net yields accurate flow-field predictions with substantial computational speed-ups, achieving up to 4x and 170x acceleration compared to conventional CFD workflows for 2D and 3D simulations, respectively. The network's flexible and scalable architecture makes it suitable for various dynamic boundary and deformation problems, with broad applications in optimization and real-time control.

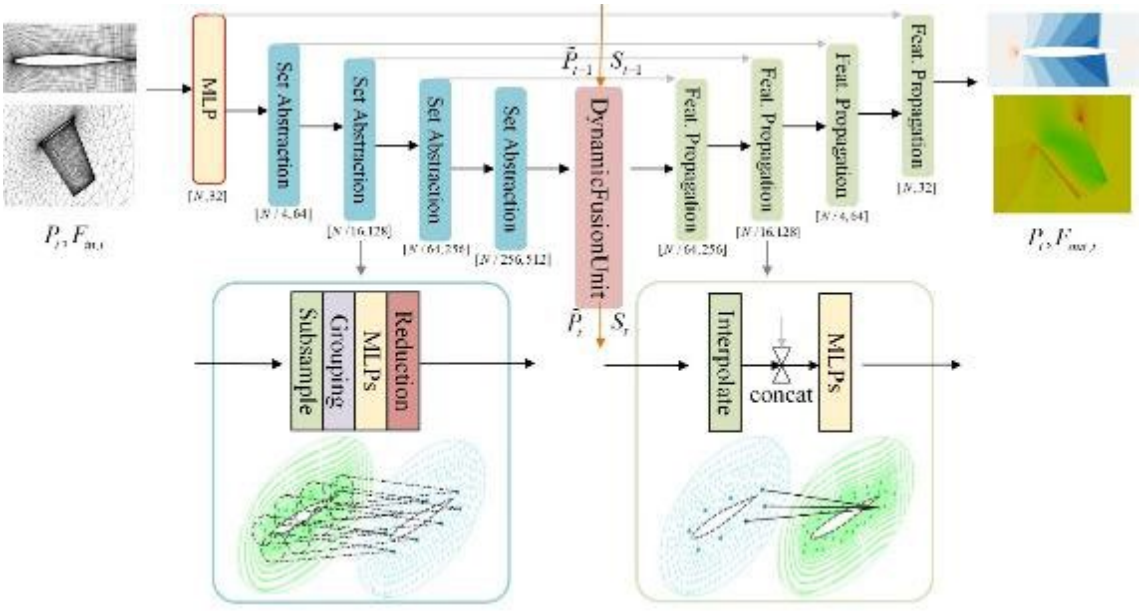

Figure 1.

Keywords: fluid-structure interaction, machine learning, Dynamic Boundary Flow Fields, Computational Acceleration

Development of a 1D ROM for Optimal Design of Deck Plates Considering Welding Depth

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In this study, a data-driven one-dimensional reduced-order model (1D ROM) was developed and evaluated for optimizing the design of H-Beam deck plates. Finite element analysis (FEA) was performed using ANSYS Mechanical, considering welding depth — a critical factor in H-beam connections — to analyze deformation, equivalent stress, and normal stress. The analysis model included two types of H-Beams (190×197×5×7 and 192×198×6×8), with welding depths set to 2, 5 and 8 mm. Additionally, six analysis conditions were established, accounting for vehicle driving direction (aligned/perpendicular) and load position, with a load magnitude of 144.4 kN. Figure 1 shows examples of the deck plate's geometric model, section of the FE model, and deformation.

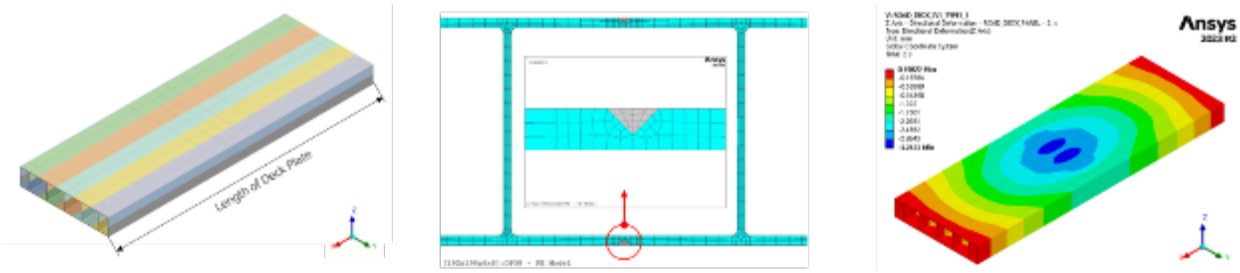

Figure 1.

Using deck plate length and welding depth as variables, 50 design points were generated through the Taguchi orthogonal array sampling method. FEA was performed on these points, and the resulting data were used to develop a data-based ROM by applying polynomial models and DFFN techniques. The ROM's accuracy was validated by comparing it with FEA results, achieving CoD adjusted and CoP of 0.991 or higher. However, due to the practical limitations of the data-based ROM, an additional, more versatile 1D ROM was developed. To ensure CoD adjusted and CoP values remained above 0.991, the DFFN sensitivity and Chebyshev polynomial coefficients were integrated to refine the equations. A comparison between the derived equations and FEA results is presented in Figure 2.

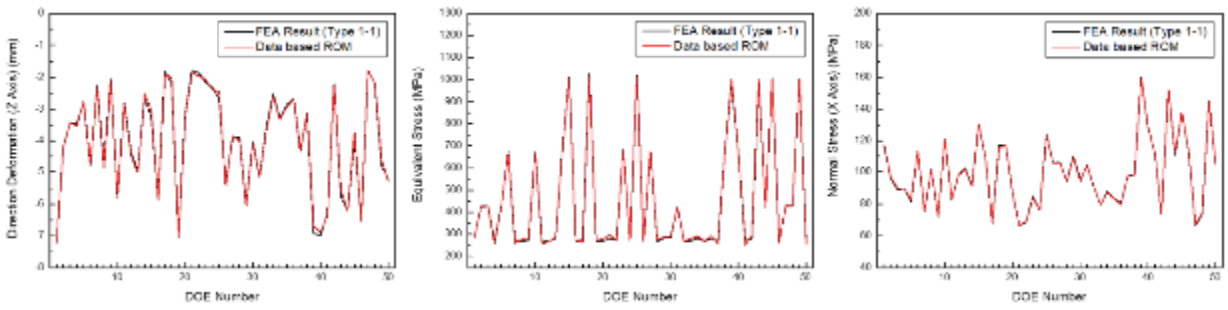

Figure 2.

In conclusion, a highly reliable deck plate design tool was developed, achieving an adjusted CoD and CoP of 0.991 or higher. This tool allows general designers, not limited to analysis experts, to calculate the optimal welding depth for deck plates in real time.

Keywords: Finite element analysis, reduced order model, design optimization, deck plate, welding

Aerodynamic performance of the wing with slotted wing tip.

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Avian wing tips are formed by a series of primary feathers. When birds such as raptors are gliding, their primary feathers at the wing tips spread and form slotted wing tips. The morphological features are well known, but the benefits of the slotted wingtips remain unclear to date due to the high degrees of freedom of such wings. In this study, we tackled the issue by evaluating the aerodynamic performance of wing with slotted wing tips through optimization in two-dimensional and three-dimensional numerical simulation. Following a previous study [1], we have modeled the primary feathers by three rectangular wings and have attached to the larger base wing. Firstly, taking advantage of the simplicity of two-dimensional computational fluid dynamics (CFD), we have optimized the relative positions and orientations of the primary feather models to maximize the lift-to-drag ratio. Next, we refined the positions of the primary feather models through three-dimensional CFD to maximize the aerodynamic performance of the slotted wingtips. Finally, by conducting a sensitivity analysis on the positions and orientations of the primary feather models obtained from the optimization, we investigated how the relative positions and orientations of the primary feather models influence the aerodynamic performance of the slotted wingtips. Optimization results indicate that there is an optimal combination of the wing angles that maximizes lift-to-drag ratio. In the three-dimensional condition, the slotted wing model was more efficient than the base wing only. Flow field around the primary feathers indicates that the slotted wings weaken wing tip vortices, increasing lift-to-drag ratio. These results provide insights into the design of flying robot and the evolution of avian wing morphology.

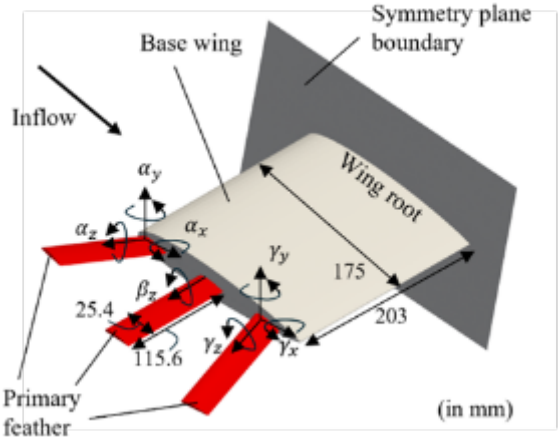

Figure 1.

Keywords: Avian flight, wing-tip slot, drag reduction, wing-tip vortex, OpenFOAM

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Morphing by Formulation of Shape Optimization Problem

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When designing automotive parts, various modifications are required to solve manufacturing problems. For example, the shape obtained by topology optimization may have too many holes, and some of them need to be filled. In such cases, it can be considered to create a model with a specified number of holes and deform it by continuous mapping so that it approaches the shape obtained by topology optimization. In this study, we formulate a shape optimization problem of domain variation type to meet these demands and present a method for solving it.

The shape optimization problem was formulated as follows: a signed distance function of the target shape was defined in an extended domain that contains the target shape, and the objective function was set to the integral of the signed distance function over the domain of the product shape. In addition, a volumetric constraint was added to ensure mass conservation. The problem was solved using the H^1 gradient method [1]. The shape gradients of the objective and constraint functions were obtained using formulas that calculate the shape derivatives of the functions with respect to the variation of domain.

(a) Target STL (b) Initial FEM model (c) Optimized FEM model

Figure 1.

A simple example is shown in Figure 1. Given the target STL shown in (a) and the initial FEM model shown in (b), the result of the FEM model being deformed to approach the target shape is shown in (c).

Keywords: Signed distance function, Shape optimization, Shape derivative, Partial differential equation, H^1 gradient method

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CFD Analysis of Building-Integrated PV Canopies for Enhancing Rooftop Wind Energy Utilization

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The rooftops of high-rise buildings in urban environments have been widely recognized for their significant wind energy potential [1-3]. Recently, the integration of Building-Integrated PV Canopies (BIPV-Canopies) has emerged as a promising strategy to optimize rooftop wind energy utilization. This study employs computational fluid dynamics (CFD) to investigate how elevated PV canopies influence wind flow patterns and enhance wind energy harvesting potential. Various canopy designs are analyzed to determine their aerodynamic effects on wind acceleration and turbulence characteristics.

Preliminary results show that the geometry of BIPV-Canopies plays a crucial role in accelerating rooftop wind flow while reducing turbulence intensity. These findings highlight the dual benefits of PV canopies—not only serving as solar energy generators but also enhancing urban wind energy utilization by optimizing airflow dynamics. As Taiwan's government has actively promoted BIPV-Canopies as a key sustainable energy solution, this study further demonstrates their potential to support Net-Zero energy buildings, offering a valuable reference for cities worldwide in advancing urban sustainability.

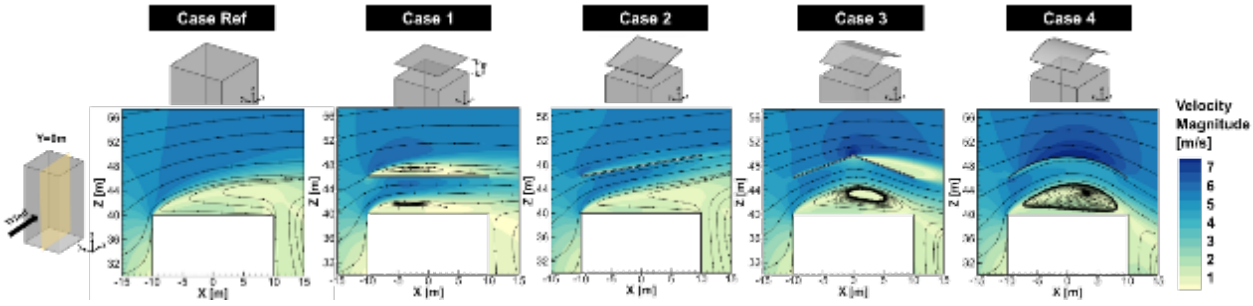

Figure 1.

Keywords: Elevated PV Canopies, Urban wind energy, Computational fluid dynamics, Net-Zero Energy Buildings, Sustainable Urban Development

Acknowledges:
The authors appreciate the financial support from National Science and Technology Council, Taiwan under grant number NSTC 113-2628-E-027-001. The authors also appreciate the financially supported by the "Research Center of Energy Conservation for New Generation of Residential, Commercial, and Industrial Sectors" from The Featured Areas Research Center Program within the framework of the Higher Education Sprout Project by the Ministry of Education in Taiwan.

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Research on Fast Calculation Model of Aerodynamic Force Based on Key Control Parameters of Streamlined Head

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In order to improve the calculation efficiency of train aerodynamic force, a fast calculation model of train aerodynamic force is developed by the method of artificial intelligence machine learning.

The development idea of this model is as follows. According to the streamlined head, a set of general three-dimensional head shape parameterization method is put forward by adopting the idea of step-by-step modelling. In this paper, the PSO method is used to realize the fast extraction of the design parameters of train three-dimensional head shape, that is to say, a train streamline head shape is controlled and calibrated by several key parameters. Based on the extracted key geometry parameters, CFD numerical calculation data and wind tunnel test data are selected as the training data. The support vector machine model (SVM)is used to construct the nonlinear implicit function model of train shape design parameters and aerodynamic forces, and a fast calculation model of train aerodynamic forces is developed.

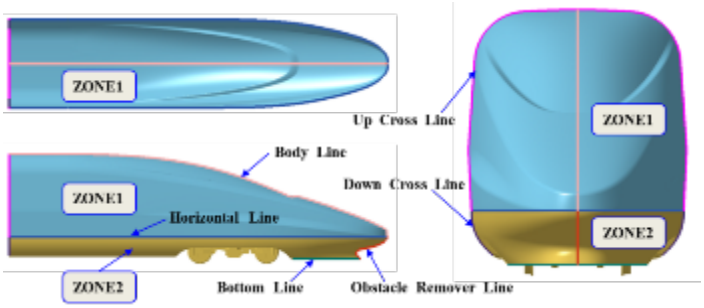

Fig 1. Key control profiles for the streamlined head

Table 1 shows the aerodynamic drag calculation results using this fast model, the maximum value of relative error is 4.49%, and the minimum value is 0.96%, both less than 5%, which is 50% less than the average error required by EN 14067-6-2018 standard [1].

	Case1	Case2	Case3	Case4
Wind Tunnel Test	/	/	**0.3394**	**0.3650**
CFD	**0.2783**	**0.3163**	0.3375	0.3536
Fast Calculation Model	0.2849	0.3021	0.3485	0.3685
Relative Error	2.37%	4.49%	2.61%	0.96%

Table 1. Calculation results of Fast Calculation Model

This calculation model is used for engineering design and aerodynamic optimization of trains. Compared with wind tunnel test and CFD method, on the premise of meeting the requirements of engineering design calculation accuracy, the calculation efficiency is increased by more than 90%. It can significantly shorten the evaluation period of train aerodynamic forces. With the increasing enrichment of wind tunnel test data and CFD calculation data, the calculation accuracy of the fast

calculation method will be improved. This will be more suitable for long-term train aerodynamic forces research and optimization.

Keywords: Aerodynamic force, SVM, High speed train, Numerical simulation, Wind tunnel test

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Study on Wind Characteristics of Balcony Glass Handrails on Building

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The architectural designs of buildings in Taiwan are becoming increasingly innovative, with a trend towards taller structures. Many residential buildings incorporate various types of balconies to enhance their aesthetic appeal. In terms of wind effects on buildings, the presence of balconies alters the wind pressure distribution on windward façades due to changes in flow separation, recirculation, and reattachment regions.

Corner balconies not only serve as architectural features but also function as passive aerodynamic devices that enhance the roughness of building surfaces, disrupt the coherence of vortex shedding, and thereby reduce crosswind forces on tall buildings. Extended corner balconies can even reduce crosswind forces by approximately 10–30%. As a result, diverse balcony designs are commonly adopted in high-rise buildings.

For better visibility and safety, glass railing systems are often used on balconies. However, the safety of these glass railings should also be considered when estimating wind loads on building façades. Unfortunately, current building codes and standards, except for guidelines related to rooftop parapets, do not provide methodologies for estimating design wind pressures on balcony glass railings. This study aims to design a mid- to high-rise residential building with various balcony configurations. Using wind tunnel test and CFD technology, it will explore the wind effects on glass railings of different balcony types and locations.

Studies have shown that the closer the balcony is to the corner of the building, the greater the net wind pressure on the balcony glass handrail. The net wind pressure on the balcony glass handrail is related to the balcony location, balcony shape, and balcony depth. The experimental results provided in this study will serve as valuable references for future balcony glass railing design, contributing to improved safety for residents.

Keywords: balconies glass railing, design wind pressures, wind tunnel test, CFD

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Peridynamic Modeling of Hydraulic Fracture in Poroelastic Media

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Hydraulic fracturing is widely utilized in engineering applications such as shale gas extraction and enhanced geothermal systems, where a porous solid is fractured through fluid injection. A critical factor influencing fracking efficiency is leak-off, which refers to the loss of fracturing fluid into the surrounding porous medium. This study introduces a novel peridynamics-based computational approach for modeling hydraulic fracturing in porous media. The model integrates a semi-Lagrangian peridynamics (PD) formulation to simulate free-flowing fluids by solving the Navier-Stokes equations and a poroelastic PD formulation using nonlocal differential operators to capture the deformation and fracturing of porous solids with fluid seepage. The fluid-solid interaction (FSI) is modeled by coupling these two PD formulations, incorporating hydraulic forces on fracture surfaces and accounting for fluid leak-off into the porous medium. The comprehensive model is then utilized to investigate the impact of permeability, confining pressure, toughness, and other factors on hydraulic fracturing efficiency, particularly in relation to fluid leak-off. Fig. 1 illustrates the hydraulic fracture process modelled by the proposed computational approach where fluid leak-off is captured together with fracture in porous solid.

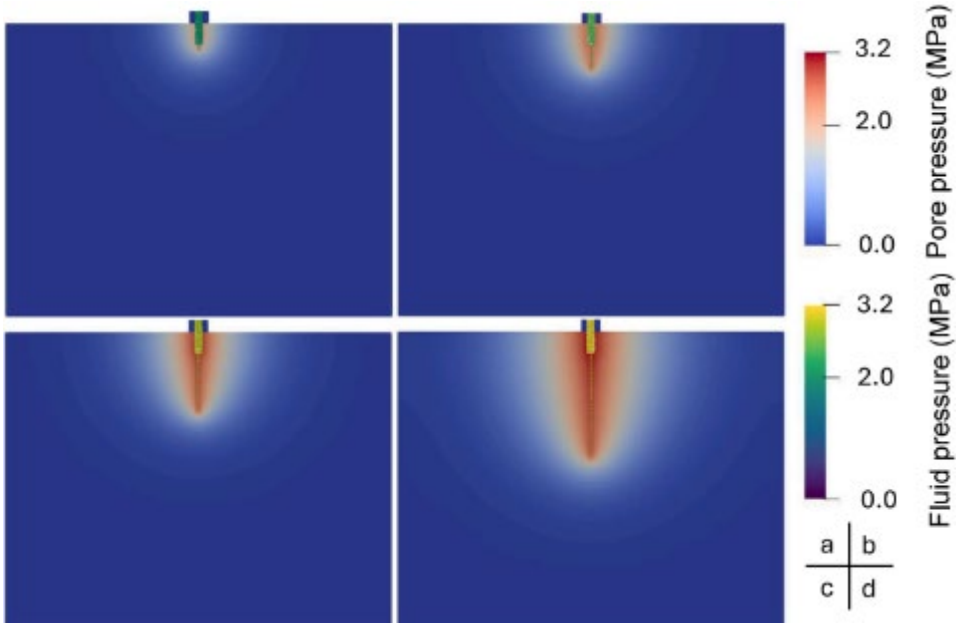

Figure 1. Simulated fluid pressure distribution at 5 ms (a), 25 ms (b), 50 ms (c) and 100 ms (d) for the leak-off dominated case

Keywords: Hydraulic fracture, Poroelastic model, Peridynamics, Leak-off, FSI

Reference:

A Semi-Concurrent Multiscale Modeling-Based Numerical Algorithm for Fluid-Structure-Fracture Interactions

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This study establishes a multi-physics partitioned coupling numerical framework, incorporating a semi-concurrent multiscale model to address the problem of dynamic crack propagation in large-scale structures under fluid-structure interaction. The framework is based on a mesh-based approach, employing the arbitrary Lagrangian-Eulerian (ALE) description for fluid dynamics calculations via the finite volume method (FVM), coupled with structural dynamics calculations based on the finite element method (FEM) and dynamic fracture analysis using the intrinsic cohesive zone Model (ICZM). This enables a multidirectional coupling analysis across multiple solvers and physical fields. To balance the time cost and computational accuracy of dynamic fracture analysis in large-scale computations, the framework introduces a semi-concurrent multiscale model, forming a fluid-solid-fracture interaction (FSFI) architecture of implicit FVM - implicit FEM - explicit FEM/ICZM. The participation of implicit FVM and implicit FEM enhances the efficiency of fluid-structure interaction calculations, while explicit dynamics is adopted for fracture simulations to ensure the robustness of crack propagation modeling. The implicit FEM serves as the primary model, extracting potential crack regions for explicit FEM calculations to analyze crack propagation. During the coupling process, a parallel implicit coupling strategy based on fixed-point iteration and quasi-Newton acceleration techniques is adopted for two-way fluid-structure interaction between implicit FVM and implicit FEM, while parallel explicit coupling is used between implicit FEM and explicit FEM/ICZM. The radial basis function (RBF) method is utilized for interpolating and mapping coupling data on non-matching meshes across solvers, with data communication facilitated through TCP/IP sockets. Based on this framework, the study conducts fluid-structure-fracture interaction calculations for a wind turbine blade under strong wind conditions, analyzing the displacement characteristics and fracture behavior of the blades under extreme conditions.

Keywords: Fluid-structure-fracture interaction, Semi-concurrent multiscale modeling, Two-way coupling, Wind turbine blade

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Molecular design of epoxy resin and the driving forces in adhesion with cementitious materials

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Epoxy resin grouted or coated in cementitious materials serves as an effective method for structural reinforcement and maintenance. However, interface debonding is the primary mode of repair failure, highlighting the need for a deeper exploration of the intrinsic adhesion mechanisms. This study analyzes the bond properties between epoxy resins and cementitious materials by semi-quantifying the mechanical interlocking (micro interface thickness) and chemical interaction (hydrogen bonds). Surface free energies and thermodynamic parameters during the adhesion process were investigated via inverse gas chromatography (IGC) and isothermal titration calorimetry (ITC) tests. Results show that the lower viscosity and higher polarity of epoxy resins lead to enhanced bond strength. The entropy change, induced by OH-π hydrophobic interactions, emerged as the primary driving force during the adhesion process, while the enthalpy change, induced by hydrogen bonds, also plays a favorable role. Moreover, the contribution of hydrates to adhesion effectiveness was determined to be C-S-H > AFt > $Ca(OH)_2$ > $CaCO_3$. Drawing on the entropy-driven thermodynamic adhesion mechanism, this study also introduces a novel approach to enhance bond strength via hydrophobic surface modification of the substrate. The treatment resulted in a 34.7% increase in flexural bond strength, with the contact angle of the substrate rising from 17.2° to 101.4°.

Keywords: Epoxy resin, Cementitious materials, Adhesion, Interface microstructure, Thermodynamic process

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Periodic Lagrangian Analysis with Mesh Reconstruction: introducing a large deformation modelling approach in computational mechanics

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Large deformation process is commonly encountered in engineering practices, particularly in geotechnical applications such as foundation installation, penetrometer test, pipeline laying and buckling, and landslides. Large deformation modelling remains one of the most challenging aspects of computational mechanics. Numerical methods developed to address large deformation issues can be categorized, based on discretization, into Lagrangian mesh-based approaches, Eulerian mesh-based approaches and particle-based approaches. Among these, Lagrangian mesh-based approaches are more established in computational mechanics due to their capability in describing solid behaviours and more straightforward treatment of boundary conditions and interface interactions, compared to the other two approaches. Lagrangian mesh-based approaches are fundamentally based on standard finite element method, specifically extended to resolve issues due to excessively distorted elements during large deformation process.

Falling within this framework, periodic Lagrangian analysis with mesh reconstruction is developed and introduced in this paper. Large deformation modelling is accomplished by mapping variables from deformed old mesh to reconstructed undistorted mesh, after which simulation resumes in the new mesh. Mapping and remeshing, two pivotal components of the proposed approach, are elaborated in this paper. An accurate and efficient mapping algorithm is proposed, with its accuracy verified through element tests. Robust remeshing capability is ensured by using constrained Delaunay triangulation and mesh decomposition technique. In addition to emphasing on mapping accuracy and remeshing robustness, the performance of periodic Lagrangian analysis with mesh reconstruction is demonstrated through several geotechnical applications: (a) anchor trajectory during plate anchor installation; (b) pipeline penetration considering soil strain rate and softening; and (c) cone penetration under various drained conditions.

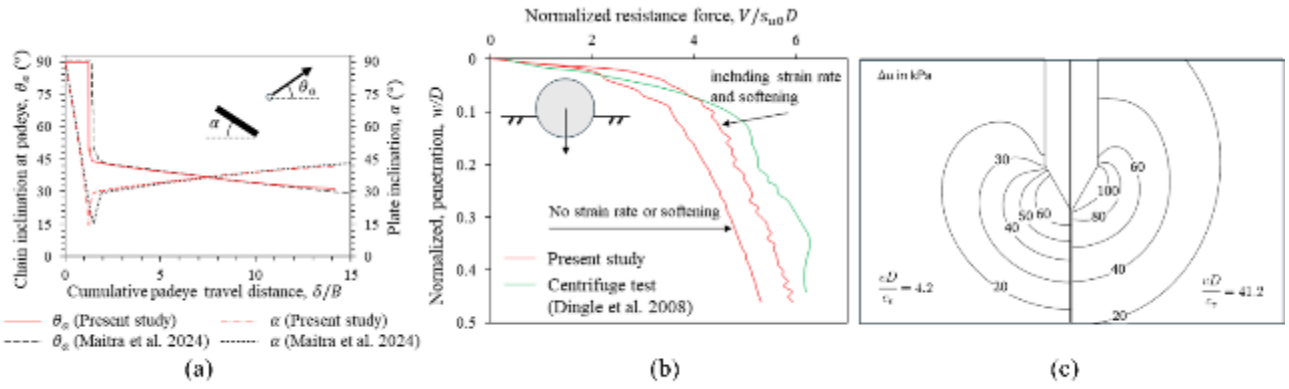

Figure 1.

Keywords: Large deformation, finite element method, Lagrangian analysis, mapping, remeshing

Particle Dispersion in the Framework of a Single-Step and Simplified Lattice Boltzmann Method

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Microparticle dispersion and deposition in flow field have wide applications in micro-contamination control, developing efficient inhalation drug delivery devices, and estimating personal exposure to particulate matters in indoor and outdoor environments. In the widely adopted Eulerian-Lagrangian computational framework, fluid is considered continuum and particles discrete. Fluid flow is solved via Navier-Stokes (NS) equations on the classical assumption where the nonlinear advection and pressure terms poses an extraordinary challenge in complex flows.

Bypassing this limitation, the Lattice Boltzmann Method (LBM) is developed based on simplified kinetic models with fictitious particle movement and collision, simulating the underlying microscopic particle interactions [1]. Here, the convection operator in the velocity space is linear and the pressure can be calculated using the equation of state, greatly simplified when compared to the traditional CFD. In Eq. (1), $\boldsymbol{e}_\alpha$ is the velocity vector of the α-th component, τ is the relaxation time factor directly related to the fluid viscosity, and $f_\alpha^{eq}(\boldsymbol{r}, t)$ is the equilibrium distribution function in the α-th direction.

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{e}_\alpha \cdot \nabla f_\alpha = \frac{1}{\tau}\left(f_\alpha^{eq} - f_\alpha\right) \tag{1}$$

Incorporating the Lattice Boltzmann Method (LBM), this study developed a new computational framework to model microparticle dynamics in 2D and 3D flow domains. Transport and dispersion of the microparticles are performed in a Lagrangian setting and the evolving fluid flow is resolved using a Single-Step Simplified Lattice Boltzmann Method (SSLBM) [2]. A case study is performed to predict the microcontaminants dispersion in an urban environment. It is shown that SSLBM has great potential for solving single- and multiphase flows with a unique view to link the multiscale interpretation.

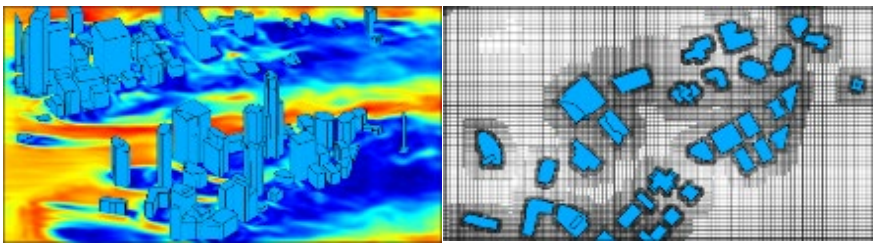

Figure 1. Microcontaminants dispersion in an urban environment.

Keywords: Microparticles, dispersion, Lattice Boltzmann Method, computational fluid dynamics

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Applying Non-ordinary State-based Peridynamics in Visco-elastoplastic Problem

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Rutting damage and cracking failure in asphalt materials represent predominant failure modes in road engineering, which not only compromise the structural service safety but also substantially escalate life-cycle maintenance costs due to recurrent rehabilitation demands. To address these challenges, this study develops a damage-coupled nonlocal visco-elastoplastic incremental constitutive model within the framework of Non-ordinary State-based Peridynamics (NOSB-PD), aiming to systematically elucidate the dynamic damage mechanisms of visco-elastoplastic materials such as asphalt.

The proposed constitutive model employs the additive decomposition principle of strain tensors to decouple the macroscopic strain into viscoelastic and plastic components through linear superposition, corresponding respectively to the viscoelastic and plastic behaviors.

The long-term viscoelastic behavior is characterized by a generalized Maxwell model based on hereditary integrals, where the temporal nonlocal response is governed by the complete history of current and past action.

Regarding plastic evolution, an incremental formulation of the linear isotropic hardening criterion is mathematically established, with plastic flow solely dependent on instantaneous elastic predictions and exhibiting temporal invariance. By rigorously adhering to the von-Mises yield criterion and associated plastic flow rule, the radial return algorithm for stress update iterations of this model is implemented, ensuring the coupling constraints of plastic flow and hardening evolution.

A time-domain explicit difference scheme is derived to formulate an incremental explicit solver for dynamic responses of visco-elastoplastic materials. Material failure is determined via a dual-point averaged stress failure criterion, while damage progression is discretely characterized using peridynamics bond-breaking criteria. Numerical validations through typical viscoelastic, elastoplastic, and visco-elastoplastic dynamic cases demonstrate the correctness, convergence, and high computational accuracy of the proposed method. Comparative analyses demonstrate that, under equivalent precision conditions, the proposed algorithm outperforms conventional finite element methods in capturing damage evolution and crack propagation phenomena within visco-elastoplastic media.

Keywords: Peridynamics, Non-ordinary State-based, visco-elastoplastic, failure criterion

References

Lightweight Auxetic Seismic Metamaterials for Low-Frequency Seismic Wave Attenuation

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Reducing seismic force input at the source is also a crucial issue for structural protection. Seismic metamaterials, periodic structures with unique wave propagation properties, utilize bandgaps to dissipate seismic wave energy. When seismic waves fall within a bandgap, energy transmission is significantly reduced, minimizing structural damage. However, achieving low-frequency bandgaps (below 10 Hz) remains a challenge. Conventional approaches rely on high-mass materials to induce local resonance, which is often impractical due to cost and implementation constraints.

This study introduces a lightweight seismic metamaterial design based on auxetic geometries, enhancing practical feasibility. The effectiveness of this design is demonstrated through comparative analysis with conventional seismic metamaterials. Key geometric parameters are investigated to optimize bandgap performance. Finite element simulations evaluate the vibration attenuation efficiency of auxetic seismic metamaterials in both time and frequency domains. Furthermore, an analytical model based on one-dimensional periodic structures establishes the relationship between mass and stiffness, and modal analysis confirms the bandgap characteristics. The proposed metamaterials are lightweight, compact, and capable of attenuating low-frequency seismic waves, offering a viable solution for practical seismic protection applications.

Keywords: auxetic; periodic structure; seismic metamaterial; auxetic geometry; bandgap

A Riemann-Solver-Free Spacetime Discontinuous Galerkin Method for Conservation Laws with Solution Enrichment via Radial Basis Functions

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This presentation introduces a Riemann-solver-free spacetime discontinuous Galerkin (DG) method designed for general conservation laws on arbitrarily unstructured meshes.

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}}{\partial x} + \frac{\partial \boldsymbol{g}}{\partial y} = \boldsymbol{s} \tag{1}$$

The method combines the strengths of the spacetime Conservation Element/Solution Element (CE/SE) method and the DG method. The key innovation lies in constructing a staggered spacetime mesh using alternate cell-centered and vertex-centered CEs within each time step. The solution within each SE is approximated by spacetime DG basis polynomials, and flux conservation is enforced inside each CE using the DG framework.

The unknowns are stored at both the vertices and cell centroids of the spatial mesh. However, the updates to the solutions at these locations are staggered in time, with updates occurring at different time levels for the vertices and cell centroids. This alternating update scheme defines the method as a Cell-Vertex Scheme (CVS).

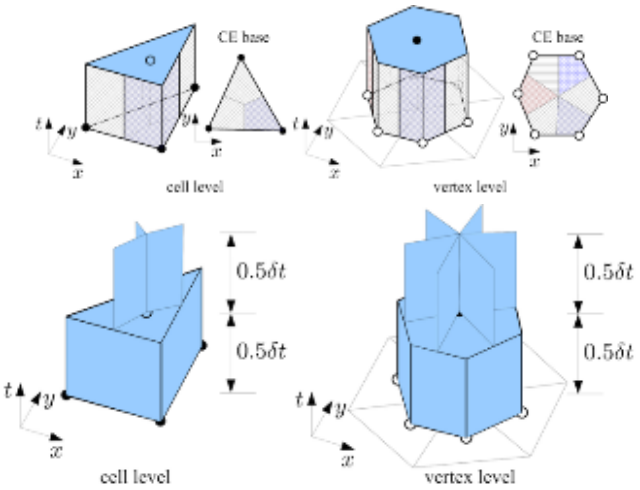

Figure 1.

Due to the staggered spacetime formulation, there is no need to define left and right states at the spacetime interface. Instead, the solution is continuous across the interface, allowing for a direct evaluation of the flux without requiring Riemann solvers. This makes the method applicable to a wide range of conservation laws. Furthermore, diffusive fluxes can be handled similarly, without the special treatments often required by other DG methods.

To ensure computational efficiency, the method employs linear DG basis functions rather than higher-degree polynomials, while enriching the solution at the end of each physical time step using radial basis functions. Several benchmark problems, including the compressible Euler equations, shallow water equations, and magnetohydrodynamics (MHD) equations, are used to demonstrate the accuracy and effectiveness of the method.

Keywords: Riemann solvers, conservation laws, discontinuous Galerkin method, spacetime methods, radial basis functions

Discussion of User-defined Parameters for Subspace-based Identification using Laboratory- and Field-data

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Real-time or online system identification techniques are improving in civil engineering, enabling the development of early warning systems and autonomous damage assessment of structures. From the viewpoint of structural engineering, online system identification can be used to track the modal parameters of structures, provide a warning message about damaged structures, and further help with post-earthquake reconnaissance and rehabilitation by identifying the dynamic characteristics and behaviors of structures and systems based on their measured data. To achieve real-time or online system identification, several techniques have been modified into a recursive formulation, such as the recursive autoregressive exogenous model, recursive instrumental variable, and recursive prediction error method. For decades, subspace-based approaches have been significantly improved and become advantageous ways for accurate estimation, data-driven framework, ease of implementation, automated modal analysis, flexibility, and adaptability. Recently, the methods related to subspace identification have been modified to recursive ones to detect the time-varying dynamic characteristics. In this study, the recursive formulations for subspace identification are first introduced. Then, the user-defined parameters used in determining modal order and managing spurious modes in field applications are carefully discussed, and the effect of those parameters on the identification results is examined. For verification of the proposed methods and user-defined parameters, two different datasets are used: one is a laboratory test of a multi-story steel frame with changes in column stiffness, and the other is seismic responses from a real building from Taiwan Strong Motion Instrumentation Program (TSMIP). The challenges of selecting the suitable model order can be verified for the online system identification techniques during the earthquake excitations. Finally, a brief summary and general suggestion on choosing suitable user-defined parameters in subspace-based identification are given, and this paper ends with a conclusion.

Keywords: subspace identification, recursive subspace identification, on-line system identification techniques

A Hybrid resolved-unresolved SPH(2)-DEM coupling scheme for fluid-graded granular materials interactions

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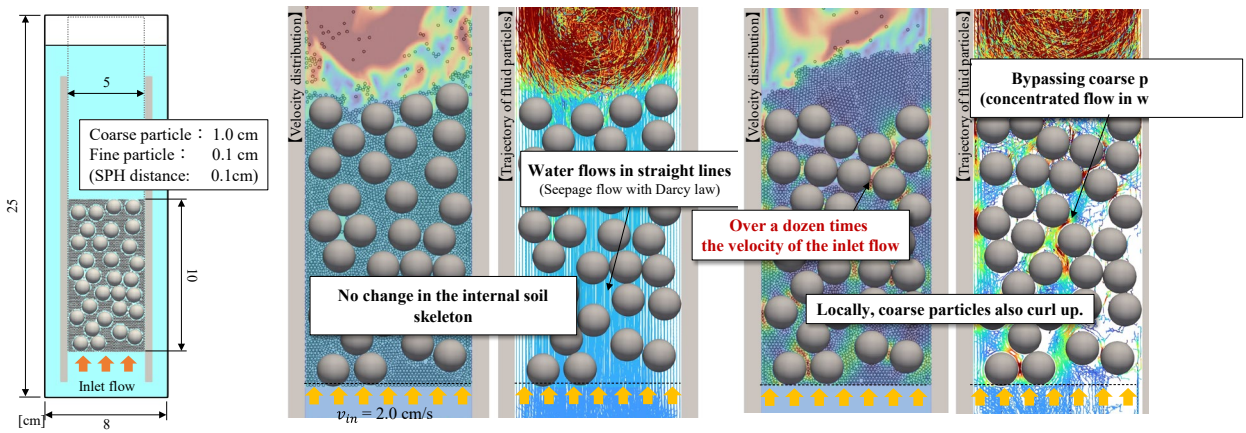
Numerical simulations of natural hazards often face challenges in designing effective coupling strategies. For example, deciding whether to treat large soil particles as moving wall boundaries can be challenging when investigating internal erosion from seepage flow in gap-graded geomaterials. Simulating debris flows, which include fine sediments, large rocks, and driftwood, is also complex. There are two main types of coupling models: the "Resolved coupling model," which provides detailed fluid dynamics, and the "Unresolved coupling model," which is based on empirical drag and seepage models. Previous studies suggest evaluating these models based on the ratio of solid particles to fluid resolution [1]. However, using the resolved model is often impractical due to computational costs for tiny solid objects, while the unresolved model struggles to represent localized failures like internal erosion.

This study proposes a hybrid coupling model for multiphase flows with gap-graded materials, in which both the resolved and unresolved models can be used simultaneously. Our method employs a resolved model based on the fictitious domain method for large objects strongly affecting the flow and an unresolved model for fine sediment. The proposed model is achieved by combining rigid-body dynamics with DEM and fluid dynamics with SPH, which is enhanced by SPH(2) and various other technologies to improve accuracy [2]. We evaluate the performance of the proposed method through numerical experiments focused on internal erosion, as illustrated in Figure 1.



(a) Simulation model and conditions (b) Results in unresolved coupling model (c) Results in proposed hybrid coupling mode

Figure 1.

Keywords: Particle method, SPH, DEM, Resolved coupling model, Unresolved coupling model

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A State-of-the-Art Review on Using the SBFEM in Water Wave – Structures Interaction: Development in Last Two Decades **and Way Forward**

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The Scaled Boundary Finite Element Method (SBFEM) has primarily been used for solving interaction problems with infinite solution domains. A recent application of this method has been to study how waves interact with fixed and floating marine structures. This type of structure is typically constructed for the purpose of protecting coastal areas and other structures, as well as providing platforms in ocean environments. This review aims to generate a detailed understanding of how SBFEM can be implemented to solve the problem of wave interaction with floating and fixed structures in the marine environment, as well as to analyze its advantages, accuracy, and limitations. According to the study, this method eliminates the shortcomings of common numerical methods and provides distinct advantages over them. Taking into consideration the advances made in this method over the past few years, this paper can be a motivation for ocean engineering researchers to incorporate this numerical-analytical method into their future research.

Keywords: Scaled Boundary Finite Element Method, Water Wave – Structure Interaction, Fixed and Floating Marine Structures

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Transgranular and intergranular fracture modelling in brittle polycrystals using the scaled boundary finite element method

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Brittle polycrystalline materials such as solar grade silicon are used in various engineering applications where understanding of failure mechanisms is of interest. The microstructural features of such material play an important role. Fracture can occur both along grain boundaries (intergranular) and through the grain (transgranular). The combined numerical modelling of both transgranular and intergranular failure modes in polycrystals is challenging for various reasons. Firstly, any model must represent the inherent anisotropic behaviour of crystalline material both with respect to elastic and fracture properties and the reduction of the fracture toughness near the grain boundaries. Secondly, robust and flexible meshing techniques are required that are tailored for polycrystal geometries. Finally, crack propagation modelling is associated with difficulties related to crack propagation criteria, re-meshing and corresponding numerical effort. To address the latter challenges, a phase-field approach to fracture modelling is used, within which both transgranular and intergranular fracture phenomena can be represented in a unified way. To get a mesh that conforms to the polycrystalline geometry, facilitate localized remeshing and thus to reduce numerical effort, polygonal meshes are employed. These are based on the scaled boundary finite element method (SBFEM), which can accommodate polygonal elements and elements with hanging nodes elegantly. The adaptive phase-field approach to fracture based on SBFEM proposed in [1,2] is extended to model the damage process in polycrystalline materials. To account for the grain orientation and anisotropy, the phase field equation is modified as suggested by Nguyen et al. [3]

$$-G_c l_0 \nabla\varphi \cdot \boldsymbol{A} \cdot \boldsymbol{\nabla}\varphi + \left[\frac{G_c}{l_0} + 2H^+\right]\varphi = 2H^+. \tag{1}$$

In Eq. (1), the symbols G_c, l_0, φ and H^+, denote the fracture thougness, length scale, phase-field variable and history variable, respectively. The fracture toughness near the grain boundaries is modelled following a smeared approach along the lines of [3]. Here, an additional phase field parameter $\alpha(\mathbf{x})$ and a corresponding length scale parameter l_α are introduced to represent the geometry of grain boundaries. The effective fracture toughness is then obtained as a function of $\alpha(\mathbf{x})$ and of the misorientation angle of adjacent grains. The proposed approach will be explained in detail and accuracy and efficiency will be illustrated using various examples.

Keywords: Polycrystalline material, transgranular / intergranular fracture, phase-field method, scaled boundary finite element method, anisotropy, grain boundaries

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FSI study of flapping wing geometry effects in compressible flows

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Inspired by insects and birds, flapping wing configurations inherit their ability to generate sufficient lift in low operational Reynolds number regions, resulting in reduced power consumption and extended flight durations. To determine the effects on aerodynamic performance in compressible flows, this study focuses on the aspect of flapping wing geometries. In particular, five different wing shapes with the first moment of area $\bar{r}_1$ values varying from 0.4 to 0.6-covering the majority of insect wing configurations-are investigated to examine the effect of geometry in compressible flow conditions. Figure 1 below represents the wing shape outlines for each wing designs.

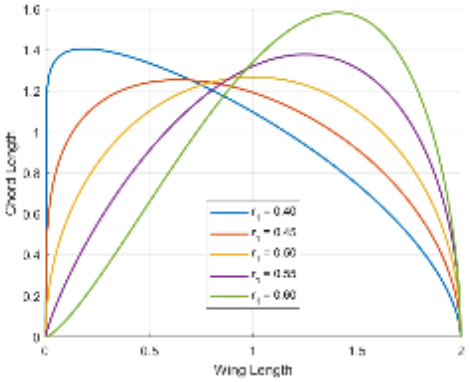

Figure 1.

For CFD simulations, a well-validated 3D immersed boundary-finite difference method solver is used to compute the aerodynamic forces, with the lift coefficient being primarily analysed to evaluate performance, and the following kinematic function is adopted to mimic insect's hovering flight:

$$\theta = \frac{A_\theta}{2} \sin(2\pi f t) \tag{1}$$

$$\phi = \frac{A_\phi}{2} \sin(2\pi f t + \frac{\pi}{2}) \tag{2}$$

Where θ is the pitch angle defined by the peak-to-peak pitch angle A_θ, ϕ the stroke angle defined by the max stroke angle A_ϕ, and f the flapping frequency.

Simulations are conducted across subsonic and supersonic flow conditions, confirming critical findings that increasing the $\bar{r}_1$ positively influences aerodynamic performance by enhancing lift generation in incompressible flows. However, as compressibility effects increasingly dominate the aerodynamic performance, while wings with higher $\bar{r}_1$ values maintain a relative advantage in lift generation over those with lower $\bar{r}_1$ values across this regime, the difference in lift coefficients between wing configurations yet diminishes progressively.

Keywords: CFD, FSI, Immersed Boundary Method, Finite Difference Method, compressible flows

The origin of Na-montmorillonite anisotropy: exploring the microstructure based on molecular dynamics under different hydration degrees

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Montmorillonite is the primary component of bentonite, and its mechanical behaviour exhibits different properties depending on the degree of hydration. This study uses molecular dynamics to simulate and investigate the atomic structure and fracture behaviour of sodium-montmorillonite (MMT). Uniaxial deformation was applied to Na-MMT at varying deformation rates under different hydration conditions. The research reveals that the mechanical behaviour of Na-MMT is anisotropic and significantly influenced by the degree of interlayer hydration. For instance, the ultimate compressive strength and Young's modulus of Na-MMT in different directions tend to decrease as the degree of hydration increases. When deformation rate is applied along two directions within the MMT layers, different deformation behaviours are observed depending on the unit cell structure. These behaviours provide a clear explanation for the origin and reasons behind the anisotropy of Na-MMT, offering important insights. This work elucidates the complex interactions between the degree of hydration, structural anisotropy, and uniaxial deformation in Na-MMT. It also provides critical scientific insights for future research on temperature effects, interlayer cations, and other mechanical responses.

The development of new analysis method for aluminum wheel rim deformation using simple tire model and discussion of test error

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During vehicle development, Various test evaluations are conducted as a part unit. Among them, permanent deformation tests are being conducted to prevent rim fracture of aluminum wheels. This test measures the permanent deformation of an aluminum wheel rim end when a load is applied to it using an inclined jig and then removed. The test method is simple, but it is difficult to accurately predict the results because tires with complex characteristics are involved.

Since tire modeling has not been possible so far, a method using normal distribution analysis has been used, but correlation problems often occur. Recently, simple tire modeling has become possible, The new rim deformation analysis method including a tire model has been developed. Although we could not create an actual tire shape, we created a finite element model with the same vertical stiffness and applied it. We performed a test-CAE analysis cross evaluation with three vendors and the test correlation of the analysis method including the tire model was better.

However, there were differences in the test results of the three vendors, and the cause was analyzed. An analysis of the causes of test dispersion by supplier was conducted, and important causes were found. As a result of reflecting the measured jig angle in the analysis model, the same results as the test were obtained.

And the permanent deformation due to the difference in tire stiffness was analyzed. The best improvement method is also presented when the rim deformation test is unsatisfied. It is expected that the analyzed research content will be helpful in determining optimal rim design conditions. In particular, it can help reduce the weight of vehicles.

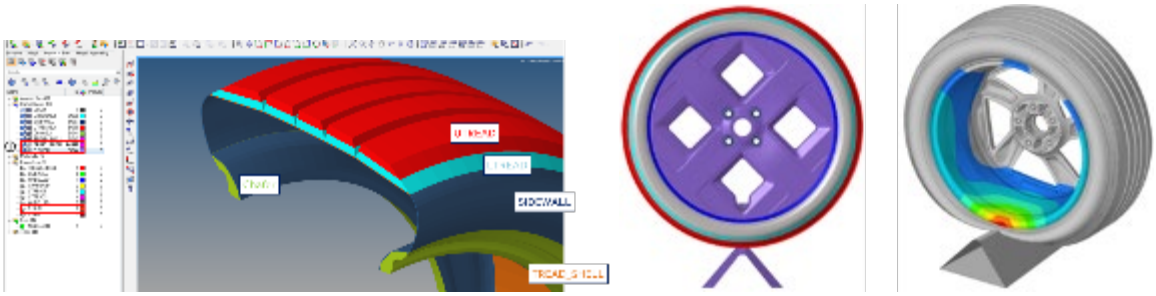

Figure 1. New analysis method of rim deformation using simple tire

Keywords: Aluminum wheel, Plasticity, Deformation, X/C fatigue, Strain analysis, FEM, Simple tire model

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A FD-SPH for robust fluid-rigid body coupling simulation

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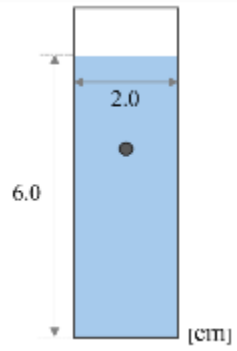
Recent torrential rains have led to severe debris flows in many countries worldwide. Fluid-rigid body coupling simulations using the particle method can be an effective approach to better understand multiphase flows that consist of large rocks, driftwood, and river water. A sophisticated multiphase flow simulation requires accurately estimating the interaction between the fluid and rigid bodies while simultaneously modeling the turbulent flow. In general fluid-rigid body interaction simulations, fluid forces are often calculated using surface integrals. However, for complex geometries, the discontinuous normal vector distributions on the surface of the objects can disrupt the stability. This study proposes an SPH based fluid-rigid body coupling simulator enhanced with SPH(2) fluid dynamics and robust interaction computation with the fictitious domain (FD) method. FD assumes that the interior of an object is filled with a fictitious fluid. By evaluating interaction forces through volume integration, this approach does not require any normal vectors on the surface of the rigid body, making it highly applicable to complex-shaped objects.

This study verifies the proposed method by simulating a circular disk's settlement. Figure 1 shows the simulation model, and the disk's settling velocity over time. The results improve with higher spatial resolution but initially do not match the reference solution by Glowinski et al. [1] due to a volume error in modeling the rigid body as particles. A correction is applied to ensure the total volume is accurate, leading to better agreement with the reference solution, even at coarser resolutions. The study will further validate the method with experimental data on settling complex-shaped objects.



gravitational acceleration	g	$-980\,\mathrm{cm/s^2}$
initial particle distance	d_x	0.01, 0.02 cm
fluid density	ρ_f	$1.00\,\mathrm{g/cm^3}$
rigid body density	ρ_s	$1.25\,\mathrm{g/cm^3}$
kinematic viscosity	ν	$0.1\,\mathrm{cm^2/s}$
time step width	Δt	5×10^{-5} s

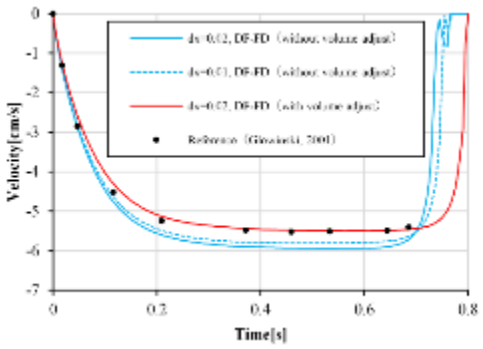


Figure1.

Keywords: Particle method, SPH, Fluid-rigid body interaction, Fictitious domain method

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Design of new interlocking elements and evaluation of their dynamic performance

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Topological interlocking (TI) is a design principle in which specially shaped elements are arranged to achieve global stability solely through their geometry, thereby establishing kinematic constraints without the need for connectors or binders. TI structures have gained attention due to their enhanced fracture resistance, superior energy absorption, and potential for reusability. This study employs a parametric design method to generate novel planar TI structures featuring curved contact interfaces, where interlocking is achieved through paired concavo-convex surface morphology. A validated numerical model is used to compare the impact performance of these TI structures against monolithic counterparts, while the influence of geometric parameters on overall structural performance is also examined. The results suggest that by adjusting geometric parameters, tunable mechanical performance can be achieved without increasing material consumption.

Keywords: Topological interlocking, curved interfaces, impact performance, tunable performance

Data-driven formulation of quasi-steady aerodynamic model of flapping wings

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Insects stay airborne by means of flapping wings, utilizing various unsteady aerodynamic mechanisms. Understanding their flight mechanisms is of great importance from biological, physical, and engineering perspectives. To investigate the flapping aerodynamics, robotic and computational simulations, which can capture the flow field and aerodynamic force with high accuracy and resolution, have been utilized, but their time-consuming natures make it unsuitable for the application to optimization or machine learning. Quasi-steady models, which explain the aerodynamic force by instantaneous attitudes and kinematics of flapping wings, can estimate the aerodynamic performance much faster, but the assumption that flapping wings rotate around their base reduces the accuracy especially when applied for free-flight. In this study, we improved the accuracy of quasi-steady models using data-driven model discovering method [1]. The ground truth data is based on the correlation between kinematics and aerodynamic force acquired by computational fluid dynamics. In the model discovering method, sparse identification was performed to explore the mathematical formula of kinematic parameters required for the aerodynamic force models. As a result, we have discovered various force generation mechanisms that have not been considered in the conventional quasi-steady models. A new quasi-steady model was built by incorporating these mechanisms, which successfully reduced errors in the estimation of aerodynamic force by flapping wings in various flight regimes and different Reynolds numbers (Figure 1). This model can be effectively applied to wing kinematics optimization, stability analysis, or reinforcement learning, for free-flying conditions including manoeuvring.

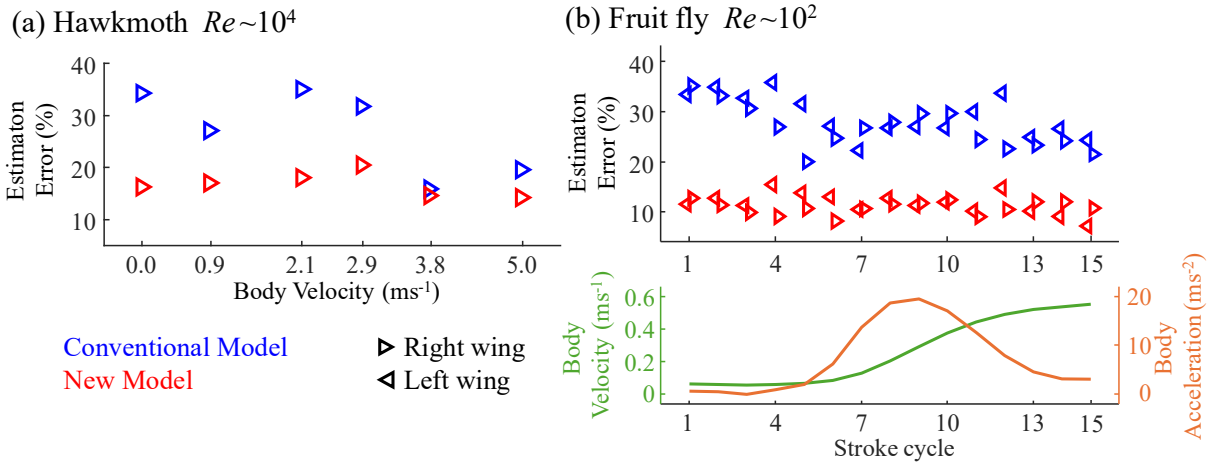

Figure 1.

Keywords: Flapping, Quasi-steady Model, Data-driven, Sparse Identification

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Integrated Topology and Path Optimization for Fiber-Reinforced Composite Structures with Concentric Printing Paths

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Fiber-reinforced additive manufacturing has emerged as a promising technique for fabricating lightweight and high-strength structures by depositing material in a layer-by-layer fashion. One of the key advantages is the ability to control fiber orientation during the printing process, which can significantly enhance mechanical performance. However, the inherent anisotropic properties of fiber-reinforced composites (FRCs), resulting from the deposition patterns and constrained by the chosen layer-by-layer printing strategy, pose substantial challenges in structural design and optimization [1]. In particular, commonly used concentric printing paths [2] coupling with structural geometries, resulting in challenges in both topology and path optimization [3].

This work presents a novel optimization framework that simultaneously determines both the optimal topology and the manufacturable printing paths of FRC structures based on concentric printing paths. Unlike conventional topology optimization methods that optimize the structure first and then apply post-processed printing paths [4, 5], our approach integrates the printing path directly into the optimization process to ensure manufacturability. First, a finite element model specialized for FRC structures with concentric paths is developed to represent the structural response. The optimization algorithm then iteratively updates both the structural topology and the corresponding printing paths in a concurrent manner, ensuring that the final design is manufacturable using fiber-reinforced 3D printing techniques.

To demonstrate the effectiveness of this approach, several numerical examples and experimental printed models are presented. The proposed framework provides a seamless integration of computational design and additive manufacturing, enabling the fabrication of highly optimized FRC structures with tailored fiber orientations. This research contributes to advancing topology optimization in the field of fiber-reinforced additive manufacturing, offering new possibilities for high-performance lightweight structures.

Keywords: Fiber-reinforced composite structures, additive manufacturing, concentric printing paths, topology optimization

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CycleGAN based 3D multiphase microstructure reconstruction method preserving real microstructural characteristics

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Composite materials, such as cementitious materials, have complex internal microstructures. These microstructures are strongly affect the performance of the materials. In this study, a method is proposed to reconstruct a virtual 3D microstructure with the same microstructural characteristics as the real multiphase microstructure of the cement paste obtained by micro-CT, as shown in Fig. 1. The reconstruction of the 3D microstructure is a two-step process based on CycleGAN [1]. The first step is to train the 2D cross-sectional images obtained by micro-CT to construct three virtual 2D images, and the second step is to generate a virtual 3D microstructure from the virtual 2D images. The process of this multiphase microstructure reconstruction based on CycleGAN (MMR-GAN) has been validated in previous work [2], and an extension is presented in this study. In this method, the phase ratios are obtained from the real microstructure and applied to the reconstructed 3D microstructure, and the characteristics of each phase distribution are quantified using probability functions. These probability functions are then compared with those of the real sample and accepted if the microstructure-based criteria are met. This method allows a virtual 3D microstructure to be reconstructed with the same microstructural characteristics as the real 3D microstructure. This method can ensure the quality of the reconstructed multiphase microstructure not only in terms of visual perspective but also in terms of material properties.

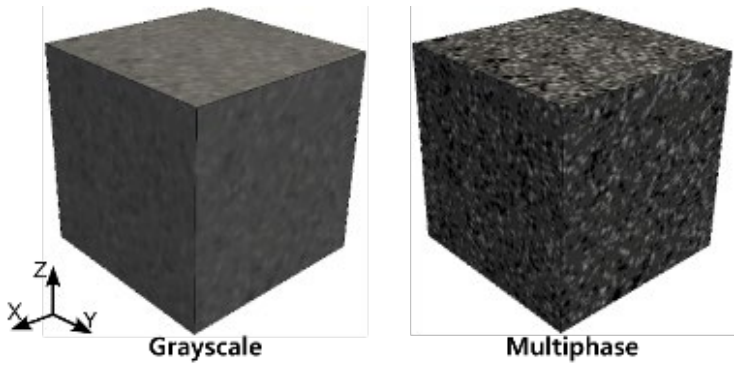

Figure 1. microstructure of cement paste obtained from micro-CT and its multiphase representation

Keywords: reconstruction, multiphase, CycleGAN, 3D microstructure, microstructural characteristics

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A Straightforward yet Effective Approach to Predict the P-I Diagrams of RC Beam during Design Process

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This research presents a straightforward yet efficacious methodology for generating bending and shear P-I diagrams for arbitrary reinforced concrete (RC) beams utilizing a linear interpolation procedure, thereby obviating the need for conducting multiple blast analyses through rigorous nonlinear time-history approaches. The bending and shear P-I diagrams for a limited number of RC beams have been constructed and serve as reference P-I diagrams for the linear interpolation process. A total of 144 representative RC beam cases have been incorporated into the database, with plans for expansion through the continual addition of RC beam data. Given that the P-I diagram is formulated based on the blast analyses of RC beams subjected to uniform blast pressure, this paper additionally proposes a method for determining the equivalent uniform pressure-time history resulting from TNT explosions, whose effects may vary along the beam span. Furthermore, this paper introduces a method to adjust for the influence of changing boundary conditions on the P-I diagrams. By utilizing the proposed methods for evaluating equivalent uniform pressure-time histories and the linear interpolation procedure, flexural and shear P-I diagrams for arbitrary RC beams can be effectively determined. The efficacy of the proposed interpolation approach has been validated through comparisons between the interpolated P-I diagrams and those directly derived from multi degree of freedom blast analyses, supplemented by additional parametric studies to investigate the influence of various design variables on the P-I diagrams. As shown in Figure 1, proposed methodology can be effectively utilized to assess the removal or retention of explosion-damaged RC beams for which flexural or shear P-I diagrams are not available, as well as in determining the sectional dimensions and steel ratios of RC beams during the preliminary stages of explosion-proof design.

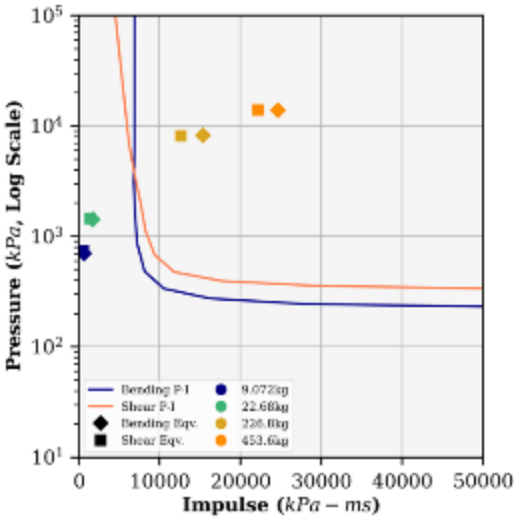

Figure 1.

Keywords: Blast analysis, Pressure-impulse diagram, TNT explosion, Moment-curvature relation

Numerical Simulation of Heat Transfer in Lattice Structure for Heat Sink Application

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Introduction: Heat sinks play a vital role in electronics, vehicles, and industrial settings by removing excess heat thereby preventing overheating. Their performance relies on factors like the surface area, the materials used, their designs, and their heat transfer efficiency. Testing different heat sinks designs using traditional method can be slow and costly. Instead, numerical simulations provide an efficient way to study and enhance their effectiveness. The integration of lattice structure in heat sink is significant because of their enhanced surface area, which facilitates efficient thermal management. This study employs numerical simulation to study the heat transfer in X-type lattice structures using ANSYS Fluent 2023 R2.

Methodology: The X-type lattice structure, as sketched in Fig. 1, was first modelled in SolidWorks and repaired in SpaceClaim. The material selected for the lattice structure was steel having a thermal conductivity of 16.25 W/(m·K). The continuity and Navier-Stokes equations were solved using the finite volume method. The turbulence was modelled by SST k-ω to capture the near wall accurately. Variation in lattice angle (α) ranges from 50 to 30 degrees. The governing equations are the continuity and Navier-Stokes equations as follows,

$$\nabla . \mathrm{V} = 0$$

$$\rho(V . \nabla)\mathrm{V} = -\nabla \mathrm{P} + \mu \nabla^2 \mathrm{V} - \nabla . (\rho \mathrm{u}' \mathrm{u}')$$

where ρ is fluid density, V is the mean velocity vector, P is the mean pressure, μ is the dynamic viscosity, and $\nabla . (\rho \mathrm{u}' \mathrm{u}')$ is the Reynolds stress terms that account for the effect of turbulence.

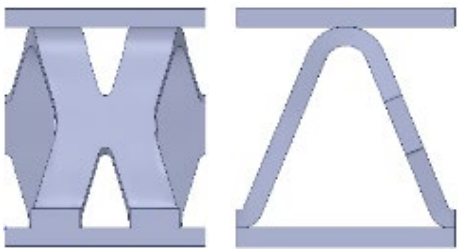

Figure 1. Schematic of a section of the X-type lattice structure considered.

Result: The result shows that the lattice angle plays a crucial role in heat dissipation. Angle 40 has the best combination of both pressure drop and heat dissipation.

Conclusion: This study demonstrated that X-type lattice structure has a high heat dissipation capability which is associated with their increased surface area.

Keywords: Heat sink, lattice structure, thermal management, numerical simulation

Stress-based Multi-material Design by Floating Projection Topology Optimization

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Ensuring structural integrity through strategic material allocation and stress control is essential for preventing engineering failures, especially in complex multi-material systems. While topology optimization has revolutionized structural design approaches, traditional methods primarily focus on global performance metrics and struggle with localized stress management. This work introduces an enhanced multi-material stress optimization framework leveraging the Floating Projection Topology Optimization [1] approach with linear interpolation functions. Breaking from conventional Solid Isotropic Material models with penalization-based interpolation, our methodology facilitates seamless material transitions and naturally extends to N-material optimization scenarios. By combining comprehensive stress evaluation techniques with floating projection principles, the framework effectively simulates binary material constraints without relying on standard material penalization methods, thereby improving material distribution clarity. Experimental results from both 2D and 3D computational test cases confirm the approach's capability to achieve optimal material configurations while minimizing stress concentrations, offering a more resilient and computationally practical framework for real-world engineering applications.

$$\begin{aligned} &\min: f = \bar{\sigma} + \sigma^{pn} = \frac{\sum_e \sigma_e^m}{\sum_e x_{e,1}} + [\Sigma_e(\sigma_e^m)^p]^{\frac{1}{p}} \\ &\text{s.t.}: \begin{cases} V_{f,i} \le V_{f,i}^* \text{ or } W_f \le W_f^* \\ x_{\min} \le x_{e,N} \le x_{e,N-1} \le \cdots \le x_{e,1} \le 1 \\ x_{e,i} = x_{min} \text{ or } 1 \text{ except for boundary} \end{cases} \end{aligned} \tag{1}$$

In Equation (1), the objective function consists of two stress measures to be minimized: $\bar{\sigma}$ represents the average stress measure, while σ^{pn} denotes the maximum stress measure, where $p > 1$ is a self-defined parameter controlling the aggregation intensity. The constraints include volume and weight limitations, where $V_{f,i}$ and $V_{f,i}^*$ denote the volume fraction of material i and its constraint value, respectively, while W_f and W_f^* represent the weight fraction of the entire structure and its corresponding constraint value. The design variable $x_{e,i}$ is defined as the summation of materials from position i to N in the material sequence, ensuring a proper material distribution throughout the optimization process.

Keywords: Topology optimization, stress minimization, linear interpolation, multiple materials, floating projection

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Assessing Potential Pressure Recovery in Coronary Tandem Stenoses

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Coronary tandem stenoses, characterised by multiple narrowed segments within a single artery, present challenges for physiological assessment using fractional flow reserve (FFR). This study investigates the hemodynamic mechanisms driving pressure recovery in tandem stenoses and its implications for FFR interpretation. A computational fluid dynamics (CFD) study was conducted using ANSYS FLUENT 2024 R1 to simulate blood flow in coronary arteries with stenotic lesions. Two cases were examined: one with a single severe stenosis (≥80% narrowing) and another with a tandem stenosis configuration where a moderate stenosis (40–70% narrowing) was located downstream of the severe stenosis. Flow parameters, including axial (Figure 1) and radial velocity contours, wall shear stress, flow vorticity, turbulent kinetic energy, and instantaneous coherent structures, were analysed to characterise flow behaviour and pressure distribution.

Results show significant pressure recovery in the tandem stenosis configuration, leading to a reduction in the apparent severity of the downstream stenosis. Increased turbulence and shear-layer interactions were observed in this region, altering local haemodynamics and influencing FFR measurements. Comparisons with the single stenosis case highlight the role of flow recirculation and turbulence-induced energy dissipation in modulating pressure distribution. These findings are consistent with previous observations reported by [1], reinforcing the need for careful interpretation of FFR in patients with multiple lesions. Understanding the impact of pressure recovery may inform clinical decision-making for treatment strategies.

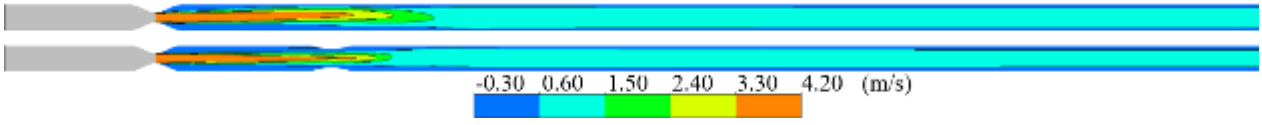

Figure 1. Axial velocity contours of two cases without (top) and with (bottom) moderate stenosis (with a degree of stenosis of 50%) located downstream of an upstream 85% severe stenosis.

Keywords: computational modelling, coronary artery, tandem lesions, pressure recovery.

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Topology Optimization Using a Fourth-Order Reaction-Diffusion Level Set Method

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This paper introduces an advanced isogeometric topology optimization framework based on a higher-order reaction-diffusion model. Unlike conventional methods that rely on the second-order Laplacian operator [1, 2], our approach incorporates a fourth-order biharmonic operator to regulate curvature variations, thereby enhancing the structural smoothness and numerical stability in optimization problems. Both the elastic equations and the reaction diffusion equation are represented using Non-Uniform Rational B-Splines (NURBS), which enables precise geometric representation of complex structures while ensuring computational robustness.

The level set function is updated using isogeometric analysis with k-refinement, which ensures higher-order continuity in the solution space, reducing numerical dissipation and enhancing computational performance compared to traditional finite element methods. The governing equation for the reaction-diffusion-based level set update is formulated as follows:

$$\frac{\partial \varphi}{\partial t} = -D\Delta^2\varphi + R(\varphi) \tag{1}$$

in which φ represents the level set function, D denotes the diffusive operator responsible for smoothing effects, and $R(\varphi)$ serves as the reaction term that drives the evolution of the topology. Compared to conventional level set methods, our framework achieves faster convergence with fewer iterations, avoiding the need for additional filtering techniques such as Gaussian convolution [2]. Furthermore, the integration of NURBS-based k-refinement allows for superior control over high-order derivatives, making it particularly suitable for applications where geometric accuracy and computational efficiency are critical. The figure illustrates the advantages of k-refinement, while the table presents the order of basis functions.

Figure 1.

case	Refinement	Order for elastic equations	Order for reaction diffusion equations
1	no-refinement	1	1
2	p- refinement	1	2
3	k- refinement	1	2

Table 1.

Keywords: Topology optimization; Biharmonic term; Isogeometric analysis; NURBS

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Analyzing elastic half-spaces with cavities under wave loads using an RK dynamic infinite meshfree method

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This study introduces the Reproducing Kernel Dynamic Infinite Meshfree Method (RK-DIMM) for analyzing elastic half-spaces with cavities subjected to seismic wave loads [1]. By integrating Reproducing Kernel Particle Method (RKPM) with Dynamic Infinite Element Methods (DIMM), RK-DIMM ensures computational efficiency and accuracy in simulating wave propagation in semi-infinite domains. The method partitions the domain into near and far fields, employing RKPM for localized accuracy and DIMM for efficiently managing wave dissipation. RK-DIMM incorporates stabilized conforming nodal integration (SCNI) and naturally stabilized nodal integration (NSNI) [2] to achieve numerical stability and precision. Benchmark comparisons confirm its ability to model seismic wave interactions and underground cavity effects. The method is further validated using 1999 Chi-Chi earthquake data, demonstrating its practical application in seismic impact assessments on infrastructure. RK-DIMM presents a robust alternative to traditional finite element methods [3], offering enhanced accuracy and efficiency for computational geomechanics

Keywords: Meshfree methods, Wave propagation, Seismic analysis, Elastic half-spaces, RK-DIMM

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Composition Design and Mechanical Properties of High-Strength and High-Toughness Zinc Alloys Based on Machine Learning

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Zinc alloys are widely used in automotive, electronics, and construction fields due to their low melting point and excellent casting properties. However, the challenge of balancing strength and toughness limits their application in high-end structural materials. In this study, machine learning algorithms were combined to design and develop a novel high-strength and high-toughness zinc alloy. Through feature engineering, key elemental features influencing the mechanical properties of zinc alloys were identified, and the XGBoost algorithm was employed to construct machine learning prediction models that correlate alloy composition with hardness, tensile strength, and elongation, respectively. The prediction accuracy of all three models on the test set exceeded 0.9. By integrating the NSGA-III multi-objective optimization algorithm, a zinc alloy that satisfies both strength and toughness requirements was designed and experimentally validated. Machine learning plays a crucial role in identifying the optimal balance among multiple mechanical performance indicators, significantly advancing the design and performance prediction of novel zinc alloys.

Keywords: Machine learning; XGBoost model; NSGA-III; Zinc alloy; Mechanical property

Acknowledgements

Authors want to thank the support of Project funded by National Natural Science Foundation of China 12302179, 22108316), Natural Science Foundation of Zhejiang Province (LY24E010001), Ningbo Natural Science Foundation (2023J102), Major Science and Technology Projects in Ningbo (2024Z070, 2024Z158).

B-spline Based Superimposing-Version of Finite Element Method for Fluid Boundary Value Problems with Nitsche's Method

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Our ultimate goal is to analyze the flapping-wing motion of a free-flying insect as a fluid–structure interaction (FSI) phenomenon. Numerical methods for handling moving boundaries in FSI analysis can be broadly classified into tracking and capturing methods. The tracking method, however, often leads to distorted meshes in the fluid domain, causing instability due to the large deformations, movements, and contact of boundaries inherent in flapping motion. In contrast, the capturing method is robust against such complex boundary motions but struggles to maintain high-resolution boundary layer meshes, resulting in reduced accuracy.

To address these challenges, we employ structured meshes based on the interface capturing method. For achieving high spatial resolution in specific local regions, we explore the application of the s-version of the finite element method (SFEM) [1], primarily studied in structural mechanics. SFEM enables efficient modeling by superimposing meshes with different spatial resolutions, offering advantages such as localized high accuracy, reduced computational cost, and simplified meshing procedures.

As an initial step, we have developed a B-spline-based SFEM (BSFEM) [2], which integrates both B-spline and Lagrange basis functions, significantly enhancing accuracy and convergence. This study aims to refine local mesh adaptation in interface capturing approaches for moving boundary problems in fluid dynamics. As a next step, BSFEM is applied to hydrodynamic problems for localized refinement, and Nitsche's method is incorporated to enforce boundary conditions. The proposed approach is validated through several 3D flow test cases.

Keywords: Localized refinement, Navier-Stokes equations, S-version of finite element method, Mesh superposition method, B-spline basis functions

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Multi-scale analysis to predict macroscopic material response associated with uncertainties of microstructure

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The purpose of this study is to propose a multi-scale method with the aim to predict macroscopic material response associated with uncertainties of microstructure. In the proposed multi-scale method, under two assumptions that the microstructure can be characterized as unit cell and the uncertainties can be represented as random variables in the unit cell, the physical quantities like the stress and strain in the macro-scale are obtained as the expected values from the unit cells corresponding to the random variables. The expected values are discretized by Stochastic Collocation (SC) method and computed by Gaussian quadrature. The physical quantities corresponding to the random variables are obtained as the volumetric averages of those in the unit cell in the line with a conventional homogenization method. In addition, the constrained conditions are imposed on the disturbance displacements on the edge of the unit cells to not only satisfy periodic boundary condition in a unit cell but also become the same values between the unit cells. Throughout several numerical examples, the capability of the proposed multi-scale method is demonstrated by comparing with the reference solution of the microstructure obtained by direct numerical simulation and the numerical results obtained by the conventional multi-scale method simply combined with the SC method and the homogenization method. From these comparisons, it can be confirmed that the proposed multi-scale method provides us with more accurate prediction for the reference solution than the convectional one.

Keywords: Multi-scale simulation; Homogenization methods; Periodic boundary conditions; Stochastic collocation method

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Die casting simulation using MPH method

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Die casting is a metal casting process in which molten metal is injected into a mold under high pressure. In general, the rapid cooling rate and high flow velocity of the molten metal often lead to defect formation, such as shrinkage porosity and abnormal microstructures, which can significantly deteriorate the mechanical properties of the final product. To improve the quality of die-cast components, optimizing the casting process and minimizing defect formation are essential. Since trial-and-error-based optimization is impractical, computer-aided modeling and numerical simulations play a crucial role in casting process design. Considering the significant fluid deformation in the die casting process, the particle method is particularly well suited for simulation, enabling continuous modeling of molten metal flow into the mold cavity and subsequent solidification.

In this study, die casting process was simulated with the MPH (Moving Particle Hydrodynamics) method [1-3], which is one of the particle methods. Some models necessary for the simulation of die casting, such as heat transfer, phase change, and temperature-dependent volume model, were introduced into the MPH method.

For heat transfer analysis, the governing equation is the equation of energy conservation:

$$\frac{\partial H}{\partial t} = \lambda \nabla^2 T, \tag{1}$$

where H is the enthalpy [J/m^3], λ is the thermal conductivity [W/(m K)], and T is the temperature [°C]. Discretising the Laplacian in Eq.(1) with the Laplacian model of the MPH method, the enthalpy of each particle is calculated. Then, the temperature and the solid fraction are calculated from the enthalpy. To express the solidification, the viscosity of the fluid varies with the solid fraction.

With the introduced model, the porosity caused by the solidification shrinkage was qualitatively observed.

Keywords: particle method, Moving Particle Hydrodynamics, multi physics analysis, solidification, die casting

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Aging behaviors of integral hydrophobic cement paste modified by stearic acid

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Integral hydrophobic concrete is developed for its anti-corrosion, excellent abrasion resistance, and hydrophobic maintaining after-cracking properties [1]. However, its performance under natural conditions such as ultraviolet (UV) radiation and extreme temperatures remains unclear [2]. Investigating the aging behaviors of integral hydrophobic concrete is essential for understanding its service behavior and predicting lifespan. This paper explores the wettability changes of hydrophobic specimens modified by stearic acid (SA) after UV and thermal aging. Results demonstrate that 16 years of equivalent UV aging develops a 1.5 mm aged layer, increasing the surface energy of the specimens from 47.7 mJ/m^2 to 73.1 mJ/m^2 due to photooxidation of SA and the formation of the polar carbonyl groups, leading to a 117.6% increase in water absorption. The photooxidation of SA mainly occurs in the depth of 0-0.5 mm, and its photooxidation degree increases with aging time. The UV aging reaction of SA is illustrated in Figure 1. Additionally, thermal aging at 70 °C primarily causes microcracks formation without sublimating or pyrolyzing the alkyl groups, thereby slightly increasing water absorption.

Keywords: Integral hydrophobic concrete; Stearic acid; Aging; Water absorption

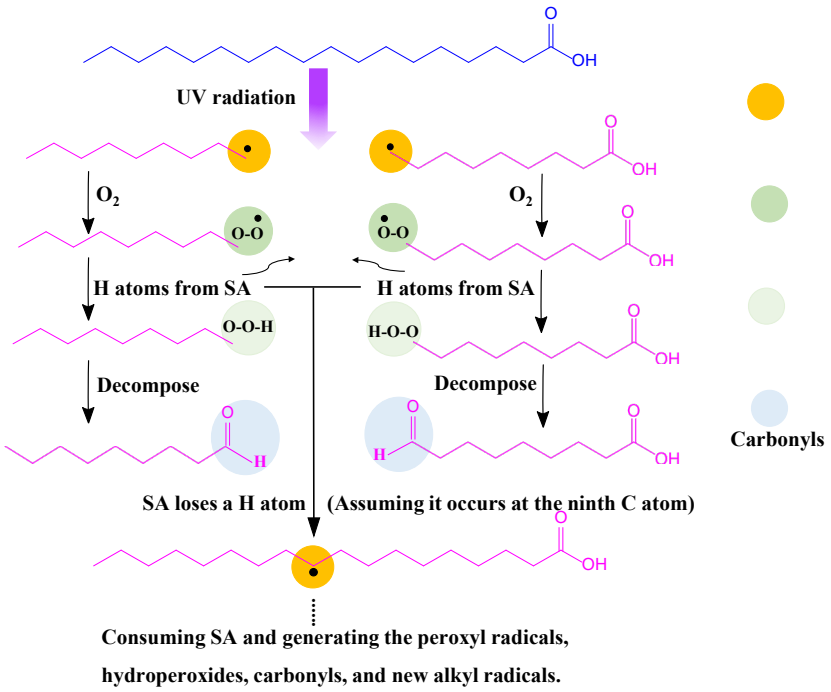

Figure 1. The UV aging process of SA.

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Insights into airflow characteristics during the onset of respiratory arrest

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The transition from active breathing to respiratory arrest presents a complex and dynamic phenomenon in the human airway physiology, with significant implications for critical care, airway management, and emergency airway drug delivery. This study employs Computational Fluid Dynamics (CFD) techniques to investigate the transient airflow behaviour within the upper airway during the cessation of breathing. Utilizing patient specific airway geometries reconstructed from CT images we simulate airflow condition under varying inspiratory and expiratory scenarios leading to respiratory arrest. Numerical studies on airway drug deposition often assume that a non-breathing patient experiences complete absence of flow; however, we aim to investigate this assumption.

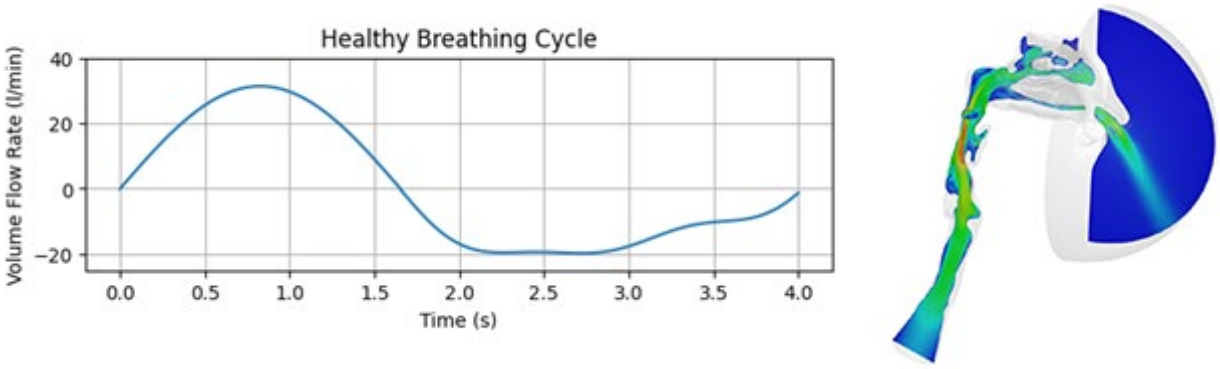

Figure 1 shows a representation of a healthy breathing cycle used in earlier numerical breathing studies and may be interrupted at various points and a velocity contour in the airway during exhalation.

Since the airflow in the airway changes rapidly with time during respiratory arrest, a transient SBES model has been selected to accurately capture peak flow characteristics and their subsequent decay. As the pressure driven flow subsides, convective flow may become influential driven by the metabolic heat of the human body. To capture this process, we employed a model which captures both the sensible and latent heat transfer on the mucus coated nasal wall.

Keywords: Human Airway, Computational Fluid Dynamics, Respiratory Arrest

Immediate Large-area Prediction Model of Rainfall-induced Landslides Using Slope Stability Analysis

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In Japan, there have been many landslides caused by heavy rainfall, and 1,433 landslides occurred, causing 56 fatalities in 2024. In order to protect lives and properties from such slope hazards, it is important to establish a framework that can accurately and quickly predict the occurrence of landslides for a wide area. Previous studies have used statistical methods based on information on slopes and prediction models based on the relationship between rainfall and actual disasters, but few studies have utilized information from detailed (slope-level) numerical analyses based on mechanics. This study develops a framework for real-time slope instability evaluation that considers the effects of rainfall-induced infiltration by incorporating a machine learning method and verifies the validity of the developed model.

For the numerical analysis, this study applies a slope stability analysis based on the three-dimensional limit equilibrium method to calculate the factor of safety [1]. The factor of safety is calculated as the ratio of the resisting force and the sliding force acting on the slip surface, as shown in the following equation,

$$F = \frac{\sum_{ij}\{cA + (N_{ij} - U_{ij}A)\tan\phi\}}{\sum_{ij} T_{ij}}, \quad (1)$$

where c is the cohesion, A is the area, N_{ij} is the normal force, U_{ij} is the pore water pressure, ϕ is the internal friction angle, and T_{ij} is the shear force. By introducing the infiltration analysis results as the pore water pressure U_{ij}, the factor of safety can be calculated, considering the effects of heavy rainfall.

This study creates a prediction model using spatial mode decomposition. A database of the factor of safety distributions is created by conducting a pre-analysis of various rainfall scenarios. By applying mode decomposition to the database, the spatial distribution characteristics (spatial modes) of the factor of safety distribution are extracted, which can be used to construct a prediction model that can extract hazardous slopes quickly without performing the analysis.

In this study, Hachinohe City, Aomori Prefecture, Japan, was selected as the target area to validate the proposed framework. The results of the prediction model were compared with those of the numerical analysis, and it was confirmed that the proposed method can reproduce the numerical results with a low computational cost and high accuracy.

Keywords: Slope Stability analysis, Limit Equilibrium Method, Landslide, Rainfall

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Determining the Representative Elementary Area for Multiphase Flow in Gas Diffusion Layers: Leveraging Tomographic Imaging with the Lattice Boltzmann Method

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Porous gas diffusion electrodes are essential for facilitating efficient mass transport in electrochemical devices such as fuel cells, electrolysers, and metal-air batteries. These electrodes consist of a porous catalyst layer supported by a conductive carbon-based gas diffusion layer with a hierarchical structure. The macroporous carbon fiber substrate facilitates bulk gas transport, while the microporous layer offers resistance to liquid penetration and supports the catalyst layer. However, cracks in the microporous layer can create pathways for liquid infiltration, thereby diminishing its capacity to prevent flooding. Liquid accumulation within the pore space remains a significant challenge, obstructing gas transport and limiting performance.

Computational modelling has emerged as a valuable tool for understanding, predicting, and optimizing multiphase flow within these structures. However, simulating an entire electrode at pore-scale resolution is impractical due to the centimeter-scale span. Consequently, determining a representative elementary volume (REV) is necessary, representing the minimum domain size required for models to capture bulk transport properties. In thin, porous materials like gas diffusion layers, the through-plane dimension is often insufficient for a meaningful REV, necessitating the definition of a representative elementary area (REA) instead. The conventional approach for determining this area relies on ensuring that average morphological properties become independent of domain size. However, this single-phase perspective does not account for the formation of complex multiphase flow patterns, which are critical to understanding flooding behavior.

To address this challenge, the phase-field lattice Boltzmann method was used to evaluate the REA for single and multiphase flow in the carbon fibre substrates of three commercially available gas diffusion layers. High-resolution X-ray computed tomography was used to reconstruct the samples and isolate the carbon fibre substrate, with single-phase permeability first determined as a baseline. The analysis examined whether the REA for single-phase permeability is comparable to that of multiphase flow and quantifies the associated error. In addition, the influence of mixed wettability, introduced by hydrophobic additives during manufacturing, is explored through stochastic generation of the phase on the reconstructed geometries. This study provides a foundation for assessing single and multiphase

transport properties in gas diffusion layers with future work looking to address the challenges associated with physically characterising their material (i.e. local hydrophobicity) and the impacts this has on electrolyser reliability.

Keywords: Lattice-Boltzmann method, multiphase flow, x-ray computed tomography, porous media, mixed wettability, electrochemical systems

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Numerical Investigation of Phase Separation Effects on Hydrodynamically Stable Flow in a Partially Miscible System

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Viscous fingering instability occurs when a less viscous fluid displaces a more viscous one in porous media or Hele-Shaw cells [1]. This instability is relevant in chromatography and secondary oil recovery [1]. In partially miscible systems, phase separation can induce instabilities even in hydrodynamically stable displacement [2]. When the concentration of injected fluid lies within the spinodal region, thermodynamic instability leads to phase separation. The spinodal region can be identified when the second derivative of free energy is negative [3]. This study investigates radial displacement where viscosity depends exponentially on concentration. Using the Cahn–Hilliard Hele-Shaw framework, we conduct nonlinear simulations with a hybrid numerical method combining pseudo-spectral and compact finite difference approaches [3]. We obtain that the instability pattern depends on the concentration of injected fluid as shown in Figure 1 [2]. These findings provide insight into how phase separation influences flow instabilities in multiphase systems. Understanding these mechanisms is crucial for applications such as enhanced oil recovery and CO_2 sequestration, where phase separation-driven instabilities can impact fluid displacement efficiency [4,5].

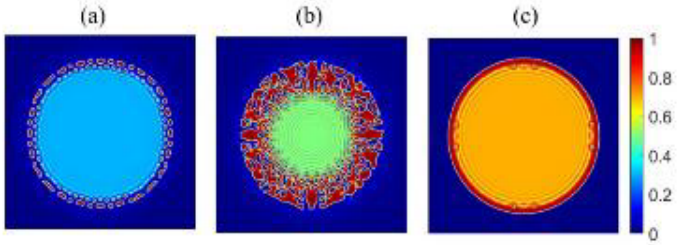

Figure 1: Density plots of concentration for different concentrations of injected fluid (c_i) for a fixed viscosity ratio between fluids. (a) $c_i=0.3$, (b) $c_i=0.5$ and (c) $c_i=0.7$.

Keywords: Cahn-Hilliard Hele-Shaw mode, partially miscible fluids, viscous fingering and phase separation.

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Dynamic experimental study and design optimisation of steel safety rails and posts used in road safety barriers

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Steel guardrails and posts are key structural components used as energy absorbers in many road safety barrier systems. In Australia, these components can be found in conventional W-beam steel guardrails and safety roller barrier systems. As energy absorbers, these components must be designed to optimise the energy absorption during a vehicle impact to minimise risks to the occupants. In this paper, the authors aimed to optimise the designs of two key components of the safety roller barrier system: safety rail, and circular post. Comprehensive experimental studies including quasi-static and dynamic three-point bending tests were conducted to investigate the dynamic behaviours of these components. Subsequently, the results were used to validate the finite element models before design optimisation successfully. A two-stage design optimisation was implemented to maximise the specific energy absorption while minimising the mass of the steel components. The Response Surface Method was used in the first stage to optimise based on the existing design of the safety rail and circular post. Then the Non-Dominated Sorting Genetic Algorithm II (NSGA-II) was employed to explore alternative safety rail designs. The results indicated that immediate improvements could be made to existing designs by modifying the components' overall dimensions, while further enhancements could be achieved with alternative designs generated by the Non-Dominated Sorting Genetic Algorithm II.

Keywords: road safety barrier, safety roller barrier, design optimisation, RSM, NSGA-II.

Topology Optimization of Mode-Converting Metamaterials for Obliquely Incident Elastic Waves

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Mode conversion between longitudinal and transverse waves is a unique phenomenon in elastic wave propagation that complicates coupling analysis, but it also enables valuable applications, such as ultrasonic flow meters. Due to its intriguing physics and practical significance, mode conversion has recently gained considerable attention. However, most research on designing elastic metamaterials for perfect or highly efficient mode conversion has focused on normally incident waves. For example, Yang and Kim [1] conducted topology optimization for mode-converting elastic metamaterials under normally incident longitudinal waves, but no extension has been made to obliquely incident waves, whether longitudinal or transverse. While the significance of oblique mode conversion has been highlighted in the retroreflection of obliquely incident longitudinal waves, no topology optimization method exists for arbitrary oblique incidence.

This study presents the topology optimization of elastic metamaterials for perfect or highly efficient mode conversion of obliquely incident elastic waves, whether longitudinal or transverse. The metamaterial is placed between two media, medium A and medium B, with wave incidence from medium A (where medium B may be identical to medium A). A density-based optimization framework is employed, utilizing the adjoint method for sensitivity analysis. Since the incident wave is oblique, special care is required to enforce periodicity along the direction normal to the interfaces between the media and the metamaterial. We explore multiple design cases involving different incident angles and metamaterial dimensions to validate the proposed optimization method and examine the effects of these parameters on the optimized microstructures. Additionally, a multi-frequency analysis is conducted to address pulse-type wave inputs. If time permits, an application of the optimized metamaterial will be presented.

Key Words: *topology optimization, metamaterial, mode conversion, oblique incidence.*

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Large-Scale Parallel Flow Analysis with Implicit Field-Based Neural Surface Reconstructions

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The interface-capturing technique is widely used in the numerical analysis of complex moving boundary problems involving fluid-structure interactions. By capturing boundary surfaces using fixed computational meshes, this method enables stable analyses even for problems involving large deformations and complicated shapes of boundaries. Though combining the technique with technology for sensing the shape of real space, such as biological structures or landscapes, may enable automatic analysis of real space, it is a challenging research problem.

In this study, we aim to develop a fluid analysis system that automates the process from analysis model creation to simulation by integrating photogrammetry techniques into the interface-capturing finite element method. For model creation, we utilize neural implicit functions obtained from NeuS[1], a photogrammetry technique incorporating neural networks. NeuS reconstructs surface geometry by learning neural implicit functions from multiple input images. These functions represent distance fields from spatial points to object surfaces and enable precise surface reconstruction. By distributing neural implicit functions on fixed computational meshes, boundary positions can be smoothly defined as analytical models. In general, interface-capturing methods face challenges in directly enforcing boundary conditions when object boundaries do not align with computational meshes. To address this, we apply the penalty method[2], a straightforward approach for approximating boundary conditions. The penalty method adds pseudo-elastic forces as penalties when function values deviate from prescribed boundary conditions, thereby approximating their satisfaction. To impose boundary conditions with high accuracy, we employ high-resolution meshes. To reduce computational time, we introduce a domain decomposition-based parallel computing approach[3].

Using an interface-capturing fluid analysis solver that combines modeling with neural implicit functions and boundary condition handling with the penalty method, we conducted simulations of incompressible viscous fluid flows.

Keywords: Neural Implicit Functions, Finite Element Method, Computational Fluid Dynamics

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Origami-Inspired Lattice Structures Enhance Ductility of Cementitious Composites

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The quasi-brittle nature and tensile strength deficiency of cementitious materials constrain their structural efficacy in advanced engineering applications. Drawing inspiration from the exceptional deployability of origami, this work presents a novel method to enhance cementitious matrices through additively manufactured Miura origami lattice inclusions. Polylactic acid (PLA) origami architectures with parametrically varied folding angles are fabricated via fused deposition modeling (FDM) technology and then embedded within cementitious matrices. Axial compression tests are conducted to quantitatively characterize the effects of origami lattice morphologies on the mechanical responses and deformation mechanisms of cementitious composites. All specimens, regardless of reinforcement ratio, exhibit smooth softening behaviors during compression. Furthermore, finite element simulations are performed to analyze the PLA reinforcement efficacy across various cementitious formulations, revealing significant improvements in energy absorption capacity for conventional Portland cement concrete, engineered cementitious composites, and ultra-high-performance concrete. Additional simulations comparing PLA, acrylonitrile butadiene styrene (ABS), and high temperature polyamide with carbon fiber reinforcement (PAHT-CF) as reinforcement constituents demonstrate that PAHT-CF exhibits the most significant reinforcement effect. It is also concluded that the reinforcement efficiency increases with decreasing origami folding angles, increasing thickness, and higher unit cell density. This research substantiates additively manufactured origami lattice architectures as an innovative approach to improving the ductility performance of cementitious composites, offering promising implications for non-corrosive reinforcement alternatives, optimized material utilization, and sustainable construction methodologies.

Keywords: Origami, additive manufacturing, cementitious composites, mechanical characterization, lattice-reinforcement

Stability analysis of annular perovskite plates based on opto-electro-thermo-mechano model

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Perovskite materials have emerged as advanced photoelectric structures and devices, while the mechanical characteristics of the structures remain not fully understood. Based on the opto-electro-thermo-mechano constitutive model, this study investigates buckling behaviors of annular perovskite plates considering photostriction, electrostriction and thermal expansion properties of hybrid perovskite $MAPbI_3$ crystals. The constitutive model is built as:

$$\{\sigma_i\}=\left[Q_{ij}\right]\left(\{\varepsilon_j\}-\{\beta_j\}I_L-\{\alpha_j\}\Delta T-\{\eta_j\}E_Z^2-\{d_{3j}\}E_Z\right) \quad (1)$$

in which $\{\sigma_i\}$ and $\{\varepsilon_j\}$ are the total stress and strain vector; $\left[Q_{ij}\right]$ is the stiffness matrix of perovskite structures; $\{\beta_j\}$, $\{\alpha_j\}$, $\{\eta_j\}$, and $\{d_{3j}\}$ represent the photostrictive coefficient vector, thermal expansion coefficient vector, electrostrictive coefficient vector, and piezoelectric coefficient vector, respectively.

The first-order shear deformation plate theory and Lagrange equation method are applied to obtain governing equations of the annular perovskite plate. The Chebyshev-Ritz method is then utilized to numerically solve the eigen equations of buckling of the annular perovskite plate. A comprehensive parametric study analyses the effects of light illumination, electric field, temperature change, and mechanical loading on elastic buckling behaviours of the annular perovskite plate with various boundary conditions under multi-physical fields. The results show that the combinations of multi-physics fields can considerably weaken the stability of perovskite structures. The critical buckling load of the plate can be greatly overestimated when multi-physics field is ignored but its influence on the buckling modes is minimal. These findings highlight the important role of the multi-physics fields including optical, electric, thermal and mechanical fields in predicting the mechanical performances of perovskite structures, which must be considered in engineering design.

Keywords: Buckling analysis, annular plate, multi-physics field, perovskite, photostriction, electrostriction

A Quick Synthetic System for Rarefied Gas Flows By Solving the Gas-kinetic Equation

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We present a quick synthetic system for finding the steady state of rarefied gas flows by solving the gas-kinetic equation across a wide range of Knudsen numbers. Conventionally, when dealing with rarefied gas, one needs to solve the Boltzmann equation, or a linearized gas-kinetic equation using iterative methods like the discrete velocity method (DVM). Conventional DVM uses implicit time stepping to treat the convection changes of the velocity distribution function (VDF), however, the relaxation term, due to its complexity, is treated explicitly. As a result, when the Knudsen number is large, the convection effects dominate, and the DVM iterations converge very quickly. In contrast, when the Knudsen number gets smaller and the flow enters the near-continuum regimes, inter-molecular collisions gain dominance, which slow down convergence rate drastically.

In the recent decade, researchers came up with the solution to use synthetic equations to accelerate the convergence of conventional DVM, especially at low Knudsen numbers. The key idea of synthetic equation is to study a much smaller system, usually the conservative quantities, to provide projections. In this way, one can predict the changes in the flow and update VDF as a whole, without calculating individual terms in the relaxation model. Existing research in the synthetic system shows that in extreme cases, the convergence rate of DVM can be 1000 times faster.

Despite the initial successes of the synthetic system, its formulation remains open to interpretations and modifications. In [1], researchers used the Euler equation and the NSF equation as the foundation of the synthetic system. In this research, we propose the use of a numerical dissipation system that is based on half-fluxes of the Maxwellian distribution. The derivation of the system is based on the steady-state conditions of the DVM under a finite-volume type space discretization. We suggest that the formulation of the synthetic system should conform to the flux of DVM in terms of conservative quantities, so that when the system reaches the steady state, the effective change brought about by the synthetic system is zero. Following this criterion, the synthetic flux of the conservation parameters by considering the integral of a Maxwellian distribution over half of the infinite velocity space. One interpretation of the proposed flux is it models the change in flux of conservative quantities when the equilibrium component of the current VDF is substituted by another. The resulting numerical system of for the synthetic equation is dissipative and has short stencil. The flux Jacobian can be directly derived in analytical forms. This makes it easier to solve compared to its Euler or NSF counterparts. In addition, we introduce an activation parameter, which is related to local cell size and the Knudsen number, to control the portion of current flow residual that gets introduced to the synthetic system. Numerical experiments in 1D rarefied gas flow fields show that fine-tuning of this parameter results in better performance compared to existing synthetic schemes.

Keywords: Gas-kinetic equation, rarefied gas, synthetic system, discrete velocity method.

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Mechanistic Investigation of KtrAB Channel Regulation via Molecular Dynamics

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Potassium ions are essential cations that play a vital role in cellular physiology. For bacteria that inhabit in highly dynamic environments, maintaining an appropriate intracellular K^+ concentration is crucial, and an efficient gating mechanism is key to preserving cellular homeostasis.

KtrAB is a nucleotide-dependent K^+ channel system composed of the cytoplasmic subunit KtrA and the transmembrane subunit KtrB. ATP binding to KtrA activates K^+ transport, whereas ADP binding inactivates it. The operation of this channel is accompanied by significant conformational changes, with the D1M2b helix of KtrB proposed as a critical component of the gating mechanism. The cryo-EM structure of ADP-bound KtrAB reveals that the D1M2b helix is fully extended, whereas ATP binding induces a helical hairpin conformation.

To gain deeper insight into the behavior of the KtrAB system, we performed molecular dynamics simulations. By analyzing hydrogen bond interactions, we identified key residues involved in channel regulation. Steered molecular dynamics simulations further confirmed the role of these residues in the gating mechanism. Since the conformational change of D1M2b was attributed to steric hindrance caused by KtrA, we constructed a model with only KtrB in the ATP-bound state embedded in a membrane. Surprisingly, we observed the extension of the D1M2b helix even in the absence of KtrA.

Figure 1.

Keywords: KtrAB, ion channel, gating mechanism, molecular dynamics, steered molecular dynamics

Hierarchical Subdomain Preconditioning Utilizing Eigenmodes in Parallel Finite Element Analysis

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This study proposes a high-performance preconditioning technique for iterative solvers in large-scale sparse linear systems, assuming parallel computation based on domain decomposition methods. In the field of preconditioning techniques for large-scale matrices, projection-based methods such as multigrid methods, domain decomposition methods, and deflation methods have been actively studied [1]. Traditionally, preconditioners based on multigrid and domain decomposition methods construct a coarse problem by applying operations equivalent to low-order approximations, such as zeroth- or first-order approximations.

In contrast, the proposed method improves preconditioning performance by approximating the solution within each subdomain using low-order eigenvectors obtained from the subdomain, which correspond to a higher-order approximation compared to conventional methods. Furthermore, this method allows independent settings of subdomains used for parallel computation and those used for obtaining low-order eigenvectors by hierarchical domain decomposition scheme. This approach can be considered a combination of hierarchical domain decomposition scheme and deflation methods [2]. By leveraging domain decomposition, the computational cost of obtaining low-order eigenmodes, which is generally expensive, can be significantly reduced.

To evaluate the effectiveness of the proposed method, numerical experiments are conducted using structural analysis problems based on the finite element method. The evaluation metrics include the number of iterations, computation time, and parallel computing performance, and the results are compared with conventional algebraic multigrid methods.

Keywords: iterative solver, preconditioning, domain decomposition, deflation, conjugate gradient method, finite element method

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Fluid Simulation of a Liquid Ring Pump by the MPS Method with Gas Backflow using a Gap Model

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The liquid ring pump is widely used in various industries, such as chemical and power industries. Numerical methods are expected to reduce the cost of product development by replacing much of the experimental testing with numerical analysis testing. The flow in a liquid ring pump exhibits a drastically changing gas-liquid interface. Due to this characteristic, the Moving Particle Semi-Implicit (MPS) method [1], a representative particle-based approach, is considered well suited for its simulation.

This study is based on the previous study [2] by Kaito et al. In the previous study, the liquid phase in a liquid ring pump was simulated in two dimensions using the MPS method. The gas phase was calculated based on the equation of state of an ideal gas. Ghost particles were placed between the impeller blades to calculate the gas volume. However, the backflow of gas through the gap between a side wall and the impeller was neglected because it was difficult to express the three-dimensional gap effects in a two-dimensional simulation.

Therefore, in this study, the gap was modeled to improve the accuracy of the gas density in a liquid ring pump simulation. In the gas density calculation based on the equation of state of an ideal gas, the gap was modeled as a backflow of gas mass caused by pressure differences between adjacent air chambers and between the air chambers and the inlet. Using the developed gap model, a liquid ring pump was simulated under various conditions, and the simulation results were compared with the experimental results.

Keywords: Computational fluid dynamics, multiphase flow, gas-liquid interaction, gas calculation, MPS method, liquid ring pump

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Turbulent heat transfer enhancement by large-scale perturbation associated with the Kelvin-Helmholtz instability

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Turbulent heat transfer enhancement by large-scale perturbation associated with the Kelvin-Helmholtz (K-H) instability is explored by means of direct numerical simulations. The flow geometry was a turbulent flow through a pipe with streamwise-aligned rib roughness, as shown in Figure 1. The friction Reynolds number was fixed at 180 while the Prandtl number was unity, with the buoyancy effects neglected. The geometry of the rib roughness, namely the rib height and spacing between the neighboring ribs, was systematically varied. The flow was periodic in the streamwise direction and driven by the pressure gradient. We prescribed the constant wall temperature at the rib surface and pipe and included the internal volumetric heating to drive the heat transfer. The set of thermal and flow boundary conditions makes the non-dimensional governing equations for heat and momentum transfer similar. For the numerical method, we employed the D3Q27 multiple-relaxation-time lattice Boltzmann method (LBM) for velocity fields while we utilized the Q19 regularized LBM for the thermal fields. The LBM method employs the regular grid with equal spacing, and the grid resolution was determined such that grid spacing in wall units was around 1.6.

The results show that the streamwise-aligned rib roughness induces the streamwise large-scale perturbations associated with the K-H instability as shown in Figure 2. The significance of the perturbation strongly depends on the geometry of the rib roughness, and some of the essential conditions are the sufficient height of the rib and moderate permeability within the rib region which are related to the development and emergence of the K-H instability, respectively. All the cases achieve the favorable breakdown of the Reynolds analogy although the breakdown is more pronounced when the perturbations are significant. To better understand the physical mechanisms behind the breakdown of the Reynolds analogy, we compare the turbulent fluxes in Figure 3. The figure confirms that the turbulent heat flux outweighs that turbulence momentum flux, i.e., Reynolds shear stress, suggesting that the turbulence plays a vital role in the breakdown of the Reynolds analogy.

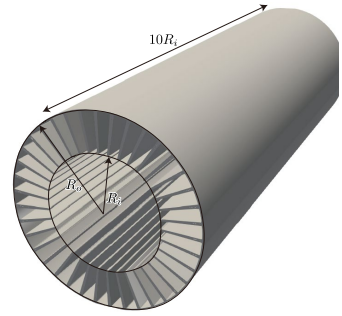

Figure 1 Flow geometry.

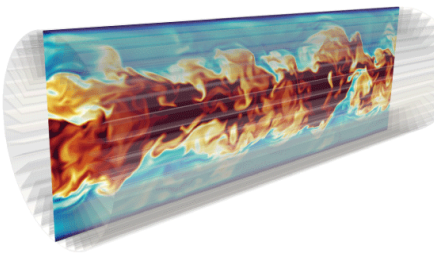

Figure 2 Instantaneous temperature

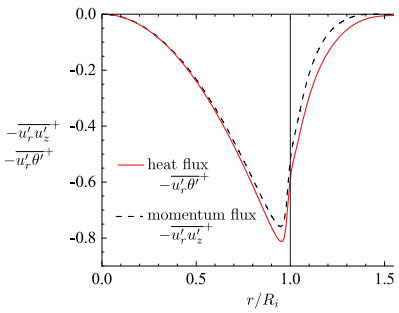

Figure 3 turbulent fluxes

Keywords: Direct numerical simulation, turbulent forced convection, Reynolds analogy, Kelvin-Helmholtz instability

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Data-driven algebraic model for turbulent heat transfer over several types of rough surfaces

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We performed large eddy simulations of turbulent heat transfer over several types of rough surfaces to derive the algebraic predictive model of the roughness effects on turbulent heat transfer. The rough surfaces under consideration were 40 surfaces including surfaces with hemisphere, hemi-ellipsoid, dimple, and irregular roughness. The flow geometry was a rough-walled open channel flow in Figure 1. The Prandtl number was 0.71. We applied the periodic boundary conditions in the streamwise and spanwise directions, and the friction Reynolds number was varied up to 1200 by adjusting the streamwise pressure gradient. For the numerical method, the velocity fields were obtained by the D3Q27 multiple-relaxation-time lattice Boltzmann method (LBM) [1] while we used the Q19 regularized LBM [2] for the thermal fields. We used the local grid refinement [3] by which we allocated finer grid block near the rough walls. The near-wall grid resolution was determined such that grid spacing in wall units was around 2.5. For the sub-grid-scale model, we used the wall-adapting local eddy viscosity model [4]. We develop the predictive model based on the correlation based on the analogy between the turbulent diffusivity of heat and momentum transfer [5]:

$$S_t = \frac{0.5C_f}{1+\sqrt{0.5}C_f g_k(k_s^+, Pr)} \tag{1}$$

where C_f is the skin friction coefficient, and the unknown correlation g_k is a function of the inner-scaled equivalent sand grain roughness, k_s^+, and the Prandtl number Pr:

$$g_k(k_s^+, Pr) = A_1((k_s^+)^{0.2} Pr^{0.44} - A_2) \tag{2}$$

where A_1 and A_2 are the coefficients. We model A_1 as a function of the morphological parameters of rough surfaces while we assume A_2 to be constant. We extract two important morphological parameters that dominantly affect A_1 with the help of the machine learning. Figure 2 shows the predictive performance, demonstrating that the model reasonably predictive the temperature roughness function which quantifies the effects of the roughness on the mean temperature.

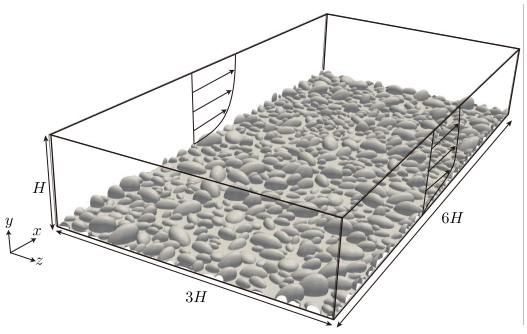

Figure 1 Geometry of rough-walled channel.

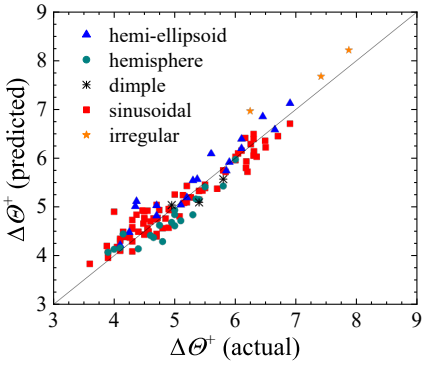

Figure 2 Predictive performance of roughness function.

Keywords: Large eddy simulation, turbulent forced convection, roughness, machine learning

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Simulation of Seawall Block Damage Using the Moving Particle Hydrodynamics (MPH) Method with Fluid-Rigid Body Interaction

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To estimate damage to seawalls under construction caused by high waves, numerical analysis is one of the approaches, along with experimental investigation. Seawall collapse due to high waves generally has three main factors [1]; (1) Horizontal force due to the difference in water level between the front and back side of the block, (2) Scour caused by overflow, (3) Decrease in the bearing capacity due to seepage flow. This study mainly focused on the factor (1). When a seawall is under construction, backfill stones are piled behind the blocks. It is known that the backfill stones influence the force to the blocks.

In this study, a fluid-structure interaction simulation was conducted to analyse the collapse of seawall blocks under construction due to high waves. The particle method was chosen for this simulation as it is well-suited for handling the large-scale motion of both fluid and rigid bodies. Specifically, Moving Particle Hydrodynamics (MPH) [2], a physically consistent particle method, was employed to simulate the interactions between the blocks, backfill stones, and fluid. Modeling methods for backfill stones and blocks were discussed. The simulation results were compared with experimental data.

Keywords: Particle method, Seawall, High wave, Fluid structure interaction, Moving particle hydrodynamics

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A multi-GPU computational framework for large-scale phase field crack simulations

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The phase field model has been proven to be a powerful approach for simulating cracks in quasi-brittle materials. However, its large computational cost is a bottleneck of this method, limiting its engineering applications. To address this issue, we develop an efficient multi-graphics processing unit (GPU) framework for computing an explicit finite element method that adopts a length scale-insensitive phase field regularized cohesive zone model [1] for accurate crack simulations. Two GPU control strategies are designed. The first strategy is based on OpenMP calls, which requires minimal modifications to the original single-GPU code, promoting excellent scalability. The second strategy is based on loop-based GPU calls, which eliminates the need for additional library call overhead and efficiently utilizes the GPU for asynchronous computations. The results demonstrate that both control strategies exhibit high and comparable efficiency. The computational domain is decomposed into subdomains, and each subdomain is distributed to one GPU card. Then, the pre-processing and all calculations are conducted on the GPU side, which fully leverages the computational capabilities of the GPU. In addition, asynchronous operations enable the overlap of computations on GPUs with data transfer, while pre-processing and stream-based data output are optimized using OpenMP, further enhancing the efficiency of the computational framework. Several benchmark tests are performed to demonstrate the performance and efficiency of developed computational framework. Finally, the capacity and reliability of the developed computational framework are demonstrated through an engineering application of progressive damage in a large-scale wind turbine blade.

Keywords: Multi-GPU parallel technology, Phase field fracture, CUDA-OpenMP hybrid model, Efficient data exchange strategy, Large-scale parallel computing

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Numerical Investigation of Influence of Airfoil Shape on Sand Erosion in a Low-Pressure Turbine

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The phenomenon of sand erosion occurs when gas-solid two-phase flow impinges on materials, causing the detachment of surface material. Sand erosion on aircraft engines poses significant economic and safety concerns. Therefore, this study aims to clarify the influence of the airfoil shape on erosion. Multi-physics numerical simulations were conducted to evaluate the erosion resistance and aerodynamic performance of an altered first-stage stator shape in the low-pressure turbine (LPT).

An in-house computational fluid dynamics (CFD) solver, UPACS, was employed. The simulation procedure comprises grid generation, flow computation, particle tracking, erosion computation, grid regeneration, and flow computation after erosion. Gas-solid two-phase flow simulations were based on the Eulerian-Lagrangian coupling method, while an empirical model (Neilson and Gilchrist, 1968) was utilized for erosion damage:

$$W = W_D + W_C = \begin{cases} \dfrac{\frac{1}{2}m_p(V\sin\alpha - K)^2}{\psi} + \dfrac{\frac{1}{2}m_p V^2\cos^2\alpha \sin n\alpha}{\varphi} & (a < a_0) \\ \dfrac{\frac{1}{2}m_p(V\sin\alpha - K)^2}{\psi} + \dfrac{\frac{1}{2}m_p V^2\cos^2\alpha}{\varphi} & (a \geq a_0) \end{cases} \quad (1)$$

where W is the weight loss, m is the mass, V is the impinging velocity, a is the attack angle, K is the threshold value of the normal velocity below which no deformation wear occurs. The parameters a_0, n, ψ, and φ are model constants. The subscripts D, C, and p refer to deformation, cutting, and particle, respectively. The elliptic-hyperbolic grid solver updated the computational grid to fit the eroded surface.

The computational target included the last stage of the high-pressure turbine (HPT), a transition duct, and the first-stage stator of the LPT to account for the effects of upstream components. Significant erosion was observed at both the midspan and tip regions, as well as at the leading edge. The pronounced erosion at the midspan and tip regions is attributed to the high frequency of particle impacts resulting from the interaction between particle motions and the upstream components. The vane shape affected the erosion resistance and aerodynamic performance.

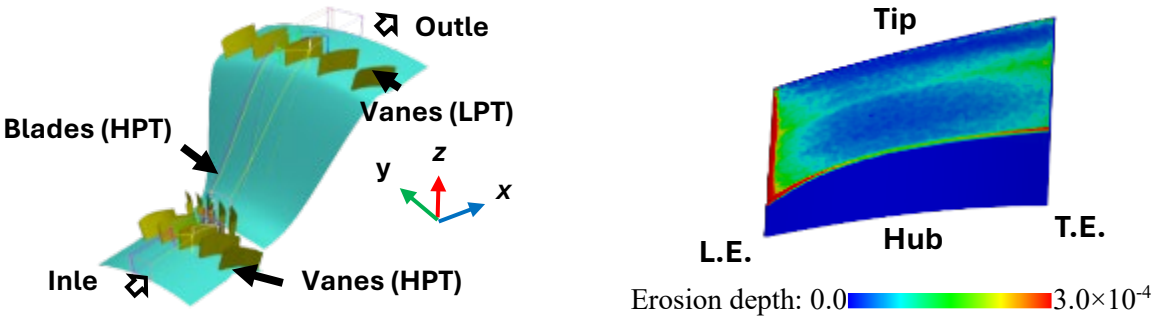

Figure 1.

Keywords: Sand Erosion, High-Pressure Turbine, Low-Pressure Turbine, Transition Duct, Numerical Simulation

Numerical Modelling of Laser Paint Stripping on Carbon Fibre Reinforced Polymer

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The removal of protective coatings from composite structure surfaces is a critical challenge in aerospace maintenance and repair operations, as traditional chemical and mechanical methods pose environmental and structural risks. Pulsed laser technology, as an emerging advanced method, offers precise material removal with minimal heat-affected zones and damage. However, despite the complex thermal and mechanical interactions between laser energy, paint layers, and composite substrates, most reported studies so far only focus on either thermal effects or mechanical behaviour in isolation, neglecting the coupled effects. This study develops a coupled thermal and mechanical model based on a finite element (FE) framework in COMSOL Multiphysics to model the laser paint stripping of carbon fibre reinforced polymer (CFRP). A three-layered structure is modelled, consisting of a polyurethane topcoat, an epoxy primer, and the CFRP substrate. A Gaussian-distributed pulsed laser is applied to simulate the temporal and spatial energy deposition on the topcoat, with laser absorption modelled using Beer-Lambert's law. The coupling between thermal and mechanical fields is achieved by solving the heat transfer and thermoelasticity equations, and the thermal response is governed by the heat transfer equation. The resulting temperature field acts as a thermal load in the thermoelasticity equations, enabling the prediction of stress evolution and potential damage to the substrate. The results from the laser test including temperature distribution and ablation depth monitored during the process are used to validate the numerical model, and the numerical results demonstrate strong agreement with the experimental data. The developed model provides insights into temperature distribution, ablation depth, and the coupled thermo-mechanical effects within the paint layers and CFRP substrate, facilitating efficient and damage-free paint removal from CFRP substrates using the optimal laser parameters.

Keywords: Finite element model, laser paint stripping, temperature distribution, stress evolution, carbon fibre reinforced polymer

Numerical study of powder agglomeration and intra-biomass temperature gradient effects in cement calciner

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Using coarse biomass as fuel in cement calciners is key for reducing carbon emissions in the cement industry [1]. However, raw meal agglomeration and temperature gradients within large biomass particles limit calcination and combustion efficiency, causing downstream blockages and quality issues [2]. Current industrial-scale models neglect inter-particle adhesive forces and intra-particle temperature gradients, failing to accurately capture essential phenomena [3]. This work develops an integrated model addressing these limitations. First, this work develops an agglomerate-based method accounting for effects on flow, heat transfer, and reactions, validated in pilot and industrial coal-fueled calciners (Figure 1(a)). Subsequently, a sub-particle scale model is developed to capture real-time effects of intra-particle temperature gradients on heat transfer, reactions, and material properties, validated with single biomass and lab-scale reactor experiments (Figure 1(b)). These models are then incorporated into an industrial-scale multifluid framework and validated in biomass-fueled cement calciners (Figure 1(c)). Finally, an optimization method is proposed to achieve efficient raw meal calcination and biomass combustion. This work aims to address practical cement calciner operational challenges and advance carbon emission reduction in the cement industry.

Keywords: Biomass; Agglomerate; Intraparticle; Cement calciner; Multi-fluid model

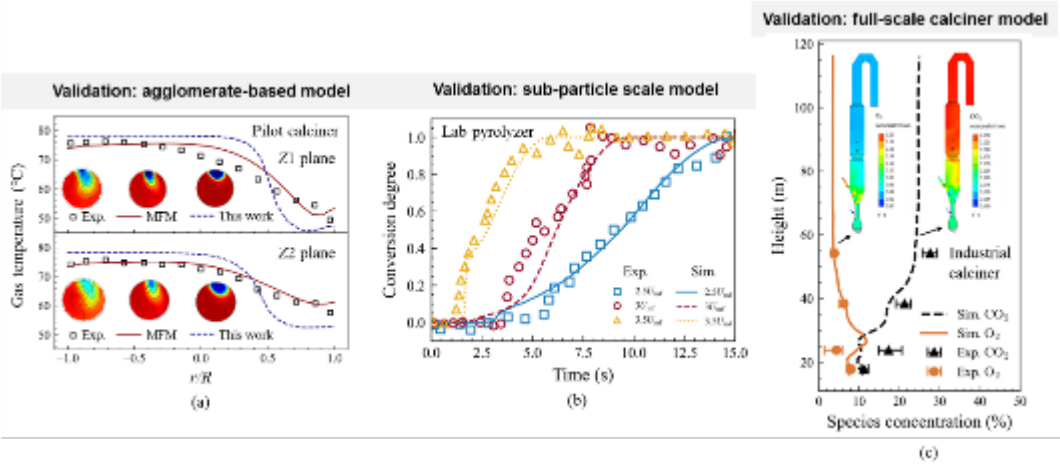

Figure 1. Model validation for (a) agglomerate-based model, (b) sub-particle scale model and (c) full-scale calciner model

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Contact point acceleration estimation via Bayesian filtering and smoothing

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This study presents a new method for estimating the contact point acceleration $\ddot{\mathbf{u}}_{\mathbf{cp}}$ solely based on vehicle measurements, assuming the vehicle model is known. The estimated contact point acceleration is useful in identifying the modal properties of the traversed bridge since the contact point response has minimum interference from the vehicle frequencies. Instead of using an analytical formula to back-calculate the contact point acceleration, this study suggests a new state-space model that links the contact point acceleration with the flexible modal responses of the vehicle. The state-space model is derived from the following relationship between the contact force $\boldsymbol{\lambda}$, contact point acceleration $\ddot{\mathbf{u}}_{\mathbf{cp}}$, and the dynamic of the vehicle flexible mode(s):

$$\boldsymbol{\lambda} = (\mathbf{W}_{\mathbf{v}}^{\mathbf{T}}\boldsymbol{\Phi}_{\mathbf{v}}\boldsymbol{\Phi}_{\mathbf{v}}^{\mathbf{T}}\mathbf{W}_{\mathbf{v}})^{-1}\left(\ddot{\mathbf{u}}_{\mathbf{cp}} + \mathbf{W}_{\mathbf{v}}^{\mathbf{T}}\boldsymbol{\Phi}_{\mathbf{v,flex}}\left(\mathbf{Z}_{\mathbf{flex}}\dot{\boldsymbol{\xi}}_{\mathbf{v,flex}} + \boldsymbol{\Lambda}_{\mathbf{flex}}\boldsymbol{\xi}_{\mathbf{v,flex}}\right)\right) \quad (1)$$

where $\boldsymbol{\Phi}_{\mathbf{v}}$ represents the mass-normalize modal shape matrix of the test vehicle, while $\mathbf{W}_{\mathbf{v}}$ is contact direction matrix of the test vehicle. $\boldsymbol{\Phi}_{\mathbf{v,flex}}$ and $\boldsymbol{\xi}_{\mathbf{v,flex}}$ are flexible modal shape matrix and displacement vector, respectively. Additionally, $\boldsymbol{\Lambda}_{\mathbf{flex}}$ and $\mathbf{Z}_{\mathbf{flex}}$ correspond to the generalized stiffness and damping matrices associated with the vehicle's flexible modes.

To solve the input-state estimation problem involved, we employ an Augmented Kalman Filter in conjunction with a Rauch-Tung-Striebel Smoother. Through numerical simulations, this study validates the proposed method, offering valuable insights into how different parameters impact the accuracy of the contact point response.

Keywords: contact point acceleration, Augmented Kalman Filter, Rauch-Tung-Striebel Smoother, vehicle scanning

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Analysis of Debris Capture Behavior in Permeable Sediment Control Dams

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In recent years, the occurrence of heavy rainfall has increased in Japan due to the effects of global warming. Heavy rainfall can lead to landslides, which cause serious damage to human life and property, making early countermeasures crucial. One effective measure is the use of sediment control dams. These dams temporarily hold back sediment and prevent its flow, thereby reducing the risk of disaster. Traditionally, impermeable sediment control dams have been used, but this type has the problem of fragmenting natural ecosystems due to its structure. On the other hand, permeable sediment control dams maintain the continuity of ecosystems and have become the mainstream in recent years. Furthermore, permeable sediment control dams capture more debris compared to impermeable ones, which makes them even more noteworthy. However, research on the behavior of debris capture and the forces acting on permeable sediment control dams is still insufficient, and many aspects remain unclear.

This study aims to develop a method for measuring the changes in force and behavior when a permeable sediment control dam captures debris. Specifically, a floating log model will be introduced into a water channel with flowing water, and the phenomenon of the sediment control dam capturing debris will be analyzed. The analysis method will use the Finite Volume Method for discretization. Additionally, the contact detection between the debris model, the dam model, and the debris models will be performed using the Discrete Element Method. The accuracy of the analysis method will be examined by comparing it with experimental data.

Equivalent Extreme Wind Load Method for Mean-Wind-Speed Profile Prediction with Python Implementation

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The mean wind speed profile constitutes a fundamental parameter for structural wind load calculations. Conventional methods directly adopt characteristics (e.g., mean values and envelope values) of measured wind data as predicted profile parameters, failing to guarantee structural wind load effects reaching required extremes. To overcome this limitation, this paper proposes the Equivalent Extreme Wind Load Method (EEWLM) [1], which establishes a physical equivalence between the mean wind speed profile and extreme wind load effects based on wind load codified principles. The EEWLM implementation framework comprises four phases: (1) preprocessing of anemometric data, (2) selection of mean wind speed profile models, (3) analysis of extreme wind loads, and (4) estimation of equivalent profile parameters. (Figure 1)

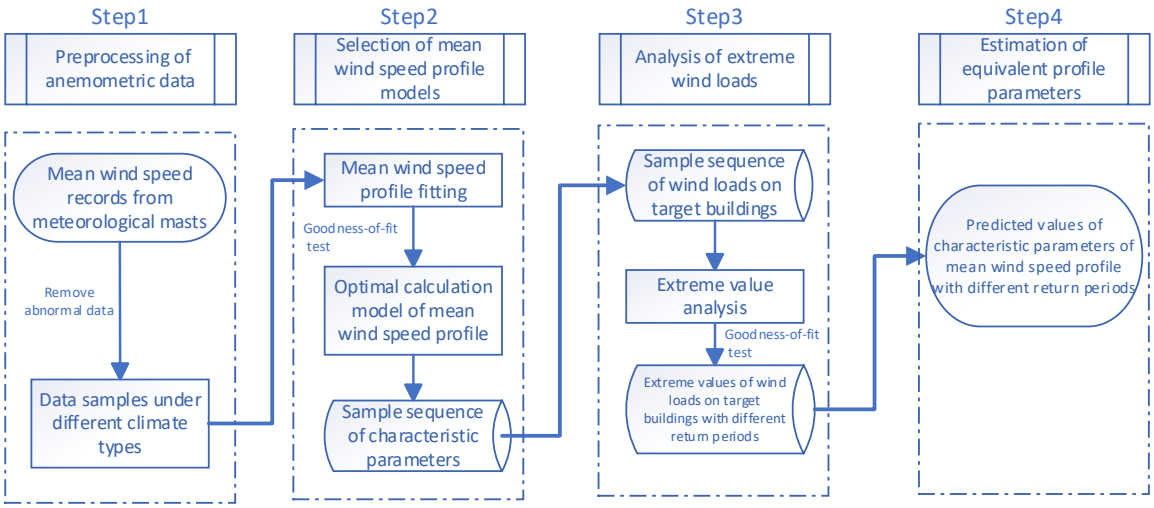

Figure 1. Flowchart of the Equivalent Extreme Wind Load Method

A Python-based data-driven system was developed using wind speed records from eight meteorological masts along the Fujian coastline and applied to a high-rise building as a case study. Results indicate that: (1). The predicted mean wind speed profile parameters incorporate the concept of recurrence period, making them more suitable for structural wind load calculations; (2).The equivalent mean wind speed profile power index (α) decreases sequentially in mixed wind climates, typhoon conditions, and monsoon climates; (3). The derived profile parameters significantly exceed both code-specified values and statistical mean values, highlighting a systemic underestimation of typhoon-induced wind loads in current Chinese standards.

Keywords: Mean wind speed profile, typhoon, recurrence period, wind load standard, python

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A comprehensive model for H_2-intensive shaft furnaces

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The hydrogen-intensive shaft furnace (SF) is considered a new technology for ironmaking, offering significant potential for achieving ultra-low CO_2 emissions. However, SF technology currently faces high operating costs due to the reliance on expensive high-grade pellets and low fuel efficiency. These limitations restrict its application, accounting for only 5% of crude steel production in 2024. To reduce costs and enhance feasibility, future developments aim to enable the use of lump ore and improve hydrogen utilization efficiency [1]. Numerical simulation is a valuable tool for evaluating the internal conditions of industrial-scale SFs and supporting process optimization. However, existing models in the literature involve major simplifications: they often focus only on the reduction zone, use one-dimensional algebraic models, simplify the iron ore reduction process, neglect major side reactions and their heat effects, and offer limited analysis of lump ore degradation. To overcome these limitations and provide more accurate predictions, we have developed a comprehensive computational fluid dynamics (CFD) model for the entire H_2-intensive SF. The model treats solid and gas flows as two single-phase flows. A porous-medium moving bed approach is applied to describe the gas-solid flow. Iron ore reduction is modeled using an improved multi-interface shrinking core model. In addition, key side reactions—including the water-gas shift reaction, methane reforming and cracking, and CO disproportionation—are incorporated along with their heat effects. Lump ore degradation is also considered by modeling the formation of fines and particle shrinkage. This comprehensive CFD model has been validated against industrial data from two SFs. The predicted effects of ore degradation align well with established understanding.

Item		Equation
Mass	gas & solid	$\nabla\cdot(\varepsilon_g\rho_g\boldsymbol{u}_g)=S_g$, $\nabla\cdot(\varepsilon_s\rho_s\boldsymbol{u}_s)=S_s$
Momentum	gas	$\nabla\cdot(\varepsilon_g\rho_g\boldsymbol{u}_g\boldsymbol{u}_g)=-\nabla(\varepsilon_g p)+\nabla\cdot(\varepsilon_g\boldsymbol{\tau}_g)+\boldsymbol{S}_{mon}$
Thermal	gas	$\nabla\cdot(\varepsilon_g\rho_g\boldsymbol{u}_g H_g)=\nabla\cdot[\varepsilon_g(\lambda_g/C_{pg})\nabla H_g]+h_{gs}a_{gs}(T_s-T_g)$
	solid	$\nabla\cdot(\varepsilon_s\rho_s\boldsymbol{u}_s H_s)=\nabla\cdot[\varepsilon_s(\lambda_{s,eff}/C_{ps})\nabla H_s]+h_{gs}a_{gs}(T_g-T_s)+S_T$
Species	gas	$\nabla\cdot(\varepsilon_g\rho_g\boldsymbol{u}_g\omega_{g,i})=\nabla\cdot(\varepsilon_g\rho_g D_{g,i}\nabla\omega_{g,i})+S_{g,i}$
	solid	$\nabla\cdot(\varepsilon_s\rho_s\boldsymbol{u}_s\omega_{s,i})=S_{s,i}$
Ore degradation		$d_{ore,i}=d_{ore,inlet}+\Sigma\Delta d_{ore,i}$, $\Delta d_{ore,i}=(\partial d_{ore}/\partial f)\|_{T_i,f_i}(f_i-f_{i-1})$

Table 1. Governing equations

Keywords: Industrial shaft furnace, comprehensive model, ore reduction, side reactions, ore degradation, internal state

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A Sharp Interface Level Set Approach without Reinitialization for High Reynolds Number Free Surface Flows

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High Reynolds number free-surface flows pose significant challenges due to the complex dynamics of moving interfaces and strong inertial effects. Traditional level set methods relying on a diffusive interface require reinitialization to maintain a signed distance function, preventing interface drift and mass loss [1]. In contrast, the proposed sharp interface approach eliminates the need for reinitialization by employing a cut cell method to directly enforce jump conditions. Like the traditional approach, the interface location is tracked by advecting a level set function ϕ using the fluid velocity field $\mathbf{u}$, governed by the following equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0, \tag{1}$$

The method then assigns physical parameters, such as density and viscosity, directly at quadrature points within cut cells, ensuring accurate representation of material properties at the interface. This approach maintains sharp discontinuities without requiring a separate redistancing procedure. The density at any point x is defined piecewise in Equation (2), where ρ(x) is the fluid density at point x, and ρ_1 and ρ_2 denote the densities of the first and second fluids, respectively:

$$\rho(x) = \begin{cases} \rho_1 \; if \; \phi(x) < 0, \\ \rho_2 \; if \; \phi(x) \geq 0. \end{cases} \tag{2}$$

Initial assessments suggest that the proposed formulation may offer promise in addressing interfacial dynamics and preserving mass conservation in high Reynolds number flows. Moreover, the proposed method enhances computational efficiency by eliminating the overhead associated with reinitialization [2]. The integration of the cut cell technique with a sharp interface representation appears to effectively preserve the discontinuities in material properties, indicating its potential versatility for future applications in simulating complex multiphase flows in hydrodynamics, including marine engineering.

Keywords: Level set method, sharp interface, high Reynolds number, free-surface flow, reinitialization, cut cell method

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Performance evaluation of safety roller barriers made of recycled rubber

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Australia has set ambitious targets within its National Road Safety Strategy 2021-2030, aiming to reduce fatalities by at least 50% and serious injuries by at least 30% in road accidents by 2030, and zero road deaths and serious injuries by 2050 [1]. Recent reports indicate significant challenges in meeting these objectives, as the current fatality rate is continuously increasing since 2021, and hospitalised injuries is on rise [2]. This situation calls for an urgent need to reevaluate traditional safety measures such as wire barriers, W-beams, and concrete barriers, which are useful but have limitations. For instance, W-beams can absorb crash energy through rail deformation but may also cause vehicle snagging, rollovers, or crossovers due to excessive deformation, and often require extensive maintenance or replacement after collisions. In contrast, the past decade has seen the rise of innovative safety roller barriers (SRB) systems, which use posts covered with polymer foam rollers to effectively absorb shock energy and direct vehicles gliding along the road, reducing the risk of severe accidents. For example, the Laverton section, equipped with SRB (Figure. 1), has experienced numerous impacts over more than eight years without a single reported death or serious injury (VicRoad Crash Data), and remarkably, has received no maintenance or replacement.

Figure 1. SRB installed at High St. Laverton, Victoria.

Original SRB uses Ethylene-Vinyl Acetate (EVA) foam material for roller. This material has many advantages such as durability and UV resistance. However, the high cost of the EVA foam roller is the main obstacle for its widespread adoption. Lower the cost may greatly facilitate its rate of deployment on roads in Australia and overseas, thereby helping Australia to achieve the road safety targets and save lives in road accidents. Recycled ground tyre rubber (GTR) has been applied for road safety applications [3,4], which is a good choice for not only reducing the cost, but also improve sustainability. Australia is currently recovering 77 per cent of used tyres. While this achievement is something to be proud of, recovering the remaining 23 per cent is critical to achieving national waste reduction goals, reducing carbon emissions, and preventing environmental hazards in the future [5].

In this study, rollers made from a new compound foam blending EVA with GTR were introduced to the SRB design. The EVA/GTR compound foam is shown in Figure 2. To evaluate the effectiveness of the SRB constructed from this innovative material, a comprehensive comparison with the original SRB model was undertaken. Initial steps involved testing the material properties of each component under both quasi-static and dynamic conditions, which were assigned to the numerical models for simulations of SRB systems impacting with passenger cars and pickups in ANSYS/LS-DYNA. The simulation model is illustrated in Figure 3, showing a passenger car collision with a segment of the safety roller barrier.

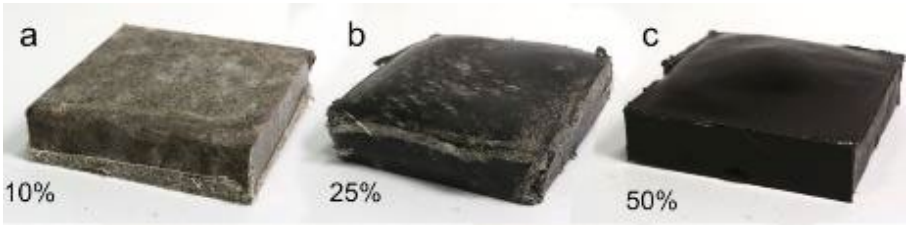
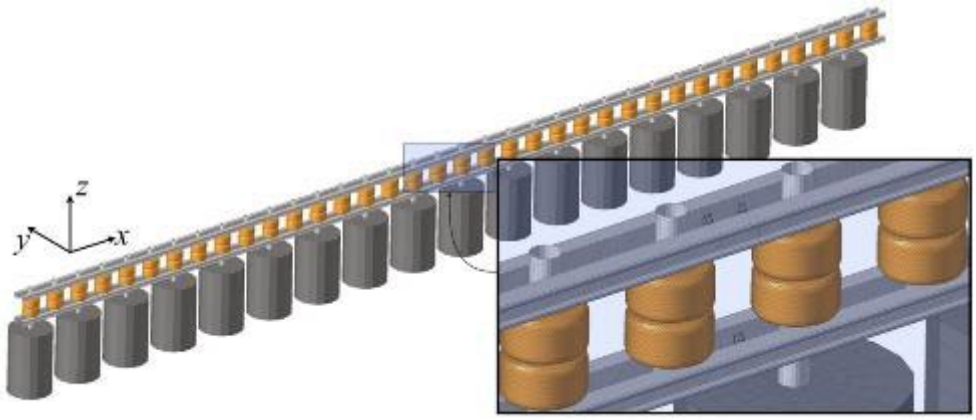
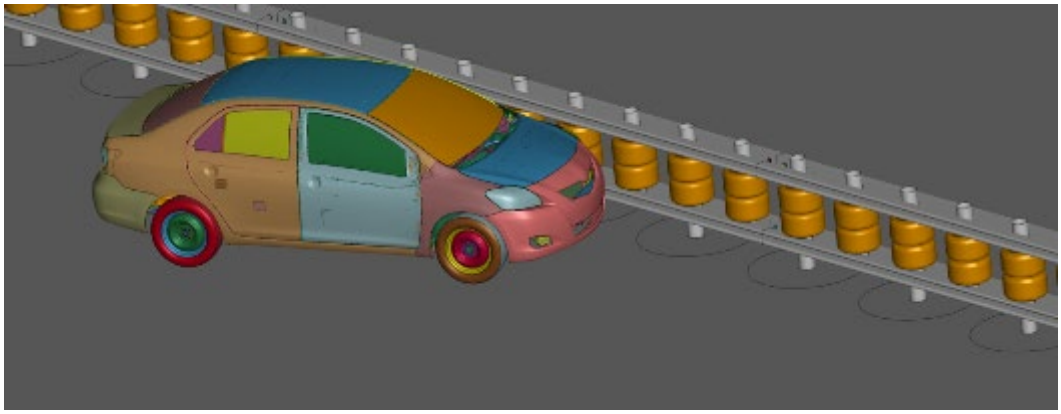


Figure 2. Photos from EVA/GTR compound foams with different GTR contents.



(a)



(b)

Figure 3. Simulation model of (a) SRB barrier and (b) Toyota Yaris crashing into a segment of safety roller barrier.

The validity of the numerical model for the existing SRB was confirmed by comparing the impact characteristics with standard MASH tests carried out in Christchurch, New Zealand, in 2012. The validated model is used to identify the key occupant risk indices in the new SRB system, such as ride-down acceleration (RA) and occupant impact velocity (OIV), derived from the simulation results of the two SRB variants. This comparative analysis aimed to assess the performance of the new SRB, utilising the EVA/GTR compound foam, against the existing system.

The results listed in Table 1 indicated that the SRBs employing the EVA/GTR compound foams exhibited performance indices comparable to those of the existing SRBs. The optimisation of geometric parameters such as post spacing, post height, and roller size to is conducted to fine-tune the performance of the new SRB. This research highlights the potential of incorporating the EVA/GTR compound foam into SRB systems, suggesting a path forward for the deployment of more cost-effective and sustainable safety barriers without compromising on performance.

Roller material	Original	10% rGTR	25% rGTR	50% rGTR
Exit velocity (km/h)	69.12	70.92	70.5	70.2
Exit angle (degree)	16.14	16.88	15.33	15.44
Working width (m)	0.154	0.154	0.153	0.156
OIV-x (m/s)	7.18	7.31	7.15	7.01
OIV-y (m/s)	8.79	8.38	8.52	8.55
RA-x (g)	6.35	5.72	6.43	5.38
RA-y (g)	8.74	10.31	8.36	9.09

Table 1. The evaluation indexes of the crash simulations

Keywords: ground tire rubber, road safety barrier, foam technology, finite element method, optimisation

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An artificial neural network interatomic potential to reproduce dislocations in silicon

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Elucidating the dislocation behavior in silicon is crucial because dislocations in silicon degrade the performance of devices [1]. Classical molecular dynamics has been used to analyze dislocations in an atomic scale. It enables us to perform large-scale simulations compared to the method using the density functional theory (DFT). Its accuracy is highly dependent on the interatomic potential Therefore, for dislocation analyses, an interatomic potential capable of accurately reproducing elastic constants and stacking fault energies is essential. However, existing interatomic potentials tend to underestimate stacking fault energy [2].

Therefore, we developed a machine learning interatomic potential (MLIP) for dislocation analyses in silicon. We employed an artificial neural network (ANN) interatomic potential as the framework of our MLIP. [3]. Unlike conventional empirical potentials, it offers a highly flexible functional form, allowing it to fit arbitrary potential energy surfaces. We used approximately 15,000 datasets derived from DFT calculations. Not only basic structures such as diamond structures but also a substantial amount of data on stacking faults and generalized stacking faults are employed to enhance the reproducibility of dislocations.

Table 1 shows the mechanical properties of our interatomic potential, conventional empirical potentials, and existing MLIPs. Our potential can reproduce the elastic constants as well as other MLIPs. Notably, our potential can reproduce mechanical properties affecting dislocation behavior such as stacking fault energy although others cannot. Also, our potential has a less computational cost compared to other MLIPs. Therefore, our potential is expected to elucidate various mechanisms regarding dislocations in silicon.

	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]	γ_{sf} [mJ/m^2]	$\gamma_{\mathrm{usf}}^{\mathrm{glide}}$ [J/m^2]	$\gamma_{\mathrm{usf}}^{\mathrm{shuffle}}$ [J/m^2]	Cost
Experiment [4][5]	168	65	80	50			
DFT	153	56	76	45	1.91	1.61	
Stilinger-Weber	151	76	56	1	3.21	1.15	0.02
Tersoff	122	86	10	0	1.84	0.97	0.05
MLIP 1	155	57	69	19	2.00	0.93	10.6
MLIP 2	148	58	70	3	1.98	1.51	449
Our potential	167	58	77	48	1.74	1.11	1

Table 1.

Keywords: Silicon, molecular dynamics, machine learning interatomic potential, dislocation

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Three-Dimensional Crack Propagation Prediction Using Transfer Learning

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It is known that more than 80% of structural failures are caused by fatigue failure. Therefore, it is important to prevent fatigue failure of structures and maintain their integrity. Fatigue crack analysis is essential to predict the remaining life after crack detection. In order to evaluate the life of structures with cracks in situ, a technology called a surrogate model, which substitutes computer simulation with machine learning, has been actively studied.

In this study, we focused on transfer learning to construct surrogate models in a shorter time to maintain prediction accuracy [1]. Transfer learning is applied to a predictor trained with two-dimensional crack propagation simulation results by adding three-dimensional crack propagation simulation results. The training dataset is obtained from the results of a crack propagation analysis using an s-version FEM [2]. The input factors are the crack tip coordinates. The incremental values of the crack propagation are predicted to reproduce the continuous crack growth. The training datasets are augmented based on histograms to account for bias in the prediction parameters. In addition to regularization by the L2 norm, a PDE-based loss function with partial differential terms composed of output and input factors, which is created using automatic differentiation is found by AI-Feynman. The combination of the loss as a weighted sum of the predicted loss and the PDE loss as regularization is expected to reduce the validation loss and improve the generalization performance [3].

The crack tip can be predicted with accuracy comparable to previous studies. In addition, the learning time was reduced by applying transition learning to 1/3 of the previous study. We would like to discuss the effectiveness of transfer learning in surrogate models.

Keywords: Transfer learning, Crack propagation, Surrogate model, Equation discovery

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Development of a Surrogate Model for Predicting Deformation of Offshore Wind Turbine Blades

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In recent years, the global demand for renewable energy has surged due to efforts to address climate change and build a sustainable society. Offshore wind power is gaining attention among renewable energy sources due to its advantages over onshore wind power. Offshore wind power benefits from stronger and more stable winds, resulting in higher power generation efficiency while also reducing noise and visual impact. Additionally, the availability of vast ocean areas facilitates large-scale deployment as part of the renewable energy infrastructure. Offshore wind power systems are classified into fixed and floating types. Floating systems, in particular, offer installation flexibility and can be deployed in deep-sea areas. However, challenges remain in reducing costs and improving durability. High maintenance costs and the difficulty of offshore operations necessitate a careful evaluation of fatigue resistance and structural integrity during the design phase.

For complex systems such as floating offshore wind turbines, numerical simulations are essential but computationally expensive. To address this challenge, using machine learning to construct high-precision surrogate models based on simulation data has gained attention. Surrogate models reduce the computational load of simulations and shorten the calculation time for optimization and design exploration. The design of floating offshore wind turbines involves complex interactions between multiple parameters, requiring significant computational resources for conventional simulations. However, surrogate models enable rapid predictions and design adjustments, and they can also be applied to condition monitoring and fault prediction during the operational phase.

In this study, we aimed to develop a surrogate model to predict the blade displacement of wind turbines based on wave and wind analysis [1]. A neural operator using a convolutional neural network [2] was constructed to create a time-evolution model, successfully achieving a prediction error within 5%.

Keywords: offshore wind power, surrogate model, machine learning, neural operator

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A ghost element coupler for fluid-structure interaction

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Numerical analysis of structural destruction is essential for disaster prevention and mitigation. The 2011 Great East Japan Earthquake and the resulting tsunami caused extensive damage to coastal infrastructure. With the risk of a future tsunami from the Nankai Trough earthquake, it is crucial to accurately assess how structures behave under tsunami impact. Building upon the work of Nakamura et al. [1], which developed a fluid-structure interaction (FSI) model coupling a free surface flow model with a rigid body solid using the finite cover method (FCM), this study extends the model by incorporating deformable structure analysis with a proposed FSI coupler and a robust strong coupling strategy to improve accuracy and stability.

The proposed FSI model employs FCM for fluid analysis and the finite element method (FEM) for structural analysis. A phase-field model (PFM) represented by the Allen-Cahn equation tracks the air-water interface, while FCM separates the physical fluid domain from the mathematical domain using a fixed mesh, enforcing velocity continuity at the fluid-structure interface via a penalty method. The level set method is applied for precise interface tracking between fluid and solid, and the stabilized FEM is used to solve the Navier-Stokes and Allen-Cahn equations [2]. Structural analysis utilizes FEM for spatial and the Newmark-Beta method for temporal discretization. To improve the accuracy of interaction force evaluation between fluid and solid, a novel coupler, the ghost element, is originally introduced. To ensure strong coupling and prevent numerical instability, an iterative partitioned method with Aitken relaxation [3] is adopted. Several numerical examples are presented to demonstrate the premise and performance of the developed technique.

Keywords: fluid-structure interaction, finite element method, free surface flow, partitioned scheme, strong coupling

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Design of SILS Architecture for Hydrogen Fuel Cell of Unmanned Underwater Vehicle

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The demand for longer endurance, greater range and specialised (complex) missions for unmanned underwater vehicles continues to grow. However, traditional battery-based power sources have limited endurance to meet these demands. The limited energy density of current battery systems does not meet the requirements of long-duration operation, so research is underway into power sources that can be used for long periods of time for unmanned underwater vehicles [1]. In particular, hybrid power sources combining underwater hydrogen fuel cells and batteries are being actively researched. Our institute is also working on the application of hybrid power sources to unmanned underwater vehicles. In this paper, a SILS(Software in the Loop Simulation) design for a hybrid power source based on an underwater hydrogen fuel cell is presented as shown in Figure 1. In particular, we are conducting research on SILS to develop a virtual digital platform, and in the future we plan to develop a digital twin by combining it with hardware. This will be used to design an unmanned underwater vehicle based on hydrogen fuel cells.

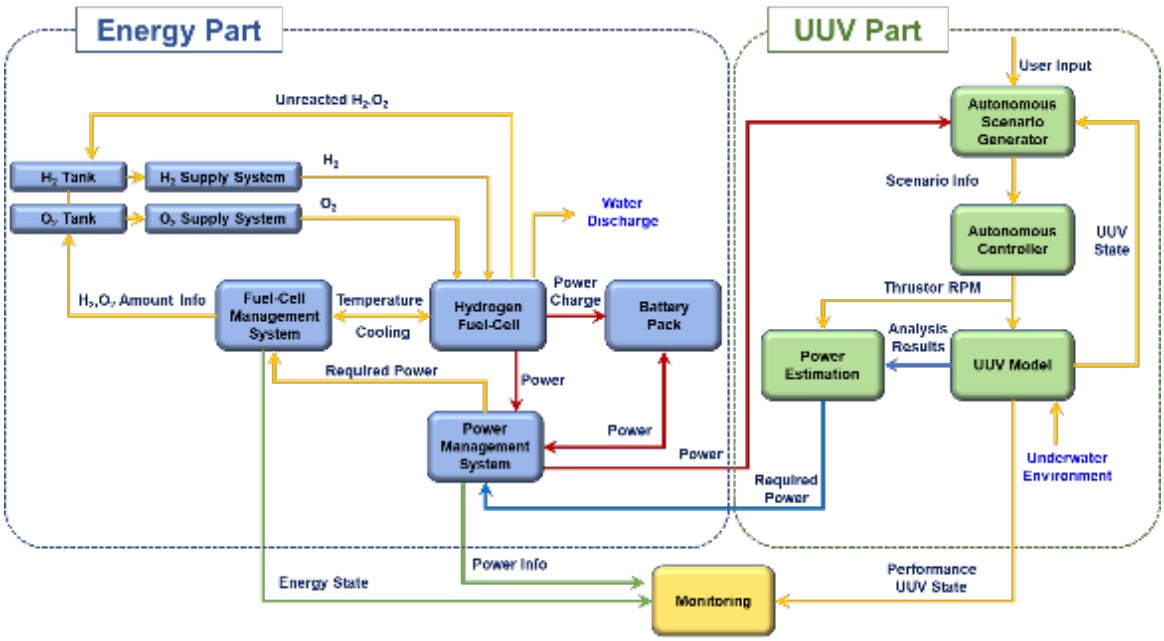

Figure 1. Architecture for hydrogen fuel cell in underwater unmanned vehicle

Keywords: Unmanned Underwater Vehicles, Hydrogen Fuel Cell, Software in the Loop Simulation, Hybrid Power Source, Digital twin

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City scale simulation-driven seismic risk assessment with dynamic fragility analysis

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Earthquakes in densely populated urban regions pose significant challenges for risk assessment and disaster management. This study introduces an integrated framework for evaluating seismic risk at a city scale by combining advanced numerical simulation, sparse sensing, and dynamic fragility analysis. Traditional methods rely on extensive sensor networks and costly computations, whereas our approach uses simulation-based scenario generation and data-driven techniques to provide rapid, reliable assessments.

The framework generates realistic earthquake scenarios via a multistage simulation process. First, a stochastic method based on Green's function simulates the propagation of seismic waves from fault zones to the engineering bedrock under various conditions. The outputs feed into a comprehensive simulation that computes surface ground motion. The generated datasets are then split into training and validation sets for further analysis.

To identify dominant spatial features from the simulation datasets, the proper orthogonal decomposition is applied to the training data, revealing the essential low-dimensional structure of the seismic responses. This information is used to derive a sensor optimal placement strategy[1], which strategically selects sensor distribution to maximize efficiency and prediction accuracy without requiring a highly dense network.

A key innovation is a hierarchical Bayesian model-based dynamic fragility analysis[2][3], which classifies buildings by structural type while also accounting for individual building characteristics. Additionally, the proposed framework supports a sequential update of the fragility functions as new data becomes available.

To evaluate the effectiveness of the proposed framework, a case study in a real city in Japan is demonstrated. The integrated simulation and sensor optimization yield reliable ground motion estimates, while the dynamic fragility analysis provides detailed insights into the vulnerability of structural groups and individual buildings. Additionally, the sequential update further enhances accuracy, making this framework a practical tool for real-time emergency response and long-term urban planning.

Keywords: Numerical simulation, Proper orthogonal decomposition, Sparse sensing, dynamic fragility analysis, Bayesian hierarchical modelling

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Research on Scour Repair and Dynamic Response of Monopiles Using Scour-Resistant Tough Solidified Soil

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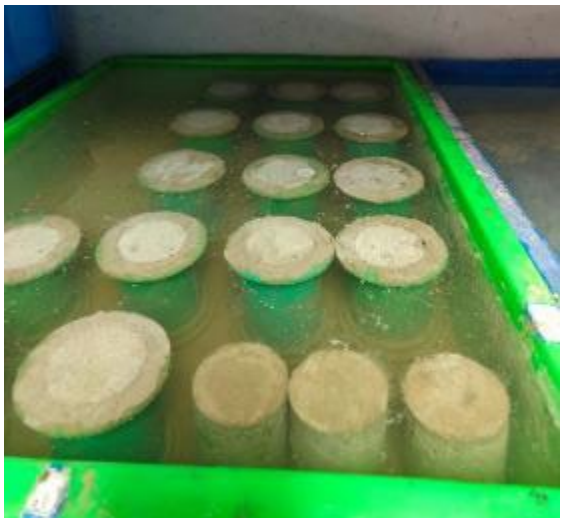
Local scour around monopiles induced by water flow is a critical factor affecting the overall stability of offshore wind turbines. To promote the application of silt solidification technology in scour protection of pile foundations, this study developed a fiber-reinforced solidified soil. Flowability tests, anti-dispersion tests, and unconfined compressive strength tests were conducted to investigate the improvement effects of fibers on solidified soil. Flume experiments were also performed to evaluate the repair effectiveness of fiber-reinforced solidified soil in scour pits around piles and its influence on the dynamic response of pile foundations after scour remediation. Experimental results demonstrate that fiber incorporation reduced the flowability while enhancing the anti-dispersion capability and strength of solidified soil. The maximum scour depth around piles in solidified soil decreased by 86.75% compared with model sand, with an additional 25.45% reduction achieved through fiber reinforcement. Affected by scour pit evolution, the vibration center at pile top initially shifted before stabilizing, and vibration amplitude exhibited an increasing-then-stabilizing trend. The solidified soil reduced pile top vibration amplitude by 18%-50%, with vibration trajectories presenting a figure-"8" pattern. It also decreased the vibration frequency by 4.4%-20.17%. Increasing cement content from 5% to 15% reduced scour loss rate by 40.72%, while extending curing time from 0.5h to 2h decreased it by 34.96%. A predictive equation for anti-scour performance was established through scour loss rate fitting.

Keywords: Pile foundation;Solidified soil; Anti-scour resistance; Scour repair



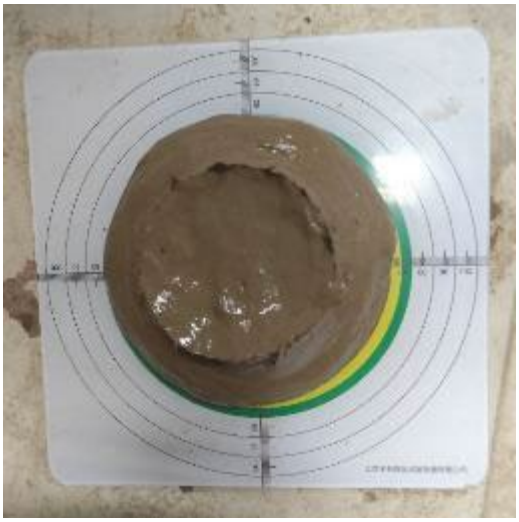


Fig.1 Preparation of solidified soil Fig.2 Flowability tests

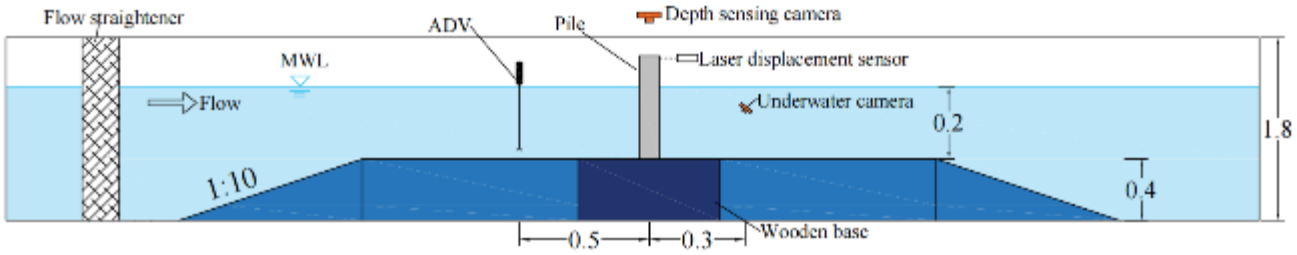


Fig.3 Flume layout

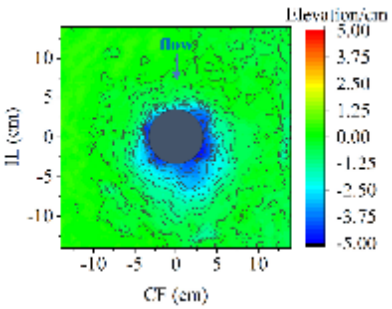


Fig.4 Measured topographic map Fig.5 Scanned topographic map

CDE based economic feasibility process for suitable site selection on wave energy converters

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Computational Design and Engineering(CDE) technologies were developed for reduction of design cost and period in various industries. Recently, these CDE technologies have been expanded through many researches to be utilized not only in the design stage but also throughout the entire product lifecycle, including planning, installation, operation and maintenance. Representative examples include building information modelling(BIM) automation and manufacturing digital twins. In particular, Korea announced that it will apply BIM automation to the entire process by 2030. It would secure the safety of buildings and construction sites and perform efficient management of entire building lifecycle using digital data. In this paper, we would like to analyze the digital data required for suitable site selection on wave energy converters and perform basic research to develop a CDE based economic feasibility process. The oscillating water column(OWC) type wave energy converters have been the center of attention as eco-friendly energy, but they are difficulties in commercialization due to low power generation efficiency compared to the production cost. Recently, the systems linked to breakwaters have been developed, and which linked to breakwaters are receiving attention again because their production costs are similar to those of existing breakwaters. The Korea Institute of Ship and Ocean Engineerings(KRISO) has designed, manufactured, and operated two wave energy conversion systems, and has secured various digital data for them [1]. The process aims to provide users with various information related to sutable site selection in real time by economic feasibility evaluation based on CDE. We expect that it will be utilized in future commercialization studies on OWC type wave energy converters.

Figure 1. OWC type wave energy converters installed and operated by KRISO

Keywords: Wave energy convertor system, Computational Design and Engineering, Economic feasibility, Conceptual Design

Acknowledgment

This research was supported by Korea Research Institute of Ships and Ocean engineering a grant from Endowment Project of “Digital platform development to support marine digital transformation” funded by Ministry of Oceans and Fisheries(2520000291).

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Rapid Uncertainty Quantification Analysis for Seismic Response of High Arch Dams Using Stochastic Scaled Boundary Finite Element Method

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The dynamic response analysis of high arch dams under seismic action has long been a hotspot in the field of seismic resistance, with significant randomness in the analysis process. A pioneering framework based on the Stochastic Scaled Boundary Finite Element Method (SSBFEM) is proposed for uncertainty quantification in seismic analysis of high arch dams, enabling the prediction of structural dynamic responses considering randomly distributed material properties. Implementing octree SSBFEM on commercial software provides accurate and convenient full order models for uncertainty quantification. For the time-consuming nature of Monte Carlos (MCs), a fast algorithm based on model order reduction (MOR) combined radial basis function (RBF) is proposed. Through the linear combination of the constructed low-order subspaces, the solution required for MCs is quickly obtained, and the computational efficiency of traditional MCs is improved. Additionally, the key objective of singular value decomposition (SVD) is to uncover the intrinsic relationships among these snapshots, extract the primary characteristics of the data, and then reduce its dimensionality. Finally, several numerical examples and a high arch dam are provided to verify the accuracy and effectiveness of the proposed algorithm.

Keywords: Scaled boundary finite element method; Monte Carlo simulation; singular value decomposition; radial basis function;

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Structural Analysis of Multi-domain System Using Deep Operator Network

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Finite Element Analysis has an inherent limitation in that the required computational resources and time increase exponentially with the number of degrees of freedom, posing significant challenges for large-scale structural analysis. As a potential alternative, surrogate models based on Physics-informed Machine Learning have been researched, demonstrating significantly higher computational efficiency than Finite Element Analysis. However, since the training data for these surrogate models depend on Finite Element Analysis simulations, its generation cost remains high. To mitigate this issue, this study explores the application of domain decomposition to Physics-informed Machine Learning based surrogate models to improve training efficiency. The surrogate model proposed in this study is constructed using a Deep Operator Network, which receives physical properties (including elastic modulus, cross-sectional area, boundary conditions) and loading conditions as input variables and predicts structural responses such as displacement. To improve training efficiency, the structural domain is partitioned into multiple sub-domains. At the interfaces between sub-domains, both displacement continuity and residual continuity, derived from partial differential equations, are enforced to ensure the physical consistency of the system. The linear equilibrium equation(1) applied in this study is given as follows:

$$\nabla \cdot \boldsymbol{\sigma} + \rho_0 \mathbf{f_b} = 0 \quad \text{in } \Omega, \tag{1}$$

where $\boldsymbol{\sigma}$ is the stress tensor, $\nabla \cdot$ is the divergence operator, ρ_0 is the mass density, $\mathbf{f_b}$ is the body force vector, and Ω is a bounded domain. To validate the proposed methodology, numerical experiments were performed on a two-dimensional structural system. As a result, this study demonstrates that the domain-decomposed Deep Operator Network can optimize computational efficiency in structural analysis. Furthermore, future work will explore its extension to large-scale structural analysis.

Keywords: structural analysis, physics-informed machine learning, Deep Operator Network, partial differential equations, surrogate model, domain decomposition

Acknowledgement

The research was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science and ICT) (NRF-2023R1A2C200375811)

A Graph-Based Generalization of Geometric Domain Decomposition Based Parallelization for Advanced Galerkin Methods

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As a strategy to achieve large-scale parallel numerical analysis for distributed-memory parallel environments, geometric domain decompositions, which geometrically partition regions and map each region to a processing element, is widely used, especially for finite element methods (FEM). This strategy often defines a weighted graph structure of a discretized target region and determines the partitioning of the region to obtain a good load balance by solving a minimal cut problem of the weighted graph utilizing graph related libraries such as METIS [1].

In this study, we generalize the idea of geometric domain decompositions using graph structures to be applicable to the s-version of FEM [2], the proper orthogonal decomposition (POD) Galerkin method using subdomains [3], and other advanced methods. In addition, we introduce how to design a library for the generalized method that can easily parallelize existing simulators. In addition, specific examples of graph constructions and decompositions for these advanced Galerkin methods are presented, and their parallelization efficiencies are measured to quantitatively evaluate the effectiveness and versatility of the generalized method and the library.

Keywords: graph structure, domain decomposition, finite element method, s-version of FEM, POD Galerkin method

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A Hybrid iFEM-NOSPD Model for Structural Health Monitoring of Damaged Structures

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Structural health monitoring (SHM) plays an essential role in ensuring the safety and longevity of engineering structures. A recently developed numerical model, called the inverse finite element method (iFEM) [1], has been extensively utilized for various SHM engineering applications. However, the iFEM model encounters considerable difficulties in monitoring stress concentrations and singularities. Thus, the non-ordinary state-based peridynamic (NOSPD) model [2], which has demonstrated its significant potential in the field of fracture mechanics, is introduced into the iFEM framework. A hybrid iFEM-NOSPD model is proposed in this study to monitor structural responses of damaged structures. Several numerical examples are presented to verify the performance of the proposed hybrid model. It is confirmed that the proposed hybrid model is capable of effectively capturing structural and fracture responses with enhanced computational efficiency.

Keywords: Inverse finite element method, Peridynamics, Structural health monitoring, Fracture mechanics

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Direct numerical simulation of turbulent thermal channel flow over riblet surface

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Much research has been done on turbulence control to improve energy efficiency. There are active and passive turbulence control methods: the former requires energy for actuation, and the latter requires only initial system processing without actuation energy. In the present study, we focus on the riblet surface, which is a typical example of passive control.

The riblet surface prevents the turbulent vortical structure from approaching the wall. The skin-friction drag is reduced since the contact between the vortical structure and the wall is suppressed. Choi *et al*.[1] performed direct numerical calculations of turbulent channel flow with the straight type of riblet surfaces. The riblet spacing must be smaller than the vortex diameter to prevent vortex structures from approaching the channel flow. Recently, Sasamori *et al*.[2, 3] investigated the three-dimensional riblet surface by experiments and direct numerical simulation. The riblet surface provides a larger drag reduction effect than the straight riblet with wide lateral spacing of the riblet walls.

On the other hand, it is well known that turbulence decreases in stable stratification and is promoted by unstable stratification. The buoyancy force can create stable stratification with heating and cooling on the wall. Therefore, we expected the riblet surface to enhance the drag reduction effect if the buoyancy force creates stable stratification in the channel flow.

In this study, we perform the direct numerical simulation of the turbulent channel flow. The riblet surface is installed on the channel walls, and the wall's heating and cooling create stable or unstable stratification. Figure 1 shows the sample results: left shows an uncontrolled flow, and right shows the flow with riblet walls. The buoyancy force is absent. The vortical structure, which increases the skin friction drag, is shifted away from the wall. In the presentation, we will report the buoyancy effect on the drag reduction effect by the riblet surface.

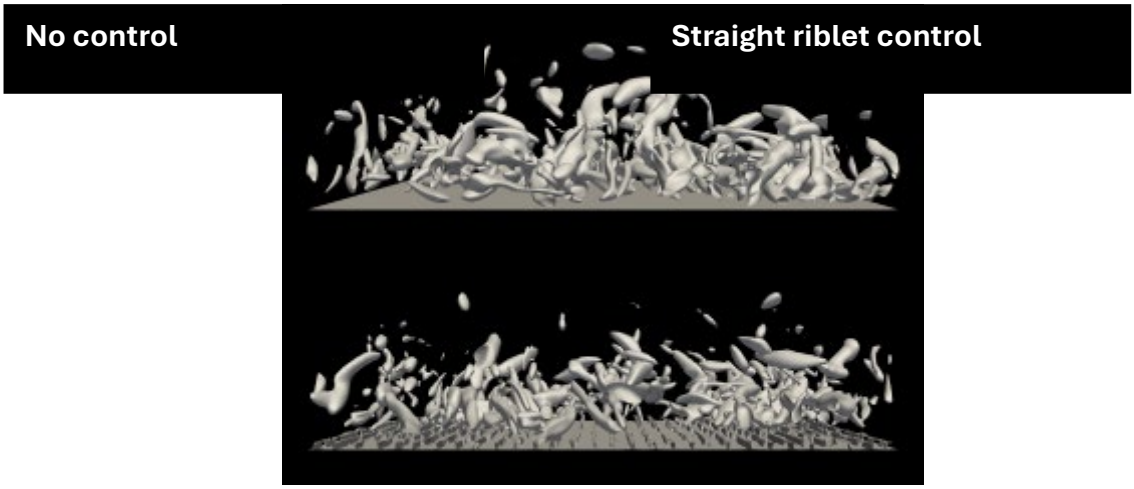

Figure 1. Visualization of the vortical structure.

Keywords: turbulent channel flow, riblet, drag reduction, direct numerical simulation, buoyancy

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Parameterization and coarse-grained molecular dynamics simulations on mechanical behaviour of semi-crystalline polymer

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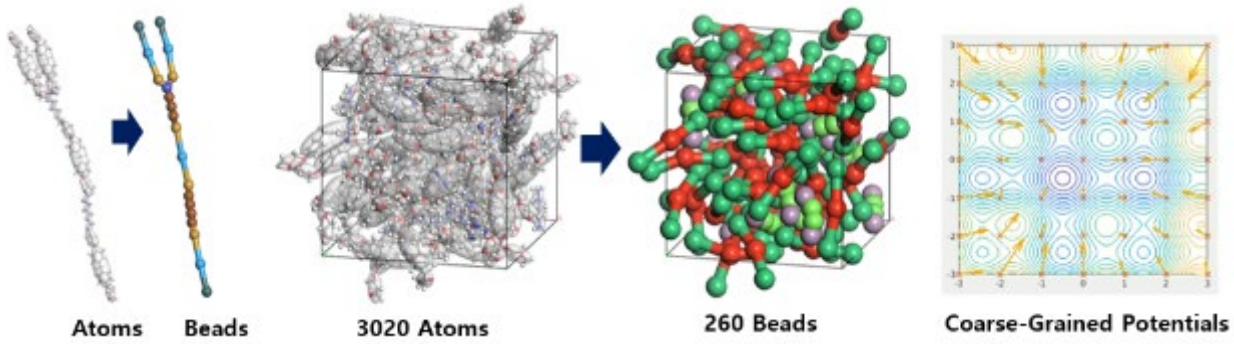
With the rapid advancements in IT, energy, and high-tech materials technology, the demand for in-silico simulation and design of polymer-based functional materials has been continuously increasing. All-atom molecular dynamics (AAMD) simulations offer a promising approach; however, due to time and length scale limitations, modelling polymers that can exhibit multiple phases within the same polymer system still remains challenging.

In this study, we parameterized coarse-grained (CG) potential models suitable for describing the behaviour of both crystalline and amorphous thermoplastic polymers. To determine the equilibrium parameters such as bond length and angles defined from CG models, the Boltzmann inversion method is applied to the linear single chain model of the polymer. To accurately predict the mechanical properties of crystalline and amorphous phase, the mechanical properties of single strand polymer and of bulk amorphous polymer are considered both in AAMD and CGMD. To optimize the CG parameters, the particle swarm optimization (PSO) algorithm is used. Using the developed CG parameters, semi-crystalline polymer unit cells including an ellipsoidal crystalline phase inside an amorphous phase are constructed and the stress-strain relation is determined according to the volume fraction of semi-crystalline domain.

$$\overrightarrow{V_i^{t+1}} = \mathrm{w}\overrightarrow{V_i^t} + c_1 r_1 \left(\overrightarrow{P_i^t} - \overrightarrow{X_i^t}\right) + c_2 r_2 \left(\overrightarrow{G^t} - \overrightarrow{X_i^t}\right) \quad (1)$$



Keywords: Coarse-Graining, Molecular simulation, optimization, multiscale, mechanical properties

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The collapse of low-saturation liquid-containing granular materials

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The flow of low-saturation liquid-containing granular materials is prevalent in nature and industrial processes, and understanding the associated transient dynamics is extremely important for exploring such complex flow processes. In this report, the collapse dynamics of wet granular column is systematically studied based on the discrete element method (DEM) for wet particles and the corresponding small-scale experiments. Furthermore, the dependence of the dynamics and flow mobility on particle size distribution is also examined, as shown in **Figure.1**, and the underlying mechanisms are explored by analyzing particle path lengths and average fidelity. Building upon the effective Bond number proposed using the mixing theory, a macroscopic cohesion parameter at the material scale is defined by considering the dependence of the collapse on system size effect. The relevance of this cohesion parameter in describing different wet polydisperse granular collapses is further validated based on our designed experimental tests and DEM simulations. The approach of constructing the cohesion parameters at different scales can be extended to characterize cohesion effects in more complex wet polydisperse granular flows and describe their associated rheological behaviors.

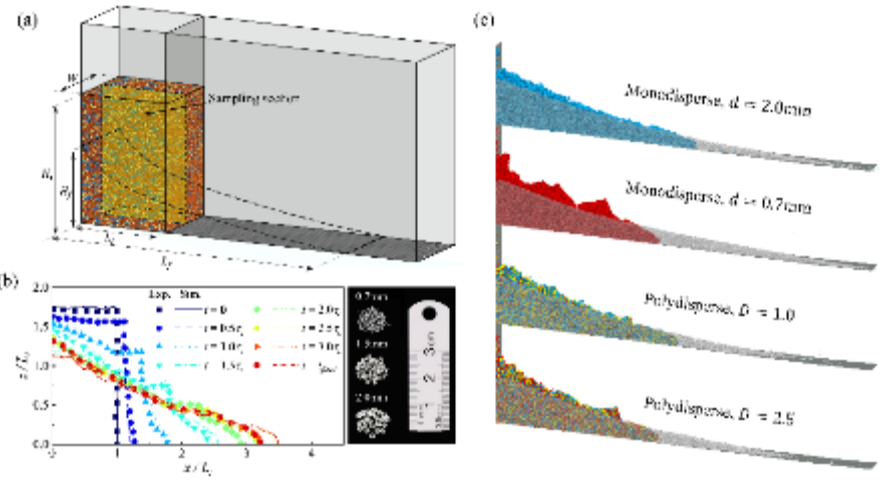

Figure. 1. The collapse of polydisperse granular columns. (a) Schematic diagram of the configuration employed. (b) Comparison of side-view deposit profiles between simulations and experiments at various moments for particle size distribution $D = 1$, and glass beads used in experiments are shown in the right column. (c) Comparison of final deposit morphologies between monodisperse and polydisperse systems.

Keywords: Wet granular materials, collapse dynamics, cohesive effects, deposit morphology, discrete element method

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Shape design optimization of magnetic actuator using isogeometric boundary element method

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A continuum-based shape design sensitivity analysis (DSA) approach is introduced for two-dimensional multi-domain magnetostatic problems using the isogeometric boundary element method (IBEM), which directly incorporates NURBS basis functions from CAD systems for response evaluation. To maintain consistency between NURBS patches in multi-domain BEM models, a discontinuous element formulation is employed. Since the magnetic potential is highly sensitive to the geometry of ferromagnetic materials, the precise multi-domain boundaries are represented using NURBS basis functions and control points in the response computation. Consequently, the proposed isogeometric shape DSA method offers more precise gradient information of the objective function, enabling efficient one-directional searches in optimization. The effectiveness of the developed discontinuous IBEM and DSA is demonstrated through numerical case studies.

Keywords: Isogeometric method, Magneto-statics, Boundary Element Method, Shape Optimization

Acknowledgement

This research was supported by Korea Research Institute of Ships and Ocean engineering a grant from Endowment Project of "Development of Basic Technologies in Eco-friendly Ship Fuel Reliability and Safety Evaluation" funded by Ministry of Oceans and Fisheries(1525014866) and the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (RS-2024-00356107)

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Membrane vesicles embedded with multiple curved proteins subjected to osmotic pressure: Monte Carlo simulations

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Biological membranes, which as physical communication mediums facilitate the transfer of mechanical signals between cells, organelles, and their surrounding environments, play important roles in many fundamental physiological processes and cellular functions, such as endocytosis, cell migration, metabolism and intercellular trafficking. The successful implementation of relevant cellular functions is closely associated with the specific cell/organelle shape defined by the biomembranes. In biological systems, in general, the curved protein and osmotic pressure would simultaneously take part in regulating the membrane shape remodelling. A fundamental question of how the curvature-sensing proteins and the osmotic pressure jointly guide the vesicle mechanics and the dynamical evolution of vesicle morphology under the action of thermal perturbation is spontaneously raised. Challenges here in describing the mechanics of membrane deformation induced by the interaction between curvature-sensing proteins and osmotic pressure are integrating the proteins distribution, the osmotic effect and the geometrical morphology of vesicle membrane. To address these challenges, in this article, we conducted dynamic Monte Carlo simulations from mesoscopic membrane model to systematically investigate the stochastic dynamical spatio-temporal evolution and the equilibrium analysis of a vesicle embedded with two distinct curvature-sensing proteins (taking account the diversity among curvature-sensing proteins) subjected to osmotic pressure based on the free energy of vesicle system. Rich morphological evolution of vesicles is observed and is sensitive to the membrane mechanics (e.g., elasticity and fluidity). Moreover, the osmotic effect would inhibit the curved proteins-induced vesicle shrinkage. These findings are consistent with previously experimental observations.

Keywords: Monte Carlo simulations, membrane vesicle, fluctuations, curvature-sensing proteins, osmotic pressure

Stress triaxiality-dependent cohesive zone model and its application to ductile crack growth analysis in C(T) specimen

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Cohesive zone modeling (CZM) has been proven to be an effective approach for predicting crack growth in ductile materials by employing a traction-separation law (TSL) to characterize the failure process in the crack tip region. The traction-separation law is primarily defined by the cohesive strength, T_0, and the cohesive energy, Γ_0, which respectively govern the crack initiation and energy dissipation due to the crack growth. Traditionally, T_0 and Γ_0 are treated as material constants and measured experimentally. However, some studies suggest that variations in stress state and plastic constraint, influenced by specimen size and loading configuration, can impact material failure. This indicates that the TSL should account for these effects [1]. In this study, a stress triaxiality-dependent CZM with a trapezoidal TSL is proposed for modeling ductile fracture behavior by regarding stress triaxiality as a meaningful parameter to describe the stress state and plastic constraint on the crack tip. The relationship between traction T and separation δ on the crack plane is expressed as follows:

$$T = \begin{cases} T_0(\eta) \cdot \dfrac{\delta}{\delta_1} & \text{for } 0 < \delta \le \delta_1 \\ T_0(\eta) & \text{for } \delta_1 < \delta \le \delta_2 \\ T_0(\eta) \cdot \dfrac{\delta_c - \delta}{\delta_c - \delta_2} & \text{for } \delta_2 < \delta \le \delta_c \end{cases} \tag{1.1}$$

$$\delta_c = \frac{2\Gamma_0(\eta)}{T_0(\eta)} - \delta_2 + \delta_1 \tag{1.2}$$

where T_0 and Γ_0 are treated as functions of local stress triaxiality η obtained from solid elements adjacent to cohesive interface elements. δ_C is the separation when material fully failure, while δ_1 and δ_2 are the relative displacements corresponding, respectively, to the onset of damage and to the beginning of stiffiness degradation.

In this presentation, the proposed CZM is implemented in the interface element used in FEM, and a three-dimensional ductile crack growth analysis in a low-carbon steel C(T) specimen is conducted. The analysis results include the obtained load-displacement relationship and propagating crack profiles, which are shown and compared with experimental results as validation.

Keywords: Ductile fracture, Cohesive zone model, Finite element method, C(T) specimen

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Topology optimization for ITR-free thermal metadevices

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Thermal cloaks and related metadevices control the heat flux around an obstacle or a domain to be protected from overheating and suppress disturbances in the surrounding temperature distribution, thus realizing innovative heat transfer control. These metadevices typically use two or more materials with different thermal conductivities, with or without metamaterials. It has been reported that when the size of the metadevice is smaller than the micro scale, interfacial thermal resistance (ITR) occurs at the interface between these different materials, degrading the performance of the thermal cloak [1]. To overcome this issue, ITR-free thermal cloak has been proposed based on the equivalent thermal conductivity scheme and the bilayer one [2]. Also, density-based topology optimization is developed for the ITR-free thermal cloak to optimize the height distribution [3]. The method of moving asymptotes (MMA) [4] is employed for optimizing height distribution as an optimizer based on the sensitivity analysis for thermal cloaking.

In this work, we present objective function(s) and constraint(s) for realizing ITR-free thermal metadevices. Density-based topology optimization is used to design ITR-free thermal metadevices and optimizers, objective function(s) and constraint(s) are discussed for designing ITR-free thermal metadevices. Performance(s), manufacturability, and the optimal configurations will be presented.

Keywords: Topology optimization, thermal cloak, interfacial thermal resistance

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Computational Fluid-Structure-Control Interaction Analysis for Insect Flight Maneuverability

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Insect flight maneuverability is a complex problem consisting of fluid-structure interaction (FSI) of wing flapping and intelligent control. It is difficult for us to understand the mechanism using experimental methods [1] because of small and high-speed phenomena. Hence, in this study, we developed a computational fluid-structure-control interaction analysis method for insect flight maneuverability using wing-body partitioning shown in Figure 1.

In the proposed method, the aerodynamic forces acting on the wings are evaluated by solving the following finite element discretised equation for the FSI:

$$ {}_{\mathrm{L}}\mathbf{Ma} + \mathbf{Cv} + \mathbf{N} + \mathbf{q}(\mathbf{u}) - \mathbf{Gp} = \mathbf{g}\,, {}_{\tau}\mathbf{Gv} = \mathbf{0} \tag{1} $$

where **M**, **C**, and **G** are the mass, diffusion, and divergence matrices, respectively; **N**, **q**, **g**, **a**, **v**, **u**, and **p** are the advection, elastic internal force, external force, acceleration, velocity, displacement, and pressure vectors, respectively; and the subscripts L and τ indicate lumping and transposition of matrices, respectively. The angular displacement of the body is evaluated by solving the equation of motion for the rigid body with the aerodynamic forces. The wing stroke angle is controlled using the following feedback control law:

$$ \Delta\Phi^{\mathrm{R}} = K_{\mathrm{p}}\dot{\Psi}_x + K_{\mathrm{i}}\Psi_x \tag{2} $$

where $K_{\mathrm{p}}, K_{\mathrm{i}}, \Delta\Phi^{\mathrm{R}}, \Psi_x, \dot{\Psi}_x$ are the proportional gain, integral gain, stroke angle between the two wings, roll angular displacement, and roll angular velocity, respectively.

A fluid-structure-control interaction analysis is conducted for recovering the body attitude of a fruit fly with the actual morphological and flight data [1]. The numerical simulation results are summarized in Table 1, which shows the flapping cycles required for recovering the body attitude. These results are very close to those of actual insects [1].

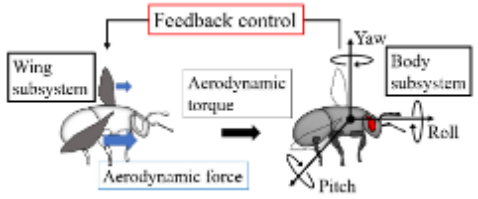

Figure 1.

Case	K_{p}	K_{i}	Flapping cycle required for the recovery of body attitude
1	0.0144	1.2	6.0368
2	0.0144	1.4	5.0852
3	0.0144	1.6	4.4896

Table 1.

Keywords: Insect flapping flight, Insect flight maneuverability, Fluid-structure-control interaction, Partitioned method, Feedback control.

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Electromagnetic Field Prediction of Electric Motor Using Deep Operator Network

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Electromagnetic field data is crucial to electric motor design and analysis, because it directly impacts performance, efficiency, and reliability. Accurate field data enables the optimization of torque production and reduction of energy losses. It also helps reduce noise and vibrations caused by magnetic forces. By utilizing electromagnetic field data, one-dimensional performance metrics, such as torque, can be obtained. For instance, the following equation calculates the axial torque, τ_z using the integral of the radial and tangential magnetic flux densities (B_ρ and B_φ), along with the length L and the permeability μ_0 [1].

$$\tau_z = L \int_0^{2\pi} \frac{\rho^2 B_\rho B_\varphi}{\mu_0} d\varphi, \tag{1}$$

Despite these advantages, the finite element method used to obtain accurate electromagnetic field data has the limitation of high computational cost. As an alternative to this, methods using machine learning are under research. However, in the machine learning methods, the image-based approach is limited by its inability to explicitly reflect physical constraints. Also, data-driven methods have the limitation of not being able to process high-dimensional data effectively. Therefore, research using data-driven method has mainly focused on one-dimensional data [2].

This study proposes a Deep Operator Network based electromagnetic field prediction method to reduce the high computational cost, which is a limitation of existing methods. This method can reflect input variations based on control. Additionally, it allows users to select an optimal balance between computational cost and prediction accuracy depending on data selection. Future research will include experiments to verify the practical effectiveness of this study.

Keywords: Deep Operator Network, Electric Motor, Electromagnetic Field, Digital Twin

Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT). (No. 2023R1A2C200375811)

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Estimation of stored energy distribution using hybrid data assimilation and in-situ observation of static recrystallization in aluminum alloy

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To develop metallic materials with desired properties, prediction and control of growth of recrystallized grains during a static recrystallization are essential. Multi-Phase-Field (MPF) method [1] has been actively used to simulate the recrystallized grain growth. The MPF method defines phase-field (PF) variable ϕ_i to describe the ith crystal grain in a polycrystalline metal. Using the PF variables, the total free energy functional of the system is defined. The time evolution equation of ϕ_i which describes the grain boundary migration is derived from the total free energy functional. In the time evolution equation of ϕ_i, the driving force for the growth of recrystallized grains is the difference of stored energy between the recrystallized grains and the deformed matrix. Therefore, the accurate stored energy distribution is required for the precise prediction of the recrystallized grain growth. However, experimental measurement of the stored energy distribution has not been established. This study focuses on a data assimilation (DA) [2] based on the Bayes' theorem for the estimation of the stored energy distribution. In this study, we developed a new hybrid DA method to estimate the stored energy distribution by integrating the sequential and non-sequential data assimilation algorithms. Furthermore, the hybrid DA developed in this study enables us to improve the prediction accuracy of the MPF simulation and estimate the uncertainty of the estimation results. **Figure 1** shows the inverse pole figure map of recrystallized microstructure in an A1100 aluminum alloy obtained by the in-situ observation and estimated using the developed DA method. The recrystallized grain growth estimated by the hybrid DA shows a better agreement with the in-situ observation data than that by the non-sequential data assimilation. The result demonstrates that the hybrid DA is a novel way to realize the precise prediction of the recrystallized grain growth.

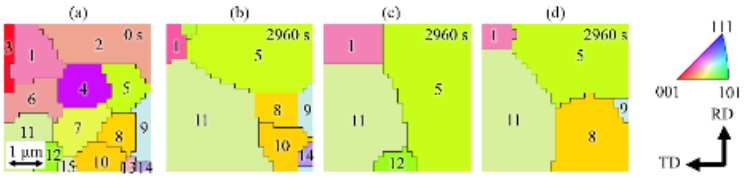

Figure 1 Inverse pole figure map of (a) deformed matrix and recrystallized microstructures in an A1100 aluminum alloy (b) obtained by the in-situ observation, (c) estimated by the non-sequential and (d) the hybrid data assimilation method.

Keywords: Data assimilation, Phase-field simulation, Static recrystallization, Stored energy

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Parameter estimation of a multi-phase field model for austenite-to-ferrite transformation in steel based on Bayesian inference

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To improve the balance between strength and ductility of steels, it is necessary to predict and control the microstructure evolution during the austenite-to-ferrite transformation. Multi-phase field method is widely used to analyze the microstructure evolution during austenite-to-ferrite transformation, parameters and physical properties included in the multi-phase field model have to be identified for more accurate prediction. In this study, we construct the framework for estimating parameters included in the multi-phase field model using Bayesian inference.

In the multi-phase field model employed in this study, we define the phase field variable f_i which represent the ith crystal grain and the k atom's concentration variable c^k and solve the time evolution of these variables. Assuming a material composed of N crystal grains and $n-1$ solute elements, the time evolution of the phase field variables is given by the following equation:

$$\frac{\partial \phi_i}{\partial t} = -\frac{1}{N}\sum_{j=1}^{N} M_{ij}^{\phi}\left(\frac{\delta G}{\delta \phi_i} - \frac{\delta G}{\delta \phi_j}\right) \tag{1}$$

where M_{ij}^{ϕ} is the phase field mobility between ith and jth grain, which is estimated by Bayesian inference in this paper. G is the total free energy of the system which is function of the chemical free energy obtained from CALPHAD data.

The numerical experiment is conducted to validate our proposed parameter estimation framework using Bayesian inference. The isothermal austenite-to-ferrite transformation of Fe-0.092C-0.68Mn-0.8Si (wt.%) alloy at 1103 K is simulated. The volume fraction of ferrite is calculated using the assumed true phase field mobility and hypothetical experimental error is introduced to the volume fraction curve to generate synthetic experimental data. Using this synthetic data, the phase field mobility is estimated based on the Metropolis-Hastings algorithm, a representative approach of the Markov chain Monte Carlo method. The volume fraction curve calculated using the estimated phase field mobility shown in **Fig. 1** closely match that obtained using the true phase field mobility, demonstrating that the proposed framework can accurately estimate the phase field mobility.

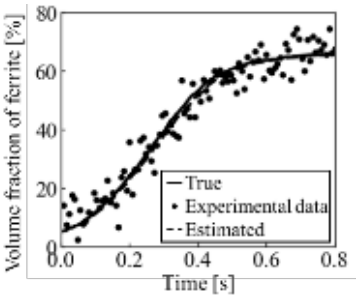

Fig. 1 The volume fraction of ferrite calculated by the multi-phase field simulation of austenite-to-ferrite transformation. The solid and dotted lines are obtained using true and estimated phase field mobility, respectively. The points represent synthetic experimental data.

Keywords: Steel, Austenite-to-ferrite transformation, Phase field simulation, Parameter estimation, Bayesian inference, Markov chain Monte Carlo method

A single-micro-convex contact model based on the assumptions of volume-invariant theory

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The problem of contact and friction has always been a major difficulty in engineering practice, and how to observe the interface in situ and accurately measure the real contact area between the two rough surface interfaces is the key to solve this problem. After hundreds of years of theoretical development, the existing theories have made different degrees of explanations and views on the above problems, but there is still a big gap between them and the real solution of the above problems. Therefore, starting from the volume-invariant form of a single micro convex body, this paper innovatively proposes a set of single micro convex contact models that are different from the previous models, and obtains a good characterization in the experimental control, and then proposes a new rough interface distribution model by introducing the distribution function of the interface, which provides a new idea for how to correctly characterize and calculate the real contact area between interfaces.

Keywords: contact, friction, rough interface, micro-convex

A large-scale phase-field lattice Boltzmann simulation of the sedimentation of multiple equiaxed dendrites

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In the casting of large products, numerous nuclei and fragments generated in the undercooled melt grow into equiaxed dendrites, which then move and settle at the bottom of the mold due to buoyancy and melt convection [1]. Macrosegregation caused by this solid motion affects the quality of the cast product, making it essential to understand the growth and motion behaviours of equiaxed dendrites. However, direct observation of dendrite growth inside a mold is challenging due to opaque and high temperature environment. Therefore, numerical simulations are essential for accurately predicting the sedimentation of equiaxed dendrites.

The phase-field (PF) method is a powerful tool for accurately representing dendrite growth. Furthermore, coupling the PF method with the lattice Boltzmann (LB) method and motion equations enable the simulations of dendrite growth with melt convection and solid motion. However, previous PF-LB simulations have been restricted to two-dimensional cases or short-range movement of a few 3D dendrites due to the high computational cost. Recently, we developed a high-performance computational method for the PF-LB model by integrating multi-GPU parallel computing with the adaptive mesh refinement (AMR). This approach successfully reproduced the long-distance sedimentation of a single 3D dendrite [2].

In this study, we introduce a computational technique that enables the representation of multiple grains using a single PF variable [3] in the PF-LB model, allowing for the simulations of polycrystalline solidification with solid motion. This developed method enables large-scale 3D simulations of growth and long-distance motion of multiple equiaxed dendrites in undercooled melt. Using the developed method, multiple simulations are performed with different numbers of dendrites in the domain, and the time evolution of the solid volume, interfacial area, and sedimentation velocity of isotropic dendrites is obtained. From the results, we evaluate the dependence of number density of dendrites on the growth and motion behaviours, demonstrating that the development method is a powerful technique for elucidating the growth and movement behaviour of dendrites inside molds.

Keywords: Phase-field lattice Boltzmann method, Multiple GPUs computation, Adaptive mesh refinement, Multiple equiaxed dendrites, Sedimentation, Casting

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Surrogate modeling of nonreciprocal mechanical behavior reflecting microscopic tension-compression asymmetry

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Mechanical nonreciprocity causes an asymmetric mechanical behavior, which has a possible application to asymmetric systems such as energy harvesting. In a nonreciprocal gel composed of a hydrogel and a nanosheet, this is attributed to the tension-compression asymmetry resulting from the buckling behavior of nanosheets[1]. Constitutive modeling of the mechanical nonreciprocity is technically challenging because the switching of the microscopic mechanical behavior occurs point by point in the microstructure.

This study presents surrogate modeling of the macroscopic constitutive model that links the microscopic tension-compression asymmetry to the macroscopic asymmetric mechanical behavior for a nonreciprocal material through a machine learning approach. The process includes numerical material testing to obtain macroscopic stress data sets and constructing the response function, which characterizes the macroscopic stress and strain relationship using a radial basis function[2]. The resulting model can be used directly in finite element analysis to solve a macroscopic boundary value problem.

Several numerical examples are solved to verify the performance of our proposed method in practical use. In this verification, we also investigate the effect of increasing the number of data sets and appropriate radial basis function on the performance of the macroscopic constitutive model. The results demonstrate the utility of our proposed method in terms of accuracy and efficiency.

Keywords: Surrogate model, Nonreciprocal, Tension-compression asymmetry, Multiscale

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Assessment of LES, IDDES, and URANS for turbulent flow around a sedan with rotating tires

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The turbulent flow past a sedan model at $Re_H = 1.02 \times 10^5$ is investigated through a combined of wind tunnel experiments and numerical simulations. This study aims to compare the predictive abilities of Large Eddy Simulation (LES), Improved Delayed Detached Eddy Simulation (IDDES), Unsteady Reynolds-Averaged Navier-Stokes (URANS), and Reynolds-Averaged Navier-Stokes (RANS) for the flow around a sedan with the consideration of rotating tires. The results indicate that LES captures most dynamic information, particularly in the near-wall region around the tires, among the numerical methods used. Compared to them, IDDES and URANS with coarser mesh can generate similar mean flows, but they are not applicable to the near wall coherent wake structures. Furthermore, IDDES is found to be unsuitable for the near-wall flow instability concerning wake dynamics, Reynolds stress, turbulent kinetic energy, and fluctuation of pressure. In summary, this study suggests that LES is suitable for the flow around the sedan with rotating tires. In addition, IDDES and URANS are applicable to the mean field of the studied flow.

Figure 1 shows the time-averaged streamwise velocity ($\bar{u}$) of the three models. Figures 1(a, b, c) illustrate the distribution of $\bar{u}$ on the mid-section plane of the sedan model, demonstrating remarkable similarity among the IDDES, URANS and LES approaches. For more quantitative comparison, Figures 1(d, e) display the averaged velocity profiles along two characteristic sampling lines. The profile comparisons reveal that while minor discrepancies exist in the absolute values predicted by the three methods, they exhibit excellent agreement in capturing the overall flow characteristics and velocity trends. This quantitative analysis confirms that all three simulation approaches are capable of predicting similar time-averaged velocity fields, despite their inherent methodological differences.

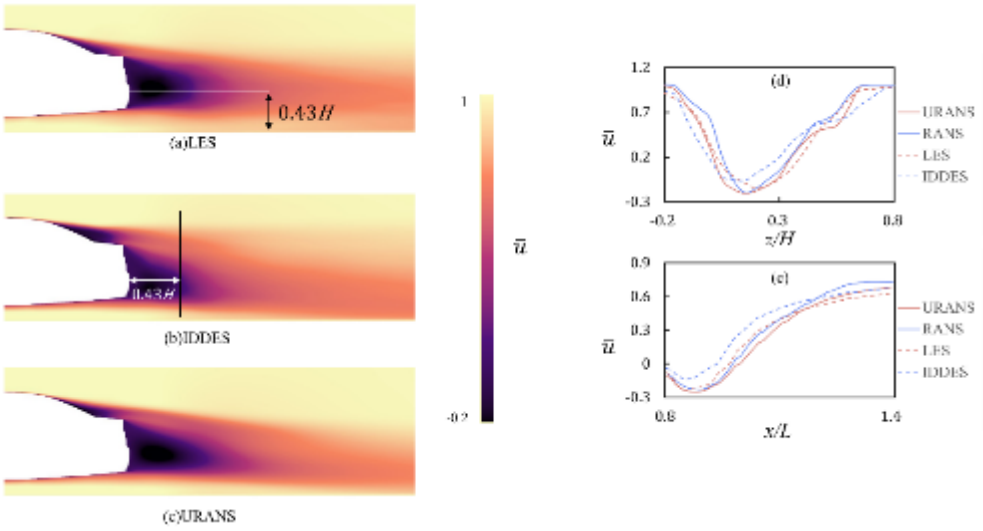

Figure 1. Time-averaged streamwise velocity distribution in the wake of the sedan model, predicted by: (a) LES, (b) IDDES, (c)URANS. Velocity profile comparisons: (d) vertical, (e) horizontal.

Keywords: Turbulence modellings, assessment, sedan, wakes, rotating tires

Elucidating the effect of off-angle on the contraction of basal plane dislocation in 4H-SiC

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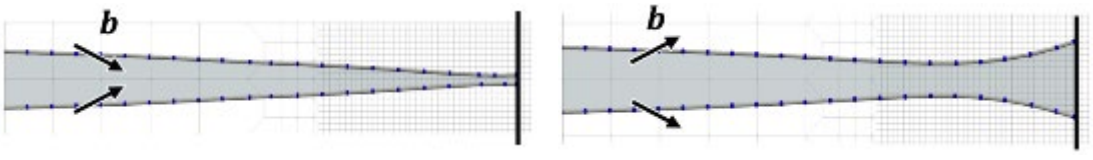
4H-SiC has recently been gaining attention as one of the next-generation materials for power semiconductors. One of the challenges for its practical application is the basal plane dislocations (BPD) in the epitaxial layer, which degrade device performance [1]. During step-controlled epitaxy at an off-angle of 4°–8°, more than 95% of BPDs are converted into threading edge dislocations (TEDs) [2], which do not affect device performance. However, some BPDs still remain in the epitaxial layer, leading to the degradation of device performance [1]. Although it is known that BPDs typically dissociate into 30°-30° or 30°-90° partial dislocation pairs, the conversion mechanism from BPD to TED remains unclear. Therefore, understanding the behavior of BPDs is crucial. Additionally, previous experiments suggested that there are some methods such as small off-angle to reduce BPDs [3]. However, the underlying mechanisms of these methods remains unclear. Since the surface has a significant influence during deposition, it is crucial to elucidate the influence of the surface on the behavior of BPDs.

In this study, dislocation dynamics analysis was conducted to clarify the behaviour of BPD pairs near the surface of 4H-SiC, which enables us to evaluate the mechanical interaction between the surface and dislocations. Based on the dislocation theory, the forces acting on the dislocation were calculated by the stress field around the dislocation near the surface obtained by the finite element method (FEM). The equilibrium position of the forces between the two partial dislocations was calculated by moving the dislocations, where the forces become zero. In the 3D analysis, FEM meshes with an off-angle were used to investigate the relationship between the off-angle and the shape of the 30°-30° partial dislocation pair. It was found that the width of partial dislocation pairs decreases as the off-angle decreases. Additionally, different trends were observed depending on the directions of the Burgers vectors. When the Burgers vector was closed toward the surface (Figure 1(a)), the 30°-30° dislocation pair was contracted near the surface. In contrast, when the Burgers vectors were open toward the surface (Figure 1(b)), the dislocation pair contracted further from the surface, and the width of the dislocation pair was larger than that of those with Burgers vectors closed toward the surface.



(a) (b)

Figure 1.

Keywords: 4H-SiC, Basal plane dislocation, Off-angle, Dislocation dynamics, Surface, Finite element method

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Elastic and In-elastic Behaviour of Silicon Carbide Crystals by Using Newly-developed Machine-learning Potential

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Silicon carbide (SiC) is one of promising ceramic materials which are used for electronics and high-temperature fields because of its high performance on crystalline stability. However, it becomes an issue that SiC crystals exhibit a polymorphism including 3C-SiC (cubic structural unit), 4H-, 2H- or 6H-SiC (hexagonal structural unit). Among them 3C-SiC is known to be very strong ceramics whose hardness is next to diamond (carbon), and so it is used as abrasives in surface finishing as well as single-crystalline semiconductor. In particular, 4H-SiC is fabricated by simple process and becomes more abundant material made of Si and C atoms. In performing mechanical process such as grinding and cutting, inadequate crystalline defects will be introduced into the material. It often leads to inferior electronic or mechanical property. However, the in-elastic behaviour of 4H- or 3C-SiC, in which dislocation motion and grain boundary sliding play an important role, is not yet well understood. Therefore, the atomic mechanism in SiC should be theoretically studied in detail. The first-principle (*ab initio*) calculation has been applied extensively to 3C- or 4H-SiC, whereas any interatomic potential function for classical molecular dynamics (MD) fully available for polymorphs of SiC has not yet developed.

In this study, based on hundreds of *ab initio* calculation data for SiC crystals, machine-learning potential is devised on the framework called “spectral neighbour analysis potential (SNAP)”. The paper assesses reproduction of elastic properties of 3C- and 4H-SiC as well as surface structure. Also, for confirming availability in in-elastic behaviour, a MD computation model with dislocation dipoles and periodic boundary is prepared and is tested for shearing. Pictures in Fig.1(A)(B) show stable core regions of edge dislocation which are obtained by using our newly-developed SNAP potential. The results shows that this machine-learning potential is sufficiently capable of being used in atomistic simulation of mechanical (elastic-plastic) deformation of 3C- and 4H-SiC materials.

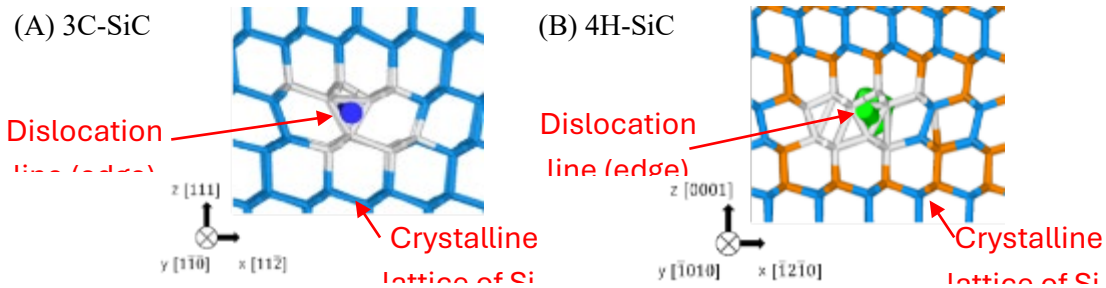

Figure 1. Core structure of edge dislocation obtained for SiC polymorphs by SNAP (machine-learning potential): dislocation line is depicted by cylinder near the centre.

Keywords: Machine-learning potential, Molecular dynamics, Silicon carbide (SiC), Dislocation

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Flow-Induced Vibrations in Compressible Flows using a Hybrid Immersed Boundary-Lattice Boltzmann Method

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Numerical methods are often employed for studying fluid-structure interactions (FSI) in high-speed flows due to their effectiveness in capturing complex flow phenomena. In this study, we employ an immersed boundary approach coupled with the lattice Boltzmann method and finite difference method (IB-LB-FDM) for compressible flows due to its robustness and efficiency. The governing equations are:

$$\frac{\partial(\rho u_j)}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0, \tag{1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j + P\delta_{ij})}{\partial x_j} = \frac{\partial(\tau_{ij})}{\partial x_j} + f_i, \tag{2}$$

$$\rho T\left(\frac{\partial s}{\partial t} + u_j \frac{\partial s}{\partial x_j}\right) = \tau_{ij}\frac{\partial u_i}{\partial x_j} - \frac{\partial}{\partial x_k}(q_k) + S, \tag{3}$$

where ρ is density, $\boldsymbol{u}$ is velocity, P is pressure, $\boldsymbol{\tau}$ is shear stress tensor, $\boldsymbol{f}$ is body force, s is entropy, T is temperature, $\mathbf{q}$ is Fourier heat-flux, and S is heat source, respectively. The mass and momentum equations (1 and 2) are solved using the LBM with appropriate corrections to account for the compressibility, while the entropy equation (3) is solved using the FDM [2]. An iterative IBM is utilized to enhance the accuracy near the fluid-structure interface. An elastically mounted cylinder with two degrees of freedom is investigated from subsonic to supersonic flow regimes *(Ma ≤ 1.5)* over a range of Reynolds number *(Re ≤ 300)*. For the first time, a heavy cylinder with a 2S (two single, oppositely rotating vortex) shedding mode is observed after an initial excitation at a *Ma* of 1.4 and a *Re* of 300 [1], as visualized in the Figure 1. At transonic flows, the intermittent lambda shock reduces the interactions between the cylinder and the wake. Compressibility effects tend to stabilize the system by reducing the force input across the range of *Ma* and *Re* considered.

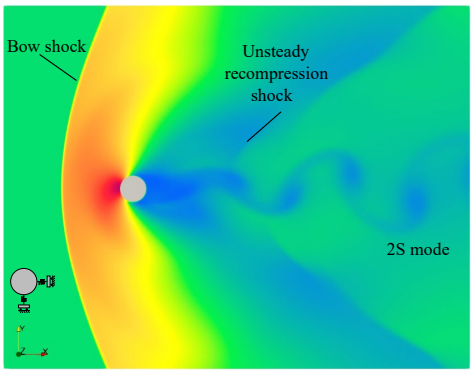

Figure 1 : Density contour of a cylinder during flow-induced vibration (FIV).

Keywords: Lattice Boltzmann method, fluid-structure interactions, flow-induced vibration, shock waves, supersonic flows, compressibility

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Dislocation dynamics analysis of size effects in alloys

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It is known that plastic deformation behavior in small volumes of materials with micro-meters is different from that in bulk, which is called size effect. Flow stress in small volumes increases with diameter decreasing because of dislocation behavior. Previous research performed compression test of micropillar including precipitates to elucidate the effect of precipitates on the size effect [2]. It found that specimens including small precipitates such as GP zone, θ' precipitates showed size effect whereas that including large precipitates such as θ'' precipitates did not. However, the relationship between precipitates size and flow stress is unclear.

Therefore, we elucidated the mechanism of size effect in alloy using computational method. We used dislocation dynamics, which can analyze the effect of dislocation behavior on the material properties by simulating dislocation behavior [3]. One previous research obtained simulated the relationship between specimen size and flow stress by using dislocation dynamics [4]. Another previous research simulated dislocation behavior in bulk material with one precipitate [5]. Therefore, we performed dislocation dynamics simulation in micropillar with a plenty of precipitates.

We simulated dislocation behavior in an alloy-micropillar. Figure 1 is snapshot at alloy-micropillar's yielding. In micropillar with no precipitates, micropillar yielded when a dislocation left pillar from the surface. On the other hand, micropillar with plenty of precipitates did not yield just when a dislocation left. Instead, it yielded when dislocations penetrate precipitates. Therefore, we observed the effect of precipitates on dislocation behavior in a micropillar.

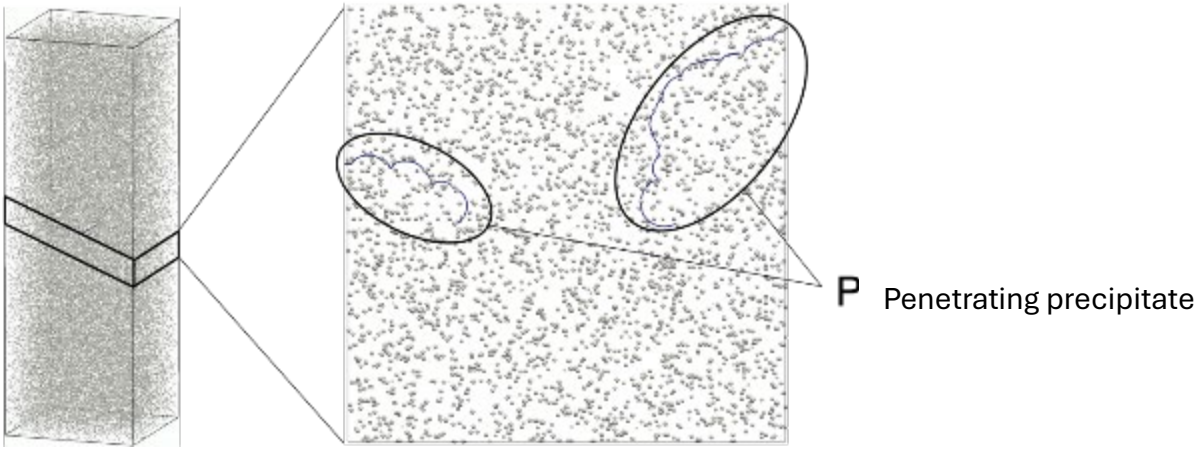

Figure 1.

Keywords: Dislocation dynamics, Micropillar, Precipitation hardening, Size effect

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Transient Analysis of Nearly Incompressible Hyperelasticity by Using Stabilized Finite Element Scheme and Mixed Time Integrator

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Explicit time integration schemes are widely employed for wave propagation simulations in finite element analyses of dynamic problems involving solid structures[1]. However, their conditional stability necessitates the selection of time step sizes based on the velocity of elastic wave propagation. In the case of nearly incompressible materials, such as rubber-like materials and biomaterials, explicit integrators encounter significant difficulties due to the requirement of exceedingly small time steps. This constraint arises from the high P-wave velocities associated with volumetric deformations. Consequently, for such materials, implicit time integration schemes, which offer unconditional stability, are often preferred to ensure computational efficiency and stability.

To overcome the aforementioned limitations, the author has proposed a novel time integration scheme that retains characteristics analogous to explicit integrators in terms of S-wave propagation for isochoric deformations[2]. The proposed method extends the Rattel scheme[3], originally developed for constrained Hamiltonian systems, to mitigate the constraints on time step size. The resulting formulation adopts a mixed time integration approach, wherein an implicit solver is utilized for volumetric deformation propagation, while an explicit solver is employed for isochoric deformation. This mixed approach effectively balances computational efficiency and stability in simulations of nearly incompressible materials.

In this study, the proposed time integration scheme is applied to the numerical analysis of large deformation problems of nearly incompressible hyperelasticity. For spatial discretization, a pressure-stabilized linear element formulation is adopted to enhance numerical stability and robustness in the large deformation range[4].

Keywords: Finite element method, dynamic problem, nearly incompressible, hyperelasticity, mixed time integrator

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Ab-initio and Molecular dynamics simulation study on BN-based Piezoelectric nanostructures

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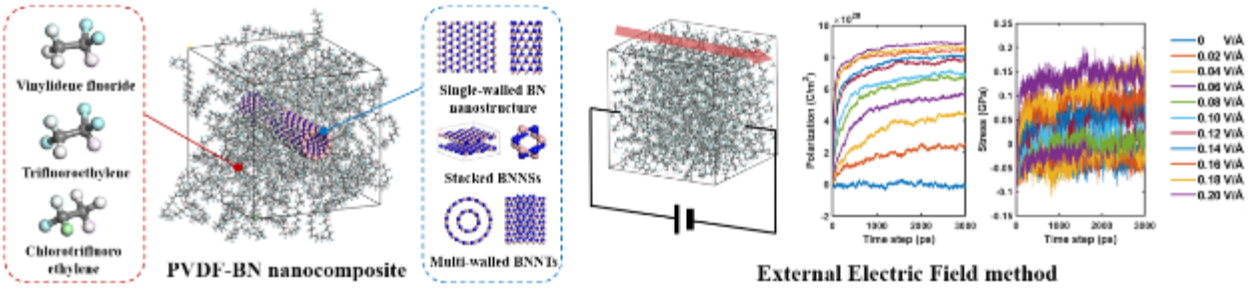
Nanoscale energy harvesting, initially driven by research on the piezoelectric effect, has recently expanded into hybrid nanocomposites for energy harvesting with the discovery and advancement of triboelectric, thermoelectric, and flexoelectric effects. Boron nitride nanotubes (BNNTs) and boron nitride nanosheets (BNNSs) have been actively studied as multifunctional nanofillers for these energy-harvesting materials due to their piezoelectricity, flexoelectricity, biocompatibility, radiation shielding properties, and high thermal conductivity. Despite these advantages, the theoretical limitations on piezoelectricity in bulk and multi-walled boron nitride, alongside the high output observed in triboelectric and flexoelectric effects, challenge the development of boron nitride-based piezoelectric nanogenerators (PENGs).

To overcome this limitation, we systematically reassess the theoretical piezoelectric properties of BNNSs and BNNTs in bulk and stacked configurations using density functional theory (DFT) calculations and molecular dynamics (MD) simulations. Based on the piezoelectric properties of the studied BN nanostructures, we performed MD simulations to investigate the electroelastic behavior of polyvinylidene fluoride (PVDF)/BNNT piezoelectric nanocomposites. In the simulation methodology, we employed an external electric field method and uniaxial tensile simulations based on the linear piezoelectric constitutive equation (1-2), incorporating the Born effective charge to evaluate the piezoelectric, dielectric, and mechanical properties of nanofillers and nanocomposites [1].

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} - e_{lij}E_l \tag{1}$$

$$D_i = e_{ikl}\varepsilon_{kl} - \kappa_{il}E_l \tag{2}$$



Keywords: Molecular dynamics simulation, Density functional theory, Piezoelectric nanogenerator (PENG), Boron nitride, PVDF, Piezoelectric nanocomposite

Acknowledgement: This research was supported by the Nano & Material Technology Development Program and Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by Ministry of Science and ICT (RS-2024-00408845) (RS-2024-00340747)

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An improved Immersed Boundary Method for studying fish-like locomotion

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Fish-like locomotion has always been a crucial part of biomimetic research, and computational fluid dynamics (CFD), as an important means of exploring fluid mechanisms, often requires a significant amount of computational resources to cope with complex fish-like locomotion. In this work, we propose a new calculation method based on the traditional direct force method. The traditional direct force method, as an important immersed boundary method, has good performance in dealing with simulation about complex shapes and movements due to its special immersion treatment different from the body-fitted mesh. However, traditional methods generally use point clouds as geometric inputs, which greatly limits the generality of this method in practical use. In this work, we introduce the kernel function and the signed distance field (SDF) to eliminate the strong correlation between geometry and grids, enabling easier and more efficient simulation of various complex fish shaped movements. And, certain improvements have been made to the calculation of the signed distance field, ensuring its effectiveness while minimizing the consumption of excessive computing resources.

In this work, we will focus on basic 2D cylinder cases and various different motion modes of fish-like locomotion, verifying its curves about aerodynamic force and analysing the flow structure to demonstrate the reliability of this method.

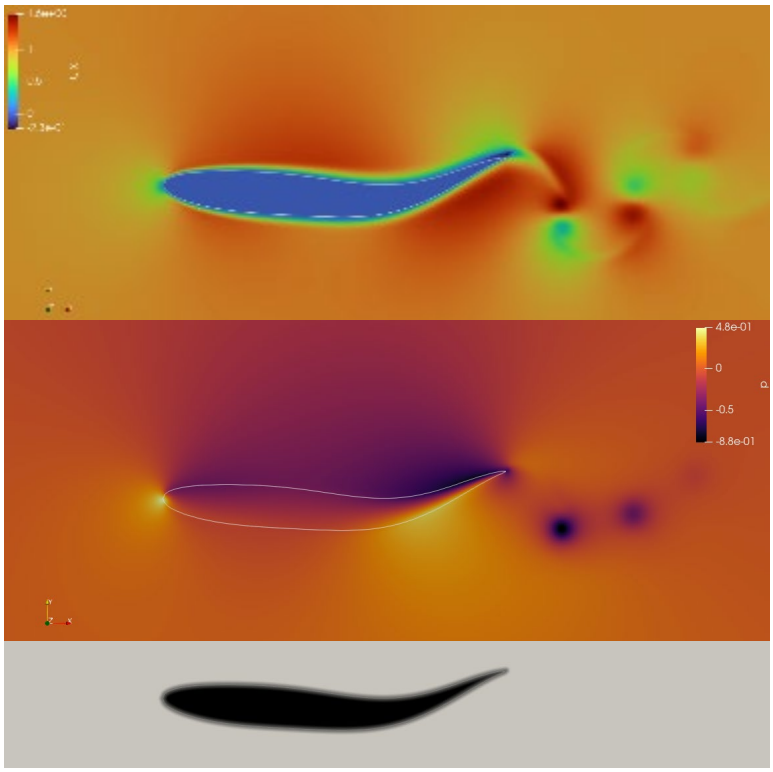

Figure 1.

Keywords: fish-like locomotion, Immersed Boundary Method, Computational Fluid Dynamics

Multiphysics Modelling of Reacting Flow in an Electric Steelmaking Furnace

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Reacting flows are prevalent in industries such as metallurgy, pharmaceuticals, and food processing, where they play a critical role in production. A notable example is the innovative use of electric furnaces for iron- and steel-making. In these reactors, direct reduced iron (DRI)—a partially reduced form of iron ore—is introduced, either alone or mixed with other feedstock. During operation, electrical energy is converted into heat, supplying the necessary energy for DRI melting and reactions, ultimately producing immiscible liquid melts. This process involves intricate multiscale and multiphysics interactions among particles, electric arcs, magnetic fields, compressible gases, and immiscible liquids with evolving free interfaces, along with phase transitions and chemical reactions. Understanding these interactions is crucial for designing and optimizing furnaces, improving electricity consumption efficiency, ensuring high-quality iron or steel production, extending furnace longevity, and minimizing electrode consumption. However, experimental research on these interactions is both costly and risky due to existing knowledge gaps. To address these challenges, developing and applying an effective computational model presents a promising alternative, despite its complexity. Building on our expertise in modelling multiphase reacting flows, we have developed a discrete element model (DEM)-based approach to simulate these processes. This model can accurately capture key phenomena, including multiphase flows, heat and mass transfer, chemical reactions, particle melting, free interface evolution, and electromagnetic-thermal conversion (Figure 1). The model has been validated against experimental data such as iron ore melting rates and reaction kinetics. This in-house computational tool serves as a robust and versatile platform for understanding, exploring, designing, and optimizing electric furnaces and similar systems, contributing to the global transition toward low-carbon economy.

Keywords: Multiphase Flow, Chemical Reactions, Electromagnetic field, Multiphysics Process

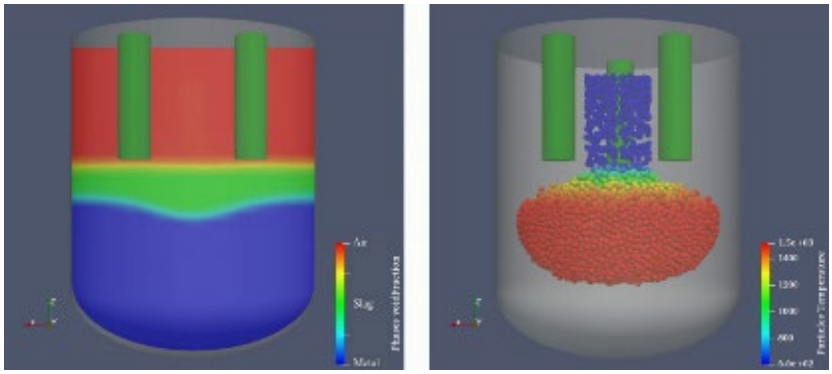

Figure 2. Predicted multiphysics phenomena in an electric furnace, including multiphase flows, heat and mass transfer, reactions, particle melting, and electromagnetic-thermal conversion.

Vortex-foil Interaction and Motion Optimization for Energy Harvesting

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Many studies have explored multiple flapping foils for energy harvesting, but achieving high efficiency for the trailing foil in the wake remains challenging. Most research focuses on sinusoidal motion and tandem configurations, with optimal performance when the trailing foil avoids the vortex generated by the leading foil[1]. Some studies suggest that increasing the heave amplitude not only reduces negative wake effects but also improves energy harvesting by using wake vortices to generate additional lift and power extraction[2]. However, the mechanism behind vortex-foil interaction is not fully understood, and there is a lack of detailed quantitative analysis. Sinusoidal motion may not be optimal for a trailing foil in a wake, as it limits beneficial vortex interactions. To address this, simulations explore the different positions of foils and vortices, angles of attack of the trailing foil, and their interaction effects on lift. The Force and Moment Partitioning Method[3] is applied to analyse force production and power extraction, helping to quantify the impact of local flow structures:

$$F = \int_B p \cdot n_i dS = -\rho \int_B \vec{n} \cdot \left(\frac{d\vec{u}}{dt}\varphi\right) dS + \rho \int_V [\nabla \cdot (\vec{u} \cdot \nabla\vec{u})]\varphi dV + \mu \int_B (\vec{\omega} \times \vec{n}) \cdot \nabla\varphi dS \quad (1)$$

The results show both destructive and constructive vortex-foil interactions. A wake vortex with the same sign as the leading-edge vortex generated by the trailing foil can affect lift differently depending on the angle of attack. For the large angle of attack, the wake vortex will disrupts the leading-edge vortex structure, leading to a drop in lift. When a vortex with the opposite sign appears in front of the foil, it strengthens the leading-edge vortex and increases lift. This study shows that a heaving motion with half the chord length amplitude can achieve the same energy extraction efficiency as a sinusoidal motion with a full chord length amplitude. These findings provide new insights into arranging multiple foils in a wake. They also help in designing better motion trajectory for foils in wake flows.

Figure 1. Force field of local flow structure

Keywords: Energy harvesting, Vortex-foil interaction, Force and Moment Partitioning Method, Lattice Boltzmann Method

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CFD-DEM study of particle triboelectrification in pneumatic conveying

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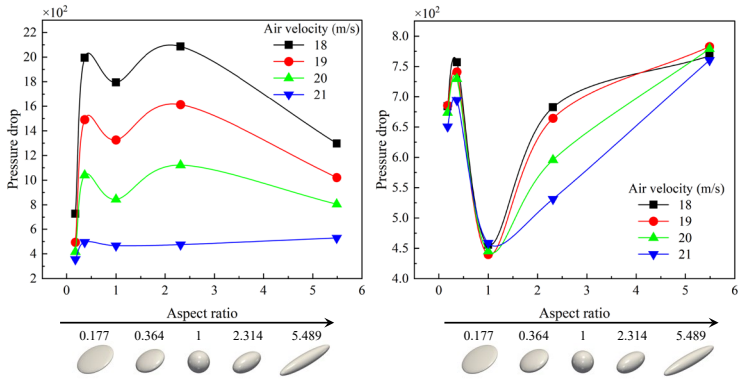
Triboelectrification in pneumatic conveying, driven by repeated particle interactions and contact with pipe walls, leads to issues such as clustering, adhesion, reduced conveying performance, and even fire or explosion risks. Strongly influenced by particle shape and pipe orientation, this phenomenon remains challenging to study due to equipment limitations and the absence of numerical models. To address this, we have developed an in-house computational code based on a combined computational fluid dynamics (CFD) and discrete element method (DEM) approach. The model incorporates a condenser model that accounts for frictional charging and enables coupling for non-spherical particles, allowing for a comprehensive evaluation of impact charge, frictional charge, and electrostatic interactions between the pipe wall and particles of varying shapes. After thorough validation, we have systematically analyzed the interactions between particle shape and triboelectrification under different conveying conditions, revealing significant dependencies. For example, the pressure drop across pipe bends is notably affected by particle shape, and more importantly, this effect differs significantly between charged and uncharged conditions (see Figure 1). Specifically, the pressure drop curves for non-charged particles exhibit an "M"-shaped trend, which flattens at higher air velocities. Particles with extreme aspect ratios (ARs) (AR = 0.177 and 5.489) tend to cause lower pressure drops as they are more easily suspended, whereas particles with moderate non-spherical shapes (AR = 0.364 and 2.314) result in higher pressure drops due to reduced flowability. When particles are fully charged (Figure 1b), both ends of the "M" shape are elevated, and pressure drops for all non-spherical particles surpass those of spherical ones due to intensified Coulomb forces. This strong interplay between particle shape and triboelectrification significantly impacts conveying performance, complicating system design and control strategies aimed at mitigating potential risks. The developed model offers a powerful tool for addressing these challenges.

Keywords: Charge transfer, triboelectrification, non-spherical particles, pneumatic conveying, CFD-DEM



(a) (b)

Figure 1. Pressure drop variations with different particle shapes of (a) no electric charge and (b) equilibrium electric charge.

Flow Characteristics of Cohesive Particles in Silos: FEM and Machine Learning

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Silos are widely utilized across diverse industries, such as additive manufacturing, agriculture, chemicals, pharmaceuticals, and food production, among others. They are primarily employed for the storage and transportation of particulate materials and are specifically engineered to facilitate stable discharge when necessary. However, gravity-driven discharge of cohesive particles frequently encounters challenges, such as consolidation phenomena caused by arching and rat-holing. This study introduces a machine learning model designed for rapid prediction and control of stress profiles and critical cohesion in silos. The model is constructed based on a modified graph neural network (GNN) and is trained using data generated from a well-established and validated Finite Element Method (FEM). This GNN-based surrogate model incorporates two modifications to improve its prediction accuracy. The first modification involves data smoothing, which mitigates the adverse effects of abrupt changes in spatial distributions. The second modification involves adjusting the loss function to incorporate stress field information derived from the FEM model. The predicted stress fields are compared against those of the original GNN and random forest (RF) models, using FEM results as the benchmark. The results demonstrate that the proposed surrogate model can accurately reproduce stress profiles in arching silos and exhibits higher accuracy than other models in predicting spatial distributions across various error metrics. These findings offer valuable insights into the role of silo design in optimizing granular flow and enhancing discharge efficiency in industrial applications.

Keywords: Flow Characteristics, cohesive particles, silos, FEM, machine learning

A CFD-DEM Based Wear Prediction Analysis for Coating Damage Considering Fluid-Particle Interactions

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Evaluating the resistance of coatings to high-speed impact wear remains a significant challenge, particularly when involving complex multi-particle dynamic interactions. The main focus of this work is to develop a computational approach that combines a numerical model with a predictive method to address this challenge. The numerical model couples Computational Fluid Dynamics and the Discrete Element Method to simulate the motion of large, irregularly shaped particles driven by high-pressure airflow in a multifunctional anti-impact tester. In this coupling method, the normal moment equation of Navier-Stokes equations is modified to consider fluid-particle interaction as follows,

$$\frac{\partial \varepsilon_f \rho_f u_f}{\partial t} + \nabla \cdot (\varepsilon_f \rho_f u_f u_f) = -\varepsilon_f \nabla p - F_p + \nabla \cdot (\varepsilon_f \tau_f) + \varepsilon_f \rho_f g, \quad (1)$$

where $\varepsilon_f, \rho_f, u_f$ are the volume fraction, density and velocity of fluid; p, g are the pressure value of fluid and the gravity acceleration; F_p is the fluid-particle interaction force, which is calculated by a drag force model. The particles are represented using discrete element method with a multi-sphere approach. The coupling strategy of fluid and particles is implemented via an open-source software project, CFDEM®project. To resolve boundary condition inconsistencies with experimental setups, a limitation stemming from the oversimplified model in prior research [1], this study develops a novel and comprehensive tee-pipe model. Furthermore, the compressibility effects of high-pressure airflow on particle dynamics are incorporated, significantly enhancing simulation accuracy.

To assess particle-induced damage, a wear assessment method is developed by integrating a particle erosion model into this coupled simulation framework. For long-term damage estimation under standard test conditions, a predictive approach based on mean-range random functions is embedded into this approach. Validation through single- and multi-particle impact simulations demonstrates good agreement with experimental data, as the presented in Table 1.

Parameter	**Method**	Average	STD.	Maximum	Minimum
Particle impact Velocity/(m/s)	Experiment	6.18	1.27	8.97	4.05
	Simulation	6.21	1.16	9.17	4.12
Particle impact angle/(°)	Experiment	130.17	6.79	144.12	116.86
	Simulation	130.33	6.45	142.27	118.69

Table 1.

Keywords: CFD-DEM, multi-sphere method, non-spherical particle

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Mechanical behaviour of 3D printed continuous fibre-reinforced composite gyroid structure under quasi-static and dynamic compression

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Triply periodic minimal surface (TPMS) sheet-based cellular structures are sheet-based metamaterials that can improve the mechanical and other engineering properties of cellular structures that use struts as their primary structural component. The range of applications of these structures is vast in the biomedical, aerospace, and automotive industries due to their ability to tailor according to specific requirements, strength-to-weight ratio, and high energy absorption. This study investigates the mechanical properties and performance enhancement strategies of 3D-printed gyroid structures fabricated using continuous fibre-reinforced composites (CFRCs). The research was conducted in two phases: first, a comparative analysis between pure Onyx gyroid structures and Onyx gyroids reinforced with glass fibres was carried out under quasi-static loading conditions in three principal directions. Results indicated significant directional dependency in the mechanical performance, with increased plateau stress and specific energy absorption (SEA) in the out-of-plane direction, while stiffness in both in-plane directions was superior to that in the out-of-plane direction. Due to the arrangements of the voids in the structures seen through the Micro CT-scan. In the second phase, strain sensitivity analyses were performed on CFRC gyroid structures made from pure Onyx, glass fibre filament (GFF), Kevlar fibre filament (KFF), and carbon fibre filament (CFF) under quasi-static and dynamic compression. It was found that higher loading speeds improved mechanical performance across all structures. The study highlighted directional loading and strain sensitivity's significant role in mechanical properties such as Young's modulus, plateau stress, and specific energy absorption (SEA). Notably, the KFF/Onyx gyroid structure demonstrated a 30% increase in dynamic plateau stress compared to its quasi-static strength. These insights are vital for optimizing the mechanical performance of CFRC gyroid structures in advanced manufacturing.

Keywords: Additive manufacturing, continuous fibre-reinforced composite, sheet-based gyroid, strain sensitivity, anisotropic properties.

AM-structural coupled analysis for accurate prediction of mechanical behavior of FDM-printed composite structures

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Recently, FDM(Fused Deposition Modeling) 3D printing technology has continuously paid attention in various engineering fields due to its geometric flexibility and material versatility. However, the parts manufactured by FDM printing inherently exhibit anisotropic properties because the filament orientation can be determined by the nozzle path. This issue becomes more pronounced when the short-fiber reinforced composite filaments are considered. Therefore, a refined analysis scheme is highly required to accurately predict the mechanical behavior of FDM-printed composite structures.

In this study, FDM-structural coupled analysis is proposed to precisely consider the anisotropic characteristics of FDM-manufactured composite structures. To this end, the effect of the nozzle path on the mechanical behavior of FDM-printed parts is analyzed based on the experimental data. Then, analytical material properties are defined by using the mean-field homogenization method. Finally, an FDM-structural coupled analysis can be reasonably performed by considering local material properties that depend on the nozzle paths in the finite element model. The numerical performance of the proposed FDM-structural coupled analysis model is demonstrated by comparing the mechanical behavior of the ASTM D638 tensile coupons.

Keywords: FDM 3D printing, Anisotropic properties, Nozzle path, AM-structural coupled analysis

Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (RS-2022-NR072163 and RS-2024-00356107)

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Octree Pattern-Based Scaled Boundary Finite Element Modelling for Static Analysis of Porous Structures

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Porous structures have attracted wide attention in recent years due to their substantial advantages, such as lightweight, vibration and noise isolation, thermal management, as well as energy absorption. However, their complex geometric features often bring significant burdens to mesh generation and computational efficiency in conventional numerical simulations [1]. The scaled boundary finite element method (SBFEM), characterised by its high flexibility in mesh generation and compatibility with the octree algorithm, offers a promising solution to these challenges. This paper presents a comparative study on different octree pattern-based SBFEM implementation strategies within commercial software for the static analysis of porous structures. First, ANSYS Fluent is adopted for pre-processing and the generation of polyhedral-balanced octree mesh. It is followed by the implementation of SBFEM framework in ABAQUS using the User Element Subroutine (UEL). In addition to the available open-source ABAQUS UEL for SBFEM [2], the scaling technique for geometrically similar octree cells [3] is further incorporated to reduce the computational effort. After verification, various implementation strategies are evaluated for their applicability and efficiency through typical porous structure examples, including both homogeneous and graded lattice structures based on triply periodic minimal surfaces. Finally, a practical guideline for the static analysis of porous structures is proposed, which enables researchers and engineers to utilise the advantages of SBFEM, thereby facilitating its application in the simulation of complex porous structures.

Keywords: porous structures, triply periodic minimal surfaces, scaled boundary finite element method, octree mesh, ABAQUS UEL

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A Modelling Study of Right Ventricular Dynamics with Valvular Regurgitation

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Introduction

Both pulmonary regurgitation (PR) and tricuspid regurgitation (TR) would lead to adverse growth and remodelling (G&R) in right ventricle (RV), causing RV dilation and ultimately RV pump function failure if untreated. Although PR is well tolerated by RV, while treatment of tricuspid valve (TV) remains unclear because of the higher risk of mortality than surgically repairing other cardiac valves. There is an urgent need to identify those patients with RV regurgitation who would benefit from correcting pulmonary valve and TV regurgitation.

Method

An RV regurgitation model based on patient-specific bi-ventricular geometry has been developed in this study, we further integrate a kinematic G&R framework with updated references to model myocardial response to the regurgitation in RV. Both PR and TR are realized by allowing the blood to leak into the pulmonary artery or the right atrium.

Result

The results show that this bi-ventricular model can capture the main characteristics of cardiac functions under PR and TR, as shown in Figure 1(a), such as increased RV filling volume, increased RV pressure, increased RV stroke work, and the bulged septum towards LV. By modelling myocardial G&R triggered by fibre stretch at end-diastole and fibre stress at peak systole, our results have further shown that the heart, especially the RV, experiences significant wall dilation and thickening (Figure 1(b,c)).

Discussion

Comprehensive experimental studies will be needed to validate this G&R model and to determine appropriate growth laws before its clinical translation. It is expected that this cardiac model, once validated, will provide important insights into RV biomechanics and dysfunction under various pathological conditions, for example, the optimal timing of tricuspid valve replacement.

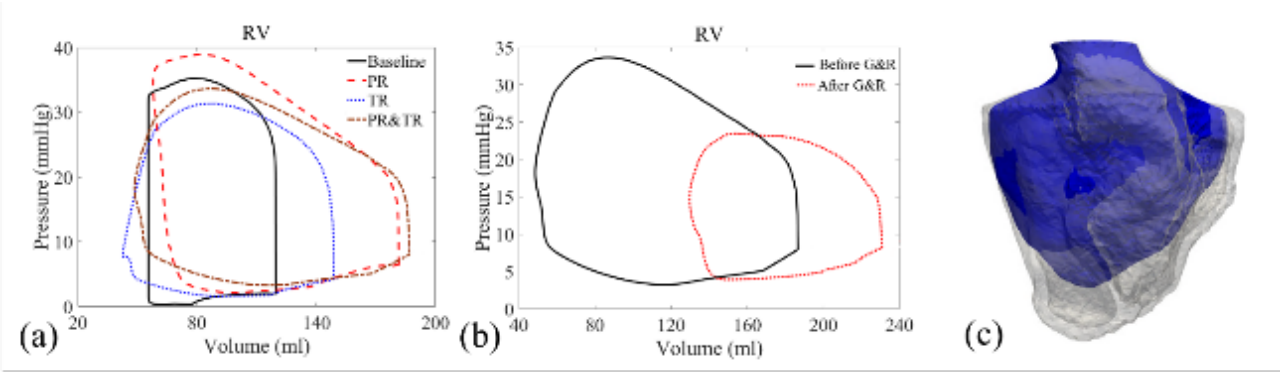

Figure 1. (a) Pressure-volume loops of the RV at baseline, with PR, with TR, and with both PR and TR, before G&R. (b) Pressure-volume loops for RV after G&R with both PR and TR, alongside the geometries before (blue) and after (grey) G&R (c).

Keywords: Computational modelling, right ventricle, valvular regurgitation, growth and remodelling.

Effect of Cross-Sectional Shape of 3-Dimensional Riblets upon Drag Reduction and Surface Stress in Turbulent Channel Flow

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Riblets are one of the wall frictional drag reduction methods that are expected to have practical applications. For example, Sasamori *et al*. [1] observed a 12% drag reduction in turbulent channel flow with sinusoidal riblets. However, Optimizing the riblet shape is difficult due to the large number of shape parameters involved. Furthermore, riblets are wall structures with longitudinal micro-grooves, so durability is an issue. Tanisho *et al*. [2] varied the riblet height and span position using a random Fourier series in the streamwise direction. Then, in addition to drag reduction, durability was evaluated using the force generated on the riblet surface. However, the cross-sectional shape remains rectangular, which is not practical from the viewpoint of durability.

In this study, we proposed a riblet with slopes on both sides and investigated the effects of drag reduction and surface stress on the riblet. Direct numerical simulations were performed on a turbulent channel flow with riblets. The riblets were represented using the immersed boundary method. The drag reduction rate R_D [%] is defined as follows:

$$R_D = \frac{C_{T,f} - C_{T,r}}{C_{T,f}} \times 100, \tag{1}$$

where the total drag coefficient for the smooth wall is represented by $C_{T,f}$, and that for the riblet wall is represented by $C_{T,r}$, respectively. Figure 1 shows the visualization results of the vortices and surface stress on the channel walls with riblets. The riblets had 30° slopes on both sides. The drag reduction R_D was 4.5%, which was lower than 10% that of a rectangular cross-section, and the stress at the top of the riblets was higher. Investigating the relationship between the slope angle and increased drag for various cross-sectional shapes would lead to the optimal cross-sectional shape.

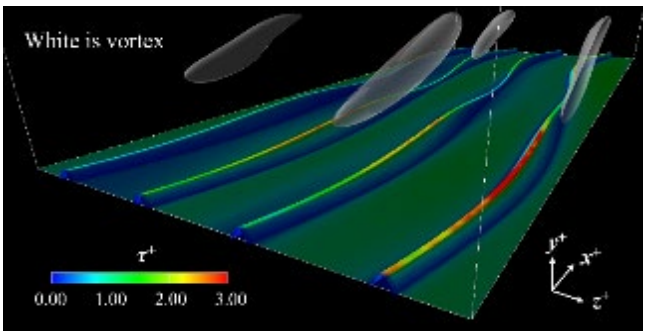

Figure 1.

Keywords: Turbulence control, Drag reduction, Direct numerical simulation, Riblets

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Flexoelectric influence on crack propagation in ferroelectric single crystal: a phase-field approach

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Ferroelectric materials, known for their inherent brittleness, are prone to brittle fracture. The pronounced strain gradient present at the crack tip necessitates consideration of the flexoelectric effect. This study introduces a sophisticated phase-field model incorporating the flexoelectric effect to elucidate its role on crack growth and domain evolution in ferroelectric single crystals. Our findings demonstrate that both crack trajectory and domain switching phenomena at the crack's forefront are substantially influenced by the magnitude and sign of the flexoelectric coefficient, as well as the initial polarization direction. Depending on the computational scenarios, the flexoelectric effect can either exacerbate or impede crack propagation. Considering cracks initiation and propagation, the total energy of ferroelectric materials can be expressed as follows:

$$F_{total}=\int_{\Omega}[(v^2+\eta_k)(f_{elas}+f_{grad}+f_{flexo})+f_{Land}+f_{elec}]dV+G_c\int_{\Omega}[\frac{(1-v)^2}{4l}+l|\nabla v|^2]dV-\int_{\partial\Omega}\boldsymbol{\tau}\cdot\mathbf{u}dS \quad (1)$$

where f_{Land}, f_{grad}, f_{elas}, f_{elec} and f_{flexo} are densities of the Landau energy, gradient energy, elastic energy, electrostatic energy, and flexoelectric energy, respectively. V denotes the volume. G_c is the critical energy release rate; $\mathbf{u}$ and $\boldsymbol{\tau}$ represent the displacement and traction force, respectively. v and ∇v represent the crack field variable and its gradient, respectively. l is a regularization parameter characterizing the width of the fracture transition region. Fig.1 shows the crack patterns as flexoelectric coefficients increase in computation condition [1].

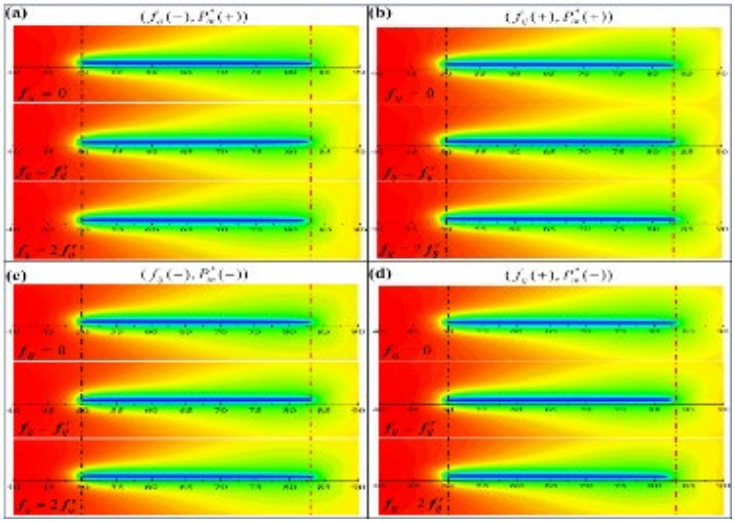

Figure 1.

Keywords:ferroelectrics, fracture and crack propagation, flexoelectric effect, phase-field modelling

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Deep Learning-Based Surrogate Model of Constitutive Equation in Viscoelastic Turbulence for Avoiding Numerical Instabilities

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Viscoelastic fluids are a type of non-Newtonian fluid. They reduce frictional drag near the wall, which is known as the Toms effect. This effect contributes to energy savings in fluid transportation applications, such as in oil pipelines. The drag reduction rate can reach a maximum of approximately 80% by increasing Weissenberg number Wi. Although numerical simulations of viscoelastic turbulence at high Reynolds numbers are industrially in demand, they are much more challenging than those of Newtonian fluids. This difficulty arises from numerical instabilities inherent in the constitutive equations of the polymer stress, known as the high Weissenberg number problem [1]. In this study, we propose a deep learning-based approach to construct a surrogate model for the constitutive equation.

To collect training datasets, we conducted direct numerical simulation (DNS) of fully developed viscoelastic turbulent channel flow. The governing equations are the incompressible Navier–Stokes equations and the Giesekus model-based constitutive equation:

$$\frac{\partial c_{ij}}{\partial t^*} + \frac{\partial u_k^+ c_{ij}}{\partial x_k^*} - \frac{\partial u_i^+}{\partial x_k^*} c_{kj} - \frac{\partial u_j^+}{\partial x_k^*} c_{ki} + \frac{Re_\tau}{Wi_\tau}\left\{c_{ij} - \delta_{ij} + \alpha(c_{ik} - \delta_{ik})\left(c_{kj} - \delta_{kj}\right)\right\} = 0, \qquad (2)$$

where c_{ij} denotes the constitutive stresses. The notations $()^+$ and $()^*$ represents normalization with friction velocity u_τ and kinematic viscosity ν, and with u_τ and the channel half-width δ. The parameters were the friction Reynolds number of $Re_\tau = u_\tau\delta/\nu = 395$, the friction Weissenberg number of $Wi_\tau = u_\tau^2\lambda/\nu = 20$, where λ indicates the polymer relaxation time. We impose non-slip and periodic boundary conditions on the wall and the stream- and span-wise directions, respectively.

We employ a 3D U-Net [2], a variant of convolutional neural network (CNN) models, as our deep learning model. The U-Net predicts the constitutive stresses c_{ij} from the velocity gradient tensor $\partial_j u_i$. The three-dimensional flow fields used for training the U-Net were decomposed into several subdomains to enhance the generalization ability of the model. The predicted subdomains were then merged using weighted linear interpolation to reconstruct the full stress field with the whole computational domain. In an a-priori test, the mean values of tr(c_{ij}) and the most significant shear component c_{xy} indicate good agreement between the surrogate model and the true DNS results. Furthermore, we conducted an a-posteriori test by integrating the deep learning model into the DNS solver (DNS-CNN simulation). We carried out the DNS-CNN simulation for 10 wash-out times from a DNS snapshot. While the mean velocity distribution agreed with the reference DNS, the prediction of the constitutive stresses were not successful. This is due to the discontinuities at the edge of neighbouring subdomains between subdomains in the constitutive stress fields.

Keywords: Viscoelastic fluid, machine learning, deep learning, convolutional neural network

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Regulating separate energy-dissipative mechanisms in constitutive modelling for quasi-brittle materials

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This research proposed an approach to constitutive modelling of quasi-brittle materials by utilising a thermodynamics-based framework to drive the dissipated energy via two distinct mechanisms that are fracture opening and frictional sliding. Traditional coupled damage-plasticity constitutive approach often treats energy dissipation as a single budget, thus, the work produced from these models, while implicitly accounting for both damage and plastic strain, lacks the ability to directly adjust each dissipative mechanism. Although this is not inherently incorrect, it overlooks the full potential of the energy aspect, often leading to reliance on additional ad-hoc parameters to achieve the desired constitutive response. To overcome this limitation, the proposed framework explicitly partitions the total energy dissipation into three key components - damage, volumetric, and shear - each directly embedded in the plasticity flow rules, allowing precise control of the model response while ensuring compliance with thermodynamic principles. Results show that increasing the contribution of fracture opening in the dissipation process enhances the brittle behaviour, leading to steeper post-peak stress drops in triaxial tests, while a higher volumetric dissipation promotes compaction and ductile responses. The ability to regulate these mechanisms proves significant in capturing key rock deformation features, such as strain softening, dilation, and residual strength evolution, across a range of stress states. By providing better control over dissipative mechanisms, this framework can be useful for developing constitutive models that accommodate complex loading cases, improving predictive accuracy in geotechnical engineering applications.

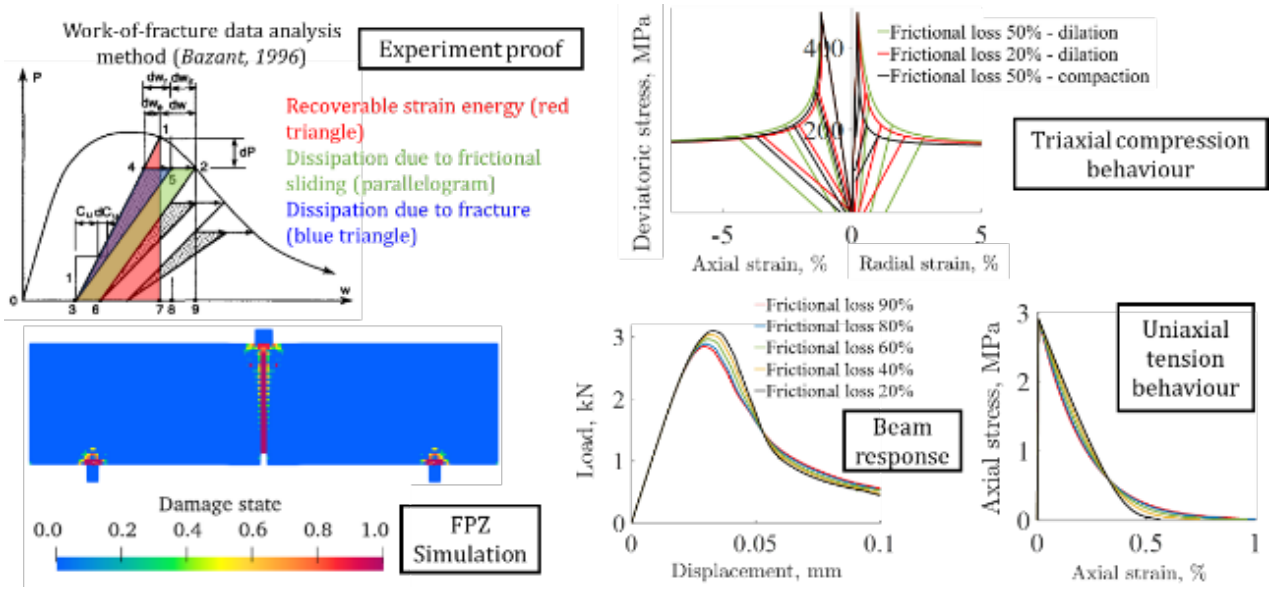

Figure 1. Controlling failure behaviour of constitutive models under different loading conditions by adjusting individual energy dissipative mechanisms.

Keywords: quasi-brittle material, thermodynamics, dissipation, enrichment, constitutive modelling, continuum, damage-plasticity, fracture process zone

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Investigation on the Pull-out Performance of Suction Anchors Considering Torsional and Trenching Effects: From Finite Element Analysis to Macroelement Model

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Torsional pull-out of suction anchors can occur during installation due to improper positioning or current-induced deviations. However, the impact of torsion on pull-out capacity has received limited attention in existing studies. Additionally, seabed trenching—a common geotechnical hazard in offshore engineering—can weaken suction anchor capacity over time, posing risks to mooring systems, while many studies simplify trench configurations for modelling convenience, which may lead to inaccurate assessments of their effects. Therefore this study numerically investigates suction anchor's pull-out capacity and failure mechanisms, considering both torsional and trenching effects. The influences of padeye depth, torsion angle, anchor aspect ratio, as well as various trench transversal and longitudinal geometric configurations including local scour phenomena are comprehensively studied. Based on the analyses results, a systematic framework is proposed to estimate pull-out capacity as trenching progresses. Furthermore, a plastic-hardening, non-associated macroelement model is developed to predict load-displacement responses (**u** is the displacement vector, **Q** is the pull-out load vector, A is the plastic resistance, F is the failure surface and g is the plastic potential) during monotonic pull-out under horizontal-vertical-torsional loading in clay. These models provide a practical tool for researchers and engineers to address torsional and trenching challenges in offshore engineering.

$$\{d\mathbf{u}\} = \frac{1}{A}\left\{\frac{\partial g}{\partial \mathbf{Q}}\right\}^{T} \{d\mathbf{Q}\}\left\{\frac{\partial F}{\partial \mathbf{Q}}\right\} \tag{1}$$

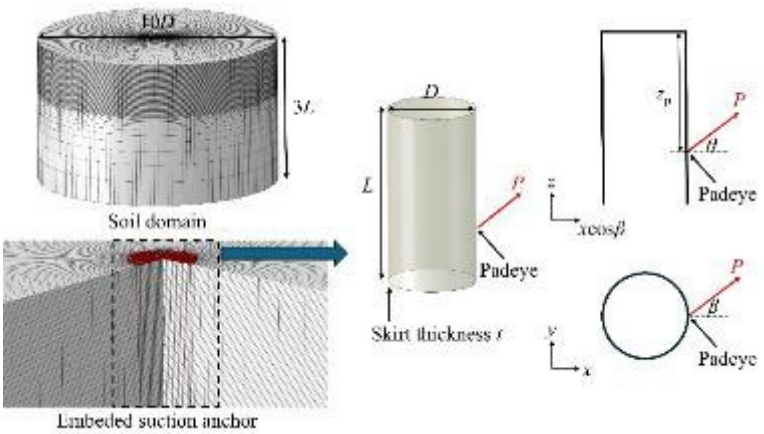

Figure 1.

Keywords: suction anchor, torsion, seabed trenches, finite element analysis, macroelement model

A Fictitious Physical Model for Multi-Observation-Point Visibility Evaluation in Structural Design

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Topology optimization is a powerful method for determining optimal structural designs within a fixed design domain under given constraints. Compared to traditional size and shape optimization, topology optimization offers the highest flexibility. It allows for simultaneous alterations to both external boundaries and interior features, including the creation, removal, merging, and sizing of holes within the structure. These comprehensive modifications can lead to significant enhancements in structural performance. Due to these advantages, topology optimization has been widely applied in a variety of contexts, such as solid, heat, fluid, and acoustics.

In real-world mechanical design scenarios, in addition to physical performance, geometric features are often required to ensure structures' manufacturability and usability. One such feature is visibility, which is crucial where operators must maintain clear sightlines for safety and operational efficiency. In practice, visibility assessment typically involves multiple observation points. Even the most basic human visual system comprises two eyes, creating binocular vision that must be accounted for in accurate visibility modelling. This natural multiplicity of observation points significantly increases the complexity of visibility evaluation. Due to this complexity, there is currently no effective model for rigorously evaluating visibility within structural design frameworks.

In this study, we propose a novel fictitious physical model that couples multiple sets of partial differential equations based on the level-set method. We establish a virtual physical field whose state variables intrinsically characterize the visibility conditions for any individual observation point as well as arbitrary combinations of multiple observation points. As a result, the visibility information is integrated within the partial differential equations. Moreover, this approach is particularly compatible with level-set method[1], enabling seamless integration with existing topology optimization frameworks.

Finally, we validate the proposed model through several numerical examples including a practical case. We will present the detail of these numerical examples and provide a comprehensive discussion of the proposed model at the conference.

Keywords: structural design, topology optimization, geometric features, visibility evaluation, finite element method, fictitious physical equations

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Algebraic Derivation of Consistent Tangent for Elastoplastic Problems in Finite Element Analysis

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The problem of structures considering material nonlinearity can be described by two different mechanical behaviors of the deformation in the structure and the nonlinear response of the materials. The structural deformation is governed by the equilibrium equation expressed in terms of the displacement field. In elastoplasticity, the evolution of the plastic strain is based on the yield condition, which depends on the stress state and a set of internal variables. Hence, the elastoplastic problems can be formulated as a coupled problem to determine the displacement field in the structures and the internal variables of the materials.

In elastoplastic problems, the staggered scheme, which includes the return mapping algorithm [1], has been widely adopted. Simo and Taylor [2] proposed a systematic procedure whereby for rate-independent plasticity. They developed an explicit form for the tangent moduli consistent with the stress integration algorithm to obtain the desired property of the iterative solution scheme. In the consistent approach [2], an effective and robust scheme for the stress integration algorithm is applied to the rate-independent constitutive equation by the return mapping algorithm, and the consistency condition is imposed by local iterative calculations. On the other hand, Ellsiepen and Hartmann [3] presented the solution scheme, which defines a system of differential–algebraic equations with the diagonally implicit Runge–Kutta methods for simultaneous updating of the displacement field and the internal variables. However, this approach requires local iterative calculations to update the internal variables.

In this work, for elastoplastic problems, we define a coupled problem of the equilibrium equation and the yield condition, and develop a numerical scheme based on the block Newton method to solve the overall structure using the finite element discretization. Based on this idea, the consistency parameter, which is the internal variable for describing the evolution of plasticity, can be condensed out from the incremental form of the equilibrium equation. In the proposed approach, the tangent moduli can be constructed algebraically by eliminating the internal variables from the coupled problem, and the internal variables are also updated algebraically without local iterative calculations. In addition, the residual of the yield condition is incorporated into the linearized equilibrium equation as the pseudo-stress, whose order is the same as the stress tensor. Some numerical examples demonstrate the effectiveness of the proposed approach by comparing the numerical results of the proposed approach with those of the return mapping algorithm.

Keywords: Block Newton method, Elastoplasticity, Finite element analysis, Backward difference scheme

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FE-PINN: A Hybrid Optimization Framework Integrating Finite Elements and Physics-Informed Neural Networks

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The Finite Element Physics-Informed Neural Network algorithm is developed to tackle the limitations of traditional Physics-Informed Neural Network in solving partial differential equations, particularly their struggles with high local errors and slow global convergence. By combining the Finite Element Method with Physics-Informed Neural Network, this approach creates a hybrid framework that improves accuracy and efficiency, especially in regions with complex behaviour. Studies on Physics-Informed Neural Network have shown their effectiveness in solving partial differential equations by integrating physical laws into neural network training. However, challenges such as significant local inaccuracies and delayed convergence in certain scenarios are well-documented. Conversely, the Finite Element Method is renowned for delivering precise local solutions through structured spatial discretization. The proposed algorithm merges these strengths to address the deficiencies of each individual method. The key innovations include

• **Hybrid Solution Space and Coupled Variational Formulation**: Construct a unified solution space $V_h \times V_\theta$ combining finite element solutions $u_h \in V_h$ and neural network solutions $u_\theta \in V_\theta$. The bilinear form is defined as:

$$a\big((u_h, u_\theta), (v_h, v_\theta)\big) = \sum_{i \in \{\text{fem,pinn,couple}\}} \lambda_i a_i(u, v) \tag{1}$$

where the coupling term $a_{\text{couple}}(u, v) = (u_h - \Pi_h u_\theta, v_h - \Pi_h v_\theta)_{L^2(\Omega)}$ with$\Pi_h: V_\theta \to V_h$ being the L^2 projection operator, and λ_i representing adaptive weighting coefficients.

• **Alternating Optimization Strategy**: Implement dynamic resource allocation through local error indicators:

$$\eta_e \propto |\mathcal{F}(u_{\text{hybrid}})|_{L^2(e)} + h_e^{1/2} |j(\nabla u_{\text{hybrid}})|_{L^2(\partial e)} \tag{2}$$

Prioritize FEM in high-error subdomains $\Omega_{\text{fem}} = \{e \in T_h \mid \eta_e > \tau\}$ while optimizing neural network parameters in low-error regions $\Omega_{\text{pinn}} = \Omega \setminus \Omega_{\text{fem}}$.

• **A Priori Error Estimation**: Establish convergence guarantees:

$$\left|u - u_{\text{hybrid}}\right|_{H^1(\Omega)} \leq C \left(h^k + \epsilon_{\text{NN}} + \lambda_{\text{couple}}^{-1/2} \delta_{\text{couple}}\right) \tag{3}$$

where h denotes the FEM mesh size, ϵ_{NN} the neural network approximation error, $\delta_{couple}$the coupling residual, and C a stability constant related to Lam´e parameters.

Keywords: Finite Element Method,Physics-Informed Neural Network, Hybrid VariationalFormulation, Residual Coupling, Adaptive Sampling, Partial Differential Equations

An integrated surface and seepage flow simulator based on ALE-SPH

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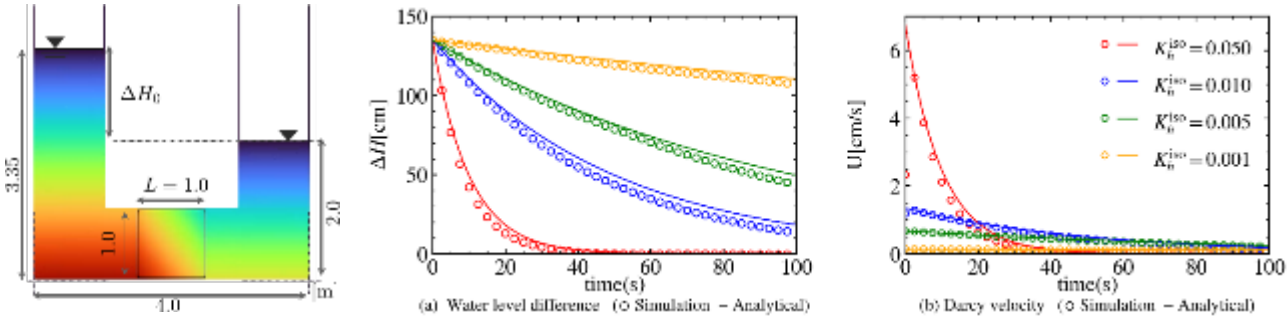
Extreme weather events linked to global warming, such as typhoons and heavy rainfall, are causing considerable damage worldwide. In Japan, crushed shells have recently been employed to mitigate the erosion of levee banks during overflow events. By applying crushed shells to a levee's back slope, overflow erosion is expected to be effectively prevented [1]. To understand the mechanical properties and limitations of applying crushed shell layers, a numerical tool is required to represent surface flow with drastic free surface deformation, and seepage flow through the shell layer simultaneously. This study presents the SPH-based surface and seepage flow simulator, which can represent such characteristics.

This study developed a numerical simulator based on the Smoothed Particle Hydrodynamics (SPH), employing the Darcy-Forchheimer-Brinkman equation, which can describe surface and seepage flows in a unified form as the governing equations to satisfy these performance requirements. In addition, SPH(2) is introduced to achieve highly accurate derivative operators, and governing equations in the Arbitrary-Lagrangian-Eulerian description are used to introduce Particle Shifting Techniques (PSTs) to improve particle configuration and volume conservation [2]. We simulated the seepage flow in a U-shaped channel with porous media to evaluate the fundamental performance of the proposed method. The Figure shows a smooth and stable pressure field over the entire area, and the pressure drop inside the porous media subjected to resistance force can be confirmed. Furthermore, comparing the theoretical solutions of the left-right head difference and the cross-sectional mean velocity obtained from the linear Darcy law differential equation with the analytical results, it was confirmed that the proposed method was able to reproduce the pressure field in general and to analyze the seepage flow stably and accurately. We plan to conduct overflow simulations on river levees with crushed shell beds.



Keywords: Particle method, ALE-SPH, SPH(2), Seepage flow, Crushed shells

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Interlocking Joints Generation Method for Multi-component Topology and Shape Optimization Using Dimensional and Interfacial Stress Constraints with Quadratic Stress Criterion

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As one of the important tools of generative design, topology optimization technology has been applied in more engineering fields with its high degree of freedom. It has gradually expanded from single component design to the field of complex assembly. Compared with the single structure, the multi-component topology-optimized structure needs to comprehensively consider the interface connection strength, manufacturability and reassembly requirements, which poses a severe problem to the traditional welding, bonding and other joints, these traditional joint methods not only increase the manufacturing complexity, but also causes stress concentration and appearance damage. To find a novel solution to the connection and joint issues in multi-component topology optimization problems, this paper proposes an interlocking joint generation method based on the dimensional constraints and interfacial stress constraints with quadratic stress criterion, which support easily reassembly and ensure the manufacturability of the optimized structure.

This study uses the extended level-set method [1] to solve the multi-component optimization problem and combines topology and shape optimization. Based on our previous work [2], this research innovatively introducing the interfacial stress constraints with quadratic stress criterion, which effectively increase the involvement range of the material interfaces for joints generation. Besides, dimensional constraints are applied to control the distribution regions of different material phases, creating continuous material interface for generating interlocking joints while ensuring the manufacturability of multi-component topology optimization. In addition, the method incorporates the dynamic response of harmonic force into the optimization system, so that the generated interlocking joint can still maintain stable performance under vibration forces.

This study has three innovations: 1. Compared to our previous research [2], a more stable and complex interlocking joint shape is generated through improved interfacial stress constraints with quadratic stress criterion, which increase the application scenarios of the interlocking joint for multi-component topology optimization; 2. The combination of shape optimization perfectly meets the requirements of multi-component topology optimization based on the extended level-set method [1]; 3. Considering the influence of vibration forces on the structure, the generated interlocking joints can resist the disturbance from different directions.

Keywords: Multi-component structures, topology optimization, shape optimization, interlocking joints, geometry constraints

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The Influence of Wood Anisotropy on Instruments

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Since the 1970s, modal analysis and acoustic analysis have been employed in the study of violins [1]. The objectives of such analyses are diverse; one notable example is the investigation into the mechanisms responsible for the distinctive tonal characteristics of the Stradivarius, an instrument crafted by the renowned Italian luthier Antonio Stradivari (1644–1737). However, in the case of antique violins such as the Stradivarius, conducting experimental procedures that involve direct physical contact or structural deformation is highly challenging. Consequently, numerical simulations, which enable non-destructive analysis, have emerged as a valuable approach.

In recent years, violin vibration analysis utilizing numerical methods such as the finite element method (FEM) and the boundary element method (BEM) has been actively investigated [2-4]. However, due to the inherent variability of wood arising from individual differences, aging effects, and anisotropy, accurately determining its physical properties remains a significant challenge. When employing representative material property values in numerical analyses, discrepancies between simulation results and experimental measurements often arise. This suggests that material property values exert a substantial influence on FEM-based analyses. If a methodology could be established to predict material properties while accounting for the anisotropic nature of wood, it would enable the derivation of results that exhibit greater consistency with experimental findings, thereby enhancing the reliability of numerical simulations. Furthermore, if material properties could be inversely identified from frequency response data, it would be possible to obtain valid physical parameters without necessitating the destruction of the instrument.

The present study aims to investigate the variability of material properties by conducting hammering tests and mechanical property evaluations in both the fiber and tangential directions of wood to improving simulation of violin. Additionally, hammering tests will be performed on plates exhibiting curvatures similar to those of a violin soundboard, allowing for the assessment of differences in transfer functions along the fiber and tangential directions.

Keywords: Vibrations, Violin, Anisotropy of wood, Fiber and tangential direction of wood

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Deterioration Mechanism and Residual Life Prediction of Cement Asphalt Mortar under the Coupled Effects of Rainwater and Mechanical Loading

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The cement asphalt mortar (CAM) serves as a critical component in high-speed railway infrastructure. However, its durability is adversely affected by the combined action of rainfall-induced erosion and dynamic train loads. In this study, a self-developed experimental platform was employed to investigate the coupled effect of rainwater and loading on the mechanical properties and microstructure of CAM. The results indicated that the leaching of calcium ions under rainfall erosion conforms to Fick's diffusion law. Three distinct layers were identified along the radial direction of the specimens, differentiated by their local calcium content. Under the combined effect of rainwater erosion and dynamic loading, calcium dissolution and surface abrasion occurred simultaneously, and both the cumulative calcium ion leaching per unit area and the thickness loss increased linearly with time, following a first-order kinetic equation. Notably, the coupling of chemical erosion and dynamic loading accelerated calcium dissolution exponentially. Additionally, through the establishment of a MATLAB-based iterative computational model, it was predicted that continuous coupled action over 20 years would result in a thickness reduction of approximately 1.5 mm in CAM.

Keywords: cement asphalt mortar, calcium leaching, coupling action of water and dynamic load, High-speed Railway.

A combined MCNP and molecular dynamics simulation study on radiation degradation of epoxy resins in nuclear power plant

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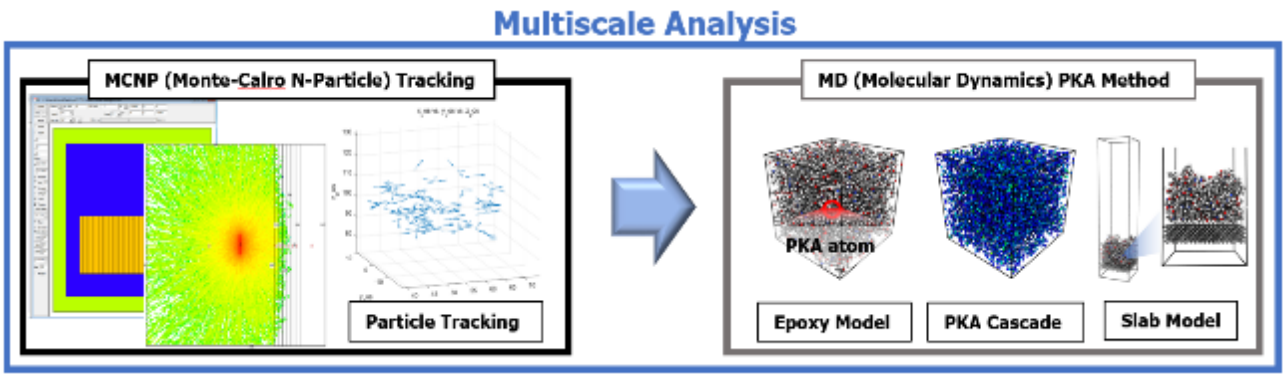
Despite their superior mechanical strength and thermal stability, the precise pathways of radiation-induced material degradation in high-performance polymers are not yet fully understood, especially compared to the extensive research on metallic materials. Here, we introduce a novel multiscale computational approach to investigate the radiation-induced degradation mechanisms of cross-lined epoxy resins, which are extensively used as protective coatings in extreme environments such as nuclear power plants. The complexity of epoxy degradation arises from intricate chemical and physical transformations under irradiation, necessitating further investigation to ensure the reliability of these materials in nuclear applications.

First, neutron and gamma-ray exposure conditions within nuclear facilities are simulated using the Monte Carlo N-Particle (MCNP) transport code to evaluate radiation dosimetry and its impact on particle interactions within the epoxy matrix. Next, molecular dynamics (MD) simulations are employed to subsequently evaluate structural modifications induced by primary knock-on atoms (PKAs), including bond dissociation in the amorphous network. To describe the reactive chemistry during irradiation-induced damage, ReaxFF simulations are performed for a detailed characterization of radiation-induced defects, atomic displacements, density reduction, and their impact on the material's insulating properties. The proposed integrative modelling framework is expected to contribute to the development of radiation-resistant epoxy coatings for enhanced durability in nuclear environments.

$$\mathrm{dpa} = \frac{\varphi \cdot \sigma \cdot E_d}{N \cdot E_{th}}, \tag{1}$$



Keywords: Monte Carlo, Primary Knock-on Atom (PKA), Molecular Dynamics (MD), Irradiation, Degradation, Epoxy

Acknowledgement: This research was supported by the Nano & Material Technology Development Program and Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by Ministry of Science and ICT (RS-2024-00408845) (RS-2024-00340747)

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MLP-Based Inverse Analysis in High-Voltage Electric Shock Simulations

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Prediction of input data from unknown outputs using an MLP trained on coupled analyses of current density and heat conduction in high-voltage electric shock scenarios, predicting input conditions based on observed thermal and electrical effects is a critical challenge for accident investigation and safety assessment. This study proposes a data-driven inverse analysis approach using a Multi-Layer Perceptron (MLP) trained on simulation data from coupled analyses of current density and heat conduction. The numerical simulations integrate quasi-static field analysis and transient heat conduction to accurately model current density distributions and Joule heating within the human body during electric shock events. To create a robust training dataset, extensive simulations were performed for multiple scenarios, including applied voltages of 100 V, 6,600 V, and 22,000 V, diverse contact locations, and varying material properties of body tissues. The simulations using the open source CAE system, ADVENTURE[1] yielded detailed outputs such as current density distributions, Joule heat generation profiles, and temporal temperature variations. These input-output pairs were used to train the MLP, enabling it to capture and generalize complex nonlinear interactions between electrical and thermal phenomena.

By leveraging machine learning, this study demonstrated strong predictive performance in accurately estimating unknown input parameters from limited observed outputs. This capability significantly enhances the accuracy and efficiency of accident investigations and safety assessments by enabling scenario reconstructions without direct measurements, thereby providing deeper insights into the dynamics of high-voltage electric shock accidents. It should be noted that this approach relies on several key assumptions and has certain limitations. Firstly, the quasi-static and transient analyses are based on idealized boundary conditions and may oversimplify the complexities encountered in real-world scenarios. Secondly, although the training dataset is extensive, it is generated under specific simulation conditions and might not cover the full range of variability present in actual accident cases, potentially affecting the generalizability of the model.

Future research directions include further refining prediction accuracy through the expansion of the training dataset to encompass broader conditions and scenarios. Additionally, incorporating advanced tissue damage and physiological response models will allow a more realistic representation of the biological impacts of electric shocks. Exploring sophisticated neural network architectures could further enhance the robustness and generalization capability of the inverse analysis model. Finally, integrating uncertainty quantification techniques to assess prediction reliability and performing sensitivity analyses

to identify critical input parameters will further advance the robustness and practical applicability of the proposed approach.

Keywords: Multi-Layer Perceptron, Inverse Analysis, Coupled Simulation, High Voltage Electric Shock, Machine Learning, Joule Heating

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Lift enhancement of a butterfly-inspired flapping wing by tip-vortex capture and streamwise ram effect

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Both butterflies and dragonflies possess four wings, yet their wing structures and movement patterns exhibit notable differences. Specifically, the distance between the forewing and hindwing in butterflies is considerably smaller compared to that in dragonflies. While earlier studies have thoroughly examined the interactions between the forewing and hindwing in dragonfly flight, this study shifts its focus to these interactions in butterfly flight. The research employs numerical simulations of the Navier–Stokes equations applied to a butterfly-inspired flapping wing model, which features an adjustable slot representing the narrow space between the forewing and hindwing. This slot is regulated by the dihedral angle formed between the forewing and hindwing. The study meticulously analyzes the lift coefficients of wings with varying slot size and position. Findings indicate that the interactions between the forewing and hindwing can substantially enhance lift when the slot is appropriately adjusted. For instance, when the forewing is elevated at a 10-degree dihedral angle relative to the hindwing during flapping, the wing produces more than 20% additional lift compared to a model without such a slot. The enhancement in lift is attributed to two primary mechanisms: the streamwise ram effect and tip-vortex capture, as elucidated by a lift decomposition formula. The streamwise ram effect diminishes the streamwise velocity beneath the forewing, thereby reducing the negative vortex lift linked to spanwise vorticity. Meanwhile, the tip-vortex capture boosts the positive vortex lift associated with streamwise vorticity, particularly when the hindwing intercepts the tip vortex shed by the forewing, as shown in figure 1.

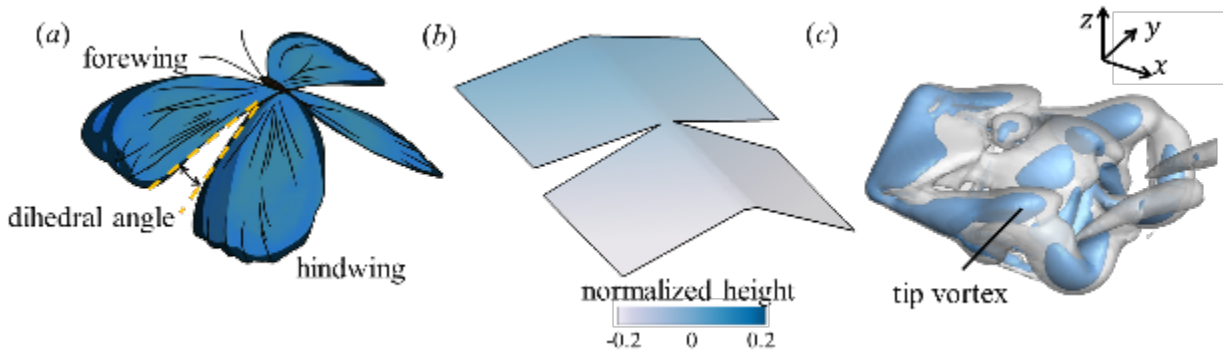

Figure 1. (a) The dihedral angle between the forewing and hindwing during flapping flight of a butterfly. (b) Snapshots of the model with dihedral angles $\beta = -10°$. During a wingbeat, the dihedral angle remains constant. The wing is coloured by the normalized height. (c) The dihedral angle between the forewing and hindwing leads to tip vortex shedding from the forewing. The tip vortex shed from the forewing passes above the hindwing, enhancing lift of the hindwing.

Keywords: flapping wing, unsteady fluid dynamics, vortex dynamics, wing-wing interaction, slotted wing, computational fluid dynamics

Motion Pictogram Generation using Generative AI and Pre-Trained Models, and Usability Evaluation

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This study explored the potential of artificial intelligence (AI) to enhance visual communication by automatically generating dynamic motion pictograms from static pictograms. Traditional static pictograms have limitations in conveying complex information and dynamic concepts. Motion pictograms, on the other hand, can facilitate more intuitive and comprehensible communication through dynamic visual representation. However, the creation of motion pictograms requires specialized skills and a great deal of effort using video software, which has prevented their widespread use. To solve this problem, this study utilizes AI to spread motion pictograms through automatic generation technology, aiming to enhance nonverbal communication and effectively convey information.

Two approaches were tried: in the LLM-based approach, a multimodal AI was given a common text prompt and a still image pictogram as input. As a result, the AI output a motion based on the meaning of the target pictogram, which was then input to a TI2V (Text-conditioned Image-to-Video generation) type AI to generate motion pictograms. In the motion transition approach with pre-trained models, generation was tried by using two pre-trained models and applying motion data from live-action video to still pictograms [1][2]. While some of the pictograms successfully produced motion pictograms of the expected or near-expected quality, some were found to be of unsuitable quality for conveying information. Since pictograms may play the role of giving instructions for action or warning of danger in the event of a disaster, a certain level of safety is required for their quality. In order to improve the effectiveness of information transmission while ensuring safety, it is necessary to establish a system that automatically evaluates the quality of output results and regenerates them as necessary.

To evaluate the effectiveness of AI-based motion pictograms in conveying information, an experiment compared three types: motion pictograms generated by TI2V-type AI (with human-inputted meanings and actions), those created by conventional video software, and still picture pictograms. Participants were asked to rate their understanding of each pictogram. The results showed that AI-created motion pictograms tended to improve comprehension compared to static pictograms, especially for dynamic concepts. However, in general, human-created motion pictograms were more comprehensible.

These results suggest that AI-generated motion pictograms offer encouraging possibilities for visual communication. However, further research is needed to carefully consider the design elements and motion characteristics that influence viewer interpretation.

Keywords: AI, image recognition, pictograms, motion graphics, user experiment

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A novel meshless formulation using a staggered variable arrangement and mesh-constrained approach for the incompressible Navier–Stokes equations

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The meshless method is a practical tool for predicting complex flows with moving boundaries. The methods are intrinsically free from topological limitations regarding to mesh reconstruction due to the feature that discrete points (DPs) with no connectivity to each other are used as unknowns, whereas they often suffer from high computational costs for stencil calculations. To address this issue, the authors have developed a novel meshless method, termed mesh-constrained discrete point (MCD) method, and shown validities in both the stationary boundary problems [1] and moving boundary problems [2]. The MCD method associates each DP with a background mesh element in a one-to-one manner to ensure spatial uniformity of DP arrangements, and this can dramatically reduce computational costs due to compact stencils and efficient memory access for stencil calculations in spatial derivatives. However, the existing approaches encountered problems that checkerboard-like numerical oscillations occur in pressure fields and the oscillations increase when the time interval Δt is reduced. One possible reason is to impose a collocated variable arrangement for the velocity and pressure at the same DP.

A meshless formulation using a staggered variable arrangement based on the moving least-squares method has been proposed for elliptic partial differential equations [3] and Stokes equations [4]. In this formulation, a radial projection of physical quantity is defined at each midpoint of stencil-centric DP and its neighbouring DPs, and then the divergence operator is taken for the radial projection quantities. This feature is crucial for meshless methods to address not only conservative forms, but also the consistent coupling of velocity and pressure in projection-type solves of the incompressible Navier-Stokes equations.

In this study, we propose a novel meshless formulation using the staggered variable arrangement for the incompressible Navier-Stokes equations based on the MCD method. In addition to the velocity and pressure as collocation quantities, an intermediate velocity is introduced as an additional unknown which is radially projected between DPs. The time evolution converting technique [5] is applied for updating the intermediate velocity in the pressure projection method. Our formulation fully satisfies the divergence-free condition in the discrete level due to the consistent coupling of velocity and pressure.

Keywords: Meshless method, mesh-constrained approach, staggered variable arrangement, velocity–pressure coupling, incompressible Navier–Stokes equations

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Data-driven geometrically exact beam elements for structural analysis of offshore wind turbines

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Recently, data-driven computational mechanics has emerged as a promising and powerful approach that enables the direct employment of raw experimental data in structural analysis, for instance data on the constitutive relations. In this work, we develop a data-driven geometrically exact beam element based on the direct approach introduced in [1] and the geometrically exact beam formulation introduced e.g. in [2,3]. We focus on the static structural analysis of offshore wind turbines and formulate our data-driven problem as a discrete-continuous quadratic optimization problem [1,2] as follows:

$$\inf_{(\mathbf{q},\mathbf{e},\mathbf{s},\tilde{\mathbf{e}},\tilde{\mathbf{s}})} \frac{c}{2}\|\mathbf{e}-\tilde{\mathbf{e}}\|_{L^2(\Omega)} + \frac{1}{2c}\|\mathbf{s}-\tilde{\mathbf{s}}\|_{L^2(\Omega)} \qquad (1)$$

$$\text{s.t. } \Phi((\lambda,\mu),(\mathbf{q},\mathbf{e},\mathbf{s});\mathbf{f}) = \langle \lambda, \mathcal{B}(\mathbf{q})^T\,\mathbf{s}-\mathbf{f}\rangle_{L^2(\Omega)} + \langle \mu, \mathcal{E}(\mathbf{q})-\mathbf{e}\rangle_{L^2(\Omega)} = 0$$

$$\forall(\lambda,\mu) \in H_0^1(\Omega)\times L^2(\Omega)$$

where c is a positive constant for unit consistency, **q** the vector consisting of the position and three directors defining the beam current configuration (see e.g. [2]), **e, s** the strain and stress fields (in Voigt notation), respectively, $(\tilde{\boldsymbol{e}}, \tilde{\boldsymbol{s}})$ the discrete-valued functions in $L^2(\Omega, \mathcal{D})$, where Ω is the domain of the beam configuration and $\mathcal{D}$ the set of available experimental data, $\mathcal{B}(\mathbf{q})$ the strain operator, $\mathcal{E}(\mathbf{q})$ the displacement-based strain fields, **f** the external force vector, and λ, μ the dual fields enforcing the equilibrium and compatibility conditions stated in Φ, respectively. Employing the direct data-driven solver introduced in [1] to solve (1) leads to the best possible phase state, i.e. the pair (**e, s**), that satisfies the two constraints considered in Φ and is closest to the data in $\mathcal{D}$. We apply the developed beam elements to the modeling of the structural components of offshore wind turbines, such as the tower and blades, while coupling these substructures in a multi-body finite element framework [4] for a static analysis of the turbines. We investigate the accuracy and robustness of our approach via numerical benchmarks and examples of wind turbines.

Keywords: Data-driven computational mechanics, geometrically exact beam, offshore wind turbines, multi-body framework.

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Hydraulic fracture simulation of meso-concrete using the SBFEM-FVM model

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This paper explores the simulation of the coupled interaction between mesoscale crack water pressure and the process of mesoscopic crack initiation and propagation in concrete, treating it as a three-phase material consisting of aggregates, mortar, and interfaces. A hybrid approach, combining the scaled boundary finite element method (SBFEM) and finite volume method (FVM), is employed at the microscale to model the interplay between crack water pressure and mesoscopic crack evolution. The cohesive crack model is applied to analyse the non-linear fracture transition zone. When multiphase materials are present within the crack tip element, the crack propagation direction is determined by generalized stress intensity factors and the fracture toughness of each phase material. Comparisons of numerical results with experimental data reveal a close correspondence between F-CMOD curves and water pressure variations under different loading conditions. The impact of crack water pressure on the mesoscopic concrete crack propagation direction is emphasized. This coupled model provides valuable insights into the interrelation of mesoscale phenomena and macroscopic behaviour in brittle concrete materials. The findings contribute to an enhanced understanding of fracture processes in concrete structures, particularly under varying environmental and loading conditions.

Keywords: concrete crack propagation, coupling; finite volume method, hydraulic fracture, scaled boundary finite element method

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Numerical Study of the Effect of Smoke Barrier Length Relative to Ceiling Height on Fire Spreading between Electric Vehicle

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The increasing adoption of electric vehicles (EVs) has introduced new challenges in fire safety, particularly in confined spaces such as underground parking facilities and tunnels. Electric vehicle fires, often linked to thermal runaway events in lithium-ion batteries, exhibit distinct characteristics compared to fires in internal combustion engine vehicles. These fires can produce intense heat, emit toxic gases, and be difficult to extinguish due to potential battery re-ignition. The study provides essential data for designing appropriate fire suppression system and minimize property damage and human casualties.Many researchers have performed study on fire spreading for fuel car. With the development of electric vehicles and charging station in underground car park,detailed study fire spreading and smoke movement to ensure safety for evacuation and fire supression are required.

This study employs numerical simulation techniques, specifically the Fire Dynamics Simulator (FDS), to analyse the interaction between smoke barriers and BEV fire dynamics. The simulations model a typical enclosed parking lot, where a BEV battery fire serves as the ignition source. A numerical study was conducted to validate the model against experimental data, leading to the development of a HRR customized simulation model for restricted fire. The study was conducted in an underground car parking lot measuring 7,800 x 7,800 x 3,250 mm, with the smoke barrier length adjusted to fractions of the ceiling height, specifically 1/5, 1/4, and 1/3 of the total ceiling height.

The results indicate that shorter smoke barriers (e.g., 1/5 of ceiling height) effectively direct temperature toward exhaust systems but allow some lateral spread due to insufficient coverage. Intermediate barrier lengths (e.g., 1/4 of ceiling height) offer an optimal balance by enhancing smoke channelling and stratification. Conversely, longer barriers (e.g., 1/3 of ceiling height) obstruct natural airflow, leading to reduced visibility in lower areas and localized smoke accumulation. Furthermore, the longest barrier length results in the highest temperature distribution due to smoke retention and heat reflection. The battery begins catch fire at approximately 300 ºC. Spreading time for longer barrier is 8 mins 30 seconds and shorter than other barriers. The figure for intermediate smoke barrier is around 9 mins 24s. The shorter smoke barrier have longest time to spreading fire to next car 10 mins 54s.

Acknowledgement

This work was supported by the Korean Planning & Evaluation Institute of Industrial Technology (KEIT) grant funded by the Korean government (Ministry of the Interior and Safety, MOIS) (RS2024-00408982), Development of intelligent fire detection and sprinkler facility technology reflecting the characteristics of logistics facilities).

Keywords: Navier-Stokes equations, FDS, Battery Fire Vehicle, Fire Spreading

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Remeshing Strategy for ALE-based FSI analysis to deal with large structural displacement

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Inspired by effective swimming and flapping flight of insects, birds, and fishes, bio-inspired artifacts mimicking their swimming and flapping flight such as robot fishes and flapping wing micro air vehicles (FWMAVs) have been developed for many years. Because numerical simulation is effective for accelerating the development of artifacts, many researchers have been working on fluid-structure interaction (FSI) simulations about swimming and flapping motion. In the previous study of my research group, the flapping motion in hovering flight was analysed by the partitioned iterative method [1]. The final goal of my research is to realize the simulation where robot fishes and FWMAVs swim and fly in a wide space freely.

The first step towards the goal is to construct the analysis system to solve FSI problems with large structural displacement. FSI analysis methods are classified into two types: interface tracking (IT) and interface capturing (IC). The representative IT method is the arbitrary Lagrangian-Eulerian (ALE) method. In general, the ALE method is accurate because the interface between fluid and structure is precisely considered. However, the classical ALE is difficult to prevent mesh distortion when the structure moves largely. In contrast, interface capturing methods such as the immersed boundary method and the immersed finite element method can cope with large structural displacement, even topology change. However, it is difficult to keep fine meshes around the structure. Therefore, the conventional IT and IC methods are incomplete to solve my target problem.

The purpose of the present study is to propose an ALE-based analysis system overcoming the difficulty of the classical ALE method. As well as the s-version FEM [2], the proposed method has two meshes: a local fine mesh to resolve the complex behaviour near the structure and a global coarse mesh to resolve relatively simple behaviour far from the structure. Then, the fine mesh is moved along with the structural motion while fixing the coarse mesh. Moving fine mesh is realized by remeshing. In my talk, the details of the proposed analysis system are explained, and numerical examples are presented as the demonstration.

Keywords: fluid-structure interaction, remeshing, finite element method, arbitrary Lagrangian-Eulerian

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Threshold of sediment particle in turbulent flow

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The transport of sediment particles in turbulent flow is widespread in nature. The turbulent entrainment of bed particle represents the first step in the formation and development of the multiphase flow [1]. According to the observed fact that the duration of fluid force acting on the particles is equally significant as the magnitude of the fluid force itself, several event-based entrainment criterions have been developed. However, these models, which is mainly based on wind tunnel or water channel experiments, only focus on the fluid forces and particle motions in the two-dimensional plane (streamwise and vertical directions). Recent studies have found that the spanwise fluid action, which depends on particle bed arrangement, is important. The semi-resloved particle Lagrangian tracking method and direct numerical simulation of wall turbulence four-way coupled with particles are employed to simulate the entrainment of individual particles for different bed arrangement and various Shields numbers. The fluid structures surrounding the particles during the entrainment process were analyzed, revealing that at lower Shields numbers, sweep events are the primary driving force for particle entrainment. Furthermore, for particles initiating motion in the spanwise direction, the surrounding spanwise velocity field is asymmetrical and larger spanwise structures form in the direction of motion. Accordingly, a three-dimensional impulse criterion for particle entrainment was developed and validated by the numerical simulation results.

Keywords: Turbulence, semi-resloved particle, four-way couple, entrainment thresold

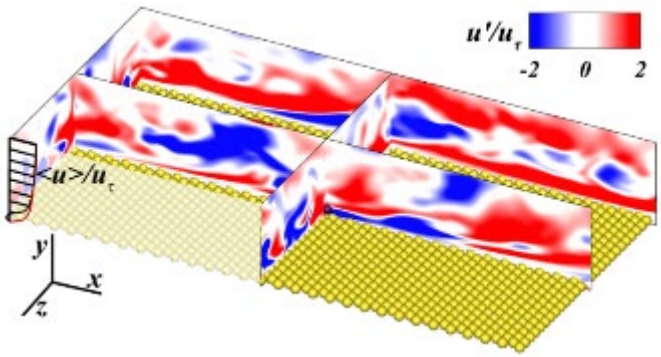

Figure 1. Instantaneous flow field over a fixed particle bed. The contours in each slice represent the streamwise fluctuation velocity u'. The red line illustrates the mean velocity profile of the single-phase flow, while the black line represents that over fixed particle bed.

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A Novel Framework for Calibrating DEM Models of Geo-materials

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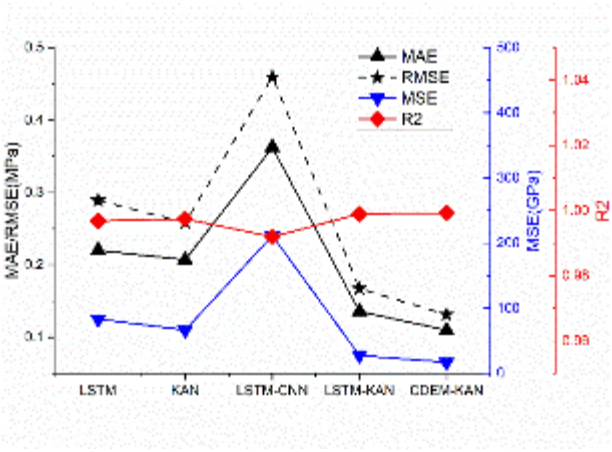
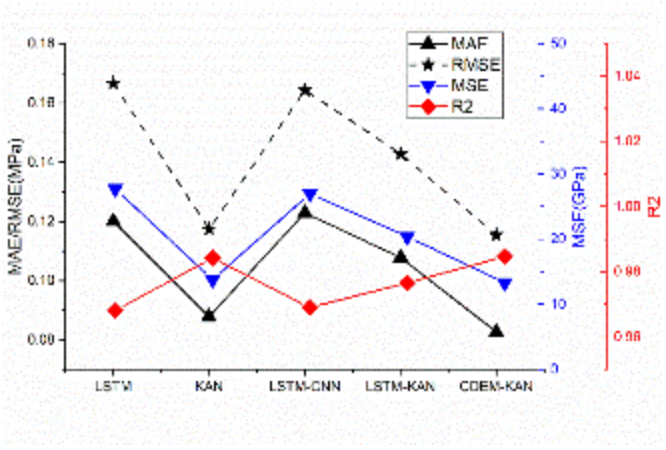
It is well known that it is challenging to efficiently calibrate micro-parameters to predict the macro-behaviors in discrete element method simulations, particularly for Uniaxial Compressive Strength (UCS) tests and Brazil Tensile (BT) tests. With the advancement of machine learning, these techniques have become powerful tools for handling complex datasets. Given the unique structure of both micro- and macro-parameters, Long Short-Term Memory (LSTM) networks have shown promise when combined with Convolutional Neural Networks (CNN) and Kolmogorov-Arnold Networks (KAN). Furthermore, a novel machine learning framework called Calibrating Discrete Element-Kolmogorov-Arnold Networks (CDEM-KAN) was proposed and applied to forecast the micro-parameters in Particle Flow Code (PFC). In addition, four other methods—KAN, LSTM, LSTM-CNN, and LSTM-KAN—were compared to validate the efficiency of CDEM-KAN. All models underwent training and hyperparameter optimization using cross-validation techniques to ensure fair and robust performance evaluation based on metrics such as Mean Squared Error (MSE), R^2, and Mean Absolute Error (MAE). Six micro-parameters, including particle contact elastic modulus, normal and tangential stiffness ratios, loading rate, contact cohesion, contact internal friction angle, and contact tensile strength (each examined at three levels), were used to derive three macro-parameters: the elastic moduli of UCS and BT, Poisson's ratio, and the strengths of UCS and BT using the PFC software. All 739 sets of results were collected, preprocessed through cleaning and normalization, and then divided into training and validation sets. The results show that CDEM-KAN has excellent predictive capability for the UCS and BT strengths across all indices, as shown in Figure 1.





(a)The evaluation index for UCS **(b) The evaluation index for BT**

Figure 1. The evaluation index of different machine learning method for UCS and BT

Keywords: discrete element method, machine learning, kolmogorov-arnold networks, uniaxial compression test, brazil tensile

Fast, large-scale tetrahedral mesh improvement on a single GPU

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Abstract. A GPU-based tetrahedral mesh improvement method is proposed for large-scale tetrahedral mesh generation. By leveraging independent vertex sets, the method achieves parallelization of vertex smoothing operation, while the locality of topological operations enables the parallelization of edge removal, multiface removal, edge collapse and edge split operations. The preliminary results show that the proposed method achieves a two-order-of-magnitude improvement in computational efficiency relative to Stellar when executed on a single RTX 4090D GPU, while maintaining mesh quality that is comparable to that of Stellar.

INtroduction

Mesh generation is the preprocessing step in numerical simulation techniques such as the Finite Element Method (FEM) [1], Finite Volume Method (FVM) [2] and Boundary Element Method (BEM) [3]. This process involves partitioning a continuous geometric domain into a finite combination of basic geometric elements, known as mesh. Commonly used element types include triangular, quadrilateral, tetrahedral and hexahedral elements. To meet the demands of high-precision simulations for complex models, the industry often employs large-scale mesh generation, which results in significant time consumption and computational resource overhead. How to rapidly generate high-quality large-scale meshes has become a pressing issue in the field of mesh generation.

The quality of the mesh is crucial for ensuring the precision and accuracy of computational results. In practical engineering applications, mesh generation for complex models requires iterative refinement and improvement to meet design and computational requirements. To satisfy these demands, vertex smoothing and topological transformation operations must be performed to improve the quality of the mesh. This process is known as Mesh Improvement. It accounts for more than 70% of the total time spent on tetrahedral mesh generation, making it the primary time bottleneck in the process of large-scale tetrahedral mesh generation.

Parallel computing technology based on Graphics Processing Unit (GPU) has provided new solutions for the generation of large-scale meshes. GPU is the processor specifically designed for graphic rendering. Differing from CPU which typically have a limited number of cores, GPU can simultaneously operate thousands or even tens of thousands of processing cores. Although the individual computational speed of these cores is relatively slow, they excel in performing the mathematical operations required for graphic rendering. This massive parallelism makes general-purpose computing on GPU possible. Recent advancements in computing power, together with the relatively low cost and wide availability of GPU, makes using GPU for tetrahedral mesh improvement become a viable option [4-5].

Methodology

The process of GPU-based tetrahedra improvement in this study is described in Alg. 1. It takes a tetrahedral mesh T as input and begins with a round of vertex smoothing. Subsequently, the algorithm enters an iterative loop of combinatorial operations, which include vertex smoothing, edge removal, multiface removal, edge collapse and edge split. It is important to note that edge collapse and edge split are only invoked when edge removal and multiface removal operations fail to further improve the mesh quality. The iteration process terminates under one of the following conditions: either the number of consecutive failures in combinatorial operations reaches 3, or the total number of iterations reaches the predefined upper limit of 27. Finally, the algorithm outputs the improved tetrahedral mesh T.

To better evaluate the effectiveness of mesh quality optimization, this study introduces two evaluation metrics: the worst element quality Q_{worst} and the penalty value for low-quality elements $S_{penalty}$ which are defined as follows:

$$Q_{worst} = \min_{t \in T} Q(t) \tag{1}$$

$$S_{penalty} = \sum_{t \in T} \max\left(0, Q_{low} - Q(t)\right) \tag{2}$$

Here, Q_{low} represents the predefined threshold for identifying low-quality elements. An element is classified as low-quality if its quality measure $Q(t)$ is lower than Q_{low}. In this study, the minimum dihedral angle is used as the criterion for evaluating mesh quality, with the low-quality threshold set to $30°$.

ALGORITHM 1 Tetrahedral mesh improvememt on GPU

Input: Tetrahedral Mesh *T*
Output: Improved Tetrahedral Mesh *T*

$n_f \leftarrow 0$
GPUVertexSmoothing
for $i \leftarrow 1$ to 27 **do**
  $Q_{worst}, S_{penalty} \leftarrow$ *EvaluateMeshQuality*
  if $n_f \geq 3$ **do**
    break
  end if
  GPUEdgeRemoval
  GPUMultiFaceRemoval
  GPUVertexSmoothing
  $Q'_{worst}, S'_{penalty} \leftarrow$ *EvaluateMeshQuality*
  if $Q'_{worst} < Q_{worst}$ **or** $S'_{penalty} < 0.999 * S_{penalty}$ **do**
    $n_f \leftarrow 0$
    continue
  end if
  GPUEdgeCollapse
  GPUEdgeSplit
  GPUVertexSmoothing
  $Q'_{worst}, S'_{penalty} \leftarrow$ *EvaluateMeshQuality*
  if $Q'_{worst} < Q_{worst}$ **or** $S'_{penalty} < 0.999 * S_{penalty}$ **do**
    $n_f \leftarrow 0$
  else
    $n_f \leftarrow n_f + 1$
  end if
end for

Preliminary results

The tests presented here are conducted on a personal computer with an Intel i9-14900KF CPU, 128GB of DDR5 RAM and an RTX 4090D GPU with 24GB of VRAM. Results obtained from the proposed method are compared with those obtained by Stellar [6] (Version 1.0.0), using the meshes illustrated in Fig. 1. In this test, the option that prohibits the change on the mesh surface is enabled for Stellar code.

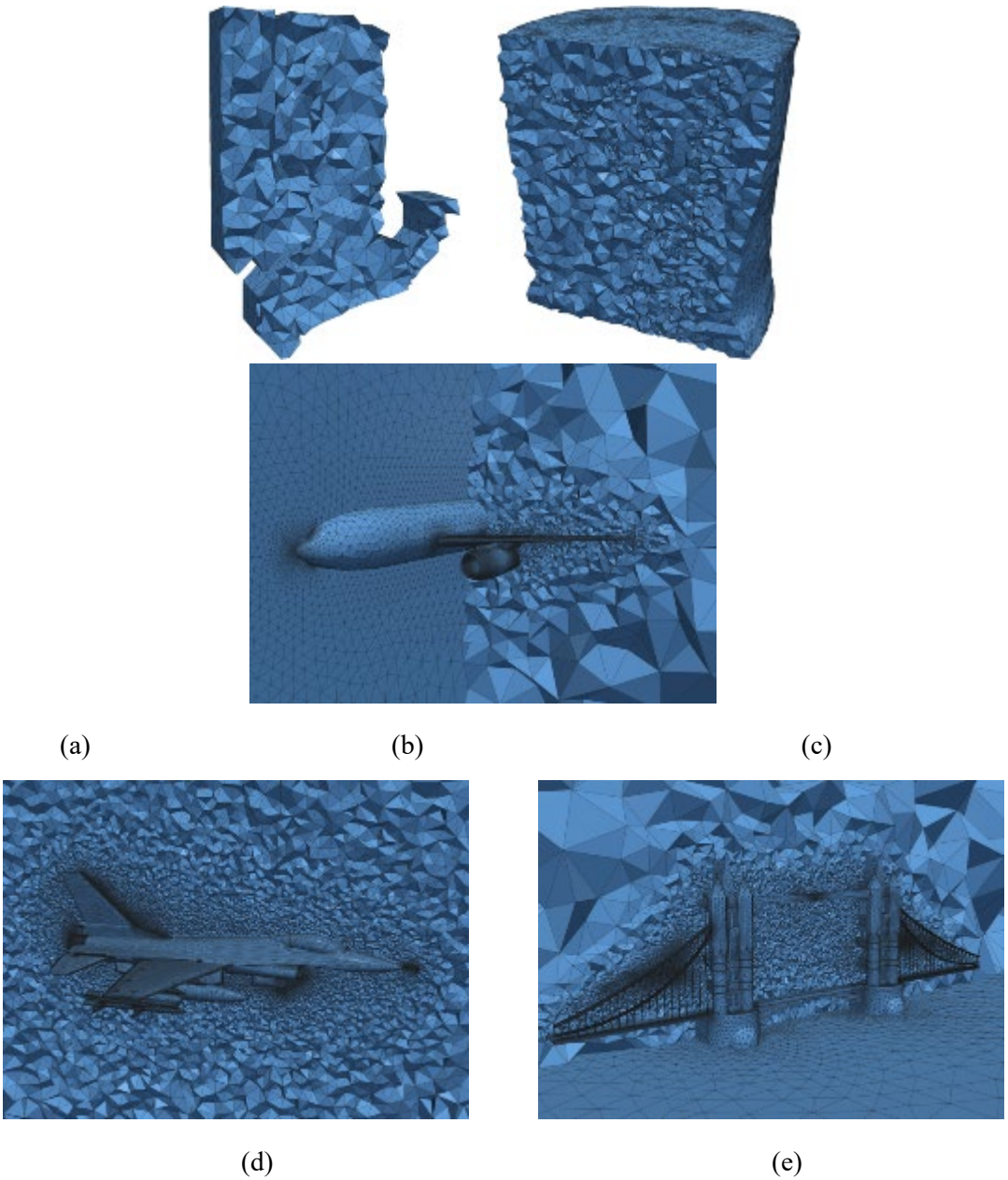

FIGURE 1 The selected meshes (a) Tire; (b) Patient-organs02; (c) F6 aircraft; (d) F16 aircraft; (e) London Tower bridge.

Table 1 lists the mesh size and the quality data statistics of the initial meshes and improved meshes, where $\theta_{\min}$ and $\theta_{\max}$ refer to the minimum and maximum dihedral angles, and λ refers to the percentage of bad dihedral angles, i.e., angles within the range of $[0, 30°]$ or $[150°, 180°]$, respectively. Meanwhile, λ_i $(i = 1 \sim 5)$ is used to evaluate the distributions of bad angles, which refers to the percentage of dihedral angles within the range of $[6(i-1), 6i)$ or $(180 - 6i, 180 - 6(i-1)]$ degrees. For instance, λ_3 refers to the percentage of dihedral angles within the range of $[12°, 18°)$ or $(162°, 168°]$.

In terms of time performance, the proposed method consistently requires the least time across all test cases. It can be seen that Stellar is 72, 817, 193, 197 and 222 times slower than the proposed method for the test cases Tire, Patient-organs02, F6, F16, and Tower Bridge, respectively. This indicates that the proposed method achieves a significant speed improvement of two orders of magnitude compared to Stellar on large-scale meshes.

In terms of mesh quality, the meshes improved by Stellar are slightly better than those optimized by the proposed method. For the test cases Tire, Patient-organs02 and F6, the proposed method still

exhibits a gap compared to Stellar, but it has successfully eliminated all bad tetrahedral elements with angles smaller than 12°. For the test cases F16 and Tower Bridge, the meshes improved by the proposed method and Stellar exhibit very close metrics in both minimum and maximum dihedral angles, with only minor differences in the distribution of bad dihedral angles. Both methods achieve mesh quality suitable for numerical simulation.

Overall, the proposed method demonstrates significant advantages over Stellar, requiring approximately one percent of the computational time while achieving comparable mesh quality.

TABLE 1. The mesh size and the quality data statistics of the initial meshes and improved meshes

Examples	Method	#tetra.	#vertices	$\theta_{\min}$	$\theta_{\max}$	λ	λ_1	λ_2	λ_3	λ_4	λ_5	Time(s)
Tire	Initial	11,098	2,570	0.66	178.88	4.58	0.12	0.46	0.77	1.28	1.96	/
	Stellar	10,636	2,600	23.43	149.79	0.13	0	0	0	0.016	0.11	49
	Ours	12,384	2,871	18.00	154.69	0.52	0	0	2.7e-3	0.06	0.45	0.68
Patient-organs02	Initial	280,911	51,124	2.89	175.23	7.65	0.0072	0.21	1.20	2.45	3.78	/
	Stellar	229,368	46,494	32.30	141.58	0	0	0	0	0	0	1,225
	Ours	278,107	54,722	12.54	156.74	0.12	0	0	1.2e-4	2.4e-3	0.12	1.5
F6	Initial	1,023,532	172,664	2.6e-13	≈180	6.65	0.23	0.68	1.19	1.82	2.73	/
	Stellar	919,401	172,113	19.14	155.65	5.4e-3	0	0	0	6.7e-4	4.7e-3	503
	Ours	955,169	173,776	14.20	167.70	0.015	0	0	4.0e-4	2.3e-3	0.012	2.6
F16	Initial	18,065,336	2,906,056	2.6e-14	≈180	6.63	0.23	0.67	1.18	1.82	2.74	/
	Stellar	16,361,969	2,910,680	3.81	174.24	0.024	6.1e-6	7.1e-6	8.0e-5	7.0e-4	0.024	5,510
	Ours	16,870,989	2,926,994	3.81	174.24	0.029	5.9e-6	2.7e-4	2.4e-4	4.6e-3	0.024	28
Bridge	Initial	37,772,656	6,205,571	2.1e-13	≈180	6.72	0.23	0.68	1.19	1.85	2.77	/
	Stellar	34,188,981	6,211,786	7.54	171.46	0.014	0	9.8e-5	4.3e-4	9.7e-4	0.013	12,891
	Ours	35,402,281	6,283,059	6.41	172.17	0.027	0	8.4e-5	3.6e-4	1.3e-3	0.025	58

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Computational Mechanics and Nanomaterial-Informed Modelling of Ship Collision Impact on Bridge Piers

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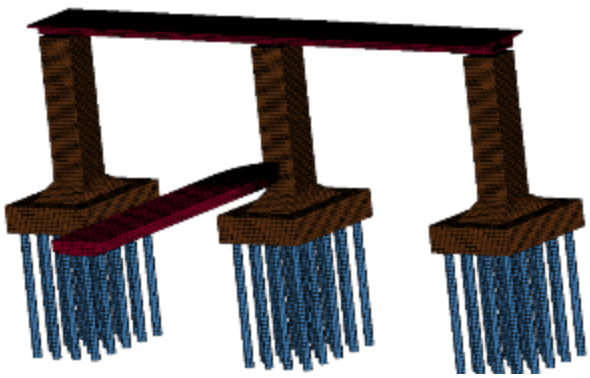
The resilience of bridge piers under extreme impact loading, such as ship collisions, is a critical aspect of modern infrastructure safety. This study integrates computational mechanics with advanced material modeling to analyze the behavior of nanomaterial-reinforced bridge piers subjected to high-energy impacts. A high-fidelity finite element (FE) model is developed using LS-DYNA to simulate a collision scenario in which a 16,000-ton vessel impacts a reinforced concrete pier at a velocity of 5 m/s.

The pier is modeled using the Johnson-Holmquist Concrete (JHC) model to accurately capture brittle failure and dynamic cracking, while steel reinforcement is defined with the Plastic Kinematic model to reflect strain hardening behavior. The impacting ship is treated as a Rigid body to isolate the structural response of the pier. Dynamic response parameters such as stress wave propagation, effective plastic strain, and crack evolution are analyzed using explicit time integration.

To enhance impact resilience, nanocomposite-reinforced concrete is introduced, accounting for nanoscale effects on fracture energy and ductility. Additionally, a Physics-Informed Machine Learning (PIML) framework employing a Multilayer Perceptron (MLP) is developed. The model is trained on FE simulation datasets to predict damage indices, crack distribution, and energy absorption levels across various collision scenarios. The MLP achieved high predictive accuracy ($R^2 \approx 0.96$), enabling rapid assessment of structural performance under diverse conditions.

This research advances the integration of computational mechanics and nanomaterial-enhanced design, providing a robust framework for improving the impact safety of bridge piers in maritime environments. The combination of material-specific FE modeling and AI-driven prediction offers a valuable pathway for future resilient infrastructure development.

Keywords: Computational mechanics, nanomaterials, finite element analysis, ship collision, machine learning, impact resilience, structural safety.



Hierarchical Domain Decomposition Parallelization for Local POD with Adaptive Basis Selection

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POD (proper orthogonal decomposition) is a technique for obtaining a basis to represent physical phenomena and has also been used in reduced-order models for rapid analysis.

To apply POD to large-scale problems, distributed-memory parallel computing, in which parallel processes are allocated to each partitioned subdomain, is effective. On the other hand, local POD [1], which obtains a basis for each partitioned subdomain, has been proposed to enhance the computational efficiency of POD.

In this study, to fundamentally address memory usage and computational bottlenecks, we propose a distributed-memory parallel computation technique for local POD, based on generalized hierarchical graph decomposition. The proposed framework comprises three layers: (i) mesh nodes, (ii) POD computation subdomains (responsible for local basis generation), and (iii) parallel computation subdomains (allocated for parallel processes). By decoupling the subdomains required for POD basis computation from those employed for parallel processing, the framework achieves robust parallel efficiency across diverse problem settings. In addition, the integration of adaptive basis selection, hyper-reduction [2], and load-balancing techniques provides the method with enhanced flexibility and scalability, thus offering a powerful approach for reduced-order modeling of large-scale numerical simulations.

Keywords: parallel computing, domain decomposition, graph structure, reduced-order modeling, proper orthogonal decomposition

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Inertia-Dominated Viscoelastic Turbulence and Fluid-Structure Interactions

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The addition of polymers to fluids in wall-bounded flows plays a crucial role in reducing turbulent drag. This modification introduces a chaotic state known as elasto-inertial turbulence (EIT), which occurs across a wide range of Reynolds numbers due to elastic instabilities in the fluid. Constitutive models, including the FENE-P and Oldroyd-B fluid models, are commonly used to represent viscoelasticity in these flows because they reflect the nonlinear elastic effects of polymers on turbulent dynamics. Although fluid-structure interactions (FSI) have many important applications in engineering and biomedical sciences, including deformable particle suspensions, bioinspired flexible designs in aerospace components, and high-speed fluidic devices, the relationship between EIT and FSI is yet unknown.

In this work, we develop a computational framework integrating lattice Boltzmann method (LBM) and immersed boundary method (IBM) with large eddy simulations (LES) to model inertia-dominated viscoelastic turbulence and its interaction with deformable structures. The governing equations for momentum and viscoelastic stress evolution are solved using a hybrid numerical approach, enabling the resolution of complex FSI phenomena in turbulent flows. The fundamental governing equations for incompressible viscoelastic flow are given by:

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla P + \nabla \cdot \tau + \rho \mathbf{g} \tag{1}$$

where $\mathbf{u}$ is the velocity vector, P is the pressure, τ is the extra stress tensor representing viscoelastic contributions, ρ is the density, and $\mathbf{g}$ is the gravitational force. The viscoelastic stress follows the constitutive equation:

$$\tau + \lambda_1 \left(\frac{D\tau}{Dt} - \tau \cdot \nabla \mathbf{u} - \nabla \mathbf{u}^T \cdot \tau \right) = 2\,\eta \mathbf{D} \tag{2}$$

where λ_1 is the relaxation time of the polymer, η is the polymeric viscosity, and $\mathbf{D}$ is the rate-of-deformation tensor. With this approach we aim to investigate how inertia-dominated viscoelastic turbulence influences the deformation of flexible structures, modifying energy transfer mechanisms and vortex dynamics. The developed framework is anticipated to offer new insights into bio-inspired propulsion, flow control strategies, and enhanced mixing in industrial processes. Future work will focus on validating the computational model against experimental and theoretical benchmarks, extending its applicability to complex geometries, and exploring data-driven approaches for turbulence closure models.

Keywords: Inertia-dominated viscoelastic turbulence, fluid-structure interaction, flexible structures, Immersed Boundary Method, Lattice Boltzmann Method, Large Eddy Simulation, computational fluid dynamics.

Meshfree method for large deformation analysis without any domain remesh- a nonlinear scheme based on stabilized collocation method

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Abstract

The Finite Element Method (FEM) and other mesh-based methods require mesh remeshing to address grid distortion issues when solving large deformation problems. In contrast, Galerkin-based meshfree methods do not request remeshing for approximation in large deformation analysis, while the integration grid still needs to be remeshed after distortion. In this work, we introduce a meshfree nonlinear solution scheme built upon Stabilized Collocation Method (SCM) and Reproducing Kernel (RK) approximation for the large deformation analysis. This method is genuinely meshfree, and no domain remeshing is required during the entire solution procedure. The total Lagrangian description is introduced for the formulations. The SCM can achieve accurate subdomain integration by using low-order Gaussian quadrature, which can significantly raise the accuracy and stability of the solutions. Lowering the condition number of the discrete matrix through subdomain integration further enhances the algorithm's stability. The subdomains for integration are determined by the particle locations, and domain deformation is represented by the movement of the particles, for which subdomains can remain regular without any deformation. Eliminating the need for remeshing can notably promote the solution efficiency. The Newton-Raphson iterative technique is conducted to address the nonlinear discrete equations. Several numerical examples of large deformation are examined, demonstrating the high accuracy, high efficiency and good stability of the proposed method for large deformation analysis. This method can handle very large deformation problems, even beyond the limit where FEM and High-order Finite Element Method (HFEM) solutions terminate. All these indicate that SCM has immense potential in addressing large deformation problems.

Keywords: stabilized collocation method; large deformation; accurate integration; accuracy; efficiency; stability

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Simulation of Concrete Compression and Shear Failure Based on Three-Dimensional Scaled Boundary Finite Element Method

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A macro-micro model integrating peri-dynamics and unified phase-field theory is utilized to investigate the damage evolution in concrete. The peri-dynamics concepts of material points and bonds are employed to analyze the micro-damage within the structure. Macroscopic topological damage is defined through the weighted integration of micro-damage within the influence domain of material points. This macroscopic damage model is incorporated into the Scaled Boundary Finite Element Method (SBFEM) framework, based on the energy degradation of the unified phase-field theory [1]. Building on prior research into the tensile damage of concrete, this study focuses on the initiation and propagation of damage in complex concrete failure scenarios, such as shear and compression. Appropriate deformation quantities are extracted from the natural strain rate to serve as deformation indicators for material point pairs, thereby driving the evolution of damage [2]. Structured strain is obtained via structured decomposition of the material points' strain tensor, resulting in structured elongation. For concrete compression failure, a masonry-style decomposition of the material points' strain tensor is used, which can more accurately simulate the crack propagation and failure mode of quasi-brittle materials under compression. For concrete shear failure, a deviatoric decomposition can be applied. Several numerical examples validate the effectiveness of the proposed method, which also exhibits weak mesh dependency.

Keywords: Scaled boundary finite element method, octree, nonlocal macro-micro damage model, compression, shear, concrete

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Anisotropic elastoplastic constitutive model considering strain softening and initial cohesion based on critical state

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To describe the three-dimensional stress-strain characteristics of heavily overconsolidated soils or asphalt mixtures, which exhibit strong initial cohesion under zero or even negative confining pressures, this paper introduces the initial relative mean effective stress p'_{r} to account for the initial cohesion based on the super-subloading surface constitutive model. The dilatancy relationship function of the new model is modified to describe the initial anisotropy in Equation (1), and a novel shape function $\Gamma(\theta)$ is employed to unify the von Mises, Mohr-Coulomb, Lade-Duncan, and Matsuoka-Nakai yield criteria for characterizing stress-induced anisotropy, thereby a new super-subloading surface constitutive model is established within the critical state framework. The stress integration algorithm of the proposed constitutive model is also developed with the incremental plastic deviatoric strain as the iterative variable, utilizing the UMAT subroutine in ABAQUS. The results show that: 1) The proposed model can describe the three-dimensional stress-strain characteristics of materials with strong cohesion and is also applicable for computational analysis under three-dimensional pure tensile stress states; 2) The proposed model can describe both initial anisotropy and stress-induced anisotropy; 3) The proposed model can simulate strain softening induced by both over-consolidated dilatancy and shrinkage due to structural damage; 4) The stress integration algorithm of the proposed model requires fewer iterations, converges rapidly, and the subroutine operates efficiently and stably.

$$\frac{\mathrm{d}\varepsilon_{\mathrm{v}}^{\mathrm{p}}}{\mathrm{d}\varepsilon_{\mathrm{d}}^{\mathrm{p}}}=\frac{\left(M\Gamma(\theta)\right)^{\chi}-\left[q/\left(p'_{r}+p'\right)\right]^{\chi}}{\left[q/\left(p'_{r}+p'\right)\right]^{\chi-1}}=\frac{\left\{\dfrac{M}{\alpha}\sec\left\{\beta\dfrac{\pi}{6}-\dfrac{1}{3}\arccos[\xi\sin(3\theta)]\right\}\right\}^{\chi}-\left[q/\left(p'_{r}+p'\right)\right]^{\chi}}{\left[q/\left(p'_{r}+p'\right)\right]^{\chi-1}} \tag{1}$$

where c is the dilatancy parameter in the dilatancy relation, p'_{r} is the initial relative mean effective stress, $\Gamma(\theta)$ is the shape function, θ is Lode angle, α 、 ξ and β can represent different yield criteria.

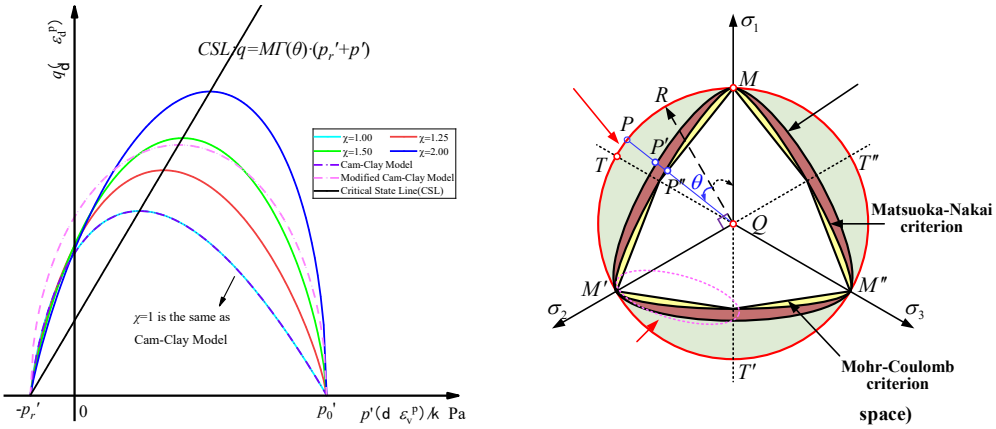

Figure 1.

Keywords: strain softening, initial cohesion, dilatancy function, stress-induced anisotropy; stress integration algorithm

A Differentiable Variational Framework for Contact and Fracture

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Numerical modelling of structural self-contact and crack propagation poses significant challenges. Traditional approaches to contact typically rely on Lagrange multipliers or penalty methods which introduce numerical complexities. Crack nucleation and propagation require careful handling to accurately capture the inherent discontinuous and non-linear nature of fractures. This work integrates failure and contact in a unified and numerically stable variational framework. The proposed framework is fully differentiable, a key component for future integration in topology optimisation methods, enabling the design of structures that explicitly account for contact and fracture. The contact phenomenon is described through the hyper-elastic Third Medium Contact model [1]. Structures are embedded in a third medium, that when compressed stiffens. This allows for the transfer of forces between structural members. Fracture is represented by a phase field which reduces the material resistance when the critical energy release rate is exceeded [2]. Careful treatment is required when coupling the two phenomena, particularly in terms of the behaviour within the void domain. The framework is validated against reference results in [3] for a notched three-point bending test presented in Figure 1.

Figure 1. Three-point bending test validation, force-displacement curve and structural depiction at discrete displacement increments

An initially detached semi-circle is brought into contact with the upper surface of the beam. The model shows nearly null reaction force up to the contact displacement and shows excellent agreement with the reference results in terms of peak force and displacement. These results demonstrate the framework's capability to accurately capture both internal contact mechanics and structural failure processes including crack initiation and propagation.

Keywords: Third Medium Contact, Phase Field, Fracture, Topology Optimisation

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A Study on Predicting the Behavior of Partitioned Structures using the Deep Neural Network

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To efficiently perform finite element analysis, parallel computing techniques utilizing multi-core processors have been widely employed. In particular, Lagrange multiplier-based methods such as FETI (finite element tearing and interconnecting) and AFETI (algebraically partitioned FETI) have been extensively studied and are now regarded as the most mature and highly accurate techniques [1, 2]. Meanwhile, driven by advancements in the deep learning technique, various studies have proposed integrating the deep learning into such parallel analytical frameworks. In this study, we aim to establish a foundation for overcoming the limitations of the computational resources while maintaining the accuracy of numerical methods by leveraging the deep learning and Lagrange multipliers. In this study, AFETI is used as a domain decomposition method which includes the local Lagrange multipliers. A schematic of AFETI is in Fig. 1.

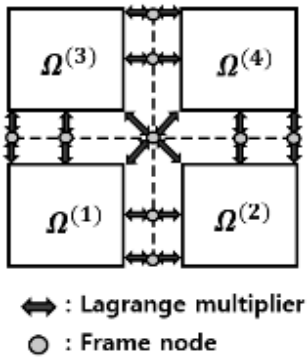

Figure 1.

where Ω^i means i^{th} subdomain. As demonstrated in Figure 1, since Lagrange multipliers possess the boundary degrees of freedom, they will be applicable to the deep learning more efficiently compared against handling the total degrees of freedom. In this study, we validate the efficiency of the proposed method by implementing several numerical techniques to confirm these advantages.

Keywords: domain decomposition method, Lagrange multipliers, deep neural network

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Particle tracking in a nasal to tracheo-bronchial airway using a scale resolving simulation

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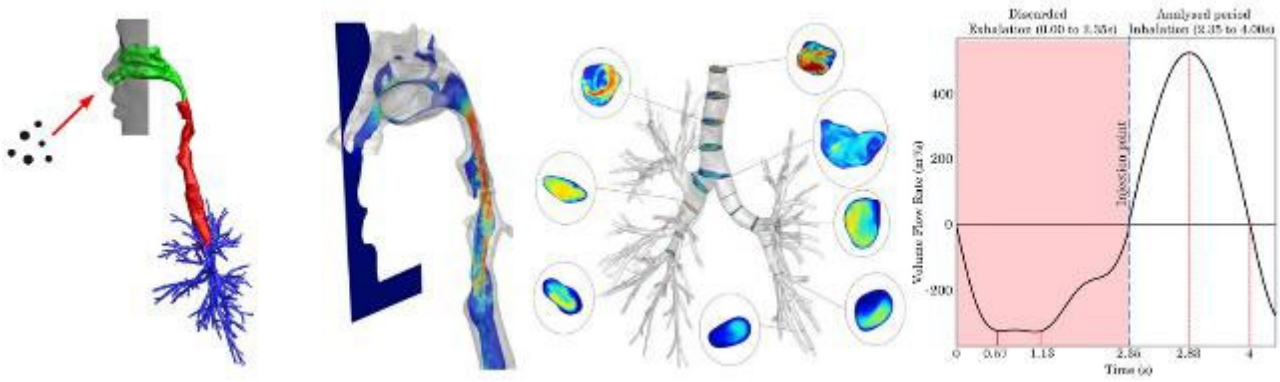
Particle deposition in the human respiratory system remains a critical factor affecting drug delivery and inhalation toxicology. Previous studies indicate that the deposition efficiency is significantly influenced by airflow patterns and particle size, with larger particles (> 5 μm) predominantly depositing in the upper airways through inertial impaction mechanisms. Whilst smaller particles (< 2 μm) are capable of penetrating deeper into the respiratory tract, often reaching the alveolar region and leading to localised toxicity

This research aims to improve the understanding of how specific inhalation patterns and airway morphology can influence the deposition of inhaled particles and identify regions of localised deposition. A realistic airway model extending from the nasal cavity to the lung bronchioles was created to investigate these issues. A transient scale resolving simulation was performed for a single inhalation event to capture the dynamics of the continuous and discrete phase in high detail.

The results further identified that larger particles depose early in the nasal cavity, whilst small particles can penetrate deeper into the distal bronchial airway. The scale resolving simulation further identified localised regions of intense mixing contributing to enhanced deposition, earlier in the respiratory airway, thereby contributing to the respiratory system's natural defence system. Ultimately, this research contributes valuable insights that could inform therapeutic strategies, particularly in the context of aerosolised medications and respiratory disease management.



Keywords: Respiratory airway, Nasal cavity, CFD, Breathing, Tracheo-bronchial tree, Inhalation Toxicology, Drug Delivery

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Numerical modelling of fracture propagation of hot dry rock with the acid fracturing fluid

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Fracture propagation in hot dry rock acid fracturing is a critical issue in geothermal resource development, significantly influencing the efficient utilization of geothermal resources and the formulation of development plans. However, the understanding of fracture propagation rules in acidized hot dry rock reservoirs remains unclear. To address this issue, this study constructs a multi-field coupling model for hot dry rock reservoirs based on the phase-field method, utilizing COMSOL Multiphysics software for numerical simulation. This study investigates the changes in fracture propagation characteristics under acid fracturing conditions, analyzing the effects of acid concentration on fracture initiation pressure and propagation speed. Additionally, simulations under different fracturing conditions reveal the impact of perforation angle, in-situ stress difference, and fracturing fluid displacement on fracture deflection and propagation. The results indicate that with increasing acid concentration, fracture propagation speed accelerates, while the impact of acid concentration on fracture initiation pressure is negligible. Perforation angle significantly affects fracture deflection; as the perforation angle increases from 0°to 75°, the fracture initiation pressure increases by 39.9%, with significant deflection occurring at angles above 45°. The in-situ stress difference markedly influences fracture initiation pressure; reducing the stress difference from 20 MPa to 5MPa increases the fracture initiation pressure by 20.6%. Increased fracturing fluid displacement promotes fracture propagation, with a corresponding increase in initiation pressure. These findings provide crucial references for optimizing fracturing design and enhancing geothermal energy extraction efficiency in hot dry rock reservoirs.

Keywords: hot dry rock, fracture propagation, acid fracturing fluid, phase-field method, COMSOL Multiphysics

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Data-driven Design of Bio-inspired Perturbated Vertex-based Hierarchical Honeycomb for Improved Energy Absorption

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While periodic honeycombs have been widely applied in energy absorption applications, non-periodic honeycombs, including perturbated honeycomb, can offer rectified stress propagation paths with even better mechanical properties and still remain underexplored. This research aims to explore how to further improve the energy absorption capability under three maximum allowable stress levels by integrating vertex-based hierarchical structures, which can further enlarge the design space of perturbed honeycomb. This novel structure is called perturbated vertex-based hierarchical (PVH) honeycomb. Bayesian optimization and Gaussian Process Regression (GPR) framework shown in Figure 1 is utilized to identify optimal PVH honeycomb structures with low computational cost. Results demonstrate that optimal energy-absorbing structures vary under different allowable stress levels. While periodic hexagonal honeycombs can still present superior energy absorption at low stress level, non-periodic honeycombs exhibit enhanced energy absorption due to their distinct hardening behaviour at medium and high stress levels. Under medium and high stress levels, optimized PVH honeycombs can achieve 146.72% and 214.77% higher energy absorption than baseline regular hexagonal honeycomb, respectively. The results reveal the effectiveness of Bayesian optimization and GPR in designing non-periodic structures with non-linear properties, and present the potential of PVH honeycombs for energy absorption devices across varying allowable stress level requirements.

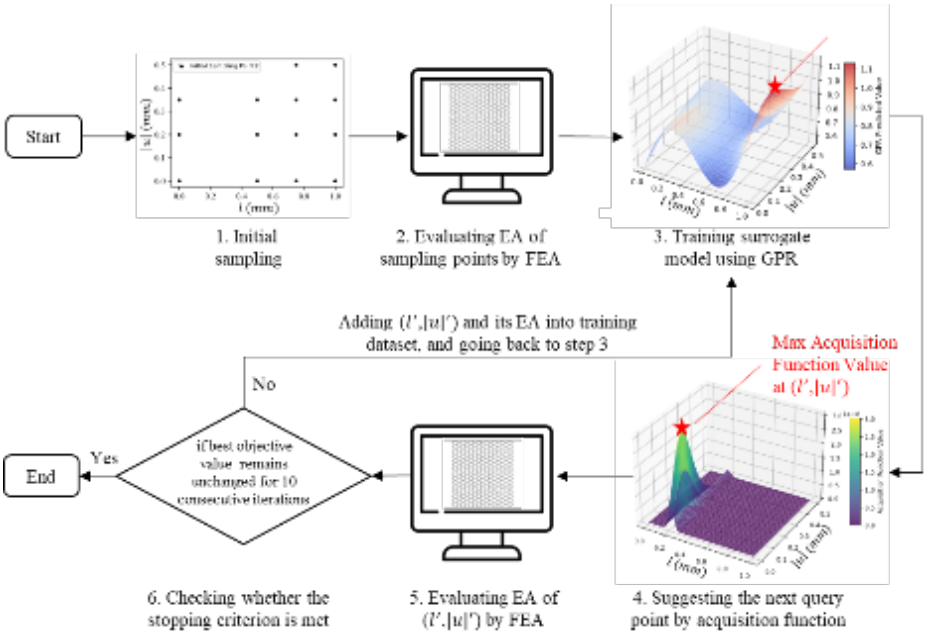

Figure 1. Design framework.

Keywords: Machine learning, Energy absorption, Metamaterial

Measurement of deformation behavior of aluminum alloy under biaxial tensile test and estimation of material model parameter using data assimilation

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Aluminum alloys are lightweight and suitable for reducing the weight of automotive components. Efficient plastic forming processing of aluminum alloys requires the prediction of the deformation behavior during the plastic forming process using a finite element (FE) simulation. To accurately predict the deformation behavior using the FE simulation, calibrating the parameters of material models is necessary. The parameters of material models have been identified based on experimental data obtained from multiple material tests, but the experimental calibration is a time-consuming task.

In this study, the distribution of the strain on a cruciform specimen during a single biaxial tensile test, measured by Digital Image Correlation, is integrated into the FE simulation of the biaxial tensile test by data assimilation to estimate the parameters of material models, avoiding the need for multiple experiments. The estimation targets all nine parameters of the Yld2000-2d yield function. This study utilizes Data assimilation method Minimizing a four-dimensional Cost function using Tree-structured Parzen Estimator [1] as the data assimilation.

To evaluate the accuracy of the optimally estimated parameters in this study, the FE simulations of the biaxial tensile test are performed twice: once with the optimally estimated parameters and once with the literature parameters identified through uniaxial tensile and hydraulic bulge tests [2], and the results of these FE simulations are compared with the experimental data. In the biaxial tensile test, the specimen fractured 866 seconds after the start of the test. **Figure 1** shows the distribution of the logarithmic strain e_{yy} just before the specimen fractured (at 865 s): (a) the experimental result, (b) the result of the FE simulation with literature parameters, and (c) the result of the FE simulation with the optimally estimated parameters. The FE simulation with the optimally estimated parameters reproduces the experimental result more accurately than the FE simulation with the literature parameters. This study improves the accuracy of the estimation of the parameters of the yield function.

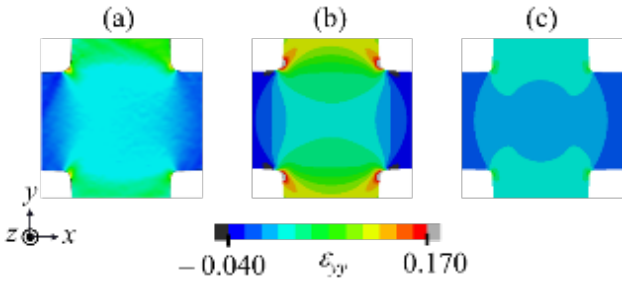

Figure 1.

Keywords: Data assimilation, Biaxial tensile test, Finite element simulation, Yield function.

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Design of Temporary Defensive Structures for Managing Wind-related Disasters

By

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Abstract

The wind-related disasters are one of the most frequent natural disasters, i.e., tornados, cyclones (Hurricanes and Typhoons), hurricanes, downbursts, Haboobs, Dust Storms etc. The global warming results in server climate changes, as a result, the occurrence of those wind-related disaster increased substantially with increasing damage intensities on civil infrastructure. As an example, the occurrence of tornado in America indicates that despite the fluctuations in tornado occurrences, with notable peaks in 2008, 2011, 2019, and 2024, the occurrence peak in 2024 with a number of 1780 comparing to an average number of 1320 in the last five years before 2024. The damage caused by those wind-related disaster will increase substantially when the debris or projectiles of buildings or hailstone were blowed in those strong winds.

Designing sacrificial deployable structures can be an effective strategy to protect buildings from various hazards, including wind-related disasters and other threats. These structures are intended to absorb or deflect the energy from such events, thereby minimizing damage to the primary building. Rapid Deployment: Deployable structures can be quickly assembled in response to imminent threats, providing timely protection. For instance, rapidly deployable protective enclosures have been developed using flexible membranes supported by inflatable frameworks. These structures serve as temporary shields during events like hurricanes, tornadoes, or even man-made threats, reducing the impact on permanent buildings. Implementing sacrificial structures can be more economical than reinforcing existing buildings to withstand extreme events, especially in high-risk areas. The design must ensure that the deployable structure can withstand the specific hazards it is intended to protect against without collapsing onto the building it protects with efficient and reliable deployment systems. Materials should be chosen based on durability, weight, and resistance to the specific hazards anticipated. The effectiveness of the sacrificial protective structures will be developed and verified using numerical simulations.

In summary, sacrificial deployable structures offer a viable solution for protecting buildings from various hazards. Their effectiveness depends on thoughtful design, appropriate material selection, and reliable deployment mechanisms tailored to the specific threats faced. The prototype of the modular components will be automatically constructed using new 3D printing technology. The impact tests with ice projectile and common wooden debris in wind will be carried out to test the performance of the design developed. The FEM will be developed to simulate the behaviour/damage of the sacrificing structures under dynamic impact identified from wind disasters.

Based on the performance of the designs, the wind-related disaster can be managed to minimize their damages on civil buildings including rapid pre-disaster deployment, post-disaster recycling, and reconstruction/restoration of those sacrificing structures to increase the community resilience and preparedness. Regular community training sessions on the deployment of these protective structures can enhance preparedness, ensuring swift and efficient responses to future wind-related threats.

XCT-Based Finite Element Modelling for Performance Degradation Mechanism in 3D Printed Continuous Carbon Fibre Reinforced Composites

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The development of 3D printed continuous fibre-reinforced composites (FRP) offers new possibilities for manufacturing complex structures. However, their mechanical performance, particularly strength and stiffness, is significantly reduced due to defects such as porosity, fibre breakage, fibre misalignment, and matrix-rich regions. Existing studies have limitations in characterizing these microstructural defects, such as measuring porosity size and quantifying fibre breakage and misalignment. Additionally, the mechanisms by which these defects affect mechanical performance remain insufficiently explored, with a lack of modelling approaches incorporating real geometric information to analyze stress distribution and fibre/matrix interactions.

This study employs micro-computed tomography (micro-CT) to achieve high-precision characterization of the internal structure of 3D printed FRP, enabling the identification of individual pores and fibre distributions. Based on CT data, numerical models are constructed to investigate stress concentration effects in realistic geometries. First, 3D printed samples are prepared and scanned using micro-CT, and the processed data is used to extract information on fibre distribution, fibre misalignment, porosity, and pore morphology. CT-based numerical models are then developed and validated through experimental mechanical tests. Finally, the effects of fibre distribution, porosity, and fibre misalignment/breakage on mechanical performance are systematically analyzed. The results reveal that matrix-rich regions cause local stress concentrations, porosity reduces overall stiffness and strength, and fibre misalignment and breakage further weaken load-bearing capacity. The CT-based numerical modelling approach proposed in this study provides an effective tool for optimizing the microstructure and predicting the mechanical properties of 3D printed continuous fibre composites.

Keywords: 3D printing, Continuous fibre-reinforced composites, Micro-CT, Finite element modelling, Manufacturing defects

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Heat transfer and fluid flow characteristics of turbulent spots in plane Couette flow under temperature stratification

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Achieving high efficiency in heat exchangers requires breaking the similarity between heat transfer and momentum transport. Turbulent spots developing in a plane Couette flow exhibit dissimilarity, which enhances the heat transfer against the momentum transport. However, the thermal stratification effect due to the buoyancy force caused by fluid temperature change has not been fully understood. This study investigates the dissimilarity of the turbulent spots affected by buoyancy due to imposed temperature stratification.

Direct numerical simulations (DNS) of the spectral method [1] were performed to investigate the emergence mechanism of dissimilarity between heat transfer and momentum transports in a plane Couette flow with temperature stratification. The objective flow is characterized by the Reynolds number $Re = U_W\delta/\nu = 450$ and the Prandtl number $Pr = 1$, where U_W is the wall velocity, δ is the channel half-width, and ν is the kinematic viscosity. The temperature stratification is characterized by the Grashof number $Gr = g\beta\Delta T(2\delta)^3/\nu^2$, where g is the gravitational acceleration, β is the thermal expansion coefficient, and ΔT is the temperature difference. Here, positive and negative Gr corresponds to stable and unstable temperature stratification, respectively. A vortex pair disturbance [2] is introduced to the laminar plane Couette flow. The momentum and heat transports were evaluated using the following friction coefficient C_f and Stanton number St.

$$C_f = 2(u_\tau/U_w)^2 \tag{1}$$

$$St = Nu/RePr \tag{2}$$

Where, u_τ is the friction velocity and Nu is the Nusselt number. According to the Chilton–Colburn analogy, an efficient heat transport state is evaluated by dissimilarity rate $(2St - C_f)/C_f$.

Figure 1 shows the time evolution of C_f and $2St$. Both values increase linearly accompanied by the growth of the turbulent spots. The dissimilarity rate shows that the efficient heat transport states are obtained in the spatial developing process of turbulent spots in all cases. The most efficient heat transport state in present cases was achieved at $Gr = -10^3$, which marks 9% efficiency. On the other hand, it was confirmed that the efficient heat transport state persisted under the stable temperature stratification. In the presentation, we will provide these mechanisms in detail.

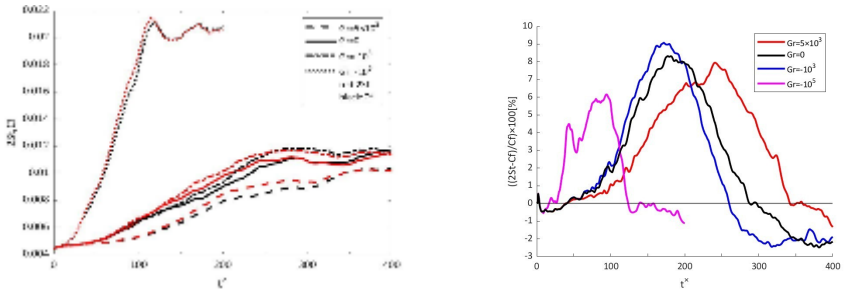

Figure 1. Time evolution of developing turbulent spots

Keywords: Dissimilarity, Turbulent Spot, Plane Couette Flow, Direct Numerical Simulation

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Improved Basis-screening Kriging Method using Penalized Maximum Likelihood Estimation for Structural Optimization

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In this study, an improved basis-screening Kriging (IBSK) surrogate model using penalized maximum likelihood estimation (PMLE) is proposed. The basis-screening based Kriging surrogate model determines the maximum order of the basis function and then sequentially selects the optimal basis set by evaluating the importance of each basis function element through cross validation error (CVE) [1]. In this process, it may fail to find the optimal hyper-parameter through maximum likelihood estimation since the likelihood function has highly nonlinear near the origin and a large flat region elsewhere even when the advanced optimization algorithm is used such as generalized pattern search (GPS) method. To solve this problem, MLE applies a penalty function with a penalty parameter [2]:

$$\psi(\boldsymbol{\theta},\lambda) = -\frac{n}{2}\ln(\sigma^2) - \frac{1}{2}\ln(|\mathbf{R}|) - np_{\lambda}(|\boldsymbol{\theta}|) \tag{1}$$

The optimal penalty parameter can be determined by CVE for a given hyper-parameter. This procedure requires iterative calculations between hyper-parameters and the penalty values. In order to avoid such iterative calculations, we proposed penalty sensitivity based method that calculates the optimal penalty value based on the CVE only when the sensitivity to the penalty value of the likelihood function is high:

$$\lambda^{(k+1)} = \lambda^{(k)} + \Delta\lambda \times sign\left(\frac{\partial\psi}{\partial\lambda}\bigg|_{\boldsymbol{\theta}=\boldsymbol{\theta}^{(k)},\lambda=\lambda^{(k)}}\right) \tag{2}$$

For given next state penalty parameter $\lambda^{(k+1)}$, the new optimal hyper-parameter of correlation function $\boldsymbol{\theta}^{(k+1)}$ is obtained using Generalized Pattern Search (GPS) algorithm. This procedure is repeated until the updated k-fold CVE is reduced. Using the proposed method, hyper-parameters can be obtained quickly and accurately regardless of their initial values. In this paper, the accuracy and efficiency of the proposed method were verified through several numerical examples.

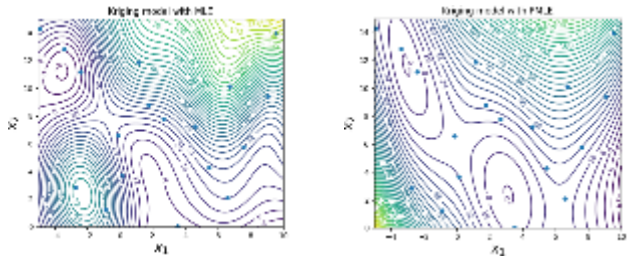

Figure 1. (a) MLE (RSME = 16.0904) (b) PMLE (RSME = 0.8099)

Keywords: Improved Basis-screening Kriging(IBSK), Penalized maximum likelihood estimation(PMLE), Correlation Hyper-parameters, Penalty Sensitivity based Method(PSM)

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Stochastic PushForward and Multi-Scale Physics-Constrained Neural Networks for Efficient Long-term Forecasting of Complex Physical Systems

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Improving long-term prediction and training efficiency stands as a central challenge for data-driven modeling of physical systems. Although purely data-driven methods have gained traction due to fast inference and reduced computational costs, their performance often degrades over long term because of error accumulation. Concurrently, physics-constrained neural networks offer enhanced robustness by incorporating physical constraints in the training process, yet can be prohibitively expensive for high-dimensional systems, especially when multi-fidelity data are involved.

To address these challenges, we propose two complementary frameworks that collectively balance accuracy, resource efficiency, and robustness. First, we introduce the Stochastic PushForward training paradigm for multi-step-ahead forecasting. Stochastic PushForward retains a one-step-ahead training structure but dynamically constructs a supplemental dataset from the model's own predictions. By stochastically drawing training inputs from both ground-truth and model-generated data, Stochastic PushForward naturally balances short- and long-term performance, while also mitigating memory overheads associated with unrolled sequences. Second, we present the Multi-Scale Physics-Constrained Neural Network [1], designed to incorporate multi-fidelity data within a unified latent space via a tailored multi-fidelity autoencoder. In Multi-Scale Physics-Constrained Neural Network, separate decoders map this shared latent space to different fidelity levels, enabling physical constraints to be computed in lower-fidelity fields—thus greatly reducing training complexity while preserving predictive accuracy.

We evaluate these methods on fluid dynamics benchmarks, including two-dimensional Burgers' and shallow water systems. Experimental results reveal that Stochastic PushForward significantly improves long-term forecasts without sacrificing short-term accuracy or requiring large memory consumption. Meanwhile, Multi-Scale Physics-Constrained Neural Network effectively leverages multi-fidelity data and cuts computational costs by enforcing physics constraints in low-fidelity fields. By combining these strategies, we offer a robust, scalable, and memory-efficient solution for forecasting complex physical systems.

Keywords: Long-term Prediction, Memory-efficient Training, Resource-constrained Environments, Dynamical systems

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Cellular aggregate formation:
continuum modelling and computational implementation

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Cellular aggregates play a crucial role in various biological processes, including tumor growth, tissue expansion, wound healing, and biofilm formation. The study of such systems necessitates an analysis of the interplay between cell–cell and cell–matrix interactions, which collectively govern the dynamics of cellular aggregates an inherently out-of-equilibrium phenomenon.
In this presentation, we introduce a nonlinear continuum mechanics framework alongside a finite element simulation approach to model the physics underlying cellular aggregate formation. As a representative case, we focus on bacterial colony formation, and conceptualize the aggregation process as an active phase separation phenomenon. The problem is formulated withi both Eulerian and Lagranfian continuum descriptions. Furthermore, a robust and efficient finite element implementation is elaborated for the computational implementation of the problem.
To further enhance numerical stability, we present our recently developed micromorphic-based artificial diffusion method to mitigate instabilities stemming from the convective nature of the problem. This approach improves the robustness of the numerical scheme while preserving the essential physics of the system.
Finally, through a series of numerical examples, we investigate how different parameters influence the dynamics of cellular aggregate formation. The proposed methodology provides a comprehensive framework for exploring the rheology and non-equilibrium behavior of cellular aggregates.

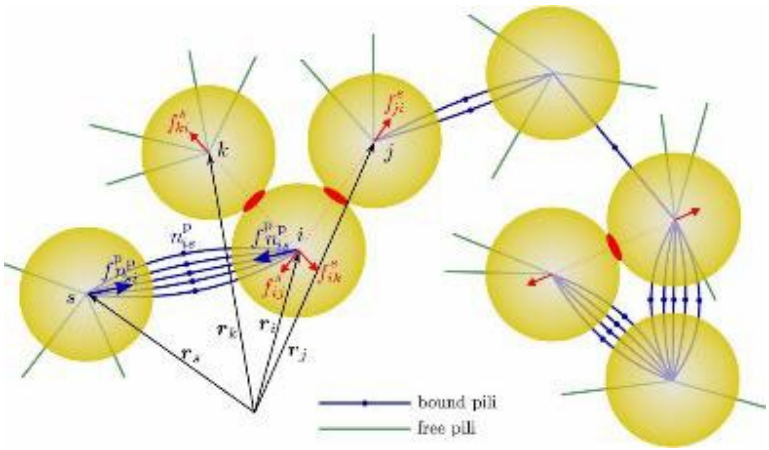

Figure 1. A sketch of N. gonorrhoeae bacteria interacting by their pili. The forces acting on each bacterium are illustrated.

Keywords: cellular aggregates, convection-diffusion equations, active phase separation, continuum modelling

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A lattice Boltzmann approach for viscoplastic shallow flows

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Viscoplastic shallow flows are essential in geophysical and engineering applications, including landslides, mudflows, and debris transport [1-2]. Traditional numerical methods often face challenges in capturing the interplay between free-surface dynamics and viscoplastic rheology. In this study, we present a lattice Boltzmann method (LBM) designed to solve two-dimensional shallow water equations (SWEs), building upon our previous model for Cauchy equations [3-4]. This approach retains the advantages of LBM while directly deriving the governing equations without relying on viscosity-dependent relaxation times or a coupled pressure-density relationship. This study builds upon our previous research on the one-dimensional Saint-Venant equations for viscoplastic fluids [5]. Our novel formulation enables the incorporation of additional stress terms relevant to viscoplastic fluids, making it a versatile tool for generalized SWEs. A key contribution of this research is the extension of the model by incorporating the Herschel-Bulkley-Papanastasiou model for viscoplastic fluids. With the exponential regularization, the method accurately captures viscoplastic flow behavior while mitigating the numerical challenges commonly encountered with shallow water equations (SWEs). Benchmark simulations validate the method's accuracy in capturing key viscoplastic flow characteristics, including yield surfaces and shear localization [7-9]. The results demonstrate the potential of the LBM as a robust and efficient framework for simulating shallow water flows with complex non-Newtonian behaviour. Figure 1 presents depth (left) and Froude number (right) contours of dam break passing three square cylinders for a viscoplastic fluid.

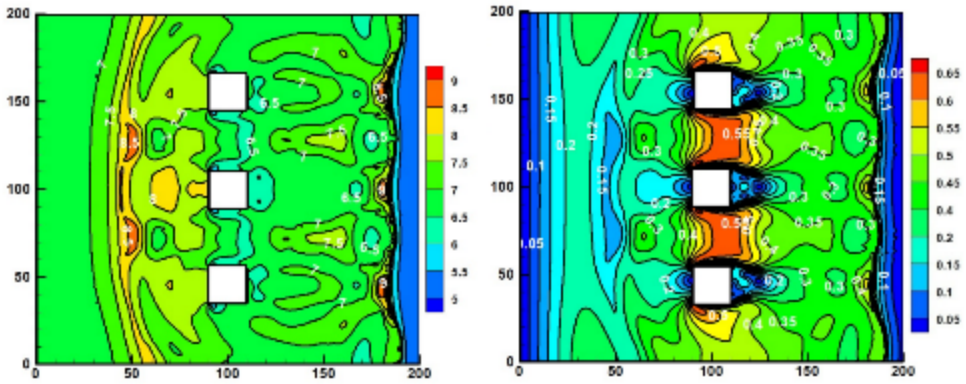

Figure 1.

Keywords: Lattice Boltzmann method (LBM), Shallow water equations (SWEs), Viscoplastic fluid

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Application of Deep Learning Model for Nonlinear Response-History Analysis in Multi-Objective Design Optimization for Base-Isolated Reinforced Concrete Structures

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Nonlinear response-history analysis (NRHA) is acknowledged as a highly accurate technique for evaluating the seismic performance of buildings, as it captures detailed insights into structural inelasticity, damage potential, and stability conditions under strong ground shaking. However, NRHA's extensive computational demands limit its popularity in practical design. To overcome this challenge, the present research introduces a Graph-based Long Short-Term Memory (GraphLSTM) [1] approach, combining spatial pattern extraction via Graph Neural Networks (GNNs) and temporal dynamic forecasting with Long Short-Term Memory (LSTM) units. This integrated method significantly accelerates predicting nonlinear seismic responses across various structural typologies. The GraphLSTM model is trained specifically for base-isolated reinforced concrete (RC) structures in this study. Following model training, a multi-objective optimization algorithm is employed for structural design. The results demonstrate the capability of GraphLSTM as an efficient and accurate surrogate for conventional NRHA. The accelerated analysis provided by GraphLSTM enables design optimization by performing extensive NRHA simulations within a relatively short timeframe. In designing base-isolated structures, increasing isolator strength typically reduces isolator displacement but simultaneously increases floor accelerations in the superstructure. By utilizing extensive NRHA simulations through the trained GraphLSTM model, the study successfully integrates multi-objective optimization techniques to identify Pareto-optimal designs, effectively addressing the inherent trade-off between minimizing superstructure accelerations and controlling isolator displacements. The resulting Pareto front provides engineers with clear insights into feasible design alternatives and meaningful information for decision-making. Ultimately, this research advances performance-based design practices for base-isolated RC structures and significantly contributes to progress in earthquake engineering.

Keywords: Nonlinear Response-History Analysis, Graph Neural Networks, Long Short-Term Memory, multi-objective optimization, base-isolated reinforced concrete buildings

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Modelling of Hybrid Carbon Black and Carbon Nanofiber Reinforced Ultra-High-Performance Concrete for Enhanced Self-Sensing Capabilities

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Abstract: This study investigates the self-sensing properties of ultra-high-performance concrete (UHPC) modified with hybrid carbon black (CB) and carbon nanofiber (CNF) fillers. Utilizing data-driven modelling techniques, the research explores the relationship between conductive network structures and piezoresistive performance under mechanical loading. Experimental investigations combined with advanced characterization methods, including X-ray diffraction (XRD), scanning electron microscopy (SEM), and AC impedance spectroscopy (ACIS), reveal the synergistic effects of CB and CNF in enhancing electrical conductivity and self-sensing behaviour. The study employs equivalent circuit modelling to characterize conductive pathways and to analyze the role of CNF in improving conductive network continuity. coefficient. Based on the analysis of the microstructure and the involved conductive behaviors, the overall equivalent circuit model is expressed as ((R_1 (C_1R_2))(R_3Q)(R_4W)) and its impedance formula is shown in the following equitation:

$$\frac{1}{Z} = \frac{1}{R_1 + \frac{R_2}{1+w^2R_2^2C_1^2} - j\cdot\frac{wR_2^2C_1}{1+w^2R_2^2C_1^2}} + \frac{1}{R_3+Z_Q} + \frac{1}{R_4+Z_W} \quad (1)$$

where Z denotes bulk UHPC impedance; C_1 represents the capacitive behaviour of the insulated matrix and CB(CNF)/matrix/CB(CNF) structures; R_1 represents the electrical behaviour of directly connected CB/CNF structures and connected pore solution; R_2 represents the electrical behaviour of directly connected CB/CNF structures and connected pore solution. Z_Q represents the electrical behaviour of complex unconnected pore structure; R_3 represents the bulk resistance in series with the unconnected pore in the direction of electrical current and 'R_3+Z_Q' is presented as 'oblique line' in the Nyquist plot; Z_W represents the electrical behaviour of ions diffusion; R_4 represents the bulk resistance in series with charge-diffusion layers in the direction of electrical current, 'R_4+Z_W' is presented as a 'depressed semi-circle' in Nyquist plot.

Results indicate that hybrid CB/CNF fillers contribute to superior mechanical strength and enhanced sensing stability under dynamic and monotonic loading conditions. The hybrid CB/CNF system achieved a compressive strength increase of approximately 15% compared to single CB-filled samples. Additionally, the resistivity decreased by nearly one order of magnitude with CNF inclusion, demonstrating enhanced conductive pathways. Data-driven modelling further demonstrates that CNF improves the continuity of conductive pathways, effectively reducing resistivity and enhancing piezoresistive sensitivity. The proposed model correlates microstructural characteristics with electrical response parameters, providing insights into optimizing conductive network formation in UHPC for intelligent infrastructure applications. This study presents a robust framework for integrating data-driven approaches with multiscale modelling techniques to improve the sensing performance of sustainable construction materials.

Keywords: Ultra-high-performance concrete, Nanofillers, Conductivity, Piezoresistive sensing, Data-driven modelling, Equivalent circuit modelling

Numerical homogenisation of porous composite materials via Scaled Boundary Finite Element Method

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Porous composite materials made of foams are gaining traction in various industrial sectors, and are featured with light weight, high specific stiffness, good energy absorption, and novel thermal, biological, acoustic characteristics. They give unique flexibility in performance-tailoring and possess great potential in multi-functional applications. Highlighted by random cellular geometries, porous materials play an important role in advancing various engineering fields. Especially in civil engineering, novel porous composite forms have found their potential in enhancing the current building and infrastructure components, by reducing the weight, promoting the structural stiffness and protection, while bringing interdisciplinary advantages. A typical example in this field is porous concrete, offering thermal and acoustic insulations for efficient temperature and noise management.

One of the key difficulties in applying porous materials lies in the lack of effective and efficient examination methods, induced by the highly irregular and complex geometries and cellular randomness. This work innovatively adopts scaled boundary finite element method (SBFEM) to assess the mechanical responses of porous materials via representative volume elements (RVEs). RVE is a commonly used approach of finite element (FE) numerical homogenisation to identify the characteristics of the overall domain by evaluating only a small representative volume, which is required to contain all the key features of target composites and implemented with periodic boundary conditions within FE calculations. The existing tools for FE homogenisation of porous materials generally include commercial software such as ANSYS and ABAQUS for simulating the mechanical behaviours. However, originated from the aforementioned complex morphologies of random porous materials, these simulations via software are often time-consuming with overly large node numbers and frequently encountered meshing failures. Applying SBFEM will effectively address this problem, leveraging its superior quad-tree and octree meshing strategies and S-element assembly.

This study will reveal the advantages of using SBFEM in porous material FE homogenisation, highlighted via a direct comparison with ANSYS/APDL, regarding the computational efficiency and accuracy, as well as the applicability in different calculation scenarios. The properties of porous composites with diverse cellular morphologies will also be discussed to quantify the impact of cell sizes, densities, and shapes on the RVE extensional stiffness and shear resistance, shedding light on porous structure designs for specific mechanical components.

Keywords: Porous composite materials, Scaled Boundary Finite Element Method, numerical homogenisation, representative volume elements, random cellular geometries

Numerical Study on the Influence of Prestressing Levels in Post-Tensioned Flat Plate Slab-Column Joints with High-Strength Concrete

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Concrete flat plate structures are widely used in multi-story buildings due to their architectural flexibility and economic efficiency. However, their inherent vulnerability to brittle punching shear failure at slab-column joints (SCJs) poses a major structural risk. Post-tensioning (PT) and high-strength concrete (HSC) have been increasingly adopted to improve structural performance by enhancing shear resistance and mitigating failure. Yet, studies on the combined impact of PT and HSC on the structural behaviour of SCJs remain limited.

This study numerically examines the influence of varying prestressing levels on the punching shear and post-punching behaviour of tested PT-HSC SCJs [1]. Three finite element models were established in LS-DYNA, with a 50 MPa HSC column zone and three prestressing levels of 1.2 MPa, 1.8 MPa, and 2.4 MPa. One model was validated using experimental data [1] to ensure accurate representation of the failure mechanisms. The punching shear behaviour at small deformations and the post-punching behaviour at large deformations of the models are given in Table 1.

Results show that increasing the prestressing levels enhances the punching shear capacity by up to 18.6% (from 1.2 MPa to 2.4 MPa) and the initial stiffness by up to 31% (from 18.80 kN/mm at 1.2 MPa to 24.63 kN/mm at 2.4 MPa) before punching shear failure occurs. However, higher prestressing levels reduce ductility, evidenced by a slight decrease in displacement capacity at punching shear failure, from 28.72 mm (1.2 MPa) to 26 mm (2.4 MPa). The results also indicate a higher post-punching load capacity at increased prestressing levels, though the rate of post-punching load resistance growth depends on the tendon anchorage, regardless of prestressing levels. This behaviour is attributed to the constant amount of through-column reinforcement and similar tendon contributions to post-punching strength.

Prestress level	Punching Shear Failure Stage		Post-Punching Failure Stage	
	Load (kN)	Displacement at punching shear failure (mm)	Load (kN)	Displacement at tendon rupture (mm)
2.4 MPa	640.30	26.00	862.50	229.20
1.8 MPa	577.85	28.68	763.31	259.03
1.2 MPa	540.04	28.72	754.98	260.49

Table 1. Numerical results for PT-HSC SCJs with varying prestressing levels.

Keywords: Post-tensioned slab-column joints, high-strength concrete, prestressing levels, punching shear resistance, finite element analysis.

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Chebyshev Polynomials Based Interval Finite Element Analysis For Interval Field Uncertainty

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In this work, we investigate the interval finite element analysis for structures with spatially varied uncertainty. Given the limited sample data available from practical engineering, the uncertainty is intuitively quantified through an uncertain-but-bounded field. The B-spline decomposed interval field model [1] is employed to reduce the complexity and dimensionality of uncertainty modeling. Then, we use the Chebyshev polynomials of the first kind to approximate the uncertainty, by which the spatially varied uncertain material properties, geometry and external loading are included. The propagation of uncertainty on the structure is then analyzed, where the upper and lower bounds of the interval of structural response can be obtained by an optimization algorithm. Finally, the Chebyshev Interval Polynomials Approximation (CIPA) method is developed in the framework of the finite element method, by which the interval finite element analysis is naturally realized. Several numerical examples are presented to illustrate the effectiveness of the proposed method, in which the uncertain material properties, geometry and loading are investigated, respectively. Compared with the conventional interval perturbation and Monte Carlo methods, the proposed method shows good potential in balancing the accuracy and efficiency of uncertainty propagation analysis, especially for large-scale uncertainties. This work also reveals that the *midpoint offset* phenomenon of the interval perturbation method when dealing with large-scale uncertainties is one of the reasons for its inaccuracy in propagation analysis.

Keywords: Uncertainty propagation, Interval field model, Chebyshev polynomial approximation, Interval finite element method

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Stagnation-shortening inexact Newton method based on unsupervised learning for highly nonlinear hyperelasticity problems on three-dimensional unstructured meshes

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Inexact Newton method is widely used in many scientific and engineering applications, but in some situations its convergence involves a long stagnation period in which the nonlinear residual doesn't decrease much and a large percentage of the total compute time is wasted. The reasons for the stagnation are quite difficult to quantify. In this work, we propose a stagnation-shortening inexact Newton algorithm with a stagnation analysis phase during the Newton iterations in which the norms of the residuals are used as a guiding curve and the vector values of the residuals are centralized and decomposed into a slow subspace and a regular subspace using an unsupervised learning method based on principal component analysis. A targeted quasi-Newton is then performed in the slow space whose solution is later projected back to the global space. We show numerically that with such an embedded learning phase the inexact Newton method converges almost quadratically. As an application, we consider the modeling of the human artery with stenosis using the hyperelasticity equation with multiple material parameters. Due to the significant difference in the material coefficients between the plaques and the healthy parts of the blood vessels, the problem is nonlinearly very difficult. Numerical experiments demonstrate that the proposed method offers significantly reduced number of nonlinear iterations and improved robustness for this rather tough hyperelasticity problem.

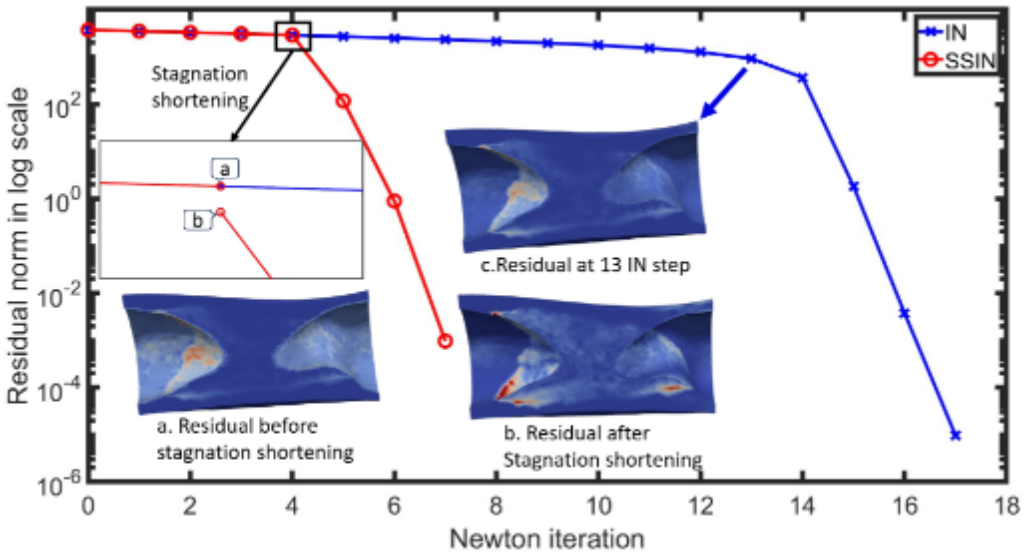

Figure 1.

Keywords: Inexact Newton, learning-based nonlinear preconditioning, principal component analysis, hyperelasticity, finite element, parallel computing

Investigation on Heat Transfer Performance of Graphene Origami/Polymer Nanocomposites Using Molecular Dynamics

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Graphene/paraffin nanocomposites are promising thermal interface materials (TIMs) to dissipate heat in electronic devices due to the high thermal conductivity (TC) of graphene and easy processing of paraffin. Recent research on graphene-based polymer nanocomposites mainly focuses on the TC improvement via interface engineering. Our previous studies have proved that origami-inspired structural modification not only improves the flexibility of graphene, but also the interfacial strength in the polymer nanocomposites.

This work reports the first study of the heat transfer performance of graphene origami (GOri) in polymer matrix. Molecular dynamics (MD) simulations reveal that GOri enhances the TC at the GOri/polymer interface (Eq 1 and 2) by nearly 300% compared to the pristine graphene fillers. This significant TC improvement is attributed to GOri morphology.

$$dT/dz = \frac{\overline{\Delta T}}{h} \tag{1}$$

$$k_{\mathrm{I}} = \frac{J}{dT/dz} \tag{2}$$

where dT/dz is the temperature gradient; $\overline{\Delta T}$ is the average temperature jump in the interface; h indicates the interface thickness; k_{I} represents the TC at the interface and J is the heat flux in nanocomposites.

From the in-depth analysis of radial distribution function (RDF), mean squared displacement (MSD) and vibrational density of states (VDOS) by using equation (3) and (4), we confirm that GOri fillers with rough surfaces and hydrogeneration contribute to strong interfacial interactions and phonon coupling at the filler-matrix interfaces.

$$MSD = < \sum_{i=1}^{N} |r_i(t) - r_i(0)|^2 > \tag{3}$$

where, <> represents the average of calculated group, $r_i(0)$ and, $r_i(t)$ are the atom position at initial and time t and N is the particles number in the composite;

$$D(\omega) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} e^{i\omega t} < \sum_{j=1}^{N} v_j(t) v_j(0) > dt \tag{4}$$

where, $D(\omega)$ is the phonon density at ω, $v_j(0)$ and $v_j(t)$ denote the atom j at initial time and at time t, respectively.

Consequently, However, the presence of creases and sp^3 bonds formed by hydrogenation in GOri give rise to more phonon scattering and thus lead to a reduction in the in-plane TC of GOri/polymer composites. Our findings indicate that GOri is an effective TC filler for improving thermal performance of polymer composites and may offer new design strategies for advanced TIMs.

Keywords: Graphene origami, Polymer nanocomposites, Thermal conductivity, Interfacial interactions, Molecular Dynamics

Finite element analysis of abnormal mechanical responses in a nonreciprocal gel

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This study conducts finite element analysis of abnormal mechanical responses in a nonreciprocal gel [1], which is a uniform composite hydrogel embedded with nanosheets. The nonreciprocal gel exhibits significant mechanical nonreciprocity owing to the buckling of embedded nanosheets. aAs a result, it exhibits distinctive mechanical behaviours including asymmetric inhomogeneous deformation under cylindrical indentation and the abnormal Poynting effect. The nonreciprocal gel is distinguished by three key characteristics: anisotropy, tension-compression asymmetry (TCA), and nonlinearity. To study the effects of these three factors, the finite element analysis of the cylindrical indentation is conducted using a nonTCA (nTCA) model, a TCA model, and a TCA-nonlinear (TCAn) model. Figure 1. shows deformed configurations and strain distributions ε_{11} at indentation depth is 2 mm. The nTCA model shows almost no asymmetric deformation. On the other hand, the TCA and TCAn models exhibit significant asymmetric deformation, and these surface profiles are in excellent agreement with the experiments. The Poynting effect is a nonlinear phenomenon, i.e., when an elastic body is subjected to simple shear or torsion, the strain occurs in the direction normal to the sheared faces or in the axial direction. We conduct plane-strain finite-element analysis under simple shear using the three models: a neo-Hookean (nH) model and two nonreciprocal gel models, vertically oriented nanosheets (NRv) and horizontally oriented nanosheets (NRh). The nH and NRv models exhibit a normal Poynting effect, i.e., negative. In contrast, the NRh model shows the abnormal Poynting effect, i.e., it starts as a negative but changes to a positive. The simple shear condition is imposed by the displacements at the sheared faces, resulting in an inhomogeneous deformation. Among the three models, only the NRh model develops a shear band, which significantly affects the Poynting effect. The strain distributions in the material coordinates reveal that the shear band is induced by the micro-buckling of nanosheets.

Figure 1.

Keywords: Nonreciprocity, tension compression asymmetry, anisotropy, Poynting effect

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Parameter estimation of material models for data assimilation using uniaxial tensile test under high-temperature condition

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During plastic forming of automotive parts, a plastic work caused by the forming increases temperature of the material. The increase of temperature changes mechanical properties and makes it difficult to predict the deformation behavior of material. Therefore, it is crucial to identify material model parameters that depend on temperature. The parameters of thermo-elastoplastic material models have been identified based on material test results obtained under various temperature conditions. However, many high-temperature tests are required to identify accurate model parameters. In this study, we developed a new data assimilation method to estimate the material model parameters for high-temperature condition using high-temperature uniaxial tensile tests. In the data assimilation method developed in this study, we define the extended state vector $\boldsymbol{x}_t$, which contains the parameters to be estimated at time t. The observation vector $\boldsymbol{y}_t$, which contains the material test data. The optimal estimated parameters are estimated by minimizing the cost function $J(\boldsymbol{x}_0)$, which represents the error between the observation and simulation results. $J(\boldsymbol{x}_0)$ is defined as:

$$J(\boldsymbol{x}_0)=\frac{1}{2}\left(\boldsymbol{x}_0-\boldsymbol{x}_0^b\right)^{\mathrm{T}}\boldsymbol{B}^{-1}(\boldsymbol{x}_0-\boldsymbol{x}_0^b)+\frac{1}{2}\sum_{t=0}^{T}\left(H_t(\boldsymbol{x}_t)-\boldsymbol{y}_t\right)^{\mathrm{T}}\boldsymbol{R}_t^{-1}(H_t(\boldsymbol{x}_t)-\boldsymbol{y}_t) \tag{1}$$

where $\boldsymbol{x}_0$ represents the initial state of $\boldsymbol{x}_t$, and $\boldsymbol{x}_0^b$ is the initial guess of $\boldsymbol{x}_0$. $\boldsymbol{B}$ and $\boldsymbol{R}_t$ are called the observation and background error covariance matrices, which represent the uncertainties of $\boldsymbol{x}_0^b$ and $\boldsymbol{y}_t$, respectively. H_t is called the observation operator, which transforms $\boldsymbol{x}_t$ to compare with $\boldsymbol{y}_t$.

In this study, we conducted the uniaxial tensile test simulation for A6061 aluminium alloy at 300 ℃. To describe the deformation behavior of the alloy, the von Mises yield criterion was employed. The parameters of Ludwik's hardening law (s, C and n) were estimated by the developed data assimilation. **Figure 1** (a), (b) and (c) show the distribution of the logarithmic strain ε_{yy} on the surface of the specimen obtained from the uniaxial tensile test, the uniaxial tensile test simulations using the initial estimated parameters (s = 88.79 MPa , C = 48.46 MPa and n = 0.55) and the optimal estimated parameters (s = 67.64 MPa , C = 77.98 MPa and n = 0.45), respectively. U_y represents the forced displacement applied to the lower edge of the specimen. When the optimal estimated parameters were used, the overestimation of the logarithmic strain relative to the uniaxial tensile test was decreased. Therefore, it is concluded that the data assimilation method developed in this study is effective to estimate the material model parameters for high-temperature condition.

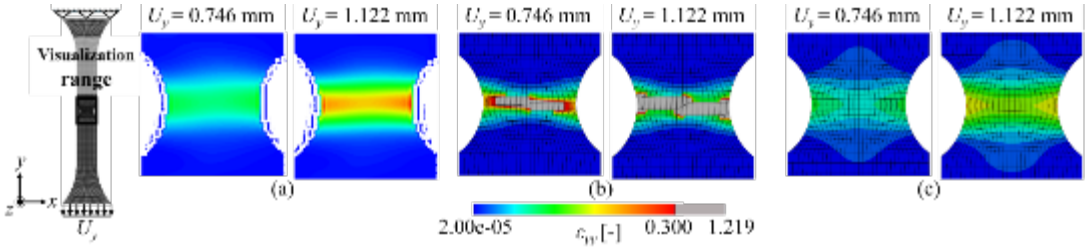

Figure 1.

Keywords: Data assimilation, Material parameter identification, High-temperature deformation behavior.

Adaptive Robust Bayesian Framework for Optimising Battery-Cooling Microchannel Heat Exchangers

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As the global battery market expands, ensuring the safety and reliability of thermal management systems becomes critical for modern energy storage applications. Advances in microchannel heat exchanger design offer numerous avenues—ranging from channel geometry modifications to the introduction of porous media and viscoelastic fluids—for boosting heat transfer. However, the interplay among these parameters is highly nonlinear, making it difficult to discover truly optimal configurations without a systematic optimisation approach.

Moreover, although numerous researchers have optimised heat exchanger performance through optimisation algorithms, few have accounted for real-world input uncertainties—such as manufacturing tolerances or variations in operating conditions—when deriving their solutions. Existing research on robust optimisation typically produces a single fixed solution under a predefined level of risk. Such an approach may fail to meet the varying requirements of practical scenarios, where one design might demand minimal risk whereas another could accommodate moderate fluctuations to further improve the expectation.

To address this limitation, this work introduces an Adaptive Robust Bayesian Optimisation framework. In this framework, the traditional robust optimisation approach Bayes' risk is utilised to quantify the input uncertainty by giving expectation and uncertainty. An adaptive scalarisation method then integrates these two factors, guided by user-defined parameters, to achieve different compromises between mean performance and variance to adapt to multiple degrees of risk tolerance. In this way, instead of returning a single robust solution, this framework generates distinct trade-off solutions for different uncertainty tolerances, thereby aligning better with realistic engineering demands. The novelty lies in enabling a flexible, context-dependent design selection, all while preserving the data-efficiency advantages of Bayesian Optimisation. Although the proposed method is validated using synthetic benchmark problems—due to the insufficiency of existing adaptive robustness test cases—it stands ready for future applications in battery cooling design and other engineering domains requiring resilience to real-world perturbations.

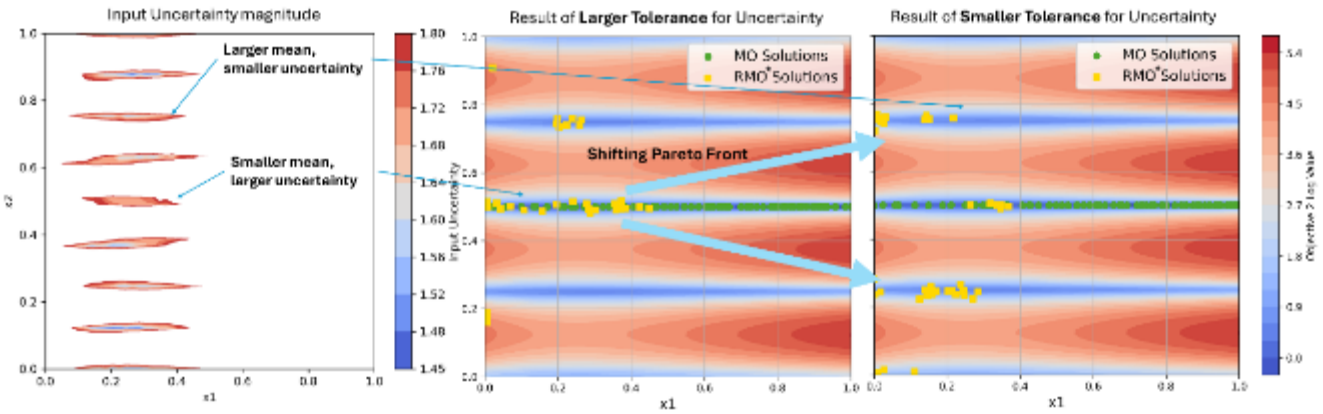

Figure 3 Comparison of Multi-Objective and Adaptive Robust Multi-Objective Solutions Under Varying Uncertainty Tolerances

Keywords: Adaptive robust optimisation, Bayesian optimisation, heat exchanger design, battery cooling

Multiscale shape and topology optimization using level set functions and trimmed meshes

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Let the subscript M and m denote macro and micro scale, whose coordinates are $\boldsymbol{x} = (x_1, x_2)^{\mathrm{T}}$ and $\boldsymbol{y} = (y_1, y_2)^{\mathrm{T}}$. In the shape and topology optimization using the level-set method, structure domains D_M, D_m and boundaries S_M, S_m of a fixed design domain Ω_M, Ω_{m} are represented by an implicit level-set function $\boldsymbol{\phi}_M(\boldsymbol{x})$, $\boldsymbol{\phi}_m(\boldsymbol{y})$ and $\boldsymbol{h}$. A macro level-set function, its trimmed mesh, a basic level-set function of the micro structure and its trimmed mesh cut by height h are described in Fig. 1.

$$\begin{cases} \boldsymbol{\phi_M(x) > 0} & \forall \boldsymbol{x \in D_M} \\ \boldsymbol{\phi_M(x) = 0} & \forall \boldsymbol{x \in S_M} \\ \boldsymbol{\phi_M(x) < 0} & \forall \boldsymbol{x \in \Omega_M} \end{cases}, \quad \begin{cases} \boldsymbol{h - \phi_m(y) > 0} & \forall \boldsymbol{y \in D_m} \\ \boldsymbol{h - \phi_m(y) = 0} & \forall \boldsymbol{y \in S_m} \\ \boldsymbol{h - \phi_m(y) < 0} & \forall \boldsymbol{y \in \Omega_m} \end{cases} \tag{1}$$

The shape and topology optimization problem is formulated by

$$\begin{aligned} &Find && \boldsymbol{\phi}_M \; and \; \boldsymbol{h} \\ &Minimize && a(\boldsymbol{u}_M, \boldsymbol{u}_M, \boldsymbol{C}_H) \\ &subject\ to && \begin{cases} a(\boldsymbol{u}_M, \boldsymbol{v}, \boldsymbol{C}_H) = b(\boldsymbol{v}) \\ \sigma_{pn} < \sigma_a \\ V(\boldsymbol{\phi}_M, \boldsymbol{h}) < V_a \end{cases}, \quad \begin{aligned} &a(\boldsymbol{u}_M, \boldsymbol{u}_M, \boldsymbol{C}_H) = \textstyle\int_{D_M} \boldsymbol{\varepsilon}(\boldsymbol{u}_M) \boldsymbol{C}_H \boldsymbol{\varepsilon}(\boldsymbol{u}_M) dD, \; b(\boldsymbol{v}) = \int_{S_N} \boldsymbol{f v} dS \\ &-1 \le \boldsymbol{\phi}_M \le 1, \; 0 \le \boldsymbol{h} \le 1 \end{aligned} \\ &\boldsymbol{u}_M \in \mathcal{U}, \; \boldsymbol{v} \in \mathcal{V} \end{aligned} \tag{2}$$

where the $\boldsymbol{\phi}_M$ is the macro level-set function, $\boldsymbol{h}$ is the height function, $\boldsymbol{C}_H$ is the homogenized elastic tensor, σ_{pn} and σ_a are the global p-norm stress and its allowable value and V is the volume of the macro structure. $\boldsymbol{u}_M$ is the solution of the constrained state equation in Equation (2), $\boldsymbol{\varepsilon}(\boldsymbol{u}_M)$ is the strain of displacement $\boldsymbol{u}_M$ and $\boldsymbol{f}$ is the external load vector.

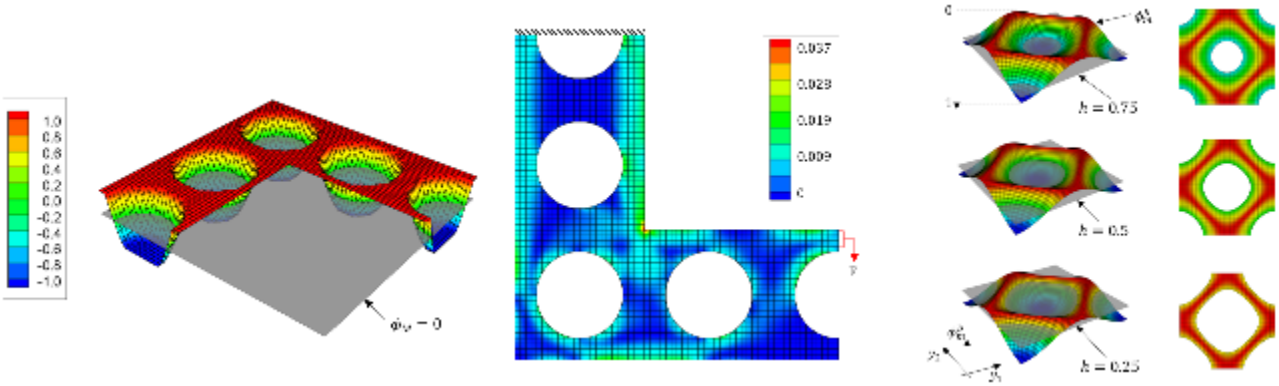

Figure 4. Level-set method for macro structure(left), macro trimmed mesh(center), and level-set method for micro structure and micro trimmed meshes cut by height h(right).

Keywords: multiscale optimization, shape and topology optimization, stress constraints, level set functions, trimmed meshes

A Parallel Implicit Algorithm for Simulating Patient-specific Human Heart

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In this talk, we discuss a highly parallel domain decomposition method for simulating the elastodynamics of a four-chamber human heart with patient-specific geometry. The heterogeneous hyperelastic model is discretized by a finite element method in space and a fully implicit adaptive method in time, and the resulting nonlinear algebraic systems are solved by a scalable domain decomposition algorithm. The deformations of the cardiac muscles are quite complex due to the realistic geometry, the heterogeneous hyperelasticity of the cardiac tissue, and the myocardial fibers with active stresses. Moreover, the deformations in different chambers and at different phases of the cardiac cycle are very different. To simulate all the muscle movements including the atrial diastole, the atrial systole, the isovolumic contraction, the ventricular ejection, the isovolumic relaxation, and the ventricular filling, the temporal-spatial mesh needs to be sufficiently fine, but not too fine so that the overall computing time is manageable, we introduce a baseline mesh in space and a two-level time stepping strategy including a uniform baseline time step size to obtain the desired time accuracy and an adaptive time stepping method within a baseline time step to guarantee the convergence of the nonlinear solver. This is a joint work with Y. Jiang.

Keywords: hyperelasticity equations, human heart, finite element, nonlinear solver, parallel computing

From Informed Optimization to Generative Intelligence: Designing the Next Frontier of 3D Architected Materials

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Architected materials have emerged as powerful platforms for achieving unprecedented mechanical performance through geometrical design at micro- and nano-scales. In this talk, we explore three converging directions in the evolution of 3D structural design: optimization, hybridization, and generative intelligence. First, we present a class of nanoarchitected carbon lattices created via multi-objective Bayesian optimization and two-photon polymerization, achieving specific strength values rivaling carbon steel at ultra-low densities [1]. These designs exploit not only optimal geometries but also leverage pyrolysis-driven atomic gradients for enhanced material properties. Next, we introduce hybrid triply periodic minimal surface-based architectured materials (HTAM), which expand the design space by superimposing multiple TPMS topologies [2]. Using Gaussian process-based Bayesian optimization with parallel hypervolume-driven acquisition strategies, we identify optimal configurations and validate their superior stiffness-to-weight ratios through macro- and microscale fabrication. Finally, we present a forward-looking approach that integrates generative AI into 3D architecture creation, enabling the synthesis of entirely new structural motifs unconstrained by traditional topological paradigms. Together, these three directions represent a paradigm shift toward high-performance, data-driven, and creativity-driven structural design—offering new opportunities in lightweight engineering, energy efficiency, and functional material innovation.

Keywords: Architected Materials, Bayesian Optimization, Triply Periodic Minimal Surfaces (TPMS), Two-Photon Polymerization, Generative AI Design

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Learning Hyperelastic Material Models via PINNs with Minimal Experimental Data

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Discovering constitutive models for hyperelastic materials is crucial yet difficult due to their nonlinear behavior and the scarcity of experimental data. Conventional methods often require extensive stress–strain or full-field data, which are impractical in many real-world scenarios. This study proposes a Physics-Informed Neural Network (PINN)-based framework that identifies constitutive models using limited data such as displacement, strain, and reaction forces—even from a single test. By integrating finite element discretization, the framework reconstructs displacement fields and selects a strain energy density function from predefined candidates while satisfying physical laws. A two-stage training strategy combines neural network optimization with sparse regression to identify concise models. Validation on benchmark problems shows the framework's ability to recover accurate constitutive models and displacement fields, even with scarce and noisy data, demonstrating its practical applicability.

Keywords: Physics-Informed Neural Networks, Hyperelastic Constitutive Modeling, Data-Driven Material Characterization

References

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Oral Inhalation: Understanding Physiologically Realistic Changes of the Human Upper Airway

Brenda Vara Almirall [1], Chun Yuen Jerry Wong [2], Hua Qian Ang [1], Daniela Traini [2], Narinder Singh [3] and Kiao Inthavong [1*]

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The role of computational fluid dynamics in visualising the invisible air during respiration or inhalation is dependent on the airway model that gets used. In recent years there has been a shift towards further realistic patient specific models. This work looks at one subject, and the changes of the airway during restful respiration, open mouth inhalation, and a head tilted back during inhalation [Fig. 1]. The aim of this work is to highlight the sensitivity of realistic airway models on the scan conditions, and to consider the implications of targeted drug delivery to the larynx.

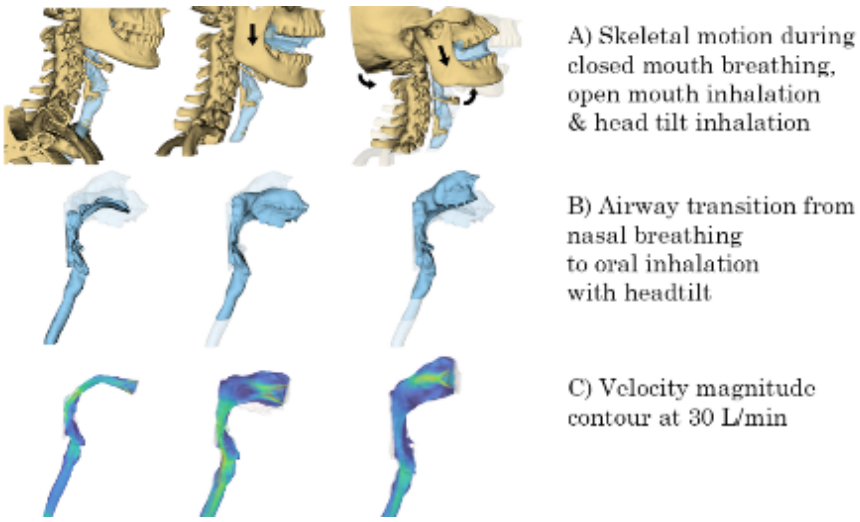

Figure 1.

The delivery method for inhaled medication has huge variation, however there is less discussion on the physiological changes of the models that strongly impact the internal particle flow. This work shows how researchers in this multidisciplinary field may use the physiological differences to better chose airway models to represent the drug inhalation.

Our results indicate that simulating a closed mouth inhalation and an open mouth inhalation (soft palate risen, tongue dropped) we can capture the maximum and minimum ranges of particle deposition in each region of the airway.

Keywords: Oral Drug Inhalation, Computational Fluid Dynamics, Particle Deposition, Experimental Validation

Transformer-Based Temporal Prediction of Hydrodynamic Forces on Ventilated Cavitating Vehicles Using Multi-Sensor Pressure Sequences

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This paper presents a novel Transformer-based framework for predicting the time-varying hydrodynamic forces acting on ventilated supercavitating vehicles using historical pressure data. The complex interaction between unsteady cavity dynamics and hydrodynamic responses poses significant challenges for conventional prediction methods. Our approach leverages the self-attention mechanism of Transformer architecture to effectively model long-range temporal dependencies in pressure sequence data, capturing critical nonlinear relationships between cavitation behavior and resultant hydrodynamic forces. The proposed model processes multi-channel pressure history measurements from strategic sensor locations as input sequences, generating multi-step predictions of axial/lateral forces and pitching moments. Through comprehensive validation using both experimental water tunnel data (Re = 5×10^6) and high-fidelity CFD simulations, the framework demonstrates superior performance compared to traditional RNN/LSTM-based approaches, achieving a 23.7% reduction in mean squared error for 5-second prediction horizons. The attention weight analysis reveals the model's capability to automatically identify critical temporal patterns in cavity pressure fluctuations that significantly influence hydrodynamic responses. This data-driven prediction method enables real-time hydrodynamic forecasting without requiring full flow field measurements, offering practical potential for guidance and control optimization of high-speed supercavitating vehicles operating in complex multiphase environments.

Keywords: transformer, ventilated cavities, hydrodynamic force

Real-Time Solutions to PDEs with Neural Operators in Scientific Machine Learning

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Recent advancements in deep learning have led to a surge in research focused on solving scientific problems under the "AI for Science." Among these efforts, Scientific Machine Learning (SciML) aims to address domain-specific data challenges and extract insights from scientific datasets through innovative methodological solutions. A particularly active area within SciML involves using neural operators to find real-time solutions to Partial Differential Equations (PDEs) as their parameters change. This presentation will discuss my latest research in this field, highlighting the significant potential of neural operators for solving complex physical phenomena. Especially, we propose the Finite Element Operator Network (FEONet), which solves parametric PDEs without labeled data by learning solution coefficients in a finite element basis:

$$\hat{u}_h(x;\omega) = \sum_k \hat{\alpha}_k(\omega)\phi_k(x)., \quad (1)$$

We establish theoretical guarantees showing that the predicted solution converges to the finite element approximation, ensuring both approximation accuracy and generalization in the operator learning framework.

Keywords: Neural Operators, Scientific Machine Learning, Parametric PDEs, Finite Element Method, Operator Learning

References

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Coupled MPM and level-set DEM and its application to modelling stone columns

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Simulating discrete-continuum interactions, especially those involving irregularly shaped particles and large-deformation continua, has historically presented significant challenges. We introduce a novel framework that effectively integrates the level-set discrete element method (DEM) with the material point method (MPM) on a graphics processing unit (GPU) architecture. This approach specifically addresses the complexities associated with arbitrarily shaped particles and their interactions with large-deformation solids. We apply the framework to model soft soil improvement using stone columns, where the soft soil is modelled by MPM and the stone column by level-set DEM. Prior to this, the parameters of both modules are determined through respective element tests. The efficacy of the integrated scheme is validated by comparing load-displacement results with experimental data. Additionally, we provide multiscale analyses of deformation and force transmission across the two regions, demonstrating the potential of this approach in tackling complex geotechnical applications.

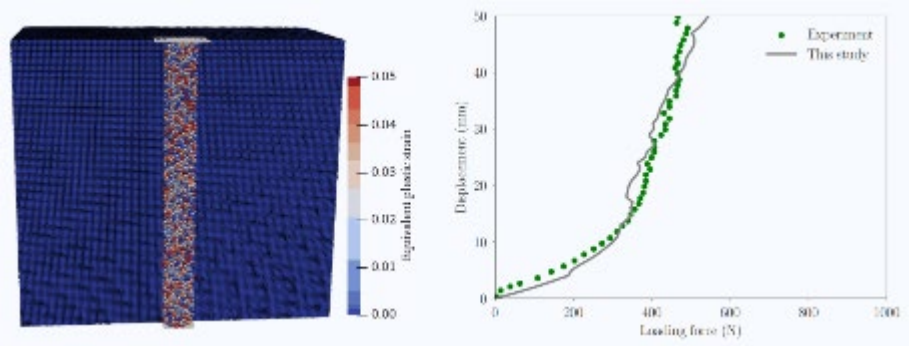

Figure 1. Modelling stone column with coupled MPM and level-set DEM

Development of polymer micromachined insect-mimetic wings using fluid-structure interaction analysis

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Insect flapping flight is governed by complex aerodynamic forces that induce cambering and pitching, making it crucial to understand their locomotion dynamics. This study employs fluid-structure interaction (FSI) analysis to develop a polymer micromachined insect-mimetic wing based on the FSI design concept. The design solution is determined through design window search using static analysis and then fabricated via polymer micromachining, incorporating actual insect and polyimide material properties. Further, a pixel model is proposed which transforms an unstructured mesh into a structured one, reducing the computational cost. The novelty lies in the development and analysis of a microfabricated wing using the FSI design concept.

A parallelized projection method using iterative algebraic splitting, stable for large elastic deformations, is employed for the FSI analysis. The monolithic equation can be written as [1]:

$$_{\mathrm{L}}\mathbf{Ma} + \mathbf{Cv} + \mathbf{N} + \mathbf{q}(\mathbf{u}) - \mathbf{Gp} = \mathbf{g}, \;\; _{\tau}\mathbf{Gv} = 0, \qquad \text{(1a, b)}$$

where $\mathbf{M, C, G}$, and $\mathbf{N}$ are the mass, diffusive, divergence operator matrices, and convective term, respectively, $\mathbf{q}$ and $\mathbf{g}$ are the internal and external forces, respectively, $\mathbf{a}, \mathbf{v}, \mathbf{u}$, and $\mathbf{p}$ are the acceleration, velocity, displacement, and pressure, respectively.

The fluid mesh is composed of P1P1 elements, while the structure uses MITC4 shell elements for partitioning. Table 1 shows the parameters, while Fig. 1 (a) shows the insect-mimetic wing employed in this setup. The details can be referred from previous studies [1].

Parameters	**Ishihara [2]**	**Vinay**
Flapping freq. [Hz]	148	148
Stroke angle [deg.]	71.4	71.4
Poisson's ratio [ν]	0.49	0.289
Membrane [Pa]	7.0×10^9	3.5×10^9
Center vein [Pa]	2.8×10^{12}	1.3×10^9
Leading edge [Pa]	3.5×10^{16}	2.5×10^9
Root vein [Pa]	5.1×10^{15}	2.3×10^9
Mass [kg]	0.49×10^{-6}	0.23×10^{-5}

Table 1.

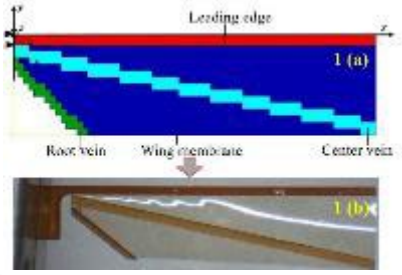

Figure 1 (a), (b).

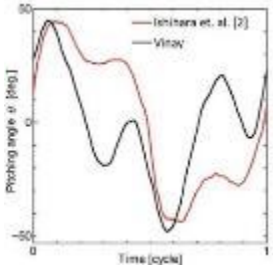

Figure 2.

Fig. 1 (b) shows the wing fabricated using polymer machining, and its flight performance is evaluated using FSI analysis. The result in Fig. 2 shows a rapid decrease in pitch angle after reaching the maximum, with lift and camber synchronized to pitching. The average lift C_L required for insect hovering is 1.19, while the present model achieved 1.0, indicating insufficient lift. Comparison with actual insects shows the model to be 4 to 5 times stiffer. Despite the model's roughness, vibration theory aligns with the numerical results, indicating further adjustments to mass and stiffness are needed. Then, modifying the membrane stiffness and flapping frequency using FSI analysis improves the aerodynamic performance, exceeding the required lift. Hence, polymer micromachined insect-mimetic wing is successfully developed using FSI analysis.

Keywords: fluid-structure interaction analysis, polymer micromachining, insect-mimetic wings

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Optimizing Energy Forecasting in Low-Energy Houses: A Data-Driven Feature Selection Approach

Gongli Li [1*], Yidie Luo[1], Zhen Luo[1], Nick Bennett[1], and Mohammad S. Islam[1]

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Accurately predicting appliance energy consumption in low-energy houses is critical for optimising energy efficiency, reducing costs, and minimising environmental impact. Household appliances constitute a substantial segment, accounting for approximately 20 to 30 % of the total electrical energy demand. In Australia, household appliances and equipment contribute around 25% of residential energy usage. Traditional approaches often focus on a limited number of variables, such as room temperature or aggregated power consumption. They overlook important features, such as indoor environmental factors, occupant-driven patterns, and external weather conditions. Building machine learning models and identifying the most relevant features can help to understand the relationships between different variables and appliances' energy consumption to assess their impact. This study proposes a novel data-driven feature selection framework to enhance predictive modelling of appliance energy consumption using a real-world experimental dataset from a low-energy house. Temperature and humidity data from wireless network sensors (WSN), weather data (temperature, pressure, humidity, windspeed, visibility, and dewpoint) gathered from a nearby weather station, and lighting fixtures energy consumption (total 25 features) are considered. Key influencing factors identified include lighting energy consumption, humidity in the kitchen, and temperature and humidity in the laundry area. Weather-related variables such as wind speed, atmospheric pressure, and humidity emerged as critical predictors, with air temperature ranking third in importance. This study highlights the effectiveness of feature selection in improving energy consumption predictions and provides insights into the most influential parameters for optimizing energy use in low-energy buildings. The findings contribute to smart energy management strategies by offering a robust, interpretable, and computationally efficient approach to appliance-level energy forecasting.

Keywords: Appliances, Energy, Low-energy house, High-dimensional data, Machine Learning, Wireless Sensor Network

Enhancing Heat Transfer with Perforated Vortex Generators

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Improving heat transfer efficiency in fin-and-tube heat exchangers is crucial for reducing energy consumption and operational costs in various industrial applications such as power generation, chemical processing, and HVAC systems. Among the different enhancement methods, rectangular winglet vortex generators have gained considerable attention due to their capability to disrupt thermal boundary layers and generate secondary flow structures, thereby improving heat transfer performance. While previous studies have demonstrated the effectiveness of rectangular winglets in enhancing thermal performance, the impact of introducing punched holes with varying shapes on vortex generation and heat transfer efficiency remains unexplored. Addressing this gap, this study investigates the underlying mechanism behind thermal performance improvement by analysing the influence of rectangular winglet vortex generators with different hole shapes in fin-and-tube heat exchangers. The turbulence effects are modelled using the k-ε RNG turbulence model, due to its accuracy in predicting Reynolds stresses under turbulent flow conditions. Simulations cover a Reynolds number range from 400 to 2400, representing both laminar and transitional flow regimes typically encountered in practical applications. Results indicate significant improvements in heat transfer coefficients and reductions in pressure drop when using rectangular winglets with punched holes compared to solid rectangular winglets. Moreover, the shape of the holes is found to significantly influence vortex formation and flow resistance, highlighting their importance in design optimisation. This research provides critical insights into advanced vortex generator designs for enhancing the thermal-hydraulic performance of fin-and-tube heat exchangers, thereby contributing to more efficient heat exchanger designs.

Keywords: Vortex generators, heat exchangers, heat transfer enhancement, vortex formation, rectangular winglets.

Active Regions of Transonic Buffet by Fluid-Structure Interactions

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Transonic buffet is a complex unsteady flow problem that involves large self-sustained shock oscillations and flow separation. It is also a nonlinear flow problem where the computational fluid simulations can reproduce the phenomena but fall short of explaining the inherent instability. A linear reduced-order model should help us to carry out the stability analysis with efficiency. Even though many researchers have investigated the active regions of transonic buffet using the global instability, local selective frequency damping method and so on, the exact regions are not fully determined.

This study incorporates the autoregressive exogenous method with the local elastic skin to establish the aeroelastic space state model of the fluid-structure interactions, as Eqn. (1) shows:

$$\begin{Bmatrix} \dot{\boldsymbol{X}}_{\boldsymbol{s}}(t) \\ \dot{\boldsymbol{x}}_a(t) \end{Bmatrix} = \begin{bmatrix} \boldsymbol{A}_s + \boldsymbol{q} \cdot \boldsymbol{B}_s \boldsymbol{D}_a \boldsymbol{C}_s & \boldsymbol{q} \cdot \boldsymbol{B}_s \boldsymbol{C}_a \\ \boldsymbol{B}_a \boldsymbol{C}_s & \boldsymbol{A}_a \end{bmatrix} \cdot \begin{Bmatrix} \boldsymbol{x}_s(t) \\ \boldsymbol{x}_a(t) \end{Bmatrix} = \boldsymbol{A}_{ae} \cdot \begin{Bmatrix} \boldsymbol{x}_s(t) \\ \boldsymbol{x}_a(t) \end{Bmatrix}, \tag{1}$$

where $\boldsymbol{x_s}(t)$ and $\boldsymbol{x}_a(t)$ are the state vectors of the structural generalized displacement and the aerodynamic force, respectively. The state matrices $\boldsymbol{A}_s$, $\boldsymbol{B}_s$ and $\boldsymbol{C}_s$ are determined by the aeroelastic governing equations based on modal coordinates while $\boldsymbol{A}_a$, $\boldsymbol{B}_a$, $\boldsymbol{C}_a$ and $\boldsymbol{D}_a$ are determined by the reduced-order model. The model is trained on the linear development stage of the unstable steady base flow with small perturbations realized by given generalized displacements of the skin generated from the Filtered White Gaussian Noise signal.

By analysing the eigenvalues of $\boldsymbol{A}_{ae}$ with varying base frequencies of the elastic skin, the root loci of the aeroelastic system are derived, whose real parts stand for the growth rates of the corresponding modes. The length of the elastic skin is set to be 0.1c (c is the chord length of the aerofoil.). Different locations of the skin are also investigated to form the contour of the growth rate as Figure 1. For validation, the responses of the generalized displacement calculated from the time domain computation are also marked in Figure 1. The zero-level contour line generally predicts the flutter boundaries and there are multiple bifurcations from 0.25c-0.5c. There are two branches of root loci at each tested skin location, where the least stable couped fluid mode can be spotted. The active regions of the buffet are estimated from 0.25c-0.5c with positive growth rate of the least stable fluid modes. These locations are related to the shock foot and the separation point, suggesting that the cause of the buffet is independent of the region near the trailing edge.

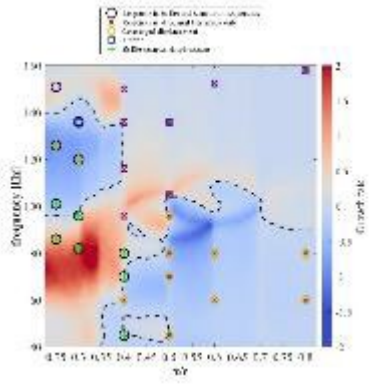

Figure 1.

Keywords: Transonic buffet, fluid-structure interactions, reduced-order model, aeroelastic instability

Template for APCOM-ACCM 2025 Abstract Submission

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High-rise and super-high-rise building structures play an important role in cities, and their seismic performance analysis is especially critical. The traditional structural dynamic analysis models based on machine learning, especially long short-term memory network, can predict the structural response quickly and efficiently, but there are a number of problems that need to be solved: excessive dependence on the quality of the data set, poor interpretability, difficult to predict the plastic deformation in high-rise and super-high-rise building structures, and the response data in the data set uniformly adopts the same length of the sequence, which is not in line with the real response of the structure in the actual engineering. The random initialization in the network training process also leads to randomness and instability in the learning process. This study aims to develop a prediction model of seismic response of super high-rise structures by integrating physical information, which combines the ground shaking intensity index and structural dynamics equations of motion with the long short-term memory network. By establishing structural response datasets with different sequence lengths, the long short-term memory network automatically fills the data with different sequence lengths when loading the data, while the characteristics of the filled part of the data are not considered during the network training process to avoid the introduction of noise, thus realizing the network's prediction of structural response with different sequence lengths. The parameters of the output layer of the network are initialized to reduce the initial training loss of the model, using the predicted values derived from the relationship equation between the ground vibration intensity index and the engineering demand parameters as a guide. The plastic deformation of the structure is predicted through the unbalanced force terms separated in the equations of motion by the substructure method, and the deformation coordination conditions of the main-substructure are utilized to physically constrain the plastic deformation. The experimental results show that, compared with other models, the dynamic analysis model established by this method not only realizes the accurate prediction of structural response, but also significantly improves the network training efficiency, and the accuracy of the prediction of structural plastic deformation reaches a fairly high level, and effectively solves the problem of the current model's limitation on the length of the data, which provides a more reliable and efficient tool for seismic design and safety assessment of super-high-rise buildings.

Keywords: Long short-term memory network, high-rise building structure, plastic deformation, intensity index, sequence length, earthquake response prediction

Enhancing Seismic Resilience in Hillside Reinforced Concrete Structures through High-Damping Rubber Bearings: A Computational Analysis

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Abstract

Buildings on hillsides with split foundations face unique seismic challenges due to uneven soil conditions. This study investigates the effectiveness of high-damping rubber bearings (HDRBs) in combination with the Deformation History Integral (DHI) model to simulate the complex nonlinearity of HDRBs and mitigate seismic risks. Using Finite Element Analysis (FEA), three structural configurations were analysed: Split Foundation (SF), Split Foundation Isolated System (SFIS), and Split Foundation Middle-story Isolated System (SFMIS) under varying earthquake intensities. The results demonstrate that base and middle-story isolation significantly reduce seismic forces, with base shear reductions ranging from 78% to 86% compared to non-isolated structures. Additionally, inter-story drifts are greatly improved, with isolated systems showing drifts below 0.30%, while non-isolated models experience drifts up to 1.5%. Roof accelerations are also substantially reduced, with isolated systems maintaining peak accelerations within the acceptable range of 0.2g to 0.3g. The integration of HDRBs, modeled with the DHI approach, effectively absorbs and dissipates energy, reducing peak accelerations, inter-story drifts, and story displacements in isolated structures. The stable hysteresis behaviour and enhanced strain stiffening of HDRBs improve their energy dissipation capacity, significantly bolstering the seismic resilience of hillside buildings. These findings underscore the importance of isolation systems, particularly in the SFMIS configuration, and highlight the value of DHI modeling in enhancing the safety and stability of hillside structures during seismic events.

Keywords: High-damping rubber bearings; hillside structures; DHI model; split foundation.

Numerical study of parametric excitation effects on a deep-sea mining riser

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In the deep-sea mining system, the mining riser is a critical component connecting the mining vessel to the buffer station. The heave motion of the mining vessel results in varying axial forces in the riser, which may induce parametric vibration of the riser. Unlike the traditional risers with hinged ends, the mining risers with the suspended state of the bottom buffer station are more prone to parametric vibration. Prolonged exposure to parametric resonance can readily lead to fatigue damage in the riser. This study employs the characteristic root method to derive and solve the parametric resonance control equation of the mining riser. The perturbation method is used to solve the Mathieu equation and determine the parametric instability zone of the mining riser. The Runge-Kutta method is employed to calculate the vibration response and dynamic characteristics of the riser. The results indicate that maximum vibration displacement occurs at the bottom, and the parametric resonance of the mining riser exhibits a mixed characteristic of standing wave and traveling wave behavior. Additionally, the vibration frequency demonstrates quasi-periodic characteristics.

This study simplifies the mining riser as an Euler beam to solve its vibration problem:

$$\frac{\partial^2}{\partial z^2}\left(EI\frac{\partial^2 x}{\partial z^2}\right)-\frac{\partial}{\partial z}\left(T(z,t)\frac{\partial x}{\partial z}\right)+m_e\frac{\partial^2 x}{\partial t^2}+\frac{1}{2}\rho_w D_o C_d\left|\frac{\partial x}{\partial t}\right|\frac{\partial x}{\partial t}=0 \tag{1}$$

where t is the time, s; EI is the bending stiffness of the riser, N.m^2; $T(z,t)$ is the axial tension, N; m_e is the equivalent mass per unit length, kg; x is the lateral displacement of the riser, m. The calculation formula for $T(z,t)$ is as follows:

$$T(z,t)=m_R g+\int_0^{L-z} w(z)dz+Ka\cos(\Omega t) \tag{2}$$

where m_R is the mass of the buffer station, kg; L is the length of the riser, m; $w(z)$ is the net weight per unit length of the mining riser, N/m; K is the equivalent spring stiffness of the tensioner, N/m; a and Ω are the amplitude and frequency of the vessel heave motion, m and rad/s, respectively.

The Mathieu equation considering the addition of damping is:

$$\ddot{x}+2\mu\dot{x}+(\delta+2\varepsilon\cos 2t)x=0 \tag{3}$$

where ε represents the strength of excitation and is a small parameter; μ is the damping coefficient; δ is the coefficient related to changes in system parameters. The perturbation method can be used to obtain periodic solutions with periods of π and 2π, thus obtaining the parametric stability diagram.

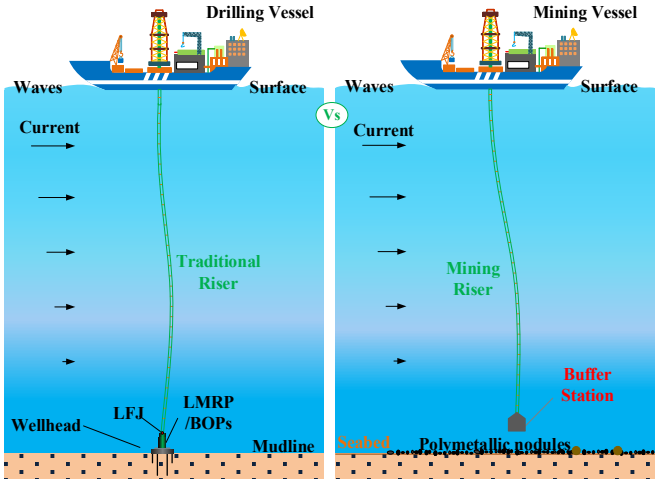

Figure 1. Schematic of the risers under: (a) the drilling riser and (b) the mining riser

Keywords: mining riser, parametric vibration, Mathieu equation, instability zone, quasi-periodic.

Gravitational Instability and Flow Reversal in Open Cavity Mixing: An Investigation using the Lattice Boltzmann Method

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The mixing of a dense passive scalar in an open cavity, driven by gravitational effects, is a critical process in fluid dynamics with applications in engineering and natural systems such as pollutant dispersion in reservoirs and CO_2 mixing during carbon sequestration. We employ the lattice Boltzmann method (LBM) to numerically investigate the dynamics of mixing and flow evolution within an open cavity, where the scalar is released from a top channel. The hydrodynamics is simulated using a D2Q9 incompressible LBM, while the advection-diffusion equation governing scalar transport is solved using a D2Q5 Multi-Relaxation-Time (MRT) LBM. The gravitational effect is modelled using the Boussinesq approximation, allowing for the analysis of buoyancy-driven instabilities that may enhance mixing efficiency.

The flow direction within the cavity, quantified by the curl of the velocity field, exhibits a striking reversal beyond a critical Rayleigh number, signalling a transition in the dominant transport mechanisms from forced convection to gravitational instability (Figure 1). Parametric simulations reveal how gravitational instability amplifies mixing and how the Rayleigh number governs the shift from one flow regime to another. This LBM-based approach provides detailed insights into the spatiotemporal evolution of the flow and scalar distribution, offering a robust framework for studying gravitationally driven mixing in confined geometries. These findings advance the understanding of buoyancy-driven mixing in confined geometries and provide a foundation for accurately modelling and predicting mixing processes in engineering and environmental applications.

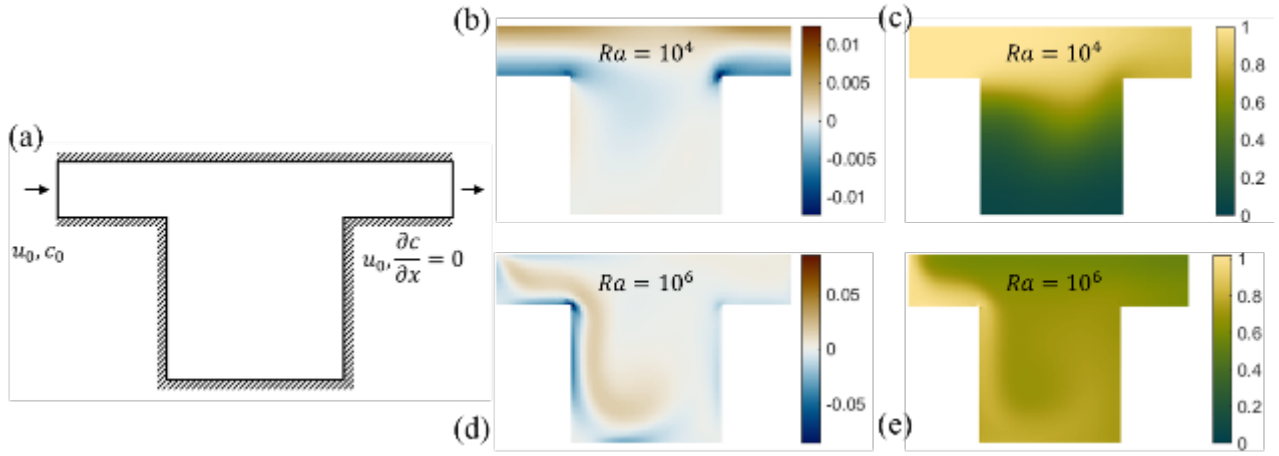

Figure 1. (a) Problem schematic. The curl (b) and concentration (c) of the flow during mixing at Rayleigh number $Ra = 10^4$. (d-e) Results at $Ra = 10^6$.

A Density Smoothing B-Spline Material Point Method for Fluid-Structure Interaction Problems

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In simulating nearly incompressible fluids, a common issue is pressure instability/oscillation for MPM/BSMPM, which arises from volumetric locking and an over-constrained system of equations. In this work, a node-based density smoothing scheme is introduced into BSMPM (referred to as ds-BSMPM) to eliminate pressure oscillations. The proposed algorithm ensures the smoothing of material particle density while simultaneously eliminating pressure oscillations in the simulation of weakly compressible fluids. In this approach, the same B-spline basis functions are used for the density smoothing, with generic form:

$$(\bullet)_p\left(\boldsymbol{x}_p,t\right)=\sum_I S_I\left(\boldsymbol{x}_p\right)\cdot(\bullet)_I\left(t\right) \tag{1}$$

$$(\bullet)_I\left(t\right)=\sum_p S_I\left(\boldsymbol{x}_p\right)\cdot(\bullet)_p\left(t\right) \tag{2}$$

In practice, a lumped mass is used to reduce the computational cost, and the nodal values of the smoothing density are approximated using

$$\bar{\rho}_I\left(t\right)=\frac{1}{m_I}\sum_p m_p\cdot S_I\left(\boldsymbol{x}_p\right)\cdot\rho_p \tag{3}$$

The smoothing density for material particles can be then obtained by

$$\bar{\rho}_p\left(t\right)=\sum_I S_I\left(\boldsymbol{x}_p\right)\cdot\bar{\rho}_I \tag{4}$$

The density smoothing B-spline Material Point Method (ds-BSMPM) with a contact approach is proposed for efficient and accurate simulations of fluid structure interaction (FSI) problems. In order to eliminate pressure instability and oscillation in the simulation of the weakly compressible fluid, a node-based density smoothing algorithm is proposed and straightforwardly implemented in the BSMPM with B-spline basis functions, which omits the need for a sophisticated particle search algorithm and ensures the smoothing of material particle density while simultaneously reducing numerical locking in the simulated flow. Therefore, pressure instability and oscillation are eliminated, and accurate water pressure and solid stress are obtained for FSI problems.

Super dislocation-precipitate interaction in Nickel-based superalloy by virtual dislocation core model

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Nickel-based superalloys are used in high-temperature environments such as gas turbine blades due to their inverse temperature dependence. One of the strengthening mechanism in them is precipitation strengthening [1]. In the γ' phase, super dislocation exists and exhibits complex stacking faults, which affects the mechanical properties in these materials [2]. Dislocation dynamics has been used to reveal the mechanism. In an existing dislocation dynamics method, the dislocation core is represented by placing fractional dislocations based on the Peierls-Nabarro model, making it possible to consider the stacking fault strengthening mechanism [3]. However, it requires a high computational cost because the placement of dozens of fractional dislocations is needed, which makes it difficult to perform large-scale analyses.

Therefore, to address this issue, this study proposes a virtual dislocation core model. In this model, we define a virtual dislocation core at each integration points along the dislocation line in one-dimension instead of fractional dislocations (Figure 1). The force generated by these virtual cores is applied to the dislocation. Therefore, this method requires only a single dislocation line to a consider dislocation core. The force acting on the dislocation can be expressed using the lattice restoring force and the elastic interaction force acting on each virtual dislocation core. The position of dislocations is calculated by using dislocation dynamics where the force is converged. Furthermore, we introduce the Fast Inertial Relaxation Engine method for the convergence calculations, achieving convergence with approximately 1/100th of the computational steps required by conventional methods [4]. Using this approach, we analyzed the interaction between super dislocation and precipitate, investigating the relationship between precipitate diameter and Critical Resolved Shear Stress.

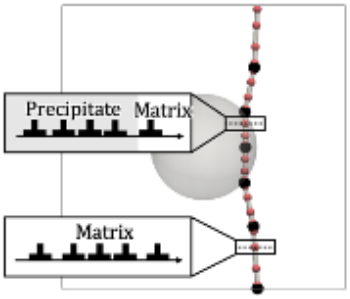

Figure 1.

Keywords: Nickel-based superalloy, dislocation dynamics, precipitation strengthening, stacking fault, super dislocation

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Next-Generation Wind Turbine Blade Repair Method using UV Curing

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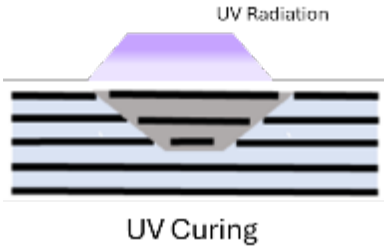
Extending the operational life of wind turbines is essential for both economic and environmental sustainability. One promising approach is the use of ultraviolet (UV) curing for repairing composite wind turbine blades. UV curing offers a fast and efficient alternative to traditional thermal curing methods, significantly reducing turbine downtime, especially in remote or offshore locations where rope-access repairs are common.

This study investigates scarf patch repairs on composite blades using UV curing (as shown in fig.), with a focus on evaluating residual stresses that develop during the repair process. A comprehensive numerical framework is developed in ABAQUS, incorporating a cure- and temperature-dependent viscoelastic material model. The resin's cure kinetics were characterized and used to simulate stress evolution during and after the curing cycle. A coupled temperature-displacement analysis captures the effects of thermal expansion and chemical shrinkage on residual stress buildup.



Custom user subroutines were employed to model chemical shrinkage, heat generation, and evolving material properties. Results show that residual stresses in the repaired region can significantly affect the blade's structural integrity and long-term performance.

Experimental validation was performed by assessing the post-repair behavior of the blade, showing good agreement with numerical predictions. Additionally, X-ray tomography of the repaired sections identified voids within the adhesive layer. Using submodeling techniques, the study evaluated how these voids influence local stress concentrations. It was found that voids can increase local stress by a factor of 2 to 2.5, underscoring the importance of minimizing void formation.

The findings highlight UV curing as a rapid, effective, and scalable repair solution for wind turbine blades. This method not only shortens repair times but also offers strong potential to enhance blade longevity, thus supporting more reliable and sustainable wind energy generation.

Keywords: Wind turbine repair; UV curing; Voids; Residual Stresses

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Comparison of two impulse loading devices applicable to VSM

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Recently, the possibility of using a moving impulse device in a form of a cogwheel together with a scanning vehicle for the drive-by identification has been proposed (see figure1) [1]. Now, a new principle of moving impulse device is designed and tested on a laboratory model. Its impact force can be easily controlled and measured which is an advantage over the cogwheel load. On the other hand, the cogwheel impulse intensity increases with the driving speed, while the impulse intensity of the new devise is constant depending only on gravity. Further advantages and disadvantages of the new operating principle are discussed with respect to various application purposes.

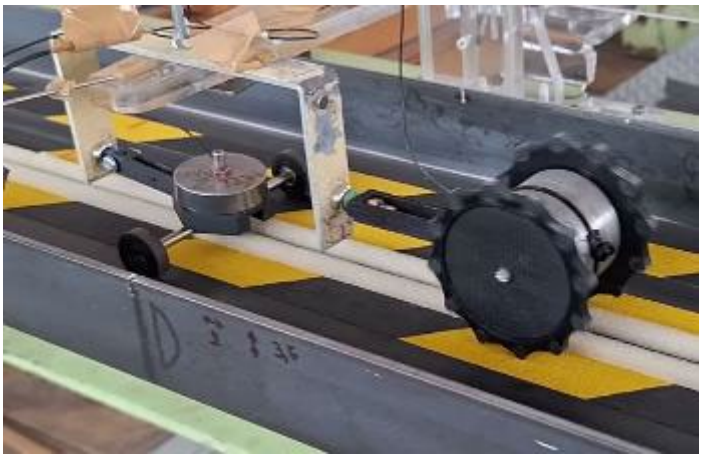

Figure 1. Scanning vehicle at the damage position with accelerometer followed by the CW and theirs common towing device

Keywords: Drive-by Identification, Vehicle Scanning Method, moving impulse load, Numerical simulations

References

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Mode Shape and Binding Behavior of Oxygen Reduction Enzymes: A Molecular Dynamics and Finite Element Methods

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In this study, we present the combination of all-atom molecular dynamics (MD) and finite element methods (FEM) to investigate the vibrational properties of oxygen reduction enzymes. Key residues at the enzyme's active site fluctuate to catalyze substrates, making it important to observe their dynamic behavior. Traditionally, these properties and binding conformations have been evaluated by Quantum Mechanics (QM) simulations using first-principles calculations. We found that mode shapes computed via normal mode analysis (NMA), particularly at the active site, correlate with catalytic activity. Surface-based FEM modeling is also computationally efficient for large biomolecules compared to MD. We solved the eigenvalue problem using ABAQUS, and supported our results with HADDOCK docking and MD trajectory analysis. Binding energies between the active site and various substrates were computed to evaluate conformational differences. Our findings suggest that mode shapes and conformations of active site residues are closely related to substrate binding and catalysis. This computational approach may guide the application of oxygen reduction enzymes such as glucose oxidase (GOx), hydrogenase, and laccase. We are further validating these findings through electrochemical experiments.

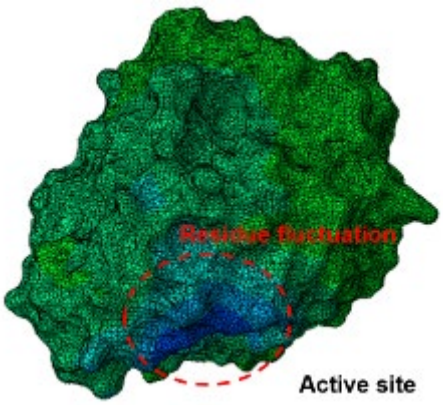

Figure 1.

Keywords: Protein vibration, Molecular dynamics, Enzymatic biofuel cell, Graphene

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Microscopic Insights into Local Scour Mechanism and Mitigation Strategies around Offshore Monopiles Using CFD-DEM

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Local scour is a critical concern for the stability and duration of offshore structures, such as bridges and wind turbines, where erosion processes under variable hydrodynamic conditions may compromise monopile foundations. This work presents a comprehensive study that integrates three complementary investigations employing a coupled computational fluid dynamics and discrete element method (CFD-DEM) framework. First, we examine the full evolution of local scour around a monopile under different hydraulic gradients. The scour process, classified into formation, sedimentation, and stabilization stages, is associated with distinct microscale phenomena including alterations in interparticle connectivity, kinetic energy, drag forces, and particle trajectories. Second, we assess the influence of monopile cross-sectional geometry by comparing circular, square, square with rounded corners, and diamond configurations. While the diamond-shaped pile produces the deepest and widest scour pits, the incorporation of rounded corners emerges as a beneficial modification, mitigating scour evolution by optimizing local flow characteristics. Third, we investigate an advanced scour mitigation approach using sacrificial piles placed in proximity to service monopiles. By analyzing key microscale attributes, such as particle momentum, Reynolds number, and rotational kinetic energy, we demonstrate that appropriately sized and positioned sacrificial piles can significantly delay scour development, with an optimal configuration proposed based on quantitative multiscale insights. Bridging macroscopic scour pit morphology with microscale sediment dynamics, this study provides novel guidelines for both the design of effective offshore monopile foundations and the implementation of robust scour countermeasures.

Keywords: Local scour, Offshore monopile, CFD-DEM, Sediment dynamics, Hydraulic conditions, Cross-sectional geometry, Scour mitigation, Sacrificial pile

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Numerically Stable Evaluation and Automatic Differentiation of Closed-Form Expressions for Eigenvalues of 3×3 Matrices

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Standard non-iterative closed-form expressions for the eigenvalues of 3×3 matrices are derived from the roots of their characteristic polynomial. However, these expressions suffer from numerical instability due to the ill-conditioning of the roots, particularly in the vicinity of eigenvalues with higher multiplicity. Despite this, the eigenvalues themselves remain well-conditioned functions of the matrix entries, as established by the Bauer-Fike theorem [1]. In this work, we propose an alternative approach that circumvents the explicit computation of the characteristic polynomial and its associated principal invariants. Instead, we employ a formulation based on more suitable matrix invariants, leveraging the matrix discriminant expansion introduced in [2] and improving earlier explicit eigenvalue expressions as introduced in [3].

For symmetric matrices, we demonstrate that this expansion yields a sum-of-squares formula for the matrix discriminant, facilitating a forward-stable evaluation. This results in a novel non-iterative algorithm for computing eigenvalues, achieving forward errors on the order of machine precision even in the limit case of matrices with an eigenvalue of multiplicity two. We extend these findings to all real-valued diagonalizable 3×3 matrices by presenting a sum-of-products approach for the matrix discriminant and analysing its numerical stability. We further establish the expected backward stability of the proposed algorithm.

Beyond the evaluation of eigenvalues, we investigate the challenges associated with automatic differentiation (AD) through eigenvalues of general 3×3 matrices. We discuss the implications of ill-conditioning at critical points and along critical paths, identifying sources of numerical instabilities. These issues are especially relevant in computational mechanics, where spectral formulations of elasticity and constitutive laws may introduce non-smooth dependencies. We present selected numerical benchmarks and applications to hyper-elastic materials, specifically Ogden-type constitutive laws, as well as inelastic material models. The stability of the proposed algorithm and its suitability for AD will be discussed through examples in finite-strain elasticity, informed by recent advancements in stable numerical formulations [4].

Keywords: Eigenvalues, Numerical stability, Finite-strain elasticity

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Intelligent Plane Schematic Design of Super High-Rise Frame Core-Tube Structures Based on Function-Stiffness Constraints

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Abstract: Intelligent building and structural design have emerged as a prominent research field [1]. As the design of super high-rise frame core-tube structures involves multi-disciplinary collaboration, conventional data-driven methods are difficult to balance building functions (e.g. space usage) and initial stiffness requirements, resulting in insufficient utility of the generated solutions. To address these limitations, datasets are classified according to code indicators, including building function, fortification intensity and height, and the key building components information are extracted through Tall-DeepLabv3+. This research employs R3GAN as the baseline to improve, and implementing a two-stage methodology. The residual blocks in original generator are replaced with multi-scale convolutional attention networks to enhance the extraction of sparse strip features in plane layout firstly. To satisfy building function requirements, the propagation path of the functional evaluation is added behind the structural design, and indicators, like space utilization rate etc., are incorporated into the functional loss. Secondly, to optimise the components features in diversify positions particularly vertical traffic and floor transition, while enabling the assembly of different functional layout to satisfy the initial stiffness, which achieved by genetic algorithm combined with simplified evaluation model that utilizes inter-story drift angle. Through pre-training and ablation experiments, the generative scheme reaches a 95.74% Intersection over Union Score. It is 4.26% higher than the highest of five mainstream networks such as StyleGAN2, and the Fréchet Inception Distance is reduced by 3.44%. These research results illustrate that the improved network can provide an efficient and practical tool for the intelligent design of frame core-tube structures.

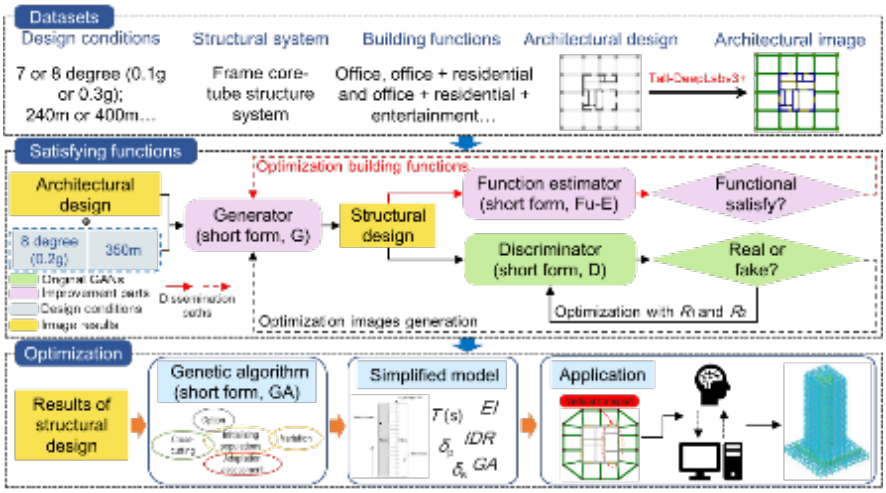

Figure 1.

Keywords: Frame core-tube structure, intelligent design, generative adversarial networks, building function, stiffness requirement.

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Mechanical metamaterials in reducing vibration level of the battery pack

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The effects of the lattice and auxetic structures in mitigating the vibration level of aluminum and polyphthalamide or high-performance/high-temperature nylon (PPA-CF) battery packs under random vibration conditions were studied using a numerical method in the present study. The results show that both structures increase the natural frequencies of the aluminum battery pack to above 200 Hz. The deformation of the original aluminum battery pack is uniformly distributed over its bottom part during longitudinal and transverse vibrations but concentrated at the center of its bottom wall during vertical vibration. With higher natural frequencies, the lattice and auxetic aluminum battery packs can mitigate approximately 97% to 99% of the vibration levels in all three directions, except for some small areas under the battery pack's extension in the transverse direction. Lattice and auxetic structures lower the natural frequencies of the PPA-CF battery packs to about 2.2 Hz to 2.8 Hz. Consequently, these mechanical metamaterials significantly enhanced the vertical vibration levels over the entire PPA-CF battery pack. They can only mitigate the longitudinal vibration levels of the PPA-CF battery pack at its top cover and center front and back walls, which are about 63.8% and 92.8% by lattice and auxetic structures, respectively. The auxetic structure manages to mitigate the transverse vibration level (39.8%) around centre of both side walls of the PPA-CF battery pack. It can be concluded that both mechanical metamaterial are effective in mitigating vibration level of an aluminum battery pack. Aluminum alloy is a better choice for battery pack's material no matter with or without the structural modification compared with PPA-CF.

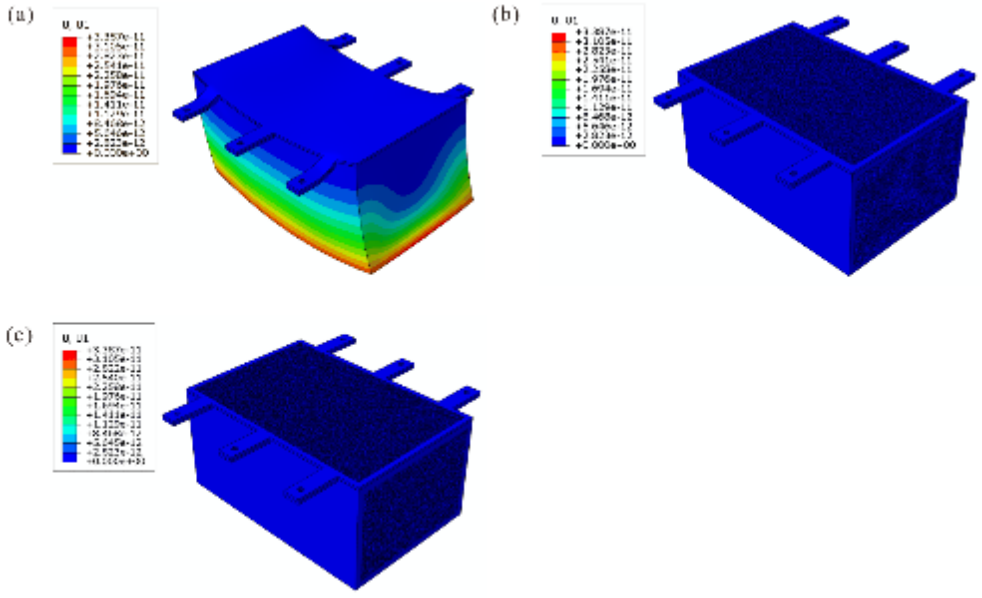

Figure 1. Longitudinal displacement (m^2/Hz) of the three different aluminum battery packs at 15 Hz. (a)Original battery pack (b)lattice battery pack (c)auxetic battery pack.

Keywords: Battery pack, lattice, auxetic, vibration

Utilizing Bayesian Inference to Quantify Model-Inherent Uncertainty in Soil Constitutive Models

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ABSTRACT: Accurately quantifying uncertainty in soil constitutive models is a complex yet crucial task for enhancing predictive accuracy. While Bayesian inference (BI) has been recognized as an effective approach for managing uncertainty, prior research has largely concentrated on uncertainties within input parameters of idealized constitutive models. However, traditional models such as Mohr-Coulomb, Cam-Clay, and Modified Cam-Clay are built on simplified assumptions that fail to fully replicate the complexities of real soil behaviour, making it impossible for them to perfectly match experimental data. This research proposes an innovative framework that utilizes BI to convert deterministic models into probabilistic models, enabling the quantification of uncertainty inherent to the models themselves. A modified variational Bayes method is employed, introducing a penalty term into the negative log-likelihood to develop a new loss function, which improves bias estimation and enhances model reliability. The framework evaluates three different assumptions for the model bias term using triaxial test data from Karlsruhe sand. The findings highlight those non-constant assumptions for the bias term led to significant improvements in model performance. Among the models analysed, the probabilistic Modified Cam-Clay model with a nonlinear bias assumption provides the best results. In contrast, the probabilistic Mohr-Coulomb model shows certain shortcomings, such as overestimating peak deviatoric stress and overfitting volumetric strain, which indicates the necessity for further model adjustments.

Keywords: Uncertainty quantification, Bayesian inference, probabilistic models, model bias, constitutive models

Structural Cross-Section Design Optimization via Graph-Based Reinforcement Learning Integrating Nonlinear Response-History Analysis

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Cross-section design plays a pivotal role in structural engineering, requiring a careful balance between strength and material cost. While thicker sections generally improve structural strength, they also increase material expenses. Despite its importance, current design practices encounter two primary challenges. First, the exploration of the design space remains inadequate. Engineers typically determine initial section configurations based on specific requirements and personal experience, making only minor adjustments through structural analysis software. This approach heavily depends on the engineer's expertise and can sometimes overlook more optimal design candidates. Second, the assessment of design strength is limited. Existing regulations do not require nonlinear response-history analysis to design regular buildings. Instead, engineers favor the less time-consuming Complete Quadratic Combination method of response spectrum analysis for design. As a result, the performance of these designs carries higher uncertainty when subjected to maximum-considered earthquake events.

The rapid advancement of deep learning has created new opportunities to address the aforementioned issues. In particular, Graph Neural Networks (GNN), with their graph-based representation and message-passing mechanisms, closely mirror the topology and force transmission characteristics of structural systems. This resemblance has driven extensive applications in structural engineering, enabling highly accurate and near real-time predictions of nonlinear response histories of buildings [1]. Reinforcement Learning (RL), which empowers agents to explore environments and learn through accumulated experience, is particularly well-suited for optimization problems due to its strong generalization capability. Combined with GNN, RL has been utilized to develop a framework for optimizing two-dimensional steel frame designs [2], minimizing material usage while meeting strength requirements. To tackle the above challenges, this study extends the existing methodologies to design three-dimensional steel buildings with varying geometric shapes. The proposed model is trained under two different code-compliant scenarios for verifying design strength: one only performs response spectrum analysis, while the other additionally conducts nonlinear response-history analysis,

emphasizing the crucial role of nonlinear analysis in structural seismic design. The results highlight the potential of this approach to derive more comprehensive and cost-efficient cross-section designs.

Keywords: graph neural network, reinforcement learning, cross-section design optimization, seismic design, nonlinear response-history analysis

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A Fast Directional BEM for Solving Wideband 3-D Half-Space Acoustic Problems

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In this talk, we will present a new wideband fast multipole boundary element method (BEM) based on a fast directional algorithm (FDA) for solving large-scale 3-D half-space acoustic wave problems. The method employs the half-space Green's function in the boundary integral equations, eliminating the need to discretize the infinite plane and avoiding truncation errors. An improved FDA is developed to expand the kernel functions, enabling efficient matrix-vector product acceleration across a wide range of frequencies. Leveraging the symmetry of the half-space problem, we introduce techniques to reduce the computational cost in fast multipole translations. Specifically, only an additional moment-to-local (M2L) translation for the image part is required, bypassing the computation and storage of other image-related translations. The iterative solver GMRES is used to further accelerate the solution in the proposed FDA-BEM. Numerical examples include large scale models with the nondimensional wavenumber above 400 and number of elements above 3 million solved successfully using the developed method. These results validate the accuracy of the method and demonstrate its nearly linear computational efficiency in solving large-scale 3-D half-space acoustic problems.

Keywords: Fast directional algorithm, fast multipole method, boundary element method, half-space problems, acoustic wave problems

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A mixed diffusive-sharp interface approach for multi-physics modeling and its application to metal additive manufacturing

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Abstract: Interface-coupled multi-physics systems are ubiquitous in natural phenomena and engineering systems. They possess all the features of bulk-coupled multi-physics counterparts: physical coupling occurs through source terms or constitutive relations at every spatial point of the problem domain. Additionally, the physics coupling occurs through an idealized interface or a narrow buffer zone through boundary conditions. Metal additive manufacturing (AM) is such a challenging system. However, existing metal AM models have difficulty handling the laser-metal interaction and associated boundary conditions (BCs) that significantly influence printed part quality. This talk presents a mixed sharp-diffusive interface computational method to overcome these challenges in multi-physics simulations of metal AM processes. The framework consists of two components. The first is a mixed interface-capturing/interface-tracking multi-physics model to explicitly track the gas-metal interface topological changes without mesh motion or remeshing. The second is an enriched immersed boundary method (EIBM) to impose the critical Neumann BCs, which are enforced in a smeared manner in current AM models, on the gas-metal interface with strong property discontinuity.

I will demonstrate how the developed model elucidates the fundamental metal AM physics (e.g., melt pool dynamics, keyhole instability, and powder spattering) and predicts critical part quality-related quantities (e.g., defect and surface roughness). The proposed framework's accuracy is assessed by thoroughly comparing the simulated results against experimental measurements from NIST and Argonne National Laboratory using in-situ high-speed, high-energy x-ray imaging. I will also report other important quantities experiments cannot measure to show the framework's predictive capability.

Bio: Jinhui Yan is an associate professor in the Department of Civil and Environmental Engineering at the University of Illinois Urbana-Champaign. He obtained his B.S., MS, and Ph.D. from Wuhan University (2009), Peking University (2012), and University of California, San Diego (2016), respectively. After a two-year postdoc at Northwestern University, he joined the faculty of CEE@UIUC. His research group broadly works on computational mechanics and its scientific and engineering applications. His honors include the ASME Robert M. and Mary Haythornthwaite Young Investigator Award in 2018 and the Gallagher Young Investigator Medal from the U.S. Association for Computational Mechanics (UASCM) in 2023. The AM model developed by his research group won two prizes in the 2022 NIST AM benchmark modeling contests. His work also won the Best Paper in Manufacturing Technology from the Vertical Flight Society in 2024. He is a Levenick Teaching Fellow and often enters the list of excellent teachers ranked by the students at UIUC. He currently serves as the vice-chair of the computational fluid dynamics (CFD) and fluid-structure interaction (FSI) technical thrust of USACM and the Computational FSI committee of ASME.

Low-dissipation Schemes for Compressible Flows Using Machine Learning Based on Boundary Variation Diminishing Principle

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This study proposes low-dissipation schemes using machine learning based on the boundary variation diminishing (BVD) principle [1] for compressible flow simulations. We consider the Euler equations written as,

$$\frac{\partial U}{\partial t}+\frac{\partial F(U)}{\partial x}=0,\quad U=[\rho \quad \rho u \quad \rho E]^{\top},\quad F(U)=[\rho u \quad \rho u^2+p \quad (\rho E+p)u]^{\top}, \tag{1}$$

where U is the conservative variable, F is flux, ρ is density, u is velocity, E is specific total energy and p is pressure given by the ideal-gas law: $p=(\gamma-1)\rho\left(E-\frac{1}{2}u^2\right)$ with a specific heat ratio γ.

In the Godunov-type finite volume method, which is a typical computational framework for compressible flows, the flux through a cell boundary is calculated by the following equation,

$$\hat{F}=\frac{1}{2}(F_{\mathrm{L}}+F_{\mathrm{R}})-\frac{1}{2}|\alpha|(U_{\mathrm{R}}-U_{\mathrm{L}}), \tag{2}$$

where subscripts L and R denote the physical quantities obtained from the reconstruction in the cells on the left-oriented and right-oriented sides of the cell boundary, respectively, and α represents characteristic speed. Since the second term on the right-hand side in the equation (2) works as artificial viscosity, the BVD principle [1] defines $|U_{\mathrm{R}}-U_{\mathrm{L}}|$ as the boundary variation (BV), and suggests that the reconstruction should minimize the value of BV to suppress the numerical dissipation error.

Several hybrid-type schemes based on the BVD principle have been developed. For example, the MUSCL-THINC-BVD method [2] uses the MUSCL method, one of the representative spatial reconstruction methods, and the THINC method, which excels in capturing discontinuous distributions, as the candidate interpolation functions, and selects an appropriate interpolation function in each cell based on the BVD principle. Recently, a method called the deepMTBVD method [3], which replaces interpolating function selection with machine learning, has been proposed to reduce the computational cost by up to 40% while maintaining the same computational accuracy as the conventional MUSCL-THINC-BVD method.

We constructed deepXTBVD ($\mathrm{X}\in \mathrm{M(MUSCL)},\mathrm{W(WENO3)}$) methods using a new learning method different from Huang's method [3]: whereas Huang's machine learning generated training data from numerical solutions of typical benchmark tests of the Euler equations, in this study, the training data is generated based on random data. We solved the benchmark tests and confirmed that the proposed methods using machine learning based on random data produce numerical results that are as low-dissipation as the conventional BVD methods.

Keywords: Computational Fluid Dynamics, Compressible Flows, Conservation Laws, Low-dissipation Method, Boundary Variation Diminishing, Machine Learning

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Prediction of Blast induced Flyrock Using an Ensemble Deep Kernel Ridge Regression model

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Blasting operations have been widely employed in civil engineering applications to excavate rocks, such as railway excavation, mining and tunnel construction, for its advantages of low cost and high flexibility. However, only a small portion of the explosive energy generated during blasting operations can be applied to the fragmentation of rock, while the remaining part is wasted which brings some negative effects. Flyrock is one of the main negative effects induced by blasting operations, causing fatal or non-fatal injuries. Therefore, the prediction of blast induced flyrock distance is necessary in order to identify the safety zone to prevent the potential injuries.

Considering the complicated relationship between flyrock and its influencing factors, the predictive accuracy of traditional empirical equations are limited. Therefore, in this study, an attempt has been made to predict blast induced flyrock distance using machine learning technique. An ensemble deep model is developed in this study, which use the combination of stacking based representation learning framework (S-RL) and kernel ridge regression (KRR). The S-RL framework is employed for representation learning purpose to develop a deep structure, whereas the MKL serve as the base learner of this framework. The proposed edKRR (Ensemble Deep KRR) model can achieve higher prediction accuracy compared with traditional machine learning methods.

Keywords: Blasting operation, Flyrock, machine learning, stacking based representation learning, kernel ridge regression

Hydrogen-Stabilized Dislocation Interactions Drive Crack/Blister Formation in BCC Metals

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Achieving tritium self-sufficiency is a critical milestone on the path to practical fusion energy. Hydrogen isotope charging in plasma-facing tungsten components is known to induce blistering, which significantly increases tritium retention and jeopardizes self-sufficiency. Despite extensive research, the atomistic mechanisms underlying hydrogen blister formation remain poorly understood, particularly for intragranular blisters observed under sub-threshold hydrogen plasma. Here, we identify the nucleation pathway of such hydrogen-induced blistering. We reveal that hydrogen promotes the interaction between two <111>/2 screw dislocations, facilitating the formation of a <001> edge dislocation junction, which is energetically unfavorable in the absence of hydrogen. This <001> dislocation exhibits exceptional stability and evolves into a <001> vacancy-type dislocation loop under applied strain. The accumulation of these loops during ongoing deformation and dislocation reactions leads to bulk fracture along {001} planes, culminating in hydrogen crack/blister formation. These findings demonstrate universal applicability across BCC metals, providing atomistic elucidation of sub-threshold blistering in tungsten observed experimentally, while delivering novel explanations for hydrogen embrittlement in BCC metals.

Keywords: Dislocation reaction; hydrogen induced damage; atomistic simulation; bcc metals;

Buckling and optimization of arches based on Hencky bar-chain model

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Abstract

This paper presents a computational framework for the in-plane buckling and optimization of elastic arches of any shape, piecewise constant cross-sectional area variation, loading and boundary conditions. The Hencky bar-chain model (HBM) and the energy approach are adopted for the buckling analysis. HBM is well-suited for arches with piecewise constant cross-sections, while the energy approach simplifies the problem by avoiding the derivation and solving of complex governing differential equations. In HBM, the arch is discretized into rigid segments connected by rotational elastic springs, whose stiffnesses depend on the cross-sectional areas—these become the decision variables in the optimization process. The computational framework will be demonstrated by analysing various arch shapes, loading and boundary conditions for their buckling loads and optimal designs for maximum buckling capacity.

Evaluating Soil Movement in Underpass Frame Bridges with Finite Element Method

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With the urbanisation of regional areas, the intersection of highways and railways has become increasingly common. The underpass construction of roads beneath railways effectively prevents level crossings between trains and motor vehicles, thereby enhancing traffic safety. As a result, it has become a widely adopted engineering solution. In recent years, the application of the jacking-in-place method for frame bridges has further facilitated the construction of underpasses beneath railways. However, after the completion of the jacking process, uneven soil movement often occurs at the connection between the abutment and the embankment. Due to the significant stiffness difference between the subgrade and the bridge structure, this issue is particularly prominent and requires in-depth research on effective mitigation measures. The study utilises finite element method to simulate the construction process of jacking-in-place frame bridges, focusing on analysing the characteristics of soil movement between the abutment and the adjacent embankment under different soil conditions. Through numerical simulations, horizontal and vertical displacements in the transition zone between the bridge and the subgrade are analysed. The findings will explore the impact of different types of foundation soils on settlement in the road-bridge transition area, providing valuable reference data for the design and construction of related engineering projects.

Keywords: Highway-railway intersection, uneven soil movement, finite element method, abutment–embankment connection

Brownian Configuration Field – Radial Basis Function meshfree method for simulating concentrated suspension flows

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The multiscale meshless method based on the Brownian Configuration Field (BCF) & Integrated RBF (IRBF) approximation for concentrated fibre suspensions in a Newtonian solvent is developed to simulate concentrated fibre suspensions ($\phi a_r^2 > a_r$), where ϕ and a_r are the volume fraction and the aspect ratio of fibres. For the research, the macro and micro processes are serially proceeded at each time step and then linked together used a kinetic model of the fibre stress. Due to the interaction between fibres, random interaction is introduced into the evolution equation for the solution of fibre configurations using the BCF method. A coupled macro-micro multiscale equation system for concentrated suspension flows in 2-D axisymmetric coordinates is given by [1]

$$\frac{1}{r}\frac{\partial^2\psi}{\partial z^2}+\frac{1}{r}\frac{\partial^2\psi}{\partial r^2}-\frac{1}{r^2}\frac{\partial\psi}{\partial r}=2\omega, \quad (1)$$

$$Re\left(\frac{\partial\omega}{\partial t}+u_z\frac{\partial\omega}{\partial z}+u_r\frac{\partial\omega}{\partial r}-\frac{u_r}{r}\omega\right)-\eta_a\left(\frac{\partial^2\omega}{\partial z^2}+\frac{\partial^2\omega}{\partial r^2}\right)=-(\eta_a-1)\left(\frac{\partial^2\omega}{\partial z^2}+\frac{\partial^2\omega}{\partial r^2}\right)+\left(\frac{1}{r}\frac{\partial\omega}{\partial r}-\frac{1}{r^2}\omega\right), \\ +\frac{1}{2}\left(\frac{\partial^2\tau_f^{rz}}{\partial r^2}-\frac{\partial^2\tau_f^{zr}}{\partial z^2}+\frac{\partial^2\tau_f^{zz}}{\partial r\partial z}-\frac{\partial^2\tau_f^{rr}}{\partial z\partial r}+\frac{1}{r}\frac{\partial\tau_f^{rz}}{\partial r}-\frac{1}{r}\frac{\partial\tau_f^{rr}}{\partial z}-\frac{1}{r^2}\tau_f^{rz}\right), \quad (2)$$

$$\frac{\partial Q_z}{\partial t}+u_z\frac{\partial Q_z}{\partial z}+u_r\frac{\partial Q_z}{\partial r}=(1-\zeta)\frac{\partial u_z}{\partial z}Q_z+\left[\frac{\partial u_z}{\partial r}-\frac{\zeta}{2}\left(\frac{\partial u_z}{\partial r}+\frac{\partial u_r}{\partial z}\right)\right]Q_z+\sqrt{2C_i\dot{\gamma}}QdW_z, \quad (3)$$

$$\frac{\partial Q_r}{\partial t}+u_z\frac{\partial Q_r}{\partial z}+u_r\frac{\partial Q_r}{\partial r}=(1-\zeta)\frac{\partial u_r}{\partial r}Q_r+\left[\frac{\partial u_r}{\partial z}-\frac{\zeta}{2}\left(\frac{\partial u_z}{\partial r}+\frac{\partial u_r}{\partial z}\right)\right]Q_z+\sqrt{2C_i\dot{\gamma}}QdW_r, \quad (4)$$

$$\tau_f^{zz}=(1-\zeta)\frac{\partial u_z}{\partial z}Q_z+\left[\frac{\partial u_z}{\partial r}-\frac{\zeta}{2}\left(\frac{\partial u_z}{\partial r}+\frac{\partial u_r}{\partial z}\right)\right]Q_z+\sqrt{2C_i\dot{\gamma}}QdW_z\,, \quad (5)$$

$$\tau_f^{rr}=(1-\zeta)\frac{\partial u_z}{\partial z}Q_z+\left[\frac{\partial u_z}{\partial r}-\frac{\zeta}{2}\left(\frac{\partial u_z}{\partial r}+\frac{\partial u_r}{\partial z}\right)\right]Q_z+\sqrt{2C_i\dot{\gamma}}QdW_z\,, \quad (6)$$

$$\tau_f^{zr}=(1-\zeta)\frac{\partial u_z}{\partial z}Q_z+\left[\frac{\partial u_z}{\partial r}-\frac{\zeta}{2}\left(\frac{\partial u_z}{\partial r}+\frac{\partial u_r}{\partial z}\right)\right]Q_z+\sqrt{2C_i\dot{\gamma}}QdW_z, \quad (7)$$

where ψ, ω are the stream and vorticity functions, respectively; u_r & u_z the velocity components on r and z directions, respectively; Re is the Reynold number and $\tau_f^{zz}, \tau_f^{zr}, \tau_f^{rr}$ the components of the fibre stress tensor $\boldsymbol{\tau}_f$ determined by the modified Phan-Thien & Graham model [2]; η_a the adaptive viscosity defined in [3]; Q_z and Q_r are the components of the configuration field **Q** and Q is the modulus of **Q**; $\dot{\gamma}$ and C_i are the general strain rate and the interaction coefficient; $\zeta = 2/(a_r^2+1)$.

The simulation method is verified with the axisymmetric expansion flows for a range of the fibre concentration of the concentrated suspension. Besides the advantages of a RBF meshless method and

the BCF approach, the present method shows a significant improvement on both the accuracy and the stability of the stochastic process.

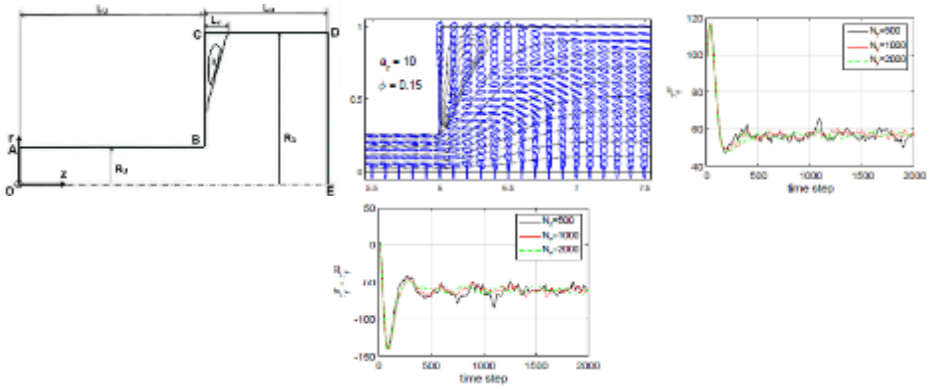

Figure 1.

Keywords: Concentrated fibre suspension, Multiscale meshless method, Brown Configuration Field, Integrated Radial Basic functions.

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Real-time predictions of primary stability in reverse shoulder arthroplasty

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The time necessary to run virtual patient models directly impacts in silico clinical trials, digital twins, and pre-operative planning because these applications all require many simulations. In silico clinical trials entail a virtual population with many plausible virtual patient models. Digital twins and pre-operative planning models consider one single patient, for which many simulations may be necessary to evaluate the patient's recovery or to determine an optimal implant configuration, respectively. This large number of simulations requires significant computational power and time, which limits the broader use of these technologies.

Surrogate modelling may reduce computational cost by training a model on simulation results [1]. This study's objective was to assess surrogate modelling feasibility on data from a previously conducted in silico clinical trial [2], where one single model would take over one hour to solve.

Methods: A subset of data from the completed in silico clinical trial was selected as input, which included 130 finite element (FE) simulations of primary stability for a humerus replacement system, modelling 45 patients with different implant sizes and surgically admissible implantations during simulated unloaded 90° arm abduction. The FE models and bone-implant relative displacement results were mapped to an iso-topological mesh. The relative significance of the peri-prosthetic bone stiffness, implant geometry and position was investigated using two distinct surrogate models. One model used the peri-prosthetic bone stiffness alone as a predictor, whereas the second model additionally included implant geometry and position to predict primary stability. A partial least squares regression (PLSR) algorithm was implemented to relate patient and surgical features to primary stability in MATLAB (Natick, MA, USA). The models were validated using a 10-fold cross-validation scheme.

Results: The goodness-of-fit was $R^2 = 0.94$ ($p < 0.0001$) and RMSE of 0.005 for both models. The peri-prosthetic bone stiffness alone model required 5ms for the prediction. The peri-prosthetic bone stiffness and stem geometry/position model required 11 ms for the prediction.

Discussion: This study demonstrates that a statistics-based surrogate model can accurately predict FE results while allowing a massive time gain, from over an hour to milliseconds. The similar goodness-of-fit of the two surrogate models suggests that peri-prosthetic bone stiffness largely determines primary stability by implicitly accounting for changes in stem size and position, resulting in a light and fast predictive model. In pre-operative planning, the surrogate model could run many simulations and provide a first indication of optimal implant placement. In silico clinical trials typically deliver an order of magnitude more virtual patients than real clinical trials. By increasing the simulation speed, surrogate modelling can enrich the clinical trial by adding several orders of magnitude of datapoints in an acceptable time frame. The study's main limitation resides in the scope of the training data. A new model should be developed for populations, devices, and processes that are different from those analysed here. The excellent fit supports the use of the model in large-scale simulations of implant stability in in-silico clinical trials, digital twins, and pre-operative planning applications.

Keywords: In silico clinical trial, Surrogate modelling, Finite element simulations, Primary stability

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Bridge and Rail Vibration Lab at Chongqing University

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The vehicle-bridge interaction (VBI) dynamics has emerged since the mid-1990s, propelled by the rapid global expansion of transportation infrastructure [1]. In 2004, Prof. Y.B. Yang and collaborators pioneered the Vehicle Scanning Method (VSM) [2], an innovative technique for evaluating bridge dynamic properties via instrumented moving vehicles, eliminating reliance on fixed on-site sensors. To validate VBI theories and accelerate the real-world deployment of VSM, the Bridge and Rail Vibration Laboratory (BRVL) is established, which consists of three zones:

(1) **Highway Bridge Test Zone**: This zone incorporates a full-scale simply supported bridge constructed with three precast reinforced concrete T-beams, spanning 25 meters with a 7.2-meter width and 1.6-meter structural depth (Fig. 1). The bridge is characterized with a vertical bending frequency of 5.3 Hz, torsional frequency of 6.4 Hz, and Class A surface roughness profile. Functioning as a controlled experimental platform, it enables systematic investigation of VBI mechanisms while yielding field-calibrated datasets essential for optimizing VSM in real scenarios.

(2) **Railway Track Test Section**: This section, spanning 25 meters in length and 6 meters in width, incorporates SK-2 double-block ballastless tracks with WJ-8B fasteners and 60 kg/m standardized rails. This section aims to systematically decode the dynamic propagation mechanisms in train-track coupled systems, and more importantly pioneers theoretical frameworks for VSM-enabled rapid inspection technologies.

(3) **Vehicle Dynamic Calibration System**: This system is equipped with eight synchronized electric actuators (5-ton load capacity, 0–20 Hz frequency range), as shown in Fig. 2, enabling precise calibration of vehicle dynamic parameters (mass, stiffness, damping) for diverse configurations, including single/double-axle inspection vehicles and multi-purpose road vehicles. It quantifies dynamic responses under programmable road roughness inputs and performs rigorous stability/durability assessments to optimize the field performance of the VSM.

BRVL is also complemented by advanced sensing devices and high-precision signal acquisition systems. This lab will play important role in advancing lifecycle performance assessment theories for transportation infrastructure and fostering next-generation lightweight intelligent maintenance solutions, bridging the gap between academic research and industrial implementation.

(a) (b)

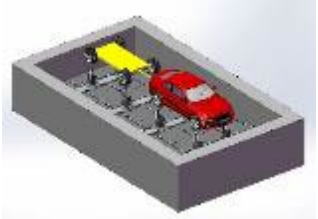

Figure 1. Highway bridge: (a) surface; (b) Underbridge view Figure 2. Vehicle dynamic calibration system

Keywords: Vehicle-bridge interaction, Vehicle scanning method, Bridge, Railway, Vibration, Lab

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Template for APCOM-ACCM 2025 Abstract Submission

First/Lead Organiser [1*], Second Organiser [1] and Third Organiser [1]

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The abstract should be given here. This should include a brief introduction and statement of the problem, a summary of the background literature, a discussion of the methods used and the main research findings. No acronyms should be used. The maximum length should be 1 page. The authors should include the main equation(s) for their problem or method of analysis, which must be centred with a number flush against the right margin:

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla P + \mu \nabla \mathbf{u} + \rho \mathbf{g}, \tag{1}$$

for which all symbols should be defined in the text. For symbol handling, it may be possible to use different symbol fonts or equation editors with this template, but this is not guaranteed. It is also possible (but not essential) to include one small figure or one small table, without caption text:

Figure 1.

Mesh	**No. of cells**	C_D	C_L'	St
M1	16,192	1.538	1.034	0.245
M2	64,792	1.546	1.053	0.241
M3	261,600	1.547	1.064	0.239

Table 1.

It is also possible (but not essential) to include a small number of references, which should be hand-numbered [1]. These are provided in the initial submission to assist the reviewers, but will need to be removed from the published version. Up to six keywords (or phrases) must also be given – these will be used to guide the selection of reviewers.

Keywords: Navier-Stokes equations, boundary-layer flows, conservation laws, machine learning, entropy production

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Neural Network Tearing and Interconnecting Methods for a Poisson problem

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Neural Network Tearing and Interconnecting Methods are developed for neural network approximation to the following Poisson model problem:

$$-\Delta u = f \text{ in } \Omega \text{ and } u = g \text{ on } \partial\Omega. \quad (1)$$

Our method is based on classical domain decomposition iterative algorithms [1]. For the problem domain Ω, a nonoverlapping subdomain partition is introduced and independent local neural networks are associated to each subdomain and each of them approximates the problem solution in each subdomain. The above problem is then partitioned into local problems where the local neural networks are trained for the given interface value as the boundary condition. The interface value is then updated by using the trained local neural network solutions to proceed the next iteration.

The update formula in our iterative method is obtained from an energy minimization problem with continuity constraints on the partitioned neural networks across the interface, of which idea was first introduced in Finite Element Tearing and Interconnecting methods [2].

The convergence of our proposed updated formula is proven for a sufficiently small step size. In addition, to speed up the iteration convergence various preconditioning schemes are developed for the iterative algorithm. The proposed iterative algorithm and its preconditioning schemes are tested for various examples to verify their convergence and efficiency.

Keywords: Poisson problem, neural network, iterative algorithm, preconditioning, domain decomposition, nonoverlapping subdomains

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A Machine Learning-Driven Multiscale Framework for Mapping Nanoindentation Data to Finite Element Model in Cement Paste

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At the microscale, cement paste is a highly heterogeneous composite material comprising multiple phases, including unhydrated clinker, calcium hydroxides (CH), various calcium-silicate-hydrates (C-S-H), and pores. While statistical nanoindentation has been widely employed to characterize its micromechanical properties, the relatively large spacing between indentation points leads to low spatial resolution, making it difficult to integrate the measured elastic moduli into multiscale models. To overcome this limitation, we present a novel two-step framework and, for the first time, develop a computational method that directly maps nanoindentation results onto a finite element (FE) model for mechanical analysis. First, Gaussian process regression (GPR) with a Matérn kernel is employed to establish spatial correlations within the nanoindentation dataset, enabling high-fidelity data densification. Then, through customized programming and secondary development, the enriched dataset is systematically mapped onto a voxel-based FE mesh, facilitating accurate mechanical analysis, possibly at the macroscale. Among various machine learning algorithms, GPR with a Matérn kernel proves particularly effective in capturing the inherent heterogeneity of cement paste. The proposed framework not only enables seamless integration of nanoindentation data into FE simulations, yielding physical stress-strain responses, homogenized elastic modulus and stress distribution, but also opens new possibilities for upscale modeling. Specifically, it allows for fracture energy estimation from nanoindentation data and provides a pathway for extrapolating 2D nanoindentation results to reconstruct 3D mechanical behavior, significantly enhancing predictive capabilities and multi-scale modeling in cementitious materials research.

Keywords: Gaussian Process Regression (GPR); Multi-scale Modeling; Finite Element Method (FEM); Micromechanic

Performance Study of Multi-Fidelity Surrogate Modeling for Flexible Utilization of Multiple Data

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Data-driven models have been widely adopted in simulation-based design optimization to enhance computational efficiency [1]. Once trained, these models require negligible computational cost for evaluation, enabling their effective use in tasks such as sensitivity analysis and optimization. However, despite advances in computing power, obtaining sufficient data remains a major challenge when simulations are computationally expensive. To address this issue, multi-fidelity surrogate modeling has emerged as a promising approach that combines high-fidelity data—accurate but costly—with low-fidelity data—less accurate but computationally inexpensive [2]. By leveraging the complementary strengths of different fidelity levels, this approach yields a synergistic effect [2]. Nonetheless, in practical scenarios, the quality of multiple low-fidelity data sources is not always reliable [3~5], and flexibly managing these diverse sources remains a significant challenge.

To tackle these issues, this study investigates the performance of a multi-fidelity surrogate modeling framework designed to adaptively utilize multiple low-fidelity data sources obtained from various domains. The proposed method estimates the relative importance of each low-fidelity source and systematically constructs a set of promising surrogate candidates based on their individual rankings. Two multi-fidelity data fusion strategies are considered: hierarchical and ensemble combination approaches. The hierarchical strategy employs a linear embedding-based multi-fidelity technique, while the ensemble strategy utilizes a multi-output technique to integrate multiple low-fidelity data sources. Finally, a multi-fidelity dataset selection algorithm is introduced to identify the best-performing surrogate among the candidates. The effectiveness of the proposed framework is validated through a series of benchmark functions and real-world engineering problems. Numerical results confirm that the proposed strategy consistently achieves higher accuracy than conventional methods under the same computational budget.

Keywords: Multi-fidelity surrogate, multiple low-fidelity data sources, rankings of the low-fidelity sources, hierarchical combination approach, ensemble combination approach

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Design optimization framework for drone-based surveillance system using flight experiment

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The demand for real-time monitoring of critical infrastructure such as military bases and energy facilities has fostered interest in unmanned aerial vehicle (UAV)-based surveillance [1]. While electric quadcopters are suitable for such applications due to their low noise, vertical takeoff and landing, and maneuverability, optimizing their operational strategy and system design remains a challenge [2]. This study proposes a framework that integrates experimental data with simulation-based optimization to minimize the surveillance gap—the time interval between consecutive drone visits to the same location—while ensuring energy efficiency and cost-effectiveness. Key design variables include the number of drones, battery capacity, cruise speed, and charging station configuration. Flight experiments using electric quadcopters measured energy consumption under varying payloads and speeds, enabling development of a surrogate model. The optimization accounts for battery degradation using an empirical C-rate dependent model. Two charging scenarios were evaluated: (S1) wireless charging and (S2) battery swapping. Under baseline conditions (20-day operation, 20-second surveillance gap), S2 reduced total cost by 20.2% compared to S1. Parametric studies showed that system cost scales sharply with increased surveillance frequency or path length, but electricity cost remains negligible (<1%), confirming the system's energy sustainability. This experiment-informed optimization framework bridges the gap between drone design and field operation by enabling adaptive surveillance planning under realistic constraints. It supports the deployment of energy-independent drone surveillance systems for long-term, high-frequency monitoring in critical domains.

Keywords: Drone-based surveillance, surveillance gap, experiment-informed optimization framework, energy efficiency, battery degradation

References

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Parallel Domain Decomposition Methods for Multi-organ Blood Flow Simulations

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The increasing demand for personalized healthcare solutions has positioned multi-organ blood flow simulations as a powerful tool for medical diagnostics and treatment planning. Capturing the complex hemodynamics across interconnected vascular systems, such as cerebral, coronary, and peripheral arteries, requires high-fidelity, patient-specific modeling. However, the resulting multiphysics problems, which may include fluid-structure interaction and nonlinear boundary conditions, lead to extremely large and ill-conditioned systems that challenge traditional numerical solvers. In this talk, we present scalable parallel domain decomposition methods tailored for multi-organ blood flow simulations. These methods partition the computational domain efficiently across processors, enabling the accurate simulation of coupled blood flow dynamics in large-scale, organ-level vascular networks. By enhancing both numerical robustness and computational scalability, our approach makes whole-body or multi-organ simulations computationally feasible within clinically relevant timeframes. We will highlight applications in cardiovascular and cerebrovascular modeling, demonstrating how these techniques can integrate patient-specific data to predict surgical outcomes and support personalized treatment strategies.

Keywords: Blood Flow Simulations, Domain Decomposition Method, Parallel Computing, Incompressible Navier-Stokes Equations

Intelligent Plane Schematic Design of Super High-Rise Frame Core-Tube Structures Based on Function-Stiffness Constraints

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Abstract: Intelligent building and structural design have emerged as a prominent research field [1]. As the design of super high-rise frame core-tube structures involves multi-disciplinary collaboration, conventional data-driven methods are difficult to balance building functions (e.g. space usage) and initial stiffness requirements, resulting in insufficient utility of the generated solutions. To address these limitations, datasets are classified according to code indicators, including building function, fortification intensity and height, and the key building components information are extracted through Tall-DeepLabv3+. This research employs R3GAN as the baseline to improve, and implementing a two-stage methodology. The residual blocks in original generator are replaced with multi-scale convolutional attention networks to enhance the extraction of sparse strip features in plane layout firstly. To satisfy building function requirements, the propagation path of the functional evaluation is added behind the structural design, and indicators, like space utilization rate etc., are incorporated into the functional loss. Secondly, to optimise the components features in diversify positions particularly vertical traffic and floor transition, while enabling the assembly of different functional layout to satisfy the initial stiffness, which achieved by genetic algorithm combined with simplified evaluation model that utilizes inter-story drift angle. Through pre-training and ablation experiments, the generative scheme reaches a 95.74% Intersection over Union Score. It is 4.26% higher than the highest of five mainstream networks such as StyleGAN2, and the Fréchet Inception Distance is reduced by 3.44%. These research results illustrate that the improved network can provide an efficient and practical tool for the intelligent design of frame core-tube structures.

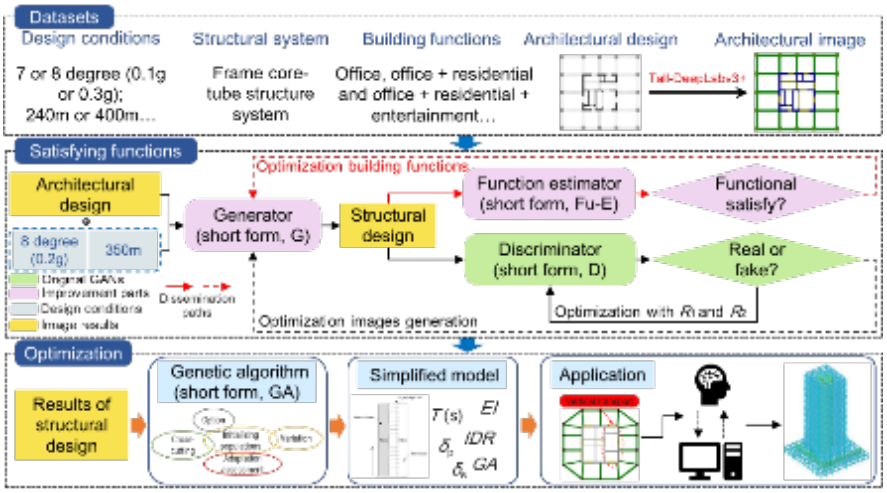

Figure 1.

Keywords: Frame core-tube structure, intelligent design, generative adversarial networks, building function, stiffness requirement.

References

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Recent advances in the scaling of small-scale passive scalar turbulence

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[2] University of Newcastle, Australia

Passive scalar transport plays a crucial role in various engineering applications, including turbulent mixing and combustion. Consequently, the scaling of the passive scalars has attracted considerable attention in the literature. In this work, we review recent advances in the scaling of small-scale passive scalars, focusing on the following three aspects: (i) The effect of a uniform mean scalar gradient on the small scales of a passive scalar field in statistically stationary homogeneous isotropic turbulence is investigated through the transport equation for the scalar fluctuation. Analytical results indicate that, for a given non-dimensional scalar gradient, the normalized odd moments of the scalar derivative tend towards isotropy as $Pe_{\lambda_\theta}^{-1}$ (Pe_{λ_θ} is the turbulent Péclet number). This is supported by DNS data at large Pe_{λ_θ} (Fig. 1a). (ii) An analytical expression, relating the mixed velocity-temperature derivative skewness -S_T and the destruction coefficient of the mean scalar dissipation rate, was derived and tested in both decaying grid turbulence and stationary forced periodic box turbulence (SFPBT). The available data agree well with the analytical results (Fig. 1b). (iii) A dual scaling of the second-order scalar structure function $\overline{(\delta\theta)^2}$, i.e. a scaling where the smaller scales scale on the Batchelor-Kolmogorov scales whilst the larger scales scale on the rms temperature θ' and the integral length scale L, is examined in the context of the transport equation for $\overline{(\delta\theta)^2}$. This dual scaling leads to the power-law relation $\overline{(\delta\theta)^2}\sim r^{\alpha}$ where α=2/3 in the overlap region when $Re_\lambda \rightarrow \infty$. The use of an empirical model for the local slope of $\overline{(\delta\theta)^2}$ (i.e. α) shows that a value of Re_λ of about 10^4 is required before the slope first approaches the value of 2/3 (Fig. 1c).

Keywords: Small-scale turbulence, scaling, passive scalar

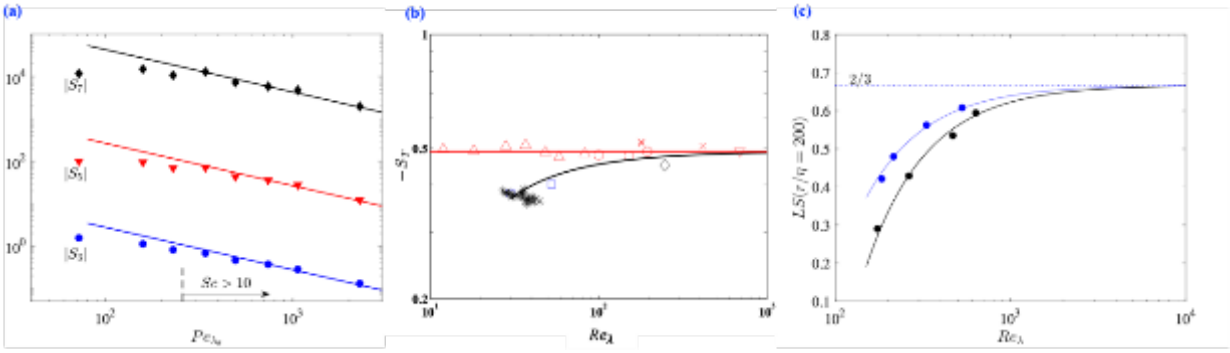

Figure 1. (a) Dependence of normalized odd moments of the scalar derivative S_3, S_5 and S_7 on Pe_{λ_θ} at Re_λ =140. Lines: $\sim Pe_{\lambda_\theta}^{-1}$. (b) Dependence of -$S_T$ on Re_λ in grid turbulence (black and blue symbols) and SFPBT (red symbols). The black and red curves, inferred from analytical expressions **[1]**, correspond to decaying grid turbulence and SFPBT, respectively. (c) Local slope of $\overline{(\delta\theta)^2}$ at r/η=200 (η is the Kolmogorov length scale). Symbols correspond to the DNS data. The black and blue curves are the fits to the data. The dotted horizontal line corresponds to the value of 2/3.

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Creep Instability Mechanism and Its Application of Residual Coal Mass after Directional Hydraulic Punching in Soft-Hard Composite Coal Seam

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Abstract: To achieve safe and efficient mining of high-gas and low-permeability coal seams, taking the soft-hard composite coal seam of Yuxi Coal Mine in China as the engineering background, the creep instability mechanism of residual coal seams after directional hydraulic flushing and the method of pressure relief and permeability enhancement in soft-hard composite coal seams were studied. Considering the influence of damage accumulation on the viscosity coefficient during the accelerated creep process, a fractional differential non-stationary creep mechanical model for coal-rock composite seams was proposed. The central difference scheme of the viscoelastic-plastic creep equation characterizing the nonlinear rheological characteristics of coal-rock composites was derived. An engineering mechanical model of soft-hard composite coal seams was established. The creep evolution and the self-adjusting distribution process of additional stresses in residual coal seams with uniform and non-uniform borehole arrangements after directional hydraulic flushing were analyzed respectively. Results show that the fractional differential non-stationary creep mechanical model for coal-rock composites can accurately characterize the non-stationary rheological properties of soft-hard composite coal seams to overcome that traditional integer-order models being difficult to describe the nonlinear characteristics of the accelerated creep stage of coal-rock composites. The Levenberg-Marquardt algorithm can be used to achieve intelligent inversion of parameters of the fractional nonlinear creep model. Based on experimental data, the accuracy and rationality of the model were verified. The nonlinear creep damage model implemented by secondary development of FLAC3D software through C++ can simulate the stress redistribution and local damage evolution process induced by hydraulic flushing during the pressure relief process of soft-hard composite coal seams. By introducing the dynamic correlation between damage variables and viscosity coefficients into the model, the coupled evolution law of micro-crack propagation and macro-deformation failure in soft-hard composite coal seams under long-term loading was revealed, providing theoretical support for predicting coal seams instability. The Boussinesq concentrated load additional stress model was used to simulate and optimize the parameters of directional hydraulic flushing holes in soft-hard composite coal seams, significantly improving the pressure relief efficiency of soft layers. The proposed new method of pressure relief and permeability enhancement by directional hydraulic flushing in composite coal seams has been successfully applied and verified by field tests. The research results provide a theoretical basis and technical support for the application of directional hydraulic flushing technology in disaster prevention and control of low-permeability and high-gas outburst coal seams.

Keywords: Soft-hard composite coal seam, directional hydraulic punching, creep equation, central difference calculation, fractional differential

A multi-scaled fracture analysis method based on BEM and PD

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A multi-scale method based on a combination of the boundary element method (BEM) and peridynamics (PD) has been verified as an efficient approach to modelling the crack propagation problems. The special feature of this method is that it can take full advantage of both the BEM and PD to achieve a higher level of accuracy and efficiency. In the implementation process, based on the scale of the structure and the location of cracks, the considered domain can be divided into non-cracked parts and cracked parts. However, for actual application, the crack propagation path cannot be predetermined. Thus, an adaptive coupling technique is necessary. In this paper, an adaptive coupling approach based on BEM-PD has been developed. A small PD domain is predesigned on the crack tips or automatically created at the largest stress part. The remaining part is modelled by the BEM. The iterative algorithm is employed by transforming the force equilibrium condition at the interfaces between two models to achieve the displacement continuously. The PD domain always moves with the crack tip moving, the created macro cracks in the PD domain will be replaced by the crack edges of BEM. This method can be used to predict the crack propagation, additionally, controlling the PD domain in a very small region is an important way to improve the efficiency of BEM-PD.

Keywords: Multi-scale crack propagation, BEM, PD, adaptive coupling, fracture analysis.

APCOM-ACCM 2025

Brisbane, Australia 7-10 December 2025

Mechanical Resilience and Rapid-Charging Capability of High- Nickel Cathodes Through Nanoscale Framework Engineering

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Nickel-based cathode materials offer high capacity but suffer from significant durability issues during fast charging due to mechanical stress and lattice deformation. Lithium-ion concentration shock fracture (CSF) simulations revealed that lithium-ion concentration imbalances intensify at fast charging rates (5C), leading to stress concentration in specific regions within the electrode. Notably, CSF was relatively suppressed in high-nickel cathodes (LiNi0.9Mn0.1O2, NM90), while more severe cracking occurred at intermediate nickel contents (NM66~NM80). H2–H3 phase transition shock fracture (HSF) analysis demonstrated that high-nickel content cathodes (≥80%) experienced rapid lattice volume contraction (up to 6%) during the H2–H3 phase transition. With increasing charging rates, this phase transition mechanism demonstrated enhanced ability to absorb and release mechanical stress, thereby minimizing particle cracking and electrode thickness variations.

The mechanical durability of high-nickel cathodes was further enhanced through an elastic framework simulation with multi-walled carbon nanotube (MWCNT) nanoscale coating. This coating effectively absorbed and released mechanical stress during charge-discharge cycles, reducing particle cracking and minimizing electrode thickness variations. Finite element analysis (FEA) demonstrated a 50% reduction in particle volume change, confirming improved durability.

When subjected to a 5C fast-charging protocol with MWCNT-coated NM90, the cathode maintained 80% capacity within 35 minutes and achieved 89% capacity retention after 100 cycles. Compared to conventional cathodes, crack formation decreased by 60%, resulting in enhanced long- term cycling stability. This research presents design principles for high-nickel cathode materials that maintain long-term stability even in fast-charging environments, potentially contributing to the commercialization of next-generation electric vehicles and energy storage systems (ESS).

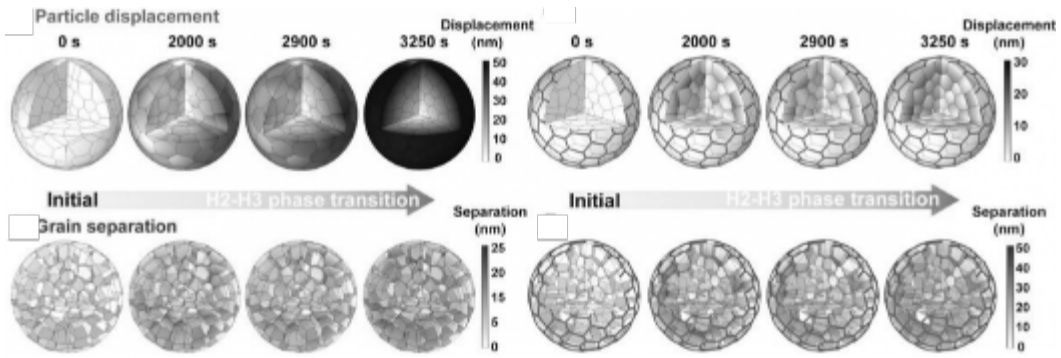

Figure 1.

Keywords: Lithium-ion Batteries, Surface Modification, Carbon Nanotube, Elastic Framework, Mechanical Resilience

References

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An implementation of the scaled boundary finite element method for three-dimensional elastoplastic analysis

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The advance in 3D modelling techniques creates a demand for highly efficient and easy-to-use numerical tools for displacement and stress analysis. These tools should significantly reduce human intervention in mesh generation for high-resolution images and complex 3D geometries. Moreover, users need to pay little attention to the selection of elements for different materials and geometries.

To this end, we present an implementation of polyhedral elements for three-dimensional elastoplastic analysis for ABAQUS users. The implementation is based on an average-strain based formulation and the scaled boundary finite element method, which is a numerical method with arbitrarily shaped polyhedral elements. The proposed implementation also uses the octree decomposition algorithm to automatically discretize complex geometries into conforming and balanced octree meshes made up by a set of regularly shaped cells. The rotating, mirroring, and scaling operations on the cells are considered for a minimized set of cell patterns. These cell patterns are implemented in ABAQUS as user elements and work like built-in finite elements.

A satisfactory computational efficiency is obtained by employing the average-strain-based formulation and the extended cell patterns. For each scaled boundary finite element, the stiffness matrix and nodal force vector of elements are computed in a quadrature-free manner and by return-mapping algorithm once per element. This feature enables fast stress analysis for various purposes.

We present examples of elastoplastic analysis on 3D models from generative design and reconstructed geometries of bio-tissues to illustrate the streamlined workflow for complex geometries. The conforming meshes of scaled boundary finite elements are regionally refined for specific analysis aims. A comparison between scaled boundary finite element and classic finite element models is given to show its accuracy and efficiency. It is concluded that the proposed implementation provides an efficient and user-friendly way for elastoplastic analysis on modern digital models.

Keywords: Scaled Boundary Finite Element Method, elastoplasticity, Octree mesh, octree cell patterns, ABAQUS

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Behavior of Simulation for Spar Type Offshore Wind Power Turbine by Particle Method

Seiya Hagihara [1*], Rikuto Ideta [1], Yuhi Uchino, Satoyuki Tanaka[2],

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Numerical calculations are needed to simulate behaviors for stabilizing for the offshore floating wind power plants and to consider safety in case of a design for the offshore floating wind power plant under the waves. The particle methods which are the smoothed particle hydrodynamics (SPH) method [1] and the moving particle semi-implicit (MPS) method [2] are recently applied to fluid dynamics analyses.

In the present study, the SPH method including the artificial viscosity coefficient and the artificial density diffusion coefficient are proposed by M.Antuono et al.[3] and D.Molteni et al.[4] that is the d-SPH method. The numerical correction terms are added to the momentum conservation equation and mass conservation equation in the delta-SPH method respectively. The 3-dimensional delta-SPH method analyses are applied to calculate the behaviour of the conventional and the new spar type wind power plant models. The new spar type has the plate for the reduction of motion. The calculated results are compared between the analyses and the experiments. The results of the simulation of the particle method were close to the experimental results of the model experiments.

Keywords: Particle Method, Wind Power Plant, Reduction of Motion

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Abstract

In recent years, the growing demand for micro-parts in aerospace, medical, and electronics industries has driven the development of microforming due to its efficiency, low cost, and environmental benefits. Titanium, widely used in advanced manufacturing, was investigated in this study to analyse the effect of grain size (33–54 μm) on its micro deep drawing (MDD) performance. Experimental results show that increasing grain size reduces tensile strength and hardness while increasing wrinkling and surface roughness (Ra: 0.24–0.84 μm). The peak drawing force decreases from 48 N to 37 N, correlating with poorer forming quality. Finite Element Method (FEM) simulations using a Voronoi polycrystalline model accurately predicted drawing forces and deformation behaviour. The simulation revealed that larger grain sizes lead to greater thickness inhomogeneity (0.042–0.071 mm), higher standard deviation in thickness distribution (1.206–1.77), and reduced maximum drawing force (33.34–21.54 N). This study demonstrates the critical role of grain size in microforming and validates the effectiveness of FEM in optimizing titanium microforming processes.

Heated Spalling and Damage of Rock Caverns Under Extreme Fire Temperatures Using the Phase Field Method

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Fire safety remains a paramount concern in the operation of underground rock caverns. To investigate the heated spalling and damage behaviours of rock caverns under extremely high temperatures, a case study in Hong Kong was simulated using the thermo-mechanical coupling phase-field method (TM-PFM). We specifically analysed various conditions, including fire scenarios, cavern burial depths, rock stiffness, and the presence of rock bolts. The results indicate that the failure of the lining and rock is significantly influenced by the fire scenario on the fire-exposed surface, while the burial depth and rock stiffness have minimal impact. Rock bolts significantly influence the spalling and damage modes of the lining and surrounding rock. They prevent excessive displacement in intact rock not exposed to high temperatures. However, as temperature rises, the thermal dilation of the rock and concrete is constrained by the bolts, increasing the risk of damage near the bolt ends.

Main equations for this problem:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = 0 \tag{1}$$

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b} = 0 \\ \left[\frac{2l_c(1-k)\mathcal{H}}{\mathcal{G}_c} + 1\right] d - l_c^2 \nabla^2 d = \frac{2(1-k)l_c\mathcal{H}}{\mathcal{G}_c} \end{cases} \tag{2}$$

where ρ and C_p are the density and heat specific capacity, respectively. T represents the temperature. $\mathbf{q}$ denotes the heat flux. $\boldsymbol{\sigma}$ is the Cauchy stress. $\mathbf{b}$ represents the body force. d represents the phase field. $\mathcal{G}_c$ is the critical energy release rate. $\mathcal{H}$ denotes the maximum positive strain energy. l_c is the scale parameter of crack width. k is a small parameter to avoid the numerical singularity.

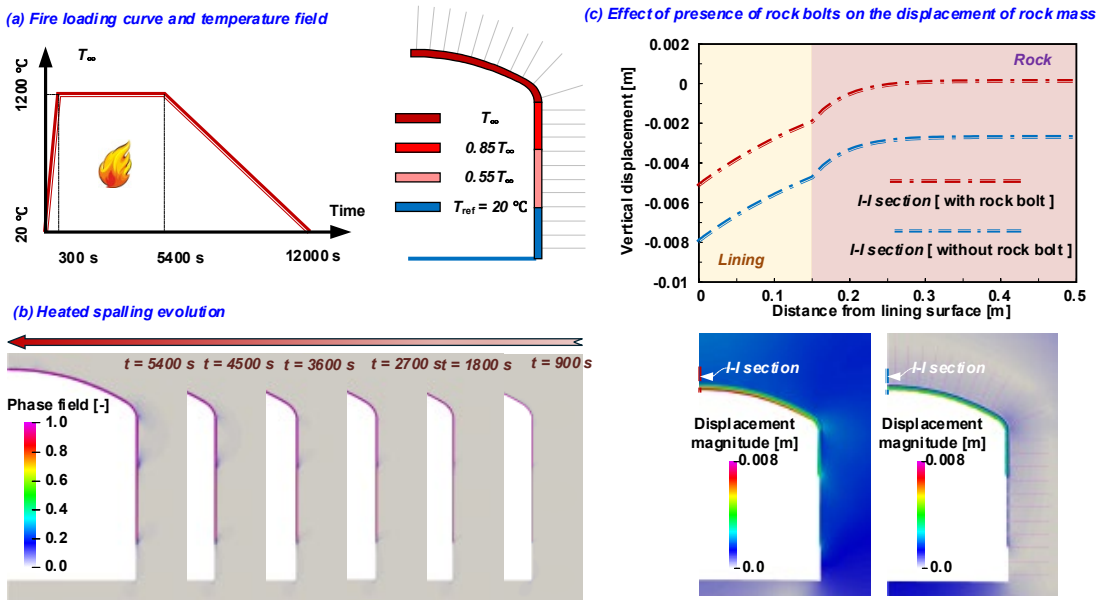

Figure 1. Some numerical results based on TM-PFM.

Keywords: Fire safety, rock cavern, heated spalling, thermo-mechanical coupling phase field method

A Matlab-Based Computer Vision-Aided Triangular Mesh Generator for High-Fidelity Grain-Based Model

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In polycrystalline rocks, constitutive behavior is highly dependent on the size, shape, and distribution of grains, and grain boundaries being pivotal in governing the properties of polycrystalline materials [1]. Consequently, high-fidelity grain-based models (GBMs) become indispensable in computer-aided engineering environments for accurate micromechanical simulations.

This paper introduces a novel modeling tool for numerical simulation preprocessing of polycrystalline rock materials. Built on Matlab, the tool leverages its widespread adoption, rich subfunctions, and robust data visualization capabilities. The tool comprises three main modules: computer vision-assisted detection of mineral grain distributions, Voronoi tessellation processing, and triangular mesh generation. To accurately capture the structural characteristics of polycrystalline materials, the mineral grain distribution detection module employs computer vision functions to obtain particle coordinates and areas (Fig. 1). Weighted Voronoi tessellation is then generated and processed based on these grain distribution features. The tool facilitates direct output of triangular meshing using polygon information, utilizing two different meshing tools.

The tool was utilized to construct GBMs for uniaxial compressive tests and Brazilian splitting tests on crystalline rocks. Numerical simulations (Fig. 1) demonstrate that GBMs generated by the tool effectively replicate the deformation, damage, and failure characteristics of polycrystalline geomaterials. The tool holds promise for numerical simulations in rock mechanics, supporting preprocessing for multiple numerical methods such as NMM, FEM, DEM, combined finite-discrete element method (FDEM), Discontinuous Deformation Analysis, and Distinct Lattice Spring Model.

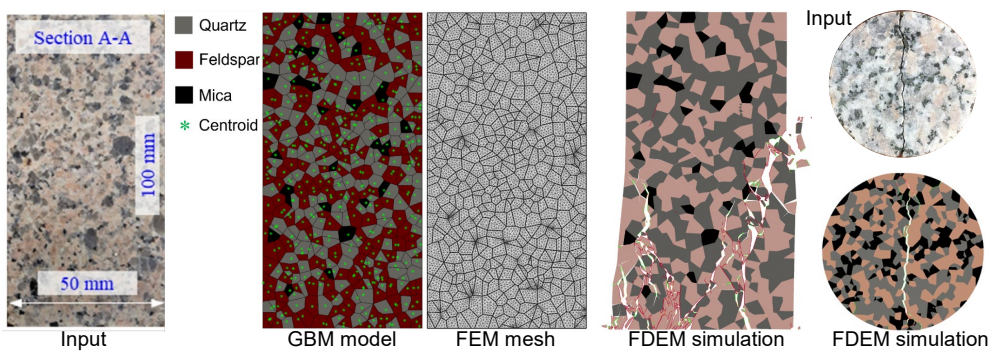

Figure 1.

Keywords: Polycrystalline Rocks, Grain-Based Model, Voronoi Tessellation, Power Diagram, Mesh-Based Methods

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Advances in Physics-informed machine learning for PDEs in computational mechanics

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In recent years, deep learning has become ubiquitous and has attracted widespread attention in empowering various fields. Physics-informed machine learning deeply integrates data with physical equations and solves partial differential equations using artificial intelligence algorithms, which has become the focus of computational mechanics research. Compared with traditional numerical methods, Physics-informed machine learning shows significant advantages in engineering inverse analysis, high-dimensional nonlinear problems and multi-physics coupling problems. This talk introduces the recent advances in physics-informed machine learning from my research group, which includes: 1) Physics-informed kernel function neural networks, 2) Curriculum-transfer learning-based physics-informed neural networks, 3) Physics-informed Kolmogorov-Arnold networks, and 4) Physics-informed kernel function operators based on Kolmogorov-Arnold networks. Several benchmark examples are presented to show the efficiency of these neural networks.

Keywords: Physics-informed machine learning, Computational mechanics, Kolmogorov-Arnold networks, Physics-informed kernel functions

Pattern-based Massively Parallel Mesh Generation and Analysis with the Scaled Boundary Finite Element Method

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Parallel computing and other digital technologies are being rapidly adopted in engineering. Developing novel numerical methods of computational mechanics are necessary to fully harness their benefits. This work presents a fully automatic high-performance numerical framework to utilize modern digital technologies in large-scale engineering applications. We propose an extended octree meshing paradigm to discretize the problem domains into polyhedral elements of a small number of patterns. The scaled boundary finite element method [1, 2] is employed to model the polyhedral elements. In the proposed framework, various formats of geometrical models, such as those employed in laser scanning, X-ray computed tomography (XCT) and 3D printing, can be robustly and efficiently meshed without surface reconstruction. The computation of element property matrices is formulated from those of the element patterns. This technique reduces memory access for iterative solvers and is efficient in parallel computing environments. The robustness as well as the accuracy are demonstrated by four numerical examples of elastostatics and elastodynamics, including complex geometries and heterogeneous problems. The results highlight the scalability and notable speedup for very large-scale simulations on high-performance computing systems.

Keywords: Mesh generation, polyhedral elements, high-performance computing, octree mesh, scaled boundary finite element method, heterogeneous domains.

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Analysing Electrochemical and Manufacturing Steps of Prelithiation for Enhancing Silicon Anode Performance

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Batteries used in electric vehicles demand high energy density and extended cycle life for optimal performance. The theoretical capacity limitation of graphite anodes (372 mAh/g) significantly constrains overall battery capabilities. Prelithiation, a process of preemptively introducing lithium into anodes, offers a promising approach to address severe volume expansion and initial lithium loss in high-capacity silicon anodes, subsequently improving capacity retention and cycling stability. The prelithiation process typically requires electrolytes distinct from those used in regular cell operation, introducing concerns about cost-effectiveness, environmental impact, and commercial viability. This investigation examines the electrochemical prelithiation process through integrated DFT/MD simulations and experimental validation, emphasizing material costs and environmental sustainability throughout the manufacturing sequence. For prelithiation solution chemistry optimization, we introduce cost-efficient lithium salts characterized by high dissociation rates, crucial for ensuring adequate lithium availability. Inevitably, the electrochemical prelithiation process generates unstable solid electrolyte interphase (SEI) layers through solvent decomposition. Our interfacial analysis establishes comprehensive solvent selection guidelines designed to minimize detrimental SEI formation.Implementation of prelithiation in practical cells necessitates a post-washing procedure. Our detailed analysis of this critical step reveals methods to suppress undesirable SEI development and maintain stable electrochemical performance. Although DFT/MD simulations are unconventional in manufacturing process analysis, we demonstrate their effectiveness in illuminating electrolyte behavior and interfacial reactions. This work presents a comprehensive strategy for enhancing silicon anode prelithiation efficiency by integrating simulation results with practical fabrication data, addressing both fundamental mechanisms and implementation challenges in commercial applications.

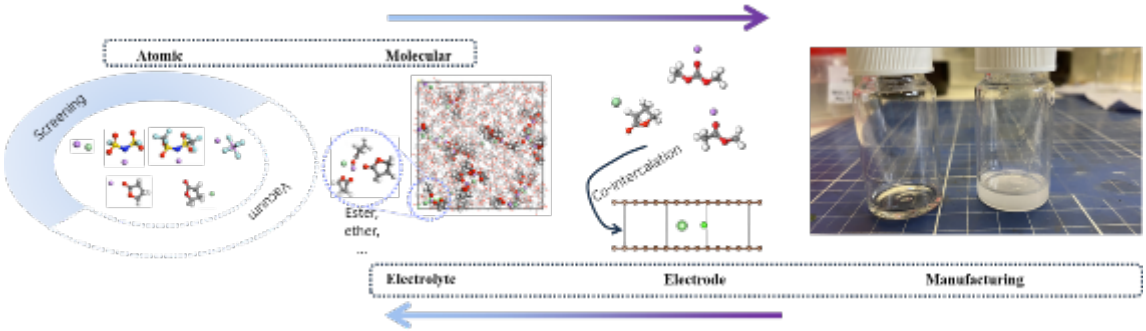

Figure 1. Schematic of Muli-Scales simulation for Prelithiation silicon anode

Keywords: Multi-Scales modelling, Prelithiation, Solvent analysis, Manufacturing process, DFT/MD simulation

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A Robust S-IGA Framework for Finite Strain Elastoplasticity Using Blending Strategies

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This paper presents the formulation and numerical implementation of S-IGA (s-version isogeometric analysis) with blending strategies for finite strain elastoplasticity. IGA, which is based on NURBS functions, is considered a high-precision numerical analysis method that may replace the finite element method (FEM). In fracture mechanics analysis, S-FEM (s-version FEM) has been proposed as a flexible and efficient modeling technique. S-IGA follows the concept of S-FEM and can easily represent local features such as circular holes and cracks. In addition, the higher-order continuity of the basis functions is expected to reduce errors introduced by the integration of the coupling stiffness matrix. In applications to elastoplastic problems, the integration error that occurs in the evaluation of internal force and consistent tangent stiffness remains to be a challenge in S-FEM. To address this issue, integrations using recursive mesh subdivision and octree meshes have been studied. However, these approaches significantly increase both computational cost and memory usage. This study focuses on addressing the integration error, which is a major issue in S-FEM elastoplastic analysis, by introducing S-IGA with blending functions. The blending functions are smooth weighting functions for both the global and local IGA models, allowing for accurate evaluation of the internal force and consistent tangent stiffness.

The blending function $f(r)$ is defined in the auxiliary domain (shown in Fig. 1) as:

$$f(r) = \begin{cases} 1 & \text{in } \Omega^L + \Omega^{fict.} \\ g(r/r_{\max}) & \text{in } \Omega^A \\ 0 & \text{in } \Omega^G - \Omega^L - \Omega^{fict.} - \Omega^A \end{cases}, \tag{1}$$

where the notations Ω^G, Ω^L, Ω^A and $\Omega^{fict.}$ denote global, local, auxiliary and fictitious domain respectively. The r is the distance from the local boundary defined in natural coordinates, and $r_{\max}$ is a positive effective domain coefficient. Examples of g are shown in Fig. 1. In nonlinear analysis, the global internal force $\boldsymbol{F}^G_{\text{int}}$ and tangent stiffness matrix $\boldsymbol{K}^{GG}$ are expressed as follows:

$$\begin{aligned} \int_\Omega \boldsymbol{F}^G_{\text{int}} \mathrm{d}\Omega &= \int_{\Omega^G} [1-f] \boldsymbol{F}^G_{\text{int}} \mathrm{d}\Omega^G + \int_{\Omega^L} \boldsymbol{F}^G_{\text{int}} \mathrm{d}\Omega^L + \int_{\Omega^A} f \boldsymbol{F}^G_{\text{int}} \mathrm{d}\Omega^A \\ \int_\Omega \boldsymbol{K}^{GG} \mathrm{d}\Omega &= \int_{\Omega^G} [1-f] \boldsymbol{K}^{GG} \mathrm{d}\Omega^G + \int_{\Omega^L} \boldsymbol{K}^{GG} \mathrm{d}\Omega^L + \int_{\Omega^A} f \boldsymbol{K}^{GG} \mathrm{d}\Omega^A. \end{aligned} \tag{2}$$

A test small strain elastoplastic analysis was performed as shown in Fig. 2. The proposed S-IGA demonstrates quadratic convergence behavior and shows good agreement in the contour plots compared with IGA.

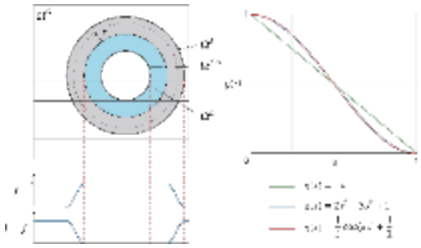

Figure 1.

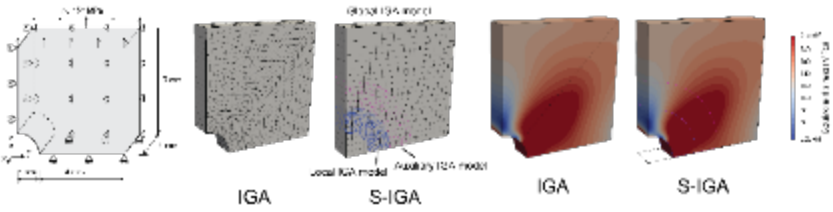

Figure 2.

Keywords: Isogeometric analysis, S-version finite element method (S-FEM), Blending functions, Extended finite element method (XFEM), Finite strain elastoplasticity

The Investigation on Coherent Transport in Graphene Phononic Crystal

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With the miniaturization of mechanical components to the nanoscale, understanding heat transfer in nanomaterials has become essential. Graphene and carbon nanotubes (CNTs), known for their exceptional thermal and electrical conductivity, have emerged as key materials for nanoscale devices. However, at these scales, heat transport deviates from classical behaviour. In particular, periodic modifications to graphene—such as phononic crystals with patterned holes—can reduce thermal conductivity while retaining electrical properties, opening new avenues in thermal management and thermoelectrics.

This study investigates coherent phonon transport in graphene phononic crystals (GPCs) with isosceles triangular holes using non-equilibrium molecular dynamics (NEMD) simulations performed in LAMMPS with the optimized Tersoff potential. The system was relaxed with a Langevin thermostat, and only the final portion of each simulation was used for data analysis. The GPC model included fixed and temperature-controlled regions, with a temperature difference of 20 K and a constant porosity of 6.67%. We varied several parameters to study their effects on thermal conductivity: unit cell lengths (1.23–7.38 nm), rotation angles of holes (0°, 60°, 120°, 180°), free slab lengths (29.5–73.6 nm), system temperatures (200–300K), and periodic arrangements (square vs. triangular). Thermal conductivity was computed using Fourier's law, and temperature was derived from kinetic energy. Results showed that conductivity increased with unit cell length from 2.46 to 7.38 nm, which is expected. Surprisingly, conductivity also increased when reducing cell length from 2.46 to 1.23 nm—an indication of coherent transport, where phonons maintain phase and travel as waves, enhancing heat transfer. This behaviour agrees with previous findings in literature [1–3]. The impact of hole orientation was notable: rotation angles of 0° and 180° yielded similar conductivities, as did 60° and 120°. Phonon correlation analysis revealed that higher thermal conductivity correlated with stronger phonon coherence, especially for low-frequency phonons, which play a dominant role in coherent transport. At 200K, coherent transport was observed in configurations like T1 (0°), while increasing the temperature to 300K suppressed coherence in T3 (120°) due to increased phonon–phonon scattering. Additionally, changing the periodic arrangement from square to triangular further reduced thermal conductivity. This emphasizes that both geometry and symmetry strongly influence phonon behaviour in GPCs. Nonlocal thermal effects were also considered in CNT-like systems, and while factors such as heat input rate and location showed minimal influence, free slab length significantly affected nonlocal transport.

In summary, coherent phonon transport in GPCs highly depends on geometry, temperature, and lattice symmetry. Both phonon correlation and dispersion curves effectively predict thermal conductivity, offering valuable guidance in the design of thermally tunable nanomaterials.

Keywords: phononic crystal, coherent transport

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Topology optimization of bi-material microstructures for achieving directional damping

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In structural design, stiffness and loss factor simultaneously influence the vibration reduction performance. We first study the concept of 'directional damping' for viscoelastic composites and develops a topology optimization model to achieve directional damping properties. Microstructures with both load-bearing capacity and dominant damping in the prescribed direction can be obtained by maximizing the loss factor while imposing stiffness constraints. We find that the optimized configurations with curved viscoelastic strips are similar to the 'suture' lines in the beaks of woodpeckers, which perform well in energy absorption. Based on the observation for directional damping design, we further present a parametric wavy strip microstructured composite, in which each wavy strip is enclosed by two sinusoidal curves. It is shown that this microstructure, resembling the wavy sutures in biological structures, provides exceptional energy absorption properties. The asymptotic homogenization method is used to calculate the equivalent complex stiffness matrices of the microstructures with different parameters. The results demonstrate that the introduction of waviness leads to a simultaneous increase in both the storage modulus and loss modulus in the X direction, achieving high stiffness and damping characteristics that approach the Ashby limit. Based on the coordinate rotation matrix and the neural network, the fitting functions between the microstructure parameters and the material properties are established. Tthen by optimizing the microstructure parameters and orientation angles, the stiffness and damping can be adjusted to achieve effective vibration damping. The effectiveness of the proposed vibration damping design method, which incorporates damping directionality, is validated through numerical examples and experimental results in plate vibration damping applications.

Keywords: *Directional damping, microstructure, vibration damping, topology optimization*

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Molecular modelling of gellan gum in bioengineering applications

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Gellan gum demonstrates excellent biocompatibility, biodegradability, and tunable mechanical properties, making it an ideal foundational material for bioprinting in bioengineering applications. It can be utilized as a bioink to fabricate biomaterial substrates with controlled mechanical and biological properties. Previous studies have shown that gellan gum modified with N-succinimidyl methacrylate exhibits improved mechanical properties and biological characteristics [1-3]. In this study, we aim to explore the molecular structure and interactions of unmodified gellan gum and gellan gum modified to varying degrees with methacrylate groups through molecular dynamics simulations at the molecular scale as shown in Figure 1. We investigate the effect of methacrylate substitution and its concentration on the number of hydrogen bonds and structural changes within our models. Our results indicate that as the degree of modification increases, the molecular chains extend further. More methacrylate modification increases intramolecular hydrogen bonding but reduces intermolecular hydrogen bonding, weakening the overall molecular interactions due to steric hindrance. Additionally, increased concentration leads to more intermolecular hydrogen bonds, indicating stronger molecular interactions. This study provides a detailed microscopic analysis that deepens our understanding of the material properties of gellan gum and highlights its potential applications in bioengineering.

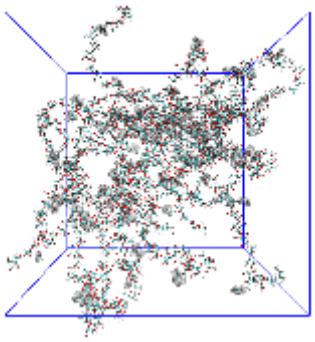

Figure1. The snapshot of the molecular model of gellan gum chains with 50% methacrylate modification.

Keywords: gellan gum, molecular dynamics simulation, methacrylate modification

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Integrated radial basis function networks for solving PDEs under the embedded boundary framework

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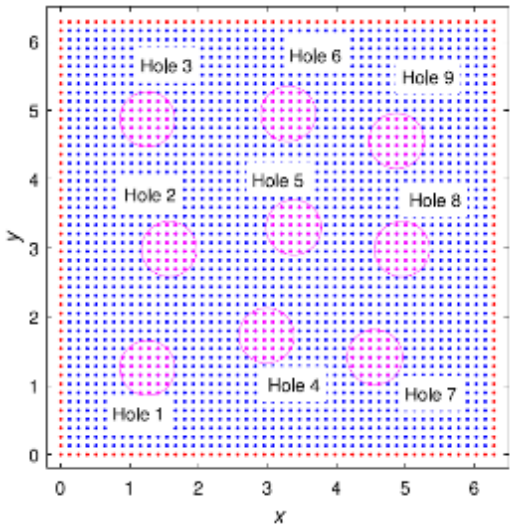
Using the conventional discretisation methods such as the finite-element, finite-volume and boundary-element methods to solve partial differential equations (PDEs) in nontrivial domains still presents a great challenge as their meshing for representing the shape of the geometry is not economic. The use of non-boundary-fitted meshes, e.g. simple structured ones, has received a great deal of attention. This paper presents an application of integrated radial basis function networks (IRBFNs) in solving the two-dimensional elliptic partial differential equations (PDEs) under the embedded boundary framework. The physical domain, which is of complex shape, is embedded in a rectangle called the computational domain. The task of mesh/grid generation in the computational domain is much simpler than that in the physical domain, resulting in a very economic preprocessing. The RBF networks are constructed locally through integration to approximate the field variable. The constants arising from the integration process are utilised to include the derivative values at the neighbouring nodes in the local approximation, which helps achieve high-order accuracy. These compact approximations are used for both the discretisation of PDE and the imposition of prescribed values on immersed boundaries. In solving the extension problem, the IRBF solution is constructed to be smooth across the immersed boundaries. Linear and nonlinear problems are considered to verify the proposed method. Highly accurate results are obtained using relatively coarse spatial discretisations.



Keywords: PDE, immersed boundary, integrated radial basis function network, high-order approximation, local approximation

Derivative Relationships of Commonly Used Numerical Methods and Their Performance Analysis of Accuracy, Stability and Efficiency

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Abstract:

In this study, the commonly used numerical methods, finite element method (FEM), finite volume method (FVM), boundary element method (BEM), mesh free method (MFM), free element method (FrEM) and finite line method (FLM), are derived from the weighted residual formulations of problem's governing differential equations. The relationships between these methods are deeply investigated, and the advantages and disadvantages of each method are described from the aspects of computational accuracy, stability and efficiency. The special attention of the study is paid on the specific treatments in each method for improving the above mentioned three aspects. It is particularly found that the distribution of the nodes within a mesh used by a numerical method has big influence on the accuracy of the method, and the number of nodes related to a computational point heavily influence the stability and efficiency of a numerical method. Besides, to improve the stability and accuracy of some methods, a few effective techniques will be proposed for these methods by extending the influence region of nodes under the same comparison condition that the total number of the discretized nodes is invariant but the accuracy and stability can be improved considerably. Some examples on thermal and mechanical problems will be given for demonstrating the mentioned factors in the commonly used methods.

Discrete element modelling of electro-mechanical behaviour in modified cementitious materials

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Cementitious materials modified with carbon black nanoparticles (CBN) exhibit self-sensing capabilities due to enhanced electrical properties, making them promising for structural health monitoring. However, current sensing mechanisms rely on macroscopic observations, limiting predictive accuracy, particularly under internal damage. This study proposes a novel modelling approach by integrating a tunnelling-effect-based mathematical model with the Discrete Element Method (DEM) to simulate the electrical behaviour of the CBN-modified cementitious materials. The framework distinguishes between elastic piezoresistivity and crack-induced resistance changes, enabling a more accurate representation of their electro-mechanical response. Piezoresistivity is characterised by the fractional resistance change (FRC), calculated as the ratio of change in the resistance (R_b) to the initial resistance (R_{b0}):

$$FRC = \frac{1}{1+\alpha}\frac{R_b - R_{b0}}{R_{b0}} \text{ with } R_b = \frac{1}{r^3 \sum \frac{1}{C_1 \frac{d_i}{r} exp(C_2 \frac{d_i}{r})}}, \quad (1)$$

here, r is particle radius, d_i is the gap between particles, and C_1, C_2, and α are material parameters controlling the resistance baseline, piezoresistive sensitivity, and initial resistance, respectively. These parameters are calibrated through DEM simulations. At the microscale, resistance is directly linked to inter-particle displacement, with bond breakage representing a local disruption in electron transfer.

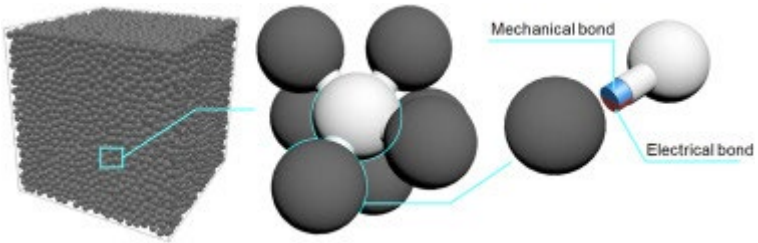

Figure 1.

The proposed model demonstrates comparable accuracy to analytical solutions in the elastic regime. More importantly, in the plastic regime, where traditional models fail due to crack development, this model maintains strong agreement with experimental results, capturing resistance changes driven by damage. These results highlight that the method can effectively capture the evolution of electrical resistance in both elastic and plastic regions, making it suitable for better understanding the mechanism of such materials for stress sensing and damage detection in practice.

Keywords: DEM; Electrical resistance; Electro-mechanical; Piezoresistivity; Self-sensing; Cementitious materials

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Analysis of impact resistance and Layer Optimization of Composite B-pillar Structure

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Carbon fiber-reinforced thermoplastic composites (CFRTP) are increasingly adopted in automotive structures due to their exceptional mechanical properties and lightweight characteristics. However, their application remains largely limited to non-load-bearing components, as systematic design methodologies for load-bearing structures are still underdeveloped. This study pioneers the application of CFRTP to load-bearing B-pillar structures, integrating layer design, layer sequence optimization, and sample fabrication. This systematic research contributes to advancing the application of composite materials in automotive structures. Firstly, the B-pillar finite element analysis (FEA) model is validated by comparing the maximum peak load obtained from the drop-weight impact test on metal B-pillars with numerical simulations. Subsequently, the impact performance of the CFRTP B-pillar with the initial layer sequence is evaluated, revealing a 45.27 % reduction in deformation and a 71.54 % decrease in mass compared to metal B-pillars, while maintaining comparable peak force levels.

To identify optimal layer sequences for dynamic impact conditions, a conditional generative adversarial network (CGAN) deep learning model is developed for layup optimization. The objective function of the CGAN generative network model is shown in Eq. (1).

$$\min_{G}\max_{D} L_{CGAN}(\boldsymbol{D},\boldsymbol{G}) = \mathsf{E}_{X\sim P_{data}(X)}[\log \mathbf{D}(X,\zeta)] + \mathsf{E}_{Z\sim P_{Z}(Z)}[\log(1-\mathbf{D}(G(X,\zeta)))] \quad (1)$$

where D and G represent the generator and discriminator, respectively. ξ is the conditional probability. $P_{data}(X)$ and $P_z(Z)$ denote the probability distributions of the training datasets and random noise, respectively, while E representing the expectation. The model successfully generates layering schemes that satisfy physical constraints. The optimized layup sequence is incorporated into the FEA, revealing an approximately 64.25 % increase in load-bearing capacity and a 41.1 % reduction in deformation. Finally, CFRTP B-pillars are prepared using the customized hot-pressing mold, and their impact resistance is evaluated through drop-weight impact tests. The results confirm superior impact mechanical properties compared to metal B-pillars. This closed-loop design process validates the feasibility of the proposed methodology and provides a robust framework for the application of CFRTP in automotive load-bearing structures.

Keywords: Carbon fiber-reinforced thermoplastic composites; Automotive; B-pillar; Impact resistance; Layup optimization; Prepared

A Validated Fluid Structure Interaction Simulation Methodology for Flow in Blood Vessels

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Biomedical studies often involve the need to model flow and its interaction with a flexible duct to determine the resulting fluid structure interaction. This process is complicated. The fluid flow is often in a transitional regime, involves a non-Newtonian fluid, such as blood, and occurs in a regime where the Womersley number effect is significant. The flexible duct is typically made from a biological material that is not rigidly constrained. Add to this the inclusion of an artificial material grafted into a blood vessel and the situation is more complicated. Furthermore, the scanned geometry is in a prestressed state, so it is essential to prestress the wall material before performing the fluid structure interaction simulation. If this is not complicated enough, it is common that separate computational fluid dynamics and finite elements solvers must be coupled iteratively to provide the time evolution of a geometry. However, once simulations are achieved, they provide very high-resolution data on the flow field, wall shear stress, stress field inside the material, propensity for fatigue and much more.

For this study, simulations were performed using the Ansys Mechanical solver coupled to the Ansys CFX fluids solver via the system coupling framework The paper focusses on presenting the numerical techniques used and most importantly the practices used to ensure stability and proper coupling. Simulations of a simple tube system are first performed and validated against *in vitro* data to establish the validity of the technique. It was then applied to the study of vascular bypass grafts, where an additional complexity is the need to model sutures.

The important generic lessons learned from these studies will be presented, making them available to those performing biomedical fluid structure interaction simulations regardless of the software they use.

Keywords: computational fluid dynamics, finite element analysis, fluid structure interaction, prestressing, hyperelastic materials.

Fast Urban Flood Model for Real-time Flood Management

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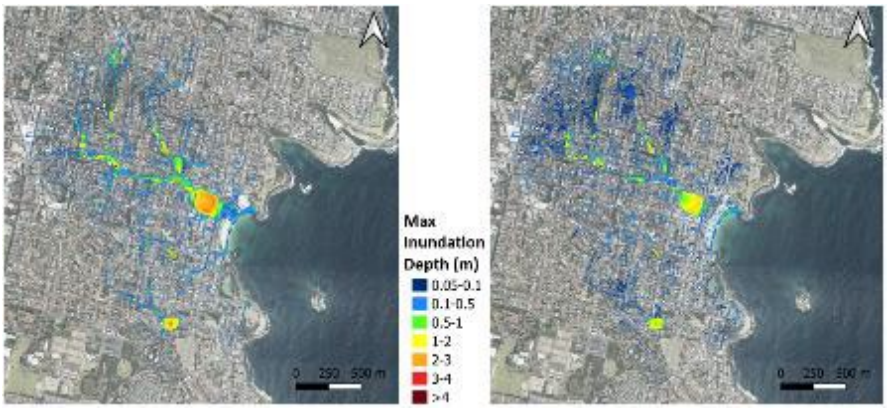
Urban flash flooding presents significant challenges due to its rapid onset and the complexity of urban drainage systems. Traditional hydrodynamic models, while accurate, are computationally intensive and time-consuming. This study introduces Dynamic CA-ffé, a hybrid 1D-2D flood evaluation model designed to address these challenges. Unlike traditional approaches that solve the full shallow water equations at a high computational cost, Dynamic CA-ffé integrates a 2D steady-state surface flow model with a 1D transient drainage model while maintaining dynamic flow exchange between them. This novel hybrid approach effectively imposes the momentum equation on the 2D surface model via the 1D drainage system, resulting in a quasi-dynamic flood simulation.

The 2D surface flow model employs a Cellular Automata (CA) approach, which simplifies the simulation of water movement across the urban landscape. In this model, the urban area is divided into a grid of cells, each representing a portion of the landscape. Water movement is simulated by applying rules based on mass conservation to determine the flow between cells. The 1D drainage system model uses the Storm Water Management Model (SWMM), developed by the United States Environmental Protection Agency. It is widely used for simulating the hydrological and hydraulic behaviour of urban drainage systems and models the flow within pipes, manholes, and channels.

The model leverages a novel parallelisation technique to enhance computational efficiency, achieving a balance between speed and accuracy. Validated in two Australian catchments, Scotchmans Creek and Coogee Bay (Figure. 1), Dynamic CA-ffé demonstrates high accuracy in predicting flood extent and depth, performing comparably to established hydrodynamic models such as MIKE Flood and TUFLOW.



a: TUFLOW **b: Dynamic CA-ffé**

Figure 1.

The findings highlight Dynamic CA-ffé's potential as a valuable tool for urban flood risk management, particularly in time-sensitive decision-making scenarios. The model achieves high accuracy in

predicting flood extent and depth, with significantly reduced simulation times compared to traditional hydrodynamic models.

Keywords: Urban Flash Flood Model, Cellular Automata, Storm Water Management, Hybrid Numerical Schemes, Shallow Water Equation

Polyhedral Discretization and Analysis for Complex Geometry

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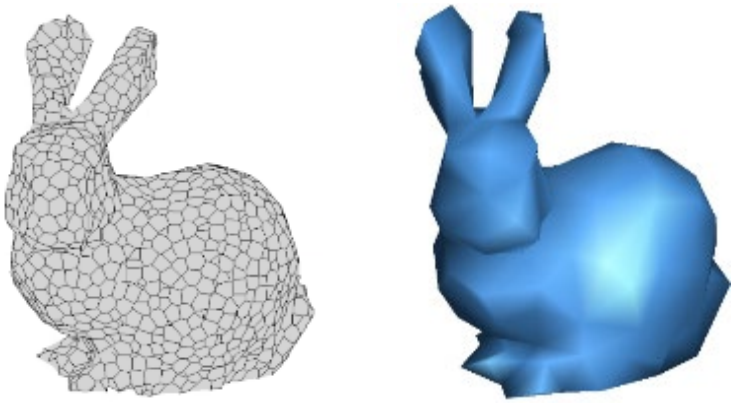
Polyhedral elements provide flexibility in domain discretization, while few mesh generation algorithms are available for them. In this study, a simple and robust method is proposed to discretize complex geometry by superimposing a polyhedral element domain and triangular surface mesh [1]. Figure 1 demonstrates an example of a polyhedral mesh generated based on the STL surface mesh of the Stanford bunny. The process consists of four steps: (1) identifying the intersection points on each edge of polyhedral elements, (2) splitting faces of polyhedral elements, (3) constructing internal faces in polyhedral elements, and (4) splitting polyhedral elements. To effectively and effectively handle the above mesh generation process, a topology-based data structure for polyhedral elements is employed, named as PolyMo [2], which provides the linear scalability on retrieving adjacency relationship. Furthermore, the discretized polyhedral mesh is analyzed using the virtual element method, which consistently handle arbitrary nonconvex polyhedral elements [3, 4].



(a) (b)

Figure 1. Example of polyhedral discretization for Stanford bunny: (a) polyhedral mesh and (b) triangular surface mesh

Keywords: Domain discretization, polyhedral elements, STL surface mesh, virtual element method

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Modeling, Simulation, and Optimization in Plastics Profile Extrusion

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Numerical optimization is an important tool in both the design of individualized components and their manufacturing processes. Despite this vital role of numerical optimization, the creative aspects of the design process are still left to the human designer. In fact, for centuries, creativity has been considered a purely human attribute, if not the defining element of a human being. Recent advances in artificial intelligence (AI) have shaken this perception to its roots. Bit by bit, creative, rational agents have made their way into our daily lives. Inspired by these advances, we will explore different ways in which machine learning algorithms can help improve numerical design, e.g., in terms of geometry parameterization, surrogate models for forward simulations and optimization strategies.

To this end, we show how machine learning tools can be included into the optimization workflow for the design of both extrusion dies and static mixers. For example, variational autoencoders (VAE) can be used to learn low-dimensional, yet feature-rich, shape representations. A VAE can discover common properties among a variety of shapes without an explicit, human-made parametric representation of the original designs. A VAE is a neural network architecture that learns the underlying structure of a 3D shape in an unsupervised manner. It infers a latent, hierarchical representation of objects. This approach promises significant improvements in both performance and variety of shapes. Furthermore, we will discuss how the resulting shape parameterization can become an input to numerical simulation, including both high-fidelity and reduced-order simulations. In this context, we will present both boundary-conforming methods, e.g., using OpenFOAM, but also immersed methods. In terms of optimization, we touch upon reinforcement learning as a means of learning optimization strategies.

Keywords: shape optimization, computational fluid dynamics, machine learning, reduced-order modeling, lattice structures

Predicting Residual Tensile Strength of Fibre Reinforced Polymer Composite Laminates Subjected to Laser Irradiation via Numerical Modelling

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Laser irradiation can cause significant damage to structures manufactured from fibre reinforced polymer composite laminates, such as ships and aircraft components. The residual strength of a fibre reinforced polymer after being subjected to laser irradiation is dependent on the laser's power, beam diameter, wavelength, and exposure duration, as well as the properties of the material. As the fibre reinforced polymer is subjected to laser irradiation, a combination of thermal, mechanical, and chemical effects occurs with damage modes including ablation, fibre-matrix separation, cracks, and internal delamination. The damage is most prominent at the location in which the laser strikes a material and progressively recedes from this region. Outer areas of the heat affected region have a reduction in the polymer matrix content, which decomposes at significantly lower temperatures compared to the fibres, resulting in limited matrix material to hold the fibres in place and distribute any applied stresses. It is critical to evaluate and understand the residual strength of composites after laser irradiation for the design, operation, and through-life support of their respective infrastructures.

In this study, a numerical modelling framework has been developed to predict the residual tensile strength of fibre reinforced polymer composite laminates subjected to continuous wave laser irradiation. The procedure involves detailed microstructural analysis of laser irradiated composite panels to develop a representative model. The representative model is used to facilitate the simulation of tensile loads on ablated composite panels using the commercial finite element analysis software ABAQUS 2022 and its 'Standard/Explicit' model. The numerical modelling framework has been validated through modelling 300 × 100 × 2 mm^3 carbon fibre reinforced polymer panels made of IM7/977-3, which were subjected to laser irradiation and then tensile loading until failure [1]. The laser irradiation applied consisted of a Gaussian beam profile with a wavelength of 1045 nm, a power output of 215 W, and beam diameters of 3 and 5 mm. The predicted tensile strengths of the composite panels from the numerical model compared well with those reported from the experiment [1], demonstrating this numerical modelling framework's ability to determine the residual tensile strength of fibre reinforced polymers.

Keywords: Fibre Reinforced Polymers, Finite Element Analysis, Laser Irradiation, Residual Strength

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Tunable compression response and enhanced mechanical properties of bio-inspired lattice structures with dual-stage stiffness

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To address the inherent contradictions among high stiffness, superior energy absorption, and stable deformation in classical lattice structures, this study draws inspiration from the microscopic configuration of skull and the root growth patterns of bamboo by integrating a tangent-arc truss with a supporting truss to construct a Y-truss unit, which are implemented in representative lattice structures including body-centered cubic (BCC), face-centered cubic (FCC), octet truss (OT), and rhombic dodecahedron (RD) structures. Samples were fabricated using stereo lithography apparatus (SLA) technology. Through combined quasi-static compression testing and numerical simulations, a systematic investigation was conducted on the Y-truss effects on deformation modes, mechanical properties, and failure mechanisms. The results show that in bending-dominated BCC and RD lattices, the Y-truss induces compressive deformation in supporting trusses, achieving remarkable enhancements in specific stiffness up to 284.3%, specific strength up to 276.0%, plateau stress up to 325.7%, and specific energy absorption (SEA) up to 259.4%. For stretching-dominated FCC and OT lattices, the Y-truss introduces bending deformation to increase structural degree of freedom (DOF), effectively suppressing initial peak stress (IPS) and stress fluctuations while improving plateau stress up to 159.5%, SEA up to 120.4%, and crushing force efficiency (CFE) up to 165.7%. Notably, the unique bending-compression dual-stage deformation mode of the Y-truss generates two stiffness responses, with secondary stiffness reaching 3.08 times the initial stiffness and stress up to 2.84 times. Further parametric studies reveal that tuning the thickness ratio between the tangent-arc and supporting truss enables flexible mechanical response modulation, facilitating performance optimization from high load-bearing to stable energy absorption. This work establishes theoretical foundations and design guidelines for developing multifunctional bio-inspired lattice structures with high stability, tunable compressive response, and dynamic adaptability.

Keywords: lattice structure; bio-inspired design; compression response; energy absorption; finite element method

Study on Dynamic Strength and Energy Dissipation Characteristics of Coal Samples under Multi-Axial Static-Dynamic Loading

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During the underground coal seam mining, the coal mass is constantly subjected to uniaxial, biaxial, and triaxial stress states. It is frequently affected by dynamic high-speed impact loads such as mine tremors, rockburst, and blast hole detonations, leading to instability and failure, accompanied by energy transformation. The Triaxial Hopkinson Bar (Tri-HB) system was employed to conduct laboratory experiments and numerical simulations on coal samples under multi-axial pre-stress conditions and dynamic loading, in order to investigate the strength variation and energy dissipation characteristics of coal samples under multi-axial static and dynamic loads. The results indicate that the dynamic response of rocks, including the stress-strain curves, dynamic strength, energy evolution, and failure modes, exhibits a strong confinement dependence, which is consistent with the experimental observations. Under uniaxial impact, multiple fractures in the coal samples interpenetrate and ultimately result in the formation of fine particles. Under biaxial impact, a typical tensile-shear composite failure characteristic is exhibited, where shear slip dominates fracture propagation, and tensile effects lead to local disintegration of the coal samples. Under triaxial impact loading, the confinement effect is significantly enhanced. The coal samples exhibit distinct shear failure characteristics, with short and dense fractures localized in specific areas, while the overall structure remains relatively intact. Additionally, the dynamic strength of the coal samples first increases and then decreases with the variation of the intermediate principal stress, with the inflection point occurring at an intermediate principal stress of 6 MPa. The relationship of energy consumption density is as follows: triaxial > biaxial > uniaxial.

Keywords: Triaxial Hopkinson bar, dynamic loading, multiaxial loads, dynamic strength, energy dissipation

Sustainability Enhancement of Biogas Plants Through Reduction of Harmful Effects of Sulfur

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This study examines how the sustainability of small-scale biogas facilities can be improved by reducing the negative consequences of sulfur emissions, particularly hydrogen sulfide (H_2S). It concerns domestic biogas units (approximately 6 m^3) in rural areas of Bangladesh (focused on Gazipur district). The primary components of biogas, consisting mainly of methane (CH_4), carbon dioxide (CO_2), oxygen (O_2), and hydrogen sulfide, were measured. An indigenous sulfur arrester, mostly made of iron oxide, was used to lessen the adverse effects of H_2S on the environment. The sulfur arrester effectively extracted sulfur from H_2S and formed iron sulfide (FeS) without releasing H_2S into the atmosphere. The sulfur arrester made the biogas safer for cooking and energy production by reducing 95% of the sulfur component. It can precipitate heavy metals like lead (Pb) and cadmium (Cd) in contaminated soils and water, lowering their mobility and toxicity; the resulting iron sulfide has a potential for secondary application, especially in environmental rehabilitation. The study, which involved 15 tiny biogas plants, produced beneficial byproducts that can be used to clean land and water, lowering hazardous emissions. Based on this idea, the process can create a massive opportunity for the country. This study offers applications for environmental remediation while putting out a strategy for reducing sulfur waste, which enhances the sustainability of biological gas systems.

Keywords: Biogas; Sustainability; Hydrogen sulfide (H_2S); Sulfur arrester; Environmental remediation; Heavy metal precipitation.

Enhancing Railway Safety and Sustainability: A Solar-Powered Automated Level Crossing System for Bangladesh

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Bangladesh has many railway-level crossings, most of which are manually operated, lack protective barriers, and have a power supply that is also not reliable, resulting in many railway-crossing accidents. The highway system with sunlight-powered automatic railroad level crossing system in this study will increase safety and operational rates, especially for rural and poorly-resourced places. A 110 Wp monocrystalline solar panel paired with a 12V deep-cycle battery provides dependable off-grid operation of the system. A PIC16F877A microcontroller controls the inputs of infrared sensors to detect train and road traffic and activate automated gates and traffic signals accordingly. For this purpose, a GSM module is used for real-time fault reporting to evoke a prompt response, leading to their transparency." The prototype undergoes testing to confirm accurate gate performance, precise detection abilities, and significant energy management, and it is capable of continuous use even in acute environments. "This would minimize collision and operational delay and encourage green and cost-effective transport solutions deployment. It applies to low-income countries with scarce infrastructure because of its modular, scalable design. Addressing significant transportation challenges, this work contributes to safer railway systems and enables cleaner energy integration. The investigation of advanced fault diagnostics and AI-based predictive maintenance for future optimizations would be the best suggestion for resilient and efficient system performance. The proposed solution is a practical, eco-friendly alternative to conventional systems, and it can even act as a prototype for updating the railway structure of underdeveloped areas.

Keywords: Solar-powered automation, Railway safety, Level crossing system, PIC microcontroller, Infrared sensor, Sustainable transportation

Applications of return-free integration to yield surface detection of cellular materials

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Cellular microstructures are observed in many biological materials, and these materials usually exhibit anisotropic features. Among natural cellular materials, some of them display asymmetric yielding in tension and compression, for example, trabecular bone. Therefore, a promising constitutive model stimulating the elastoplastic behavior with asymmetric yielding as well as nonlinear isotropic-kinematic hardening/softening is welcome. On the other hand, this comprehensive elastoplastic model needs an accurate plastic integration to compute the exact model response. In the present study, we developed finite element models of cellular materials with hexagonal microstructures and the call wall, which is made by an elastoplastic material with asymmetric and anisotropic yield surface as well as nonlinear isotropic-kinematic hardening/softening. In order to compute the exact response, the return-free integration [1] was adopted and embedded into the finite element computation. Based on the finite element model of cellular materials, its initial yield surface as well as the subsequent yield surfaces under different preloading paths were detected numerically. The yield surface evolution of cellular materials such as trabecular bone was investigated according to the finite element simulation.

Keywords: Cellular materials, elastoplasticity, yielding asymmetry, anisotropic-isotropic-kinematic hardening, yield surface evolution, return-free integration.

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Dynamic Properties Analysis and Elastic Lateral Stiffness estimate for Frame-Core Tube Structures with Multiple Viscously-Damped Outriggers

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Abstract: Frame-core tube structures with multiple viscously-damped outriggers are increasingly adopted in super-tall buildings for their enhanced lateral drift control and seismic energy dissipation capabilities. However, as the number of outriggers and damper configurations increases, accurately predicting structural vibrations becomes challenging, and a unified design theory remains lacking. This study proposes a generalized analytical model for multiple viscously-damped outrigger systems, offering a unified framework to handle various outrigger quantities and damper types. Using Euler-Bernoulli beam theory, the core tube's bending vibration equation is established, allowing closed-form solutions for natural frequencies and mode shapes. Outriggers are modeled as distributed rotational stiffness elements along the height, and an equivalent stiffness matrix accounting for damper energy dissipation is introduced to capture the interaction between outriggers and the core tube. A generalized eigenvalue formulation and a transcendental equation system incorporating outrigger parameters enable semi-analytical solutions for modal characteristics. Statistical analysis of super-tall frame-core tube buildings yielded empirical relationships for the first two modal periods, leading to code-oriented stiffness design strategies. Validation against finite element models of three super-tall structures shows the proposed model achieves higher accuracy and efficiency than traditional methods. The proposed analytical model overcomes traditional limitations regarding outrigger quantities and damping configurations, while providing an efficient, rational, and conservative assessment methodology for lateral displacement control through integration with code-specified design spectra and modal decomposition approaches.

Keywords: closed-form analytical solution, Frame-core tube structures, lateral displacement control, multiple viscously -damped outriggers, simplified mechanical model

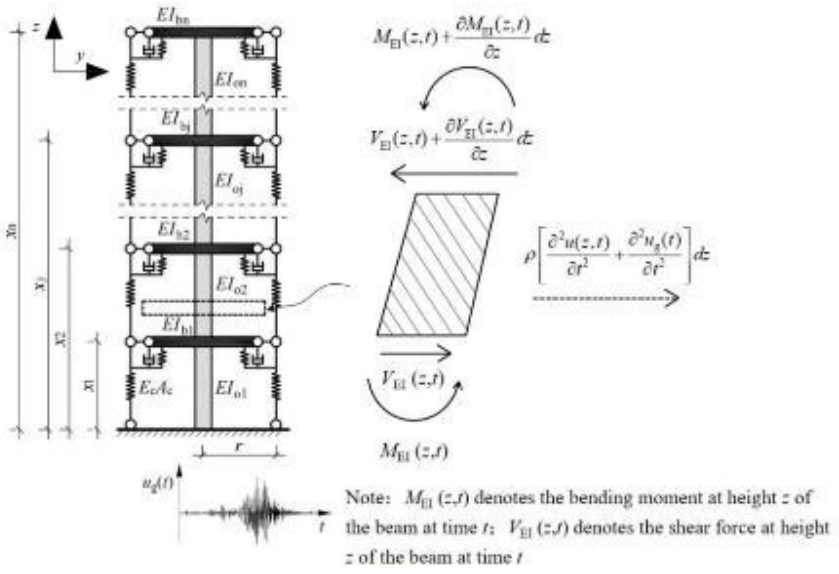

Figure. Simplified mechanical model and force analysis of an infinitesimal segment

$$\frac{d^2}{dx^2}\left[S_{\mathrm{EI}}(x)\frac{d^2\phi_{i,j}(x)}{dx^2}\right]-\omega_i^2\,\frac{\rho_0 S_{\rho}(x)H^4}{EI_0}\phi_{i,j}(x)=0$$

A three-stage identification of Viscoelastic Properties for Nacre-like materials

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Nacre, mother-of-pearl, attracts many researchers due to its excellent property of mechanics including high strength and high toughness. These characteristics are recognized as originating in the microstructure of nacre by Jäger & Fratzl [1]. In the present study, we first developed a micromechanical model of nacre taking into account its microstructure as well as the viscoelastic properties. Then we extended the model to analyze the viscoelastic property of nacre-like materials which mimics the microstructure of nacre. Due to the complexity of the micromechanical model, the model parameters are not estimated easily. To tackle this issue, we proposed a three-stage identification based on the Prony's method and the analytical response of the nacre-like materials under the stepwise, monotonic, and cyclic loadings. The proposed identification was applied to estimate the model parameters from the experimental data of uniaxial and three-point fending tests.

Keywords: Nacre-like materials, viscoelasticity, Prony's method, parameter identification, analytical response.

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Influence of solid phase homogeneity on the properties of foamed concrete using numerical analysis

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Concrete is a representative multi-phase and heterogeneous material. Among various types of concrete, lightweight foamed concrete is specifically designed to enhance thermal insulation. Due to its highly porous nature, the pore structure of foamed concrete plays a dominant role in determining key material properties such as density, strength, and thermal conductivity, and several studies have investigated the pore characteristics of foamed concrete. In contrast, comparatively few studies have focused on the solid phases within foamed concrete. Given that more than 50% of the volume of foamed concrete comprises solid phases, it is equally important to assess how the characteristics of the solid structure influence the material's performance. In actual foamed concrete, the solid phase consists of multiple components, including calcium silicate hydrates, portlandite, and unhydrated cement particles-each possessing distinct properties [1]. Nevertheless, these different solid phases are often treated as a homogenized phase for simplification in numerical and analytical studies.

This study investigates the influence of solid phase homogeneity on the mechanical properties of foamed concrete. A foamed concrete specimen with a specific target density was prepared, and the heterogeneity of its solid structure was examined using micro-computed tomography (micro-CT). Subsequently, a series of virtual specimens with varying degrees of solid phase homogenization was generated based on the relationship between material density and the pixel values in the micro-CT images. The relative compressive strength and stiffness of these virtual specimens were evaluated through finite element (FE) analysis using a concrete damage plasticity model.

$$\boldsymbol{\sigma} = (1 - d)\boldsymbol{D}^{el} : \left(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{pl}\right), \tag{1}$$

where σ is the stress tensor, d is the scalar stiffness degradation variable which can take values from 0 (undamaged material) to 1 (fully damaged material). D^{el}, ϵ, and ϵ^{pl} denote the degraded elastic stiffness, the total strain tensor, and the plastic strain tensor, respectively.

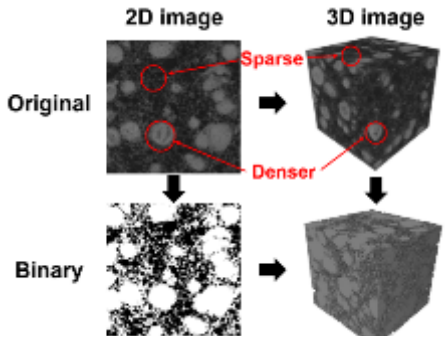

Figure 1. Micro-CT imaging for segmenting pores and solids of foamed concrete

Keywords: Foamed concrete, concrete damage plasticity model, segmentation, multi-phase model

Reference

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Point-based Diffusion Model for Predicting Spatio-Temporal Dynamics in Physical Systems

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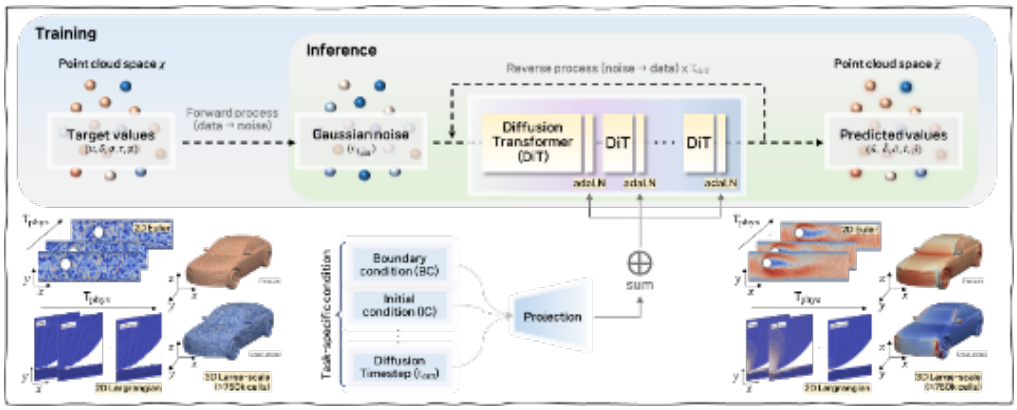

Figure 1.

Scientific machine learning (SciML) presents promising avenues for accelerating complex simulations and enabling real-time prediction. Among these, mesh-agnostic models, which learn representations independent of the underlying spatial discretization, are particularly attractive for handling diverse geometries. However, current state-of-the-art methods face significant limitations. For instance, MeshGraphNet[1] effectively preserves spatial relationships and physical constraints but incurs high message-passing costs and suffers from error accumulation in autoregressive predictions. Alternatively, DeepONet[2] achieves efficient inference through learned function representations but exhibits spectral bias, hindering its ability to capture fine-scale details. To overcome these challenges, we introduce a Point-based Diffusion model. Our approach utilizes the diffusion process to effectively model high-frequency components, inherently eliminates mesh dependency by operating on point sets, and circumvents error accumulation through single-step inference (**Figure 1**). We employ denoising diffusion implicit models[3] for sampling, drastically reducing inference time towards real-time capabilities. Comparative evaluations show that our model significantly outperforms existing methods in robustness and generalization when predicting dynamics for unseen geometries across 2D Eulerian, Lagrangian, and large-scale 3D systems.

Keywords: Scientific Machine Learning (SciML), Point-based Diffusion Model, Mesh-Agnostic, Physics Simulation (2D Spatio-Temporal, 3D Large-Scale), Shape Variations

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Characterization Of Vegetable Oil-Based Copper Nano-Lubricant on Tribological Properties

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Abstract: This study presents the development and tribological evaluation of eco-friendly copper nanoparticle (CuNP) enhanced vegetable oil-based nano-lubricants. Four biodegradable vegetable oils—mustard, soybean, palm, and sunflower—were selected as base oils due to their favorable fatty acid compositions and environmental compatibility. $CuNP_s$ were incorporated into these oils at concentrations of 0.15%, 0.30%, 0.45%, 0.60%, and 0.90% by weight, utilizing a two-step dispersion method involving mechanical stirring and ultrasonication to ensure homogeneous and stable nanoparticle distribution. Tribological assessments conducted under controlled conditions (15 rpm, 1.14 kg load, 5-minute duration) revealed that the 0.45% CuNP concentration yielded the lowest coefficient of friction and wear rate among all formulations. Scanning Electron Microscopy (SEM) analysis corroborated these findings, showing smoother wear tracks and minimal surface degradation at this concentration. Physicochemical characterizations, including electrical conductivity, flash and fire points, cloud and pour points, and p^H measurements, were performed by ASTM standards. The 0.45% CuNP formulations exhibited optimal conductivity, thermal resistance, and p^H stability, indicating robust performance under various operational conditions. Compared with conventional petroleum-based lubricants, these nano-lubricants exhibited desirable efficiency, eco-friendliness, and cost-effectiveness that signify their potential for industrial and automotive applications. CuNP concentrations > 0.45% induced nanoparticle agglomeration and decreased lubricating performance. The strong correlation indicates a key role of both the concentration of nanoparticles and the degree of tribological enhancement. It facilitates the design of green lubricants and/or additives at high-temperature and high-load conditions. The study demonstrates the potential of these bio-based nano-lubricants and establishes that 0.45% of CuNP-confined vegetable oils are promising and eco-friendly alternatives to conventional lubricants. Additional long-term stability, oxidation resistance, and engine material compatibility studies could be carried out to validate their actual field usefulness further.

Keywords: Copper Nanoparticles ($CuNP_s$); Vegetable Oil-Based Nano-Lubricants; Tribological Properties; Eco-Friendly Lubrication; Nanoparticle Dispersion Techniques; Physicochemical Characterization.

Fluid-Structure Interaction Analysis of Bioinspired Polymeric Heart Valves with Experimental Validation

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Valvular heart disease, when not addressed adequately, can result in heart failure, serious heart-related health problems, and in some cases, death. Polymeric heart valves (PHVs) are promising valve replacement technologies that may offer improved durability and better biological performance. Notably, PHVs have the potential to accommodate highly innovative valve designs. Given this feature of PHVs, it is important to shortlist the best performing valve designs prior to committing to extensive in vitro hemodynamic validation prototypes. This study presents a computational fluid-structure interaction (FSI) workflow to simulate the hemodynamic performance of PHVs under physiological conditions. The model accurately predicts cardiac output, effective orifice area and regurgitant fraction and these predictions have been successfully validated using experimental data. Detailed analysis of flow patterns, wall shear stress, valve opening and closing behaviours, and mechanical stress distribution are presented. This work demonstrates the potential of FSI simulations in predicting the hydrodynamic and mechanical behaviour of PHVs, offering valuable insights into valve durability and design optimization for improved patient outcomes.

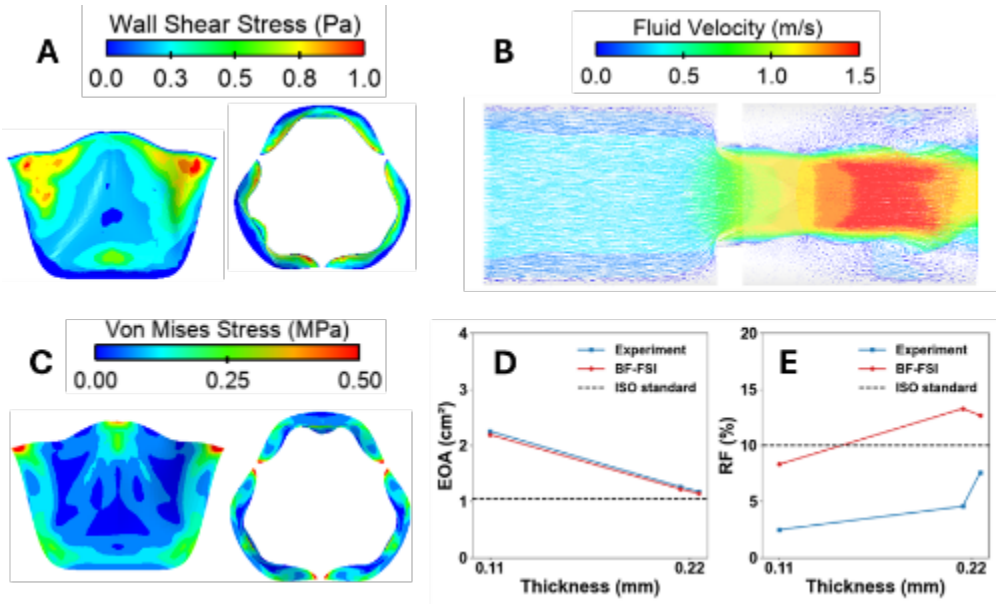

Figure 1. FSI analysis of bioinspired polymeric heart valves. (A) Wall shear stress; (B) Velocity pattern; (C) Mechanical stress; (D) Effective orifice area, and (E) Regurgitant fraction

Keywords: Polymeric heart valve, Hydrodynamic performance, Fluid structure interaction, Computational fluid dynamics, Body-fitted method

Stabilized Reproducing Kernel Enhanced Material Point Method for Air Flow and Air-Structure Interaction with Shocks

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Mesh-based methods, such as the finite element method within a Lagrangian framework, face significant challenges in modeling air flows and air-structure interaction (ASI) problems involving shock waves, primarily due to excessive mesh entanglement and distortion. In contrast, meshfree methods such as the Reproducing Kernel Particle Method (RKPM) and the Material Point Method (MPM) have proven effective, as their particle-based descriptions naturally avoid singularities caused by mesh distortion. However, these meshfree methods still suffer from various numerical artifacts to differing degrees. Additionally, when modeling air flows with shocks, appropriate numerical stabilization is crucial. To address these limitations, we propose a Reproducing Kernel Enhanced Material Point Method (RK-MPM) for simulating inviscid compressible flows with ASI. In this framework, a mixed MPM formulation is employed to solve the Lagrangian momentum and energy conservation equations, while the Reproducing Kernel (RK) approximation [1,2] is used to alleviate cell-crossing instabilities within MPM. To further suppress shock-induced oscillations, we enhance the classical artificial viscosity by introducing tensorial formulations of the diffusion and divergence operators, guided by the vorticity modulus. This approach blends numerical dissipation between the dilatational and deviatoric components to achieve improved stabilization [3]. Finally, we incorporate a point-to-structure contact algorithm to model the ASI system. The proposed method is validated through a series of benchmark problems, including shock waves, vortical flows, and air-structure interaction scenarios.

Keywords: inviscid compressible flow, reproducing kernel approximation, material point method, artificial viscosity, air-structure interaction

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Direct FE^2 multiscale modeling of hydrogen-induced cracking in reactor pressure vessels

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Leveraging the Direct FE^2 simulation method, we propose a strategy for the multiscale analysis of hydrogen-induced cracking in reactor pressure vessels that considers micro-voids, their influences on hydrogen diffusion as well as the operating pressure of the vessel [1]. In the finite element analysis, the nodal lattice hydrogen concentration and displacements are exchanged bi-directionally between the macroscale and microscale within a monolithic solution procedure. During the analysis, the voids are shown to cause non-uniform lattice hydrogen diffusion and the trapping effect, resulting in inter-void hydrogen accumulation, is demonstrated. Based on the hydrogen concentration on the void surfaces, the void hydrogen pressure was calculated for the hydrogen-induced cracking analysis. It was found that both internal shearing and necking failure modes exhibited micro-structure dependence. The internal shearing mode caused oriented through-wall propagation of cracks in the vessel pressure while the internal necking mode promoted void nucleation in the reactor pressure vessel. As a result, during the early stages of void evolution, the oriented internal shearing of the dispersed small voids showed a high possibility to induce through-wall failure of the reactor pressure vessel.

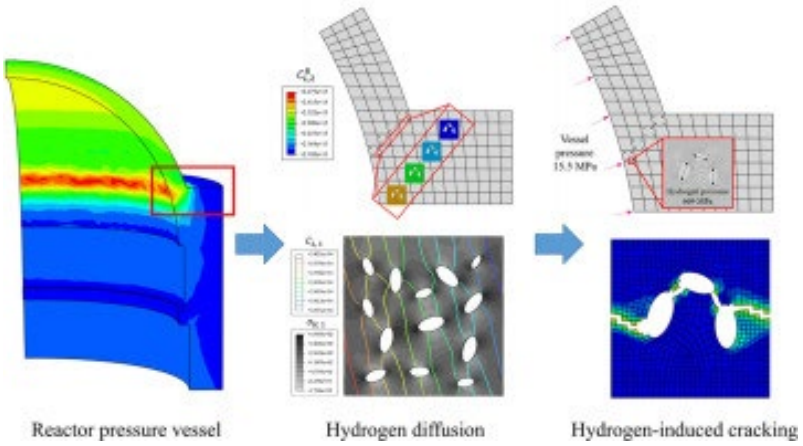

Figure 1.

Keywords: Direct FE^2, Reactor pressure vessel, Hydrogen diffusion, Hydrogen-induced cracking, Voids

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Hydration Process and Mechanical Properties of Low-Clinker LC^3

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Abstract: This study systematically investigates the effects of composite modification with calcium hydroxide ($Ca(OH)_2$) and calcium silicate hydrate (C-S-H) seeding on the hydration mechanism and mechanical properties of low-clinker calcined clay limestone cement. Experimental systems with varying metakaolin (MK) contents (20%, 40%, 60%) were designed, revealing that adding $Ca(OH)_2$ alone effectively enhances later-age compressive strength but has limited impact on early strength. The introduction of C-S-H seeds creates a synergistic effect: seeds promote early nucleation, while $Ca(OH)_2$ ensures sufficient pozzolanic reaction in the later stages. Specifically, nanoscale C-S-H seeds accelerate the early hydration nucleation process, and slow-release $Ca(OH)_2$ sustains an alkaline environment to support prolonged pozzolanic reactions. Microscopic analysis shows that this composite modification simultaneously enhances the crystallinity of carboaluminate phases and the polymerization degree of C-S-H gel, with more pronounced effects in low-clinker systems with higher MK contents (40%-60%). The proposed "nucleation-guided, sustained-release" composite modification strategy offers an innovative solution for developing high-performance ultra-low-carbon cement and provides an effective pathway for reducing carbon emissions in cement production.

Keywords: LC^3; C-S-H seeding; $Ca(OH)_2$; mechanical properties; hydration reaction.

Computational Fluid Dynamics Analysis of Metal Hydride Hydrogen Storage Performance

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Abstract

Metal hydride hydrogen storage systems are recognised for their advantages over other storage methods, though they are often limited by slow hydrogen charging and discharging due to poor reaction kinetics. Enhancing heat transfer within the storage system is a key strategy to address this limitation, as efficient heat removal accelerates hydrogen absorption, while effective heat addition enhances desorption. This study explores the use of combined internal and external heat exchangers to improve the thermal performance and reaction kinetics of metal hydride storage. An internal heat exchanger with a U-type tube is investigated and compared across three storage designs using numerical simulations in ANSYS Fluent 2024 R2. A comprehensive grid refinement is performed for the computational mesh, and the computational results are validated against experimental and numerical findings available in the literature. A detailed parametric study is conducted for both the charging and discharging processes of the metal hydride hydrogen storage system. The underlying mechanisms of liquid fraction dynamics, temperature changes, and hydrogen concentration profiles are analysed. The proposed heat exchanger design significantly improves the overall thermal performance of the system. The findings demonstrate that integrating internal and external thermal management systems greatly enhances both charging and discharging behaviour. The inclusion of a thermal cooling blanket within the heat exchanger design results in improved performance compared to the original configurations. This study contributes to advancing the understanding of thermal management in hydrogen storage systems and offers valuable design insights for developing more efficient and responsive hydrogen energy solutions.

Keywords: Hydrogen storage, Charging and discharging, Heat exchanger, Cooling blanket.

APCOM-ACCM 2025
Brisbane, Australia
7-10 December 2025

Advancing Knowledge on HMPV Spread: A CFD-Based Study of Airway Deposition

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Human metapneumovirus (HMPV) is a significant respiratory pathogen responsible for infections ranging from mild upper respiratory illnesses to severe bronchitis and pneumonia. Understanding the movement and deposition of HMPV within the human airways is critical for assessing infection risks and developing targeted therapeutic strategies. Previous studies have primarily focused on the epidemiology, molecular characteristics, and immune response to HMPV, with particular emphasis on its genetic lineages, seasonal variations, and vaccine development efforts. However, no attention has been given to the detailed particle deposition patterns in the tracheobronchial tree under different breathing conditions. This study employs computational fluid dynamics simulations using ANSYS and the discrete phase model approach to analyze the transport and deposition of HMPV-laden droplets in the human airways (see Fig.1), spanning from the trachea to generation 15.

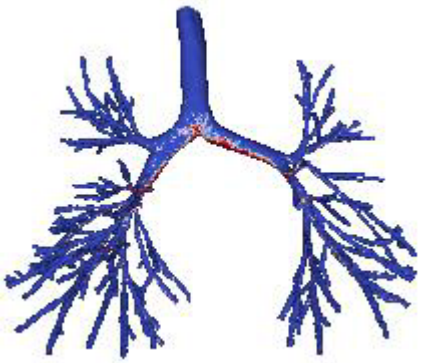

Figure 5.

The model simulates airflow in realistic airways using the Navier-Stokes equations and tracks HMPV-laden droplets with the Lagrangian method for the complete breathing cycle, considering drag, gravity, lift, Brownian forces and turbulence. Deposition efficiency is analyzed across different breathing conditions, particle sizes, and airway generations. The key results indicate that 10 nm virus particles deposit slightly more in the tracheobronchial generations compared to 250 nm particles. At a flow rate of 7.5 L/min, the deposition efficiency is 6.3% for 10 nm particles and 5.7% for 250 nm particles, while at 15 L/min, it increases to 12.4% and 11.9%, respectively. Additionally, particle trapping predominantly occurs in the earlier airway generations, from the trachea to G6, with peak deposition observed in G1 and G6. Furthermore, virus particles exhibit significantly higher deposition during the inhalation phase of the breathing cycle. The findings provide a comprehensive understanding of HMPV transport dynamics and can contribute to improved infection control measures and therapeutic strategies.

Keywords: HMPV, virus transport, human airways, respiratory treatment, computational fluid dynamics

On flexural behavior of 3D-printed continuous hybrid fiber reinforced composites: Experimental and multiscale modeling study

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3D-printed continuous hybrid fiber reinforced composites (cHFRC) present great advantages in terms of balanced design between material cost, weight reduction, and mechanical properties. Nevertheless, the lack of an effective design methodology has so far limited its large-scale application. This paper aims to provide a high-fidelity multiscale modeling strategy for 3D-printed cHFRC and achieved a micro-meso-macro matched optimization design.

To unite the models in three scales, the stress amplification factor played a crucial role. In the multiscale analysis of continuous fiber 3D-printed composites, two stages of stress amplification factor $\boldsymbol{M_{meso}}$, $\boldsymbol{M_{micro}}$ were included as shown in Eqs. (1) and (2) [1, 2].

$$\boldsymbol{\sigma_{meso}} = \boldsymbol{M_{meso}}\boldsymbol{\sigma_{macro}} \tag{1}$$

$$\boldsymbol{\sigma_{micro}} = \boldsymbol{M_{micro}}\boldsymbol{\sigma_{meso}} \tag{2}$$

where $\boldsymbol{\sigma_{micro}}$, $\boldsymbol{\sigma_{meso}}$, and $\boldsymbol{\sigma_{macro}}$ denoted microscopic stress, mesoscopic stress, and macroscopic stress, respectively. $\boldsymbol{M_{micro}}$ and $\boldsymbol{M_{meso}}$ were the microscopic and mesoscopic stress amplification factor matrix. The stress of each scale and stress amplification factor matrix $\boldsymbol{M_{\sigma}}$ were shown in Eqs. (3), (4).

$$\begin{cases} \boldsymbol{\sigma_{micro}} = [\sigma_1 \ \ \sigma_2 \ \ \sigma_3 \ \ \sigma_{12} \ \ \sigma_{23} \ \ \sigma_{13}]^T \\ \boldsymbol{\sigma_{meso}} = [\sigma_1 \ \ \sigma_2 \ \ \sigma_3 \ \ \sigma_{12} \ \ \sigma_{23} \ \ \sigma_{13}]^T \\ \boldsymbol{\sigma_{macro}} = [\sigma_1 \ \ \sigma_2 \ \ \sigma_3 \ \ \sigma_{12} \ \ \sigma_{23} \ \ \sigma_{13}]^T \end{cases} \tag{3}$$

$$\boldsymbol{M}_{\sigma} = \boldsymbol{M_{meso}}/\boldsymbol{M_{micro}} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & M_{14} & M_{15} & M_{16} \\ M_{21} & M_{22} & M_{23} & M_{24} & M_{25} & M_{26} \\ M_{31} & M_{32} & M_{33} & M_{34} & M_{35} & M_{36} \\ M_{41} & M_{42} & M_{43} & M_{44} & M_{45} & M_{46} \\ M_{51} & M_{52} & M_{53} & M_{54} & M_{55} & M_{56} \\ M_{61} & M_{62} & M_{63} & M_{64} & M_{65} & M_{66} \end{bmatrix} \tag{4}$$

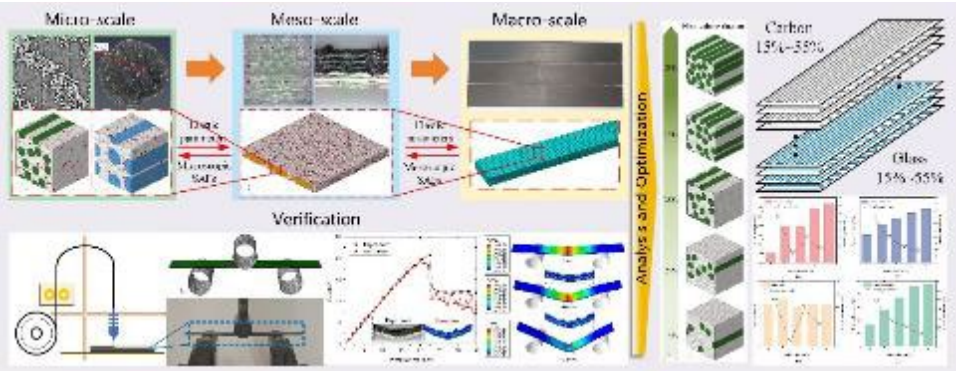

Figure 1.

Keywords: Continuous fiber 3D printing, Multiscale modeling, Flexural behavior

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Leveraging dielectrophoresis in inertial flow for versatile manipulation of micro and nanoparticles

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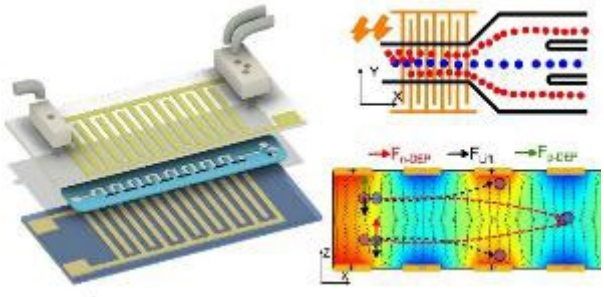
The manipulation of micro and nanoparticles has extensive applications in biomedical research, clinical diagnostics, environmental monitoring, drug discovery, and the mining industry. Dielectrophoresis (DEP) utilises nonuniform electric fields to manipulate particles, offering a label-free, high-precision, and non-invasive method for both natural and synthetic particles. DEP manipulation has been well studied in the Stokes flow region with ultra-low Reynolds numbers (Re $\ll$ 1), where viscous effects dominate. However, its application in the inertial flow regime remains largely unexplored. This study aims to bridge the gap by coupling DEP and inertial flow for the manipulation of particles across micro and nano scales. First, we theoretically analysed the physical coupling of DEP and inertial lift forces along the vertical direction in microchannels, utilising symmetrical interdigitated electrode (IDE) arrays patterned on the top and bottom channel surfaces. We then experimentally investigated how the vertical coupling of DEP and inertial lift forces affects particle lateral focusing properties. The effects of DEP along the vertical direction were leveraged and amplified by the inertial effects along the lateral direction. Finally, we applied DEP in the inertial flow regime for size-based and dielectric property-based separation of particles and cells, as well as nanoparticle focusing and filtration. Leveraging DEP in inertial flow will advance the field by providing a versatile and powerful method for the manipulation of micro and nanoparticles.[1]



Keywords: microfluidics, micro and nanoparticles, separation of particles and cells, dielectrophoresis, inertial flows, physical coupling

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A novel thermomechanical coupling continuous-discontinuous method for geomaterials based on FDEM

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Thermomechanical (TM) coupling is a hot research topic in geomechanics due to its significant relevance to natural geological processes and implications for underground engineering and energy projects. The combined finite-discrete element method (FDEM) is a powerful numerical method that integrates continuum mechanics concepts with DEM algorithms. FDEM can capture progressive damage and failure processes in brittle materials, making it an effective modeling tool for deep underground engineering applications. However, the current FDEM-based model's heat transfer calculations for thermal contact are mainly based on a single edge of the contact area rather than the entire overlapping region, and they are unable to handle the continuous-discontinuous transition processes in thermal field calculation under quasi-static and dynamic conditions.

A new thermomechanical (TM) coupled finite-discrete element method (FDEM) model has been developed for continuous and discontinuous geomaterials, incorporating heat conduction, thermal cracking, and contact heat transfer. This model features a heat conduction framework that accurately calculates the thermal field during continuous-discontinuous transition processes. Additionally, a modified contact heat transfer model is included, accounting for the entire contact area of discrete bodies. To align with the finite strain theory used in the FDEM mechanics module, the TM coupling module is based on the multiplicative decomposition of the deformation gradient.

The model has been applied to various scenarios, such as heat conduction in continuous and discontinuous media during transient states, thermal-induced strain and stress, and thermal cracking conditions. Validation of the thermal field calculation and TM coupling models has been achieved by comparing numerical results with experimental findings and analytical solutions (Figure 1). These numerical cases convincingly demonstrate the reliability of the proposed model, making it suitable for a wide range of continuous and discontinuous media.

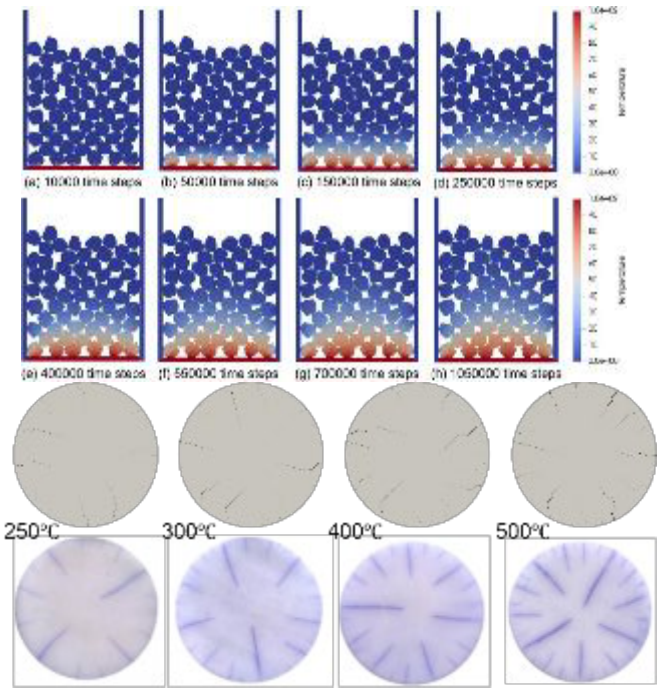

Figure 1.

Keywords: Finite-discrete element method (FDEM), Thermomechanical (TM) coupling, Thermal cracking, Contact heat transfer, Geomaterials

Optimization of a thermal flow surrogate model for liquid cooling systems based on machine learning

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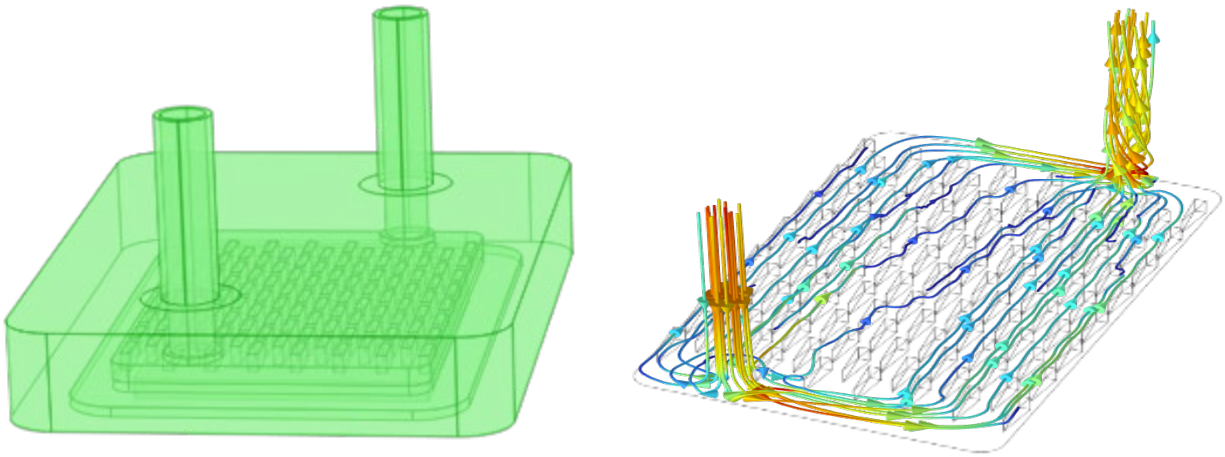
This study aims to construct an efficient surrogate model for liquid cooling systems, as shown in Figure 1, using machine learning techniques and to enable rapid design iterations and parameter optimization through optimization algorithms. The research process is divided into four main stages. First, OpenSCAD and Python are employed to achieve automated 3D modeling, generating adjustable 3D models based on key design parameters such as nozzle size and cold plate structure. Second, single-phase flow and thermal flow simulations are performed using COMSOL Multiphysics to establish a coupled multiphysics system, thereby generating a comprehensive dataset of thermal flow information. Third, machine learning techniques are utilized to train the surrogate model, with cross-validation used to verify its predictive accuracy. Finally, global optimization methods are applied to rapidly iterate design parameters and identify optimal design solutions. This research is expected to significantly reduce simulation time and computational resource requirements. By establishing a surrogate model with high predictive accuracy, a more precise and reliable design process for liquid cooling systems can be realized. Furthermore, the integration of optimization algorithms allows for the rapid identification of optimal design solutions, thereby shortening the development cycle and reducing costs for liquid cooling system design.



(a) Finite element model (b) Flow lines

Figure 1. Liquid cooling system

Keywords: liquid cooling, multiphysics simulation, machine learning, optimization, parameter design

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Discrete Element Modeling of Irregular-Shaped, Deformable Biomass Particle Flow

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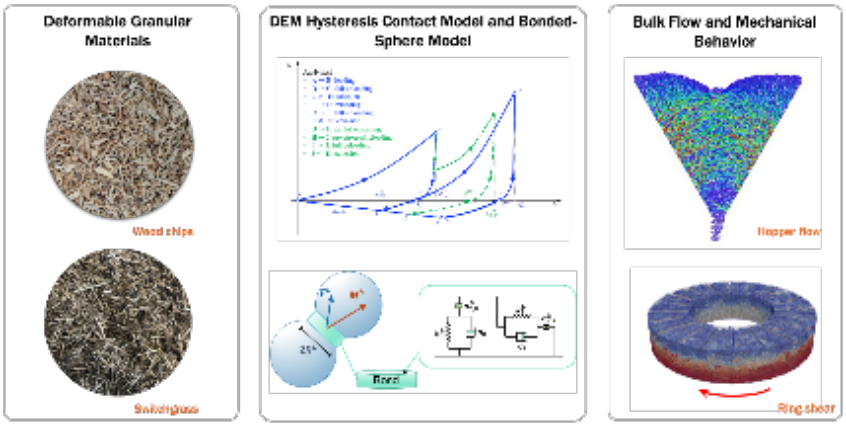
Many natural and engineered granular materials have relatively deformable particles. An example of such material is woody biomass, which is one commonly used biomass feedstock for bioenergy conversion. For these materials, particle size, shape, and deformability are all factors that may significantly impact the material's flow behavior. In this work, the flow of irregular-shaped deformable woody biomass particles is investigated using discrete element simulations. A bonded-sphere model is developed to simultaneously capture irregular particle shapes and particle-wise deformations (e.g., compression, deflection, and distortion) [1,2]. Quantitative analysis of the effects of irregular shapes and particle deformations shows that the increase in particle stiffness tends to increase initial packing porosity and decrease the flow rate in the hopper. Rigid particles tend to have clogging issues, whereas deformable particles have less chance to, indicating particle deformation reduces the critical bridging width in the hopper flow. Moreover, an alternative approach is also discussed, where, instead of explicitly modeling particle shapes and deformability, spherical particles with a novel contact model are used to capture the flow behavior of such material [3]. Parametric studies of hopper discharge over varying hopper processing parameters and pine material attributes are conducted to understand different processing parameters and material attributes on flow behavior [4].



Keywords: Discrete element method; deformable particle; particle shape; hopper flow.

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Enhanced Iterative Solvers for Coupled Problems: Overcoming the Slow Convergence of Staggered Schemes

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The staggered algorithm is one of the most widely used iteration schemes for multi-field coupled problems. It is often stable and robust in solving for the individual fields; however, it sometimes requires many iterations between the fields, leading to high computational costs. This presentation reveals the deciding factor for the convergence behaviors of the staggered scheme. This deciding factor is a parameter coined the degree of coupling (DOC). The DOC is defined based on the blocks of the Jacobian matrix (or tangent stiffness matrix). It can be proven that the staggered scheme exhibits first-order convergence, with the reduction factor of the residual and the error equal to the DOC. Consequently, when the DOC is close to 0, the staggered scheme quickly converges; when the DOC is less than but close to 1, the convergence is slow; when the DOC is greater than or equal to 1, the staggered scheme is not guaranteed to converge. For instance, in the case of phase-field model for fracture, the DOC increases with loading displacement until it oscillates slightly below 1. Thus, while convergence is guaranteed, it may require many iterations.

Based on the DOC, an efficient scheme is developed to boost the staggered scheme. The core of the proposed scheme is to employ the Schur complement to take the coupling of the fields into account when updating one of the fields. The proposed scheme significantly reduces the number of required iterations and CPU time. The efficiency of this scheme is demonstrated through benchmark examples of phase field fracture problems and a thermo-mechanical coupled fracture problem. Compared with existing schemes such as the staggered scheme and the L-BFGS scheme, the proposed scheme needs the least iterations and CPU time.

Keywords: Phase field approach to fracture, degree of coupling, Schur-complement, multi-field coupled problems, staggered scheme

Coupled Multiphysics Simulation of CO_2 Storage in Saline Aquifers: Analysing the impacts of Multiphase Flow, Fracture Network, and Geochemical Impacts

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This study presents a comprehensive coupled multiphysics model to simulate CO_2 storage in saline aquifers. The model integrates multiphase flow dynamics, non-isothermal conditions, and geochemical effects to provide a holistic understanding of the processes involved in CO_2 sequestration. By accurately simulating the behavior of CO_2 and brine within the aquifer, the model captures the complex interactions between fluid phases and the porous medium. The influence of temperature variations on the flow and storage processes is investigated, highlighting the significance of thermal gradients on CO_2 migration and stability. Additionally, the geochemical effects on the aquifer, including changes in permeability and porosity due to CO_2 injection, are investigated, with particular attention to the evolution of permeability in relation to the stress-strain responses of the reservoir rocks. The convective dissolution of CO_2 into the brine is examined, providing insights into the long-term stability and trapping mechanisms of the sequestered CO_2. Furthermore, the impact of geochemical factors on the evolution of the CO_2 plume is assessed, offering a detailed understanding of plume dynamics and potential leakage pathways. The results of this study demonstrate the critical importance of considering coupled multiphysics processes in the accurate prediction of CO_2 behavior in subsurface reservoirs. By incorporating thermal, hydrodynamic, and mechanical interactions, this model offers a robust framework for optimizing CO_2 storage strategies and ensuring the long-term integrity of saline aquifers as storage sites.

Keywords: CO_2 storage, saline aquifer, multiphase flow, non-isothermal effects, geochemical, permeability evolution, convective dissolution, plume evolution.

Hierarchical Evolutionary Renewables Optimisation in mineral processing

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The mining sector is aligning with global decarbonization trends by integrating variable renewable energy (VRE) to reduce operational costs and emissions. In Western Australia, companies like Gold Fields and Sandfire Resources are leading this transformation, with projects such as the St Ives Renewable Energy initiative supplying up to 73% of site energy needs.

However, mineral processing—the most energy-intensive stage of mining—remains a key challenge, particularly the semi-autogenous grinding (SAG) process. Our research introduces a novel AI-based approach to address this challenge by combining reinforcement learning (RL) with solar-powered grinding systems. This integration enables real-time adaptation to VRE availability, optimizing energy use and production efficiency.

We propose **Hierarchical Evolutionary Renewables Optimization (HERO)**, a three-level framework that includes:

1. **Simulation Adaptation** – responsive models of process dynamics.
2. **Supply-Demand Optimization** – neural-network-based energy allocation.
3. **Collective Intelligence Selection** – evolutionary selection of optimal strategies using swarm intelligence.

These levels operate at different sampling rates and interact through a biomimetic, agent-based architecture. Inspired by the fact that natural brains themselves are the products of an evolutionary process [1] each agent's replication is governed by an energy-based reserve fitness model designed to counteract entropic decay. The agent's reserve accumulation is described by:

$$\frac{dR}{dt} = \max\left(0, \frac{\beta\left(\psi - \frac{d\psi}{dt}\right) - \eta P + \alpha\theta_T}{(1+\gamma)}\right) \qquad (1)$$

Where:

- α, β, γ – represent the agent's degradation rate, energy acquisition capacity, and replication cost.
- ψ – agent fitness; P – power available; η – efficiency of power transfer; θ_T – production target

HERO offers multiple applications, such as early-stage impurity identification and energy-aware material selection, which improve energy efficiency, reduce mechanical wear, and lower processing costs.

Keywords: Artificial evolutionary models, renewables optimization, swarm intelligence, genetic algorithms, reinforcement learning.

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Numerical Study of the Periodic Deformation Behaviour of a Single RBC

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This study presents a computational investigation into the periodic deformation behaviour of a single red blood cell (RBC) subjected to microfluidic flow, employing the open-source numerical framework Hemocell. The primary objective is to elucidate the dynamic deformation characteristics of RBCs under varying hemodynamic conditions, with a particular focus on the periodic nature of their mechanical response. RBC deformation is quantitatively characterised through geometric configurations, dynamic motion, and force interactions, while Fourier transform techniques are applied to extract and analyse the frequency components underlying deformation periodicity. A parametric analysis is conducted to assess the effects of key fluidic parameters—namely, fluid viscosity and Reynolds number—on the deformation dynamics of RBCs. The findings demonstrate that RBCs exhibit robust periodic deformation patterns, whose frequency and amplitude are significantly influenced by the surrounding flow conditions. Increases in fluid viscosity and variations in Reynolds number induce notable changes in both the frequency content and magnitude of cell deformation, highlighting the intricate interplay between intracellular mechanical properties and external fluid forces. The results provide valuable insights into RBC biomechanics and support the development of quantitative models for RBC behaviour in microcirculatory flow. The findings also highlight that hyper viscous conditions can compromise RBC mechanical stability, with important implications for blood rheology in pathological conditions involving altered viscosity. This study enhances the current understanding of RBC deformation under flow and establishes a basis for future research into RBC mechanobiology in both healthy and diseased states.

Keywords: Erythrocyte deformation, red blood cells (RBCs), Blood rheology, Hyper viscous flow conditions, Cell integrity.

A Compressed Sensing based Framework for Surface Pressure Field Reconstruction from Sparse Measurement

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In this presentation, a compressed sensing based framework has been proposed to investigate the reconstruction of the original surface pressure field from extremely sparse measurement data, as shown in Figure 1. The proposed framework integrates the generalized proper orthogonal decomposition (GPOD) method for flow field dimensionality reduction, the compressed sensing (CS) technique for accurate reconstruction of the original signal, and the particle swarm optimization (PSO) algorithm for optimizing sensor placement strategies. Unlike image and unsteady flow field reconstructions, the method presented in this paper has been successful in reconstructing surface pressure fields of high-speed train under various conditions. Based on the accurate reconstruction of surface pressure fields, further aerodynamic load data can be obtained. Additionally, this paper optimizes the traditional pressure sensor layout using a particle swarm optimization method, which not only improves reconstruction accuracy but also significantly reduces the deployment of redundant sensors. Moreover, traditional point selection strategies based on human experience can still be incorporated into the pressure sensor layout scheme and effectively reduce reconstruction errors under crosswind conditions.

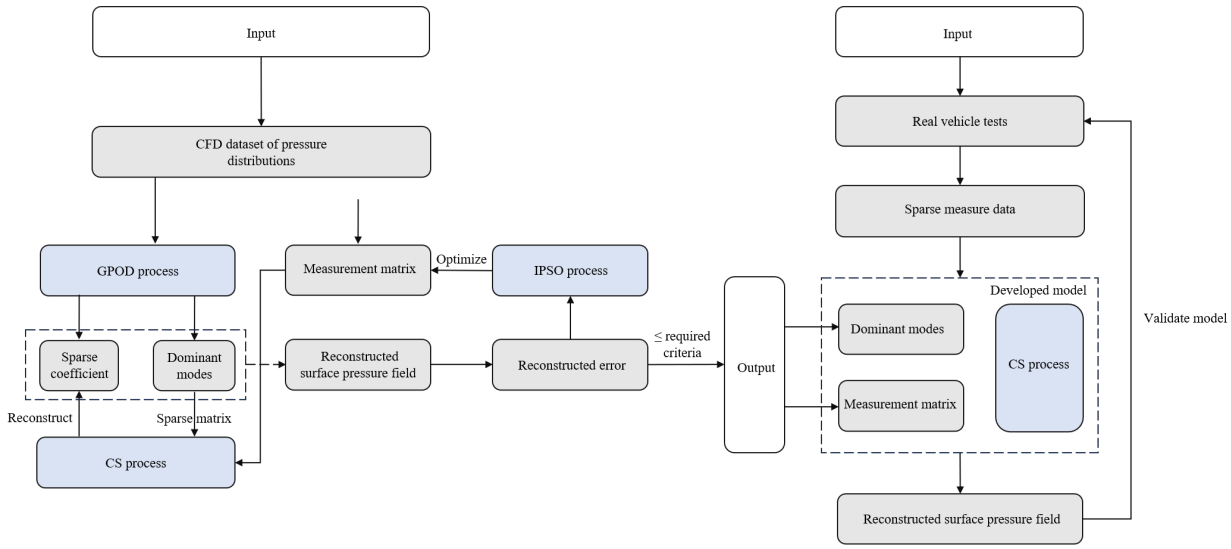

Figure 1.

Keywords: Surface pressure reconstruction, compressed sensing, proper orthogonal decomposition, particle swarm optimization

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3D Geometry Augmentation Guided by Engineering Uncertainty

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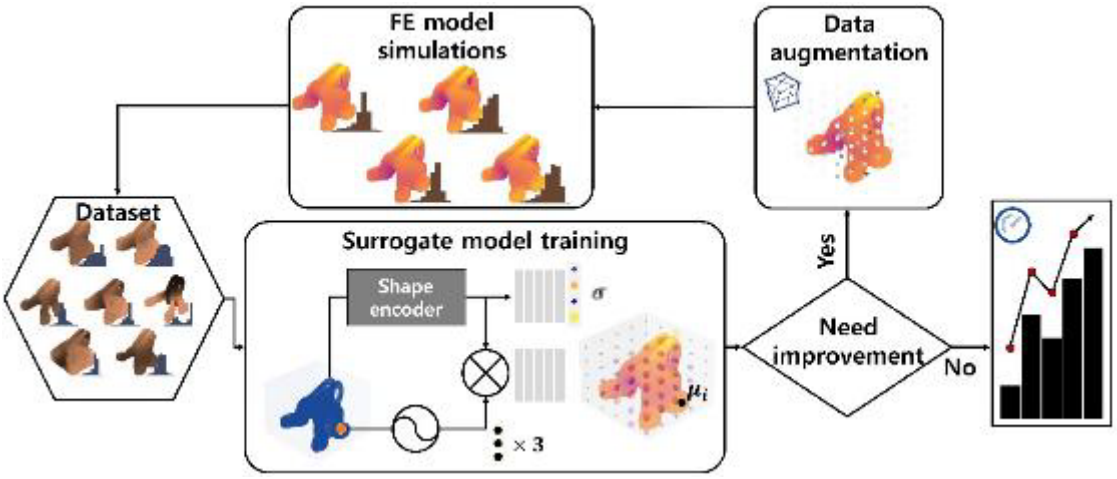

Figure 1.

In the conceptual design stage, fast and accurate shape evaluation is crucial for efficient product development. While simulation-based performance evaluation is commonly adopted, its high computational cost has motivated the development of more efficient surrogate models that leverage deep learning for rapid inference and effective handling of nonlinear, high-dimensional data. However, acquiring large-scale three-dimensional datasets in the industry is challenging. Augmentation-based active learning emerges as a viable alternative. But mere geometric diversity does not guarantee corresponding performance diversity, highlighting the need for data augmentation that considers geometry and performance [1]. This study addresses this challenge by proposing an integrated framework that combines geometry-based uncertainty quantification with free form deformation augmentation. Uncertainty quantification is achieved using a deep ensemble model that incorporates a novel architecture comprised of two regressors: an explicit uncertainty regressor to quantify aleatory uncertainty and a performance regressor to predict performance. The epistemic uncertainty extracted from this model is then leveraged to actively explore the regions necessary for the effective training of a surrogate model. Using the public three-dimensional bracket dataset, we initially built a surrogate model with a subset of the data and subsequently augmented the dataset with samples generated by our framework. This approach employs an active learning framework that accounts for both performance and geometric diversity. Experimental results confirm that the augmented dataset exhibits superior performance. Performance-aware three-dimensional shape augmentation has strong potential for industrial applications. In addition, the proposed framework can be applied not only to meshes but also to images, and other forms of representation.

Keywords: data augmentation, artificial intelligence, active learning, uncertainty quantification

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Crashworthiness analysis and multi-objective optimization design for foam-filled spiral tube

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Thin-walled structures, due to their favorable mechanical properties and exceptional energy absorption capabilities, find extensive applications across various engineering fields. This study, drawing inspiration from natural spiral structures, introduces a novel foam-filled spiral tube (FFST) to further enhance the crashworthiness of thin-walled structures. The spiral tubes (STs) and random foam are additively manufactured. Quasi-static compression tests are undertaken to investigate the energy absorption properties of STs, foam and FFSTs. Unlike conventional methods, this study adopts micro-computed tomography (micro-CT) technology to understand the mechanisms of interaction between the foam and ST. The parametric study is performed based on the finite element model to evaluate the influence of meso-structure properties of tubes and foam fillers on the crashworthiness and deformation modes. The experimental results indicate that an increase in the wall thickness of both the ST and foam leads to a simultaneous increase in specific energy absorption (SEA) and initial peak crushing force (IPCF). Conversely, a decrease in the wavelength and an increase in the amplitude of waves results in the reduction of both SEA and IPCF, along with an enhancement of crushing force efficiency (CFE). Micro-CT images indicate mutual extrusion between the foam and ST and with a reduction in wavelength, the number of folds in the samples increased, thus enhancing the energy-dissipation capacity. The numerical results reveal a strengthening of interaction between the foam and ST with decreasing wavelength and increasing foam cell wall thickness. A theoretical model is proposed for predicting the plateau stress of FFSTs based on the energy conservation principle and the plastic hinge theory. Comparisons between theoretical and test results exhibit good agreement. Comparing the FFST obtained through multi-objective optimization design with an ST featuring same structural parameters, it is observed that the IPCF increases by 8.00%, SEA increases by 18.10%, and the undulation of load-carrying capacity (ULC) decreases by 31.96%. Finally, through a comparative analysis with other energy-absorbing structures, the outstanding performance of this structure is established. This study offers a new approach for investigating interaction effects and provides useful guidelines for the design of future high-performance light-weight materials and structures.

Keywords: Foam-filled tube, crashworthiness, multi-objective optimization, micro-CT scan, interaction effect, meso-structure properties

Machine Learning-Based Assessment of Liver Fibrosis Using Animal Models and Human Clinical Data"

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Liver diseases consistently rank among the top ten causes of death in Taiwan. Generally, the progression of liver diseases can be categorized into three stages: liver fibrosis, liver cirrhosis, and liver cancer. This study aims to advance current non-invasive diagnostic methods for the early detection of liver fibrosis by introducing a machine learning (ML) approach for prediction. The research comprises two components: experiments conducted on mice and the analysis of clinical data from human subjects.

Mouse Experiment: Mice were categorized into healthy (A0), mild (A1), moderate (A2), or severe (A3) liver fibrosis stages. Support Vector Machines (SVM) were employed as classifiers using two types of features: Euler numbers and estimated porosity related to liver fibrosis. Model comparisons included SVM models with solely estimated porosity, exclusively Euler numbers, and a combination of all features. Binary and grayscale images were used to train Convolutional Neural Network (CNN) models in the baseline. The basic idea behind these feature extractions stems from the geometric and topological properties of liver imaging. After parameter tuning, the final model comparisons showed that using the two features separately for binary (Acc=63.2%) and grayscale (Acc=64.5%) images for training CNN models, as well as on SVM models using different features—solely estimated porosity (Acc=93.3%), solely Eulercharacteristic numbers (Acc=74.6%), and all features combined (Acc=90.9%). The model using solely estimated porosity as a feature outperformed other models' overall performance across the four categories, particularly excelling in the mild (A1) category.

Human Clinical Data: Clinical data from 62 patients, including blood tests and dynamic contrast-enhanced magnetic resonance imaging (DCE-MRI) signal curves, were utilized for human liver fibrosis classification. New features simulating liver properties were introduced, such as porosity, diffusion rate, and flow speeds of the portal vein and hepatic artery. K- Nearest Neighbors (KNN) and Naive Bayes (NB) models were employed, focusing on F0-3 vs F4-6 and F0-5 vs F6 classifications. The ML models achieved excellent results in F0-3 vs F4-6 and F0-5 vs. F6 classifications, with an overall three-class accuracy of 69.4%. The introduction of simulated liver signal concentration models significantly enhanced accuracy in liver fibrosis assessment.

This study highlights the promise of machine learning techniques, specifically SVM, KNN and NB, in predicting the stages of liver fibrosis. By utilizing simulated liver properties as features in human data, the research enhances our understanding of liver fibrosis and opens new avenues for exploration, potentially improving diagnostic accuracy. The findings emphasize the importance of machine learning applications in advancing the assessment and treatment of liver diseases.

A Novel Method for the Quantitative Characterization of Rock Block Systems to Enhance Rockfall Hazard Prediction

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Abstract: Rockfalls represent a significant geological hazard, making the analysis of their motion essential for effective risk prevention and mitigation. Accurate rockfall behavior prediction requires a comprehensive understanding of rock mass structures, which can be understood as either structural plane (joint) systems or rock block systems. Among these, rock blocks are critical in evaluating rock mass stability and rockfall kinematics. Quantitative characterization of block systems is key to assessing the influence of block geometry on rockfall trajectories. However, existing methods for characterizing block shapes are qualitative, limiting their application in rockfall motion prediction. To address this, we propose a novel quantitative approach for characterizing block systems using shape clustering analysis. The Shape Similarity Index (SSI) is introduced as a metric to quantitatively assess the shape similarity between two blocks. After normalizing the volumes of the target blocks, SSI is calculated as the ratio of the maximum overlapping volume (V_o) to the normalized volume (V_p):

$$\mathrm{SSI} = \frac{V_o}{V_p} \tag{1}$$

A shape similarity matrix for the entire block system is then constructed based on SSI values between all block pairs. Spectral clustering is applied to group the blocks, and a representative block is generated for each group, reflecting the shape and size characteristics of the blocks within the respective group. This method is demonstrated through a case study in an open-pit mine in the United States, where it is used to simulate rockfall trajectories and assess hazard potential. Compared to traditional methods, this approach captures the intricate shape variations of blocks. We anticipate that our method bridges the gap between theoretical geometric characterization of block systems and the precise prediction of rockfall behavior.

Keywords: rock mass structure, rock block characterization, rock block system, rock block shape, rockfall hazards, rockfall trajectory

Physics-informed neural network-based Topology optimization framework for geometrically nonlinear structures

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This study presents a Physics-Informed Neural Network-based Topology Optimization (PINNTO) framework for geometrically nonlinear structures. By leveraging the mesh-free nature of PINNs, the proposed approach effectively models nonlinear partial differential equations (PDEs) while addressing the numerical instabilities inherent in conventional nonlinear topology optimization methods. The framework integrates two key components: the Deep Energy Method (DEM) and a neural reparameterization scheme, which replace finite element analysis (FEA) and traditional sensitivity analysis, respectively. The DEM solves the forward hyperelasticity problem by embedding the principle of minimum potential energy as the natural loss of the network [1]. Sensitivity analysis is then conducted through automatic differentiation using the neural reparameterization. Unlike conventional methods that require energy interpolation or relaxation techniques to handle large deformations, our approach ensures stability without additional technique [2]. Moreover, incorporating Fourier feature embedding and periodic activation functions significantly accelerates PINN training, leading to faster computation times compared to benchmark FEA-based topology optimization methods [3]. The proposed method is validated through several benchmark problems, demonstrating both computational efficiency and accuracy. These results underscore the potential of PINNs as a robust and efficient alternative for topology optimization in geometrically nonlinear systems.

Keywords: Topology optimization, Physics-informed neural networks, Machine Learning, Nonlinearity, Fourier feature mapping

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Learning Axial Green's Function via Neural Networks for Elliptic Problems with Variable Coefficients

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The Axial Green Function Method (AGM) is a powerful computational framework for solving multidimensional elliptic boundary value problems by systematically decomposing them into a set of one-dimensional problems. [1] While AGM avoids the complexity of full-dimensional Green's functions, its applicability is limited when analytic forms of the 1D Green's functions are unavailable due to variable coefficients. In this work, we propose a neural network-based approach to overcome this limitation by learning the one-dimensional Green's function within the AGM framework. The neural Green's function $G(x,s)$ is designed to satisfy homogeneous Dirichlet boundary conditions and the differential operator in a weak sense. Specifically, we represent the Green's function as a hybrid formulation comprising an analytically defined singular kernel and an MLP-based residual component. The neural network learns the smooth non-singular part, while singular structures are handled explicitly through classical Poisson kernels.

We applied our approach to the following one-dimensional second-order linear elliptic partial differential equation:

$$Lu(x) = -\frac{d}{dx}\left(a(x)\frac{du(x)}{dx}\right) + b(x)\frac{du(x)}{dx} + c(x)u(x) = f(x). \quad (1)$$

Here, $a(x)$, $b(x)$, and $c(x)$ are continuous coefficient functions and $f(x)$ is a given source term. The objective of this study is to approximate the corresponding Green's function using a neural network and to integrate it within the AGM to efficiently compute solutions. The training is performed using supervised data composed of source-solution pair (f,u), and the learned Green's function is used in integral representations to reconstruct the solution. We demonstrate the effectiveness of the method on benchmark elliptic problems with variable coefficients, and confirm that the structure and convergence properties of the original AGM are preserved. This hybrid approach integrates data-driven modelling with analytical numerical methods, and provides a more flexible and scalable extension of the Axial Green Function Method.

Keywords: Axial Green Function Method, neural Green's function, elliptic PDE, variable coefficients, data-driven numerical methods

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Mixing Thixotropic Fluids with Yield Stress in a Static Mixer

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Thixotropic fluids are a class of non-Newtonian fluids that exhibit time-dependent viscosity changes under applied shear stress. When shear is applied, the internal microstructure breaks down, leading to a reduction in viscosity; upon removal of the stress, the microstructure gradually recovers via Brownian motion, resulting in increased viscosity. These fluids also exhibit a yield stress, adding complexity to both experimental and numerical analyses. Efficiently mixing thixotropic fluids is critical in various industrial applications, including batteries, rocket propellants, biotechnology, and more. In this study, the flow and mixing characteristics of a thixotropic fluid with yield stress inside a static mixer were investigated numerically. The static mixer consists of helical mixing elements inserted within a circular pipe, optimized to promote chaotic mixing under the creeping flow condition of Newtonian fluids. To model the thixotropic behavior, a structure-kinetics equation was employed, in which the degree of microstructure breakdown is described by a structural parameter λ:

$$\frac{d\lambda}{dt} = -k_{\mathrm{d}}\lambda\dot{\gamma} + k_{\mathrm{a}}(1-\lambda), \text{ for } 0 \le \lambda \le 1 \qquad (1)$$

where k_{d} and k_{a} are is the destruction and the structure formation parameters, respectively, and $\dot{\gamma}$ is the shear rate. The Toorman thixotropy model was adopted, in which viscosity is expressed as a function of λ and the yield stress τ_y:

$$\eta = \frac{\tau_y \lambda}{\dot{\gamma}} + (\eta_\infty + C\lambda) \qquad (2)$$

where η_∞ and C are constants representing structural contributions to the viscosity. A dimensionless, known as the thixotropy number (Th) is defined to quantify thixotropic effect, defined by $\mathrm{Th} = k_d\dot{\gamma}_c/k_a$, where $\dot{\gamma}_c$ is the characteristics shear rate associated with a specific flow condition. This, the key parameters governing the thixotropic flow are Th, k_{d}, and τ_y. Numerical simulations for a model thixotropic fluid revealed that mixing characteristics are highly sensitive to variations in these parameters. In this study, mixing performance was quantitatively assessed using the intensity of segregation. Figure 1 illustrates the evolution of concentration profiles along the downstream direction, visualized through cross-sectional concentrations, as influenced by τ_y, at fixed values of Th and k_{d}. The Reynolds number was set to 10 in all cases.

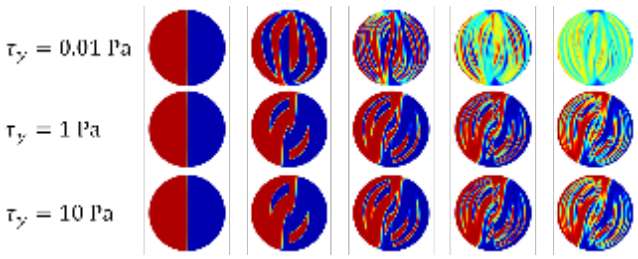

Figure 1.

At fixed values of Th and k_d, increasing τ_y reduced mixing efficiency, while lower τ_y enhanced mixing performance. These findings highlights that, in addition to Th and k_d, the yield stress τ_y plays a critical role in governing the mixing behaviour of thixotropic fluids. This insight offers valuable guidance for the design and optimization of mixers handling thixotropic systems.

Keywords: Thixotropic fluid, yield stress, chaotic mixing, static mixer, numerical simulation

Forecasting Long-term Spatial-temporal Dynamics with Generative Transformer Networks

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The accurate prediction of spatiotemporal physical dynamics is central to a wide range of scientific and engineering disciplines, yet traditional physics-based solvers remain computationally expensive, and standard deep learning models often lack long-term stability and physical consistency [1]. This study introduces DynamicGPT, a novel generative Vision Transformer (ViT)-based framework that forecasts high-dimensional physical fields by integrating multi-scale spatial encoding, temporal attention modules, and conditional generative adversarial learning. Unlike PINNs, DynamicGPT does not rely on prior knowledge of governing equations but instead learns directly from observed data. The core predictive task involves solving general classes of partial differential equations (PDEs), abstractly expressed as

$$\varphi_t = F(x, \nabla_x \varphi, \nabla_x^2 \varphi, \varphi \cdot \nabla_x \varphi, \dots), \quad (1)$$

where φ(x,t) denotes the evolving physical field and F represents the unknown nonlinear operator governing its dynamics. The model architecture embeds spatiotemporal fields into low-dimensional latent patches via a multi-kernel autoencoder, refines temporal patterns through a hybrid ConvGRU–ViT temporal network, and reconstructs future states using a trained decoder. Spatial and temporal discriminators ensure fidelity and coherence across dimensions.

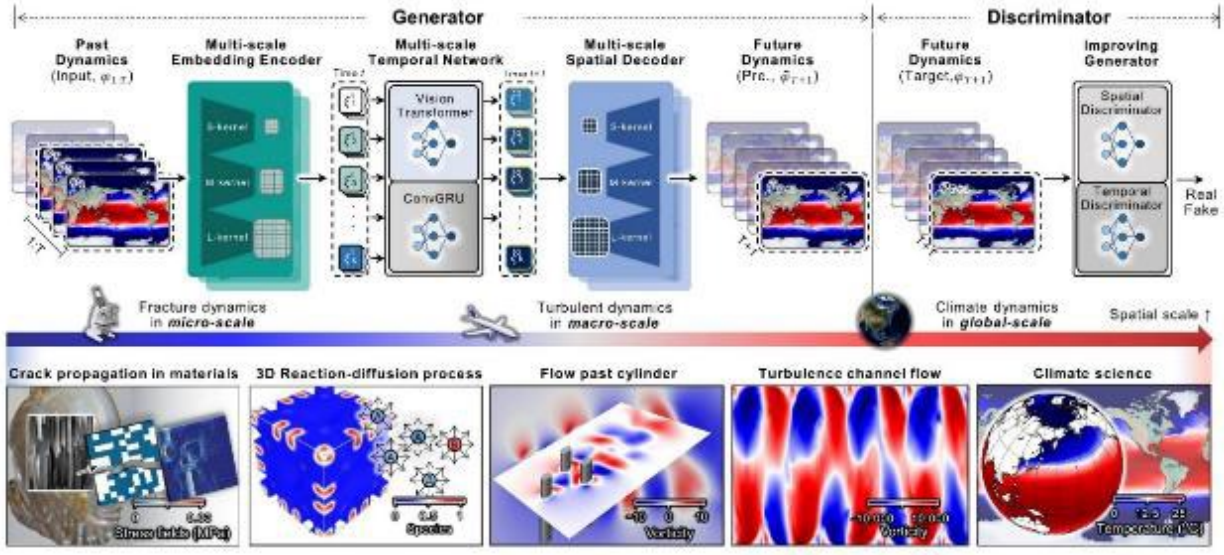

Figure 1.

The effectiveness of DynamicGPT is demonstrated across four complex physical systems: brittle fracture in composites, turbulent unsteady flow, global sea surface temperature (SST) forecasting, and 3D reaction–diffusion processes.

Keywords: Spatiotemporal dynamics, Generative transformer models, Numerical simulation, Deep learning

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Robust Topology Design of Negative Poisson's Ratio Metamaterials Considering Material Randomness

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The traditional deterministic topology optimization optimizes a deterministic objective function, for example, the error between the homogenized and target elasticity matrices. However, in practical applications, material properties are inherently uncertain. As a result, the objective value also presents the feature of randomness, and different realizations of material uncertainty can lead to significantly different optimized topologies, some of which may be non-manufacturable or highly sensitive to defects. To tackle this practice-stimulated challenge, an advanced robust topology optimization framework is proposed by minimizing a statistically defined robust objective. This objective integrates statistical information, such as a weighted combination of the mean and standard deviation, derived from the original deterministic objective. To improve computational efficiency, machine learning algorithms are embedded into the optimization process. At each iteration, a limited number of finite element-based homogenization simulations are conducted to generate training data. These data are used to construct surrogate models that capture the relationships between system uncertainties, the robust objective value, and its sensitivities. The surrogate models are then used to perform large-scale evaluations of the robust objective at significantly reduced computational costs. This proposed framework is highly flexible, supporting various uncertainty parameters, distribution types, and other statistical characteristics. Furthermore, it enables gradual structural adjustments through trade-off parameters within the robust objective and encourages the generation of topologies that are less sensitive to manufacturing imperfections.

Keywords: Robust topology optimization; Machine learning; Metamaterial design; Negative Poisson's ratio; material uncertainty.

Design and evaluation of a helical chiral lattice meta-material with enhanced impact protection and WAAM manufacturability

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Abstract

Lattice structures have attracted significant attention for their superior mechanical properties and lightweight characteristics. However, many existing designs either rely on overly complex geometries that compromise manufacturability or exhibit high stiffness that limits their energy absorption and lightweight performance. Moreover, traditional lattice structures often underperform in impact and blast protection scenarios. To address these challenges, this study proposes a three-dimensional helical chiral lattice (HCL) structure that balances structural performance with manufacturability, particularly under wire arc additive manufacturing (WAAM) constraints. Inspired by traditional pyramidal lattices and DNA-like double-helix biomimetic forms, the HCL introduces a compression-torsion coupling mechanism to enhance protective performance. Quasi-static compression tests, dynamic impact tests, and finite element simulations were conducted to compare the HCL with conventional pyramidal lattices. Results show that the HCL structure, under equivalent weight, exhibits superior protective and mechanical properties: the maximum central deflection (D_{max}) of the backing plate is reduced by 46%, and the crushing force efficiency (CFE) increases from 50% to 90%. This work effectively addresses the trade-off between structural stiffness and impact resistance in lattice design, offering new insights for blast-resistant structural applications.

Keywords: Helical chiral lattice (HCL), impact protection, WAAM, compression-torsion coupling, crushing force efficiency (CFE)

A δ^+-ULPH model: higher accuracy and lower numerical dissipation

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A δ^+- Updated Lagrangian Particle Hydrodynamics (ULPH) model is proposed, aiming to address the excessive numerical dissipation of the Smoothed Particle Hydrodynamics (SPH) model when the neighboring particles are insufficient. The governing equations of the δ^+-ULPH model are written as:

$$\begin{cases} \dfrac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \sum_j W_{ij} \left(\boldsymbol{u}_j - \boldsymbol{u}_i\right) \cdot \left(\boldsymbol{D}_i^{-1} \boldsymbol{r}_{ji}\right) V_j - \rho_i \left\langle \nabla \cdot \delta \boldsymbol{u} \right\rangle_i + \left\langle \nabla \cdot \left(\rho \delta \boldsymbol{u}\right) \right\rangle_i + \Phi_i \\ \Phi_i = \delta h c_0 \sum_j W_{ij} \left[\dfrac{2\left(\rho_j - \rho_i\right) \boldsymbol{r}_{ji}}{\left\| \boldsymbol{r}_{ji} \right\|^2} - \left(\left\langle \nabla \rho \right\rangle_i + \left\langle \nabla \rho \right\rangle_j \right) \right] \cdot \left(\dfrac{\boldsymbol{M}_i^{-1} + \boldsymbol{M}_j^{-1}}{2} \boldsymbol{r}_{ji} \right) V_j \\ \dfrac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t} = -\dfrac{1}{\rho_i} \sum_j W_{ij} \left(p_i \boldsymbol{M}_i^{-1} + p_j \boldsymbol{M}_j^{-1} \right) \boldsymbol{r}_{ji} V_j + \dfrac{1}{\rho_i} \left\langle \nabla \cdot \left(\rho \boldsymbol{u} \otimes \delta \boldsymbol{u}\right) \right\rangle_i + \dfrac{1}{\rho_i} \boldsymbol{F}_i^v + \dfrac{1}{\rho_i} \boldsymbol{F}_i^{ad} + \boldsymbol{g} \\ \boldsymbol{F}_i^v = \alpha h c_0 \rho_0 \sum_j W_{ij} \dfrac{\left(\boldsymbol{u}_j - \boldsymbol{u}_i\right) \cdot \boldsymbol{r}_{ji}}{\left\| \boldsymbol{r}_{ji} \right\|^2 + \left(0.1h\right)^2} \left(\dfrac{\boldsymbol{M}_i^{-1} + \boldsymbol{M}_j^{-1}}{2} \boldsymbol{r}_{ji} \right) V_j \\ \dfrac{\mathrm{d}\boldsymbol{r}_i}{\mathrm{d}t} = \boldsymbol{u}_i + \delta \boldsymbol{u}_i, \quad p_i = c_0^2 \left(\rho_i - \rho_0\right), \quad \boldsymbol{M}_i = \sum_j W_{ij} \boldsymbol{r}_{ji} \otimes \boldsymbol{r}_{ji} V_j, \quad \boldsymbol{r}_{ji} = \boldsymbol{r}_j - \boldsymbol{r}_i \end{cases} \tag{1}$$

where ρ_i, p_i, $\boldsymbol{u}_i$, $\delta\boldsymbol{u}_i$, and $\boldsymbol{r}_i$ represent the density, pressure, velocity vector, shifting velocity vector, and position vector of fluid particle i, respectively. c_0, ρ_0, and V are the sound speed, initial fluid density, and particle volume, respectively. W_{ij} is the kernel function. The matrix $\boldsymbol{D}_i$ is obtained by neglecting the off-diagonal elements and taking the average of the main diagonal elements of $\boldsymbol{M}_i$. $\langle \nabla \cdot \delta \boldsymbol{u} \rangle_i$, $\langle \nabla \cdot (\rho \delta \boldsymbol{u}) \rangle_i$, and $\langle \nabla \cdot (\rho \boldsymbol{u} \otimes \delta \boldsymbol{u}) \rangle_i$ are introduced to maintain the conservation (Sun et al., 2019). $\boldsymbol{F}_i^{ad}$ is the acoustic damper term (Sun et al., 2023).

Wave propagation is simulated to validate the proposed model. Figure 1 shows the pressure field of the δ^+-ULPH model. Figure 2 shows the free-surface elevations at x = 6.37 m (η_1) and 15 m (η_2). The results of the consistent δ^+-SPH model (Sun et al., 2019) with smooth length h = 1.35dx and 2dx and the experiment (Huang et al., 2022) are plotted for comparison. The particle resolution dx is 0.004 m.

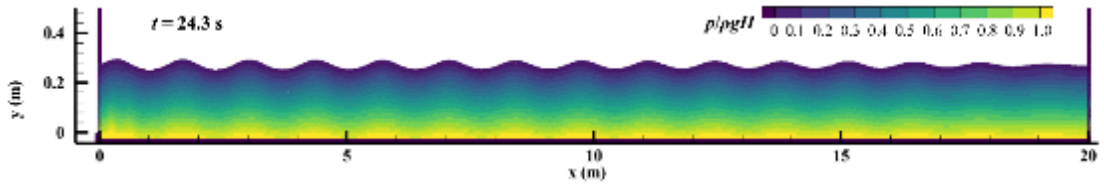

Figure 1.

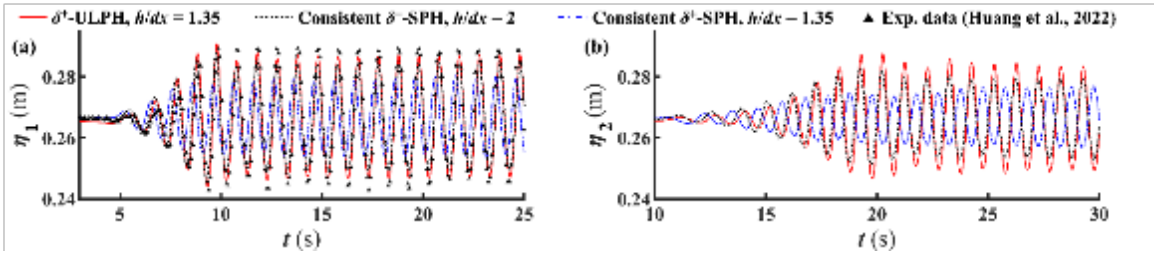

Figure 2.

Results indicate that the δ^+-ULPH model with fewer neighboring particles shows higher accuracy and lower numerical dissipation, even in long-term and long-distance simulations. Furthermore, the computational efficiency is visibly accelerated, attributed to the fewer neighboring particles.

Keywords: Updated Lagrangian Particle Hydrodynamics (ULPH), numerical dissipation

Robust path-following and branch-switching in isogeometric nonlinear bifurcation analysis of variable angle tow panels with cutouts under compression

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Advanced automated fiber placement technologies enable tow trajectories to be steered in curvilinear manner, offering novel reinforcement strategies for perforated panel structures. Nevertheless, the cutout-induced stress singularities in variable angle tow panel structures pose great challenges to the existing numerical analysis tools in resolving nonlinear bifurcation phenomena. The objective of this paper is to develop a hybrid FCM-IGA framework integrating robust path-following and branch-switching capabilities to investigate the nonlinear bifurcation behaviors of perforated VAT panels under compression. This is achieved by implementing Reddy's third-order shear deformation theory with von Kármán's geometric nonlinearity into isogeometric analysis formulations, in which higher-order NURBS basis functions satisfy the C^1 continuity requirement inherent in Reddy's model. Meanwhile, the geometric discontinuities induced by complex cutouts is handled through adaptive quadrature refinement of finite cell method. The nonlinear bifurcation equations under force/displacement-controlled edge loadings are separately derived based on the principle of virtual work and thereafter solved through robust path-following and branch-switching techniques. This paper presents three novel contributions in the proposed isogeometric nonlinear analysis framework: (i) Resolution of snap-through/snap-back instabilities via adaptive force/displacement-controlled arc-length scheme; (ii) Detection of singular points at a quadratically convergent rate via force/displacement-controlled pinpointing scheme; and (iii) Automatic branch-switching at bifurcation points without requiring any artificial perturbations. The effectiveness and robustness of the developed hybrid FCM-IGA framework is verified by comparing against FEA results obtained using ABAQUS. Effects of loading condition, hole size and fiber angle on the nonlinear bifurcation behaviors of the perforated VAT panels loaded in compression are also discussed in numerical examples. It is found that the benign load redistribution mechanism offered by favourable variable-stiffness configurations still remains in effect even there exists holes within the panel structures. The results reported herein may be beneficial for the design of perforated thin-walled structures loaded in compression.

Keywords: Bifurcation, Path-following, Branch-switching, isogeometric analysis, finite cell method, variable angle tow panels

Template for APCOM-ACCM 2025 Abstract Submission

Study on failure mechanism and energy evolution of coal-rock combination under different gas pressures

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The abstract The gas pressure has a significant effect on the energy accumulation and release and failure mode of the coal-rock combination. Under different gas pressures, the coal-rock combination exhibits significantly different mechanical and acoustic emission characteristics. In this study, the coal-rock combination of a coal mine in Maiduoshan, Ningxia was taken as the research object. The failure mechanism of coal-rock combination under different gas pressure conditions was systematically expounded from macro to micro by means of indoor test and numerical simulation, and the interaction between stress and energy accumulation was discussed in depth. The results show that: (1) With the increase of gas pressure, the compressive strength and elastic modulus of coal-rock combination decrease significantly, while the peak strain increases significantly. (2) The analysis of acoustic emission characteristics shows that the increase of gas pressure leads to the decrease of cumulative energy of acoustic emission, which indicates that gas pressure has a significant deterioration effect on the failure process of coal-rock combination. (3) Numerical simulation further reveals the influence of gas pressure on the stress distribution and elastic energy accumulation of coal-rock combination. With the increase of gas pressure, the stress value of coal-rock combination decreases from 2.98×10^8 N/m2 to 2.95×10^8 N/m^2, and the elastic energy density decreases from 9.38×10^6 J/m^3 to 9.2×10^6 J/m^3, indicating that the increase of gas pressure will aggravate the phenomenon of stress concentration and reduce the overall stability of coal-rock combination. The research results provide a theoretical basis for interface damage early warning and collaborative prevention and control of deep coal-rock gas dynamic disasters.

Keywords: Uniaxial compression; Acoustic emission; Gas-bearing coal-rock combination; Coal seam thickness; Energy.

Influence of Mesh as a Virtual Elastic Material in Free Surface Flow Computation

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Free surface flows are common in various industries. Accurate numerical methods are crucial for predicting transient changes in these free surfaces. One of the key boundary conditions in computations is the kinematic condition, which is based on mass conservation. In finite element methods that employ interface tracking, this condition can be implemented as a Dirichlet condition at the nodes of the free surface:

$$\bar{\mathbf{d}} = \mathbf{a}\Delta t \frac{\mathbf{u}\cdot\mathbf{n}}{\mathbf{a}\cdot\mathbf{n}}, \tag{1}$$

where $\bar{\mathbf{d}}$ is the imposed displacement vector, $\mathbf{a}$ is an arbitrary directional vector of the displacement, Δt is the timestep size, $\mathbf{u}$ is the fluid's velocity, and $\mathbf{n}$ is the unit outward normal vector at the free-surficial node.

However, imposing the Dirichlet condition strongly can lead to issues due to the uncertainty of the nodal normal vector, particularly on surfaces with high curvature. One possible solution is to apply the Dirichlet condition weakly at quadrature points, which each have a unique normal vector, rather than at the nodes.

One widely used mesh update method in the interface tracking category is the linear elastic mesh update method:

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{d}) = \mathbf{0}, \tag{2}$$

where $\mathbf{d}$ is the nodal displacement vector to be solved, and $\boldsymbol{\sigma}(\mathbf{d})$ is the linear elastic stress resulting from the strain caused by the nodal displacement. This method treats the mesh as a virtual linear elastic material, displacing the internal nodes in response to external deformation. While the mesh properties, such as Lamé parameters and local stiffening, affect only the distribution of internal nodes under strong imposition, they also influence the external nodes under weak imposition, thereby changing the time-dependent behaviour of free surfaces.

This research investigates the effect of mesh properties on free-surface flow computation, partitioning the problem into incompressible Newtonian fluid flow and linear elastic mesh update. Nitsche's method for linear elasticity [1] is utilized for weak imposition. Model problems, such as a sloshing tank and a sessile drop, are computed, and their transient behaviours are analysed. A physical interpretation is provided, considering the mesh's compressibility and stiffness.

Keywords: Computational fluid dynamics, finite element method, free surface flow, interface tracking, linear elastic mesh update method

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Data-driven Surrogate Modelling using Attention-based Deep Operator Network for Active Noise Control

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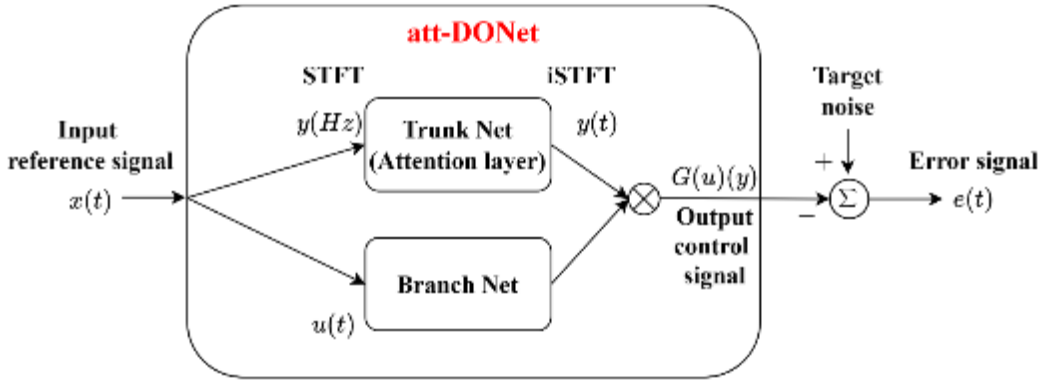
Academic and industrial research related to electric, autonomous vehicles, and urban air mobility has been increasing rapidly nowadays since the advancement of future promising mobility industry. A quite interior environment in the driving vehicle is one of the most important aspects considered for those transportations. Hence, active noise cancellation or Active Noise Control (ANC) is one of the advanced technologies to bring that necessary demand to customers. In this paper, a fully adaptive time-frequency coupling forecasting model using self-attention mechanisms based on the Deep Operator Network (att-DONet) will be implemented to rapidly and accurately nonlinear noise signal. The performance of proposed method will be evaluated by forecasting interior noise considering acceleration and signals both in terms of time-frequency coupling measured through actual driving tests.

A deep learning-based nonlinear ANC model is constructed as a simplification version to predict the noise transmitted to the mobility interior from the primary vibration transmission path.



By learning through both time and frequency domains, the att-DONet model is able to acquire noise signal patterns from a broader range. The model can learn continuous nonlinear behavior in infinite-dimensional spaces. Specifically, input data to the Trunk net are transformed into the frequency domain using Short Time Fourier Transform (STFT), and then, relationships between different frequencies are learned across the multi-head attention mechanism. The data are then converted back to the time domain using the inverse Short Time Fourier Transform (iSTFT). Besides, the Branch net learns the time-domain patterns before dot production is applied to the Trunk net and Branch net to achieve multi-scale learning for noise signal predicting. Finally, the output control signal from att-DONet is subtracted by target noise signal to achieve and minimize the error signal.

Keywords: Active Control Signal, Self-Attention Mechanism, Deep Operator Network

Multi-fidelity surrogate for mechanical properties of short fiber reinforced plastics: leveraging information from theory to experiment

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This study presents a multi-fidelity surrogate modelling approach for predicting the mechanical properties of short fiber reinforced plastics (SFRPs) by combining low-cost micromechanics-based theoretical predictions with high-fidelity experimental data. Using axisymmetric orientation-averaged Mori-Tanaka theory and second-moment strength estimates, low-fidelity stiffness and strength data are generated. These are integrated with tensile test results from injection-molded polypropylene-glass fiber composites, covering different material properties and fiber volume fractions. The model maps material parameters – modulus ratio, fiber volume fraction, and aspect ratio – to effective properties, using *k*-fold cross validation to assess performance. While the cross-validation accuracy was comparable across models, single-fidelity (SF) surrogates tends to overfit the limited available data and performed poorly in extrapolation regions. In contrast, multi-fidelity (MF) models leveraged low-fidelity theoretical trends to provide more stable predictions in extrapolative regimes, through sometimes at the cost of reduced accuracy on training data. These results suggest that MF modelling offers a more generalizable and robust framework for property prediction in data-scarce material design problems. The figure presents experimental results versus surrogate predictions for single-fidelity Gaussian process (SFGP), nonlinear multi-fidelity Gaussian process (NMFGP), single-fidelity neural network (SFNN), and multi-fidelity neural network (MFNN) for effective stiffness and strength from material A to F.

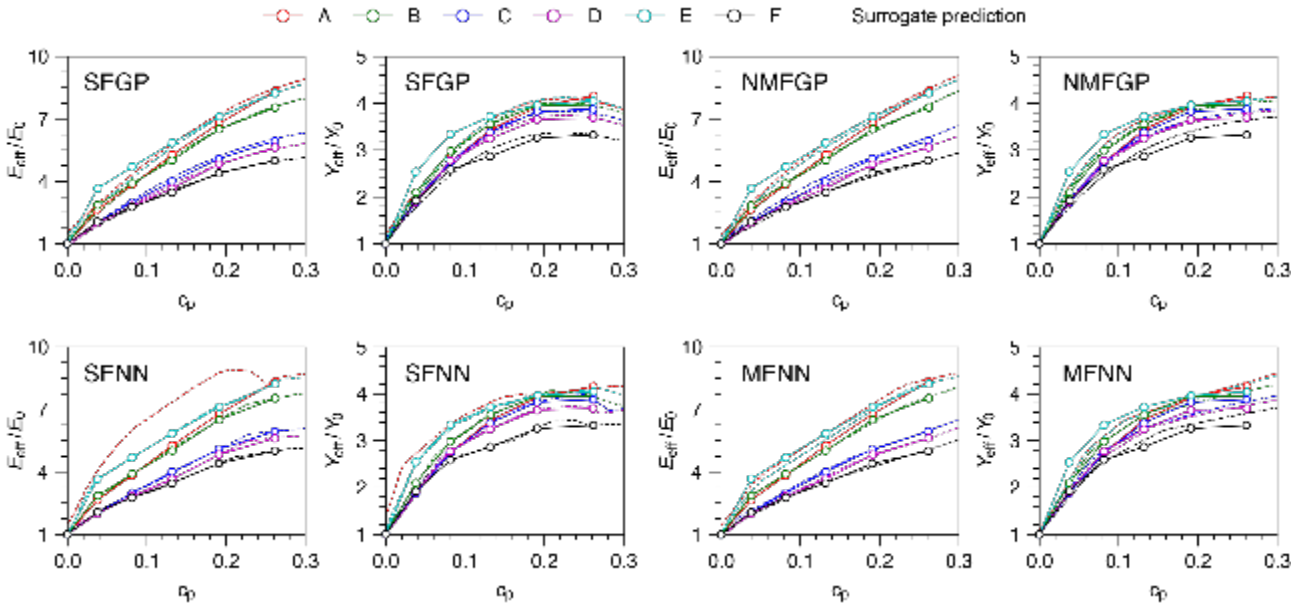

Figure 1.

Keywords: SFRP, Micromechanics, Machine learning, Multi-fidelity

Exploring Quantum Annealing for Coupled Structural Analysis Problems

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We develop and explore a novel method for using quantum annealing to solve coupled structural analysis problems, specifically focusing on fluid structure interaction problems. These problems involve the interaction between a fluid and a structural domain, making them computationally demanding. When combined with design optimization tasks, they form complex optimization problems that are difficult to solve using classical methods, creating the need to explore alternative strategies such as quantum annealing.

Quantum annealing is an emerging computational technique that utilizes quantum mechanical effects to solve complex optimization problems much faster and more efficiently than classical approaches. To optimize fluid structure interaction problems using quantum annealing, it is first necessary to develop methods that allow using quantum annealing to solve fluid structure interaction problems themselves, which is the focus of our work.

Our proposed method is based on the partitioned approach, where the fluid and structural subproblems are treated separately. To solve the structural subproblem via quantum annealing, we reformulate it as an energy minimization problem. Specifically, the system's potential energy is expressed in the form of a quadratic unconstrained binary optimization model:

$$H = \sum_i Q_{ii} q_i + \sum_{i<j} Q_{ij} q_i q_j, \tag{1}$$

where $q_i \in \{0,1\}$ are binary decision variables representing the discretized solution. The coefficients Q_{ii} and Q_{ij} are derived from the structural energy formulation, representing linear and quadratic contributions, respectively.

We apply our approach to a one-dimensional, static fluid structure interaction problem and validate the method on a state-of-the-art D-Wave quantum annealer by comparing the obtained results to analytical solutions. Additionally, we analyze the capabilities and limitations of current quantum annealing hardware for these types of problems and explore strategies to overcome existing constraints. In conclusion, we demonstrate that the proposed formulation is suitable for solving simple fluid structure interaction problems using quantum annealing.

Keywords: quantum annealing, fluid structure interaction, energy minimization, partitioned approach, QUBO formulation

Obliquely interacting solitary waves and wave wakes in free-surface flows

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We present the weakly nonlinear isotropic bi-directional Benney-Luke (BL) equation, which is used to describe oceanic surface and internal waves in shallow water, with a particular focus on soliton dynamics. Using the Whitham modulation theory, we derive the modulation equations associated with the BL equation that describe the evolution of soliton amplitude and slope. By analyzing rarefaction waves and shock waves within these modulation equations, we derive the Riemann invariants and modified Rankine--Hugoniot conditions. These expressions help characterize the Mach expansion and Mach reflection phenomena of bent and reverse bent solitons. We also derive analytical formulas for the critical angle and the Mach stem amplitude, showing that as the soliton speed is in the vicinity of unity, the results from the BL equation align closely with those of the Kadomtsev-Petviashvili (KP) equation. Corresponding numerical results are obtained and show excellent agreement with theoretical predictions. Furthermore, as a far-field approximation for the forced BL equation -- which models wave and flow interactions with local topography -- the modulation equations yield a slowly varying similarity solution. This solution indicates that the precursor wavefronts created by topography moving at subcritical or critical speeds take the shape of a circular arc, in contrast to the parabolic wavefronts observed in the forced KP equation.

Keywords: solitary waves, surface gravity waves, isotropism

References

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A two dimensional ordinary state based Peridynamic model for dynamic fracture

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Dynamic fracture involving fast crack propagation and fragmentation presents a significant challenge to classical continuum mechanics, which relies on spatial derivatives and is ill-posed for problems with discontinuities. In this work, we present an efficient two-dimensional ordinary state-based peridynamic model for efficient dynamic fracture simulation in brittle materials. Based on integral equations, a nonlocal continuum theory called peridynamics removes the need for explicit crack tracking, thus providing a solid framework for the modeling of crack initiation and propagation [1]. Previous peridynamic studies have investigated bond-based and state-based systems [2], however the conventional models require modifications to enable reliable simulations of dynamic fracture within two-dimensional domains. We use an ordinary state-based peridynamic (refer Figure 1) formulation in this research that includes a critical stretch criterion for bond rupture to simulate dynamic brittle fracture for a range of loading scenarios. A direct time integration procedure is used to represent the evolution of brittle crack growth in time explicitly. Crack branching is seen in Figure 2 where local damage variable is plotted (1 represents complete failure and 0.1 represents damage initiation). The model is validated against a set of predefined benchmark problems. These results demonstrate the models ability to accurately capture fracture initiation and propagation/branching, as well as the evolution of local damage fields. In addition, a parametric study is performed to explore the effects of peridynamic parameters on the fracture behavior..

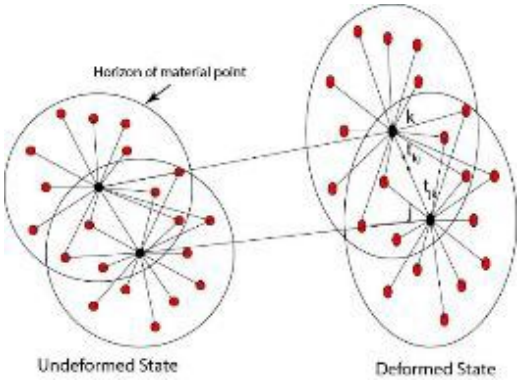

Figure 1. Ordinary state based Peridynamic

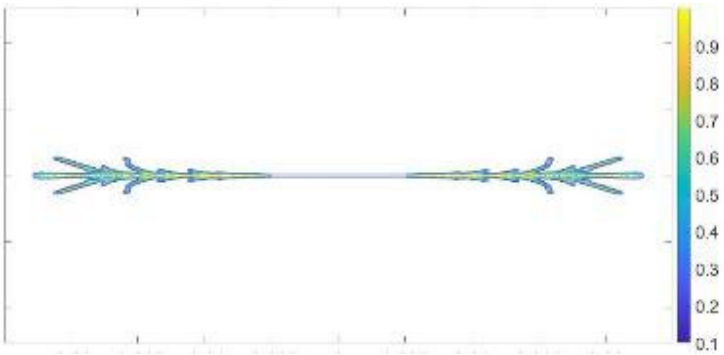

Figure 2. Dynamic fracture simulated by Peridynamic model

Keywords: Peridynamics, damage, crack propagation, nonlocal, dynamic loading, rate effects.

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RITTER-KRIŽAIĆ itteracion method of FLAT TRUSS CONSTRUCTIONS

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The optimization of construction planning is constantly evolving. Today, FEM technology dominates with the development of evolutionary and other various methods that are implemented with algorithms in computer simulations of static models of objects. The problem with these methods is the solution of large differential equations, which is inconceivable without a computer and a large memory. The iterative method Ritter-Križaić ∞ (RK FEM ∞) [1, 2] according to inclined grids is developed in and flat grids to popular beam models and scaled or mesh surfaces. This is done by adding the geometric properties of the meshes and the external actions to the line equations in an iterative element called RK-IEM ∞ with a loop in n-dimension with five force terms in the grid members in the lower and upper webs and in the vertical and shear (NDi, NGi, NVi, NKiH, NKiV):

$$N_{Di} = 1/h_{ni}\left(A \cdot\ n \cdot\ c\ - \left(\sum_{i=0}^{n} P \cdot i \cdot c\right)\right) \quad (1)$$

$$N_{Gi} = 1/l_{\perp}\left(A \cdot (n-1) \cdot\ c\ - \left(\sum_{i=0}^{n-1} P \cdot i \cdot c\right)\right) \quad (2)$$

$$N_{Vi} = -A + (\mathrm{i}+1) \cdot P \quad (3)$$

$$N_{KiH} = N_{Di} - N_{Di0} \quad (4)$$

$$N_{KiV} = N_{KiH} \cdot \Delta a \quad (5)$$

$$\mathrm{RKIEM}\infty_{i+1} = \mathrm{RKIEM}\infty_{i} \quad (6)$$

The union of the above bars defines an iterative lattice model [3,4] called RK-IEM COD. The data from the loop defines the discrete data transformed by the Gaussian least squares method into functional parabolic curves for each member of the truss, using the monogram [5] RK-IEM ∞ technology. RK-IEM COD is therefore used to create simulation games that explain many logical phenomena in the design of external and internal actions of beam members and can be compared as an RK array with spider threads or ice plate structures. The matrix-free calculation enables almost ∞ all constructions in space that continue a continuous series of iterations even in spaces of the universe.

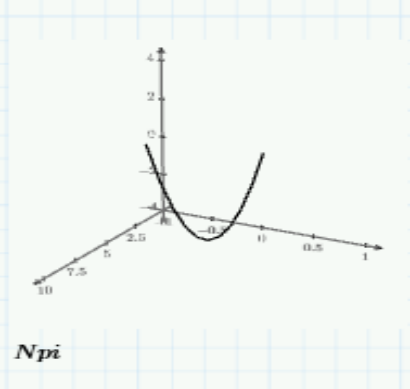

Figure 1.

KEYWORDS: FLAT truss constructions, RK-IEM∞ COD, spider thread, SPACES OF THE UNIVERSE

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Three-dimensional phase-field simulation for banded microstructure formation during rapid solidification

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In metal solidification, dendrite growth is observed up to a solidification rate of ~0.1 m/s, and planar interface growth is observed from ~10 m/s. In the intermediate rate range, a banded microstructure is formed in which dendrite and planer interface growth occur alternately [1]. This banded structure is one of the characteristic microstructures observed in rapid solidification during laser welding and 3D printing. Numerical simulation of banded structures requires the consideration of solute trapping, which depends on the solidification rate. This effect influences solute partitioning at the solid-liquid interface and must be incorporated into the simulation model. The phase-field model is a powerful tool for simulating dendrite growth, and it can express the solid-liquid interface migration considering the solute trapping effect quantitatively by using nanometer-scale phase-field interface [2]. Although two-dimensional PF simulations of banded microstructure formation were performed, the requirements of nanometer-scale grid size make it challenging to set a wide computational domain. Previous 3D PF simulations were restricted to single dendrite arm simulations due to computational limitations [3]. In this study, we aim to accelerate PF computation for rapid solidification to enable a quantitative evaluation of 3D banded structures. We apply a nonlinear preconditioning [4] to the PF model, enabling stable computation with a coarser grid while maintaining accuracy, thereby reducing computational costs. To further enhance computational efficiency, we introduce block-structured adaptive mesh refinement (AMR), which dynamically assigns fine numerical grids only around the interface while using coarser grids elsewhere [5]. Moreover, parallel computation using multiple GPUs accelerates PF simulations with AMR, further improving scalability [5]. Using the developed method, we reproduce the 3D banded structure and quantitatively evaluate the variation of band spacing under different temperature conditions and crystal orientations. These results demonstrate that the proposed approach is a powerful tool for predicting 3D rapid solidification microstructures.

Keywords: rapid solidification, banded microstructure, phase-field method, multiple GPU computation, adaptive mesh refinement

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Validation of Two-Phase Lattice Boltzmann Simulation for Gas Entrainment Using a Quasi-Steady Vortex Flow Under Varying Inlet and Outlet Conditions

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Gas entrainment (GE) is a critical phenomenon in sodium-cooled fast reactors, where the argon cover gas is entrained into the primary coolant by the free-surface vortices and disrupt the reactor performance [1]. Accurate numerical methods are essential to predict this geometry-sensitive phenomenon. Previous efforts using incompressible two-phase Navier-Stokes simulations, however, were found to be computationally expensive. To address this, we developed a two-phase Lattice Boltzmann Method (LBM) to deliver high-resolution results within a few days. Herein, we validated our model using a quasi-steady vortex flow under varying inlet and outlet conditions.

The LBM for fluid simulation solves the following discrete kinetic equation:

$$f_\alpha(\boldsymbol{x} + \boldsymbol{e}_\alpha \delta t, t + \delta t) = f_\alpha(\boldsymbol{x}, t) + \Omega_\alpha(\boldsymbol{x}, t) + F_\alpha(\boldsymbol{x}, t), \quad (1)$$

where f_α is the discrete particle distribution function, Ω_α the collision operator, F_α external forces, $\boldsymbol{e}_\alpha$ the lattice direction, $\boldsymbol{x}$ the position, and t the time. LBM offers a simple and highly parallelizable algorithm, avoiding the computationally expensive pressure Poisson equation typical of traditional CFD methods. To model two-phase flows, we use an extended version of LBM developed in our work [2].

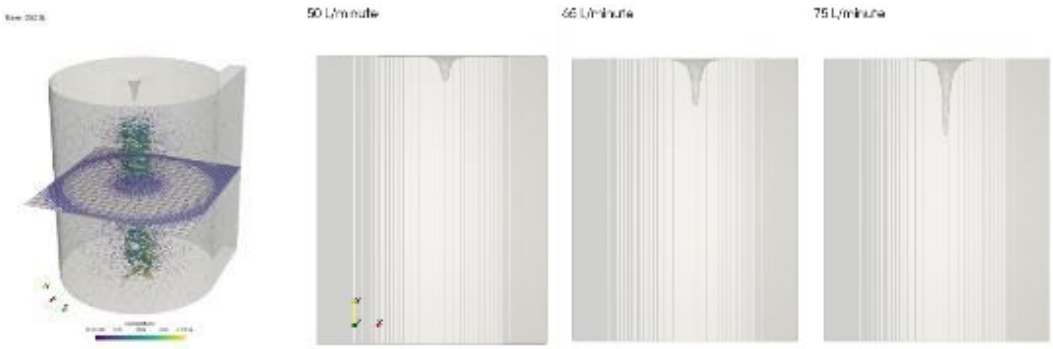

Figure 1.

We have validated our two-phase LBM model [2] using the quasi-steady vortex with an inlet flow rate of 50 L/min and an outlet diameter of 5 cm, as shown in Fig. 1 (left). Using a grid spacing of $\Delta x <$ 0.625 mm, the simulation accurately reproduced the flow profiles and gas entrainment (GE) depths. The predicted GE depth was approximately 8 cm, compared to 11 cm observed in the experiment. For cases with varying inlet and outlet conditions, preliminary tests indicate that the GE depth is highly sensitive to the inlet velocity, consistent with experimental observations (Fig. 1 (right)). A more detailed comparison with experimental results will be reported in the presentation.

Keywords: Two-phase, lattice Boltzmann method, gas entrainment, simulation, quasi-steady vortex

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Investigation of Velocity Effects on Large-Scale Hydrogen Combustion Modelling for Industrial Drying Applications

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The drying process has traditionally relied on fossil fuel-based heating methods, making it a significant contributor to environmental emissions. Hydrogen fuel presents a promising alternative due to its clean combustion and favourable properties such as high diffusivity and a wide flammability range. However, the complex interactions of hydrogen combustion kinetics with turbulent flow typical of industrial applications pose challenges in developing accurate and efficient simulation models. This research aims to establish a robust computational fluid dynamics (CFD) model for large-scale hydrogen combustion, specifically tailored for industrial drying processes. The model utilizes a non-premixed combustion approach, incorporating the standard k-ω turbulence model and a detailed chemical kinetic mechanism comprising 9 species and 19 reversible reactions [1]. The objective is to evaluate combustion efficiency, maximizing energy efficiency, and emission characteristics, with a focus on reducing greenhouse gas emissions and enhancing thermal performance. The CFD model investigates the effects of key operating parameters, including hydrogen and air flow velocities (ranging from 5–20 m/s and 1–10 m/s respectively) on NOx emissions, species concentrations, and temperature distribution. A representative large-scale combustion chamber geometry (as shown in Figure 1) is used to analyse these effects under realistic conditions. Model validation is conducted through comparison with established experimental and numerical results to ensure simulation accuracy. The findings highlight the potential of CFD modelling in optimizing hydrogen-based combustion conditions for drying applications. The insights gained from this work can guide the development of next generation drying technologies powered by hydrogen, contributing to a cleaner and more efficient industrial landscape.

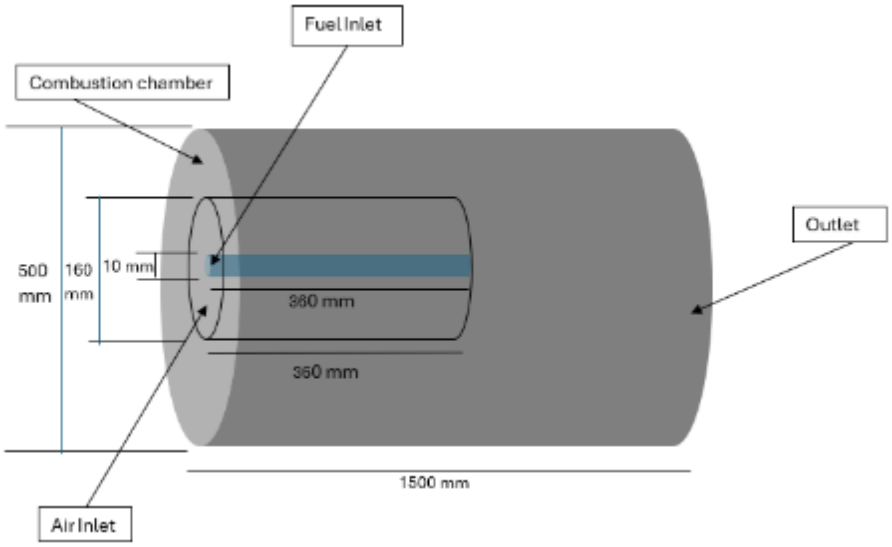

Figure 1. A schematic view of H2 combustion chamber for Agri dry dryers Pvt Ltd

Keywords: Drying process, large-scale combustor, hydrogen combustion, CFD model, non-premixed model.

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Effects of Material Properties on Plaque Vulnerability Assessment Using Fluid-Structure Interaction Analysis

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Risk of plaque rupture has been associated with its composition, internal structural stress, and external blood flow-induced shear stress. However, identifying vulnerable plaques by fluid-structure interaction is still hampered by great uncertainties in the material properties of plaques assumed, which we aimed to address with this work.

We generated an idealised coronary left main bifurcation with a 50% asymmetric stenosis in the left anterior descending artery using Morphman (Open source, Github) (Figure 1a). The bifurcation angle was 60° and the arterial wall had a thickness of 0.4 mm. We modelled the arterial wall and plaque as isotropic and hyperelastic materials with the five-parameter Mooney-Rivlin model:

$$W = C_{10}(\bar{I}_1 - 3) + C_{01}(\bar{I}_2 - 3) + C_{11}(\bar{I}_1 - 3)(\bar{I}_2 - 3) + C_{20}(\bar{I}_1 - 3)^2 + C_{02}(\bar{I}_2 - 3)^2 + \frac{1}{d}(J - 1)^2, \quad (1)$$

here C_{10}, C_{01}, C_{20}, C_{11}, and C_{02} are material constants; $\bar{I}_X$ is the Xth left Caunchy-Green deformation tensor invariant; d is the material incompressibility parameter; and J is the elastic deformation gradient determinant. Different parameter combinations were derived from literature to reflect the distinctive stiffness of three types of plaques—calcified, hypocellular, and cellular. Fluid-structure interaction simulations were performed assuming a pulsatile pressure profile at the inlet and velocity profiles at the outlet following a flow-spilt strategy. We assessed the impact of assuming different plaque material properties on the resulting time-averaged wall shear stress and first principal stress.

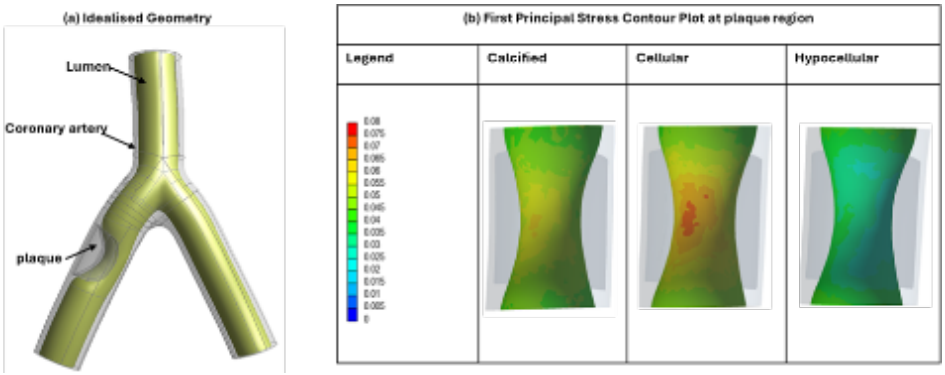

Figure 1

The plaque's material properties significantly impacted the first principal stress, with a maximum difference of 17 kPa at the plaque region (Figure 1b), given that the threshold to predict plaque rupture

is 30kPa. In contrast, assuming plaques with different stiffness in fluid structure interaction had a negligible impact on the resulting time-averaged wall shear stress, with a maximum difference of only 0.21 Pa.

Our results indicate that the haemodynamic results are less sensitive to the material properties assumed for plaque in fluid-structure interaction, whereas the plaque stiffness has to be carefully determined when the structural stress is to be analysed.

Keywords: plaque stiffness, fluid-structure interaction, stenosis, coronary artery

Three-dimensional Grain-Based Hybrid Finite-Discrete Element Modelling of Shear Fracturing of Heterogeneous Rocks under Coupled Static and Dynamic Loads

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Combined finite-discrete element method (FDEM) is becoming increasingly prevalent among the research community for modelling rock dynamics fractures and is receiving widespread recognition. Recent developments of hybrid finite-discrete element method (HFDEM), which is the authors' version of FDEM, have resulted in its increased convenience, ease of use, and reduced computational cost and time, in comparison to other FDEMs and other hybrid computational methods. This study models the shear fracturing behaviours of heterogeneous rocks under coupled static and dynamic loads in triaxial Hopkinson pressure bar-based dynamic shear tests with a grain-based three-dimensional (3D) HFDEM, as shown in Figure 1. The grain-based model is used to illustrate the mineralogical complexity of granite and to identify fracturing that occur at numerous scales under dynamic shear stresses. Initially, it is noted that the grain-based model depicts the mineralogical heterogeneity of granite and to reveal multi-scale fracturing under dynamic shear loads. Furthermore, the recently implemented nodal intensity-based contact interaction model is verified to effectively represent the interactions between discrete bodies through a series of dynamic shear tests. The results produced by this model are compared with those derived from other contact interaction models and laboratory experiments, thereby solidifying the practicability and effectiveness of the implemented contact interaction models. In conclusion, the grain-based HFDEM3D effectively captures the fundamental dynamic fracturing behaviours of heterogeneous rocks under coupled static and dynamic loads, as well as the propagation of stress waves in both metal bars and rocks.

Keywords: Grain-based modelling, 3D FDEM, Contact calculation, Parallel computing, Rock fracture, Dynamic shear test

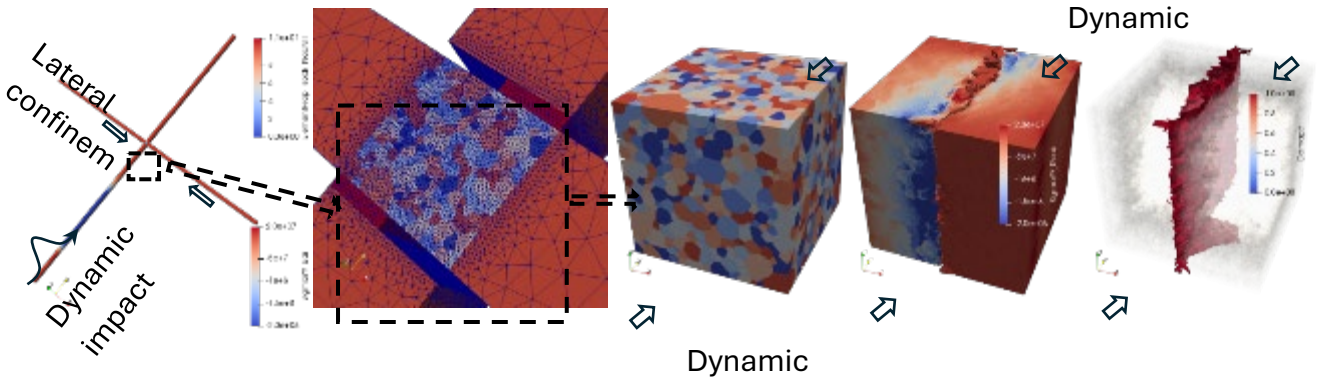

Figure 1. Grain-based 3D modelling of the dynamic fracture of heterogeneous rocks in triaxial Hopkinson bar based dynamic shear tests

Homogenization-based Multiscale Topology Optimization for Heat Sinks with Functionally Graded Structures

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With the increasing performance and integration of electronic devices, effective thermal management has become essential, highlighting the importance of heat sink design. In particular, recent studies have actively explored the application of functionally graded structures. However, the spatial variation of microstructures poses significant challenges to their design. To address this issue, homogenization-based multiscale topology optimization, which considers macro- and microscale structures, has gained attention. This method offers high computational efficiency by utilizing effective material properties of pre-defined unit cells, but it is limited in reflecting complex microstructural features due to the simple unit cell geometry. Such limitations restrict the potential for further enhancement of cooling performance. In this study, the homogenization-based multiscale topology optimization with explicit de-homogenization enabling diverse microstructural representation is proposed. First, two surrogate models on effective material properties, homogenized thermal conductivity $\tilde{k}_{ij}^{H}$ and homogenized inverse permeability $\tilde{C}_{ij}^{-1,H}$, are generated.

$$\tilde{k}_{ij}^{H} = \tilde{k}_{ij}^{H}\left(\gamma_{\phi}(\mathbf{x}), d_{l_1}(\mathbf{x}), d_{l_2}(\mathbf{x}), d_{l_3}(\mathbf{x}), d_{l_4}(\mathbf{x}), d_{\xi}(\mathbf{x}), d_{\eta}(\mathbf{x}), d_{x_2}(\mathbf{x}), d_{y_2}(\mathbf{x})\right) \quad (1)$$

$$\tilde{C}_{ij}^{-1,H} = \tilde{C}_{ij}^{-1,H}\left(\gamma_{\phi}(\mathbf{x}), d_{l_1}(\mathbf{x}), d_{l_2}(\mathbf{x}), d_{l_3}(\mathbf{x}), d_{l_4}(\mathbf{x}), d_{\xi}(\mathbf{x}), d_{\eta}(\mathbf{x}), d_{x_2}(\mathbf{x}), d_{y_2}(\mathbf{x})\right) \quad (2)$$

Here, γ_{ϕ} denotes the macrostructure design variable; d_{l_1}, d_{l_2}, d_{l_3}, d_{l_4} are microstructural size variables; and d_{ξ}, d_{η} are orientation variables. To account for spatial arrangement of microstructures, additional variables d_{x_2}, d_{y_2} are included in the surrogate models. After optimization, the resulting distribution of microstructural design variables is converted to predefined unit cell geometries at the macroscopic scale shown in Figure 1.

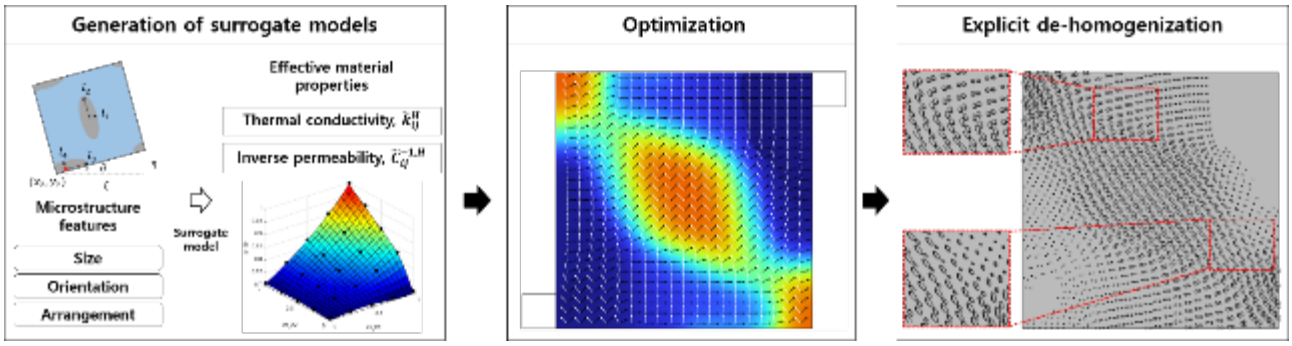

Figure 1.

Keywords: Homogenization-based multiscale topology optimization, functionally graded structure, explicit de-homogenization, multi-physics optimization, heat sink,

Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT). (No. 2023R1A2C200375811)

Machine Learning-aided Robust Optimization of Frequency Selective Surfaces with Ultrawide Passbands

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One promising class of electromagnetic metamaterials is frequency selective surfaces, which are periodic planar structures composed of metallic array elements on dielectric substrates. By carefully designing the unit cell, frequency selective surfaces can exhibit remarkable frequency selectivity and offer powerful capabilities to manipulate electromagnetic waves across an ultrawide frequency spectrum. Various design optimization strategies, including parametric, structural, and topological optimization frameworks, have been employed on frequency selective surfaces for obtaining ultrawide passbands and achieving a broad range of applications, such as radar domes, electromagnetic absorbers, transmission arrays, and Fabry–Pérot antennas. However, the performance of these planar structures is inherently sensitive to material properties and unit cell configurations. System uncertainties arising from sources such as raw material variability, manufacturing imperfections, and environmental influences, can lead to inevitable discrepancies between the designed and fabricated structures. Without properly accounting for these uncertainties, the designs may perform suboptimally in real-world conditions. To address this challenge, this paper develops a robust optimization framework for frequency selective surfaces, aiming at simultaneously broadening the passband and minimize performance variability. To efficiently estimate the statistical information of the bandwidths under uncertainty, a surrogate model is developed to capture the relationship between structural parameters and concerned structural responses. The optimization problem is solved using a recently proposed optimization algorithm, namely adaptively high-order mutation-based particle swarm optimization. A numerical case study on a frequency selective surface is conducted to demonstrate the effectiveness of the proposed framework. The frequency selective surface under optimization demonstrates significant bandwidth enhancement coupled with improved robustness of the optimal design.

Keywords: Robust design optimization, Machine learning, Electromagnetic metamaterial, Uncertainty quantification

Computational Models of Porosity-Dependent Bone Mineralisation and their Link to Bone Mechanical Properties

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The mineral content is an important determinant of the mechanical properties of bone, particularly the modulus of elasticity, which influences structural integrity and potential susceptibility to fracture [1]. The relationship between bone mineralisation and porosity is complex since it varies between different bone compartments and is altered in pathological conditions. Experimental analysis of this relationship remains difficult as mineralisation is a continuous, long-term process and imaging techniques are mostly limited to static snapshots. In this work, computational approaches to modelling porosity-dependent bone mineralisation are evaluated to gain a better understanding of the site-specific mechanical properties of bone. We analyse each model's suitability for the explicit inclusion of porosity dependencies and computational efficiency.

We focus on two computational frameworks: (1) a hybrid discrete-continuous model employing a queueing algorithm for tracking bone patch age combined with continuous ordinary differential equations describing cellular dynamics [1], for which we established explicit dependencies on bone volume fraction in our previous work; and (2) a partial differential equation model characterising Bone Mineral Density Distribution curves through mineralisation, formation, and resorption processes [2]. Our analysis confirms that mineral apposition rate and turnover rate are primary determinants of porosity-dependent mineralisation patterns. We found an inverse relationship between apposition rate and porosity and that turnover as a function of the available bone remodelling surface determines the differences in mineralisation dynamics, consistent with recent findings [3]. With our further developments, these models are explicitly porosity-dependent and allow site-specific determination of mineral content in different bone compartments.

In this work, we present an intermediate step toward developing comprehensive biomechanical models. The analysis of porosity-dependent mineralisation models forms the basis for future finite element modelling with spatially resolved mechanical properties derived from local mineralisation patterns. Such models can then be used to simulate disease progression under habitual loading or underloading conditions and to identify the bone regions most susceptible to bone loss.

Keywords: Bone mineralisation; Computational modelling; Porosity; Bone remodelling; Bone turnover; Mineral apposition rate

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Modelling Density-driven Segregation in Submerged Granular Shear Flows

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Density contrasts between particles in sheared granular mixtures can induce segregation, controlling the particle layering and phase separation. In fully saturated granular flows, however, interstitial fluid effects introduce additional viscous and inertial forces that fundamentally modify the segregation dynamics compared to the dry systems. In this study, we employed coupled CFD-DEM simulations to investigate the segregation behaviour of mono-sized particles with varying density contrast in submerged granular shear flows. By systematically investigating the combined effects of the particle-fluid density ratio, fluid viscosity, and shear rate, we examine how the competition between fluid and particle inertia influences segregation dynamics. In particular, the Stokes number emerges as a key dimensionless parameter that characterises the transition between viscous- and inertia-dominated regimes. Building on these findings, we develop a continuum model for the segregation velocity, which captures the combined effects of viscous resistance and inertial enhancement. This model provides a unified framework for predicting density-driven segregation in submerged granular shear flows, offering new perspectives for understanding the rheology and transport of particle-laden flows in fluid-saturated environments.

Key Words: Granular flow; Density-driven segregation; Fluid-solid interaction; CFD-DEM

Modelling Capillary Interactions between Flexible Substrates

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Elastocapillarity, a coupled effect of solid deformation and capillary interactions, has gained increased interest due to its relevance in biological systems and flexible engineering devices. A droplet confined between slender elastic structures forms a liquid bridge that can provide a sufficient capillary force to deform structures at small scales. This study presents a phase-field numerical framework to simulate a liquid bridge between two thin flexible substrates that are being separated at controlled motion. The model captures two-phase fluid interface dynamics coupled with substrate bendability, capable of capturing force evolution during loading. We focus on investigating effects of substrate flexibility on the capillary force–displacement relation. We identify that the capillary force evolution during liquid bridge stretching and the separation distance for bridge rupture is governed by the bendability of substrates, substrate configuration, contact angle, and droplet geometry. Additionally, we find that droplet aspect ratio also affects capillary force direction and can cause convex deformation of the substrates instead of concave, resulting from the sign switching of internal Young-Laplace pressure. Our framework provides a new numerical capability to explore the interplay between soft substrates and capillary interactions.

Keywords: Elastocapillarity, capillary bridge, surface tension, fluid-structure interaction, Phase-field method.

A Novel Two-Body Topology Optimization Framework for Strain Energy Minimization Problem

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Since the research paper by Bendsøe and Kikuchi [1], topology optimization has been widely used in various engineering fields. Most studies on topology optimization focus only on the design of a single body, where the material distribution is optimized according to its own mechanical behaviour in the design domain. In other words, the interactions between bodies in a multi-body system are not considered. This is referred to as *self-based topology optimization*.

A novel topology optimization framework proposed in this study is termed the *two-body-based topology optimization* method. In the two-body system illustrated in Figure.1, body A is designated as the target body, and body B is designated as the design domain. The main feature of this system is the ability to minimize the internal strain energy of body A by optimizing the structure in the body B. This method is developed based on the Solid Isotropic Material with Penalization (SIMP) scheme [2] and incorporates not only a standard volume constraint but also additional constraints related to displacement or compliance.

Furthermore, a Node-To-Node (NTN) frictionless contact model [3] is introduced in this study. This model can be imported into both the analysis of two-body contact problem and the topology optimization method [4]. Therefore, the interaction between the two bodies be analyzed more accurately.

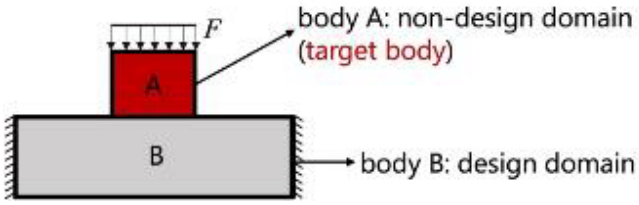

Figure 1.

Keywords: Topology Optimization, Contact analysis, Two-body system

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Lock-In Phenomena on Transonic Buffet Flow

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Transonic buffet flow on the supercritical airfoil OAT15A in fixed and pitching conditions are simulated with Unsteady Reynolds averaged Navier-Stokes (URANS) with SST-Kωturbulence mode. Firstly, the dynamic mode decomposition (DMD) is used to analyse the transonic buffet characteristics. It is indicated that the region of shock movement in pitching condition is larger than that of the fixed case, and there is chaotic flow rather than periodic flow in its wake.

Further, the buffet lock-in phenomena under pitching conditions near the buffet onset are studied by evaluating the energy exchange based on the pitching component of the moment coefficients as well as the normalized relative phase map between the pitching moment component and the airfoil angular velocity as shown in Fig. 1. It is indicated that the zero energy transfer branches in the energy map fail to predict the lock-in boundaries, while the normalized phase map generally outlines the lock-in boundaries for small pitch amplitudes near the buffet onset, which suggests that the lock-in occurs where the moment is in phase with the angular velocity at small pitch amplitudes near the buffet onset. For pitch amplitudes larger than 0.4°, the lock-in onset deviates from the phase shift, possibly due to the fact the instantaneous angle of attack can be lower than the buffet onset where the buffet phenomena may vanish.

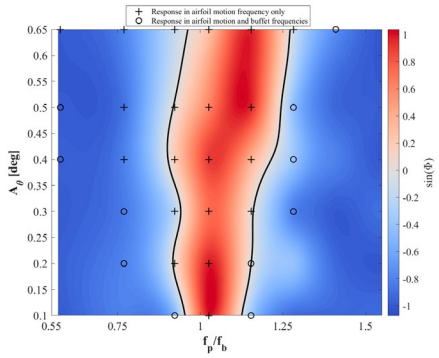

Fig. 1 Normalized relative phase map and the frequency response of the moment coefficient

Keywords: Transonic buffet, Lock-in, URANS, DMD, Phase map

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Influence of Particle Morphology on Segregation Rate in Vertically Vibrated Granular Beds

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The Brazil nut effect (BNE) describes a segregation phenomenon in which larger particles preferentially ascend to the surface of a granular mixture under external pertubations. Although extensively investigated, previous studies predominantly utilised spherical or smooth particles for simplicity, leaving a knowledge gap regarding the influence of particle shape irregularity on segregation dynamics. This study systematically addresses this gap by examining the effect of particle morphology on segregation rates through combined physical experiments and discrete element method (DEM) simulations. Specifically, a single large ceramic particle with controlled variations in shape irregularity was embedded within a vertically vibrating bed of smaller spherical glass beads. The segregation rates were quantitatively assessed by measuring the ascent velocity of the large particle of various morphological features. Experimental and DEM simulation results consistently indicated a notable reduction in segregation rates associated with increasing particle shape irregularity. Under identical vibration conditions, non-spherical particles exhibited significantly lower ascent velocities compared to spherical counterparts, primarily due to enhanced drag and frictional interactions, as well as the altered buoyancy conditions, leading to increased energy dissipation during upward migration. These findings underscore the crucial role of particle morphology in granular segregation processes and provide insights relevant to mitigating segregation-related geological hazards, such as landslides and debris flows, and providing better handling processes in material handling.

Keywords: Discrete element method, granular segregation, non-spherical particles

Simulation of Crack Path Instabilities in Quenched Glass Plate

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Understanding the onset of crack path instabilities in brittle materials under thermal loading is a long-standing challenge in fracture mechanics. While dynamic fracture has received significant attention due to its complex and unstable behavior, quasi-static crack propagation also exhibits nontrivial morphological transitions of crack paths, highlighting unresolved questions in fracture mechanics. A particularly notable example is crack growth in thermally quenched glass plates, where experiments have revealed controllable transitions from straight to oscillatory and branching cracks depending on quenching speed and plate geometry.

In this study, we perform two-dimensional numerical simulations using the Particle Discretization Scheme Finite Element Method (PDS-FEM) developed by the authors. PDS-FEM is one of the fracture analysis methods that can precisely evaluate the release of thermal stress due to fracture. PDS-FEM uses conjugate geometry (i.e., Voronoi and Delaunay tessellation) and discontinuous and non-overlapping shape functions for the discretization of field variables. The Delaunay tessellation corresponding to triangular or tetrahedral elements in conventional FEM. The governing equation for the deformation due to thermal stress is written as follows in the framework of PDS-FEM:

$$\sum_{\gamma=1}^{N} K_{ik}^{\alpha\gamma} u_k^{\gamma} = \sum_{\beta=1}^{M} B_i^{\beta\alpha} c_{ijkl}^{\beta} \epsilon_{kl}^{\mathrm{h}\beta} \Psi^{\beta}, \quad (1)$$

where $K_{ik}^{\alpha\gamma}$ is a stiffness matrix, u_k^{γ} is a displacement vector of the γ-th node, and N, M are the number of nodes and elements, respectively. $B_i^{\beta\alpha}$, c_{ijkl}^{β}, $\epsilon_{kl}^{\mathrm{h}\beta}$, Ψ^{β} are a strain-displacement matrix, an elastic moduli, a thermal strain, and a volume of the β-th element, respectively.

The simulations reproduce key features of experimental observations, including the emergence of straight, oscillatory, and branching cracks depending on the glass plate's width and its moving velocity. Our model allows for the identification of critical widths associated with morphological transitions and demonstrates how these critical values vary systematically with quenching speed.

Furthermore, detailed analysis of the stress field at the crack tip confirms that crack propagation in this context is governed predominantly by mode-I fracture mechanics. Our results show that while the crack path follows the Maximum Energy Release (MER) criterion, it also aligns with predictions from the Maximum Principal Stress (MPS) criterion due to their convergence under mode-I-dominant conditions.

By capturing complex crack morphologies in a thermally stressed brittle material, this study offers a predictive computational approach to crack path instability. These findings help bridge the gap between

experimental observations and theoretical modeling, contributing to the broader understanding of thermoelastic fracture phenomena.

Keywords: fracture analysis, thermal stress, brittle material, crack instability

Modelling of electro-thermo-convection problem based on physics informed neural network with Fourier features

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Heat transfer enhancement plays a critical role in a wide range of scientific and engineering applications. Among various control strategies, the use of electric fields has emerged as an effective and efficient approach due to its rapid response, ease of implementation, and lack of moving components [1]. In this work, a Physics-Informed Neural Network (PINN) is employed to address a multiphysics problem involving coupled hydrodynamic, thermal, and electric fields. To improve the network's ability to capture complex and localized features—particularly in cases with multi-scale behavior or high-frequency components—Fourier feature embeddings are integrated into the PINN architecture [2,3]. The performance of the proposed framework is evaluated by simulating thermal convection in a square cavity under varying Rayleigh numbers Ra and electric field strength T. The results highlight the potential of deep neural networks in solving complex multiphysics problems, offering a promising alternative to traditional numerical solvers.

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Vibrational characteristics of diamane nanosheets for mass-sensing applications

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A two-dimensional form of diamond with a bilayer sp^3 carbon nanostructure – diamane has attracted increasing attention recently, due to its unique properties and appealing applications. [1-3] This novel nanostructure has been initially predicted in 2009, [4] while its experimental synthesis has only been reported in 2019. [5]

This work carries out a comprehensive study on the vibrational properties of diamane nanosheets targeting the mass-sensing applications. Based on Kirchhoff plate model and molecular dynamics simulations, the vibrational characteristics of diamane nanosheets are investigated. The results show that the natural frequencies and corresponding modal shapes of the diamane nanosheets predicted by the Kirchhoff plate model agree well with that obtained from the molecular dynamics simulations. Furthermore, the vibrational characteristics of diamane nanosheet with attached mass are studied. It is found that diamane has higher mass sensitivity than single-layer graphene with the same size. Increasing pre-strain can significantly increase the natural frequency of diamane and enhance their sensitivity.

This work provides a comprehensive understanding of the vibrational properties of diamane nanosheets, which should be beneficial to the design and fabrication of nano mass sensor.

Keywords: Diamane nanosheets, molecular dynamics simulations, Kirchhoff plate model, mass-sensing

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Functionalization of wood composites using two-dimensional layered double hydroxides: An atomistic approach

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The integration of wood-based biocomposites in sustainable construction is limited by their flammability and microbial susceptibility. While hydrophobic surface treatments for wood have shown effects, the demand for active antimicrobial functionality remains, and conventional fluorinated silane-based flame retardants pose environmental concerns. This study proposes layered double hydroxides (LDHs), biocompatible 2D materials with tunable metal hydroxide layers, exchangeable interlayer, and high surface area, as a multifunctional solution to synergistically enhance flame retardancy and microbial resistance in wood. To overcome limitations of traditional trial-and-error methods, molecular dynamics (MD) simulations are employed to elucidate atomic-scale interfacial interactions within LDH-modified wood systems, with the basic theory shown in Equation (1) [1, 2]. Mg-Al, Ca-Al, and Zn-Al LDHs intercalated with different antimicrobial anions such as benzoate and cinnamic acid are modelled alongside low-surface-energy fatty acid modifiers (stearic, lauric, and myristic acids) to optimize hydrophobicity. The forcefields involve hybrid CVFF/CLAYFF (Equation 2) for LDH-cellulose- adhesion and CHARMM for fungal glycoproteins and phospholipid bilayers dynamics, resolving key interactions: (1) LDH-cellulose binding governed by electrostatic/hydrogen-bond networks, (2) hydrophobic modifier adsorption capacities on LDH surfaces, and (3) contact-kill antimicrobial mechanisms via membrane disruption. Simulations aim to predict the optimal LDH compositions that balance cellulose compatibility, surface hydrophobicity, and antimicrobial efficacy, establishing a structure-function framework for the rational design of multifunctional wood coatings. By replacing toxic additives with functionalized LDHs, this work advances the development of eco-friendly wood biocomposites with integrated fire and microbial protection. The simulation-guided methodology is broadly applicable to the design of 2D nanomaterial-based coatings, accelerating innovations in sustainable construction materials [3].

$$F_i = m_i \cdot d^2 r_i / dt^2 \tag{1}$$

where F_i is force acting on particle i; m_i and r_i are mass and positions of particles i; $d^2 r_i / dt^2$ is acceleration of particle i.

$$E_{\text{total_clayff}} = E_{\text{coulombic}} + E_{\text{vdw}} + E_{\text{bondstretch}} + E_{\text{anglebond}} \tag{2}$$

Keywords: Antimicrobial coatings; Flame retardancy; Layered double hydroxides; Molecular dynamics; Wood; Biocomposites

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Artificial Intelligence-Assisted Geometric Compensation and Finite Element Optimization for Patient-Specific Dental Implant Design

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. Three-dimensional (3D) printing has become a widely adopted technique in the medical field due to its exceptional flexibility in fabricating geometrically complex components. However, physical factors such as thermal strain, build orientation, and photopolymerization time during manufacturing often cause geometric deviations between the printed products and their original digital designs [1]. To address this, we propose a deep learning framework based on a 3D U-Net architecture [2] to predict and compensate for such deviations before printing. The model is trained on volumetric surface patches extracted from previously printed dental and mandibular models, enabling pre-correction of the original designs. This approach significantly improves the dimensional fidelity of the printed anatomy, providing a more accurate foundation for subsequent implant design.

Building upon these high-fidelity physical models, this study further presents the design optimization of a custom-made dental implant tailored for patients with severe mandibular atrophy and long-term tooth loss, where conventional implants carry a high risk of nerve damage [3,4]. Finite element analysis (FEA) was employed to assess and compare the mechanical performance of short implants, subperiosteal implants, and the proposed custom-made design under various loading conditions. The custom implant features a monolithic structure with an integrated stress-relief plate, exhibiting improved stress distribution and maintaining stress levels below the yield limits of both implant material and surrounding bone. Compared to conventional types, the optimized design effectively reduces localized stress concentrations, minimizing the risk of bone damage.

Together, these results demonstrate the potential of combining AI-assisted geometric compensation with simulation-based design to develop precise and patient-specific dental implant solutions. This integrated approach enhances both the manufacturing accuracy of anatomical models and the biomechanical reliability of the final implant.

Keywords: 3D printing, Deep learning, Error Precorrection, Finite Element Method, Implants, Custom-Made, Subperiosteal Implants

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Mechanochemical Influence of Vibrations on Electrode Interfaces in Lithium-Based Batteries

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Batteries are increasingly being used under diverse conditions, including a wide range of temperatures, and dynamic environments. To understand how such environmental factors affect the electrochemical behavior of batteries, numerous studies have been conducted. However, most of these studies have focused on stationary conditions, such as temperature, pressure, and charge/discharge rates [1,2]. Given that batteries are predominantly employed in electric vehicles and other mobile systems operating under dynamic conditions, it is essential to investigate how dynamic stimuli affect battery performance. In this study, we explore the effects of both low-frequency (7 Hz) and high-frequency (40 kHz) vibrations on lithium-based batteries through a combination of computational mechanics and electrochemical measurements. We demonstrate that mechanical vibrations induce a transition of the solid electrolyte interphase toward a more inorganic-rich composition, driven by the differing mechanical stabilities of the interfacial components. Furthermore, Li dendrites exhibited flattened morphology under 7 Hz, and complete dendrite breakage under 40 kHz vibration. The underlying mechanisms are systematically investigated using finite element analysis and density functional theory. These findings provide valuable insights into the computational understanding of how mechanical stimuli affect electrode surfaces in batteries operating under dynamic conditions.

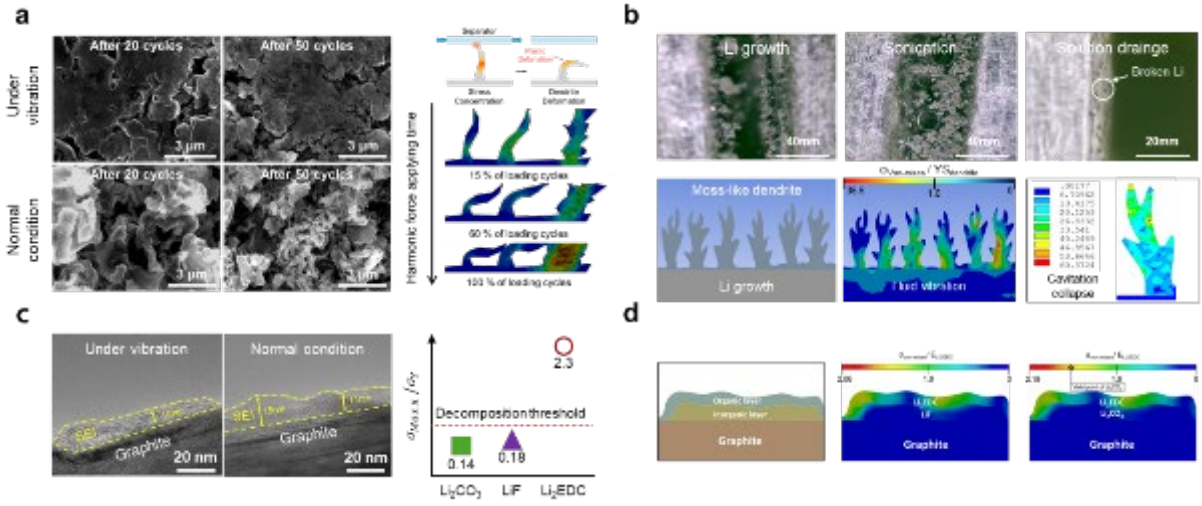

Figure 1. (a) Scanning electron microscopy images of Li after plating and stripping test with and without 7Hz vibration and finite element analysis demonstrating Li dendrite bending. **(b)** Digital images showing breakage of dendrites by ultrasound, and stress analysis illustrating cavity collapse within the dendrites. **(c)** Transmission electron microscopy images showing graphite anodes under different conditions, and stability analysis of various components under vibration. **(d)** Stress analysis of graphite electrode under 40kHz fluid motion.

Keywords: Lithium batteries, Solid electrolyte interface, Linear vibration, Finite element analysis

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Modelling Frictional Behaviour of Expansive Clay: Insights into Microscopic Mechanics of Montmorillonite

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Hydration lubrication plays a significant role in reducing sliding friction in various moving systems, from geological faults to molecular materials systems, but the mechanism of lubrication on microscopic friction remains poorly understood. In this study, we introduce a microscopic friction model that calculates the relationship between shear stress and normal stress across varying water contents. A scale-up approach is proposed to translate the microscopic friction coefficient into a macroscopic context, thereby validating the model's effectiveness. The proposed model successfully captures variations in the friction coefficient un-der different water contents, offering an innovative tool for understanding the fundamental mechanisms of hydration lubrication.

Keywords: Friction, hydration lubrication, clay mineral, molecular simulation.

Offshore Floating Photovoltaics: From Hydroelastic Response to Energy Yield Correction

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With the accelerated transition to renewable energy, Offshore Floating Photovoltaic (OFPV) is increasingly becoming an important solution to promote. However, most of the current mainstream research treats structural response and power generation performance separately, making it difficult to accurately predict the actual power generation capacity and economics of the system in real-world environment in the ocean. There is little study handling commercial scale deployment of floating PVs which consist of thousands of panel arrays, where physical coupling and system integration need to be taken into account.

This study proposes a comprehensive framework that establishes a fully coupled pathway from environmental forcing, hydro-elastic response of floating structures, and multi-module attitude variation, to irradiance loss estimation, motion-corrected power output, and final economic performance metrics. The method has been experimentally validated in a wave basin under regular wave conditions, demonstrating excellent agreement between numerical predictions and measured hydroelastic responses, confirming its accuracy and robustness [1].

The resulting structural responses are subsequently mapped to module-level tilt variations, which dynamically influence irradiance incidence, temperature-related efficiency, and partial shading effects—thus forming a motion-coupled energy yield prediction model.

Preliminary simulations conducted on a representative 300 m × 60 m OFPV platform suggest that platform motions may lead to non-negligible reductions in energy yield, which—if left unaccounted for—could result in systematic underestimation of the levelised cost of energy (LCOE). To address this issue, we propose a Motion Correction Factor (MCF) to quantify the influence of structural dynamics on power output. This factor is incorporated into the economic evaluation workflow, forming a closed-loop paradigm that connects hydrodynamic response with energy performance metrics in OFPV systems.

By bridging physical response and energy output, the proposed approach lays the groundwork for motion-aware design, planning, and investment evaluation of next-generation offshore solar farms.

Keywords: Offshore floating photovoltaics, hydroelasticity, energy yield correction, techno-economic assessment

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Damage and repair assessment of transmission tower under different seasonal loads and support movement: Discussion of member damages and ultimate strength recovery

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Transmission towers are essential components for electric power supply, but recent serious hazards cause collapse accidents and power outages. Moreover, climate change may increase disaster damage. Therefore, we must develop countermeasures to prevent structural damages and repair methods to restore damaged towers [1]. In the Asian region, including Japan, member damages and whole tower failure are caused by excessive loads due to strong winds and ice/snow accretion, as well as support movement due to ground deformation. This study performs finite element (FE) analysis simulating damage behavior and repair method of transmission towers to evaluate the ultimate strengths at initial state without damage, after damage, and after repair, which are denoted by k_{ult}^{0}, $k_{\mathrm{ult}}^{\mathrm{dam}}$, and $k_{\mathrm{ult}}^{\mathrm{rep}}$, respectively. We set three types of seasonal loads: high temperature season (H-load), low-temperature season (L-load), and heavy ice/snow accretion (S-load). We also consider the damage due to support movement of specific magnitudes in horizontal and vertical directions. In addition, the damage degradation after damage, R_{dam}, and strength recovery after repair, R_{rep}, are evaluated by:

$$R_{\mathrm{dam}} = \left(k_{\mathrm{ult}}^{0} - k_{\mathrm{ult}}^{\mathrm{dam}}/k_{\mathrm{ult}}^{0}\right),\ R_{\mathrm{rep}} = \left(k_{\mathrm{ult}}^{\mathrm{rep}} - k_{\mathrm{ult}}^{\mathrm{dam}}/k_{\mathrm{ult}}^{0} - k_{\mathrm{ult}}^{\mathrm{dam}}\right). \tag{1}$$

Table 1 shows the result of damage and repair analysis under excessive seasonal loads. We assume two repair methods: Repair method A1 replaces two of the most damaged main members, while Repair method A2 replaces two of the most damaged web members. The ultimate strength is recovered effectively by Repair method A1, whereas Repair method A2 provides no effects. This result implies choosing an appropriate repair method according to the damaged state is important.

	H-load	L-load	S-load
Initial	$k_{ult}^{0} = 3.32$	$k_{ult}^{0} = 3.83$	$k_{ult}^{0} = 2.23$
Damaged	$k_{ult}^{dam} = 2.59,\ R_{dam} = 22.0\%$	$k_{ult}^{dam} = 2.98,\ R_{dam} = 22.4\%$	$k_{ult}^{dam} = 1.55,\ R_{dam} = 30.0\%$
Repaired			
Repair method A1	$k_{ult}^{rep} = 2.93,\ R_{rep} = 46.3\%$	$k_{ult}^{rep} = 3.65,\ R_{rep} = 79.1\%$	$k_{ult}^{rep} = 1.98,\ R_{rep} = 63.1\%$
Repair method A2	$k_{ult}^{rep} = 2.58,\ R_{rep} = -1.48\%$	$k_{ult}^{rep} = 2.27,\ R_{rep} = -82.3\%$	$k_{ult}^{rep} = 1.54,\ R_{rep} = -0.35\%$

Table 1.

Keywords: transmission tower, seasonal load, support movement, ultimate strength, member damage, damage and repair simulation

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Structural Determinants of Permeability in 3D-Printed Bone Scaffolds

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Bone regeneration is essential for treating fractures, tumours, infections, and other causes of bone loss. Scaffold permeability plays a vital role by enabling nutrient delivery and waste removal. An optimally permeable scaffold promotes efficient fluid transport, accelerating tissue ingrowth and healing. Conversely, insufficient permeability may limit waste clearance, while excessively high permeability can affect cell proliferation, ultimately reducing scaffold performance [1].

Size of the pores and structural porosity are major scaffold parameters that determines the permeability of the bone scaffold among other minor contributors such as material, surface finish, etc. Therefore, permeability should be maintained within the range of human bones ranging between 2.56 x 10^{-11} to 7.43 x 10^{-09} m^2 for cancellous bones and 2.20 x 10^{-10} to 3.49 x 10^{-09} m^2 for cortical bones.

This study investigates the influence of scaffold architecture on permeability through numerical analysis. Five lattice scaffold structures with distinct structural characteristics and porosity of 65% ± 0.5% were designed using SolidWorks. Fluid domains were created for all scaffold structures using ANSYS SpaceClaim. Following a mesh convergence study, Computational Fluid Dynamics (CFD) simulations were performed in ANSYS Fluent under defined boundary conditions to evaluate fluid flow through each scaffold structure.

All scaffold structures exhibited permeability values within the physiological range of human bone. Among them, the Gyroid structure demonstrated the highest permeability at 2.17 × 10^{-10} m^2, which closely approaches the lower bound of cortical bone permeability. This can be attributed to its continuous diagonal internal pathways that facilitate fluid flow more effectively than other geometries.

Both the Lattice and Schwarz Primitive structures also exhibited relatively higher permeability compared to the remaining designs, suggesting favourable flow characteristics. Overall, the results indicate that a structural porosity of 65% is sufficient to maintain scaffold permeability within the acceptable range for both cancellous and cortical bone. Furthermore, lattice designs with more open and directional pathways may offer enhanced permeability performance, despite the geometric differences across scaffold types.

Keywords: Permeability, Bone Scaffold, Permeability, Computational Fluid Dynamics (CFD), Additive Manufacturing

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A Neumann-Neumann Acceleration with Coarse Space for Domain Decomposition of Extreme Learning Machines

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Extreme learning machines (ELMs), which preset hidden layer parameters and solve for last layer coefficients via a least squares method, can typically solve partial differential equations faster and more accurately than Physics Informed Neural Networks. However, they remain computationally expensive when high accuracy requires large least squares problems to be solved. Domain decomposition methods (DDMs) for ELMs have allowed parallel computation to reduce training times of large systems. In this talk, we present a coarse space for ELMs, which enables further acceleration of their training. By partitioning interface variables into coarse and non-coarse variables, selective elimination introduces a Schur complement system on the non-coarse variables with the coarse problem embedded. Key to the performance of the proposed method is a Neumann-Neumann acceleration that utilizes the coarse space. Numerical experiments demonstrate significant speedup compared to a previous DDM method for ELMs.

Keywords: Extreme learning machine, Neumann-Neumann method, coarse space, domain decomposition

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An efficient finite element method for recertification of aircraft component after repair

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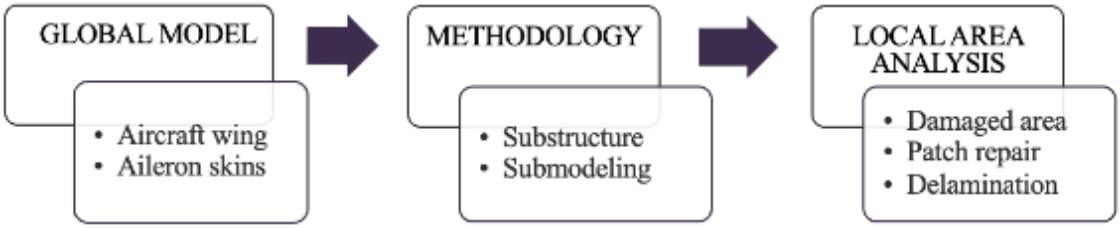
Maintenance and repair processes of aircraft structures have been essential aspects of the aerospace industry. The use of Finite Element Analysis (FEA) to address the challenges associated with aircraft maintenance and repair has recently attracted significant attention, driven by improvements in computing power and advancements in numerical approaches. However, there remain challenges in the implementation of FEA, including the complexity of modeling real-world boundary conditions, the high computational cost associated with large scale structures, and the difficulty of accurately incorporating composite material damage and defects.[1][2] This research seeks to address these issues by developing a FEA model capable of predicting the remaining lifespan of composite aerospace components. The proposed model aims to enhance maintenance decisions and contribute to the broader integration of digital twin technologies, ultimately enhancing the effectiveness of maintenance and repair operations.



Keywords: Finite element analysis, Aerospace components, Digital-Twin

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Effective property method for efficient modelling of non-uniform tissue support in fluid–structure interaction simulation of blood flows

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In fluid-structure interaction analysis of blood flow, surrounding tissue support is vital for accurately simulating physiological constraints, reproducing realistic vessel wall motion, and eliminating non-physiological oscillations. The generalized Robin boundary condition, which uses a spring-damper model to simulate tissue support, can complicate pre-processing and numerical computations when dealing with non-uniform tissue support. To address this, we propose an effective property method for modelling non-uniform tissue support and quantitatively analysing its contribution to vascular wall deformation. Based on linear viscoelasticity theory, we discovered that the parameters of the generalized Robin boundary condition can be integrated into the effective properties of the vessel wall:

$$(Eh)' = Eh + \frac{3R^2}{4}\,k, \quad (\eta h)' = \eta h + \frac{3R^2}{4}\,c, \tag{1}$$

where E is the elastic modulus, h is the wall thickness, η is the solid viscosity, and R is the lumen radius; k and c are the elastic and damping parameters of the generalized Robin boundary condition; $(\cdot)'$ denotes the effective properties. The theoretical analysis indicates that tissue support enhances the apparent stiffness and viscosity of the vessel wall, with the extent of this increase depending on the vessel radius. Furthermore, we extend the coupled momentum method [1], originally applicable only to elastic problems, to account for the viscoelasticity of the vessel wall.

We apply the effective property method to numerical simulations of a patient-specific aortic model, comparing it with cases using the Robin boundary condition. As shown in Figure 1, the results verify the method, showing maximum relative errors of less than 2.2% for flow and 0.7% for pressure, demonstrating its effectiveness for complex, non-axisymmetric tissue support distributions.

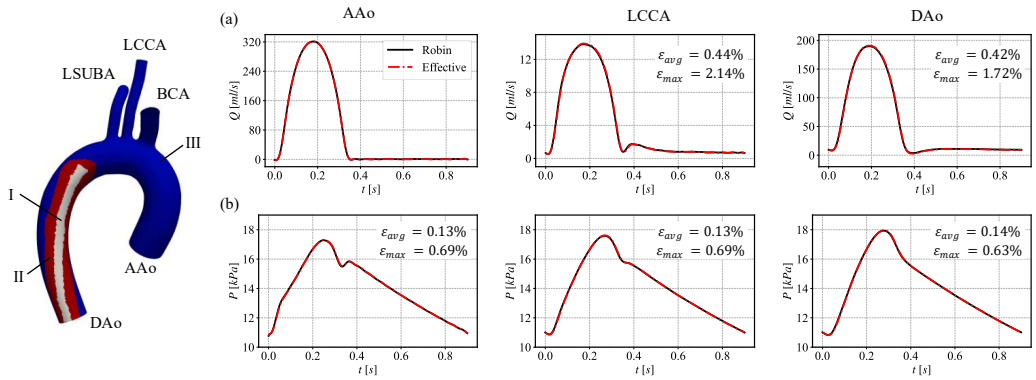

Figure 1. Patient-specific aorta model with non-uniform tissue support

Keywords: Fluid–structure interaction, tissue support, blood flow, biomechanics

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The Breakup of Earth: From Rock Failure Modeling to Earth Evolution Exploration

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The history of Earth's evolution is a chronicle of gradual thermal decay amidst cyclical shifts between cold and heat. The continuous interplay between the fragmentation-aggregation of the lithosphere and the Earth's thermal fluctuations has driven a series of surface transformations characterized by warming and cooling, expansion and contraction, melting and solidification[1]. This study, grounded in the fundamental principles of thermodynamics, physics, and mechanics, focuses on the formation mechanism of tectonic cracks to propose a novel theory of Earth's evolution driven by its own thermal equilibrium. This includes the development of an Earth simulator for modeling lithospheric rupture and the discovery of a "tessellation-fracture" pattern in plate origins through simulation—particularly the simulated formation process of mid-ocean ridge rifts. Additionally, by establishing a thermal equilibrium equation for the Earth system, the study elucidates the thermal evolution mechanism whereby lithospheric rupture triggers intrinsic cold-hot fluctuations. Furthermore, building on the observed correlation between major geological events and thermal fluctuations in Earth's evolution, the research presents reflections on the possible existence of a common driving force behind significant geological events, along with prospects for future investigation.

Keywords: Earth's evolution, Earth simulator, lithospheric rupture, mid-ocean ridge rift, thermal fluctuation

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A Multi-Agent LLM Framework for Improving Knowledge Transfer in Injection Molding

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The injection molding industry, a core sector in global manufacturing, relies heavily on tacit, experience-based knowledge to manage complex production variables and ensure product quality. Traditional knowledge transfer methods, including manuals and apprenticeship systems, face growing limitations due to an aging workforce and declining new labor inflow. Although prior studies have employed expert systems and machine learning approaches to encode domain expertise, these systems often struggle with flexibility, real-time adaptability, and accessibility for less experienced operators.

Recent advances in large language models (LLMs) have demonstrated strong capabilities in reasoning, natural language understanding, and decision-making, offering potential for scalable and human-centric knowledge support. However, limitations such as hallucination and the inability to integrate live data or domain-specific context remain challenges for pre-trained LLMs.

This study introduces a domain-specific, multi-agent LLM framework designed for effective knowledge transfer in the injection molding industry. The framework employs retrieval-augmented generation (RAG), tool integration, and role-specialized agents (e.g., retrieval, reasoning, execution), enabling both general and injection molding-specific tasks to be handled through a modular and interpretable architecture. By incorporating various knowledge sources such as operator databases, manuals, and simulation models, this framwork facilitates adaptive, data-driven decision-making while enhancing communication and learning for diverse user groups. The proposed approach addresses the limitations of monolithic LLM systems and traditional expert systems, offering a scalable, maintainable, and context-aware solution for industrial knowledge transfer.

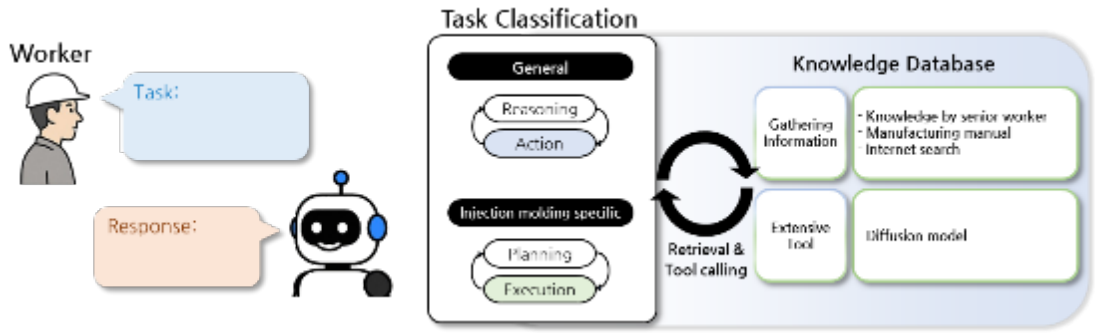

Figure 1. Overview of the Multi-agent LLM framework for knowledge transfer in the injection molding industry.

Keywords: Injection Molding, Knowledge Transfer, Large Language Model, Artificial Intelligence

Topology optimization of open radiation shielding structures

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In radiation environments, electronic devices are susceptible to failure due to irradiation damage from γ-rays, X-rays, and other radiation. To ensure reliable operation, shielding structures are typically employed to absorb radiation energy and reduce the dose rate at the device location. For instance, lead is commonly used to attenuate γ-rays. However, in specialized applications (e.g., radiation-resistant cameras), functional openings, such as optical windows, must be integrated into the shielding structure. These openings create localized weak points where direct radiation exposure significantly degrades shielding effectiveness.

There are two main strategies to protect the devices in open structures: First, fold the open path to prevent direct radiation exposure; second, optimize the shielding structure to improve the shielding efficiency. Existing design methods for shielding structure typically rely on Monte Carlo Methods for radiation transport analysis, combined with machine learning methods to get the optimal multilayer plate/shell structures. However, few studies have specifically addressed open structures. Moreover, Monte Carlo methods are computationally expensive, and machine learning methods lack physical interpretability.

This work introduces a simplified analytical model based on both energy flux conservation and experimentally validated exponential attenuation law. The model describes the attenuation of radiation intensity I from a point source. We developed a topology optimization method specifically for radiation-shielding structures base on the analytical model. It's verified that our method exhibits good convergence. Under a constrained shielding mass (10 kg of lead) and a predefined folded opening path, our optimized structure achieves about 15% higher radiation shielding efficiency compared to conventional designs.

Keywords: Topology optimization, Radiation shielding, Open structures

Analysing Rock Fracturing Process with The Discontinuous Deformation and Displacement (DDD) Method

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This study presents the discontinuous deformation and displacement (DDD) method, a novel computational approach for simulating the nonlinear deformation and failure mechanisms of jointed rock masses. Building upon the foundations of continuum mechanics, statistical damage theory, and contact mechanics, the DDD method synthesizes the key advantages of both the rock failure process analysis (RFPA) and discontinuous deformation analysis (DDA) methods. The proposed framework provides a unified solution for simulating: (1) the complete deformation process, including crack initiation and propagation, and (2) rigid body motion encompassing translation, rotation, and block interactions. The core of the DDD method lies a derived unified global equilibrium equation that simultaneously resolves both continuous and discontinuous problems within a single computational scheme. This innovative formulation enables: (1) concurrent simulation of mechanical responses in intact rock matrix and along discontinuities, (2) automatic transition from continuous to discontinuous media through implementation of a physics-based fracture propagation algorithm, and (3) seamless integration of small-strain fracture processes with large-displacement block dynamics. The resulting analytical framework achieves comprehensive simulation of the complete rock failure sequence, from initial microcracking to ultimate instability.

Keywords: rock fracture, crack propagation, discontinuous deformation, jointed rock mass, failure mechanism

Extreme-Scale Simulation of Thermal Transport in Silicon Nanostructures and Devices

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Thermal transport in low-dimensional silicon nanostructures play a crucial role in determining the performance and stability of some devices, such as field-effect transistors, thermoelectric arrays, and integrated circuits. Molecular dynamics simulation serves as a powerful tool for describing the thermal behavior of silicon nanostructures and devices. However, due to huge computational workload involved in atomistic simulation, the simulated characteristic sizes of nanostructures are significantly smaller than those fabricated experimentally, and the finite size effect of thermal conductivity in non-equilibrium molecular dynamics simulation (NEMD) is difficult to overcome. For some transistor devices, such nanoscale factors as doping, thin dielectric layer, surfaces and interfaces are also difficult to handle.

To address these issues, we realized extreme-scale non-equilibrium molecular dynamics simulation. Regarding silicon nanostructures, the simulated characteristic size reached the experimental scale, while the longitudinal size was beyond millimeters. And based on the surmounted size effect of NEMD simulation, a novel thermal conductivity prediction model of silicon nanostructures was presented. For transistor devices, different circuit modules covering multiple nanoscale factors such as surface, interface, doping, dielectric layer, gate, and layout, were calculated with tens of thousands of nano-transistors and more than one trillion atoms by using about 40 million processor cores for the massively parallel computation [1,2].

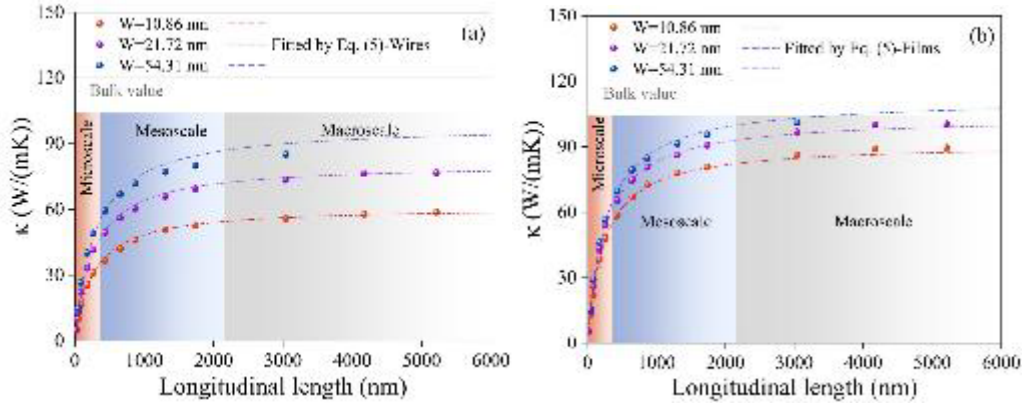

Figure 1.

Furthermore, a suite of corrected phonon relaxation time models was developed to solve the phonon Boltzmann transfer equation with a lattice Boltzmann method (LBM) scheme for larger nanostructures and devices [3]. These above simulations pave a promising way to advance nanotechnology and microelectronics.

Keywords: nanowires, nanofilms, devices, silicon, thermal transport, size effect

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Obliquely Interacting Solitary Waves and Wave Wakes in Free-Surface Flows

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Mach reflection was initially discovered and named by the physicist Ernst Mach when studying shock wave interactions at the wavefront in gas dynamics. This phenomenon was also observed in oceanic surface waves. A comprehensive theoretical explanation of Mach reflection in water waves was not achieved until the pioneering contributions of Miles, who examined the interaction of two obliquely colliding solitons in surface gravity waves and proposed that the dynamics depend on their incident angles and amplitudes. A weakly interacting scenario occurs when the incident angles are sufficiently small, allowing the two solitons to approximately linearly superpose, resulting in regular reflection. As the incident angle increases, the solitons undergo Mach reflection, leading to the formation of the Miles resonant soliton.

The previous discussions on Mach reflection of solitons are predominantly based on the Kadomtsev-Petviashvili (KP) equation, which is inherently anisotropic and describes unidirectional wave propagation. This limitation means it does not effectively capture wave phenomena with significant transverse variations in the ocean. In this talk, we investigate the Mach reflection phenomenon with the weakly nonlinear isotropic bi-directional Benney-Luke (BL) equation. Using the Whitham theory, we derive the associated modulation equations describing soliton amplitude and slope evolutions. By analyzing rarefaction waves and shock waves within these modulation equations, we derive the Riemann invariants and modified Rankine-Hugoniot conditions. These expressions help characterize the Mach expansion and Mach reflection phenomena of bent and reverse bent solitons. We also derive analytical formulas for the critical angle and the Mach stem amplitude, showing that as the soliton speed is in the vicinity of unity, the results from the BL equation align closely with those of the KP equation. Corresponding numerical results are obtained and show excellent agreement with theoretical predictions. Furthermore, as a far-field approximation for the forced BL equation - which models wave and flow interactions with local topography - the modulation equations yield a slowly varying similarity solution. This solution indicates that the precursor wavefronts created by topography moving at subcritical or critical speeds take the shape of a circular arc, in contrast to the parabolic wavefronts observed in the forced KP equation. For two topographies, depending on their selected amplitudes and speeds, Mach reflection may also occur between the two wakes

Keywords: solitary waves, equations, surface gravity waves, Whitham modulation theory, Benney-Luke equation

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An Efficient Surrogate Model Construction for Large-Scale Fluid Simulations Based on Dimensionality Reduction and FFX Method

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In computational fluid dynamics (CFD), traditional grid-based methods, such as Finite Volume Methods (FVM), and particle-based methods, such as Smoothed Particle Hydrodynamics (SPH), are widely used. However, these methods face significant challenges in large-scale simulations which require large computational cost. To address these issues, we propose an innovative and efficient surrogate model based on Dimensionality Reduction (DR) and Fast Function Extraction (FFX).

Dimensionality reduction allows for effective reduction of data complexity, and saves computational costs while preserving the essential physical information. On the other hand, the FFX method accelerates the simulation process by rapidly generating symbolic regression models. Its intrinsic path regularization process further mitigates overfitting, ensuring robust generalization and accuracy. Compared to traditional techniques, the proposed surrogate model can not only substantially save simulation time but also can be used to rapidly predict key model parameters and physical phenomena of dynamic scenarios. The surrogate model performs well in a variety of complex scenarios in large-scale fluid simulations. Numerical experimental show that this surrogate model sharply reduces computational costs while maintaining high prediction accuracy.

Keywords: Smoothed Particle Hydrodynamics, Large-Scale Fluid Simulations, Surrogate Model Regularization Techniques, Fast Function Extraction, Dimensionality Reduction

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Hybrid Self-Attention and Graph-Recurrent Neural Network for Damage Classification in a Bridge Structure

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Abstract:

Civil structures can be vulnerable to damage over time due to aging, design flaws, and environmental factors. Recent advancements in machine learning provide a robust foundation for enhancing structural damage identification capabilities. However, traditional machine learning-based damage identification methods often fall short in large structures like bridges, where varying operational conditions and complex damage patterns require more dynamic and adaptable solutions. In this study, we aim to develop a damage identification model in large-scale civil structures by leveraging the unique capabilities of autoencoder Long Short-Term Memory (LSTM) and Graph Neural Networks (GNN). The LSTM, enhanced with Multi-Resolution Wavelet Transform (MODWT) layers, extracts hidden features from raw acceleration signals across both temporal and spectral domains. This extraction is crucial as it reveals subtle patterns and variations in signal behaviour that are indicative of structural damage or anomalies. Concurrently, the GNN, employing a graph attention network (GAN), transforms the features extracted by the LSTM into dynamic, high-level graph-structured features. This transformation provides a comprehensive representation of the interconnected sensor systems on the structure, allowing the GNN to map sensor data and their relationships into a graph structure, which enables the model to dynamically update its parameters based on new data. This multi-tasking learning integration not only leverages the strengths of both neural network architectures but also combines their loss functions to effectively classify the anomalies in complex civil structures in a varying environment. The proposed framework has been validated with the acceleration data obtained from a real bridge. Results demonstrate it feasibility in detecting and classifying anomalies in bridge structures, and show better performance compared to existing methods.

Coarse-Grained Molecular Dynamics Method for Stress-Strain Prediction in Alloys

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Many important physical processes in deforming metals occur at the mesoscale. While molecular dynamics has proven a useful tool in understanding atomic-scale mechanisms in metals, and continuum mechanics provides the basis for larger scale models, there remains considerable difficulty in predicting the behaviour of materials at the scale of 1-100 μm. Motivated by the problem of optimizing high-entropy alloy coatings via cold-spray deposition, we develop a coarse-grained molecular dynamics method for complex metallic materials at the mesoscale. Previous attempts to coarse grain crystalline solids using force matching approaches accurately reproduce the radial distribution function of the material, but fail to capture the stress-strain behaviour. Energy-renormalization based methods such as the quasi-coarse-grained dynamics method assume a homogeneous deformation and thus cannot capture lattice distortion, which is essential for multi-component materials. In our approach, we combine force matching with energy regularization using a neural network ensemble-based potential. We show that this method can more accurately reproduce stress-strain behaviour of single- and multi-element metallic materials than the quasi-coarse-grained dynamics method at a reduced computational cost. Additionally, we find that even when training the method on high-strain-rate atomic simulations, it correctly predicts the stress-strain behaviour at strain rates three orders of magnitude lower. This work provides a novel method for upscaling atomistic simulations of alloys into the mesoscopic scale, offering great potential for modelling microscale deformation processes of new advanced materials.

Keywords: Coarse-grained molecular dynamics, machine learning, high-entropy alloys, mesoscale modelling

AI-powered approximation for fast and accurate prediction of nonlinear interactions in wave forecasting

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Accurate wave forecasting is crucial for various applications, such as optimising vessel route planning by avoiding rough seas, saving time and fuel consumption, ensuring safe and efficient maintenance periods at offshore wind farms, and designing robust and economical coastal structures. However, this requires an accurate and efficient computation of nonlinear wave–wave interactions, which involve solving a six-dimensional Boltzmann integral. This is an extremely time-consuming process that has challenged researchers for over half a century. To enable practical applications, almost all state-of-the-art operational wave models rely on simplified approximation with known deficiencies.

In this study, we present a data-driven approach that could enable fast and accurate predictions of nonlinear wave–wave interaction terms. Our method employs a U-net model that directly maps discrete wave spectra and Discrete Interaction Approximation onto their corresponding full nonlinear interaction terms. The model was trained using European Centre for Medium-Range Weather Forecasts reanalysis wave spectra spanning various locations and time periods. To assess the model's robustness, we further evaluate its ability to extrapolate beyond its generalization ability with model integrations. Practical possibilities for further improvements are also suggested and discussed.

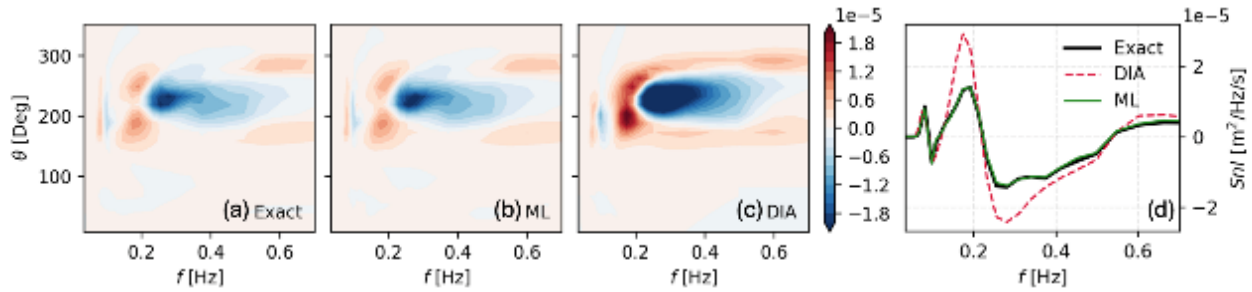

Figure 1. Comparison of the two-dimensional non-linear transfer rate between (a–c) exact, machine learning and Discrete Interaction Approximation and (d) directional integrated transfer rate.

Keywords: Nonlinear interactions, Machine learning, Wave model

Integrating Classical Numerical Methods into Deep Operator Networks for Elliptic PDEs

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Partial differential equations (PDEs) have long played a crucial role in the mathematical modeling and prediction of complex physical phenomena. In various fields of science and engineering, accurate numerical solutions to PDEs are essential. Classical numerical methods—such as the finite difference method (FDM), finite element method (FEM), and discontinuous Galerkin (DG) method—along with their variations are theoretically well-established and offer guarantees of convergence and stability. However, these methods have notable limitations when applied to complex geometries, nonlinearities, or high-dimensional problems. Recent advances in scientific machine learning offer new opportunities to address these limitations. Physics informed neural networks (PINNs) [1] and operator learning models such as DeepONet [2] have shown promise by incorporating the structural information from PDEs into the learning process, thereby reducing mesh dependency and enhancing computational efficiency. Nevertheless, these models also face inherent challenges, including difficulties in optimization, sensitivity to data quality and quantity, and potential violations of physical laws.

In this talk, we introduce a deep operator network designed to solve second-order elliptic problems. The proposed model adopts a physics-informed DeepONet approach that integrates traditional numerical methods such as FDM and FEM, enabling operator learning even under mixed Dirichlet and Neumann boundary conditions. Unlike the standard DeepONet, which consists of two neural networks—a branch network and a trunk network—to learn the operator, the recently proposed FEONet [3] leverages FEM basis functions and focuses on predicting only the solution coefficients, allowing for more efficient and accurate inference using a single network. However, achieving fine-scale solutions requires an increased number of input and output nodes, which results in a large number of trainable parameters. To address this issue, we introduce an encoder-decoder architecture that represents both input and output as images. Each pixel in these images corresponds to a node in the mesh, allowing the model to incorporate spatial information effectively. Several numerical experiments are presented to demonstrate the effectiveness and efficiency of the proposed approach.

Keywords: Partial Differential Equations, Deep Operator Network, Physics-Informed Learning, Finite Difference/Element Method, Convolutional Neural Networks

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Dynamic Glucose-Enhanced MRI for Tumor Microenvironment Characterization: LSTM-Based Time Series Analysis, SOM Clustering, and Compartmental Modeling

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Dynamic Glucose-Enhanced (DGE) MRI offers promising capabilities for non-invasively characterizing tumor metabolism and perfusion at the organ level, yet the extraction of meaningful biomarkers from complex temporal image data remains challenging. In this study, we present an integrated computational approach combining Long Short-Term Memory (LSTM) neural networks, Self-Organizing Maps (SOM), and compartmental modeling to comprehensively analyze DGE MRI data for tumor microenvironment characterization.

We employed LSTM models to analyze voxel-wise temporal MRI intensity patterns, effectively capturing dynamic differences in glucose uptake and wash-out kinetics. These time-series features provided sensitive biomarkers, enabling distinction between tumor and normal tissues and characterization of intratumoral heterogeneity. To facilitate unbiased spatial classification, SOM clustering was applied to segment regions based on similarity in their DGE kinetic profiles, effectively visualizing metabolic heterogeneity without the need for prior labeling.

To enhance physiological interpretability, we constructed a compartmental transport model simulating glucose diffusion and uptake across vascular, extracellular, and intracellular compartments within the tumor-bearing organ. Model predictions aligned closely with SOM-based clustering results and were validated against histopathological data, demonstrating accurate representation of tumor physiological states.

The synergistic integration of AI-driven temporal analysis (LSTM), unsupervised spatial segmentation (SOM), and mechanistic physiological modeling provides a robust framework for organ-level modeling of tumor environments. This approach advances quantitative MRI biomarker extraction and contributes to our understanding of tumor biology, potentially supporting clinical decision-making.

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Keywords: Dynamic MRI, Dynamic Glucose-Enhanced (DGE) MRI, Tumor Microenvironment, Long Short-Term Memory (LSTM), Self-Organizing Maps (SOM), Compartmental Modeling

Effective Finite Element Modelling of Composite Scarf Repairs

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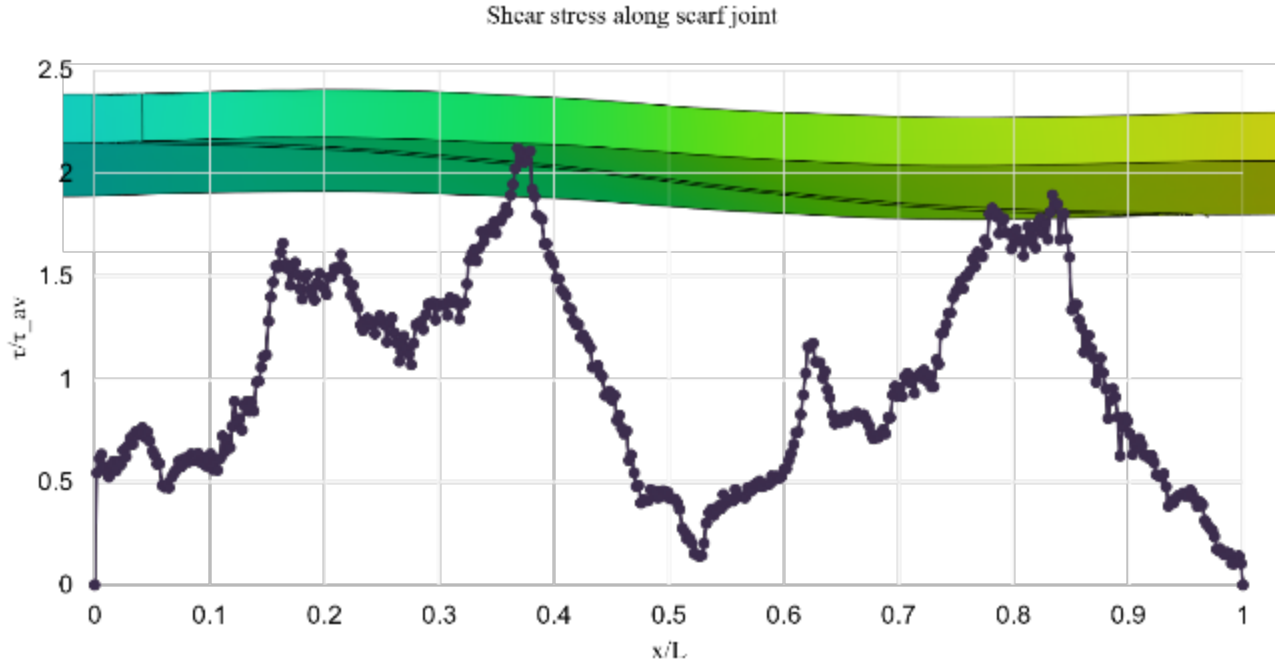
As the application of composite materials in modern commercial aircraft continues to expand, the demand for efficient and reliable composite repair methods has grown substantially. Major maintenance, repair, and overhaul (MRO) facilities face critical challenges, including ensuring damage tolerance, enhancing repair efficiency, maintaining structural integrity, and minimizing operational costs. This study presents a robust finite element analysis (FEA) approach for evaluating the structural performance of scarf repairs on carbon fibre composite panels. Through a series of benchmark simulations, it is demonstrated that modelling the composite components using continuum shell elements, in combination with solid elements for the adhesive layer, provides a highly efficient and accurate strategy. This hybrid element formulation significantly reduces computational time while maintaining high fidelity in stress distribution and damage prediction across the repair region. The proposed modelling strategy is particularly well-suited for integration into digital twinning frameworks, where rapid and reliable FEA schemes are critical. Its application enables streamlined parametric studies, supports automated process composer workflows, and facilitates near real-time model updating, which are key capabilities for predictive maintenance and adaptive decision-making in aerospace and high-performance structural applications.



Keywords: adhesive, continuum shell, composite repair, digital twin, FEA, scarf.

Application of real-time inundation prediction model with dimensional compression to multiple locations

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In recent years, flood damage caused by extreme weather events has become frequent. In order to counteract such damage, the real-time prediction of flooded areas has attracted attention as one of the effective disaster prevention measures. However, as the conventional numerical analysis methods have high computational costs, it is difficult to perform real-time forecasting. In order to solve this problem, the researches using deep learning are being conducted into flood area prediction. The present author developed a real-time predictions method by applying deep learning and dimensionality reduction techniques [1], but there were issues with its versatility because it assumed that there was only one flood point.

This paper presents a real-time flood prediction model that can account for overflow from multiple points by incorporating dimensionality reduction techniques into deep neural networks. Three dimensionality reduction methods are employed: singular value decomposition [2], nonnegative matrix factorization [3], and auto encoder [4]. To verify the computational efficiency and prediction accuracy of the proposed model, we evaluated it using flood simulation data of the Arakawa River in Tokyo. We compared the three dimensionality reduction methods in terms of prediction accuracy and computational efficiency. We also quantitatively examined the dependency on mesh resolution. It can be concluded that the proposed method can significantly reduce calculation time with sufficient accuracy compared to conventional flood simulation methods.

Keywords: Deep Learning, Flood Prediction, Dimensionality Reduction, Singular value decomposition, Nonnegative Matrix Factorization, Autoencoder

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Numerical Simulation of SH Guided Wave Propagation and Scattering in a Plate Using the Method of Fundamental Solutions

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The method of fundamental solutions (MFS) is a mesh-free technique for numerically solving partial differential equations. MFS has been widely used to solve wave scattering problems in acoustics and elastodynamics [1]. However, its application to the analysis of guided waves, which are propagation modes in waveguides such as plates and cylinders, has not been fully explored. Therefore, in this study, we extend the MFS to analyze SH guided waves propagating in a plate.

In the proposed MFS, the displacement component in the anti-plane direction on the analysis plane is approximated by the following equation:

$$\tilde{u}_3(\mathbf{x},\omega) = \sum_{k=1}^{N_y} \tilde{U}\left(\mathbf{x},\mathbf{y}^k,\omega\right)\tilde{c}^k; \mathbf{x} \in V \cup \partial V, \mathbf{y}^k \in V_c, \tag{1}$$

where $\tilde{c}^k$ is the approximation coefficient and ω is the angular frequency. V denotes a finite region in an infinite plate, ∂V is its boundary, and V_c is the complementary domain of V. Since SH wave propagation is considered, V is a two-dimensional region. $\tilde{U}(\mathbf{x},\mathbf{y},\omega)$ reprensents the fundamental solution of displacement for the SH wave equation as follows:

$$\tilde{U}(\mathbf{x},\mathbf{y},\omega) = \frac{\mathrm{i}}{4\mu} H_0^{(1)}(k_T r), \tag{2}$$

where $\mathbf{x}$ is the observation point and $\mathbf{y}$ is the source point. μ is the shear modulus, k_T is the wavenumber of SH wave, $H_n^{(1)}(\cdot)$ is the Hankel function of the first kind of order n. Moreover, $r = |\mathbf{x}-\mathbf{y}|$ and $i = \sqrt{-1}$. We assume that a defect exists only within V and the remaining part of the plate is undamaged. In the undamaged region, the displacement component is expressed as a linear combination of modal functions of SH guided waves in a plate. The approximation coefficients for both the fundamental solutions and modal functions are determined by the boundary conditions on ∂V.

Numerical examples demonstrate that the proposed method effectively simulates SH guided wave scattering. We consider several cases with different ranges of the region V, and compare the displacement components within the finite region computed by the proposed method. Based on this comparison, we assess the validity of the proposed formulation. Additionally, we evaluate the scattering characteristics by computing the amplitude ratios of the incident and scattered guided waves.

Keywords: the method of fundamental solutions, wave scattering, guided wave, SH wave

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Data assimilation using phase-field simulation to estimate polycrystalline equiaxed dendritic structures

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Dendrites are a typical growth morphology that form during alloy solidification, and their growth patterns directly influence the properties of the resulting products. Since dendritic growth occurs under high-temperature and opaque conditions, simulation studies using the phase-field method have been widely conducted. However, a major challenge lies in the lack of necessary material properties required as input for such simulations. To address this issue, we are developing a data assimilation system that incorporates time-resolved in situ X-ray observations (4D-CT) obtained at large synchrotron radiation facilities into phase-field simulations [1]. This approach aims not only to estimate physical properties but also to overcome the limitations of temporal and spatial resolution inherent in 4D-CT. While, in this study, we focus on columnar dendrites in single crystals, additional challenges arise in polycrystalline equiaxed microstructure. Alloys such as magnesium and zinc nucleate easily and therefore tend to form equiaxed polycrystals. In such cases, when the number of grains exceeds approximately ten, accurately estimating the crystal orientations becomes challenging. Therefore, this study aims to construct a data assimilation system for polycrystalline equiaxed microstructures and simultaneously estimate a large number of crystal orientations. As the data assimilation method, we employ the ensemble transform Kalman filter, a type of ensemble Kalman filter. Furthermore, to accelerate data assimilation using large-scale three-dimensional phase-field simulations, localization is introduced to reduce the ensemble size, and parallel computations are performed on a GPU supercomputer.

Keywords: data assimilation, polycrystalline equiaxed dendrites, phase-field simulation

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Learning a generalized multiscale prolongation operator

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Multigrid preconditioners are one of the most powerful techniques for solving large sparse linear systems. In this talk, we present Darcy flow problems with random permeability using iterative solvers, enhanced by a two-grid preconditioner based on a generalized multiscale prolongation operator, which has been demonstrated to be stable for high contrast profiles. To circumvent the need for repeatedly solving spectral problems with varying coefficients, we harness deep learning techniques to expedite the construction of the generalized multiscale prolongation operator. Considering linear transformations on multiscale basis have no impact on the performance of the preconditioner, we devise a loss function by the coefficient-based distance between subspaces instead of the plain L2-norm of the difference of the corresponding multiscale bases. We discover that leveraging the inherent symmetry in the local spectral problem can effectively accelerate the neural network training process. In scenarios where training data are limited, we utilize the Karhunen--Loeve expansion to augment the dataset. Extensive numerical experiments with various types of random coefficient models are exhibited, showing that the proposed method can significantly reduce the time required to generate the prolongation operator while maintaining the original efficiency of the two-grid preconditioner. Notably, the neural network demonstrates strong generalization capabilities, as evidenced by its satisfactory performance on unseen random permeability fields. The research is partially supported by the Hong Kong RGC General Research Fund (Projects: 14305423 and 14305222).

Keywords: Darcy flow, multiscale finite element method, prolongation operator, machine learning, two-grid preconditioner

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Y Liu, S Fu, Y Zhou, C Ye, ET Chung - arXiv preprint arXiv:2410.06832, 2024

Contact Wear Analysis Based on Variable Friction Coefficient Models

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Contact and wear phenomena are prevalent in mechanical systems, and their precise modeling is critical for preventing wear-induced failures. This study presents a comprehensive numerical simulation framework for contact and wear analysis that simultaneously addresses geometric, material, and boundary nonlinearities. The framework integrates the penalty function contact algorithm with Archard's wear theory, incorporating Coulomb friction models with three distinct pressure-dependent friction coefficients: constant, linear, and exponential variations. To address convergence challenges posed by variable friction coefficient models, we develop an adaptive penalty factor algorithm and validate its effectiveness through contact wear simulations involving both linear elastic and Mooney-Rivlin hyperelastic materials.

Numerical experiments reveal two key findings: (1) Under large-slip conditions, the adaptive penalty factor algorithm achieves a 15% improvement in computational convergence while reducing normal penetration and adhesive slip by 25% compared to conventional methods; (2) Friction model selection demonstrates material-dependent effects. For linear elastic materials under small-slip wear, different friction models primarily affect wear volume and stress distribution (with variations up to 18%), but show limited influence (<5% difference) on wear location and contact pressure. Conversely, in hyperelastic materials under large-slip conditions, friction model selection significantly alters all measured parameters: wear volume variations exceed 30%, wear location shifts become apparent, and contact pressure differences amplify progressively (up to 22% divergence) with increasing cyclic loading.

Keywords: contact wear, pressure-dependent variable friction coefficients, adaptive penalty factor algorithm, hyperelastic material

Augmenting On-Site Intuition: A Fully Coupled FEM with Contact and Fuzzy Intelligence for Real-Time Ground Assessment

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This research presents an innovative numerical modelling framework based on a fully coupled Finite Element Method with contact mechanics, designed to simulate the mechanical behaviour of unsaturated soils during field deflection testing. Unlike conventional models, this approach captures the complex interactions among water, air, and soil particles, offering a more realistic representation of soil response under loading.

$$\mathbf{M_u}\ddot{\mathbf{U}} + \mathbf{C}\dot{\mathbf{U}} + \mathbf{K}\mathbf{U} + \bigcup_{i=1}^{n_s}\mathbf{K}_{NC_i} - \mathbf{Q_w}\mathbf{P_w} - \mathbf{Q_c^*}\mathbf{P_c} = \mathbf{F_u} + \bigcup_{i=1}^{n_s}\mathbf{F}_{NC_i} \quad (1)$$

$$\mathbf{M_w}\ddot{\mathbf{U}} + \mathbf{Q_w^T}\dot{\mathbf{U}} + \mathbf{C_{ww}}\dot{\mathbf{P}}_\mathbf{w} + \mathbf{C_{wc}}\dot{\mathbf{P}}_\mathbf{c} + \mathbf{H_{ww}}\mathbf{P_w} + \mathbf{H_{wc}}\mathbf{P_c} = \mathbf{F_w} \quad (2)$$

$$\mathbf{M_c}\ddot{\mathbf{U}} + \mathbf{R_c^T}\dot{\mathbf{U}} + \mathbf{C_{cw}}\dot{\mathbf{P}}_\mathbf{w} + \mathbf{C_{cc}}\dot{\mathbf{P}}_\mathbf{c} + \mathbf{H_{wc}^T}\mathbf{P_w} + \mathbf{H_{cc}}\mathbf{P_c} = \mathbf{F_c} \quad (3)$$

Ground condition assessment in unsaturated soils is often hindered by missing or incomplete data, such as gravimetric water content and soil suction, both of which are critical for reliable interpretation. Existing practices typically rely on expert judgment, which can be variable under pressure, or data-driven computational models that require complete, high-quality inputs rarely available in field settings.

To overcome these limitations, this study employs an augmented intelligence framework that integrates numerical modelling with human expertise and data-driven reasoning. The system applies fuzzy logic to interpret uncertain human estimates of water content and incorporates a self-adaptive learning mechanism that estimates missing suction values based on calibration-derived insights. This hybrid approach combines the strengths of engineering intuition and computational analysis to deliver consistent and robust ground assessments even in the presence of data uncertainty. Field validation using recent trial data confirms that the framework improves accuracy in assessing unsaturated soils.

Keywords: Unsaturated Soils, Augmented Intelligence, Contact Mechanics, Fully Coupled Simulations.

Well-entangled polymer melts flow simulations using multiscale simulation method and machine-learned constitutive relation

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The processing polymer melt flows in a typical entangled state. Numerical simulations play to unveil the dynamics over multiple length- and time- scales. From the viewpoint of rheology, the hysteresis of the mechanical properties originating from the slow degrees of freedom is analyzed by so-called multi-scale simulation (MSS). The simulation with the molecular-based microscopic dynamics, even coarse-grained, using a coarse-grained model, requests extraordinary computational resources. We proposed the machine-learning (ML) based simulation scheme to contract to a constitutive relation based on the statistical evaluations of polymer conformations. Fig.1 summarizes the procedure of the proposed scheme for a polymer system as three steps: 1. Generate the training data, 2. Learn the constitutive relation, 3. Simulate the polymeric flows. The constitutive relation is assumed to be an explicit function of the time derivative of stress determined by the stress and velocity gradient approximately. This approach has previously described the linear and nonlinear rheology for the constitutive relation of the polymer models for single (shear) deformation mode and performed the flow predictions for a much shorter computation time than the conventional MSS.

In this study, we extend the methodology to the general two-dimensional flows of an entangled polymer model in considering the multi-deformation modes, then assess the accuracy and the computational efficiency. We extended our proposed machine learning-based simulation scheme to predict 2D flows of well-entangled polymer melts. The simulation scheme, which assumes that the stress and the velocity gradient determine the time derivative of the (total) stress, was previously applied to the single (shear) deformation mode flows. Under material objectivity, the extended approach is adapted to the multi-deformation modes (shears and elongations) by replacing the velocity gradient with the strain rate, then the scheme is assessed by the pressure-gap-driven flow in the contraction expansion channel.

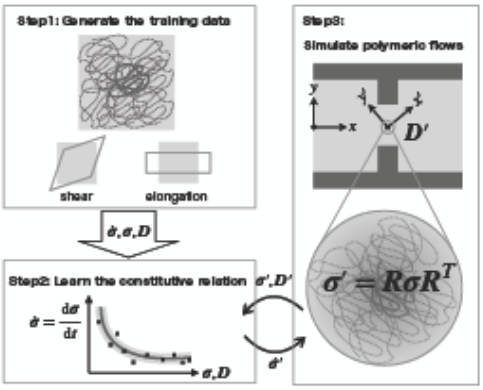

Figure 1. Schematic illustration of our proposed simulation framework for polymeric fluid with a ML constitutive relation.

Keywords: Multiscale simulation method, well-entangled polymer melt, machine learning, constitutive relation.

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Numerical simulation of droplet breakup in extensional flow using a particle method

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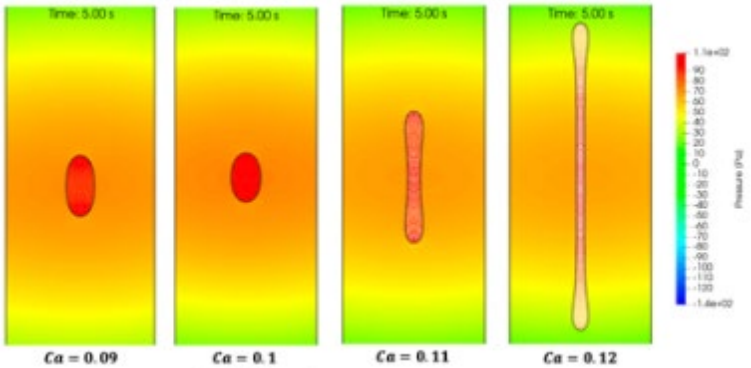
Although droplet breakup under simple shear flow has been investigated by numerous studies, the understanding of droplet breakup in extensional flow remains relatively limited. This study aims to accurately simulate droplet behavior under uniaxial extensional flow of the surrounding fluid and numerically analyze the droplet dynamics, including breakup, by using a particle method specially designed for these purposes.

In this study, we employ the moving surface mesh particle method with extensions for two-phase flow [1][2]. The spatial discretization is based on the least squares moving semi-implicit scheme[3]. Boundaries are explicitly represented by surface meshes, on which physical variables are computed based on the boundary conditions. This approach allows for the accurate simulation of droplet interface behavior and surface tension, which are significant factors in this problem.

We analyze the droplet breakup under uniaxial extensional flow of an incompressible Newtonian fluid in an axisymmetric coordinate system. In the computational domain, a droplet and the surrounding fluid are set, and the droplet surface and the outer boundary are represented by a surface mesh. This outer boundary is an inflow/outflow boundary where a constant velocity is imposed. The dimensionless parameters in this problem are the capillary number and the Reynolds number of the dispersed phase, the ratios of the viscosity and density between the dispersed and continuous phases. We examine the droplet behaviour for various sets of dimensionless parameters.

The simulation results clearly showed the instability of droplet as illustrated in Figure 1. Furthermore, the droplet deformation and the critical capillary number for breakup were in good agreement with reference values found in the literature.



Simulation results($Re = 1, \tilde{\mu} = 1, \tilde{\rho} = 1$)

Figure 1.

Keywords: Computational fluid dynamics, Newtonian fluid, Axisymmetric coordinate system, LSMPS method, Surface tension, Critical capillary number

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Phase Transitions of Poly (vinylidene fluoride) under Coupled Electric-Strain Field

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Poly(vinylidene fluoride) is a pivotal piezoelectric polymeric building block for advanced electronics, whose piezoelectric properties are determined by the proportion of the polar β phase. Molecular Dynamics simulations are computational methods used to study the physical movements of atoms and molecules. The cornerstone of Molecular Dynamics simulations is Newton's second law.

$$\boldsymbol{F} = -\nabla E = m\boldsymbol{a} \tag{1}$$

Based on molecular dynamics simulations, this work assessed the phase transition behaviors of PVDF from α phase to β phase under a coupled electric-strain field [1]. It is found that the presence of strain can significantly reduce the threshold strength of the electric field that triggers robust and stable phase transitions. Similarly, the presence of electric field will reduce the required stress or strain that initiates phase transitions. The findings obtained in this work could provide useful guidelines for manipulating PVDF with required piezoelectric properties.

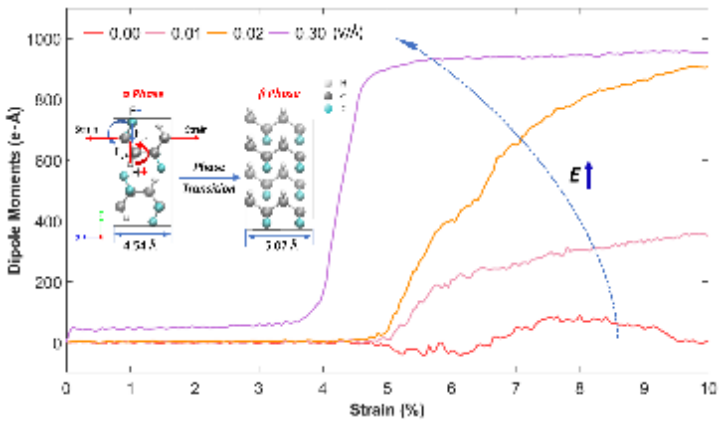

Figure 1.

Keywords: Molecular Dynamics Simulations, Poly(vinylidene fluoride), Phase Transitions, Electric-strain Coupled Field

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Study on Formation Pressure Formation Mechanism and Three-Dimensional Modeling of Manas Anticline

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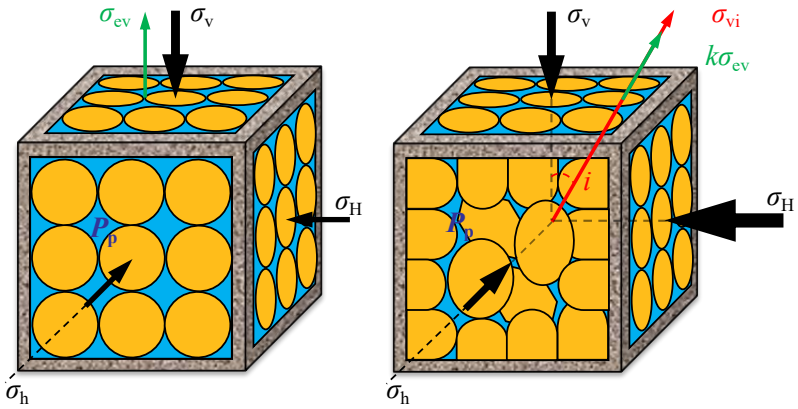
The Manas anticline has formed complex formation pore pressure under multi-stage tectonic movements, and the risk of overflow and leakage during drilling is increased. In order to clarify the causes of abnormal high pressure, the acoustic velocity-density intersection chart was improved, and the data change characteristics under multi-factor control were added. The sand-mud micro-element model is used to clarify the changes in the mechanical properties of the formation caused by tectonic compression. Based on the one-dimensional compaction theory, the influence of horizontal tectonic stress on vertical effective stress is considered, and a three-dimensional multi-factor control is formed. The calculation model of formation pore pressure is verified by the measured pressure point and drilling mud density. The results show that : (1) The abnormal high pressure is controlled by the combination of tectonic compression, fluid expansion and undercompaction. (2) Affected by the slip fault, the stress distribution of the formation and the mechanical properties of the rock deflect to the horizontal direction. The pore fluid absorbs the tectonic stress to a certain extent and reduces the bearing of the skeleton stress. (3) Compared with the one-dimensional effective stress model, the three-dimensional modified model takes the relationship between tectonic compression and fluid pressure into account, and realizes the prediction of abnormal high pressure under multi-cause combination.

$$P_p = \sigma_{vi} - k\sigma_{ev} = \sqrt{\sigma_v^2 + \sigma_H^2 + \sigma_h^2} - \frac{\sqrt{V_{pv}^2+V_{px}^2+V_{py}^2}}{V_{pv}}\sigma_{ev} \quad (1)$$

$$V_{ph(\mathrm{n})} = \left(\frac{Den_n}{Den_{s1}}\beta_1 + \left(\frac{GR_n}{GR_{s1}}\right)\beta_2\right)V_{ph(s1)}\frac{H_{s2}-H_n}{H_{s2}-H_{s1}} + \left(\frac{Den_n}{Den_{s2}}\beta_1 + \left(\frac{GR_n}{GR_{s2}}\right)\beta_2\right)V_{ph(s2)}\frac{H_n-H_{s1}}{H_{s2}-H_{s1}} \quad (2)$$

In the formula: P_p is formation pore pressure, σ_{vi} is principal stress in i direction, k is pressure coefficient of structure, σ_{ev} is vertical effective stress, $V_{ph(n)}$ is the horizontal wave velocity of mudstone section.



(a) Principle of normal compaction effective stress (b) Principle of effective stress of tectonic extrusion

Figure 1. Structural compression formation pressure correction model

Keywords: wellbore stability, formation pressure, tectonic compression, rock mechanics, three-dimensional model

Utilizing Bayesian Inference to Quantify Model-Inherent Uncertainty in Soil Constitutive Models

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ABSTRACT: Accurately quantifying uncertainty in soil constitutive models is a complex yet crucial task for enhancing predictive accuracy. While Bayesian inference (BI) has been recognized as an effective approach for managing uncertainty, prior research has largely concentrated on uncertainties within input parameters of idealized constitutive models. However, traditional models such as Mohr-Coulomb, Cam-Clay, and Modified Cam-Clay are built on simplified assumptions that fail to fully replicate the complexities of real soil behaviour, making it impossible for them to perfectly match experimental data. This research proposes an innovative framework that utilizes BI to convert deterministic models into probabilistic models, enabling the quantification of uncertainty inherent to the models themselves. A modified variational Bayes method is employed, introducing a penalty term into the negative log-likelihood to develop a new loss function, which improves bias estimation and enhances model reliability. The framework evaluates three different assumptions for the model bias term using triaxial test data from Karlsruhe sand. The findings highlight those non-constant assumptions for the bias term led to significant improvements in model performance. Among the models analysed, the probabilistic Modified Cam-Clay model with a nonlinear bias assumption provides the best results. In contrast, the probabilistic Mohr-Coulomb model shows certain shortcomings, such as overestimating peak deviatoric stress and overfitting volumetric strain, which indicates the necessity for further model adjustments.

Keywords: Uncertainty quantification, Bayesian inference, probabilistic models, model bias, constitutive models

A Multi-scale CFD-DEM approach for particulate flows

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Particulate flows can be found in a wide range of industrial application scenarios and are often modelled with coupled Computational Fluid Dynamics - Discrete Element Method (CFD–DEM) approaches. However, accurately simulating multi-scale particle systems remains a challenge for existing numerical methods. In current simulations, different CFD-DEM methods were used in the particulate flow simulations according to the ratio of the grid size to the particle diameter [1], i.e. (Δ/d). The resolved method [2] is employed for simulating particle flows with small size-ratio (Δ/d<0.1), the semi-resolved method [3] is utilized for particle flows with medium size-ratio (0.1<Δ/d<3), and the unresolved method is applied to simulate particle flows with large ratio (3<Δ/d). In this study, a multi-scale CFD-DEM approach is developed, which integrates the three different CFD-DEM methods in one modelling framework. According to the size ratio, the appropriate method can automatically be selected for different scenarios. Specifically, the resolved method based on the immersed boundary method is used for cases the small size-ratio, the semi-resolved method for cases with medium size-ratio, and the unresolved method for cases with large size-ratio, respectively.

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u}) = 0 \tag{1}$$

$$\frac{\partial \rho \varepsilon \mathbf{u}}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u}\mathbf{u}) = -\varepsilon \nabla p + \varepsilon \nabla \cdot \boldsymbol{\tau} + \mathbf{F}_{s \cup m} + \mathbf{F}_l \tag{2}$$

$$\mathbf{u} = \mathbf{u}_l + (1-h)\mathbf{u} \tag{3}$$

$$\varepsilon \mathbf{u} = \varepsilon \mathbf{u} - \nabla \varphi \tag{4}$$

$$\nabla^2 \varphi = \nabla \cdot (\varepsilon \mathbf{u}) + \frac{\partial \varepsilon}{\partial t} \tag{5}$$

$$\nabla \cdot (\frac{\Delta t \varepsilon}{\rho} \nabla \Delta p) = \nabla \cdot [(1-h)\nabla \varphi] \tag{6}$$

In the first stage, the governing equations (Eq. (1) and Eq. (2)) are solved with the body force of large-sized particle $\mathbf{F}_l$ being set to be zero. Stage 2 we incorporate the immersed boundary method to account for the influence of the large particle. Specifically, the fluid velocity within the region of the large particle (h) is explicitly set to be the velocity of large particle $\mathbf{u}_l$ (Eq. (3)). The velocity discontinuity at the boundary of the large particle domain can be removed by using a scalar field φ (Eq. (4) and Eq. (5)). After continuity modification, the pressure field is redistributed by using a pressure increment Δp to guarantee the momentum balance (Eq. (6)). A series of numerical simulations have been carried out, and the numerical results were compared with experimental data. It is demonstrated that the multi-scale CFD-DEM approach can accurately capture the interaction between cross-scale particle systems and fluids.

Keywords: Multi-scale; CFD-DEM; Resolved method; Semi-resolved method; Unresolved method; Particulate flow

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Virtual Specimen Generation of Heterogeneous Materials Incorporating Microstructural and Interfacial Characteristics

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In general, the interfacial properties of multi-material specimens play a critical role in determining their mechanical performance and durability. When combining two or more materials (or specimens), their bonding behaviour at the interface depends on interface morphology. Moreover, the interfacial region, where discontinuities in microstructural characteristics occur, can easily become a failure point. Therefore, it is essential to understand not only the distinct characteristics of each material but also those of their interface.

This study aims to generate virtual specimens composed of two different cement-based materials by incorporating their microstructures and interfacial characteristics. The two materials were produced using different methods: conventional casting and 3D printing. Due to the differences in manufacturing methods, their microstructures, particularly the pore distributions, vary significantly. Therefore, these pore distribution characteristics were identified using both probabilistic and deterministic approaches.

The virtual specimens were reconstructed based on actual pore datasets for each material. For each randomly selected location within the region of interest, the material type was identified using a segmentation mask. Then, a pore was randomly selected from the dataset corresponding to that material, reflecting its specific pore characteristics, and placed at the designated position. In this manner, the spatial distribution of pores realistically represents the microstructural features of each material.

To investigate the effect of interfacial morphology on bonding behaviour, interface shapes were introduced as a design parameter. Specifically, layered interfaces with varying depths and curvatures were applied for the 3D printed samples. By generating virtual specimens considering the interfacial features, preliminary evaluations can be conducted in advance, thereby accelerating the design of multi-material systems with improved bonding performance.

Keywords: Virtual specimen, heterogeneous, reconstruction, pore characteristics, interfacial characteristics

Acknowledgement

This work supported by KOREA & NUCLEAR POWER CO., LTD (No. 24-Tech-05)

A direct link between ultrasonic NDT and FE modelling toward SHM and a digital twin of the scarf repair.

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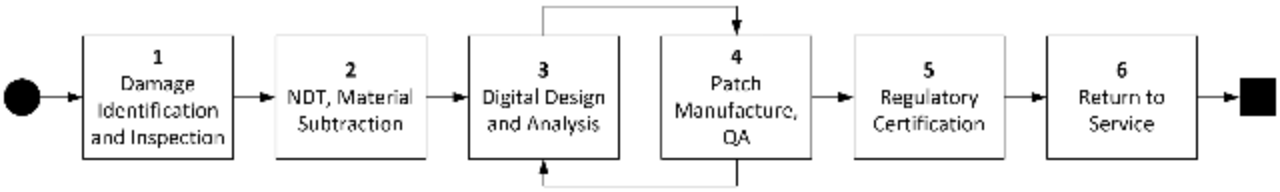
Recent decades have seen the rise of composite materials like carbon fibre reinforced polymers as dominant materials in primary aircraft structures, as well as increased requirements for safety and cost effectiveness in commercial aviation. These necessitate standardised, easy to carry out inspection practices for repair and maintenance. Current paradigms are slow, paper-based, lack optimisation techniques like finite element modelling and require highly trained technicians to carry out. Digital twins and digital threads present an opportunity to streamline these repairs, making them faster and more accessible to lesser skilled personnel as well as enabling numerical optimisation for improved repairs. Crucial to implementing these methods is a smooth link between non-destructive testing (NDT) and finite element modelling (FEM) for repair optimisation, and this is currently an underdeveloped link in industry. In this study, we present a data flow and storage architecture leveraging the digital thread philosophy linking the physical NDT space to digital FEM. Real ultrasonic A- and C-scan data is fed through a Dassault Systèmes 3DExperience-enabled workflow to construct a 3D representation of a damaged laminate and modify the pristine model to a damaged state. The proposed methodology paves the way for more effective structural health monitoring and realising a fully connected, optimised digital twin and thread of the composite scarf repair process.



Keywords: Composite materials, non-destructive testing, ultrasonic, digital twin, digital thread, structural health monitoring

Quasistatic Thermomechanical Simulation with Peridynamics

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Structures exposed to extreme environments are often subjected to continuous thermal loading. However, the thermomechanical behaviors of construction materials under such conditions have not been extensively investigated. Peridynamics, a nonlocal continuum theory, offers a promising framework for analyzing materials with discontinuities and undergoing large deformations. In this study, we propose a peridynamic methodology to simulate the quasistatic deformation of construction materials under thermal loads. The governing equations are formulated by coupling the thermal diffusion equation with the equilibrium equations of the solid as

$$\rho c_v \dot{T} = k_T \frac{\partial^2 T}{\partial x_j^2} - \alpha(3\lambda + 2\mu) T_0 \dot{\varepsilon}_{kk} + S_T \,, \tag{1}$$

$$\rho \ddot{u}_i = \frac{\partial \sigma_{ij}}{\partial x_j} + b_i = \frac{\partial}{\partial x_j}\left(2\mu\varepsilon_{ij} + \left(\lambda\varepsilon_{kk} - \alpha(3\lambda + 2\mu)(T - T_0)\right)\delta_{ij}\right) + b_i \,, \tag{2}$$

where ρ, λ, and μ are the density and Lamé constants, and k_T, c_v, and α represent the thermal conductivity, specific heat, and coefficient of thermal expansion of the material, respectively. T_0 is the reference temperature and S_T and b_i are volumetric heat source and body force [1]. Temperature and displacement fields, denoted by T and u, are calculated iteratively by a staggered approach. Heat transfer is solved using peridynamic differential operators, while mechanical responses are solved with a non-ordinary state-based peridynamic formulation. As a result, the displacement fields obtained through peridynamics are in good agreement with those from the finite element method (FEM). Additionally, peridynamics effectively captures thermomechanical responses in materials including cracks.

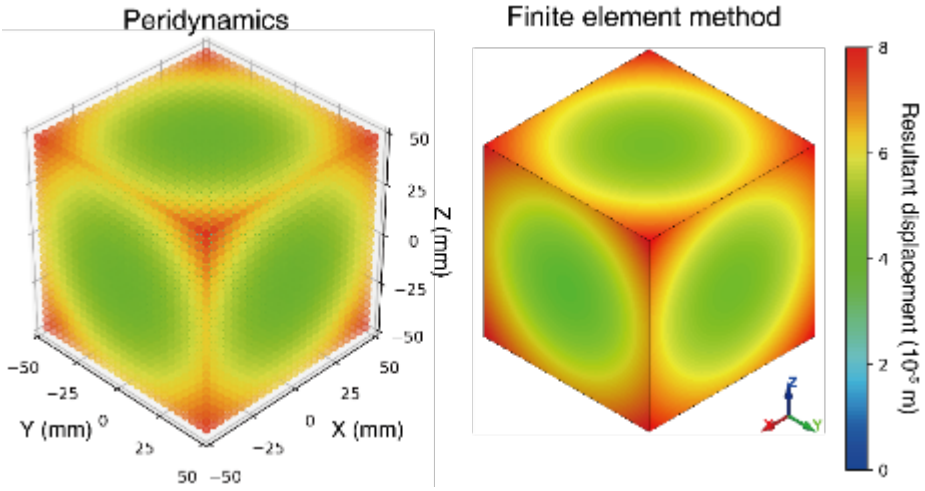

Figure 1.

Keywords: Peridynamics, thermomechanics, non-ordinary state-based peridynamics, peridynamic differential operators

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Composite Airframe Structural Repair Patch Topology Optimisation

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Composite materials have revolutionised aerostructures, introducing benefits including high specific mechanical properties and design flexibility. However, damage modes pose concerns from an aircraft maintenance, repair, and overhaul perspective. In this discussion, repair patch topology optimisation plays a crucial role. Conventional circular conical frustum scarfs require extensive machining operations, influencing parent residual structural integrity far greater than the original damage footprint. Extensive parametric studies examining the effect of various shapes with respect to the resultant repair footprint and stress concentration/intensity factors have been conducted. From these research efforts, optimisation revolves around complex, conflicting, multi-objective design criteria such as the damage aspect ratio, cut-out geometry, and patch alignment relative to the applied stress field. Thus, there is a need to ascertain custom topologies for select damage characteristics, thereby minimising design conservativeness whilst ensuring adequate safety margins.

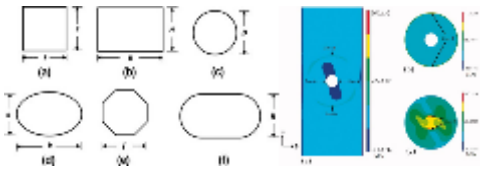

Figure 1. [1, 2]

This work will present the state-of-the-art centred around the impact of specific patch geometrical configurations on the resulting stress distributions and thus structural performance under various loading conditions. Favourable topological design elements can then be realised and taken forward as input to enable a broader-scale digital twin-driven patch repair optimisation framework.

Keywords: Composite Patch Repair, Design Space Exploration, Digital Twin, Parametric Design, Shape/Topology Optimisation

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Numerical Simulation of Air Knife Flow Field for Coating Thickness Control in Hot-Dip Galvanization

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Hot-dip galvanizing is a widely used method for corrosion protection in the steel industry. Precise control of the thickness of the galvanized layer is critical for product performance and cost efficiency. In the study, a numerical model of the air knife system was developed to investigate the air flow characteristics and its effect on coating formation. The air knife, located above the zinc bath, directs high-speed jets toward the steel strip to remove excess molten zinc, and its performance directly affects coating uniformity and thickness.

The model was constructed using ANSYS Fluent based on the Navier–Stokes equations for compressible turbulent flow. A three-dimensional symmetric geometry was employed to capture essential flow features. The standard $k-\varepsilon$ turbulence model was adopted, and boundary conditions were set to reflect typical industrial parameters. The governing equations can be summarized as:

$$\rho\left(\frac{\partial u}{\partial t}+u\cdot\nabla u\right)=-\nabla p+\nabla\cdot(\mu\nabla u)+\mathrm{F}, \tag{1}$$

Where ρ is the fluid density, u is the velocity vector, p is the pressure, μ is the dynamic viscosity, and F represents body forces. Initial simulation results show that the velocity field is highly sensitive to the nozzle gap and inlet pressure. The high-velocity jet strikes the substrate and forms a symmetric stagnation zone, beyond which the flow diverges to form a lateral recirculation zone. These characteristics are closely related to variations in coating thickness in practical operation. A representative velocity is shown in Figure 1.

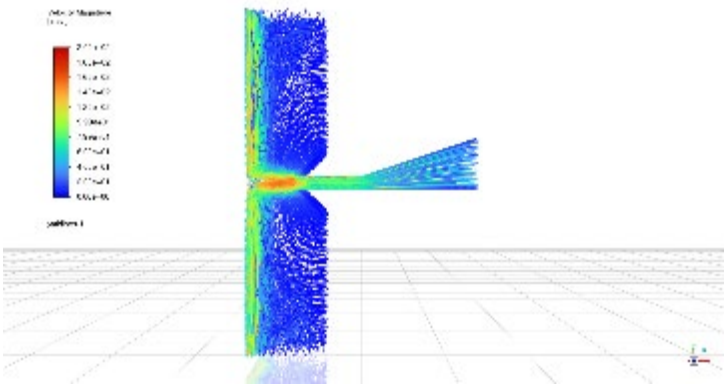

Figure 1.

Further parametric studies are planned to evaluate the effect of spray angle, strip speed and spacing on plating results. This study aims to provide a simulation-based framework for optimizing the coating control strategy of a continuous galvanizing line.

Keywords: hot-dip galvanization, Navier-Stokes equations, air knife, CFD, coating control, compressible flow, numerical simulation

Statistical Shape Modelling of Coronary Arteries for Population-Specific Synthetic Dataset Generation

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Coronary artery disease is a leading cause of mortality and morbidity among all demographics, yet risk and coronary geometry vary between populations. Simulations of the coronaries must either use idealized models, which cannot capture the nuance of geometric dependencies, or patient-specific datasets, which are typically limited by patient counts, but both limitations pose challenges for population-based analysis. The aim of this study is to design a methodology capable of generating and simulating realistic synthetic models considering the characteristics of distinct populations.

We used statistical shape modelling to group common variation patterns into principal components, which describe the relationship of variance of a dataset. Each principal component (i) of the left coronary arteries were measured to record the standard deviation (σ) of selected dimensions (D). Each principal component also has an explained variance ratio (EV), which describes its proportionality. Combining the deviations for each dimension from each principal component, as with Equation 1, enables generating new dimensions within the scope of the statistical shape model based on weighting factors (W). The weighting factors can be curated to produce realistic extreme dimensions for a population with preserved geometric dependencies.

$$D_{new} = \bar{D} + \sum_{i=1}^{n} \sigma_{D,i} \times EV_i \times W_i \quad (1)$$

This methodology was utilized to compare male and female models from a dataset of 110 left coronary arteries models (39 male, 71 female) consisting of the left main, left anterior descending, and left circumflex branches up to 30mm downstream of the bifurcation. Our principal component results showed distinct shape modes for male and female cases, particularly for bifurcation angle. Figure 1 shows the steps by which representative models of statistically large and small bifurcation angles were generated and simulated respectively for male (M) and female (F) populations.

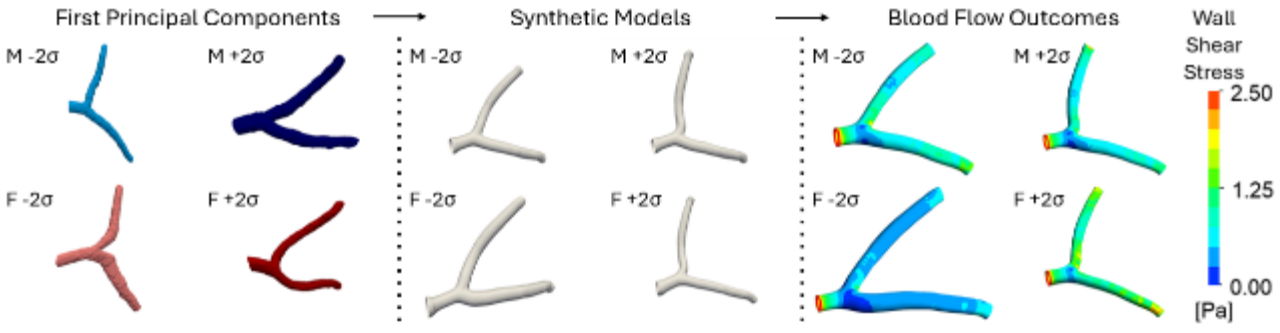

Figure 1.

When evaluating low wall shear stress, an indicator of coronary artery disease risk, the blood flow outcomes showed that the higher bifurcation angle variance of female patients informed greater variance in wall shear stress. This suggests that the haemodynamic significance of bifurcation angle depends on other sex-dependent features. Analysis of more geometric features may provide insight into population-dependent disease risk. Furthermore, this methodology enables the creation of more population-specific synthetic models for haemodynamic evaluations of geometric features.

Keywords: statistical shape model, coronary artery disease, haemodynamics, synthetic data

Shape Analysis on Coating Layer Edge Profiles

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This study investigates the non-uniform profiles near the edges of battery electrode coating layers over planar substrate using shape analysis by curve similarity. The recent growth of the lithium-ion battery market has increased the demand for high-quality electrodes. Electrodes are typically produced by applying a liquid slurry onto metal foil using slot coating. One key factor affecting electrode quality is its uniformity. During the process, surface tension induces flow within the liquid layer towards its contact line, often resulting non-uniform profiles in its edges. In practice, the edge profile exhibits a wide variety of shapes due to several factors, such as liquid properties and process parameters. Therefore, recent studies have focused on optimizing shape features obtained from experiments.

One of the limitations of the previous approaches is that shape features cannot describe the full shape of the profile. Alternative approach is constructing a data-driven model for the full profile. However, intrinsic nonlinearity and mis-matching domains across the profile data makes this a challenging task for classical statistics which treats response variables as vectors. In this study, the edge profiles are modelled by the Fréchet regression [1] where response variables are allowed to be in general metric space. The distance between two normalized profiles f and g is measured by Fréchet distance:

$$d_F(f,g) = \inf_{\alpha,\beta} \sup_{\mathrm{t}} \left\| f\left(\alpha(t)\right) - g\left(\beta(t)\right) \right\|, \tag{1}$$

where $\alpha(t)$ and $\beta(t)$ are reparameterizations of each curve. A distance matrix between profiles in the metric space Ω is constructed, and then mapped to a vector space by manifold learning. Then, a continuous transition of one profile to another is modelled using the Fréchet regression [1]:

$$m_{\oplus}(x) = \underset{\omega \in \Omega}{\operatorname{argmin}}\, \mathbb{E}(d_W^2(Y,\omega) \mid X = x), \tag{2}$$

where $X = x$ is a predictor variable in vector space, Y is population of normalized profiles and d_W is the Wasserstein distance. The model can then be used to predict the full profile given a process variable [2]. Experimental data are analysed, and compared to the results from previous studies.

Keywords: Coating process, Shape analysis, Metric space, Manifold learning

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Deep-Sea Video Stabilisation: An LSTM-Based Predictive Approach with Explainable AI Analysis

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Deep-water imaging is crucial for studying marine biodiversity, and institutions such as CSIRO have a long history of deploying towed imaging platforms at depths of up to 4000 meters [1–3]. These systems enable the collection of environmental data—particularly in deep water where fibre-optic transmission is essential for conducting real-time, large-area surveys under communication constraints. However, the complex interaction between the towing cable and the towed platform, especially in the presence of currents, poses significant challenges to maintaining platform stability, and, by extension, video image quality. Stability is key for acquiring high-quality, distortion-free imagery, ensuring consistent coverage of marine habitats, and safeguarding operational safety. The camera's steadiness is perturbed by factors such as ship motion or towing vessel speed, surface waves, ocean currents, and cable tension. A robust method of predicting the dynamic camera viewpoint angle as a function of these parameters would allow the real-time modulation of one of these parameters, typically the cable length, to obtain stable images.

We focus on the underwater camera platform, Deep Towed Camera (DTC) system, tethered to the ship, CSIRO Research Vessel Investigator (RV) [4], by a cable. In this work, we propose a Long Short-Term Memory (LSTM)–based machine learning approach that predicts the dynamic stability of the underwater camera using inertial measurement unit (IMU) data and other sensor readings from the vessel and winch [5]. Furthermore, we employ explainable AI techniques to visualise which temporal segments and sensor signals most significantly influence camera stability.

The insights gained from our study are expected to facilitate the development of real-time control systems that dynamically adjust cable tension, thereby enhancing underwater video quality for marine biodiversity research.

Keywords: Long Short-Term Memory, Explainable AI, Sensor Fusion, Machine Learning, Deep-Sea Imaging

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Dynamic Fracture Analysis by Polygonal Scaled Boundary Finite Element Method

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With the large-scale development of China's western region, many high concrete gravity dams have been or are being built in this seismically active region. The Scaled Boundary Finite Element Method (SBFEM) can solve the stress and displacement field semi-analytically in the vicinity of a crack tip without any enrichment. Therefore, based on the theory of linear elastic fracture mechanics, it achieves the determination of dynamic fracture parameters by proposing a time-domain method of generalized dynamic stress intensity factors using polygonal scaled boundary elements. Combined with the maximum tangential stress criterion, the crack propagation process was simulated to determine the crack stability in real time. The dynamic stress intensity factor of three-point bending beams under impact loading was calculated. The crack propagation process of three-point bending beams under impact loading was simulated using the local remeshing algorithm for polygons, and the dynamic stress intensity factor and crack length were obtained. The effects of the time step, mesh density and damping coefficient are also investigated. In addition, a dynamic contact simulation algorithm for crack opening and closure behaviour was developed using Koyna gravity dam as a research object, considering dam and reservoir under earthquake, and the fracture paths were obtained by using polygonal local remeshing technique to simulate the crack propagation process. The results show that the mesh density has a small effect on the dynamic stress intensity factor and crack propagation process; the larger the damping is, the smaller the dynamic stress intensity factor is. The crack propagation process of Koyna gravity dam under seismic loading obtained by using the scaled boundary finite element method is close to the boundary elements and experiments. The numerical examples demonstrate the simplicity, effectiveness and high accuracy of the proposed models, and the research findings presented above provide powerful technical means for the dynamic fracture analysis of practical concrete dams .

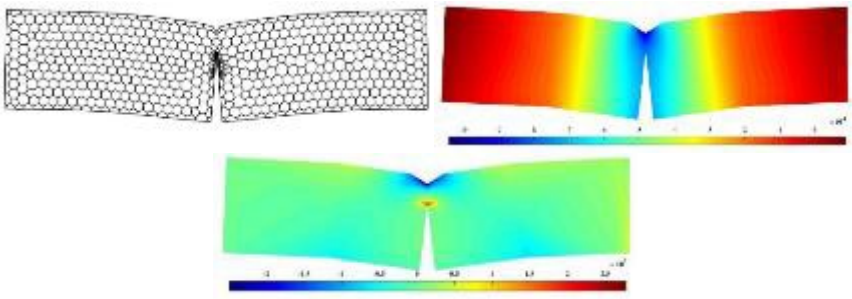

Figure 1.

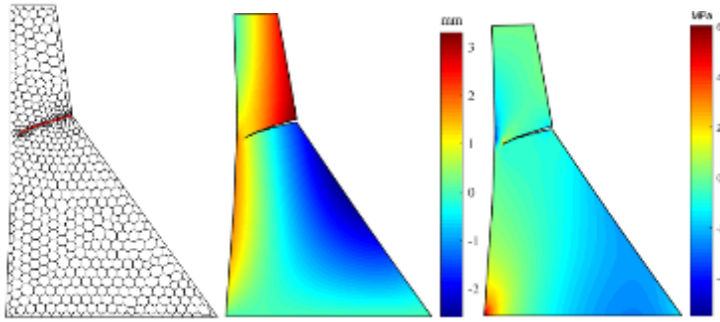

Figure 2.

Keywords: Polygonal scaled boundary finite element method; dynamic stress intensity factor; crack propagation; concrete gravity dams; local remeshing algorithm

Investigation of Curvature and Stretch Effects on NOx formation in Turbulent Ammonia-Methane Blended Flames by DNS

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Ammonia and its blended fuels are attracting attention as carbon-free alternatives to fossil fuels for reducing greenhouse gas emissions. While ammonia is advantageous in terms of production, transportation, and storage, its low reactivity and high NOx emissions pose significant challenges for practical implementation in current combustion systems. Blending ammonia with more reactive fuels, such as methane or hydrogen, can substantially improve flame stability and combustion performance. Unlike hydrogen, methane is already widely adopted in existing infrastructures, enabling smoother fuel switching with minimal infrastructure modification to the system. To support the practical use of ammonia-methane blends, accurate prediction of turbulent flame behaviour is essential. Local flame structures such as curvature and stretch significantly affect turbulent burning velocity and NOx formation, highlighting the importance of detailed analysis using direct numerical simulations.

To achieve a fundamental understanding of the effects of ammonia blending-ratio and turbulence-flame interactions on flame structure in turbulent ammonia-methane blended combustions, direct numerical simulations of turbulent premixed methane-ammonia-air jet flames were conducted. Two premixed methane-ammonia-air mixtures with ammonia mole fractions of 20% and 50% are considered. The equivalence ratio, temperature and pressure of unburnt mixture are set to 1.0, 700K and 0.1MPa, respectively.

The analysis of the computational results highlights the local effects of flame front curvature and tangential strain rate on flame structure. Figure1 shows the distribution of the heat release rate. The flame front mean curvature, k_M, is defined by equation (1). The current results show that, both the heat release rate and NO formation rate exhibit stronger correlations with flame front curvature, particularly increasing in regions where the flame surface is convex toward the burnt side. The enhanced NO formation due to flame front curvature constitutes crucial insights for predicting NOx emissions in turbulent ammonia combustion flames.

$$k_M = \nabla \cdot \left(\frac{\nabla Y_{fuel}}{|\nabla Y_{fuel}|}\right), Y_{fuel} = Y_{CH_4} + Y_{NH_3} \quad (1)$$

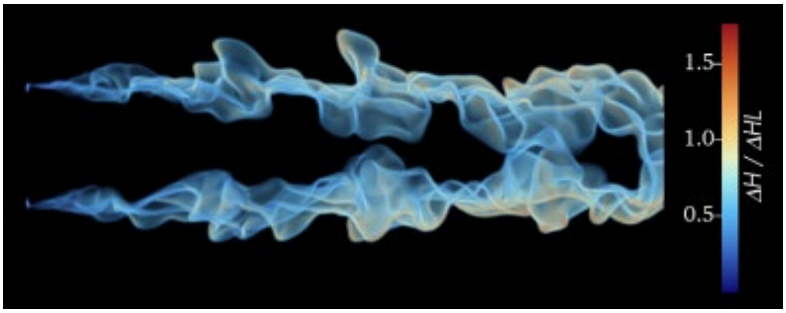

Figure 1.

Keywords: Direct numerical simulation, Ammonia, Methane, Turbulent premixed flame

A neural network-enhanced radial point interpolation method (RPIM-NNS) for modeling brittle fracture

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This paper presents a neural network-enhanced Radial Point Interpolation Method (RPIM-NNS) for the efficient and accurate resolution of crack problems. By integrating radial basis function interpolation with neural network-based optimization algorithms, a novel computational framework is established, grounded in the principle of energy minimization. This approach effectively addresses the limitations of traditional methods in capturing crack-tip singularities and offers greater flexibility in handling complex fracture scenarios. The methodology employs an adaptive, irregular node distribution strategy combined with asymptotic displacement fields to accurately characterize the singular stress field near the crack tip, a key challenge for conventional methods. Additionally, background mesh integration significantly improves computational efficiency, reducing overall computational cost while maintaining high accuracy. The neural network solver plays a crucial role in enabling efficient modeling of complex fracture behaviors, adapting to various loading conditions and crack geometries. Numerical experiments demonstrate that RPIM-NNS exhibits high accuracy, stability, and convergence in both classical linear elastic fracture analysis and crack propagation simulations. This method introduces a novel paradigm that seamlessly integrates physical modeling with advanced computational techniques, providing a powerful tool for crack behavior analysis and prediction.

Numerical Modeling of Coupled Geomechanics and Two-Phase Flow in Unsaturated Porous Media using the Discontinuous Galerkin Finite Element Method

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Geotechnical engineering problems often involve complex interactions, such as multiphase and multi-field coupling in unsaturated porous media. These problems are crucial in understanding the behavior of soils and rocks under various environmental and loading conditions. This paper develops a model for solving the fully coupled two-phase flow and geomechanics in deformable unsaturated porous media problem based on the generalized Biot model, which considers the interaction of skeleton displacement, water pressure, and air pressure.[1,2] The coupled nonlinear system is solved using the discontinuous Galerkin (DG) finite element method, which offers significant advantages in handling complex geometries and heterogeneous media. The DG method has been successfully applied to two-phase flows due to its local mass conservation and flexibility.[3,4] Nitsche's method is used to enforce Dirichlet boundary conditions and weak discontinuity conditions across mesh interfaces.[5] The effectiveness of the algorithms is validated through several benchmark problems in unsaturated porous media, demonstrating their optimal convergence and robustness. Finally, the practical application of the developed model is illustrated through simulations of footing and slope stability problems, which highlight the potential and utility of the proposed approach in realistic geotechnical engineering scenarios.[6,7]

Keywords: Discontinuous Galerkin method; unsaturated porous media; two-phase fluid flow; coupled processes

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Topographical Effects in a Fully Saturated Alluvial Valley

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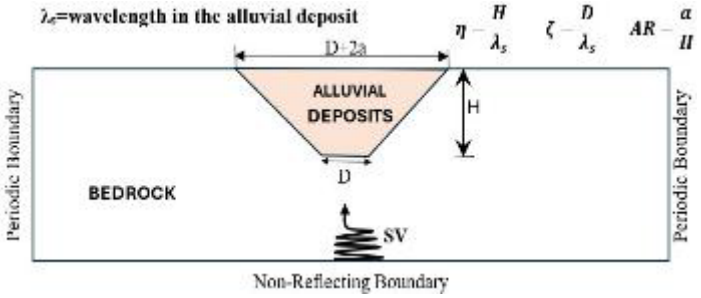
The dynamic response of soft alluvial valleys has been extensively studied in the past due to its practical significance. However, most existing studies model the domain as a single-phase dry medium. Due to the presence of rivers in alluvial valleys the pores in the soil are saturated with water for a significant portion of the year, so it is realistic to consider the domain as a fluid-saturated porous medium. While topographic irregularities can significantly alter wave interference patterns, leading to amplification or de-amplification of seismic waves, the presence of water within the soil medium can also modify wave propagation characteristics. This study investigates the combined effect of topography and saturation on the dynamic response and identifies critical geometric and material parameters that govern the response through a systematic parametric analysis.

All simulations are performed using the open-source software **MASTODON** [1], which is built on the finite element (FE) framework **MOOSE**. Wave propagation through the saturated medium is modelled using the **three-field** u-p-w **formulation,** which can capture high-frequency loading and accounts for relative fluid movement. The governing equations for wave propagation are provided equation (1). To model an infinite domain and ensure a free-flow condition, a **non-reflecting boundary condition** for the saturated medium is implemented in the MOOSE framework and applied at the bottom boundary.



$$\begin{aligned} \sigma_{ij,j} - \rho\ddot{u}_i - \rho_f\dot{w}_i &= 0 \\ P_{,i} + R_i + \rho_f\ddot{u}_i + \frac{\rho_f\dot{w}_i}{n} &= 0 \\ w_{,i} + \alpha\dot{\epsilon}_{ii} + \frac{\dot{P}}{Q} &= 0 \end{aligned} \quad (1)$$

Figure 1. Problem

where **u** is the solid displacement, **σ** is the total Cauchy stress tensor, **w** is the relative velocity of the fluid phase, **P** is the pore fluid pressure, **R** is the viscous drag vector between the solid and fluid phases, **Q** represents the combined compressibility, **α** is the Biot's coefficient, **ϵ** is the strain tensor , and **ρ** and **ρ_f** are the total and fluid densities, respectively.

The dynamic response of both fully saturated and dry alluvial valleys were estimated for a wide range of geometrical and material parameters and compared with each other. The response of a saturated valley was found to be significantly different from that of a dry one. In addition to the dimensionless parameters that govern a dry alluvial valley (η, ζ, AR, Ψ) an additional parameter, non-dimensional permeability (ωK/g), was identified to be controlling the dynamic behaviour of a fully saturated alluvial valley.

Keywords: saturated porous medium, alluvial valleys, wave amplification, topographical effects.

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THM coupling in unsaturated soils and its applications in sustainable geotechnical infrastructure under climate change

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Unequivocal global warming has led to significant and ongoing changes in the Earth's climate system. According to the Intergovernmental Panel on Climate Change, climate change is expected to bring about rising temperatures and alterations in the global water cycle, potentially resulting in more frequent extreme events such as prolonged droughts, intense rainfall, and freeze–thaw cycles. These developments raise critical questions: (1) Can existing geotechnical infrastructure, such as high-speed railway lines constructed on soil embankments, withstand these extreme weather conditions? (2) How should future geotechnical infrastructure be designed under varying greenhouse gas emissions scenarios?

Over the past two decades, research into the potential impacts of climate change on embankments and slopes has grown substantially. From a computational perspective, the hydro-mechanical behaviour of soil slopes has been extensively studied within the framework of unsaturated soil mechanics, particularly due to the role of rainfall as a major trigger for slope failures. Previous studies have also shown that soil–atmosphere interactions tend to influence soil temperature at greater depths compared to volumetric water content. However, the thermo-mechanical behaviour of unsaturated soils in slope contexts remains insufficiently understood, despite numerous experimental and constitutive modelling efforts in element scale.

To address this gap, the present study develops a novel cyclic thermo-mechanical model for unsaturated soils, grounded in bounding surface plasticity theory. Based on this model, a multi-physics coupled finite element framework is established to analyse complex atmosphere–slope interactions. Following validation, this advanced computational tool offers a robust means to investigate the fundamental mechanisms driving slope behaviour and provides valuable insights for the resilient design of geotechnical infrastructure under the influence of climate change. Simulation cases for embankments and slopes under both current and projected extreme climate conditions will be presented and discussed.

Keywords: Multi-physics coupling, geotechnical infrastructure, climate change, unsaturated soil

Investigation of Phase-field Data Assimilation for Obtaining Computational and Material Parameters from Limited Experimental Data

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Understanding and predicting material microstructures is crucial for controlling the properties of metal products. Numerical simulations have been employed for this purpose; however, a major challenge lies in the lack of sufficient input information required for accurate simulations. To address this issue, data assimilation has recently attracted increasing attention in materials science [1]. Data assimilation is a technique that integrates experimental observations into numerical simulations to enhance the simulation accuracy. Our research group is developing a data assimilation system that incorporates time-resolved in situ X-ray observations (4D-CT) of dendritic growth during alloy solidification into phase-field simulations [2]. While 4D-CT enables observation of the temporal evolution of three-dimensional dendrite, it requires large-scale radiation facilities, making it difficult to systematically vary materials and process conditions. In contrast, surface observation of materials is a more accessible and common method for capturing microstructural evolution. If the information required for numerical simulations can be obtained from such surface observations, it would represent a breakthrough in materials science. Considering the above, this study investigates a data assimilation framework that utilizes surface microstructural changes during material evolution as observational data. Specifically, we attempt to apply a sequential data assimilation approach based on the particle filter, as it is less susceptible to computational instability. The phase-field method is employed as the numerical simulation technique.

Keywords: phase-field method, data assimilation, particle filter, ensemble Kalman filter, material parameter, material microstructure

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A Numerical Study on the Effect of Sample Dimensions on Bender Element Test Results

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Bender element testing is a convenient and versatile non-destructive technique for determining the maximum shear modulus of geomaterials under various laboratory conditions. Despite its advantages, this method faces significant challenges in the interpretation of results. The arrival time of the shear wave, which travels directly from the transmitter to the receiver element, is not easily identifiable due to distortions in the received signal. These distortions are often attributed to near-field effects, as well as the reflection and refraction of shear and compressional waves at the boundaries of the test specimen. Although numerous studies have proposed methods to identify the shear wave arrival time, no universally accepted technique currently exists. One contributing factor to this ongoing debate is the often-overlooked influence of sample dimensions, which play a critical role in signal interpretation. In this study, a three-dimensional numerical simulation was conducted using a coupled electro-mechanical model to investigate the response of three commonly used triaxial sample dimensions: 35 × 70 mm, 50 × 100 mm, and 70 × 140 mm (diameter × height). These dimensions are widely employed in both research and practice. The errors in determining the shear wave arrival time using different methods were compared across these sample sizes at various shear wave velocities (100, 200, 300, and 400 m/s). The results demonstrate that these factors can lead to either overestimation or underestimation of the shear wave velocity. A range of conditions were studied, and the corresponding errors under each scenario are discussed.

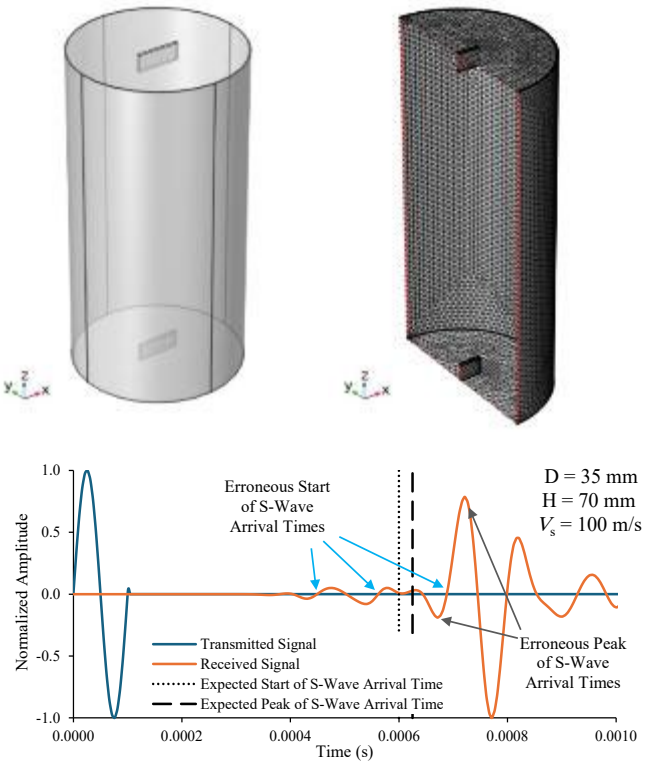

Figure 1.

Keywords: Bender Element Test, Shear Wave Arrival Time, Numerical Simulation, Sample Dimensions, Signal Interpretation Errors

Quantum algorithm for simulating solid vibration analysis

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Quantum computers are next generation computers that can solve certain problems super-fast. To leverage quantum computers, some applications in computational mechanics have been verified in recent years [1]. However, there are few examples of the applications to solid mechanics, that is essential in the fields of manufacturing, infrastructure, disaster prevention and so on. In this study, to begin with, we propose a method for simulating simple harmonic motion of structures made of a linearly elastic material as a first step by the application of relevant quantum algorithms to perform corresponding Hamiltonian simulations.

The Newton's equation of motion of a structure is discretized by the application of the finite element method and then the discreteized version of equation of motion can be expressed as

$$\boldsymbol{M}\frac{\partial^2 \boldsymbol{u}(t,\boldsymbol{x})}{\partial t^2} + \boldsymbol{K}\boldsymbol{u}(t,\boldsymbol{x}) = 0, \tag{1}$$

where t is the time, $\boldsymbol{x}$ is the spatial coordinate, $\boldsymbol{u}$ is the displacements, and $\boldsymbol{K}$ and $\boldsymbol{M}$ are the stiffness matrix and mass matrix, respectively. Obviously, this is not in the form of the Schrödinger equation, so that we transform the equation into the following form:

$$\frac{\partial \boldsymbol{\psi}(t,\boldsymbol{x})}{\partial t} = iH\boldsymbol{\psi}(t,\boldsymbol{x}). \tag{2}$$

where $\boldsymbol{\psi}(t,\boldsymbol{x})$ and $\boldsymbol{H}$ are defined as, respectively,

$$\boldsymbol{\psi}(t,\boldsymbol{x}) = \begin{Bmatrix} \dfrac{\partial \boldsymbol{u}(t,\boldsymbol{x})}{\partial t} \\ \sqrt{\dfrac{\boldsymbol{K}}{\boldsymbol{M}}}\boldsymbol{u}(t,\boldsymbol{x}) \end{Bmatrix}, \qquad \boldsymbol{H} = i\begin{pmatrix} 0 & -\sqrt{\dfrac{\boldsymbol{K}}{\boldsymbol{M}}} \\ \sqrt{\dfrac{\boldsymbol{K}}{\boldsymbol{M}}} & 0 \end{pmatrix}. \tag{3}$$

This transformation is analogous to the transformation in Ref [2] and satisfies original Newton's equation of motion when expressed in the form of the Schrödinger equation. Using this form, we calculate the time history response of the nodal displacement.

We implement the above equation to the quantum circuit and verify accuracy and computational complexity. This method can be extended to non-conservative systems with damping and is a foundation for the use of quantum computers in computational solid mechanics.

Keywords: quantum computing, Newton's equation of motion, Schrödinger equation, vibration analysis, Hamiltonian simulation

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Contact Modelling and Optimization of Contact Pressure in Joining of Thermoplastic Composite Novel Joint

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Thermoplastic composites have received increasing attention in many industries due to their reprocessability, and capability for fusion bonding. Fusion bonding is a joining process that applies heat and pressure to fuse the interface, allowing polymer chains to entangle and form a bond [1]. However, the current joining setup utilized the external equipment to apply pressure and ensure the alignment. Therefore, this presentation introduces the concept of self-supported joint for fusion bonding of thermoplastic composites by using stiffness of the geometry itself generate consolidation pressure and self-align without using external equipment. The proposed geometry is the π-joint configuration which consists of base plate, pre-consolidated heating element on reclined L-bracket, and web.

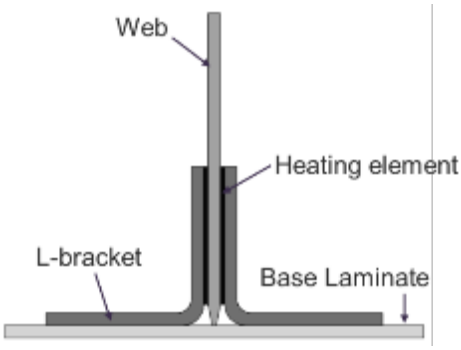

Figure 1: π-joint configuration

The contact pressure between heating element and web represents the consolidation pressure, and it is affected by four geometric parameters including thickness of the L-bracket, recline angle of L-bracket, L-bracket length, and gap between L-brackets and web. Meanwhile, other parameters are kept constant during the optimization. This study focusses on contact modelling based on Finite Element Method to simulate the contact pressure distribution, which is then experimentally validated by using pressure mapping sensor. Furthermore, geometric parameters are optimized to achieve the uniform contact pressure and complete contact at the interface by using response surface methodology, specifically face-centered central composite design experimental framework to generate the response function. Genetic algorithm is used to optimize the response function with additional constraints and boundaries. This work ensures sufficient and uniform pressure to generate high quality bonding without squeezing out the melted polymer.

Keywords: Fusion bonding, contact modelling, optimization, thermoplastic composites, Response Surface Methodology

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Utilizing an Explicit Projection Method Combined with the Immersed Boundary Method for Moving Boundary Problems on Multi-GPU Clusters

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The interaction between fluid flow and solid structures is central to many physical processes, such as sediment transport, blood flow dynamics, and fish locomotion. Traditional mesh-conforming methods are inefficient for moving boundaries, motivating the use of the sharp-interfaced immersed boundary method introduced by Liao et al. [1], which solves the fluid equations on a fixed Cartesian grid. For incompressible flows, the projection method proposed by Kim and Moin [2] couples velocity and pressure using a pressure Poisson equation. To accelerate convergence of the pressure Poisson equation, particularly in large-scale problems, the multigrid technique is adopted [3]. While each method has been widely applied, a combined implementation of sharp-interfaced immersed boundary, projection, and multigrid methods on a multi-graphics processing unit computing platform remains unavailable. This study presents such a solver and verifies it through benchmark problems including oscillating solids and particle settling. Simulations involving up to 20,000 particles settling demonstrate the method's feasibility of the proposed approach.

In the present study, the projection method is chosen for coupling velocity and pressure. To implement this method on a multi-GPU system, we employ a four-step explicit fractional-step approach [2], which is combined with multigrid acceleration. To resolve the velocity near solid boundaries, we utilize the velocity-interpolated forcing method developed by Liao et al. [1].

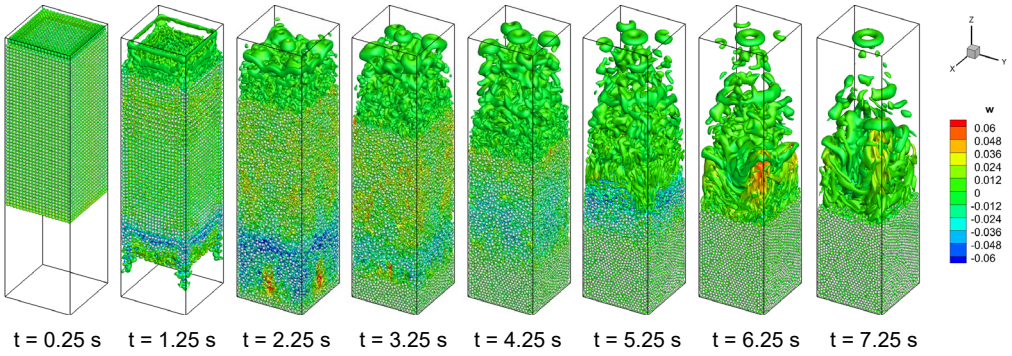

Figure 1.

Figure 1 illustrates the vortex structures generated by the settling of 20,000 particles. The present method successfully captures the upward jet flows that form between particles, demonstrating the effectiveness of the developed framework, which integrates the immersed boundary method, the Projection method, and the multigrid solver on a multi-GPU cluster.

Keywords: Fluid-structure interaction, multi-GPU cluster, Multigrid method, Immersed boundary method, Projection method

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Deep Learning-Based Flow Field Prediction: A Hybrid Learning Framework with Multi-Head Attention Mechanism

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In recent years, with the rapid development of artificial intelligence, deep learning techniques are widely and deeply penetrating into the field of fluid mechanics. Various types of neural networks, such as Convolutional Neural Networks, Physics-Informed Neural Networks, and Long Short-Term Memory networks, have played significant roles in this domain. However, a large number of studies have shown that independent neural network frameworks have their own shortcomings, such as the poor interpretability of fully data-based Convolutional Neural Networks for predictive modeling, and the insufficient performance of Physics-Informed Neural Networks models for learning temporal information as well as model generalization. In order to cope with these problems, combining different neural networks to construct a hybrid deep neural network is an effective strategy, which can further improve the overall comprehensive performance of the model by combining the advantages of different models in flow field prediction. In this paper, a hybrid neural network framework is proposed for two-dimensional flow field prediction. The model integrates Convolutional Neural Networks, Multi-Head Attention mechanisms, and Long Short-Term Memory networks, and consists of a data loss term and a physical loss term to form the loss function of the model. The model adopts Convolutional Neural Networks to extract features from the flow field information, introduces Multi-Head Attention mechanisms to weight the information in the complex flow field region, applies Long Short-Term Memory networks to learn the temporal relationship in the flow field information at different moments, realizes the reconstruction of the flow field through the deconvolution, and further optimizes the model by calculating the physical residuals and the data loss in the loss function, so as to improve the prediction accuracy and generalization ability of the model. The model is applied to learn and predict the two-dimensional cylindrical winding flow model under different initial conditions, and compared with the traditional deep learning methods. From the results, the model has an excellent performance in learning the flow features and predicting the flow field accuracy, especially the introduction of Multi-Head Attention mechanisms makes the model capture the details of the vortex shedding region better than the traditional methods. This study provides an efficient deep learning solution for the study of multi-scale and complex flow fields in fluid dynamics.

Keywords: Flow Field Prediction, Hybrid Neural Network, Multi-Head Attention Mechanism

Influence of Particle Shape on Non-linear Hydraulic Behaviour in Dense Granular Materials

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Granular materials, exhibiting permeable packing structures, commonly exist in geological formations in relation to various applications, ranging from underground oil and gas reservoirs, underground gas storage, to groundwater flow. The packing structures are usually anisotropic in the natural formations, attribute to the anisotropic pressure conditions, as well as non-uniform grain features such as size distributions, general shapes, and fine morphology. Due to the opaque nature of overwhelming parts of natural grains, instant changes of tortuosity and porosity reflected by inter-connected pore geometry are hard to quantify experimentally. To bypass the difficulty, numerical studies were often conducted on the porosity and permeability of granular media influenced by the general shape of irregular particles. Our numerical study focuses on the effect of anisotropic packing structure and grain morphology features on the hydraulic conductivity in transition flow. A discrete element method (DEM) is applied to assemble mono-dispersed granular packings at various compaction stages, where all realistic shaped particles are uniquely generated using the inverse analysis of spherical harmonics. Thereafter, we converted the compacted packing structures into voxel representations to compute multi-directional permeability using the lattice Boltzmann method (LBM) for the fluid fields within the pore space. The lattice size and the region of interest are carefully selected to balance computation efficiency and accuracy. We observed the grain rearrangement and rotation during the compaction process that alter the packing structure, e.g., decreased porosity, anisotropic features, and increased global pore tortuosity, and therefore suppressing the permeability. Our findings will contribute to the understanding of effects of grain shapes and compaction on anisotropic permeability, beneficial to the engineering applications concerning the fluid flow in various types of porous materials.

Keywords: Lattice Boltzmann methods, non-spherical particles, anisotropic permeability.

Evolution Characteristics and Integrated Prevention Measures of Coal and Gas Outbursts from the Perspective of Geodynamic Systems

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Abstract: Coal and gas outbursts represent a significant hazard to the safety of underground coal mining operations, with their occurrence governed by complex mechanisms influenced by various geological conditions. In this study, criteria for the formation and instability of a geodynamic system associated with coal and gas outbursts are established, and a coupled stress–damage–seepage model for gas-bearing coal is developed. The model is employed to simulate the spatiotemporal evolution characteristics of coal and gas outbursts under different geological conditions, and to identify the dominant factors controlling their occurrence and evolutionary patterns at various stages. The results demonstrate that the occurrence of coal and gas outbursts is closely related to factors such as geological stress, coal seam structure, gas pressure, and coal body strength. In regions with variable coal seam thickness, stress distribution becomes uneven, increasing outburst risks. Fold and fault zones, characterized by concentrated tectonic stress, are particularly susceptible to outbursts. Additionally, areas with weak coal bodies exhibit lower strength, making them more prone to fragmentation and thereby promoting gas desorption and migration. In response to the characteristics of coal and gas outbursts under different geological conditions, a comprehensive prevention strategy is proposed, Stress unloading-pressure reduce-coal reinforcement measures. Stress unloading methods, such as protective layer mining and large-diameter stress-relief drilling, aim to reduce geological stress and prevent the formation of an outburst-prone geodynamic system. Pressure reduces measures involve pre-drainage of coal seam gas and gas extraction ahead of the working face to lower gas pressure and content, thereby maintaining system stability. Coal reinforcement strength increases the fragmentation threshold, raising the energy barrier required for outburst initiation. These integrated measures offer an effective approach to mitigating coal and gas outbursts and enhancing the overall safety of coal mining operations.

Keywords: Coal and gas outbursts; Geodynamic system; Stress–damage–seepage coupling model; Dominant factor; Outburst prevention strategy

Generalizable Deep Material Networks for Polycrystalline and Composite Materials: Incorporating Graph Neural Networks and Foundation Models

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Multiscale modeling is essential for linking microstructural features to macroscopic material responses, yet its widespread adoption is limited by substantial computational costs. Deep material networks (DMNs) have emerged as powerful surrogate models capable of efficiently capturing complex material behaviours and performing nonlinear extrapolation. However, existing DMNs, including advanced variants such as the orientation-aware interaction-based DMN (ODMN) [1], require retraining when applied to previously unseen microstructures. This constraint significantly limits their applicability in industrial settings characterized by diverse microstructural morphologies. To overcome this limitation, we propose a dual-track framework that improves DMN generalization across different material systems. In the first track, we proposed a GNN-ODMN framework specifically for polycrystalline materials. The representative volume element (RVE) is explicitly represented as a graph: nodes encode crystallographic orientations, and edges capture geometric connectivity. A graph neural network (GNN) is employed to embed these microstructural features and predict the parameters of the ODMN. This architecture demonstrates strong consistency with direct numerical simulation (DNS) results, even for microstructures not seen during training. In the second track, we proposed FM-ODMN, a foundation model-based approach that leverages a 3D masked autoencoder pretrained on 100,000 microstructures sampled from a crystallographic texture design space. The model learns transferable latent representations, enabling rapid adaptation to downstream tasks with minimal labeled data. Notably, FM-ODMN achieves performance comparable to, and in some cases exceeding, that of GNN-ODMN—even without relying on explicit graph-based encoding. We further generalize this approach to composite materials by pretraining on a diverse dataset of matrix–inclusion microstructures, which enables accurate DMN parameter prediction across a broad range of morphologies [2]. The resulting DMN outputs closely match DNS responses, underscoring the scalability and adaptability of foundation model-based architectures in multiscale material modeling. It is worth noting that the current foundation model is trained with relatively modest architectures and datasets. Based on established scaling laws in foundation model research, we anticipate that increasing model capacity and diversifying microstructural datasets will further enhance generalization capabilities and unlock new opportunities for universal surrogate modeling in computational mechanics.

Keywords: Deep material networks, Foundation models, Graph neural networks, Multiscale material modeling, Crystal plasticity, Composite materials

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Particle Infiltration Depth in Granular Filters: Observed Trends from CFD-DEM Simulations

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Granular filters are particularly important in zoned embankment dams, where filter drains are constructed to mitigate the transport of finer base particles. The design of granular filters is governed by hydraulic and geometric conditions. The hydraulic condition specifies the required flow velocity or hydraulic gradient for the onset and transport of base particles, while the geometric condition specifies whether the pore space is large enough to permit the migration of base particles. Coupled CFD-DEM, which combines Computational Fluid Dynamics (CFD) to model fluid behaviour with the Discrete Element Method (DEM) to model particle behaviour, is well suited to addressing both the geometric and hydraulic conditions that govern the performance of filters.

The infiltration depth of base particles with seepage flow is an important element when considering the performance of filters. Effective filters only result in minimal to no infiltration, while ineffective granular filters can experience significant and even continuing infiltration. As such, the infiltration depth provides a pathway to understand the effectiveness of a granular filter, and this can be quantitatively explored using CFD-DEM. Simulations were conducted with finer base particles underlying a coarser granular filter with upward seepage flow perpendicular to the base-filter interface. To explore the geometric condition, a wide range of size ratios were considered, from $R = 5$ to $R = 10$, where R is the ratio of the maximum to minimum particle diameter. For each size ratio, three different ramping accelerations for the upward seepage flow was considered to investigate the hydraulic condition. The key outcome was that the time-dependent infiltration depth of transported base particles was observed to be universal with respect to a newly proposed dimensionless time parameter, which is given by $\tilde{t} = t \cdot a_{flow}/d_{f,100}$, where t is the physical time, a_{flow} is the acceleration of the upward seepage flow, and $d_{f,100}\}$ is the maximum size of the granular filter. However, it is noted that the universality is only observed during the early stages of infiltration.

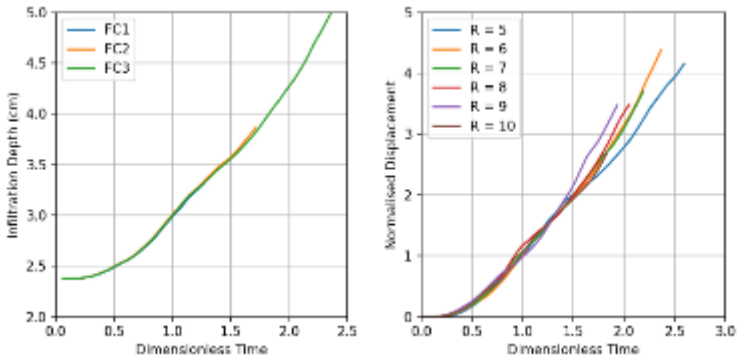

Figure 1.

Keywords: CFD-DEM, granular filters, internal erosion, infiltration, seepage

Efficient multi-body transient simulation via the displacement-based partitioned equation

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Multi-body dynamic analysis has been widely utilized in various fields such as automotive, aerospace, and robotics. However, due to the necessity of predicting the coupled motion of large-scale system, the computational cost can be significantly high. Additionally, the use of Lagrange multipliers for enforcing multiple constraints can complicates the solution process.

To address these challenges, this study utilizes the displacement-based partitioned (DP) equations [1] which essentially eliminates Lagrange multipliers through a coupling projector to ensure displacement compatibility between the subdomains, resulting in efficient implementation of multiple-point constraints, such as the tied contact and various types of the joints. The key feature of the proposed work is to exploits the unassembled mass and stiffness matrix which allows each multi-body component to be treated independently. This approach will facilitate the handling of rigid-flexible coupling and localized nonlinearities, enabling focus on specific component and improving computational efficiency.

To validate the effectiveness of the proposed approach as applied to multi-body dynamic simulations with the DP equations, a three-dimensional main rotor system of a rotary-wing aircraft will be considered. The main rotor system consists of various constraints, including the spherical and revolute joints, as well as nonmatching contacts, along with multiple components such as the blades, hinges/dampers, and control systems [2], while effectively accomplishing the desired coupling among the model elements. To handle large deformations of flexible elements, a corotational coordinate system along closed-loop control. It is shown that the solution of resulting equations can be efficiently achieved via parallel computing procedures.

Keywords: multi-body dynamic simulation, DP (displacement-based partitioned) equations, multiple constraints, main rotor system

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Influence of Flaw Geometry on the Mechanical Behaviour of Ice-filled Frozen Fractured Rock: Insights from Experiments and RFPA Simulation

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Abstract

Understanding the static mechanical behaviour of frozen fractured rock masses is essential for the design, construction, and safety evaluation of geotechnical projects in cold regions. This study investigates how the geometric characteristics of ice-filled flaws, including flaw angle, width, and length, influence the uniaxial compressive strength and failure mechanisms of frozen rocks. Laboratory experiments were conducted on specimens with and without flaw ice. To further interpret the test results, numerical simulations were carried out using the Realistic Failure Process Analysis (RFPA) method, which enables detailed analysis of stress distribution and crack evolution. The results show that the compressive strength increases with flaw angle but decreases with increasing flaw width and length. Flaw angle also exerts a strong influence on fracture morphology, affecting both the location of crack initiation and the orientation of failure planes. Compared with ice-free specimens, those containing flaw ice exhibit enhanced compressive strength, primarily due to the ice's role in alleviating stress concentrations and locally bridging mechanical discontinuities. This leads to improved structural integrity and delayed crack propagation, though the final fracture pattern remains largely unchanged. The numerical results obtained using RFPA are in good agreement with the experimental findings and help elucidate internal failure processes that are difficult to observe directly. This combined experimental–numerical approach enhances the understanding of damage evolution in frozen fractured rocks and provides a reliable framework for mechanical analysis under cold regions. This study offers new insights into the mechanical response and failure characteristics of frozen fractured rock as governed by flaw ice geometry. The findings contribute to improved design and performance evaluation of rock engineering systems in seasonally or permanently frozen ground.

Keywords: frozen fractured rock mass; ice-filled flaw geometry; fracture behaviour; RFPA simulation; cold region mechanics

Partitioned Neural Network Approximation for Partial Differential Equations with Enhanced Strategies

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Partitioned neural networks are employed to approximate solutions to elliptic partial differential equations (PDEs). The computational domain is decomposed into multiple non-overlapping subdomains, each equipped with a dedicated neural network approximation. To achieve convergence, continuity conditions across subdomain interfaces are explicitly integrated into the loss function, guiding the training of the neural network parameters. By defining suitable interface values, the global loss function is reformulated into a sum of localized loss functions, allowing each subdomain network to be trained independently.

The augmented Lagrangian method enriches each localized loss function by explicitly imposing interface and boundary conditions as constraints using Lagrange multipliers. Consequently, optimization addresses both local neural network parameters and multipliers. An iterative algorithm tailored for parallel computational environments leverages the localized loss function structure, enhancing computational efficiency and scalability.

The key contribution of this work lies in demonstrating the effectiveness of partitioned neural networks for solving challenging interface problems that are typically difficult to approximate using a single global neural network. Numerical experiments involving elliptic PDEs with complex interfaces and discontinuous coefficients validate the practicality and robustness of the proposed partitioned approach. The proposed algorithm significantly reduces inter-subdomain communication overhead compared to alternative methods, which becomes increasingly critical when scaling to larger domain decompositions where data transfer would otherwise become a computational bottleneck.

Keywords: Partitioned neural networks, Non-overlapping domain decomposition, Lagrangian multipliers, Localized loss function, Partial differential equations

Tilting of vortex rings in the oblique collision reduces the aerodynamic sound

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The sound in turbulent flows is closely related to the complex interactions of vortical structures, such as the unsteady convection, reconnecting and deforming of vortical structures. We study the impacts of those interactions on the sound generation during the oblique collision of two vortex rings. The vortical flow is governed by the unsteady Navier-Stokes equations for incompressible flows and the far-field sound is predicted by the vortex sound formula based on the matched asymptotic expansion proposed by Kambe *et al.* [1]. The sound generated by the oblique collision of two vortex rings is featured by the longitudinal quadrupole mode, the lateral quadrupole mode and the longitudinal octupole mode. We proposed a new vortex sound formula that relates the far-field sound pressure to equivalent circulations and vorticity centroids, which incorporate the effects of unsteady convection, tilting and reconnecting of vortex rings

$$
\begin{aligned}
A_1 &= \frac{\rho_0 L_0}{12\pi c_0^2 r}\left(y_{12}y_{32}\Gamma_2 - y_{21}y_{31}\Gamma_1\right)^{(3)}, \\
A_2 &= \frac{\rho_0 L_0}{24\pi c_0^2 r}\left(y_{13}y_{23}\Gamma_3\right)^{(3)}, \\
B_1 &= \frac{\rho_0 L_0}{40\pi c_0^3 r}\left(y_{12}y_{32}^2\Gamma_2 + y_{11}^2 y_{21}\Gamma_1 - y_{21}y_{31}^2\Gamma_1 - y_{12}y_{22}^2\Gamma_2\right)^{(4)}, \\
B_2 &= \frac{\rho_0 L_0}{240\pi c_0^3 r}\left(2y_{12}y_{23}y_{33}\Gamma_3 - y_{11}^2 y_{21}\Gamma_1 - y_{12}y_{22}^2\Gamma_2\right)^{(4)}.
\end{aligned}
\tag{1}
$$

A_1, A_2, B_1, B_2 are the coefficient functions of the longitudinal quadrupole mode, the lateral quadrupole mode, the longitudinal octupole mode and the lateral octupole mode, respectively. The symbols ρ_0, c_0 are the sound speed and density of the fluid in the undisturbed flow, respectively. r is the distance between the observer points and the original point. L_0 is the characteristic length taken as the initial diameter of the vortex rings. Γ_i is the equivalent circulation which is defined by the volume integral of the i-th component of the vorticity and y_{ij} is the i-th component of the centroids position vector for the j-th component of the vorticity. The equivalent circulations are changed due to the tilting, reconnecting and deforming of vortex rings. The changed of equivalent circulations due to the tilting is out of phase with that due to the reconnecting and deforming of vortex rings. Tilting of vortex rings reduces the sound generated by the oblique collision of two vortex rings.

Keywords: vortex sound, vortex rings, tilting, unsteady convection, reconnecting

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Near-field Behaviour of Filtered Water Discharge from Deep-sea Mining Operations in Marine Environments

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A systematic analysis is conducted on the near-field behaviour of solid-laden discharge fluids during the release of filtered water from deep-sea mining vessels into thermohaline stratified marine environments. A three-dimensional multiphase numerical model is established based on actual deep-sea environmental parameters, employing a coupled Large Eddy Simulation (LES) and Finite Volume Method to investigate buoyancy-driven flow, turbulent diffusion, and particle transport mechanisms under thermohaline stratification. By quantifying the synergistic effects of temperature-salinity gradients on buoyancy frequency, the evolutionary patterns of discharge plumes driven by density differences are revealed. Numerical results demonstrate that under linear stratification, the plume rise height is governed by the buoyancy-modified Froude number (Fr′), with stratification intensity and discharge momentum jointly regulating entrainment rates and horizontal dispersion extent. Nonlinear stratification triggers intermittent gravitational collapse phenomena, forming localized vortex breakdown structures that enhance particle settling rates by over 40%. Parametric analysis indicates that the contribution of salinity gradients to buoyancy effects reaches 2.3 times that of temperature gradients in deep high-density water masses. A flow regime criterion based on the Richardson number threshold is proposed, elucidating the mechanism of particle-turbulence interactions on stratification interface penetration. The findings provide theoretical support for environmental risk assessment in deep-sea mining and optimization of discharge systems, while offering new insights for multiphysics-coupled simulation methodologies in complex stratified environments.

Keywords: Buoyancy-driven flow, Thermohaline stratification, Double-diffusive convection, Particle transport, Deep-sea mining

Suppression of Thermal-Induced Performance Degradation in Magnetorheological Elastomer Dampers via Bio-inspired Heat Dissipation Structure Optimization

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Magnetorheological elastomer (MRE) dampers hold significant application value in active vibration control due to their magnetic field-adjustable mechanical properties. However, Joule heating generated by electromagnets during operation induces temperature field distortion within the damper, leading to material degradation of the MRE and consequent attenuation of vibration control efficacy. This study proposes a bio-inspired topological optimization method for heat dissipation, employing a multi-objective genetic algorithm to iteratively optimize the damper's cooling channels and establish a composite thermal management system with gradient thermal conductivity characteristics. Using electromagnetic-thermal multiphysics coupling modeling, the temperature field evolution and magnetic field distribution of the enhanced damper under sustained excitation are systematically analyzed. Experimental results demonstrate that the optimized bio-inspired heat dissipation structure reduces the steady-state operating temperature by 15.2% compared to conventional designs while maintaining magnetic field intensity fluctuations below 5%. The research elucidates the coupling mechanism among temperature, magnetic field, and mechanical performance, providing theoretical foundations and engineering solutions for thermal management design of magnetorheological devices in high-power operating conditions.

Keywords: Magnetorheological elastomer; Bio-inspired heat dissipation structure; Multiphysics coupling; Thermal-induced performance degradation; Temperature regulation

Data-Physics-Driven Optimization Method for Fracture Stage-Cluster Design Based on Gradient Feature Clustering

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The precise design of multi-stage/multi-cluster parameters in horizontal well hydraulic fracturing critically impacts stimulation effectiveness and hydrocarbon production, playing a pivotal role in achieving efficient and safe exploitation of unconventional shale resources. To address the issues of over-reliance on empirical formulas in shale fracturing design and the lack of physical interpretability in traditional data-driven approaches, this study treats logging and shale evaluation data as time series, proposing a data-physics-driven optimization method that integrates spatiotemporal gradient features with geomechanical constraints. The algorithm incorporates penalty terms to prevent adjacent measurement points from being segmented separately, ensuring superior continuity and interpretability of partitioning results while enhancing the scientific rationality of fracture stage-cluster design. By improving the Histogram of Oriented Gradients (HOG) algorithm to extract spatiotemporal heterogeneous features from logging data and employing K-means++ dynamic clustering to construct lithology-property symbolic sequences, this work innovatively introduces physical constraints including geostress abrupt change detection, rock brittleness thresholds, and stage length limitations. A joint loss function is designed to synergistically optimize data distribution and mechanical principles.

$$L = \underset{\Theta\in\Gamma,\mathrm{P}}{argmin}\sum_{i=1}^{K}\left[\overbrace{\left\|\lambda\circ\Theta_i\right\|_1}^{Sparsity}+\sum_{X_t\in P_i}\left(\overbrace{-\ell\ell(X_t,\Theta_i)}^{Log-Likelihood}+\overbrace{\beta\mathbf{1}(X_{t-1}\notin P_i)}^{Time\ Continuity}\right)\right] \quad (1)$$

Validation using horizontal well data from the Sichuan Basin shale gas field in China demonstrates that compared with conventional engineering methods, the proposed approach reduces intra-stage stress variation by 28% (mean 8.7→5.1 MPa) and improves brittleness consistency by 29%. Furthermore, it achieves a 36% increase in simulated reservoir stimulation volume over purely data-driven models. This method establishes an interpretable and generalizable decision-making framework for intelligent fracturing design in unconventional reservoirs.

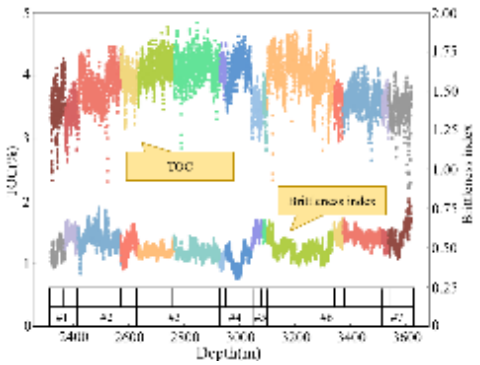

Figure 1. Segmentation clustering results in mapping organic carbon content and brittleness index

Keywords: Fracture stage-cluster optimization, Gradient histogram features, data-physics-driven, Unsupervised learning, Reservoir stimulation

Physics-Informed Laplace Neural Operator for Learning Differential Equations

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Differential equations are fundamental for modeling complex scientific and engineering processes. Operator learning offers a powerful framework for approximating the mapping from parametric inputs such as initial/boundary conditions or forcings to the corresponding solutions. However, purely data-driven operator learning methods such as the Laplace Neural Operator (LNO) typically require large training datasets and exhibit limited extrapolation capabilities. We propose the Physics-Informed Laplace Neural Operator (PILNO), which embeds the governing physical laws directly within the learning process. This physics-informed approach reduces data dependency, enabling effective learning in small-data regimes and enhancing generalization to out-of-distribution inputs where purely data-driven LNOs often fail. By leveraging both data (when available) and physics, PILNO offers a more robust and data-efficient pathway to learning solution operators. We demonstrate advantages of PILNO across diverse parametric differential equation problems, highlighting its improved data efficiency and extrapolation performance.

Keywords: physics-informed machine learning, neural operator, partial differential equations

References

Multiscale Mechanics of Cells and Biological Tissues

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Some experimental and theoretical researches conducted by the speaker's group on the multiscale biomechanics of biological tissues and cells at multiple length scales will be introduced. Particular attention is given to the biomechanical mechanisms underlying the morphogenesis of developing embryos and tumors. First, a multiscale chemomechanical model and the corresponding computational method are presented for studying the dynamic behaviors of a single cells and interconnecting collective cells. Second, we investigate the dynamic instability that occur in biological systems at different tempospatial scales and involve mechanical, biological and chemical coupling mechanisms. Third, we address, both experimentally and theoretically, the migration of collective cells. On the basis of experimental measurements and theoretical analysis, time-independent statistical laws are derived.

Keywords: Cell, biological tissue, Mechnobiology, Multiscale modeling

Machine learning-assisted multi gas sensor for enhanced selectivity and quantitative performance

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Quantitative information is vital for deriving accurate and sensitive diagnosis toward the practical application of multi gas sensor devices. This study presents the development of an artificial intelligence (AI)-based model to enhance the selectivity and sensing performance of room-temperature multi gas sensors. A MXene/graphene nanocomposite foam was synthesized and employed as the sensing material, offering high surface area, porosity, and electrical conductivity suitable for gas detection. Dynamic response data from the nanocomposite sensor were experimentally obtained for multiple target gases and used to train and validate the machine learning model. The AI model, developed using supervised learning techniques, demonstrated high accuracy in identifying and quantifying various gases based on real sensor signals. The integration of experimental sensor data with algorithmic analysis enabled improved gas discrimination, reduced cross-sensitivity, and enhanced real-time performance. This work highlights the potential of combining advanced nanomaterials with AI-driven analytics to realize intelligent, selective, and scalable multi gas sensing platforms

Keywords: Artificial Intelligence, Gas sensor, MXene, Graphene, Nanofoam

Molecular Dynamics Investigation of Splicing Interfaces Between YAG and Silica at various Temperatures

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Fusion splicing is the process of creating joints between two very small optical materials through various heat sources. The advantages of splice joints include optimized splice losses and mechanical strength with extremely small space, which make it attractive for optimizing optical systems such as silicon photonic chips. Understanding the interface mechanical behavior is crucial for designing the long-term reliability of the optical systems. Furthermore, fusion splices become challenging when applied in different optical media with discrepancies between the material properties. In this study, the fusion splicing between yttrium aluminum garnet (YAG) and silica is investigated by molecular dynamics simulations. Fig. 1(a) shows the initial models for two interfaces at 300 K, including YAG/splice region-Y (interface 1) and silica/splice region-S (interface 2). Those materials are modeled to be amorphous because they are rapidly cooled from a molten state. The amorphous configurations of these regions are prepared using the melt and quench technique. The atomic interactions are described using the partial charge pairwise potentials that consist of a short range Buckingham and long range Coulomb term. The uniaxial tensile loading is applied by moving the constrained splice region atoms at a constant speed of 0.002Å/ps, while keeping the YAG or silica atoms fixed. We are interested in the interface mechanical behavior at a maximum acceptable fiber core temperature of 600 K. As shown in Fig. 1(b), the snapshots and stress-strain curves of interfaces 1 and 2 are presented at various temperatures, indicating that temperature has an effect on the mechanical properties of those systems. Both of the yield strength slightly decreases with the increase in temperature. As the temperature increases from 300 to 600 K, the elastic constant of interface 1 decreases by 13.7 % from 113.2 to 97.7 GPa, while the elastic constant of interface 2 decreases by 3.8 % from 103.9 to 100.0 GPa.

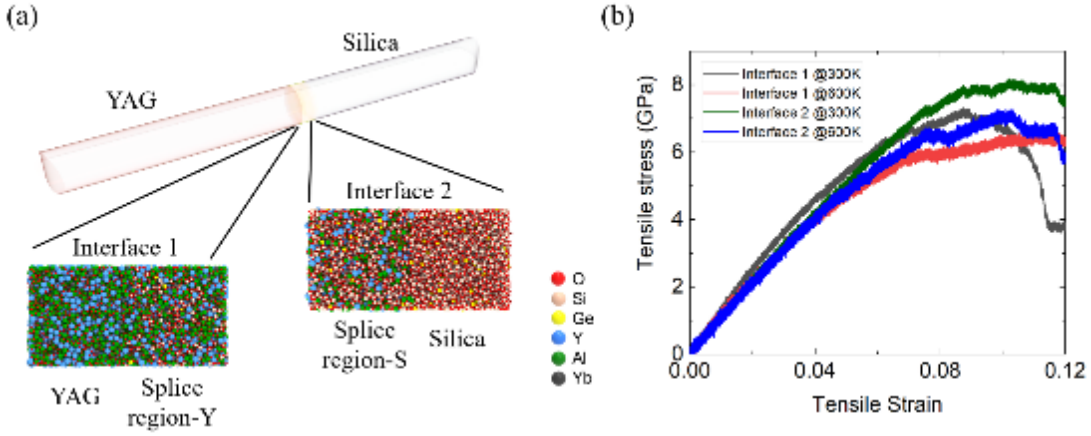

Figure 1.

Keywords: fiber fusion splicing, molecular dynamics simulations, mechanical properties, machine learning, entropy production

CFD-Based Analysis of Porosity Effects on Transport Phenomena and Hydrogen Production in PEM Electrolysers

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Hydrogen is a critical component of the global energy transition, offering a clean and sustainable alternative to fossil fuels across various sectors. Among hydrogen production technologies, Proton Exchange Membrane Electrolysers (PEMECs) have gained prominence due to their high efficiency, rapid adaptability to renewable energy fluctuations, and ability to produce high-purity hydrogen at lower temperatures [1]. These electrolysers rely on porous transport layers (PTLs) and catalyst layers (CLs), whose porosity is fundamental in determining mass transport characteristics, reactant distribution, and overall electrochemical performance. The transport and electrochemical processes in PEMECs involve fluid dynamics, species transport, and electrochemical kinetics, where porosity-dependent terms influence the governing equations [2]. Porosity (ε_p) is defined as the ratio of the pore volume (V_{pore}) to the total volume (V_{total}), influencing mass transport and water distribution within the cell

$$\varepsilon_p = \frac{V_{pore}}{V_{total}} = \frac{V_{pore}}{V_{solid+}V_{pore}} \quad (1)$$

Table 1 presents the typical porosity ranges for PTLs and CLs in PEMECs based on literature data.

Porous component	Porosity Values	Typical thickness range
Anode & Cathode CL	0.2-0.5	250 µm - 1.1 mm
Anode PTL	0.3-0.6	12 - 30 µm
Cathode PTL	0.3-0.5	12 - 30 µm

Table 1. Typical porosity ranges for CL and PTL in PEM electrolysis cells [2-3]

This study employs a 3D CFD-based numerical model in COMSOL Multiphysics to systematically investigate the impact of constant porosity variations on PEMEC performance, with a focus on fluid flow and transport mechanisms in porous layers. Using the typical porosity values of CLs and PTLs from Table 1, the model evaluates the influence of fixed porosity values on mass transport resistance, reactant penetration, and electrochemical efficiency. The polarization curve is used as a key performance indicator alongside a detailed analysis of reactant distribution and electrolyte potential across the cell. The findings provide quantitative insights into the role of porosity in optimizing mass transport and thermal distribution within PEMECs. These insights contribute to the development of more efficient PEMEC designs for enhanced green hydrogen production.

Keywords: Green hydrogen production, CFD modeling, PEM electrolysis, Porous layer engineering

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APCOM-ACCM 2025
Brisbane, Australia
7-10 December 2025

Concentration-Dependent Interaction of Polystyrene Nanoplastic with Alveolar Fluid Mediated Lung Surfactant Monolayer

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Abstract

Environmentally ubiquitous micro (MPs) and nano plastics (NPs) can be breathed in and travel through the branching air passages to reach the alveoli where they initially interact with the lung surfactant monolayer, the most crucial structure for maintaining optimum respiratory mechanics. Examining the minimum concentration of NPs necessary to impact the physiochemistry of lung surfactant and changes to the typical structure of the surfactant monolayer, as well as how different NP concentrations impact the degree of disruption in lung surfactant structure and function, is an important part of this subject area. The presence of NPs and their detrimental effects on human lung airways are demonstrated by previous research, but the mechanism of interaction with lung deep airways is still mostly unknown. In this work, we used coarse-grained molecular dynamics simulation to examine the NP interaction and aggregation mechanism on the lung surfactant monolayer. The findings from this investigation revealed that lung surfactant monolayer components spontaneously adsorb onto NPs, endowing the NPs and forming an adsorption layer that can be described as lipid corona. It is also observed by the structural and compressibility analysis, the increasing concentration of polystyrene NPs progressively reduces the order parameter of the monolayer lipids, leading to a more disordered orientation of lipids, impaired monolayer compressibility, which may disrupt the ability of the surfactant to reduce surface tension, effectively. Furthermore, density map analysis of polystyrene NPs on the surfactant layer shows that with high Polystyrene concentrations, NPs dominate the monolayer, causing extensive aggregation and severe structural damage that induces the monolayer to collapse. These structural abnormalities of the monolayer point to potential threats of respiratory dysfunction and alveolar collapse. This research advances our knowledge on the effects of NPs on respiratory health by offering molecular-level insights into how they affect lung surfactant monolayer stability for healthy breathing.

Keywords: Nano plastics, Lung Surfactant monolayer, Polystyrene, Molecular dynamics simulation, Respiratory health.

Breathing Cold Air: A Large Eddy Simulation Numerical Study in a CT-based Respiratory Tract

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Rapid inhalation of cold air poses significant thermoregulatory challenges for individuals engaged in sports and other high-intensity activities. Although the effects of cold air inhalation on the upper respiratory tract have been recognized, the comprehensive impact on the entire respiratory system remains underexplored. This study addresses that gap by employing advanced Computational Fluid Dynamics (CFD) techniques to investigate the heat transfer and flow characteristics within a realistic nasal-to-lung model derived from computer tomography scans.

The numerical framework is built upon Large Eddy Simulation (LES), integrating the subgrid-scale model to capture turbulence effects at spatial scales unresolved by the grid. The governing equations are: (1) the continuity equation; (2) the momentum equation; (3) the energy equation; and (4) the eddy viscosity equation, which provides the subgrid-scale turbulent viscosity modelling.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0 \tag{1}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot (\bar{\bar{\tau}}) + \rho \boldsymbol{g} \tag{2}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\boldsymbol{u}(\rho E + p)) = \nabla \left(k_{eff} \nabla T - \sum_j h_j \boldsymbol{J}_j + \left(\bar{\bar{\tau}}_{eff} \cdot \boldsymbol{u}\right) \right) \tag{3}$$

$$v_t = \rho \; min \left[(\kappa d_w)^2, \left(C_{Smag} V^{1/3}\right)^2 \right] \sqrt{2 \bar{S}_{ij} \bar{S}_{ji}} \tag{4}$$

Where t is the time variable, ρ is the fluid density, $\boldsymbol{u}$ is the velocity field, and p is the static pressure. The term g represents gravitational acceleration, while E denotes the total energy. The symbols h_j and $J_j$are the enthalpy and diffusion flux, respectively, of species j. The quantity k_{eff} is the effective (often thermal) conductivity, and $\bar{\bar{\tau}}$ or $\bar{\bar{\tau}}_{eff}$ is the stress (or effective stress) tensor capturing viscous and possibly turbulent contributions. The parameter d_w is the distance to the nearest wall, κ is the von Karman constant, which equals 0.41, and the V is the volume of the cell. The tensor $\bar{S}_{ij}$ indicates the strain rate, and C_{Smag} is the Smagorinsky constant used in subgrid-scale modeling.

Three cold ambient conditions, 5°C, -5°C and -20°C, are simulated to evaluate the extent of thermal stress under increasingly challenging scenarios. Boundary conditions are prescribed to reflect physiological inhalation rates typical of athletic activities, and the internal geometry of the nasal passage,

trachea, and lung branches is reconstructed from actual patient-specific computed tomography data to ensure anatomical fidelity. The simulations generate detailed spatiotemporal fields of temperature, velocity, and pressure, allowing for the quantification of localized heat flux and the identification of regions most susceptible to thermal injury.

Keywords: Computational fluid dynamic, large eddy simulation, human respiratory system, health

Research on poromechanical problems of hydrate sediment during phase transition process

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During the hydrate mining process, the decomposition of gas hydrate products the deformation of sediments due to the accumulation of pore pressure, which usually contributes to geological disasters. This paper establishes a theoretical model of reservoir deformation evolution during the hydrate decomposition process and implements this model through numerical simulations. The model combines the phase equilibrium equation and the unsaturated thermos-poromechanical constitutive law, considering the significant capillary effect of fine-grained hydrate sediments. Through this model, the evolution of reservoir deformation during thermal recovery under undrained conditions are analysed. The result shows the significant tensile strain occurs at the high level of pressure due to the hydrate decomposition, and this phenomenon is attributed to the density difference between the fluid and hydrate. Also, after the completed thermal stimulation, the deformation first decreases and then increases as the initial hydrate saturation increased. It is worth noting that the deformation is tensile but even at lower initial saturations. Thus, it is necessary to pay attention to the tensile failure of the reservoir.

Keywords: Poromechanics, Phase equilibrium, Hydrate, Deformation.

NiTi Neural Network Interatomic Potential for Defect Mechanics

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Nickel-titanium shape memory alloys (NiTi SMAs) are widely utilized in various applications. However, molecular dynamics (MD) simulations of fatigue, degradation, and other related phenomena remain challenging due to the absence of an interatomic potential capable of accurately predicting the behaviours of defects. This study introduces a neural network interatomic potential (NNIP) for an equiatomic Ni-Ti system, developed using a database derived from density functional theory (DFT) calculations with the PBE functional. The inclusion of defective structures, such as dislocations, grain boundaries, and twin boundaries, in database enhances the potential accuracy in predicting defect-related properties. The reliability of the NNIP is assessed by systematically analysing various properties, with the temperature–Helmholtz free energy and stress-strain curve diagrams confirming its accuracy in both energetic and mechanical predictions. The results demonstrate that the NNIP achieves a high level of agreement with experimental data and DFT calculations. The proposed NNIP enables more accurate MD simulations of degradation, fatigue, and other defect-related phenomena in NiTi SMAs, offering a valuable tool for further research.

Keywords: NiTi SMA, Dislocation, Grain boundary, Twin boundary, Phase transformation.

Filtration and clogging behaviour: a systematic definition on the pore network

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In geotechnical engineering, the structural integrity of embankment dams depends on the ability of filters to mitigate the risk of internal erosion failure. Granular filters are designed to trap finer base particles within the pore space of coarser filter particles. This entrapment of base particles occurs at the particle-scale through a clogging process. Yet, limited studies have considered particle-scale investigation of filtration despite such particle scale data being readily available from simulation and experimental imaging techniques. A common challenge limiting the uptake of particle-scale investigations of filtration is how to process and analyse the large amount of data generated to extract the valuable information necessary to understand and accurately model filtration behaviour.

The use of graph concepts provides a novel framework to integrate the large amount of particle-scale data to better understand filtration and clogging in the filter pore network. A graph representation of the pore space of the filter is built from particle-scale data by simplifying the geometrically complex void space into a set of individual pores (graph nodes), connected via constrictions (graph edges). Additionally, the base particle contact graph at the steady state holds force equilibrium information representing the resistive forces responsible for the clogging of base particle. By combining this information in a *hyper-graph* (Figure 1), a higher-level representation of filtration is obtained from which filtration behaviours are identified: the clogging of constrictions for base particle retention; and the pore capacity influencing backward filtration.

This systematic and widely applicable identification framework allows investigations into the filtration and clogging behaviours, necessary to implement accurate models. Preliminary findings on monodisperse samples include:

- The need for an improved clogging criteria to consider base particle group effects;
- The importance of pore capacity investigations to complement clogging behaviour;
- The existence of meso-scale relationships to inform validation of filtration models.

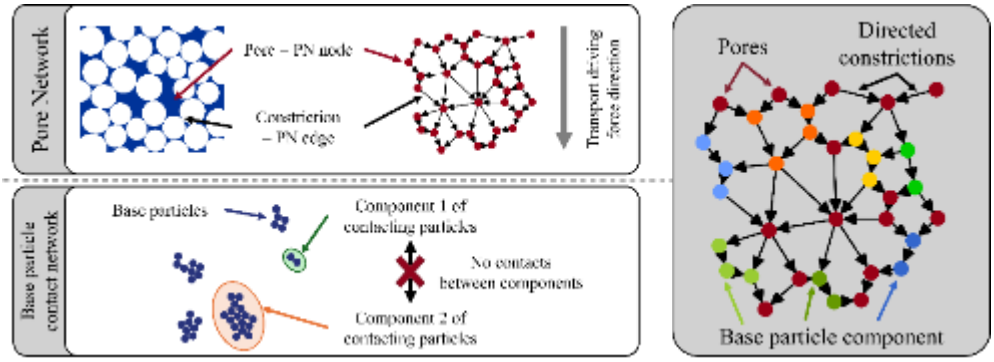

Figure 1.

Keywords: Network modelling, Granular filter, Pore capacity, Constriction clogging, Internal erosion, Graph concepts

Finite element analysis of wrinkle deformations in film–substrate bilayers induced by water droplets

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When a water droplet is deposited on a compliant substrate, capillary forces at the three-phase contact line can induce significant deformations in the substrate surface. This phenomenon, known as elastocapillary deformation or soft wetting, is markedly different from that observed on rigid substrates and has been widely studied for its unique interfacial mechanics [1]. Recent experimental studies have shown that water droplets can deform instability-induced wrinkle patterns in film–substrate bilayers, causing either wrinkle flattening or morphological transitions into localized folds near the contact line [2,3]. Such wrinkle deformations are crucial for manipulating surface morphologies and attaining controlled surface functional properties for engineering applications. However, the underlying mechanisms of these elastocapillarity-induced morphological transitions remain unclear. In this study, we perform plane-strain finite element simulations to investigate the wrinkle flattening phenomenon, which is schematically illustrated in Figure 1. The computational model comprises an incompressible neo-Hookean hyperelastic substrate and a linear elastic thin film. Our results suggest that the wrinkle flattening behavior is primarily controlled by several factors, including the film thickness, elastic modulus ratio between the film and substrate, compressive strain required for wrinkle formation, and surface wettability. These findings provide insights into soft wetting in film–substrate bilayers and facilitate the rational design of reconfigurable functional surfaces with programmable wetting properties.

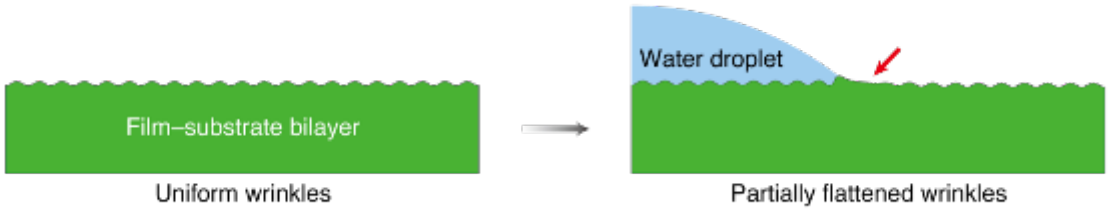

Figure 1.

Keywords: Surface instability, thin films, wrinkles, elastocapillarity, water

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Optimization Framework for Sintering Conditions Combining Phase-field Simulation and Bayesian Optimization

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Several properties of sintered materials strongly depend on the compact density and microstructure morphology. The optimal density and microstructure vary depending on the type and application of the target materials. For example, many structural and functional materials require a dense structure, whereas porous ceramics require a sparse structure with high strength and stiffness. Therefore, controlling the densification and microstructural evolution during sintering is crucial to achieve the optimal structure/microstructure and improving the material properties.

The phase-field (PF) method is one of the most promising approaches to predict the compact densification and microstructural evolution during sintering. Recent advances in computational techniques and computer power have made it possible to perform three-dimensional PF simulations of sintering with several hundred particles at a reasonable computational cost. Such large-scale simulations allow the statistical evaluation of the simulation result to calculate macroscopic density and mean grain size. These statistical data are useful for optimizing the sintering process.

This study developed a framework to optimize the sintering conditions to obtain the desired structure/microstructure by combining PF simulation of sintering and Bayesian optimization. To construct the optimization framework and verify its effectiveness, this study used a conventional PF model of solid-state sintering proposed by Wang [1]. In this model, two types of PF variables are defined: r represents the probability of particle existence, and h_i identifies the individual particle geometry, where i is an identification number of the sintered particles. The time evolutions of r and h_i are solved by the following equations.

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left\{ M_\rho \nabla \left(\frac{\partial f_{\text{bulk}}}{\partial \rho} - \kappa_\rho \nabla^2 \rho \right) - \rho \sum_i^N \boldsymbol{v}_i \right\} \tag{1}$$

$$\frac{\partial \eta_i}{\partial t} = -M_\eta \left(\frac{\partial f_{\text{bulk}}}{\partial \eta_i} - \kappa_\eta \nabla^2 \eta_i \right) - \nabla \cdot \left(\eta_i \boldsymbol{v}_i \right) \tag{2}$$

where f_{bulk} denotes the chemical free-energy density in the bulk. k_r and k_h are the gradient energy coefficients. M_r and M_h are the atomic diffusion mobility and the grain boundary migration-related mobility, respectively. $\boldsymbol{v}_i$ is the advection velocity that describes the rigid-body motion of the sintered particle.

Keywords: phase-field simulation, Bayesian optimization, sintering, microstructure

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Shear Wave Propagation in Unsaturated Porous Media

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Wave propagation in porous media is a subject of great interest in various fields of science and engineering, including geotechnical engineering, geophysics, seismology, acoustics, biomechanics, hydrogeology, and reservoir engineering. This research work presents simple yet rigorous analytical solutions for the propagation and attenuation of shear waves in saturated and unsaturated porous media. The solutions are obtained based on the mixture theory, taking into account the inertial coupling effects amongst the phases. Correlations are obtained between the velocity and attenuation of shear waves with the excitation frequency, soil shear stiffness, hydraulic conductivities of the fluid phases, and volume fractions and densities of the constituents [1]. These analytical solutions enable the evaluation of dynamic properties of unsaturated geomaterials, correlation of results from different frequency-dependent laboratory and field tests, subsurface imaging in oil and gas exploration, non-destructive integrity assessment of multiphase porous materials, and energy loss assessment critical for ground motion prediction and earthquake risk analysis. The simulation results and their comparisons with the experimental data are presented demonstrating the application of the derived analytical solutions.

Keywords: Porous media, Unsaturated, Shear wave propagation, Attenuation

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Numerical analysis on the thermal performance of circular and elliptical micro-pin-fin heat sinks with same perimeter

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For the last three decays, the flow and thermal characteristics of micro-pin-fin heat sinks have been extensively studied [1]. Previously, many studies investigated on the effect of micro-pin-fin with various shapes on the thermal performance [2]. Because the perimeters with the same characteristic length for various shapes are different, the contact area of micro-pin-fin with the working fluid varies. In the present study, numerical analysis on thermal performance of both circular and elliptical micro-pin-fin heat sinks with the same perimeter. Ansys-Fluent is employed for the investigation. Therefore, the influence of flow induced by various geometries of miro-pin-fin on the thermal performance of heat sinks can be investigated with the same convective area. The perimeter of an ellipse can be estimated by using Ramanujan formulas and listed as the following:

$$C \approx \pi\left[3(a+b) - \sqrt{(3a+b)(a+3b)}\right] \tag{1}$$

where a and b be the semi-major and semi-minor axes of an ellipse with perimeter C. There are three values of perimeters for circular and elliptical micro-pin-fin heat sinks. The physical model of the micro-pin-fin heat sink and the micro-pin-fin array are displayed in Fig. 1. The arrangement of micro-pin-fin array and number of micro-pin-fin are kept the same for circular and elliptical micro-pin-fin heat sinks. Results indicate that the elliptical micro-pin-fin heat sink demonstrated better thermal performance than that with circular micro-pin-fin for the same perimeter.

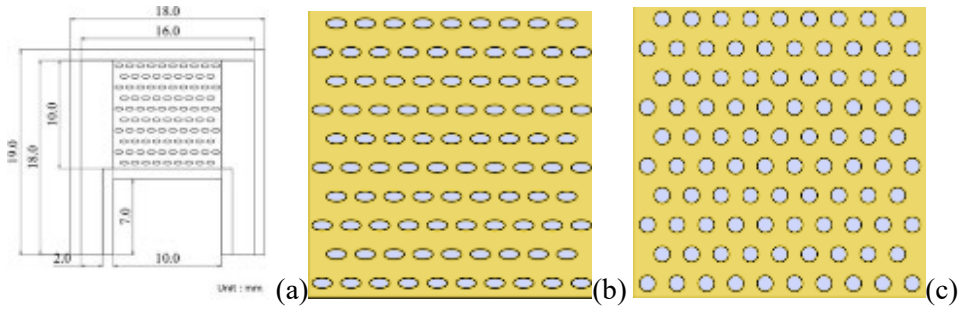

Figure 1. (a)geometry of the heat sink; (b)the array of elliptical micro-pin-fin in the heat sink with a=350□m, b=175□m; (c) the array of circular micro-pin-fin in the heat sink with the same perimeter as (b)

Keywords: micro-pin-fin heat sink, flow maldistribution, cooling performance, numerical analysis

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Physics-Informed Deep Inverse Operator Networks for solving PDE inverse problems

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This talk will introduce Physics-Informed Deep Inverse Operator Networks (PI-DIONs) for solving PDE-based inverse problems. Traditional operator learning methods typically require large amounts of labeled training data, which is often impractical in real-world applications. PI-DIONs, however, learn the solution operator without relying on labeled data. Experimental results show that PI-DIONs enable real-time inference across various inverse problems, achieving test errors comparable to supervised models. Additionally, we extend stability estimates from the inverse problem literature to the operator learning framework, providing a robust theoretical foundation for PI-DIONs.

Analytical solutions for thermo-hydro-mechanical coupled problems in layered saturated porous media

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The thermo-hydro-mechanical coupling is very important for many engineering problems, such as energy piles. Therefore, studying the coupled effect between temperature, seepage, and strain fields has become an important research topic. In terms of analytical research, Laplace, Hankel, and Fourier transforms are commonly used, which will make results not precise enough, and the boundary conditions are specific and singular. So far, none of the existing analytical solutions have considered the influence of soil layering. This study proposes a new solving method called the eigenfunction expansion method to solve thermos-hydro-mechanical coupled problems in multiple soil layers. This method can obtain accurate solutions and applies to various boundary conditions.

Keywords: Thermo-hydro-mechanical, analytical solution, layered.

Asymptotic Crack-tip Enriched Neural Network for Modeling Brittle Fracture Problems

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The analysis and prediction of brittle material fracture remain critical and long-standing challenges in solid mechanics due to stress singularities, complex crack paths, and the high computational cost of traditional numerical methods. Although conventional finite element methods are well-established, they often require intensive local mesh refinement to model sharp cracks and stress concentrations, leading to significant computational expense. Physics-informed neural networks (PINNs) [1] have emerged as an alternative for solving partial differential equations (PDEs) by incorporating PDE residuals into the loss function of a neural network. Their mesh-free nature offers advantages in flexibility and discretization. However, PINNs struggle with problems involving localized features such as cracks, as fully connected networks have limited ability to capture high-frequency components like stress concentrations or steep gradients near crack tips. Furthermore, they can be memory-intensive and computationally inefficient. To overcome these issues, this work proposes a model-based machine learning approach inspired by physics-augmented neural networks [2] and asymptotic crack-tip enrichment [3]. In this framework, known as the model-based neural network (MBNN), neural network components are constructed from analytical solutions, with asymptotic crack-tip functions embedded directly into the architecture to better capture localized behavior. The MBNN is further integrated into the PINN framework to enhance predictive accuracy in brittle fracture problems. Benchmark tests, including double cantilever beams and edge-cracked plates, validate the method's accuracy and robustness. Results show strong agreement with theoretical or analytical solutions, demonstrating the effectiveness of the proposed approach in capturing fracture behavior.

Keywords: Brittle fracture, Physics-informed neural networks, Model-based neural networks, Asymptotic crack-tip enrichment

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Rogue wave (RW) patterns are nonlinear wave phenomena universally present in integrable systems. When one or more free internal parameters in the exact RW

solutions of integrable systems like the nonlinear Schrödinger (NLS) equation are sufficiently large, the RW exhibit unique geometric patterns fully determined by the zero structure of the Yablonskii-Vorob'ev (Y-V) polynomial hierarchy. In this paper, we propose a deep learning-based "Polynomial Extractor for Rogue Wave Patterns" (PERWP). This approach replaces traditional asymptotic analysis of high-order RW solutions under largeparameter conditions, enabling automatic and precise identification of polynomial characteristics within RW patterns. We introduce a generalized polynomial hierarchy with parameters $\gamma_{k,j}$ that encompasses all Y-V polynomials relevant to RW patterns, serving as the target objective for PE-RWP. The unique dual-branch network architecture (with a regression branch for determining parameter values and a classification branch for identifying corresponding polynomial types) enables PE-RWP to effectively output this generalized polynomial hierarchy and recognize RW patterns subjected to arbitrary scaling and rotational transformations.

Furthermore, as an application based on the mathematical theory of RW patterns, we leverage the Y-V polynomials output by PE-RWP to achieve unsupervised localization of Peregrine through deep learning methods. Finally, through extensive experimental evaluation, both problems-polynomial extraction and Peregrine wave localization-are effectively solved with high accuracy

Generating Solutions for Partial Differential Equation by using Physics-Guided Generative Adversarial Networks

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Numerical analysis is essential across industries; however, in traditional finite element methods (FEM), computational time grows dramatically as the grid is refined or extended to three dimensions, and every change in boundary conditions necessitates a full re-computation. Recently, deep neural networks (DNNs) have been proposed and applied across many fields: although their training time can be long, their inference is fast. In mechanical engineering, DNNs have been used to obtain surrogate models. One approach is to infer the solution directly from specified boundary conditions [1], while another is super-resolution, where a low-resolution result is first obtained via numerical computation and then upscaled by a DNN to high resolution [2]. In this study, we adopt the former approach of inferring field variables from boundary conditions.

In this work, we extend that boundary-condition-to-solution approach to a broad class of steady partial differential equations (PDEs): namely, the two-dimensional Laplace equation, cavity flow, and back-step flow. For each case, high-resolution training data were generated using the finite element method (via the Python FeniCS library) or the finite volume method (via OpenFOAM with a k–ε turbulence model).

First, a generative adversarial network (GAN) is pretrained on this dataset, then refined using the physics-guided GAN (PG-GAN) framework [3]. Our approach decouples the generator's outputs from the neural network's computation graph, evaluates the physical residuals externally, and uses them to train the GAN. Unlike physics-informed methods, this allows arbitrary external solvers to enforce physical laws without embedding PDE operators inside the network, guiding the generator toward physically admissible solutions.

Finally, we perform quantitative evaluations of both interpolation within the training domain and extrapolation beyond it using a physics-informed GAN (PI-GAN) and a hybrid PI-PG-GAN. Moreover, PG-GAN's independent management of PDE and boundary-condition residual thresholds simplifies balancing these physical constraints. These results demonstrate that PG-GAN offers a versatile and extensible framework for learning solutions to general PDEs.

Keywords: Navier-Stokes equations, machine learning

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Multiscale Topology Optimization for Thermal-Fluid Systems
Using Variational Autoencoders

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Multiscale topology optimization (MTO) has emerged as a powerful design paradigm across a variety of engineering fields that require precise control over both microscale structure and macroscale behavior. By explicitly embedding microscale geometries—such as pores, fibers, or periodic cellular structures—within larger-scale domains, MTO enables the manipulation of effective material properties. These homogenized properties can exhibit anisotropic behavior.

Among these application areas, multiscale topology optimization in fluid systems has enabled the consideration of contact area as a design objective, opening possibilities for applications where fluid–solid interaction is critical, such as biosensing and microfluidic cell sorting, where increased interface area can improve detection sensitivity and capture efficiency [1].

To overcome the computational challenges of resolving microscale behavior at each optimization step, TOMAS [1] incorporates a variational autoencoder (VAE) that encodes key microstructural properties—such as supershape parameters, porosity, perimeter, and the permeability tensor $\boldsymbol{C}$—into a low-dimensional latent space $Z \in \mathbb{R}^2$, enabling rapid and efficient macro-scale optimization. While TOMAS lays the foundation for fluid-only systems, its extension to thermal-fluid coupling remains largely unexplored. This study proposes a VAE-based multiscale optimization framework for steady-state thermal-fluid systems

To model steady-state fluid flow through porous structures, we adopt a **Brinkman penalized formulation.** $\boldsymbol{u}$ is the velocity field, P is the pressure, and μ is the dynamic viscosity.
The term $\boldsymbol{C}^{-1}\boldsymbol{u}$ represents the Darcy drag induced by a porous microstructure, where **C** is the permeability tensor. This tensor captures anisotropic flow resistance. The corresponding heat transfer behavior is modeled using a **homogenized anisotropic conduction equation.**
T is the temperature field, Q is a volumetric heat source term, and $\boldsymbol{K}_{eff}$ is the **effective thermal conductivity tensor,** which captures thermal anisotropy**.** This tensor captures **thermal anisotropy** as well. ρ is the fluid density, and c_p is the specific heat capacity at constant pressure.

$$-\ \boldsymbol{\nabla} P + \mu \Delta \boldsymbol{u} - \boldsymbol{C}^{-1}\boldsymbol{u} = \boldsymbol{0}\ ,\ \boldsymbol{\nabla}\cdot\boldsymbol{u} = 0 \tag{1}$$

$$-\boldsymbol{\nabla}\cdot\left(\boldsymbol{K}_{eff}\boldsymbol{\nabla} T\right) + \rho c_p \boldsymbol{u}\cdot\boldsymbol{\nabla} T = \mathrm{Q} \tag{2}$$

Keywords: Topology optimization, Multiscale, Variational auto-encoders, Thermal fluid coupling

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A study on a database-driven conversational system for specific individuals

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This study explores the utilization of generative artificial intelligence (AI) to record personal data and develop interactive digital avatars that embody an individual's episodic memories, personality traits, and basic information. The primary objective is to uncover new value in personal data by enabling meaningful interactions with these avatars, which are designed to replicate the individual's characteristics and conversational style.

The research begins with a review of advancements in digital technology and generative AI, particularly the evolution of large language models (LLMs) such as ChatGPT, which have enabled human-like conversational capabilities.[1] Building on this foundation, the study proposes a method for creating digital avatars using personal data collected from social media, and other digital platforms. A prototype named "AI Zhu" was developed using Python, incorporating a database of 30 episodic memories and 68 related images.

Text vectorization was performed using BERT and text-embedding-3-small models, with the latter demonstrating superior performance in handling semantically similar queries. To retrieve the most relevant episodic memories, the system applies cosine similarity, a common method in natural language processing that compares the angle between two vectors to measure their semantic closeness. Higher values indicate a greater similarity between the query and stored memories.

Experimental results revealed that text-embedding-3-small outperformed BERT in accuracy for queries with similar meanings but different expressions. Prompt engineering was refined to enhance response naturalness, incorporating personality settings and guidelines for memory retrieval. The study also extended its scope to literary applications by vectorizing over 7,000 paragraphs from Romance of the Three Kingdoms, enabling interactive dialogues with characters.

This research highlights the potential of generative AI in personal data applications and immersive interactive experiences, while also identifying challenges such as multilingual search accuracy and ethical considerations. Future work will focus on improving data processing models, and providing users with an immersive experience that simulates direct dialogue with characters from Romance of the Three Kingdoms.

Keywords: generative AI, digital avatars, text vectorization, cosine similarity, interactive systems

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A stabilized LSMPS for three-dimensional complex free-surface flow with moving wall

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This study proposes a stabilized LSMPS method for simulating free surface flows with moving wall. In this stabilized LSMPS method, a novel wall velocity model is proposed for velocity divergence calculation and velocity interpolation.

$$\tilde{\mathbf{u}}_j = \mathbf{u}_i - (\mathbf{n}_{wall}^{n+1\,T} \cdot \mathbf{u}_i)\mathbf{n}_{wall}^{n+1} + (\mathbf{n}_{wall}^{n+1\,T} \cdot \mathbf{u}_{wall}^{n})\mathbf{n}_{wall}^{n+1}. \quad (1)$$

The proposed method also combines type-A and type-B LSMPS to enhance both accuracy and stability. Type-A LSMPS is applied to internal particles, while type-B scheme is used for free-surface and sub-free-surface particles. Additionally, type-B LSMPS is employed to interpolate the velocity after particle shifting. The stability of both type-A and type-B schemes is enhanced by the incorporation of positive values into the diagonal element of the least-squares matrix. To verify the developed LSMPS method, several three-dimensional numerical simulations are conducted. Fig. 1 shows the simulation results of dam break and sloshing compared with the experimental result. Rotating disk and gearbox is also simulated to further verify the developed method.

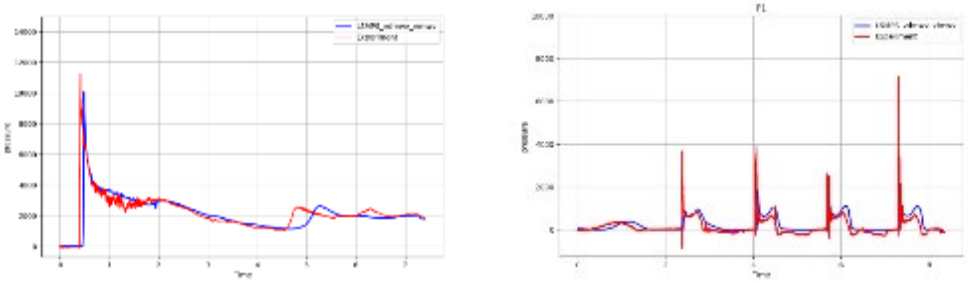

Figure 1. Calculated pressure profile in the dam break and sloshing problem.

Keywords: particle method; free surface; LSMPS

Comparative Study of Kirchhoff and Mindlin Plate Theories for Moving Load-Induced Response in Plate Structures

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This study investigates the time-dependent reactions of plate structures under moving loads by analyzing Kirchhoff (classical thin plate theory) and Mindlin-Reissner (first-order shear deformation theory). The focus is to determine how plate thickness and load velocity affect deflection and stress results in both theoretical models. A parametric framework based on finite element simulation models simply supported and cantilevered rectangular plates under constant-speed moving point loads. The Kirchhoff theory shows poor accuracy in displacement response predictions for medium to thick plates when load velocities increase because it ignores transverse shear deformation. The Mindlin theory generates more precise results throughout various thickness-to-span ratio values. The research demonstrates that thin plate assumptions fail to accurately predict responses during dynamic loading conditions while establishing selection criteria for suitable theories in moving load engineering applications, including pavements, bridge decks, and floor systems. The future research will broaden the current framework by adding damping effects and studying layered composite plates as well as their interaction with elastic foundations.

Keywords: Plate theory, moving load, vehicle bridge interaction, structural dynamics

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Numerical Investigation of the Aerodynamics and Performance of a Magnus Effect VAWT at Different Solidity and Tip Speed Ratios

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The Magnus vertical-axis wind turbine (VAWT) is designed to harness strong winds, including those from typhoons, and operates effectively across a wide wind speed range of 4 to 40 m/s, broader than that of conventional horizontal-axis wind turbines. However, due to the complex flow physics involved and the relatively recent emergence of the Magnus VAWT concept, research on its performance remains limited. To ensure consistent power generation across all cylinder positions while avoiding excessive energy input for spinning, a passive flow enhancement is employed, in which a flat plate is placed near each cylinder with a small gap [1]. This study investigates the aerodynamics and performance of a Magnus effect VAWT at varying solidity and tip speed ratios.

Three-dimensional, time-dependent fluid-structure interaction simulations were performed at a moderate Reynolds number using an in-house code that combines the direct-forcing immersed boundary method with the finite volume method and a large eddy simulation turbulence model. The governing equations are the incompressible filtered Navier–Stokes equations with an additional virtual force term, and the continuity equations. Meanwhile, the solid motion is defined as:

$$\boldsymbol{u}_c = (\boldsymbol{\omega}_R \times \boldsymbol{R}) + (\boldsymbol{\omega}_c \times \boldsymbol{r}) \text{ and } \boldsymbol{u}_p = \boldsymbol{\omega}_R \times \boldsymbol{R}, \quad (1)$$

where $\boldsymbol{u}_c$ and $\boldsymbol{u}_p$ represent the velocities of the cylinder and the flat plate, respectively. $\boldsymbol{\omega}_R$ and $\boldsymbol{R}$ denote the angular velocity and radius of the rotor, while $\boldsymbol{\omega}_c$ and $\boldsymbol{r}$ refer to the angular velocity and radius of the cylinder, respectively. All computations in this study were performed on the GPU cluster at the National Center for High-performance Computing, Taiwan.

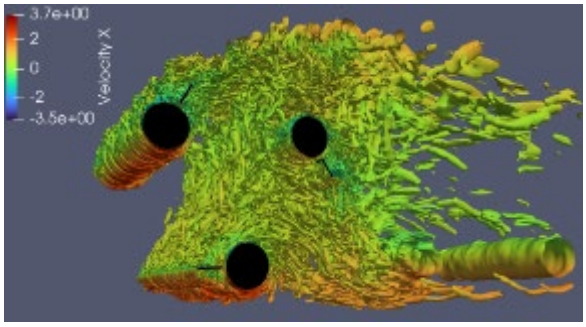

Figure 1.

The results indicate that the power coefficient is relatively high at low tip speed ratios, suggesting that with an optimal solidity ratio, the Magnus VAWT can respond efficiently in environments with frequent fluctuations in wind speed or direction, thereby maintaining a more stable power output.

Keywords: Fluid-structure Interaction, direct-forcing immersed boundary method, Magnus effect wind turbine, GPU computing

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A Physics-Informed Gaussian Process Regression Method to Infer Stokes Flows: Theory and Applications

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Stokes, or low-Reynolds number flows, characteristic of flows at small length scales or high-viscosity fluids, are ubiquitous in biology and applied sciences (e.g., microfluidics). In the case of an incompressible Newtonian fluid (viscosity μ), the equations that need to be solved, given appropriate boundary conditions, are the force balance (Stokes) and continuity equations,

$$\mu\nabla^2\mathbf{u} - \nabla p + \mathbf{f} = \mathbf{0}, \quad (1)$$

$$\nabla \cdot \mathbf{u} = \mathbf{0}, \quad (2)$$

with $\mathbf{u}$, $\mathbf{f}$, and p the velocity, external force, and pressure fields, respectively. While several numerical methods exist for solving this set of equations (e.g., Green's functions, Boundary Element, Stokesian Dynamics), they are not directly applicable to solving the inverse problem, i.e., that of reconstructing/inferring the flow field from missing and/or noisy data. For this, we have proposed a machine-learning method based on a physics-informed Gaussian Process (GP) regression scheme [1], which we refer to as a Stokesian Process (SP). Our method exactly incorporates the physics, given by equations (1) and (2), into the inference, as encoded in the GP kernel and the training data used to condition the resulting probability distribution.

This approach has been validated on simple 2D flows, where it was shown to be able to reliably infer the full flow solution from sparse and noisy data, and to outperform alternative machine-learning approaches (e.g., physics-informed neural networks) [2]. In this study, we extend the method to consider 3D flows with complex boundaries, which makes it an ideal method for analysing experimental data (e.g., inferring 3D flow/pressure fields from Particle Image Velocimetry measurements providing 2D components of the velocity field in a 2D domain).

Keywords: Stokes equation, Gaussian Processes, physics-informed, machine learning, Bayesian inference

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Data-Driven Forecasting of Subsurface Moisture in Unbound Pavements Using Climate Inputs

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Effective pavement management in regions prone to intense rainfall, such as Queensland, Australia, requires an in-depth understanding of moisture behaviour within unbound granular layers, especially when thin sprayed seals are present or absent. Excessive moisture ingress accelerates pavement deterioration, leading to structural failures. This study focuses on capturing and predicting the temporal variability of subsurface moisture, which is highly sensitive to climatic factors such as rainfall (RF), air temperature (AT), and relative humidity (RH). Accurate prediction of these variations is essential for both real-time decision-making and climate-resilient pavement design.

To address this challenge, the study investigates five classical machine learning (ML) algorithms, K-Nearest Neighbours (KNN), Decision Trees, Random Forests, Support Vector Machines (SVM), and Gaussian Process Regression (GPR). These models are trained on high-resolution data from a field-instrumented pavement site in Brisbane, incorporating real-time Volumetric Moisture Content (VMC) measurements and concurrent climatic variables. Unlike models using aggregated or averaged data, this approach utilizes actual time-step values and incorporates cyclical time components (daily and annual patterns), as reflected in the custom input structure:

$$VMC_t = f(Time, VMC_{t-1}, RF_t, AT_t, RH_t) \quad (1)$$

Model performance is evaluated using standard metrics: Coefficient of Determination (R^2), Mean Squared Error (MSE), Root Mean Squared Error (RMSE) and Mean Absolute Percentage Error (MAPE). Among the tested models, the Medium Random Forest algorithm achieved the highest predictive accuracy ($R^2 > 0.98$, RMSE < 0.15, MAPE < 2%). KNN (with N=15), Medium Decision Tree, Coarse SVM, and a basic GPR configuration also showed strong performance. Furthermore, the study identifies optimal hyperparameter settings for each model, offering practical implementation guidance for pavement monitoring applications.

This work demonstrates the value of machine learning-based tools in forecasting subsurface moisture under dynamic climatic conditions, supporting more robust pavement design and proactive maintenance strategies.

Keywords: Pavement moisture prediction, unbound granular materials, Machine learning, Climatic factors, Real-time monitoring

Numerical Simulation of Bone Regeneration in Architecturally Heterogeneous Scaffolds for Large Segmental Defects

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Bone tissue scaffolds play a pivotal role in regenerating critical-sized defects by providing a structural environment conducive to cellular infiltration and new tissue formation. Among various architectural strategies, designs that vary spatially in porosity and pore size have attracted considerable interest for their potential to mimic the hierarchical structure of native bone. However, the effectiveness of such advanced scaffold architectures in promoting bone regeneration across large segmental defects remains poorly understood. This study employs computational modeling to investigate how spatial variations in scaffold architecture influence bone healing in large defects.

We integrate finite element analysis (FEA) with agent-based modeling (ABM) to simulate bone regeneration within anatomically relevant tibial defects in sheep over 3, 6, and 12 months. The ABM captures essential cellular behaviors—including proliferation, migration, apoptosis, and differentiation—within a discretized 3D environment, with cell fate determined by local mechanical stimuli according to a mechano-regulation algorithm. The FEA component models the evolving mechanical environment using a biphasic poroelastic formulation that incorporates scaffold geometry and fixation hardware to closely mimic in vivo loading conditions.

Scaffold architectures with spatial variation in pore characteristics along both radial and axial directions are examined to determine their influence on bone formation and mechanical stability. The scaffolds' mechanical properties are also compared to investigate how these spatial variations in pore characteristics affect their load-bearing capacity.

The results demonstrate how scaffold architectures with spatially varying features affect the rate and pattern of bone ingrowth across time. Differences in gradient orientation significantly influence bone volume and mechanical performance. These findings offer valuable insights into the design of porous scaffolds with tailored internal architectures to enhance bone repair, providing a computational framework to guide the development of more effective treatment strategies for critical-sized bone defects.

Keywords: Finite element analysis (FEA); Agent-based modelling (ABM), Bone scaffold; Tissue regeneration

Numerical Study on Hemodynamics Affected by Flow-Diverter Stent Placement Position

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An intracranial aneurysm is a cerebrovascular disorder characterized by a localized, balloon-like dilation of a cerebral artery. Among the available endovascular therapies, the Flow-diverter Stent a cylindrical device woven from metallic wires has gained wide acceptance. This stent is delivered via microcatheter and deployed across the aneurysm neck to redirect blood flow and initiate gradual occlusion. However, clinical outcomes remain suboptimal in large or complex aneurysms due to the inherent variability in treatment response [1].

Recent studies emphasize that achieving effective flow diversion depends heavily on precise deployment of the device [2,3]. Improper positioning can alter intra-aneurysmal hemodynamics, potentially leading to elevated flow or pressure that compromises occlusion stability. Such adverse conditions may partly explain the inconsistent efficacy observed in the treatment of giant aneurysms.

This work evaluates the hemodynamic effects of stent placement configurations and proposes a deployment strategy to enhance therapeutic performance. As shown in Fig. 1, stent expansion was modeled using the Finite Element Method, followed by flow analysis via the second-generation Particle Finite Element Method. Blood rheology was captured using the Carreau model to represent its shear-thinning behavior. The simulation results elucidate the relationship between device location, flow velocity, and pressure distribution, and comparative assessments across aneurysm types are discussed.

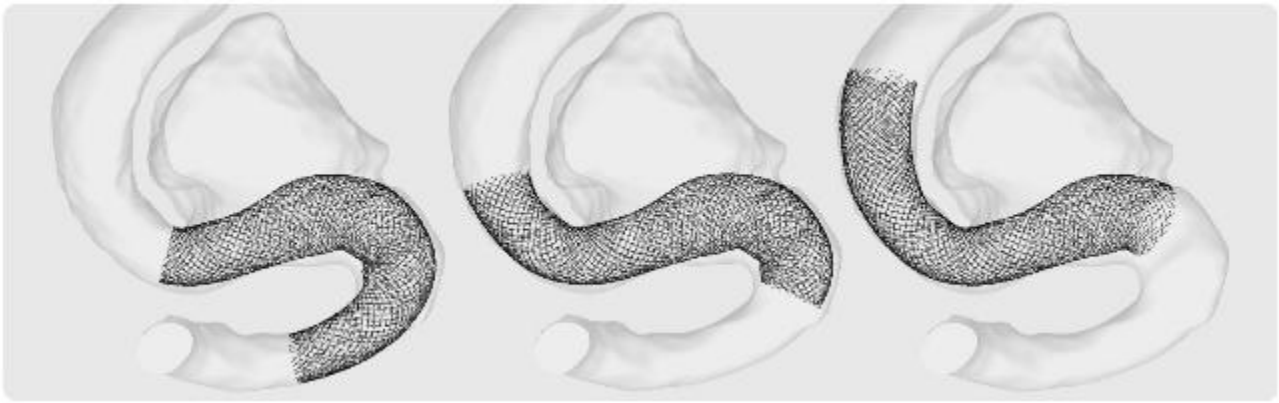

Figure 1.

Keywords: Cerebral aneurysm, Flow diverter, Stent, FEM, PFEM-2, Placement position

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Acoustic Drug Delivery to Paranasal Sinuses: Particle Size Impact

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Chronic rhinosinusitis (CRS) is a common inflammatory condition affecting approximately 10% of the global population [1]. Topical drug delivery methods, such as nasal irrigation with squeeze bottles, nasal sprays, and nebulisers, are frequently employed for CRS treatment. However, current techniques exhibit significant limitations. Squeeze bottles demonstrate low efficiency, with drug delivery efficiencies often below 3% [2]. Nasal sprays typically produce large particles (50–100 microns) that predominantly deposit in the anterior nasal regions, resulting in negligible sinus penetration [3]. Nebulisers, particularly when combined with acoustic waves (acoustic drug delivery), have shown improved drug delivery efficiencies [4].

This study investigates the impact of nebulised particle size on the effectiveness of acoustic drug delivery to the paranasal sinuses. Computational Fluid Dynamics (CFD) and direct Computational Aero-Acoustics simulations were employed to: (1) determine the resonance frequency of the sinonasal cavity and (2) analyse how particle size influences drug delivery efficiency. Two particle distributions were evaluated: mono-dispersed and poly-dispersed. Mono-dispersed particle sizes ranged from 4 to 16 microns in increments of 4 microns, while poly-dispersed particles were modelled using a Rosin-Rammler distribution with mean particle diameters ranging similarly from 4 to 16 microns. Simulations employed laminar flow conditions, considering bidirectional delivery—particles entered through one nostril and exited via the opposite nostril. The Euler-Lagrange discrete phase model (DPM) was used to simulate two-way coupling interactions between airflow and particles.

Results indicated that particle size significantly affects both the acoustic Stokes number and particle entrainment coefficient. Specifically, increasing particle size reduces the acoustic Stokes number, meaning larger particles are less responsive to acoustic oscillations and thus exhibit reduced penetration into the sinuses. Consequently, optimal particle sizing is critical for maximising the efficacy of acoustic drug delivery in treating CRS.

Keywords: Keywords: Acoustic drug delivery, Particle tracking, Particle size optimisation, Computational fluid dynamics

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Engineering Direct-Write Ultrasonic Sensors for NDT and SHM: Challenges and Solutions

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Direct-write (DW) ultrasonic sensors are an emerging and specialized type of ultrasonic sensor that offer significant advantages over conventional designs. These sensors are typically thin, lightweight, and flexible, and can be directly printed onto non-planar, curved, or complex surfaces without requiring traditional packaging, bonding, or coupling layers. This enables seamless integration into a wide range of structural components, making them highly attractive for next-generation sensing systems.

To further develop DW ultrasonic sensors for practical applications across various industries, it is essential to understand and optimize ultrasonic wave generation, propagation, and signal processing. This work is supported through close collaboration with industry partners throughout the supply chain, facilitating the delivery of structural health monitoring (SHM) solutions by local engineering and manufacturing firms.

In this study, we focus on three key areas: (a) the generation and detection of zero-group-velocity (ZGV) Lamb waves for advanced non-destructive testing (NDT); (b) the development of robust algorithms for effective SHM; and (c) the application of data-driven methods for material characterization.

These advancements collectively contribute to the growing potential of DW ultrasonic sensors in real-world scenarios, offering a scalable, customizable, and cost-effective solution for long-term structural integrity monitoring.

Keywords: Lamb waves, direct-write ultrasonic sensors, non-destructive testing, machine learning, material characterization

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Analysis of the initiation of motion of alluvial river-beds of different particle size using CFD-DEM approach

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This study employs numerical method to analyse the first stage of the sediment transport process commonly known as 'Initiation of Motion'. This study applies the microscopic approach of continuum-particulate modelling for the fluid-particle interaction, which couples computational fluid dynamics and discrete element method (CFD-DEM) by using the coupling of OpenFOAM and LIGGGHTS packages for the coarse-grained approach. Unlike the fine-grained approach where the flow around the particle is resolved, the coarse-grained approach allows large number of particles to be simulated which is appropriate sediment transport applications.

The simulation setup is represented in the Figure 1 with the simulations carried out with different flow and bed properties to achieve hydrodynamically smooth, buffer and rough flows with uniformly distributed bed of particle 0.1mm, 1mm and 10mm respectively. These different sized particles also represent the three different zones in the Shields diagram i.e. laminar (0.1mm), buffer (1mm) and turbulent (10mm) zone.

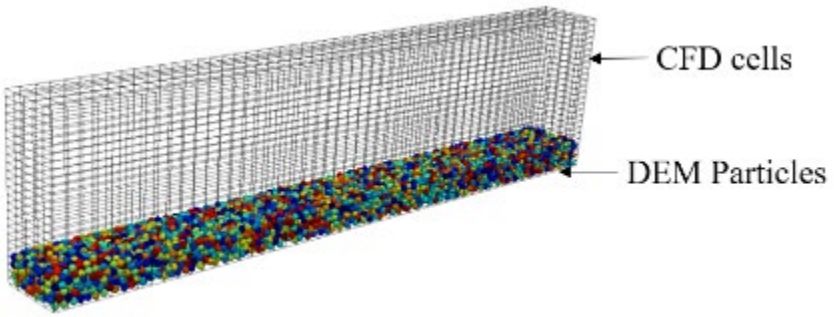

Figure 6 Simulation setup with CFD cells and DEM particles

The fluid flow profiles which is applied in the model was analyzed with the turbulence parameters which is validated with analytical data. The shear stress at the bed surface calculation is carried out with the incorporation of the wall models based on the near bed distance (y+). With the current approach, there is good agreement with the function of initiation of motion in the Shields diagram proposed by Soulsby and Whitehouse (1997) for different particle sizes. Hence, the coarse-grained approach shows potential for the application of CFD-DEM in the field of sediment transport.

Keywords: Sediment transport, Navier-Stokes equations, Computational Fluid Dynamics, Discrete Element Modelling

Reference:

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Study on mechanics test and simulation of layered rock under impact loading

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Layered rock mass is a complex natural mineral composite, with different rock bodies containing varying mineral compositions and various internal defects. Consequently, it exhibits heterogeneity and anisotropy in mechanical properties. These characteristics significantly influence the mechanical behaviors of rock, such as deformation capacity, strength, fracture toughness, and failure modes, playing a crucial role in determining the structural stability of rock under various loads. This study employs RFPA-dynamic to meticulously reproduce the entire process of crack initiation, propagation, and coalescence in layered rock mass models under dynamic impact loading. Furthermore, a series of physical experiments involving static loading, dynamic loading, and combined static-dynamic loading for rock fragmentation were conducted to validate the developed numerical model. The results from both approaches align well, demonstrating that the established numerical model can effectively simulate the complex macroscopic anisotropic phenomena of rock and reproduce the rock fragmentation process as well as crack distribution patterns. This work addresses the current gaps in most experimental and numerical studies regarding the insufficient understanding of stress accumulation, stress release, and stress transfer (SSS) processes induced by variations in bedding spacing, stress wave peak values, and pre-stress magnitudes.

2D incompressible viscous flow analysis based on NURBS-Enhanced FEM (NEFEM)

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Recently, digital fabrication technologies have gained attention in the civil engineering field. 3D printers enable the creation of complex shapes, and Isogeometric Analysis (IGA) [1] is used for analyzing arbitrary shapes. While IGA uses NURBS Spline functions from CAD software, these higher-order functions require substantial computation time. To address this issue, NURBS-Enhanced Finite Element Method (NEFEM) [2][3] has emerged as a solution. NEFEM applies linear interpolation for internal elements (like traditional FEM) while using Spline interpolation for boundary elements, allowing accurate shape representation with reduced computational load.

This paper presents the flow around a cylinder, which is a benchmark problem in incompressible viscous flow analysis, and the validity and effectiveness of the NEFEM fluid analysis method using the Navier-Stokes equations are examined. The flow velocities in the direction of flow were visualized by both NEFEM and linear FEM. It was confirmed that periodic Kalman vortices were generated behind the cylinder. It was confirmed that similar analytical results were obtained by both methods, although qualitatively. As a quantitative evaluation, the relative error of the drag coefficient around a cylinder to the reference solution and the computation time were compared for both NEFEM and FEM methods. It can be concluded that the NEFEM showed an accuracy improvement of about 4% compared to the FEM, confirming its usefulness. In the future, we plan to use NEFEM to perform fluid analysis around structures with complex geometries.

Keywords: Navier-Stokes equations, NURBS, NURBS-Enhanced FEM, NEFEM, FEM, IGA

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Breakdown of soft food solids in the stomach from coupled mechanical and chemical processes using an SPH based model

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Human digestion of food is substantially performed by the stomach. This involves coupled mechanical, fluid and particle dynamics as well as chemical and enzymic dissolution processes. This is computationally challenging with broad array of physical processes on a range of timescales. Digestive processes are driven by large amplitude waves in the stomach walls providing a complex agitation of the multiphase stomach content as well as mechanical interactions with soft foods. Acid and enzyme generation, mixing and transport also play an important role controlling dissolution and softening of solids allowing them to be physically broken down by the mechanical processes with compression and extrusion and/or fracture of sufficiently soft and degraded food matrix structures. Once smaller food particulates are generated then these are preferentially able to discharge through the pylorus. The fluid-particle-wall interactions around the open pylorus also affect this selection process which then controls the residence time of food being retained in the stomach for breakdown.

In this paper, a biomechanical SPH model with DEM based particulate components is used to model all parts of this important system. The basic model was proposed in [1] and has been extended to include mechanical breakdown [2] and acid transport and mixing [3]. Here, an initial model for the chemical dissolution and softening of the solid food bodies has been added to the model which allows effects from the softening and degradation of the food to be included in the simulations. This allows exploration of important coupled breakdown mechanisms. In addition, fluid dynamic stratification and its contribution to gastric sieving are explored. Figure 1 shows gastric sieving predicted using a coupled SPH+DEM method. This is a consequence of vertical stratification of solids with larger solids accumulating at the bottom of the stomach where they can be mechanically degraded with smaller solids located higher in the stomach and proximate to the pylorus allowing their preferential discharge.

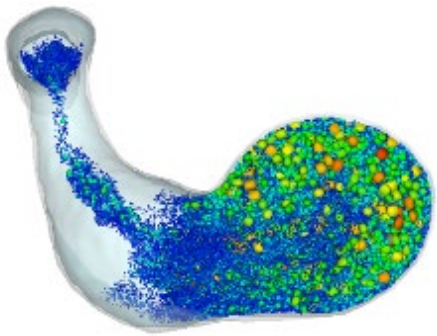

Figure 1. Gastric sieving predicted using a coupled SPH+DEM method.

Keywords: Human digestion, SPH, DEM, fluid dynamics, mixing, solid deformation

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Physics-guided computational model for airborne inhaled transmission of pox viruses

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Inhalation of airborne virus-laden aerosols and droplets can be a significant transmission route for poxviruses, even without direct contact between an infected host and an exposed individual. Understanding how airflow physics influences the movement of these particulates within the respiratory tract is crucial for elucidating the mechanism behind such infections. This study uses smallpox (caused by the variola virus) as a representative pathogen of the orthopoxvirus family, where the virus affects the oropharyngeal tissues (the lower part of the pharynx) and subsequently spreads throughout the tracheobronchial region of the respiratory system. Is it possible to identify the inhaled particulates that would land at the infective tissue sites along the airway and the viral load carried by them? More critically, what could be the critical exposure duration for such an infection onset? Our study addresses these central questions with a numerical model that captures physiologically realistic inhaled transmission. We employ high-fidelity Large Eddy Simulations of airflow and particulate motion within anatomically realistic respiratory domains reconstructed from medical-grade computed tomography imaging. Our projections for the critical exposure duration necessary for infection onset, derived from integrating flow physics trends with viral concentration in inhaled particulates and individual immunological factors, range from 0.4 to 12.0 hours, which is consistent with existing literature on smallpox. This finding underscores the potential applicability of our mechanics-driven in silico framework for realistically modeling the transmission dynamics of other emerging pathogens in the poxvirus family, such as mpox. Furthermore, we validate the numerically simulated transmission trends through physical experiments conducted within 3D-printed anatomical airway casts and with a reduced-order analytical framework that examines the effects of local vortex instability on tracheobronchial transport.

The quantification of domain effect in external flow simulations using physics informed neural network

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The effect of domain size in external fluid structure interaction simulations are difficult to quantify. Domain size affects the location of the boundary. For asymptotic boundaries such as uniform velocity inlet, or symmetry, these boundaries are mathematically only correct in an infinitely large domain. Applying it on a finite domain may cause some error in the simulation.

After successfully quantifying the effect of mesh using physics informed neural network (PINN) [1], we now aim to quantify the effect of domain by using PINN as well. This is done by making the PINN resolve the same problem as the numerical simulation with the original governing equation and a parameterized governing equation that parameterize all spatial coordinates using a sigmoid function, changing the infinite domain into a finite space. Using triangle inequality, it is possible to convert these two PINN error estimations to obtain the effect of the domain exclusively.

To evaluate this concept, we tested it on a manufactured one-dimensional diffusion & a two-dimensional swirling flow, which we both know the analytical of. An example of this error estimation is shown in figure (1), which shows that the PINN estimation is always accurate and it is possible to quantify the effect of the domain. We also found that the estimation can be done on coarse mesh, although fine mesh simulations produce a better estimate. Additional testing on a flow past cylinder would also be conducted for a practical demonstration.

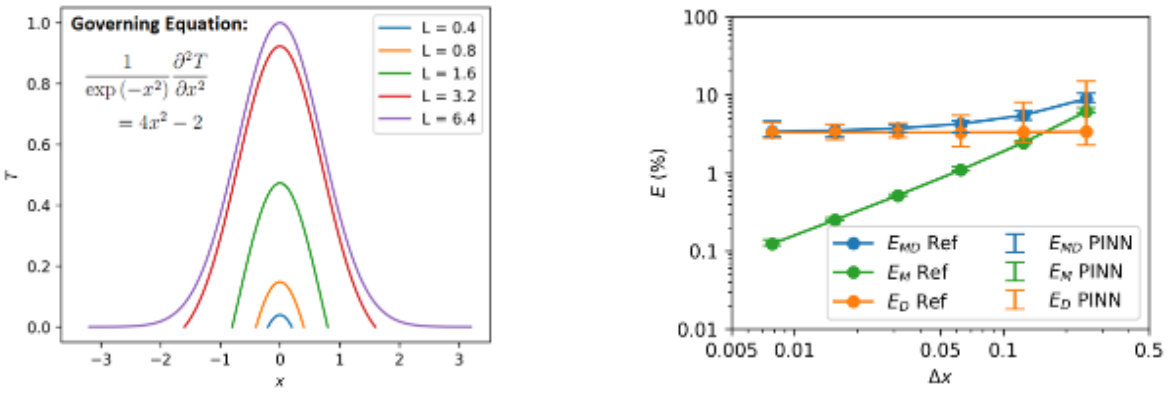

Figure 1. The results of the a one-dimensional diffusion case. (Left) The analytical solution at different length. (Right) The error estimation at $L = 4$. E_{MD} is the error due to mesh and domain, E_M is the effect due to mesh and E_D is the effect due domain only.

Keywords: Domain Independence, External Flow Simulation, Verification & Validation, Physics-Informed Neural Network, Fluid Structure Interaction

Acknowledgment: The first author would like to acknowledge the Research Attachment Programme research grant from the Agency for Science, Technology and Research (A*STAR) Singapore.

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Data-Driven Forecasting of Subsurface Moisture in Unbound Pavements Using Climate Inputs

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Effective pavement management in regions prone to intense rainfall, such as Queensland, Australia, requires an in-depth understanding of moisture behaviour within unbound granular layers, especially when thin sprayed seals are present or absent. Excessive moisture ingress accelerates pavement deterioration, leading to structural failures. This study focuses on capturing and predicting the temporal variability of subsurface moisture, which is highly sensitive to climatic factors such as rainfall (RF), air temperature (AT), and relative humidity (RH). Accurate prediction of these variations is essential for both real-time decision-making and climate-resilient pavement design.

To address this challenge, the study investigates five classical machine learning (ML) algorithms, K-Nearest Neighbours (KNN), Decision Trees, Random Forests, Support Vector Machines (SVM), and Gaussian Process Regression (GPR). These models are trained on high-resolution data from a field-instrumented pavement site in Brisbane, incorporating real-time Volumetric Moisture Content (VMC) measurements and concurrent climatic variables. Unlike models using aggregated or averaged data, this approach utilizes actual time-step values and incorporates cyclical time components (daily and annual patterns), as reflected in the custom input structure:

$$VMC_t = f(Time, VMC_{t-1}, RF_t, AT_t, RH_t) \quad (1)$$

Model performance is evaluated using standard metrics: Coefficient of Determination (R^2), Mean Squared Error (MSE), Root Mean Squared Error (RMSE) and Mean Absolute Percentage Error (MAPE). Among the tested models, the Medium Random Forest algorithm achieved the highest predictive accuracy ($R^2 > 0.98$, RMSE < 0.15, MAPE < 2%). KNN (with N=15), Medium Decision Tree, Coarse SVM, and a basic GPR configuration also showed strong performance. Furthermore, the study identifies optimal hyperparameter settings for each model, offering practical implementation guidance for pavement monitoring applications.

This work demonstrates the value of machine learning-based tools in forecasting subsurface moisture under dynamic climatic conditions, supporting more robust pavement design and proactive maintenance strategies.

Keywords: Pavement moisture prediction, unbound granular materials, Machine learning, Climatic factors, Real-time monitoring

Physics-Augmented Neural Network for Constitutive Modelling of Meniscal Root with Meshfree Simulation of Knee Joint Contact

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Meniscal roots are ligament-like structures that anchor the menisci to the tibia. They are essential for maintaining hoop stress and enabling effective load transmission [1]. Accurate modelling of these composite-like structures, including both hardening and softening behaviour, is critical for evaluating knee function and informing surgical repair strategies. Traditional constitutive models based on common hyperelastic formulations and empirical damage laws can capture nonlinear behaviour, but they often fail to match experimental data accurately, limiting their ability to reflect the underlying tissue mechanisms. Recently developed machine learning tools, such as deep neural networks (DNNs), offer greater flexibility in fitting experimental observations. However, these machine learning tools lack physical grounding and perform poorly in extrapolation, making them less effective during simulations. To address these challenges, we developed a physics-augmented neural network (PANN) framework that integrates constitutive artificial neural network [2] with mechanics-inspired progressive damage architecture to better capture the mechanics of meniscal roots at different stages of loading. The progressive damage formulation is based on building blocks of conventional linear, polynomial and exponential softening law, with embedded physical constraints, such as irreversibility. The effectiveness of the proposed model is evaluated by comparing it with conventional phenomenological models and DNN-based fittings using experimental data (Figure 1). The PANN framework shows improved accuracy in capturing nonlinear and softening responses while preserving physical consistency. Finally, we incorporate the learned meniscal root model into our meshfree formulation [3] to investigate knee joint contact mechanics, demonstrating the meshfree method's effectiveness for soft tissue modelling due to its ability to handle extreme deformations and complex contact interactions without mesh distortion. This integration enables joint-level biomechanical analysis and supports surgical repair planning.

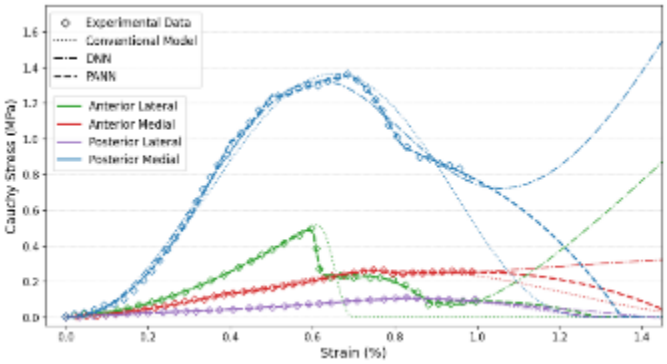

Figure 1.

Keywords: Meniscal root, constitutive models, physics-augmented neural network, progressive damage model, meshfree method

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An Implicit Gradient Regularized RK-MPM for Micro-Crack Informed Damage Simulation via Physics-Augmented Neural Networks

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Modeling cross-scale fracture-to-damage transitions remains a fundamental challenge in extreme event simulations. Capturing macroscale damage parameters informed by microscale fracture mechanics and crack patterns requires not only a deep understanding of multiscale mechanisms, but also a robust numerical tool capable of mitigating discretization sensitivity and pathological strain localization resulting from insufficient regularization. In this study, we present a length-scale regularized meshfree framework for simulating damage localization, where damage evolution is informed by microcrack data through physics-augmented neural networks. Our approach builds upon the concept of constitutive artificial neural networks [1], using neural network building blocks to generalize damage mechanisms derived from microcrack patterns [2]. This microcrack-informed damage model is embedded within our previously developed reproducing kernel-enhanced material point method (RK-MPM) [3], enabling accurate modeling of material separation due to damage. Numerical instabilities typical of standard MPM are addressed through RK enhancements and stabilization strategies, as detailed in [3]. However, unregularized damage formulations in RK-MPM remain prone to strain localization and mesh dependency. To overcome this, we incorporate implicit gradient regularization [4], introducing an intrinsic length scale via a nonlocal strain approximation. This addition effectively mitigates mesh sensitivity while preserving computational efficiency. The resulting framework—integrating RK-MPM, implicit gradient regularization, and machine learning-enhanced micro-to-macro damage modeling—is validated through benchmark problems. Results demonstrate improved accuracy, robustness, and computational efficiency, highlighting strong potential for simulating complex multiscale failure phenomena.

Keywords: Implicit gradient, physics-augmented neural networks, damage localization, reproducing kernel (RK) approximation, material point method (MPM)

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Template for APCOM-ACCM 2025 Abstract Submission

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A hybrid energy extraction system of a floating offshore wind turbine and tidal current turbine is promising for levelized cost reduction in the wind-tidal co-existed area[1]. An evaluation of such a system is quite important before practical application but are not well done due to limited simulation tools[2-3]. To investigate the dynamic response and power output performance of such a system, a novel coupled aero-hydro-servo-elastic tool based on OpenFAST-AQWA framework together with a code that can deal with the coupling between tidal hydrodynamic load and platform motions. A novel WindFloat based wind-tidal hybrid system is proposed as a representative to validate the tool. Motions, mooring loads, blade response, tower response and power output of the hybrid system are investigated under different wind-wave-current combined conditions to examine the interactions between tidal turbine, platform, wind turbine and mooring system. Results showed that the tidal turbine brings no harm to the stability of the system and the wind turbine power output has been increased by 3.83% and the power output oscillation decreased by 6.7%. The motion and mooring load oscillation have been reduced due to the extra damping originated from the tidal current turbine, while the average load of the mooring line parallel to the wind direction has been enlarged. Besides, the structure response of the tower and blade benefited from the tidal current turbine especially for the tower base load. This study demonstrated the advantage of integrated system in energy extraction and provided a novel performance evaluation tool for similar wind-tidal hybrid system.

Keywords: Wind-tidal hybrid system; floating wind turbine; tidal current turbine; coupled analysis; dynamic response, power output

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Application of Neural Operators to Inverse Problems in Solid Mechanics Based on Randomly Generated Training Data

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Fundamental performances of Neural Operators as surrogate models are presented for analysis of inverse problems associated with complex physical phenomena characterized by heterogeneous spatial distributions. The primary objective is to enhance computational efficiency by using Fourier Neural Operators (FNO) [1] with training data based on randomly generated material property distributions [2]. Inverse analyses, including topology optimization and the estimation of heterogeneous material properties, were conducted to assess the performance of the surrogate model, that is trained using FNO. The results indicate that FNO outperformed conventional Convolutional Neural Network, such as ResNet, under specific conditions. The correlation length and exponent settings for generating random distribution significantly impacted model accuracy. Moreover, the superiority of the FNO extends beyond model accuracy to the outcomes of inverse analyses. Surrogate models constructed with FNO provided optimization results closer to the reference solution, as illustrated in Figure 1. This study confirms the potential of Neural Operators to achieve near-global optimal solutions in inverse problems that are otherwise challenging to solve, highlighting their applicability to real-world engineering challenges. Future research should explore the broader applicability of this approach to more complicated nonlinear problems.

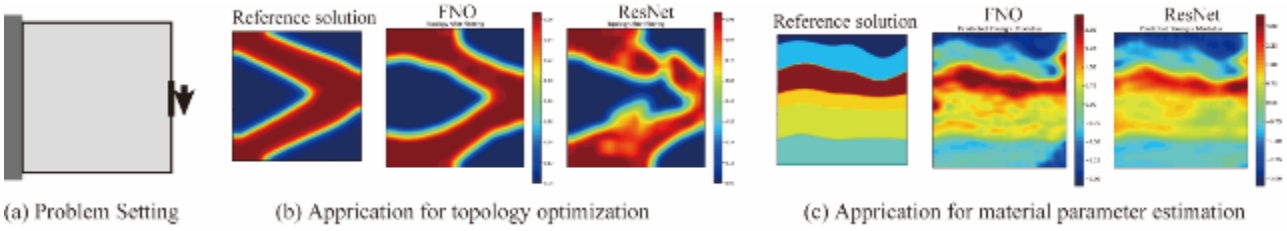

Figure 1. The results of inverse analysis using surrogate models

Keywords: Fourier Neural Operator, Topology Optimization, Heterogeneous Field Estimation

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Edge-Dislocation Behaviour under Wide Range of Hydrogen Concentrations and Mechanical Conditions: DFT, MD and Theoretical Analyses

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To effectively and safely use metallic materials under hydrogen environments, the clarification of the mechanisms of hydrogen embrittlement (HE) is crucial. The microscopic origin of HE is the modification of mobility and stability of lattice defects. The dislocation-hydrogen interaction has been attracted large attention since it is quite important for plastic deformation and fracture. Many literatures have been published which treated the behaviours of edge and screw dislocations in Fe and steels under hydrogen environments.

In this study, we treat edge dislocations in bcc-Fe since an edge dislocation has a much stronger interaction energy with hydrogen than a screw dislocation has, and an edge dislocation is densely decorated by hydrogen atoms when a screw dislocation traps hydrogen. In literatures, hydrogen enhanced mobility [1], dislocation pinning by hydrogen and depinning [1-3], hydrogen dragging by dislocation [1, 2, 4], and twinning initiation from pinned dislocation were discussed [5]. Here we treat the transition between these behaviours, especially pinning and depinning, dragging, and twinning, by molecular dynamics (MD) simulations, density functional theory (DFT) calculations, and theoretical modelling. The long-term MD simulations over micro-seconds clarified the transitions between three different behaviours as a function of temperature, dislocation velocity, and hydrogen concentration. The comprehensive large-scale DFT calculations of hundreds Fe atoms clarified the qualitative trap behaviour of hydrogen atoms around the dislocation core. The theoretical models based on the transition state theory for three different interactions were developed. After the validation of the theoretical models through the comparison with MD results, some parameters in the theoretical models were fine-tuned by using DFT results and the dislocation behaviour at practical conditions were predicted. The theoretical models are applicable for other additives such as carbon and nitrogen atoms through DFT evaluation of parameters.

Keywords: hydrogen, dislocation, diffusion, iron, molecular dynamics, density functional theory

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Large deformation behavior of lattice structure in compression: Experiments, finite element analysis and analytical modelling

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Lattice structures have garnered significant attention in industrial applications due to their exceptional mechanical properties and superior energy absorption capabilities. The nonlinear response of these structures under extreme loading conditions can critically influence their mechanical performance and safety. While previous studies have predominantly focused on the parametric properties of lattice structures in the linear elastic phase, there has been limited exploration of their plastic large deformation behavior. In this study, the BCC lattice structure was selected, and several samples were fabricated by selective laser melting (SLM) method using 316L stainless steel (316L SS) to systematically analyze the compressive behavior of the structure during the plastic large deformation stage. A theoretical model was developed based on an idealized deformation mechanism and subsequently validated through finite element (FE) analysis and experimental methods. The influence of geometrical parameters on the compression response of lattice structures was thoroughly investigated, and the applicability of the theoretical model was critically discussed.

Keywords: Additive manufacturing; Lattice structure; Rigid-perfectly plastic; Large deformation; Compressive response; Experiment and simulation

A phase-field model for fault rupture and growth

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Numerical simulation of fault rupture processes is becoming increasingly popular as a means for studying earthquake mechanics. However, these simulations are difficult to perform due to the complexities of fault geometry and off-fault damage, among other reasons. This talk introduces a new phase-field approach for modelling fault rupture and growth under in-plane and anti-plane conditions [1,2]. Built on a phase-field formulation for frictional fractures [3,4], the new phase-field model incorporates rate- and state-dependent friction, radiation damping, and stress-dependent fault nucleation and propagation criteria. The resultant formulation can represent complex fault growth without sophisticated crack-tracking algorithms. Additionally, it can capture off-fault damage within a single framework. We verify the phase-field model with a discontinuous method for fault rupture simulations. We also demonstrate the capabilities of the phase-field model by simulating complex fault nucleation and growth processes with structural and material complexities.

Keywords: Earthquake, Fault rupture, Fault nucleation and propagation, Phase-field modelling, Radiation damping, Rate-and-state friction

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Prior Knowledge-Informed Adaptive Federated Dual Scenario Graph Neural Network for Boil-Off Gas Generation Prediction

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Abstract

Liquefied Natural Gas (LNG) evaporates and generates Boil-Off Gas (BOG) during storage in tanks. Accurately predicting BOG is crucial for optimizing operational efficiency and maximizing the economic benefits of LNG receiving stations. Existing physics-informed neural networks incorporate physical information into the constraints of the loss function, resulting in slow convergence and limited interpretability. Additionally, different receiving stations encounter challenges in improving model performance by sharing their data due to data privacy protection clauses. We proposed the architecture of the Prior Knowledge-Informed Adaptive Federated Dual Scenario Graph Neural Network (PKI-AFDSGNN), which embedded the Prior Knowledge(PK) from real industrial systems into the training process of neural networks from a novel perspective. First, we analyzed the heat transfer phenomenon of the BOG generation process within the LNG tank system to formulate the PK for unloading and non-unloading scenarios. Second, we developed a node-dependent weight self-learning algorithm based on PK, which facilitated the training of graph neural networks in a more interpretable manner. Additionally, based on the federated learning framework, we adaptively determined whether to perform uploading and downloading operations on the client and server sides, depending on the model performance of the current round under unloading and non-unloading conditions, to enhance the prediction capability of the model on each client side. Finally, we predicted the BOG generation using a real dataset from a receiving station in China, thereby verifying the effectiveness of PKI-AFDSGNN and demonstrating the necessity of its components through numerous comparative experiments.

Keywords:

Prior knowledge, Federated learning, Graph neural network, Physics-informed neural networks, BOG generation prediction

Fluid-structure interactions: multiple filaments, inflating balloon, badminton shuttlecock

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The vortex-induced vibration of flexible filaments attached behind an array of side-by-side stationary cylinder is studied. We explore the response of the filaments for a wide range of flexibility and inertia. Lock-in with the various normal modes of the filament, each in a different regime of reduced speed, is observed. Several branches, based on response of the filaments, are identified. The transition between different branches is found to be hysteretic and intermittent. The flow exhibits a variety of vortex-shedding patterns. The inflation and deflation of a balloon is modeled via a membrane. Ovalling oscillations are observed during inflation. A simple model for failure of balloon is proposed. The aerodynamics of a badminton shuttlecock is investigated. It is shown that the deformation of the shuttle impacts the flow and drag very significantly. The skirt of the shuttle undergoes buckling followed by vibrations with increase in speed.

Keywords: Navier-Stokes equations, stabilized finite element methods, sports aerodynamics, fluid-structure interactions, lock-in

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Finite Element Method–Boundary Element Method Analysis of Vibroacoustic Coupling in a Biomimetic Robotic Fish Model

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The integration of computational mechanics in the design and development of bionic equipment represents a significant frontier in biomedical engineering, robotics, and materials science. Bionics seeks to augment or replace human body functions with mechanical devices, and computational mechanics plays a pivotal role in improving their functionality, safety, and efficiency. Against this background, our team has developed a biomimetic robotic fish inspired by the morphology of manta rays [1]. This bionic device exhibits excellent biocompatibility, stealth, flexibility, and maneuverability, making it highly suitable for a range of marine applications, including aquaculture management and fish migration guidance. However, during underwater operations, the robotic fish may emit noise radiation or reflect incident acoustic waves, resulting in significant vibroacoustic coupling effects that degrade its acoustic stealth performance. To address this challenge, a comprehensive investigation into the vibration and noise reduction characteristics of the robotic fish was carried out using a coupled finite element method–boundary element method (FEM-BEM).

$$\nabla \cdot \sigma(\mathbf{x}) + \omega^2 \rho_s \mathbf{u}(\mathbf{x}) = 0 \qquad \mathbf{x} \in \Omega_s \tag{1}$$

$$\nabla^2 p(\mathbf{x}) + k^2 p(\mathbf{x}) = 0 \qquad \mathbf{x} \in \Omega_f \tag{2}$$

Eqs. (1) and (2) are the primary equations that determine the structure of sound fields. ∇ represents the Laplace operator, σ represents the stress tensor, $\mathbf{u}$ the displacements, ρ_s the shell's density, $p(\mathbf{x})$ the sound pressure, Ω_s is thin shell structure, Ω_f is infinite fluid domain, and $k = \omega / c$ the wave numbe, where c is an acoustic wave's propagation velocity in the fluid domain. The vibration of thin-shell structure is analyzed using the finite element method (FEM) with Kirchhoff– Love shell elements. Exterior acoustic fields associated with seabed reflection is simulated by the boundary element method (BEM) with half-space fundamental solutions. Then the FEM and BEM are coupled to simulate interaction between acoustics wave and shell vibration in the context of isogeometric analysis. The fast multipole method is formulated for the coupled system to accelerate computation and reduce memory storage [2].

Keywords: Biomimetic device, robotic fishes, vibroacoustic coupling, finite element method-boundary element method

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A Meshless Runge-Kutta-based Physics-Informed Neural Network Framework for Structural Vibration Analysis

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Abstract.

In recent years, Physics-Informed Neural Networks (PINN) have emerged as powerful meshless numerical methods for solving partial differential equations (PDEs) in engineering and science, including the field of structural vibration [1], [2]. However, PINN struggles due to the when the target PDEs exhibit high-frequency features [3], [4]. In this work, a meshless Runge-Kutta-based PINN (R-KPINN) framework for structural vibration modelling is proposed for the first time. In the framework, the meshless features of traditional PINN are retained while applying Runge-Kutta (R-K) time integration to discretise the temporal domain, thereby reducing computational demands and enhancing temporal flexibility. Besides, the proposed R-KPINN allows for segmental training of PINN, reducing the dimensionality of the structural vibration problems and offering accurate solutions to relatively high-frequency functions. Through numerical examples including free, damped, and forced vibration of Euler-Bernoulli beams, the proposed framework provides effective and precise solutions for predicting the responses of structures. In summary, the proposed R-KPINN framework provides a flexible, efficient, and interpretable meshless method for solving structural vibration problems with state-of-the-art PINN techniques.

Keywords: Physics-informed neural network; Computational structural dynamics; Meshless method; Runge-Kutta method.

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Dynamic analysis of the diaphragm's fracture in hypersonic impulse facilities

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The shock tunnel is a key land-based test facility used to study the aerodynamic performance of supersonic aircraft. The diaphragm is an essential component of the shock tunnel test, which acts as the trigger device. The critical rupture pressure of the diaphragm is significant because it determines the operating conditions for the shock tunnel test. However, when the diaphragm ruptures, it generates fragments that can pose risks to the safe operation of the test equipment. The finite element method (FEM) is the most commonly used approach for analyzing the dynamic response of diaphragm rupture. While FEM can accurately predict the critical rupture pressure and rupture time, it has limitations in simulating the fragments produced during the rupture process. This paper proposes a method for calculating the dynamic response of a shock tunnel diaphragm rupture by combining the finite element method and smoothed particle hydrodynamics (FEM-SPH) to address this limitation. This method has been verified for its accuracy in predicting critical rupture pressure and time. Additionally, the paper introduces a research method for characterizing the fragments using aggregated SPH particles. It analyzes the dynamic response characteristics of the diaphragm and the pieces during the rupture process.

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla P + \mu \nabla \mathbf{u} + \rho \mathbf{g}, \tag{1}$$

for which all symbols should be defined in the text. For symbol handling, it may be possible to use different symbol fonts or equation editors with this template, but this is not guaranteed. It is also possible (but not essential) to include one small figure or one small table, without caption text:

Figure 1.

Mesh	**No. of cells**	C_D	C_L'	St
M1	16,192	1.538	1.034	0.245
M2	64,792	1.546	1.053	0.241
M3	261,600	1.547	1.064	0.239

Table 1.

It is also possible (but not essential) to include a small number of references, which should be hand-numbered [1]. These are provided in the initial submission to assist the reviewers, but will need to be removed from the published version. Up to six keywords (or phrases) must also be given – these will be used to guide the selection of reviewers.

Keywords: Navier-Stokes equations, boundary-layer flows, conservation laws, machine learning, entropy production

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Analysis of Phase Change Materials Undergoing Close-Contact Melting for Thermal Management Applications

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Phase Change Materials have received a large focus due to their immense latent heat which has potential for both Thermal Management and Latent Heat Storage Systems and offer advantages such as passive operation, cheaper costs, less maintenance, and high cooling capacity. Most research has focused on addressing the key limitation of low thermal conductivity by developing composite materials and tailored structures. However, the implementation of Close-Contact Melting has demonstrated to bypass the need for material modification while simultaneously achieving high power densities, although the literature struggles to provide accurate and reliable methods for modelling the process. This study explores both numerical and experimental investigations into CCM, with a focus on identifying key mechanisms that govern the melting behaviour and interface movement. Preliminary results offer insights into the coupled effects of heat transfer, fluid motion, and mechanical interaction, suggesting pathways toward improved predictive capability. These findings contribute to a better understanding of the melting process and support future development of PCM-based thermal management systems.

Keywords: close contact melting, phase change materials, thermal management, latent heat, cooling, COMSOL, simulation, computational fluid dynamics, experiment, ANSYS

Multistable origamis inspired by avian feet

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Abstract

Systems with reprogrammable stable shapes post-fabrication and preservable stiffness are desired in numerous applications, including robotics, wearable, and biomedical devices. Origamis, auxetic metamaterials, shape-memory materials, and patterned beams or plates have been used for this purpose. However, combining stiffness and large shape changes, preserving stiffness at different configurations, and stiffness tunability are challenging. Inspired by avian feet, we provide a simple and effective solution: connecting rods by multistable interlocked hinges. The elements can rotate relative to each other and the hinges transform into different stable configurations, resulting in various stable shapes. The number of stable configurations is unlimited, and locking configurations can be tailored to alter the stiffness over several orders of magnitude. Analytical modelling was used to predict the moment-rotation behavior of the hinges and prevent yielding during shape transformations. To validate the models, the origamis were printed using stereolithography and were tested in bending under in-situ imaging. Our origamis can be used for a perching or pick-and-place device that can be actuated just by being pushed on an object with various shapes and sizes.

Pulse Dynamics as Indicators of Musculoskeletal Pain

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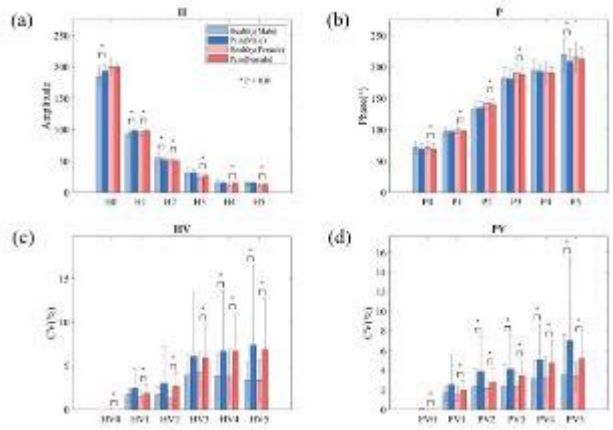
Pain is a complex condition that affects both physical and mental health, significantly impacting quality of life. Accurately assessing pain remains difficult and requires multidisciplinary approaches, combining neurobiological insights, signal processing, and wearable technologies. While self-reports are widely used, physiological measures like heart rate, blood pressure, and skin conductance are also important, especially for acute pain. Recent studies have explored heart rate variability (HRV) as a pain indicator, though results are inconsistent. Arterial pulse waveforms, which are easier to measure than HRV, may provide useful insights into pain through time- and frequency-domain analysis [1].

In this study, participants were screened by a physician, signed informed consent, and provided medical histories. They rested for 10 minutes and avoided food, coffee, or tea for at least 30 minutes before measurement. Pulse signals were collected from the left wrist using the HL158HA device, which maintains constant pressure and records at 500 Hz for 24 seconds. Pulse harmonic data were analysed to compare differences between healthy individuals.

Figure 1 shows the differences in the FFT pulse wave peaks (harmonics) between the healthy and pain groups. Males are shown in blue, females in red; lighter colors represent the healthy group, and darker colors represent the pain group. Asterisks (*) indicate p-values < 0.01. For visibility, the H_0 value in Figure 1a was scaled down to 1/20. Significant differences were found in males for H_0, H_1, and H_2, and in females for H_1 to H_5. In the pain group, both males and females showed higher H_1 and lower H_2 values. Figure 1b shows phase differences, with males differing at P_5 and females at P_0 to P_3, where the pain group had lower phase values than the healthy group. Figures 1c and 1d display the coefficients of variation for amplitude (HV) and phase (PV). Significant differences were observed in HV_4 and HV_5 for males, and HV_0 to HV_5 for females.

This study demonstrates that harmonic features of radial pulse waveforms differ significantly between healthy individuals and those with musculoskeletal pain. Higher variability and distinct changes in amplitude and phase were observed in the pain group, especially among female participants. These findings suggest that pulse waveform analysis could serve as a promising, non-invasive tool for assessing pain-related physiological changes,



offering potential applications for objective pain monitoring and personalized clinical management.

Keywords: Pulse waveform analysis, musculoskeletal pain, harmonic analysis, radial artery pulse, non-invasive pain assessment

Figure 1. Harmonic differences between the healthy and pain groups: (a) FFT amplitude, (b) FFT phase, (c) coefficient of variation of

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Rotorcraft Gearbox Housing Design using Additive Manufacturing and TPMS Lattice Structure

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This study investigates design optimization and additive manufacturing to achieve lightweight and structurally efficient gearbox housings. Since the gear contact status is affected by the housing stiffness in the bearing part, an integrated analysis model was developed, accounting for the interaction among gears, shafts, bearings, and the housing, simultaneously. The integrated model incorporated a finite element representation of the housing makes it possible to evaluate system performance and assess the load distribution across gear tooth surfaces. The gear performance is described by following face load distribution factor:

$$K_{H\beta} = \frac{\max\left(\frac{F}{b}\right)}{F_m/b} \tag{1}$$

where F and F_m are the load at an arbitrary position of the tooth flank and the mean (average) load, respectively. The closer $K_{H\beta}$ is to 1, the better the gear contact performance. To achieve this, the housing stiffness must be maintained at a certain level during the housing design process. In this study, a design process is proposed to minimize the housing weight while maintaining gear contact performance. During the optimization process, the stiffness of the bearing part of the housing was obtained using the Craig-Bampton method, and the stiffness of the housing was maintained using displacement constraints in this part[1, 2]. To derive the optimal geometry, topology optimization and Triply Periodic Minimal Surface (TPMS) lattice structures were applied. Structural integrity was verified based on the vibration fatigue criteria defined in MIL-STD-810G. The additive manufacturability of the designed housing was also evaluated.

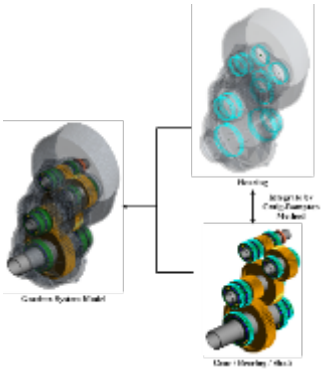

Figure 1. Housing-Gearbox Integrated Analysis

Figure 2. Optimal housing geometry with TPMS

Keywords: Gearbox Design, Topology Optimization, Additive Manufacturing, Triply Periodic Minimal Surface

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Moisture migration in unsaturated soils in non-isothermal conditions

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There are two common approaches to model moisture migration in unsaturated soils under non-isothermal conditions: the equilibrium phase change (EPC) and non-equilibrium phase change (NEPC) approaches. The two formulations adopt different assumptions and approaches to incorporating phase change phenomena. This study aims to provide insights into the application of these two methods in a fully coupled hydro-thermal numerical model for unsaturated soils. The governing equations are first presented for both approaches, followed by their implementation in a finite element-based platform, and validation against experimental data from the literature. A parallel comparison is then made between the two approaches through the estimation of variation in the degree of saturation in unsaturated soils when subjected to thermal gradients. The suitability of the two approaches for numerical modelling of unsaturated soils in the context of ground heat exchangers is then discussed. Considering the uncertainties in parameter identification, the results indicate that the EPC approach is sufficiently accurate and is often preferred over the NEPC approach in hydro-thermal modelling of ground heat exchangers in unsaturated soils.

Keywords: Unsaturated soils, hydro-thermal coupling, phase change, vapour transport

Effect of Packing Structure on SWRC in Silty Sands: A Discrete-Continuum Modelling Approach

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In this study, a pore-scale modelling approach for simulating the soil-water retention curves (SWRCs) of silty sands using a pore network model (PNM) applied to artificially generated non-uniform sphere packs is first developed and validated against experimental data from the literature. The approach is then adopted to investigate the influence of packing structure, arising from different sample preparation techniques, on the SWRCs of silty sands. DEM simulations are used to prepare samples to the same void ratio, but formed along different stress path, hence producing distinct initial fabric structures. The SWRC of these samples are then simulated and compared to analyse the role of packing structure on the SWRC. The results highlight the cases in which the sample preparation method, and the associated fabric, may have a considerable effect on the SWRC, particularly on the air entry value, which plays a critical role in unsaturated soil behaviour.

Keywords: Soil water retention curve (SWRC), unsaturated soils, discrete element method (DEM), pore network model (PNM), soil fabric.

A Lagrange multiplier/cohesive zone model for low-cycle fatigue analysis of laminated structures

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The main purpose of this work is to develop a Lagrange multiplier/cohesive zone model for low-cycle fatigue simulations of laminated structures. We introduce the concept of Lagrange multiplier to fulfil the displacement compatibility condition at finite element nodes before crack onset under dynamic cyclic loads. In doing so, the so-called artificial compliance issue arising in traditional intrinsic cohesive zone models can be well addressed. The nodal constraints are smoothly switched to cohesive forces after a defined criterion is satisfied. The adopted cohesive zone model considers the reduction of cohesive strength caused by repeated loading to account for fatigue effects. The accuracy and capacity of the developed approach in simulating fatigue behaviours of laminated composites are well demonstrated via several benchmark examples.

Keywords: Coupling method, Lagrange multiplier, Cohesive zone model, Low-cycle fatigue, Laminated structures

2-D Pure Anti-Plane Anisotropic Elastic Wave Scattering Analysis Using Deep Learning and Its Validation by the Boundary Element Method

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The boundary element method (BEM) has been widely used as an effective numerical approach for wave analysis in infinite domains. Since the BEM requires discretization only along the boundary of the analysis domain, preprocessing and postprocessing can be relatively straightforward. However, the BEM formulation becomes extremely complex for anisotropic elastodynamic problems, since the fundamental solutions required in the BEM cannot be expressed in a closed form. Moreover, the numerical evaluation of the fundamental solutions requires much computational time, which significantly increases the overall computational cost of the BEM. In this study, we develop a numerical method for 2-D pure anti-plane anisotropic elastic wave scattering problems using deep learning, in which only the boundary of the analysis domain is discritized, similar to the BEM. The proposed method satisfies not only the governing equation and physical boundary conditions, but also the radiation condition at infinity, as in the BEM. Numerical results are shown to validate the proposed method and are compared with those obtained by the BEM. The results in Fig. 1 are obtained using the proposed method by setting the elastic constants $C_{44} = C_{55} = 1.0$, which corresponds to the isotropic case.

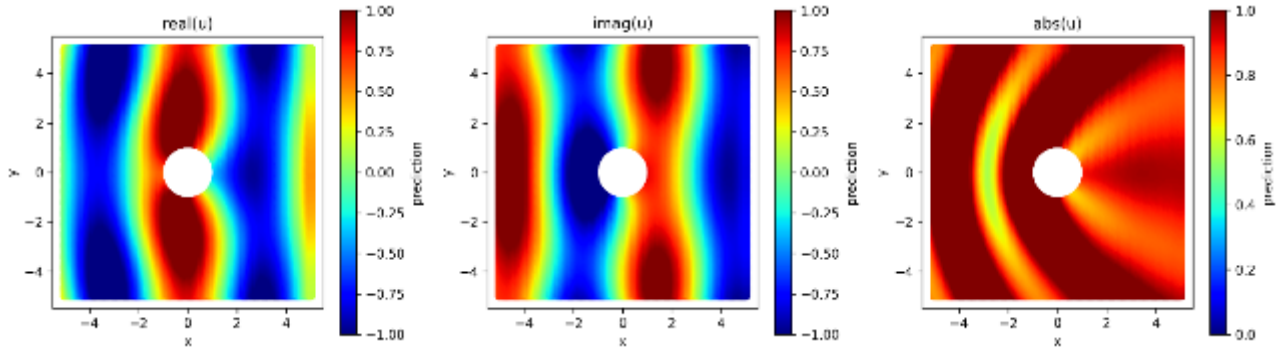

Figure 1. 2-D anti-plane elastic wave scattering by a cavity when the elastic constant $C_{44} = C_{55}$=1.0 for the proposed method.

Keywords: Deep learning, Boundary Element Method (BEM), Pure anti-plane anisotropic elastic wave propagation, Frequency-domain, Scattering problem

Acknowledgement: This work was supported by Joint Usage/Research Center for Interdisciplinary Large-scale Information Infrastructures and High Performance Computing Infrastructure in Japan (Project ID: jh250070) and JSPS KAKENHI (Grant Number: 24K0096601).

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Precision actuation of flexoelectric laminated structures under non-contact ultraviolet light illumination

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In the recent development toward building flexible aerospace structural systems and micro/nano electromechanical systems (MEMS/NEMS), actuation and vibration control based on smart materials is of great importance to their high-demanding performance. Among various smart materials and structures, photo-driven actuators exhibit many advantages, including wireless remote actuation and immunity from electric/magnetic interference, small size, etc. Flexoelectric materials do not rely on prepoling and could avoid the aging problems encountered in piezoelectric materials after prepolarization. Thus, the flexoelectric effect has received great attentions in the last few decades. According to the converse flexoelectric effect, where the electric field gradient induces stress inside the materials, flexoelectric materials can be applied to precision actuation of flexible structures. This study presents actuation control of flexoelectric laminated structures driven by light illumination. By using a photovoltaic generator to drive a flexoelectric actuator, the actuator can induce actuation stress via the converse flexoelectric effect under ultraviolet (UV) light illumination. Distribution of the flexoelectric induced control moment and its variation with time are calculated. It is observed that the flexoelectric control moment only exists in a very small region, and it is affected by the light intensity and illumination time. With the increase of illumination time, the control moment rises rapidly at first, and then gradually reaches stable. Results demonstrate that this actuation method can also effectively attenuate oscillations. The influences of several design parameters on the control effect are also investigated, such as the illumination time, the light intensity and the actuator location.

Keywords: flexoelectric effect; photovoltaic; actuation behaviour; vibration control

Hydrodynamic Modelling of a Generic Offshore Aquaculture System

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The United Nations Sustainable Development Goals (SDGs) explicitly aim to "end hunger, achieve food security, improve nutrition, and promote sustainable agriculture" (SDG 2) and to "conserve and sustainably use the oceans, seas, and marine resources" (SDG 14) by 2030. This global initiative has stimulated significant research on balancing efficient aquaculture with the sustainability of marine ecosystems amid growing food demand. As global populations and living standards rise, the increasing demand for high-quality protein places unprecedented pressure on aquaculture, a critical food source for humanity.

Currently, aquaculture operations in terrestrial and coastal areas are reaching saturation due to resource limitations and environmental constraints. Therefore, expanding aquaculture activities into more open, cleaner, and highly dynamic offshore areas has become an essential trend for global aquaculture upgrading.

However, offshore environments typically present severe and dynamically changing ocean conditions, posing significant challenges to the structural stability and operational safety of large aquaculture cages and mooring systems. Under extreme marine conditions, structural failures may lead to fish escapes, equipment damage, considerable economic losses, and environmental risks, highlighting the necessity for early identification and effective mitigation.

Against this backdrop, this study aims to develop an efficient hydrodynamic modelling method applicable to generic offshore aquaculture cage systems to enhance predictions of their dynamic responses under wave action. Firstly, a time-domain numerical model coupling linear potential flow theory with Morison's equation was established to simulate hydrodynamic loads and the motion response of aquaculture structures under typical wave conditions. Subsequently, the proposed model was systematically validated through coupled wave-structure interaction simulations performed using commercial software. Further analyses were conducted on the structural responses under varying marine conditions, including extreme events, to investigate the influence of critical ocean parameters on structural stability.

Results demonstrate that the proposed modelling approach achieves satisfactory computational efficiency and predictive accuracy. This provides theoretical support for the structural design of offshore aquaculture platforms and mooring system optimization, laying a foundation for further studies involving nonlinear wave effects and more complex scenarios. This research significantly contributes to advancing sustainable development and technological progress in offshore aquaculture systems.

Numerical simulations of flow past elliptical cylinders

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A bluff body may undergo vortex-induced vibration (VIV) when it interacts with a fluid flow. The circular cylinder has been adopted as the standard model for VIV research due to its simple geometry and various engineering applications. Fundamental insights gained from investigating the circular case have laid the foundation for studying VIV characteristics of other geometric shapes. The geometries of interest in the present study are elliptical cylinders. Very recently, Lo et al. (2023) [1] experimentally studied the effect of structural damping on the transverse flow-induced vibration of a thin elliptical cylinder with an aspect ratio of 5 at intermediate Reynolds numbers. Here, the aspect ratio is defined as the ratio of the major axis length to the minor axis length. Remarkably, they observed a hyper-branch exhibiting a maximum vibration amplitude of seven diameters of the cylinder with low damping ratios. This hyper-branch response is significantly different from the VIV response of a circular cylinder, where the maximum vibration amplitude is typically of the order of one diameter, e.g. [2]. On the other hand, Kushwaha *et al.* (2020) [3] examined the effect of aspect ratio on VIV at low Reynolds number and zero damping and found the maximum vibration amplitude to be close to one diameter of the cylinder. From these studies, it is evident that the hyper-branch phenomenon is a combined effect of the aspect ratio and Reynolds number. Nevertheless, how the vibration amplitude branch evolves as the shape transitions from a circular cross-section (aspect ratio = 1) to a flat plate (aspect ratio approaching infinity) remains unclear. This study addresses that gap by investigating the flow-induced vibration of elliptical cylinders with varying aspect ratios (1 to infinity). The Navier-Stokes equations and the cylinder motion equation are solved using the OpenFOAM-based vivicoFoam solver developed by [4]. The effects of Reynolds number on fluid forces, vibration amplitude, and vortex shedding regimes are investigated for various aspect ratios.

Keywords: Fluid-structure interaction, vortex-induced vibration, cylinder

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Energy-Based Virtual Element Method for Nonlinear Problems with the Assistance of Automatic Differentiation

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The Virtual Element Method (VEM) has gained significant attention recently. By expanding the space of approximation functions with a "virtual" function that preserves polynomials at the boundaries and ensures that the Laplacian is polynomial, VEM is applicable to arbitrary polyhedra, whether convex or concave. With the assistance of automatic differentiation, we can derive the discretization form starting from the energy functional, which simplifies the implementation. In this talk, we discuss the implementation of VEM for nonlinear problems, including contact modeling for elasto-plastic materials under large deformation. Since VEM is suitable for arbitrary polyhedra, we also apply it to model polycrystal plasticity. Additionally, some issues and improvements in the VEM algorithm, such as the integration of arbitrary polygons, will be discussed for convenience.

Keywords: Virtual Element Method, Polycrystal plasticity, Contact problem, Automatic Differentiation

An SPH-based RFT Framework for Rapid and Accurate Prediction of Spudcan Resistance

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Accurate prediction of spudcan resistance is essential for the design optimisation and on-site operation of jack-up rigs, particularly to avoid hazardous events such as punch-through or leg-run. However, available prediction approaches are often insufficiently accurate or rely on oversimplified models with ad hoc assumptions regarding soil conditions and spudcan geometry. Numerical analyses using mesh-based methods, such as Finite Element modelling, are computationally intensive, prone to instabilities (e.g., volumetric locking under undrained conditions), and struggle with tracking the free surface of the seabed. This study introduces a novel framework to address two key research questions: (i) how to accurately model the dynamic interactions between spudcan foundations and seabed soils, and (ii) how to enable rapid resistance prediction to support timely operational decisions. To this end, we propose a soil-structure interaction modelling framework based on the Smoothed Particle Hydrodynamics (SSI-SPH) approach, designed to simulate the large deformation and highly non-linear spudcan penetration in granular media under varied conditions. The effectiveness of this framework is demonstrated through validation against both numerical simulations and experimental data, which show strong agreement. Additionally, spudcan penetration can be conceptualised as the intrusion of a rigid object into a granular medium, where the object boundary can be discretised into infinitesimal areas and the total resistive force is calculated using a simple superposition law known as Resistive Force Theory (RFT) [1]. By applying the proposed SSI-SPH framework, stress coefficient diagrams required for RFT force calculations are generated, subsequently enabling rapid and precise estimation of the reactive forces acting on the spudcan. Comparison between SPH-RFT predictions and experimental results demonstrates that the SPH-RFT approach offers a computationally efficient and versatile method for estimating spudcan resistance, with broad applicability across varying soil conditions and spudcan geometries while also showing promise for broader geotechnical engineering applications in predicting resistive forces in various soil-structure interaction scenarios.

Keywords: Smoothed particles hydrodynamics, soil-structure interaction, spudcan penetration, resistive force theory, offshore engineering

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Neural PDE Solver for Geotechnical Applications: Solving Discrete-Time Problems with Dynamic Boundary Conditions

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Modelling complex geomechanics problems remains a significant challenge due to the highly nonlinear behaviour of soils and the difficulty of tracking evolving boundaries under complex loading and large deformation conditions. While recent advances in neural network-based solvers have shown promise in approximating solutions to Partial Differential Equations (PDEs), most existing frameworks are limited to continuous spatiotemporal domains with fixed or pre-defined boundaries, restricting their applicability to fluid flow and solid mechanics [1]. In this work, we present a first-of-its-kind neural-based computational framework tailored for geomechanical applications, capable of solving discrete-time PDEs with dynamically evolving domains. By integrating a high-order time integration scheme with an adaptive surface detection algorithm for boundary tracking, the method enables continuous boundary evolution throughout the simulation. The framework is validated through comparisons with experimental data and Smoothed Particle Hydrodynamics (SPH) simulations, demonstrating strong agreement and achieving accuracy comparable to, or exceeding, that of conventional solvers. It also supports the integration of field observation data, preserving fidelity to both physical measurements and governing equations. While the training phase is computationally intensive, the framework offers rapid inference and a flexible network architecture, making it well-suited for near real-time geotechnical prediction tasks, facilitating rapid response and recovery amid growing global climate-related hazards.

Keywords: Neural PDE solver, soil modelling, large deformation, real-time prediction.

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Unifying Trace, Planar Discontinuity, and Block Identification in Rock Masses via Foundation Models

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Traces, discontinuity planes, and blocks together constitute the complete spectrum of observable rock mass structures from outcrops, providing essential geometric inputs—from 2D projections to 3D discontinuities and volumetric blocks—for computational modelling in rock mass stability analysis. However, conventional digital techniques often struggle with generalization, scalability, and annotation efficiency, particularly in the face of complex geological scenes. In this study, we present a unified vision-based framework that leverages foundation models—specifically the Segment Anything Model (SAM) and its extensions—for intelligent identification of rock mass features across three levels of abstraction. First, we address trace detection by introducing a thin-object segmentation perspective, enabling high-precision delineation of linear features using SegTrace and scalable deployment via SegTraceNet. Second, we demonstrate the application of interactive SAM prompting for efficient segmentation of surface-type discontinuities, validated on over 2,000 instances from diverse outcrops. Third, we extend this methodology to the volumetric block level, proposing SA4B-3D—a novel approach that converts 3D point cloud segmentation into a 2D image task, thereby enabling intelligent in-situ block identification. By integrating these strategies with Structure-from-Motion workflows, we ensure consistent transfer between image and spatial domains, making the pipeline device-agnostic and field-deployable. Our experiments reveal significant gains in segmentation accuracy (avg. precision > 0.9) and annotation efficiency, achieving over 7,000 volumetric observations in previously intractable scenarios. This cross-scale, AI-driven approach redefines digital geological surveying and paves the way for rapid, safe, and scalable detection in engineering geoscience and hazard assessment applications.

Keywords: Rock Mass Structures; Discontinuity; In-situ Block; Digital Outcrop Model (DOM); Foundation Models (FMs); Discrete Fracture Network (DFN)

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Computational Design Assessment of Innovative Static Mixers for Gas-Liquid Flow Applications

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Mixing is essential in many industries and accounts for significant energy and cost demands. Using non-rotating mixers can lower costs, save space, and improve safety. In multiphase mixing, dispersing immiscible fluids is challenging due to surface tension and density differences. This study aimed to evaluate the mixing performance of Kenics, High-Efficiency Vortex generator (HEV), and two other novel static mixers for improving phase dispersion in gas-liquid flows. The interFoam solver in OpenFOAM is used for the simulations, where it is developed based on the Volume of Fluid (VOF) approach for two-phase flow. Both phases are considered immiscible and incompressible and share the same velocity. Therefore, one set of Navier-Stokes equations can describe the mass and momentum conservation for both phases. The distinction between phases is established through an extra transport equation that employs the volume fraction (α) as an indicator to characterise how the phases are distributed across the domain. The equation is as follows:

$$\frac{\partial \alpha}{\partial t} + \nabla(\alpha \vec{V}) = 0 \tag{1}$$

First, based on the results obtained from the CFD simulations, the gas flow stream was evaluated qualitatively. Additionally, the weighted relative coefficient of variation ($RCoV_w$) of the gas phase volume fraction is calculated at various locations within the static mixers and compared to assess the meso-mixing performance of each mixer. Finally, the friction factor is examined to gain insight into the energy requirements of each static mixer. The results indicate that the addition of curved blades to the HEV improved its performance while caused bubble accumulation in some regions of Kenics static mixers. Furthermore, pressure drop correlates strongly with improved bubble breakup and uniformity in distribution. These findings offer insights into optimising mixer designs for efficient multiphase processing, with potential benefits in reducing energy consumption and operational costs.

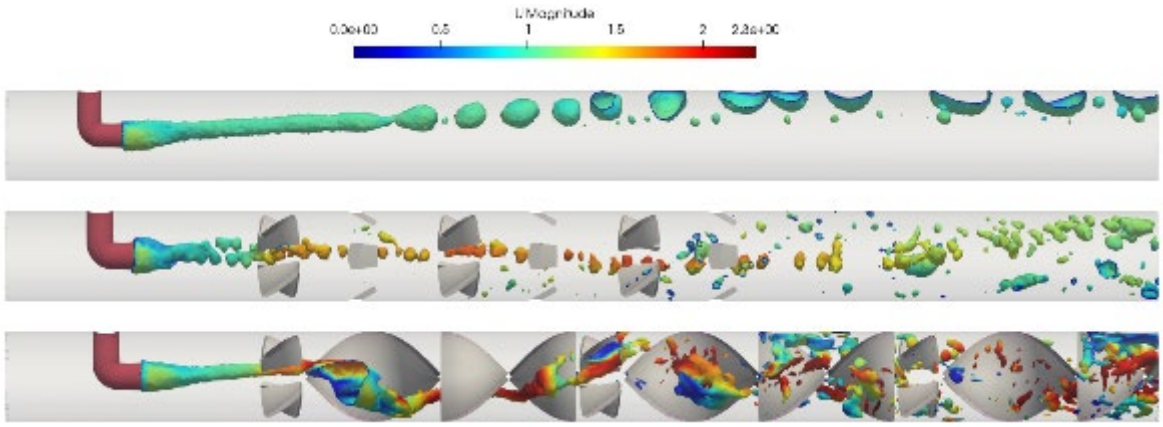

Figure 1

Keywords: multiphase flow, Volume of Fluid (VOF), static mixer, weighted relative coefficient of variation, pressure drop

DEEP LEARNING-BASED DESIGN OF DIFFERENTIAL THICKNESS SHEET TENSILE SPECIMENS AND PREDICTION OF THIN-WALLED TUBE STRUCTURAL TOUGHNESS WITH THICKNESS GRADIENT OPTIMIZATION

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Received: XXXX Accepted: XXXX

ABSTRACT

As demand for lightweight and safe automotive designs grows, tailor rolled blank (TRB) technology has become a research hotspot due to its potential for weight reduction and performance optimization.

However, due to the non-uniform characteristics of TRB, the deformation in the transition zone of traditional tensile specimens becomes highly non-uniform during axial loading. Therefore, it is necessary to optimize the transition zone of standard tensile specimens to achieve more uniform deformation during axial loading. In this paper, a novel design method for tensile specimens of TRB is proposed based on convolutional neural networks (CNN). By optimizing the width-thickness function of the transition zone, the method ensures more uniform deformation during the tensile process, thereby obtaining more material stress-strain data from different thickness regions. The effectiveness of the optimized specimens in tensile tests is verified through experiments using the digital image correlation (DIC) method. The results demonstrate the feasibility and efficiency of the optimization algorithm in practical applications. This innovation not only enhances the accuracy of TRB material performance evaluation but also provides new ideas for testing non-homogeneous materials.

Uniform-thickness thin-walled tube structures can no longer meet the growing demands for high material utilization and crashworthiness. This is because different parts of the structure absorb energy at varying efficiencies impact during. Therefore, using variable-thickness thin-walled tubes can not only further reduce weight for lightweight design but also effectively improve material and thickness utilization. In this paper, a novel method based on deep learning is proposed for predicting crashworthiness parameters and optimizing thickness gradients of TRB vehicle thin-walled tube energy-absorbing structures. The method is applied to optimize the crashworthiness performance of Functionally Graded Thickness (FGT) and Functionally Graded Width (FGW) square tubes under axial loading conditions. Finally, the proposed optimization method achieves high-precision prediction of crashworthiness indicators and simultaneous optimization of thickness gradient distribution. The effectiveness of the method is verified through experiments on FGT and FGW square tubes, and the results show that the optimized thin-walled tubes achieve a better balance between collision safety and material utilization. These results indicate that deep learning can effectively address the complexity of TRB structures, providing a practical tool for automotive safety design.

KEYWORDS

Tailor Rolled Blank; deep learning; thin-walled vehicle body structures; novel TRB specimen

Efficient modelling and simulation of 3D time-domain seismic plane P and SV waves in multilayered half-space with arbitrary incident

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Most studies assume the vertically propagated compressional (P) or shear (SV) waves when analyzing the seismic response of structures, relying on the assumption that the seismic waves originate from deep bedrock and travel across multiple soft soil layers, resulting in nearly vertical incidence angle in surface layer due to Snell's law. In reality, however, this assumption can be problematic on account of many facts, e.g., when soil stratigraphy is not horizontal, surface topography is not fact, or near-fault motions are considered. In particular, besides the difference in wave oscillation direction compared to its travel direction, one main distinction between SV and other types of body waves, such as P and SH waves, is that the SV wave will have exponentially decaying (evanescent) components in the vertical direction when its incident angle exceeds the critical angle. Such evanescent waves will intensify the shaking levels on the ground surface and hence pose a high risk for both super- and near-surface underground structures. Nevertheless, very limited existing research in the literature considered the case where the incident angle of the SV wave is greater than the critical angle, mainly due to computational complexity. In this study, we first developed the analytical solution for 3D time-domain free-field seismic waves when subjected to arbitrarily inclined incident plane P and SV waves, then inject them into a multilayered half-space via Domain Reduction Method (DRM). Furthermore, we applied the Perfectly Matched Layer (PML) outside the DRM layer to efficiently absorb any outgoing scattered waves that may be generated due to material homogeneities, soil-structure interaction (SSI), and topography irregularities. The proposed method is fully verified and validated against various analytical and numerical solutions. In the end, we created 2D and 3D models with idealized bell-shaped hills and simulated the seismic wave propagation subjected to inclined plane P and SV waves with varying incident angles in both horizontal and vertical directions, with the aim of preliminarily investigating the effects of surface topography and incident angles on ground motion intensities.

Meshfree method for large deformation analysis without any domain remesh- a nonlinear scheme based on stabilized collocation method

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Abstract

The Finite Element Method (FEM) and other mesh-based methods require mesh remeshing to address grid distortion issues when solving large deformation problems. In contrast, Galerkin-based meshfree methods do not request remeshing for approximation in large deformation analysis, while the integration grid still needs to be remeshed after distortion. In this work, we introduce a meshfree nonlinear solution scheme built upon Stabilized Collocation Method (SCM) and Reproducing Kernel (RK) approximation for the large deformation analysis. This method is genuinely meshfree, and no domain remeshing is required during the entire solution procedure. The total Lagrangian description is introduced for the formulations. The SCM can achieve accurate subdomain integration by using low-order Gaussian quadrature, which can significantly raise the accuracy and stability of the solutions. Lowering the condition number of the discrete matrix through subdomain integration further enhances the algorithm's stability. The subdomains for integration are determined by the particle locations, and domain deformation is represented by the movement of the particles, for which subdomains can remain regular without any deformation. Eliminating the need for remeshing can notably promote the solution efficiency. The Newton-Raphson iterative technique is conducted to address the nonlinear discrete equations. Several numerical examples of large deformation are examined, demonstrating the high accuracy, high efficiency and good stability of the proposed method for large deformation analysis. This method can handle very large deformation problems, even beyond the limit where FEM and High-order Finite Element Method (HFEM) solutions terminate. All these indicate that SCM has immense potential in addressing large deformation problems.

Keywords: stabilized collocation method; large deformation; accurate integration; accuracy; efficiency; stability

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A Localizing Gradient Damage Model with Adaptive Refinement for Fracture Prediction

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Nonlocal and gradient-enhanced models are widely employed to mitigate mesh dependency in continuum damage models. However, while these models ensure that the structural response remains mesh independent, they often exhibit spurious damage growth. To address this limitation n, Poh and Sun [1] proposed the localizing gradient damage model, where the interaction domain decreases as damage progresses. This approach is motivated by the fracture process in quasi-brittle materials, which typically begins as a diffuse network of microcracks before localizing into a macroscopic crack.. The constitutive response is described by the stress-strain relation:

$$\boldsymbol{\sigma} = (1-\omega)\boldsymbol{C}:\boldsymbol{\varepsilon} + h(e-\tilde{e})\mathbf{n} \qquad (1)$$

where $\boldsymbol{\sigma}$ is the stress tensor, ω the scalar damage variable, $\boldsymbol{C}$ is the stiffness tensor, $\boldsymbol{\varepsilon}$, the Lagrangian strain, e, the equivalent strain, and $\tilde{e}$, a morphic variable capturing microscale fluctuations. The evolution of $\tilde{e}$ is dictated by a microforce balance equation:

$$e - \tilde{e} = \nabla.(ghl^2\nabla\tilde{e}) \qquad (2)$$

To model this fracture process efficiently, we extend the localizing gradient damage model to incorporate adaptive mesh refinement Thermodynamic consistency is maintained via a micromorphic framework, leading to governing equations structurally similar to those in classical gradient models. This refinement scheme utilizes an error indicator derived from both the displacement field and the morphic variable. The adaptive refinement is coupled with quadtree decomposition to generate a hierarchical mesh structure.

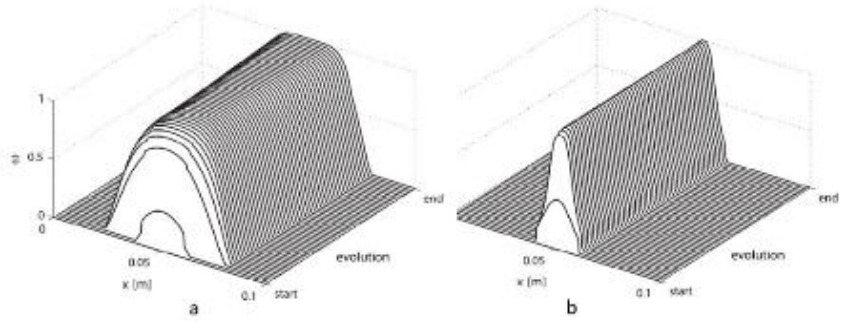

Figure 1. **Comparison of Damage Evolution** (a) Conventional gradient damage model (b) Localizing gradient damage model.

The evolution of the damage field is illustrated in **Figure 1**. Panel (a) shows the gradual and widespread damage growth typical of conventional gradient models, while panel (b) highlights the sharper and more localized damage characteristic of the localizing gradient model.

Keywords: Localizing gradient damage model, Adaptive mesh refinement, Quadtree decomposition, Gradient-enhanced regularization.

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Numerical modelling approach for tunnelling forces on excavation pit wall supports in soft soil using 2D hydro mechanical FE model

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This paper presents a significant contribution to computational mechanics in infrastructure engineering through a numerical modelling study focused on the tunnelling through and jacking forces on sheet pile walls using a 2D hydro mechanical finite element (FE) model. The primary objective of this research is to develop a robust model that meets the safety criteria of sheet pile walls while in soft soil environments impacted by both hydraulic and mechanical pressures. Literature highlights the critical challenges in excavation and tunnelling within soft, saturated soils. Studies on pipe jacking forces in soft ground emphasise the significant stresses exerted on support structures [1]. Numerical simulations of deep foundation pit excavations reveal substantial soil deformation and potential impacts on adjacent structures [2]. Additionally, modelling using PLAXIS underscores the importance of detailed support system analysis in weak geological conditions [3]. Through the review, there is a clear gap in the modelling of the working pit's stability during pipe jacking initiated to begin the tunnel excavation. These findings collectively indicate a pressing need for advanced numerical models to evaluate the structural performance of sheet piles under high jacking forces and saturated soft soil conditions, ensuring stability and safety in excavation projects.

The proposed model is designed to withstand a number of geotechnical challenges within a singular model, including water uplift and heave in the excavation pit, and sheet pile wall failure from tunnelling forces and surrounding soft soil. The computational approach used included Plaxis 2D, user-defined interfaces, and a specific construction sequence, all supported by geotechnical and structural theory [4]. The findings demonstrate the efficacy of the Plaxis 2D software in accurately modelling multifaceted subsurface deformation, consolidation, and the challenges posed by tunnelling. Through the developed comprehensive and reliable model, this study enhances the understanding and management of sheet pile wall supported excavation pits designed for tunnel initiation, thereby contributing to the advancement of computational mechanics in geotechnical engineering.

Keywords: Tunnel jacking force, Plaxis 2D, hydro mechanical laws, excavation pit, soft soil

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Topology Optimization of Creep Deformation Minimization Problems Based on Norton Model

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This study proposes a topology optimization method that accounts for the Norton constitutive law [1], which incorporates material nonlinearity. Mechanical structures operating under high-temperature environments, such as gas turbines and rocket engines, are susceptible to time-dependent deformation known as creep. Excessive creep can lead to performance degradation and structural damage, making its suppression a key design requirement. Due to the inherent time-dependent material nonlinearity, conventional, experiment-based design methods face difficulties in identifying optimal structures. To address this challenge, we apply topology optimization to derive structural layouts that minimize creep deformation.

The Norton model, a widely used constitutive model for creep, represents an inelastic material behavior with creep strain treated as an internal variable. In topology optimization, the design sensitivity—used to guide the optimization—is typically derived analytically. However, inelastic models like creep require sensitivity formulations that account for both time dependence and internal variables, making them particularly complex [2]. To overcome this, we employ automatic differentiation [3], which enables accurate sensitivity computation without explicitly deriving complicated expressions.

A density-based topology optimization method assuming two material phases is presented, incorporating nonlinear finite element analysis with the Norton law and sensitivity analysis using automatic differentiation. To formulate the creep minimization problem, objective and constraint functions are defined. Numerical examples are provided to validate the accuracy of the automatic differentiation-based sensitivity analysis and to discuss the associated computational memory requirements. Finally, a 2D topology optimization example is demonstrated, and the influence of the Norton law on the resulting optimal structure is examined.

Keywords: Topology optimization, Creep, Norton model, Automatic differentiation

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Topology Optimization of Nonlinear Structures for Stiffness–Vibration Duality Using Curve–Fitted Load Response Design

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This study presents a topology optimization method for designing nonlinear structures that suppress unwanted vibrations while maintaining sufficient stiffness for steering stability in automotive suspension systems. Rubber bushings offer damping but face a trade–off between vibration isolation and rigidity, especially under dynamic conditions. To overcome this problem, we exploit the difference in external force levels associated with vibration reduction and handling stability, aiming for structures with deformation–dependent stiffness that achieve both within a single design.

The optimization uses a curve–fitting approach to match the nonlinear load–displacement response to a target curve. Based on the method by Li et al. [1], the formulation accounts for large deformations and uses hyperelastic material. The target curve specifies low stiffness for small loads and high stiffness for large loads, enabling dual–functional performance.

The objective function Π is defined as the squared deviation between the target and actual load–displacement responses over a series of load or displacement inputs. $\boldsymbol{F}_k$ or $\boldsymbol{u}_k$ is given as an input.

$$\Pi \equiv \max_k \left\{ w_k \left(\frac{f_k - {f_k}^{\mathrm{obj}}}{{f_k}^{\mathrm{obj}}} \right)^2 \right\} \tag{1}$$

$$f_k = {\boldsymbol{F}_k}^T \boldsymbol{u}_k \tag{2}$$

Here, w_k, $\boldsymbol{F}_k$, and $\boldsymbol{u}_k$ represent the weighting parameter, the load vector, and the displacement vector at the k–th load step, respectively. In addition, f_k and f_k^{obj} denote the averaged mean–compliance obtained from structural analysis and the target averaged mean–compliance, respectively. The objective function in Equation (1) aims to minimize the maximum error between f_k and f_k^{obj} over all load steps.

The presence of nonlinearity in the response may contribute to improved vibration reduction by enabling more complex dynamic interactions that are not achievable through linear systems.

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Impact of Activation Functions Across Differential Equations in Physics-informed Neural Networks (PINNs)

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Physics-informed neural network is an emerging and rapidly advancing machine learning framework that utilizes neural network capabilities to predict solutions for differential equations. Activation functions play a key role by incorporating required non-linearities to model the complex physical behaviours of physics-informed neural networks. Different physics-informed neural network models require distinct characteristics of activation functions for effective performance where there is no systematic approach to match the activation function's characteristics with the underline physics of a given physics-informed neural network model. The objective of this study is to examine the performance of different activation functions with respect to the order of differential equations in physics-informed neural networks. In this study, several physics-informed neural network models consisting of different ordinary and partial differential equations were used to compare dissimilar seedings with a set of activation functions. Results show that different physics-informed neural network models attain diverse performances for different activation and seeding options. Remarkably, physics-informed neural network models for higher-order ordinary and partial differential equations exhibit varying levels of performances related to different activation functions. It reveals the fact that the higher-order derivatives of differential equations of physics-informed neural network models significantly influences the effectiveness of activation functions, which is an interesting avenue for further study in the domain of machine learning.

Keywords: Physics-Informed Neural Networks (PINNs), Activation Functions, Solving Differential Equations, Machine Learning

Performance Evaluation of Carbon Fibre Plate-Inserted Shoes through Human-Shoe Coupled Dynamic Analysis

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In this study, performance of carbon fibre plate-inserted shoes was evaluated through human-shoe coupled dynamic analysis. Dynamic finite element analysis (FEA) in the running motion was simulated to evaluate the impact of structural differences in running shoes on running performance.

In 2017, carbon fibre plate-inserted shoes were developed. Compared to conventional shoes, the carbon fibre plate-inserted shoes exhibit several distinctive features, such as a curved carbon plate, a thick midsole, and the use of highly energy-returning midsole materials. It remains unclear which specific features have contributed to these performance improvements. By using FEA, it is possible to obtain results on shoe performance without being influenced by the runner or the usage conditions of the running shoes.

In this study, the foot model was extracted from the human body model THUMS. THUMS, which was developed by Toyota Motor Corporation, has been provided freely for the purpose of enhancing human safety. The shoe was modelled with an outsole, midsole, an upper part and shoelace. A form material model with a non-linear stress-strain relationship was applied to the midsole, while an elastic material model was used for the upper part. Three midsole models were created by varying the presence and insertion position of the carbon plate. The carbon plate was modelled as an isotropic elastic material.

Figure 1 presents an overview of the simulation model. First, a finite element analysis was conducted in which a shoe model was fitted onto a human body model. By applying tension to the shoelace components, the shoe and the human body model were successfully integrated using only friction and contact pressure. Subsequently, finite element analyses were conducted to simulate running motion by applying initial and angular velocity to the foot model in the shod condition.

As a result, the ground reaction forces obtained from the dynamic FEA were generally consistent with experimental data reported in previous studies, supporting the validity of the model. Furthermore, this approach enabled the evaluation of running shoes while considering the interaction between the shoes and the human body.

This research was supported in part by a grant 2025 from Advanced Research Initiative for Human High Performance (ARIHHP), University of Tsukuba.

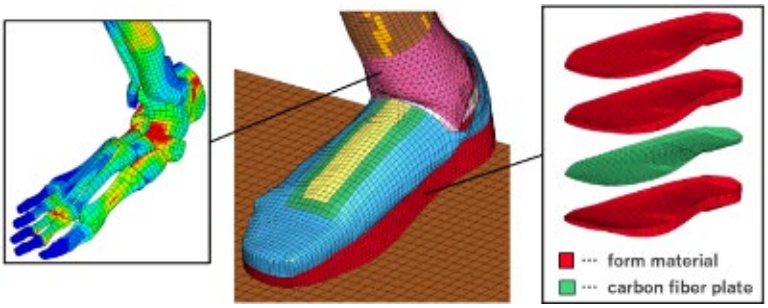

Figure 1

Keywords: Running Shoe, Carbon Fibre Plate, FEM, Ground reaction force, Human body

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Effect of vortex-induced rotation on the aerodynamic coefficients of a rigid rectangular cylinder

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A numerical investigation of vortex-induced rotations and their effect on the aerodynamic coefficients of a rigid rectangular cylinder, free to rotate azimuthally in a two-dimensional uniform cross-flow, is presented. Recent studies in the literature have identified characteristic regimes of rotation across Reynolds numbers, compared drag, lift and torque coefficients across static and dynamic modes. The dynamic response of a freely rotating square cylinder has been investigated with varying Reynolds number. However, aerodynamic response of freely rotatable rectangular cylinders under varying aspect ratios remains poorly understood. This study aims to characterize the aerodynamic coefficients in static and dynamic modes for rectangular cylinders with ten aspect ratios in the range of 0.02–1.0 at Reynolds number 100 and fluid-to-body density ratio 1/10. An in-house immersed boundary–regularized lattice Boltzmann solver with a multi-block technique is used, based on the governing equation of the distribution function, $f(x,\xi,t)$, in the configuration (x) and velocity (ξ) spaces at time t

$$\frac{\partial f}{\partial t} + \xi_\alpha \frac{\partial f}{\partial x_\alpha} + \frac{F_\alpha}{\rho}\frac{\partial f}{\partial \xi_\alpha} = \Omega, \qquad (1)$$

where ρ is the density, $\alpha\epsilon\{x,y,z\}$, F_α is the body force in the direction α, and Ω is the collision operator. Newton's second law is used for the rotational motion of the cylinder. A computational domain of 100D×100D, where D is the reference diameter.

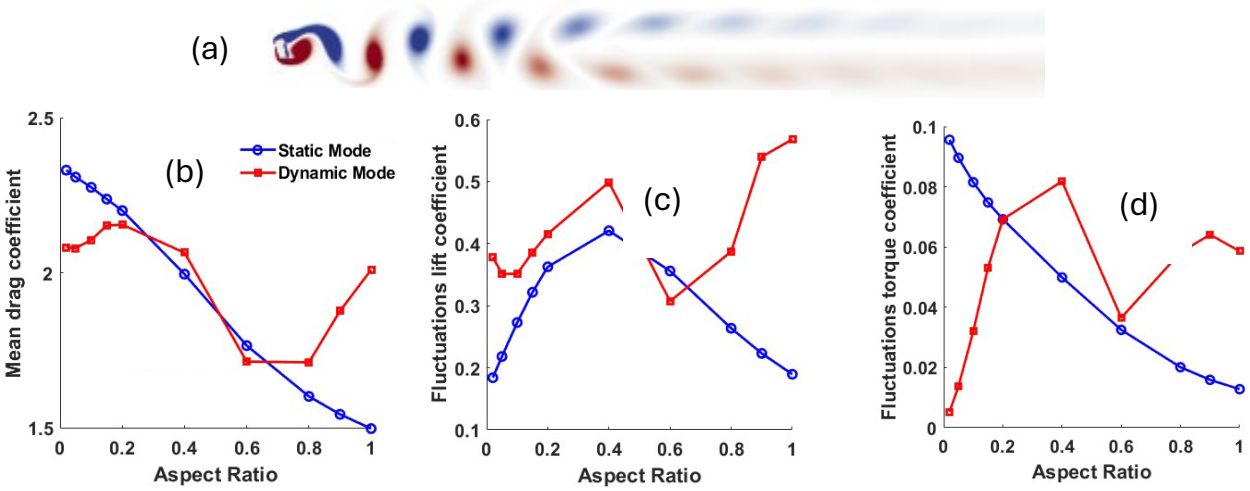

Figure 1. Simulation Results at a Reynolds number of 100: (a) contours of vorticity at aspect ratio=0.4, variation of the coefficient of (b) drag, (c) lift, and (d) torque with the aspect ratio.

Simulation results show that vortex-induced rotation significantly influences the statistics of drag, lift, and torque coefficients. Overall, the dynamic aerodynamic coefficients exhibit notable variations. This work will be extended to investigate the effects of Reynolds number on the aerodynamic coefficient in two- and three-dimensional bluff bodies in various shape, with a view to developing a drag, lift and torque model for long range irregular particle transport, such as transport of firebrand in a bushfire.

Keywords: fluid–structure interaction, vortex-induced rotation, aerodynamics

Adaptive isogeometric boundary element method for the fluid–structure interaction analysis of the hyperelastic thin sheet

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Many biological tissues are sheet-like and form complex shapes through surface area change due to growth. Viscous fluids fill almost all the spaces around tissues, and can affect the deformation of the tissues. We have developed an isogeometric boundary integral method for the deformation of a sheet in a viscous fluid, where growth is modeled as spontaneous plastic deformation. However, adaptive mesh refinement method is needed for some problems, including the development of protrusions on cell membranes. Therefore, we develop an adaptive isogeometric boundary element method for the fluid–structure interaction analysis of a hyperelastic sheet with spontaneous plastic deformation.

We use the isogeometric boundary element method. The sheet configuration is described by the Kirchhoff–Love shell theory. The spontaneous plastic deformation is formulated by the finite growth theory [1]. By the principle of virtual work, the weak foam is formulated. The fluid flow is formulated by the boundary integral method.

$$\boldsymbol{u}(\boldsymbol{x}) = \int_S \boldsymbol{J}(\boldsymbol{x},\boldsymbol{y}) \cdot \boldsymbol{q}(\boldsymbol{y}) \mathrm{d}s(\boldsymbol{y}), \tag{1}$$

where $\boldsymbol{u}$ is the flow velocity, $\boldsymbol{J}$ is the stokeslet, $\boldsymbol{q}$ is the load, $\boldsymbol{x}$ is the observation point, $\boldsymbol{y}$ is the integral point, s is the surface. Discretization is done by the isogeometric analysis with the T-spline surface [2]. The 4th order adaptive mesh refinement method is used to refine and coarse the surface mesh. Time integration is done by the 2nd order Runge–Kutta method.

As a demonstration of the developed method, we simulate the protrusion extension on a hyperelastic sheet in a viscous fluid (Fig. 1). $\dot{\theta}_0 t$ is the non-dimensional time. When the surface area of the sheet increases, a protrusion is formed on the sheet. With the protrusion extension, the computational mesh is refined at the top of the protrusion. By the adaptive mesh refinement, the mesh size is almost constant during the simulation.

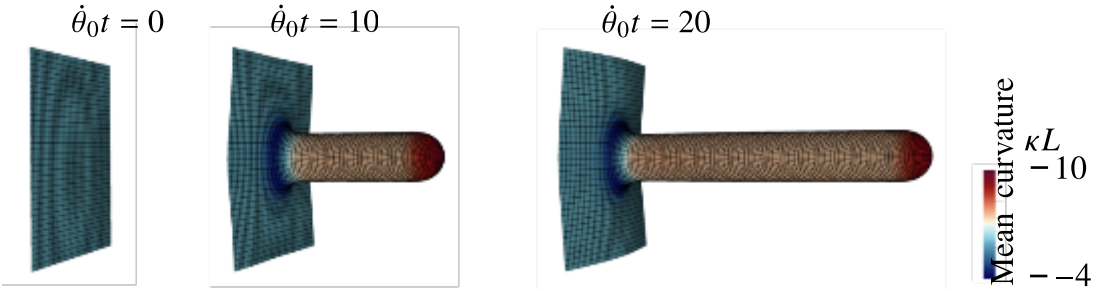

Figure 1.

Keywords: Isogeometric analysis, adaptive mesh refinement method, boundary integral method, Kirchhof–Love shell theory, fluid–structure interaction analysis

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Impact of Iron-Reducing Bacteria on Underground Hydrogen Storage Performance in the Otway Basin

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Underground hydrogen storage (UHS) in depleted gas reservoirs is emerging as a key strategy to buffer renewable-energy variability. The Otway Basin—an extensively characterised sedimentary system with proven depleted gas fields and high-porosity sandstone formations—is considered as an ideal candidate for UHS. Covering approximately 150,000 km² from southeastern South Australia to southwestern Victoria, it was formed during multi-stage Gondwana rifting (Late Jurassic–Late Cretaceous) and has hosted commercial gas production. However, a technical report by Power & Goldie Divko [1] documented high concentrations of iron oxides in Otway sandstones, suggesting that biogeochemical iron-reduction reactions could alter grain cementation and pore-throat geometry, thereby impacting porosity, permeability, H_2 injectivity, storage capacity, and long-term performance.

We employ the open-source DuMu^x framework on a corner-point grid representing Otway sandstone (initial porosity 18 %, permeability 500 mD) to simulate the coupled flow, transport, and Monod-type Fe(III) reduction over a 10-year window. Hydrogen injection and withdrawal are imposed via constant bottom-hole pressure in repeated cycles. The core reaction is given below

$$3Fe_2O_3 + H_2 \rightarrow 2Fe_3O_4 + H_2O. \quad (1)$$

The reaction rate is governed by a Monod-type expression with parameters from the literature [2]:

$$r = \mu_{max} C_m \frac{C_{H_2}}{K_{H_2}+C_{H_2}} \frac{C_{Fe(III)}}{K_{Fe(III)}+C_{Fe(III)}}, \quad (2)$$

where C_{H_2} and $C_{Fe^{III}}$ are the dissolved H_2 and Fe(III) concentrations; K_{H_2} and $K_{Fe^{III}}$ are half-saturation constants of H_2 and Fe(III); μ_{max} and C_m are the maximum microbial activity rate and microbial concentration, respectively. Model outputs track porosity, permeability, and gas recovery efficiency versus cumulative H_2 injected.

Our preliminary results include how iron-reduction alters reservoir properties on decadal timescales, quantify thresholds where storage performance degrades, and provide guidance for UHS project design in the Otway Basin by highlighting the need to account for microbial rock alteration in operational planning and risk assessment.

Keywords: Iron-reducing bacteria; Porosity evolution; Permeability; Underground hydrogen storage; Otway Basin; Reservoir performance

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Image-Physics Driven Topology Optimization Method with Integrating Biological Features

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Biological structures are renowned for their multifunctionality, with honeycomb structures being a prime example, known for their lightweight and directional superior energy absorption capabilities. To integrate biological features into structures and achieve adjustable feature scales, an Image-Physics driven Topology Optimization method (IPTO) is proposed. In this method, "image" represents the biological feature, while "physics" refers to the optimization process based on the Solid Isotropic Material with Penalization (SIMP) framework. The VGG19 convolutional neural network (CNN) is employed to extract biological features, such as honeycombs and fish scales, and integrate them into the SIMP framework to minimize compliance, thereby embedding biological features into materials. To adjust the size of biological features in the generated structure, a multi-block complete coverage filling strategy is adopted. Features extracted by the CNN are adaptively reduced with network depth l, and empty regions are filled to achieve a stepwise reduction of feature size with increasing depth. To adjust the density of biological features in the generated structure, a biological feature density control weight β is introduced, allowing effective adjustments to the density of the biological features. In addition, refer to images of earthworm skin, cuttlebone, teeth, and a combination of cuttlebone and teeth to further validate the effectiveness of the suggested method. Finally, static pressure tests are conducted to assess the energy absorption advantages of biological features, taking the optimized honeycomb structure as an example. Compared to the traditional SIMP structure, the optimized honeycomb structure has a 17.4% improvement in energy absorption, with only a 2.3% increase in compliance. These results demonstrate the potential of IPTO for optimization of multifunctional structures.

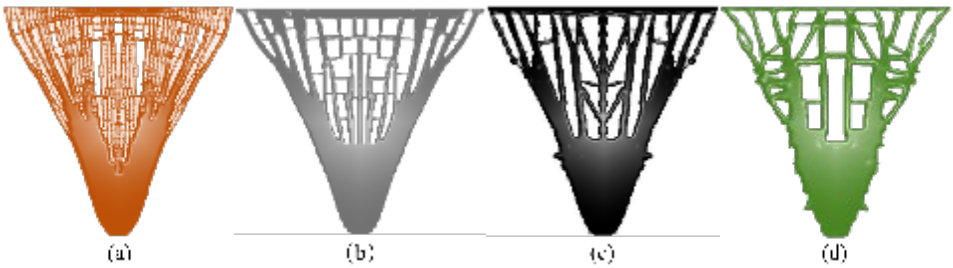

Figure 1. Design result from IPTO method

(a) Integrating earthworm skin feature, C =20.8; (b) Integrating cuttlebone feature, C =20.4; (c) Integrating teeth feature, C =19.5; (d) Integrating cuttlebone-teeth junction feature, C =20.1

Keywords: Image-physics driven design, Topology optimization, Biological features, Convolutional neural network.

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Micro-CT bone analysis via deep learning: A case study on the effects of risedronate and mechanical loading on aged mice

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We present a fully automated deep learning-based pipeline for the analysis of mouse tibiae using high-resolution micro-computed tomography (micro-CT) imaging. It enables efficient, detailed assessment of cortical and trabecular bone, supporting preclinical research such as in drug treatments and mechanical loading studies. As a case study, we applied the pipeline to investigate the combined effects of risedronate treatment and mechanical loading in aged female mice (see Fig. 1). Risedronate had a positive effect on cortical bone properties (Ct.Ar, Ct.Th, $p \leq 0.05$) and affected trabecular structure (higher Tb.Th, lower Tb.Pf, $p \leq 0.05$) without altering BV/TV. Importantly, risedronate did not impair the osteogenic response to mechanical loading in old mice. This suggests that concurrent treatment with bisphosphonates and exercise is not contraindicated. The automated pipeline enabled reproducible analysis of micro-CT scans of mouse tibiae accelerating preclinical skeletal research.

Keywords: Deep learning; Micro-CT; Osteoporosis; Bone; Preclinical research; Old mice.

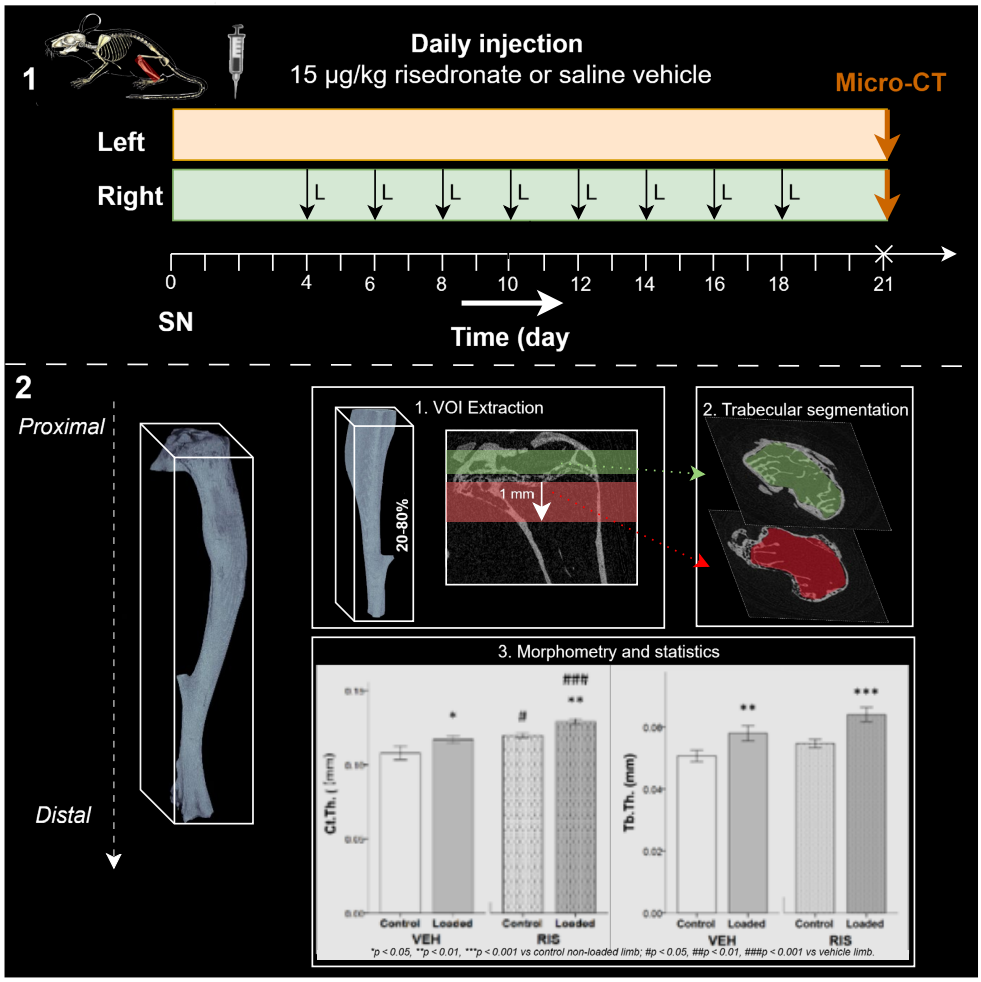

Figure 1. (1) Schematic of the study design: risedronate and mechanical loading in aged mice. (2) Deep learning analysis of cortical and trabecular bone using micro-CT imaging of mouse tibiae.

Quasi-potential model for nonlinear wind-induced water waves

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Wind-waves are one of the most common phenomena in the marine environment and have garnered significant attention since the last century. Numerous theoretical, experimental, and numerical studies have sought to clarify the complex dynamics. However, the interactions remain only partially understood due to the strong coupling, which complicates predictions and makes these interactions a challenging subject of study. This study presents an improved model for wind-driven water waves by incorporating both wind pressure and tangential viscous stress. The model referred to as quasi-potential theory is expressed as:

$$\begin{gathered}\phi_{xx}+\phi_{yy}=0, \quad -h<y<\eta(x,t)\\ \phi_y=0, \quad y=-h\\ \eta_t+\eta_x\phi_x=\phi_y+2\nu\eta_{xx}-\int_0^t\frac{\Gamma}{\rho}\eta_x dt, \quad y=\eta(x,t)\\ \phi_t+\frac{1}{2}\left[(\phi_x)^2+(\phi_y)^2\right]+g\eta+\frac{p}{\rho}=-2\nu\phi_{xx}, \quad y=\eta(x,t)\end{gathered} \tag{1}$$

where (x,y) denotes the horizontal and vertical coordinates, with subscripts indicating derivatives in the corresponding directions. h is the water depth, $\eta(x,t)$ is the surface elevation, ϕ is the velocity potential, g is the gravity, ρ is the water density, and ν is the water viscosity. p represents the wind pressure and Γ is a parameter characterizing wind tangential viscous stress. Based on numerical simulations of turbulent flow over slowing moving wave boundaries, the wind pressure p and tangential viscous stress τ are modelled as

$$\begin{aligned}p&=r\rho_a u^2 k\eta(kx+\theta,t),\\ \tau&=s\rho_a u^2 k\eta(kx+\beta,t),\end{aligned} \tag{2}$$

where r,s are parameters related to the magnitude of wind forces, ρ_a is the air density, u is the air velocity, k is the wave number, θ is the phase shift between pressure and wave elevation, and β is the phase shift between tangential viscous stress and wave elevation. A multi-scale asymptotic expansion gives the theoretical solution of the proposed system, where a crucial time-dependent parameter quantifying the wind effect on wave evolution appears, which can also be characterized as the growth rate. An unsteady numerical method based on a conformal mapping technique aligns the growth rate well with the theoretical prediction. Furthermore, the third-order statistical moments of wind-waves are established theoretically and show improved alignment with laboratory and marine observations in predicting wind-wave skewness and asymmetry.

Keywords: gravity waves, wind-wave interaction

Neural Network-Based Constitutive Model for Porous Solid Materials

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Multi-scale homogenization is a numerical method to study the behavior of heterogeneous materials at different length scales. In recent times, machine learning methods have demonstrated impressive potential in modeling material behavior [1,2]. In this work a novel neural network-based methods for simulating the complex nonlinear relations of porous solid material is proposed. To achieve this objective, an artificial neural network is used to learn path-dependent inelastic behavior. The network is constructed utilizing a general internal variable formalism, with the selection of internal variables being dependent on the nature of the problem and the desired level of accuracy.

The training data are generated with multi-scale homogenisation numerical simulation on a representative volume element including void volume fraction of $f=10\%$ with elasto-plastic von Mises material characteristics under plane strain condition and imposed to linear boundary conditions and random cyclic loading. The obtained results with neural networks have been compared against the RVE numerically generated data and shown a potential of describe the material stress/strain relationship with high accuracy. In addition, the quantities of hydrostatic pressure P and the norm of the deviatoric stress Q have been studied and compared against Gurson's model.

Keywords: Neural Network, Constitutive Modelling, Plastic Deformation, Gurson Model

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Developments of Auxetic Pile-type Metamaterials for Seismic Wave Attenuation

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This study presents a novel approach to enhancing seismic metamaterials by integrating auxetic structures to improve earthquake wave attenuation. Focusing on local resonance, the proposed design embeds auxetic geometries into pile-type metamaterials to achieve broader and lower-frequency band gaps suitable for seismic applications. Auxetic materials, known for their negative Poisson's ratio, contribute to strong energy attenuation and wide omnidirectional band gaps. Both one-fifteenth scaled experiments and corresponding three-dimensional numerical models demonstrate that the auxetic-based metamaterial can effectively block primary seismic waves. Results show excellent alignment between the predicted and observed attenuation zones, with distinct local resonance patterns identified through kinetic energy distribution analysis. A parametric study further confirms that periodic arrangements are critical for achieving the desired band gap. In sum, this research introduces a three-dimensional auxetic-concrete seismic metamaterial, validated by both simulation and experiment, highlighting its practical potential for future seismic protection systems.

Keywords: Seismic metamaterial, band gap, auxetics, local resonance, finite element analysis, laboratory-scale test

High-accuracy isoparametric closure boundary elements and their applications in mechanics analysis

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ABSTRACT

Recently, a series of isoparametric closure boundary elements have been constructed to simulate the shape of holes, tubes, disks, rings and spheres based on the Lagrange interpolation formulation and the closure condition at two ends of an arc. These elements can simulate the models which contain the shapes mentioned above with less nodes and less elements than the conventional boundary elements. However, the basis of those elements, i.e., hole elements, have the poor accuracy when the number of nodes is less than 8. To improve these elements, two kinds of improvements are proposed in this study. The first one constructs the element by 'repeated winding' a Lagrange line element over the hole. The second one let trigonometric functions be the bases of shape functions to substitute the Lagrange polynomial. Two kinds of hole elements and their derived tube, disk, ring and sphere element are used to simulate the structures containing holes, cylinders, and spheres, such as fiber reinforced composites and particle reinforced composites etc. Through those simulation, it can be found that two kinds of newly proposed hole elements and their derived elements both perform very well in the discretization of the geometry and the interpolation of physical variables.

Key words: *Boundary element method, Isoparametric element, Fiber reinforced composites, Particle reinforced composites*

Nature's Design: Optimal Functional Balance Behind Fractal Morphology of Leaf Veins

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The veins serve as the functional skeleton in plant leaves, providing deformation resistance to external loads and substance transportation channels for water and organics [1-2]. Different species of broad-leaved plants possess the similar branching vein structure, indicating some form of general and critical design principle in nature. To this end, we developed a multi objective collaborative optimization method to reveal the underlying dominant rule that suggests the fractal tree like vein morphology in broad leaves: natural plant growth requires leaves to seek the balance between the functionalities of veins on bending stiffness and substance transportation efficiency. The leaf veins have a hierarchical structure with the stronger low-order veins as main leaf skeleton to ensure sufficient illuminated area for photosynthesis; on the other hand, the high-order veins with thinner channels yet greater total length are efficient in conveying synthesized matters such as sucrose over the leaf to the branches and the trunk. Despite the variety in plant growth period, physiological structure and environment, the hierarchical vein structure remains consistent by adopting a unique balance point between bending stiffness and transportation efficiency. The consistency in vein morphology is demonstrated by the observation of close fractal dimension values for both natural and optimized leaf veins. The design principle of numerous vein structures in nature can be accounted for through the fractal tree model following specific construction rules in different conditions. The proposed optimization method provides a powerful tool for the design of optimal structures considering the collaborative functions in mechanics and transportation, and can be readily extended to the optimization problems for otherwise objectives.

Keywords: Plant leaf veins, structural optimization, fractal tree, substance transportation, bending stiffness

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Computational Optimisation of Heat Convective Structures

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This paper presents a computational approach for the shape optimization of heat sink configurations utilized in central processing unit (CPU) thermal management, with the objective of enhancing convective heat transfer efficiency. As electronic systems continue to increase in power density, effective thermal regulation becomes critical, particularly within confined design domains where both natural and forced convection mechanisms can be considered. The present research specifically addresses the challenge of designing lightweight, compact heat sink structures that minimize thermal resistance while preserving efficient airflow distribution across varying flow regimes. A comprehensive review of existing literature highlights the significance of the Reynolds number and Nusselt number in characterizing flow behaviour and convective heat transfer. The implementation of the k–ε turbulence model enables accurate modelling of turbulent boundary layers, which is essential for resolving flow separation, quantifying pressure drop and ensuring uniform thermal distribution. The fluid dynamics are governed by the Navier–Stokes equations, and the Knudsen number is considered to assess the validity of continuum assumptions in microscale heat sinks where rarefaction effects may arise. The computational framework developed in this research employs ANSYS Fluent, utilizing both steady-state and transient solvers to perform conjugate thermal-fluid simulations. The numerical models incorporate volumetric heat generation, realistic boundary conditions, and parametric variations in inlet velocity to replicate operational CPU environments. The impact of flow regime transitions on cooling efficiency is captured by systematically analysing key thermal and fluid performance measures across a range of Reynolds numbers, including temperature distribution, convective heat transfer coefficient, pressure drop, and total thermal resistance.

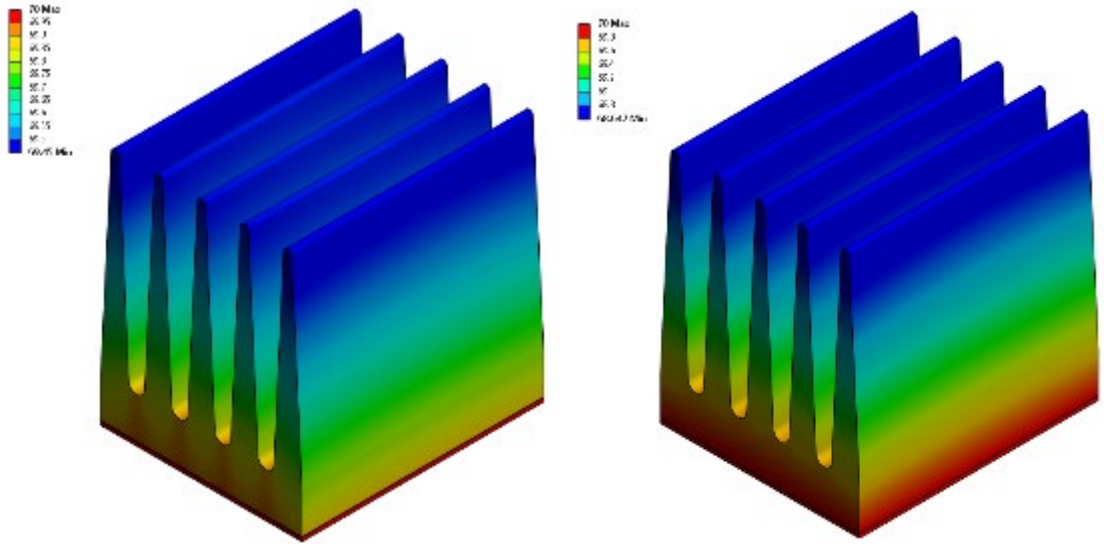

Figure 1.

Keywords: Convective heat transfer, Heat sink optimization, Computational Fluid Dynamics, k–ε turbulence model, Thermal resistance

An efficient and mesh-independent simulation framework for tunnel-induced rock failure based on the Scaled Boundary Finite Element Method

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Tunnel excavation through brittle rock is often accompanied by fracturing of the surrounding rock mass. Understanding and predicting the extent of rock fracturing during excavation is crucial for the safety and efficiency of the underground structure. Rock fracturing and collapse, induced by excavation, is a complex process involving changes in mechanical properties, stress redistribution and release after macroscopic cracking and scale effects and is strongly dependent on the stress path [1, 2]. Advanced numerical methods are commonly used in engineering practice to simulate the complex fracturing behaviour of rock masses. Among these methods, continuum- and mesh-based models are widely used for their efficiency and finite-element code compatibility. These typically treat rock masses as homogeneous continua with phenomenological constitutive laws. However, these models cannot explicitly capture macroscopic fractures or rock block separation, and their results often suffer from mesh dependency issues. To address this, this study presents a mesh-independent fracture mechanics framework for simulating tunnel-induced failure. A coupled damage–phase field formulation is adopted to describe the multiscale fracture evolution in the rock mass. With this the initiation of microcracks and the development of the fracture process zone are captured by a damage-like sub-problem. The macroscopic crack path is then regularised by the phase-field governing equations, leading to mesh-independent results:

$$\frac{\phi}{l_0} - l_0(\nabla^p)^2\phi = 2(1-\phi)F, \tag{1}$$

where ∇^p is the scalar differential operator, l_0 is the characteristic length, ϕ is the phase-field variable. F is the crack driving force. New scaling techniques are also proposed to define the characteristic length from laboratory to field-scale problems, allowing simulations with relatively coarse meshes and significantly improving computational efficiency for tunnel-scale analyses [3]:

$$\frac{l_{field}}{l_{lab}} = \left(\frac{D_{field}}{D_{lab}}\right)^{\frac{2n}{m_w}}, \tag{2}$$

where l_{lab} and l_{field} denote the characteristic lengths at the laboratory and tunnel scales respectively, while D_{lab} and D_{field} represent the corresponding characteristic sizes; n is the problem dimension, and m_w is the Weibull modulus. In addition, the proposed model is implemented based on the Scaled Boundary Finite Element Method and combined with a hierarchical quadtree meshing algorithm, enabling an automated modelling technique for excavation profiles. Validation through tunnel case studies demonstrates the model's ability to accurately predict the extent of failure zones.

Keywords: Tunnel excavation, Failure mechanism, Fracture mechanics, Phase-field modelling

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APCOM-ACCM 2025

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Numerical Evaluation of a Novel Mechanical Heart Valve Design

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The bileaflet mechanical heart valve (BMHV) remains the gold-standard prosthetic for aortic valve replacement in younger patients (< 60 years) owing to its exceptional durability, with 25-year survival rates exceeding 80% compared to bioprosthetic alternatives. However, its intrinsic design - featuring two rigid pyrolytic carbon leaflets mounted within a titanium alloy housing -generates non-physiological hemodynamics characterized by systolic triple-jet flows (Reynolds number $Re > 12{,}000$) and diastolic hinge leakage jets. These hemodynamic anomalies induce shear stresses exceeding 60 dyn/cm^2, a threshold implicated in platelet activation, thrombin generation, and subsequent thromboembolic complications. Legacy BMHVs like the St. Jude Medical Regent exhibit peak systolic shear stresses > 100 dyn/cm^2 and regurgitant velocities of 6–15 m/s during closure, triggering platelet activation. These hemodynamic shortcomings necessitate lifelong anticoagulation, exposing patients to annual bleeding risks of 1.5–2.5% and thromboembolic event rates of 1–4%, underscoring the critical need for design innovations that reconcile mechanical durability with improved hemocompatibility. To address these limitations, we propose a novel BMHV design incorporating elastic leaflet hinges (Figure 1 (a)). The design introduces a torsional spring at the pivot axis to modulate leaflet kinematics, reducing closure-phase rebound and associated regurgitant flows. Fluid-structure interaction simulations were conducted using an in-house immersed boundary-lattice Boltzmann method solver [1]. Leaflet dynamics are governed by the angular momentum balance:

$$J_o\ddot{\theta}(t) + c\dot{\theta}(t) + k_s\theta(t) = T_o(t), \quad (1)$$

where J_0 is the leaflet's moment of inertial, $\ddot{\theta}$ is the angular acceleration of the leaflet, c is the damping, k_s is the spring stiffness, and T_0 is the total moment of fluid force exerted on the leaflet. Figure 1 (b) demonstrates the hemodynamic impact of spring integration, showing a 82% reduction in diastolic minimum leaflet opening angle (4.5^o vs 23.2^o for rigid hinges). This kinematic optimisation attenuates regurgitant jet velocity, potentially lowering shear stress exposure below the threshold.

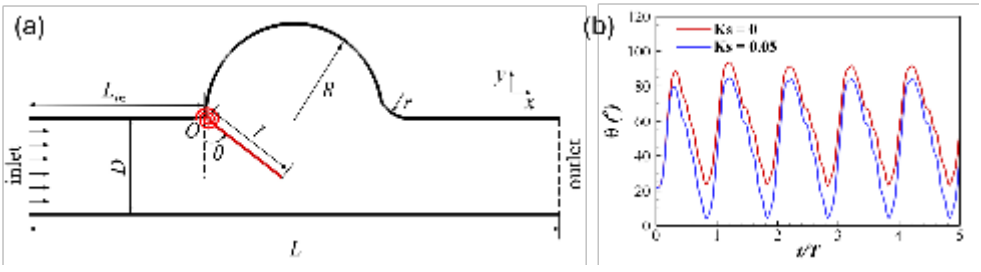

Figure 1. Proof of concept of a new mechanical heart valve design: (a) a spring is installed at the root to provide elasticity; (b) evolution in time of the opening angle of leaflets with and without spring.

Key words: Bileaflet mechanical heart valve, fluid-structure interactions, lattice Boltzmann method

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Design Optimization of Cylindrical Battery Thermal Management System for Uniform Temperature

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Temperature uniformity in Lithium-ion battery thermal management systems (BTMS) is crucial for achieving thermal safety and optimal performance in electric vehicles. Therefore, an effective battery thermal management system (BTMS) is essential to maintain safe operation by regulating the battery temperature within safe limits.

This study proposes optimization method to enhance the temperature uniformity of a liquid-cooled BTMS for cylindrical battery. The heat generation rate of the battery was determined based on voltage and current data, followed by thermal-fluid coupled multi-physics analysis to evaluate the cooling performance. Design variables include the outer and inner dimensions of the cooling plate and the coolant flow rate, constrained by the BTMS mass. The combined approach resulted in a significant reduction in temperature and showed the effectiveness of this optimization strategy in improving the thermal management of Lithium-ion battery modules.

Fig. 1. Cylindrical battery module

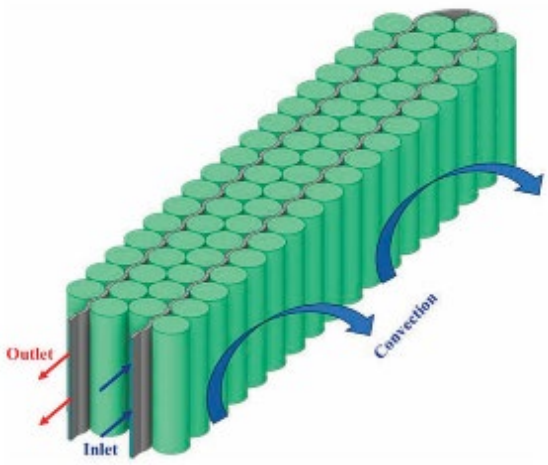

Fig. 2. Schematic of cylindrical battery module

Keywords: Lithium-ion battery, Battery thermal management system, uniform temperature, Optimization

Acknowledgements

This study was supported by National Research Foundation of Korea (NRF) grant funded by the Korea government the Ministry of Science, ICT & Future Planning (RS-2024-00352401) and by the Technology Innovation Program (RS-2024-00444961) funded By the Ministry of Trade, Industry & Energy(MOTIE, Korea).

Biomechanical Analysis of Resection Angles in Mandibular Reconstruction

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Mandibular reconstruction induced by trauma and cancer treatments involves a complex set of surgical considerations. It is essential to adequately remove malignant tissues while preserving the maximal integrity of the native bone and surrounding muscular attachments. While clinical studies have underscored the importance of osteotomy geometry in surgical planning [1], there remains a lack of systematic and quantitative analyses evaluating the biomechanical consequences of different resection angles. Angled mandibular osteotomies are particularly important due to their surgical applicability and potential impact on postoperative stability. Nevertheless, clinical evaluation is typically limited to a single surgical scenario per patient, highlighting the value of computational simulations in exploring alternative surgical strategies.

In this study, finite element analysis (FEA) was utilized to quantitatively assess the biomechanical implications of various anterior and posterior resection plane angles in mandibular reconstruction, using a single patient-specific model with preliminary bone union conditions. The methodology involves three main steps: (1) constructing a patient-specific 3D mandibular model from medical imaging data, (2) generating virtual surgical plans with systematic variations in both anterior and posterior resection plane angles, and (3) conducting finite element simulations to quantitatively compare biomechanical performance of different surgical designs relative to each other and against the native mandible.

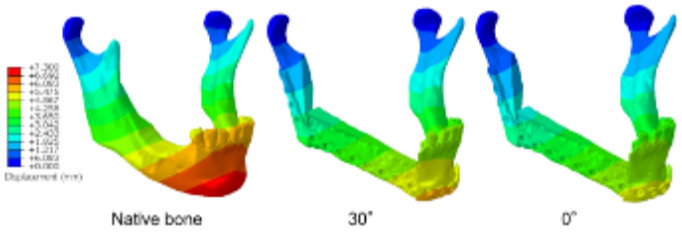

Figure 1. Finite element analysis models

The comparative analysis of different resection designs revealed that the configuration featuring both anterior and posterior resection planes angled 30 degrees inferiorly toward the midpoint of the graft yielded biomechanical behaviour most closely resembling that of the native mandible, as evidenced by reduced displacement and relatively lower stress distributions compared to alternative designs. These findings highlight a potentially optimal surgical approach, offering valuable guidance for surgeons to enhance postoperative structural and functional stability.

Keywords: Mandibular reconstruction, resection plane angles, virtual surgical planning, finite element analysis.

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Microscopic Traffic Flow Simulation Considering Electric Vehicles Charging Fee Strategy

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One of the key challenges in the widespread adoption of electric vehicles (EVs), which are expected to play a significant role in reducing environmental impact, is the development and efficient utilization of charging stations (CSs). Charging EVs at CSs takes much longer than refuelling gasoline-powered vehicles, potentially leading to waiting times and disruptions in surrounding traffic. One possible strategy to minimize the impact on traffic flow is to promote the distributed use of CSs through pricing incentives. This study examines the effect of pricing incentives on the distribution of CS usage within a simulation model capable of reproducing vehicle interactions. To analyze its impact on CS utilization patterns, a charging fee strategy algorithm [1] represented by equations (1) to (3) is integrated into ADVENTURE_Mates [2], which is a microscopic traffic flow simulator capable of modelling vehicle interactions. $P_K(T_r)$ is the charging fee, $G_K(T_r)$ is the queue of EVs charging at the CS, $M_K(T_r)$ is the queue of EVs that need to be charged but have not yet reached the CS, and U_K is the number of CSs. In addition, P_0 is the fee of electricity that the CS purchases from the power grid, P_s is the basic service fee at the CS, T_w is the waiting time in line for EVs at the CS, and E_{re} is the amount of charging per EV at the CS. η is a fee adjustment coefficient, which is a parameter for calculating the additional fee based on the waiting time in line T_w, and θ is a parameter for adjusting the basic fee according to the utilization rate of the CS.

$$\text{(i)}\ \ 0 \le G_K(T_r) + M_K(T_r) < \frac{1}{\eta}U_K \qquad P_K(T_r) = P_0 + P_s \tag{1}$$

$$\text{(ii)}\ \ \frac{1}{\eta}U_K \le G_K(T_r) + M_K(T_r) < U_K \qquad P_K(T_r) = P_0 + \eta P_s \times \frac{G_K(T_r) + M_K(T_r)}{U_K} \tag{2}$$

$$\text{(iii)}\ \ U_K \le G_K(T_r) + M_K(T_r) \qquad P_K(T_r) = P_0 + \eta P_s + \frac{\theta T_w}{E_{re}} \tag{3}$$

The simulation was conducted by installing CS1 and CS2 facing the main road, and CS3 and CS4 located away from the main road. Table 1 shows the average number of vehicles waiting to charge at each CS. From Table 1, introducing the charging fee strategy algorithm helped prevent overcrowding at CSs near the main road and promoted more use of CSs farther away. This significantly reduced the number of vehicles waiting to charge at CSs near the main road, minimizing traffic disruptions in surrounding areas.

Table 1.

	CS1	CS2	CS3	CS 4
w/o strategy	13.4	17.0	0	0
w strategy	4.3	4.1	2.4	3.8

Keywords: electric vehicle, charging station, traffic flow, microscopic simulation

Reference

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Failure-Aware Topology Optimization of CFRP Structures for Additive Manufacturing: Integrating the Tsai-Wu Criterion

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Additive manufacturing (AM) opens new pathways for designing carbon fiber reinforced polymer (CFRP) structures by enabling tailored fiber paths and complex topologies. However, compliance-only topology optimization may yield structures susceptible to failure. This study presents a novel topology optimization framework for CFRP structures that integrates the Tsai-Wu failure criterion to enhance structural integrity while ensuring manufacturability. The proposed framework utilizes the discrete material and thickness optimization (DMTO) method to simultaneously optimize material layout and fiber orientations across layers. A p-norm function aggregates local failure indices to balance computational efficiency and failure sensitivity. Two case studies—a cantilevered L-shaped structure and a three-point bending plate—demonstrate the effectiveness of the failure-aware approach. In the L-shaped design, failure-aware optimization reduced the maximum failure index by 59.6% by smoothing stress concentrations at the corner fillet. In the three-point bending example, the failure-aware design exhibited a 63.6% reduction in the failure index and a 32.5% increase in load-bearing capacity in experiments compared to compliance-only designs. The optimized CFRP samples were fabricated using a Markforged printer and experimentally validated under loading. Results confirm that accounting for failure during optimization significantly improves load-carrying performance and robustness. This study provides a practical and efficient strategy for designing CFRP components optimized for strength and manufacturability via AM, marking a step forward in high-performance composite structure design.

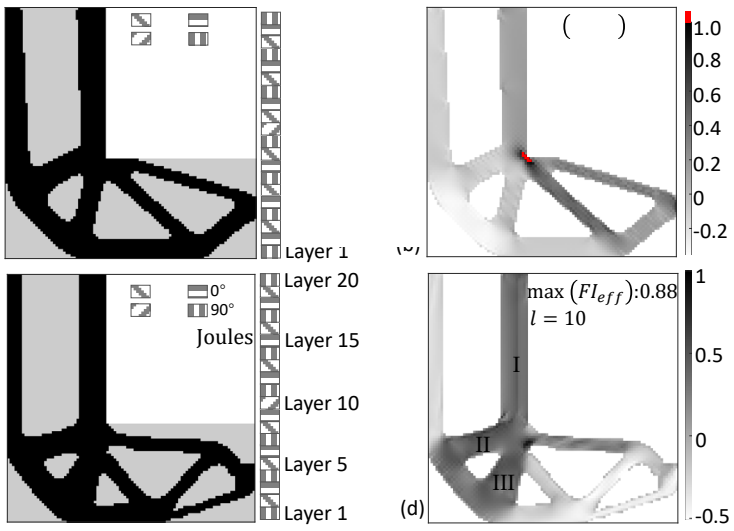

Figure 1.

Keywords: Topology optimization, CFRP composite structure, Additive manufacturing, Failure criterion

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Multiscale quadtree/octree scaled boundary finite element method

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A new numerical model is proposed by combining the framework of the extended multiscale FEM and the scaled boundary finite element method (SBFEM) for the multiscale heterogeneous analysis of mechanical and heat transfer problems. Scaled Boundary Finite Element (SBFE) and image-based quadtree or octree gridding, the construction of base functions can be conveniently and efficiently conducted particularly for the heterogeneous media with complex geometries or singularity of stress or heat flux at the small-scale, and the solution accuracy at the large-scale can be improved by increasing nodes of coarse element only without increasing new nodes inside. Consequently, the SBFEM based solutions at the large-scale can be solved with a reduced order and sufficient accuracy, and the solutions at the small-scale can be achieved using SBFEM based base functions. We have applied the proposed method into steady and transient heat transfer problems, elastic and viscoelastic problems, and developed special computational scheme for nonlinear problems, and both 2D and 3D problems can be solved. The proposed method provides an efficient approach for multiscale analysis with automatic mesh generation and fast computation in different scales, having potential in a serials of important engineering problems.

Keywords: Multiscale analysis, quadtree/octree SBFEM, image-based multiscale analysis, numerical based function, heat transfer analysis, elastic and viscoelastic analysis

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Polarization-dependent Elastic Wave Control by A Novel Honeycomb Topological Metamaterials

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Abstract

The manipulation of elastic waves through topological metamaterials has garnered significant research attention due to its promising industrial applications. However, the complexity introduced by intense wave polarization poses challenges, particularly in the realm of mono-polarized waves, thereby hindering the advancement of topological elastic metamaterials. In response to this limitation, we introduce a novel frame structure configured as a hexagonal lattice, which exhibits independent control over in-plane and out-of-plane polarized bandgaps through the utilization of accidental Dirac cones. Our in-depth investigations reveal that these accidental Dirac cones stratify the parametric space into four distinct regions, each characterized by unique valley Chern numbers. By integrating unit cells from these diverse regions, we achieve polarization-dependent topological protected interface modes, enabling scenarios where only in-plane or out-of-plane modes are supported, as well as those accommodating both. Leveraging this unique property, our study demonstrates polarization-dependent waveguiding and wave separation. To validate our theoretical findings, we fabricated one of the designed models using 3D printing and conducted experimental verification of polarization-dependent waveguiding. Further analysis confirms the independence of in-plane and out-of-plane waveguiding, even in the presence of intersections in their pathways. This discovery paves the way for the design of innovative elastic devices capable of carrying and encrypting information, as exemplified by several prototypes presented in this paper. Our work not only broadens the application scope of topological elastic metamaterials from mono-polarized to dual-polarized waves but also holds immense potential for the exploration and development of more advanced elastic devices for wave manipulation.

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Preliminary investigation of a multi-phase-field simulation method for semi-solid deformation introducing gas-liquid two-phase flow

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In casting processes, deformation of semi-solid materials due to various factors can lead to solidification defects such as segregation, porosity, and cracking [1][2]. A detailed understanding of semi-solid deformation is essential to mitigate these defects. However, direct observation of such phenomena is challenging, making numerical simulation indispensable. We has developed a multi-phase-field lattice Boltzmann model to simulate shear deformation of semi-solid systems, enabling detailed analysis of segregation formation [3]. To further address porosity and cracking, we introduced free surface as boundary conditions, and conducted compression deformation simulations incorporating a gas phase, as shown in Fig. 1. This allowed us to represent free surface behavior and successfully reproduce the initial stage of porosity formation—namely, gas entrapment—during compression of high-solid-fraction semi-solids [4]. Nevertheless, more advanced modeling is required to account for surface tension effects and internal gas generation. In this study, we investigate a deformation simulation method for semi-solid materials by incorporating a gas–liquid two-phase lattice Boltzmann model, enabling more accurate treatment of gas-phase dynamics.

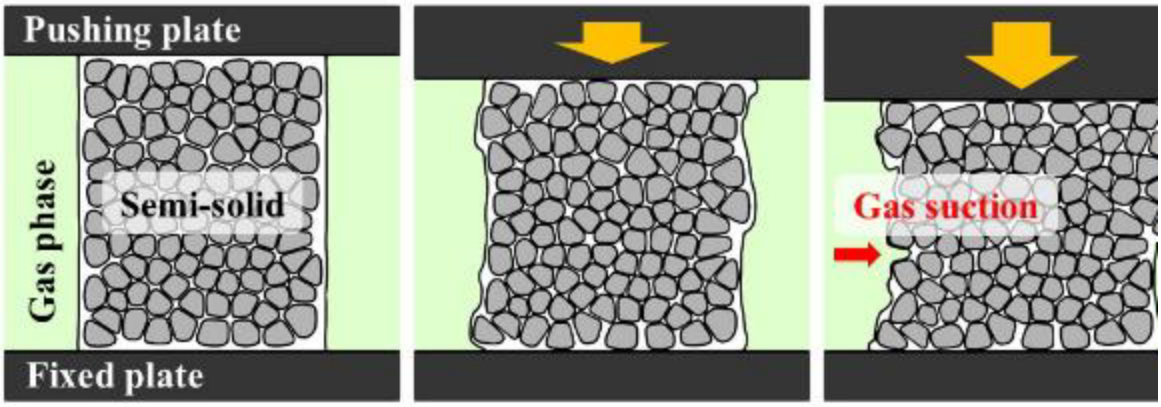

Figure 1. Compression simulation of a semi-solid body incorporating the free surface [4].

Keywords: phase-field method, Lattice Boltzmann method, two-phase flow, semi-solid deformation, solidification defect

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A Study on High-Quality Slow-motion Video Generation for Running Analysis

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In skill acquisition, particularly in sports involving running, trainers support the learning process by accurately assessing an athlete's condition and providing appropriate movement guidance. To aid in this process, athletes often review videos of their training sessions to better understand the movements and make immediate adjustments. In everyday situations, cameras built into consumer video devices or smartphones typically record at 30 to 60 frames per second (fps). However, when analyzing fast-paced sports movements, such frame rates are insufficient to produce smooth video, making it difficult to capture and reproduce motion accurately. High-speed cameras, with record at 120 to 240 fps, are more suitable for this propose but are often prohibitively expensive. To address this issue, our research aims to develop a frame interpolation tool to capable of generating high-frame-rate slow-motion video from footage recorded with standard low-frame-rate cameras.

In this study, we specifically focus on the motion of running as our primary research target. We build upon the Real-Time Intermediate Flow Estimation (RIFE) [1] model, a mature and widely adopted framework for frame interpolation at arbitrary magnification levels. To further improve interpolation quality and reduce common issues such as ghosting and blurring, we integrate the Keypoint-Aware Loss based on ViTPose [2] and the Segmentation-Aware Loss based on Mask2Former [3], following the approach proposed in the SportsSloMo framework [4]. By focusing on running motion, our method provides strong technical support for generating high-quality, low-cost slow-motion videos tailored for running performance analysis.

Keywords: Video frame interpolation, human-aware loss, slow-motion generation, running motion analysis

Acknowledgement

This work was supported by JSPS KAKENHI Grant Number JP24K14538.

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Origins of Mixed Quantum Well Width in 2D Perovskite from Machine Learning-enabled Multiscale Simulations

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Two-dimensional (2D) lead-halide perovskites have attracted significant attention due to their superior environmental stability and tunable optoelectronic properties, which can be precisely controlled by varying the quantum well (QW) width (denoted by the integer n). However, the commonly observed phenomenon of mixed QW width distributions poses a substantial challenge to achieving optimal device performance. This necessitates a comprehensive understanding of the dependence of QW width distributions on chemical composition and thermodynamic stability. In this study, we develop a robust machine learning (ML)-based energy model [1], rigorously benchmarked against first-principles calculations, enabling extensive molecular-level simulations of 2D perovskites with butylammonium (BA) and phenethylammonium (PEA) spacer cations. Through hybrid Monte Carlo simulations capable of modeling significantly larger system sizes compared to traditional first-principles methods, we demonstrate a universal and rapid transition from initially homogeneous single-phase QW structures toward energetically favoured mixed-phase distributions. Notably, the formation of these mixed phases arises primarily due to the enhanced thermodynamic stability of low-n layers, driven by the strong affinity of self-assembled spacer cations to the inorganic PbI_6 octahedra framework relative to methylammonium cations. Our findings underscore how machine learning-powered multiscale modelling provides unprecedented insights into complex 2D perovskite microstructures, thereby offering valuable guidelines for the rational design and molecular engineering of next-generation perovskite-based optoelectronic devices.

Keywords: Machine Learning, 2D Perovskite, Monte Carlo Simulations, Microstructure

References

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Effect of Image Resolution on the Accuracy of AI Pose Estimation in Sprinting

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From the perspectives of performance improvement and injury prevention, recording and quantitatively analyzing the body's movements during running is considered an effective method. Recent advancements in AI-based pose estimation technologies have enabled motion capture without markers, offering a cost-effective and accessible alternative to traditional optical systems.

This paper explores the influence of input video resolution on the accuracy of motion analysis using AI-based systems, with a specific focus on running motion. To validate the reliability of these systems, we compared their performance with that of a high-precision marker-based optical motion capture system, which serves as the ground truth. The keypoint coordinates obtained from OpenPose[1] exhibited some frames with detection failures (coordinates = 0), and misrecognitions occurred due to the recording being from the subject's right side, causing left-right reversal when the feet crossed.

To address these issues, interpolation and correction were applied to the predicted coordinates. The smoothed coordinates were then normalized. Furthermore, we also compare OpenPose's performance with that of other AI-based motion capture software.

Keywords: Motion capture, deep learning, sprint running, human motion recognition

Acknowledgement

This work was supported by JSPS KAKENHI Grant Number JP24K14538.

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Differentiable Programming for Solving Nonlinear Inverse Problems

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Differentiable programming enables the automatic computation of gradients across complex computational workflows, leveraging frameworks like JAX or Taichi to optimize parameters in neural networks, physics simulations, or hybrid models. Differentiable programming solves inverse problems by enabling gradient-based optimization of a forward model's parameters. By encoding the physical/observational process as a differentiable function, gradients of the mismatch between predictions and observations (loss) can be backpropagated to efficiently infer unknown inputs (e.g., material properties, initial conditions), avoiding brute-force search. In the context of differentiable programming, gradients become "free lunch" and the workflow can be fully automatic, enabling systematic solutions to inverse problems for complicated physical systems with strong nonlinear behaviors. This presentation will introduce JAX-FEM (https://github.com/deepmodeling/jax-fem), an open-source differentiable finite element framework built on JAX, designed to solve nonlinear inverse problems in computational mechanics by integrating automatic differentiation (AD) with traditional finite element methods (FEM). The library enables gradient computation through physics-based simulations, allowing users to efficiently infer unknown parameters by optimizing discrepancies between model predictions and observed data. By embedding constitutive laws as differentiable operators, JAX-FEM preserves gradients during partial differential equation solutions, facilitating applications like material identification from deformation measurements or topology optimization for structural design. This presentation will review existing features of JAX-FEM, discuss some ongoing efforts, and look into possible future developments. Two prominent applications of differentiable programming for solving inverse problems will be presented: parameter identification for Lithium-ion batteries and calibration of crystal plasticity finite element models. Also, some recent progress of differentiable programming for uncertainty quantification will be discussed.

Robust Topology Optimization of FRP Composite Structures under Dynamic Load Uncertainties

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This study addresses the uncertainties associated with design of fibre reinforced plastic (FRP) composite structures under dynamic loads, particularly those related to excitation amplitude and direction, which can lead to excessive deformation and significantly degraded structural performance [1]. To tackle this challenge, a robust design framework is proposed for the topology optimization of fibre-reinforced plastic composite structures, which takes into account the stochastic nature of excitation amplitude and direction. The study employs the Discrete Material and Thickness Optimization (DMTO) method, which addresses the optimization of both topology and morphological variables through parametrization. The optimization objective is to minimize the mean and standard deviation of the structural dynamic compliance response, which can be rewritten as,

$$\text{Min} \quad J(\chi, \rho_e, x_{ec}) = \mu\left(\left|\mathbf{F}^{\mathrm{T}}(\chi)\mathbf{U}(\chi)\right|\right) + \kappa\sigma\left(\left|\mathbf{F}^{\mathrm{T}}(\chi)\mathbf{U}(\chi)\right|\right), \tag{1}$$

As shown in Fig.1, through the 2D cases study, the impact of dynamic load uncertainties on optimization results is explored, and further robust optimization of a composite beam under multiple loading conditions is investigated. Additionally, the study evaluates the potential application of the proposed method in complex structural components by conducting robust optimization of the dynamic performance of a 3D laminated plate.

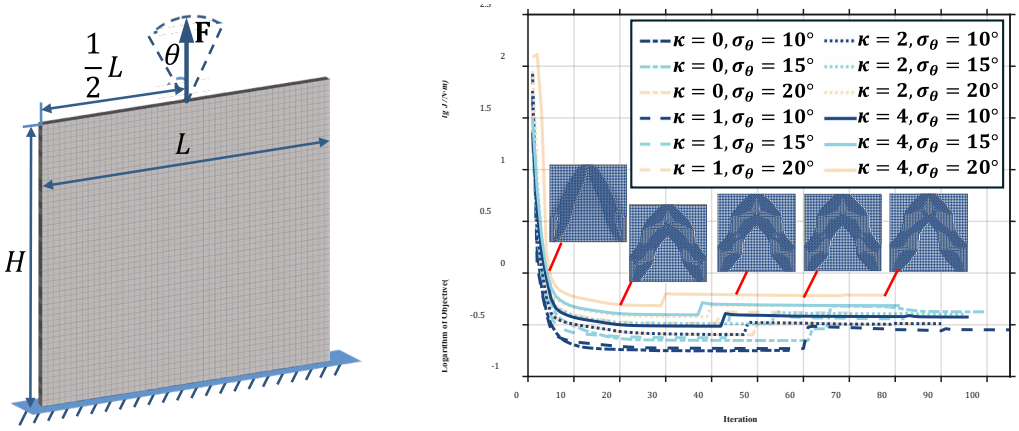

Figure 1.

Keywords: Robust optimization, Fiber-reinforced plastic composites, Discrete material and thickness optimization (DMTO), Dynamic response, Excitation forces uncertainty.

References

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The Influence of Fibre Angle Variation on Impact Resistance of Variable Stiffness Composite Laminates

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The Variable Stiffness Composite laminates which are fabricated by laying fibres in curved patterns can achieve the tailored design of stiffness distribution. In comparison to traditional composite laminates, the variable stiffness composite laminates not only achieve better designability but also enhance the performance of the structures. This study investigates the effect of curvilinear fibres on the impact resistance of variable stiffness composite laminates through proposing a novel numerical simulation method, in which a structured mesh model that accounts for the geometry of curved fibres is utilized to enhance the computational efficiency and accuracy. The proposed model is firstly validated by comparing the numerical predicted impact resistance of composite laminates with existing experimental data from the straight-fibre specimens. After that, the parametric analysis is carried out and the results indicate that the stress, damage and out-of-plane displacement distribution has significant fibre direction-dependent characteristics. Furthermore, the results also show that the variable stiffness composite laminates have superior impact performance compared to traditional composite laminates: 6-21% increase in energy absorption capacity through optimizing the fibre trajectory. The main reason is the curvilinear fibre architecture induces in-plane stiffness variation within the variable stiffness composite laminates and enable more materials to participate in deformation and failure processes so as to absorb more impact energy.

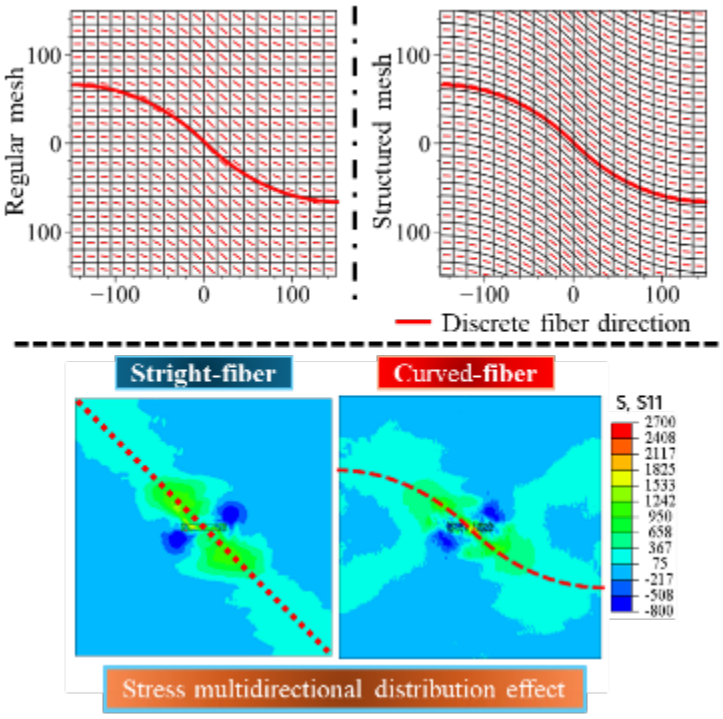

Figure 1.

Keywords: Variable Stiffness Composite, curvilinear fibre, high-velocity impact, failure mechanism

Performance Prediction of Cooling Impeller via Machine Learning

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This study proposes a machine learning (ML) framework for forecasting the performance of an impeller operating in a single-phase cooling system, where the approach of computational fluid dynamics (CFD) is employed for the impeller performance prediction and the method of deep neural networks (DNN) is adopted to establish the dependence of impeller performance on the design parameters. Geometric parameters for the impeller design as well as for the machine learning training, such as the camber, thickness, and pitch angle distribution of blade section along the radial direction as well as the impeller diameter and rotational speed, are selected as design parameters. The impeller configurations defined by design parameters are first simulated using STAR-CCM+ with a Multiple Reference Frame (MRF) approach to predict their mean performance in operation, such as the delivered flowrate across the impeller, the required torque and the efficiency at the designated rotation speed. An impeller design and its predicted flow field distribution in operation are illustrated in Figure 1. The simulation outputs, i.e., flowrate, torque and efficiency, are then used to train a DNN model, where the optimized number of the hidden layer along with the corresponding neuron number of each hidden layer is determined with the help of an iterative process as shown in Figure 2. K-fold cross-validation is employed to assess the model stability. The numerical results indicate that the blade pitch angle has a profound influence on both flow rate and torque compared to other parameters. In particular, the configurations with small pitch angle near tip and large pitch angle near hub tend to achieve better efficiency, as this configuration leads to a favorable local angle of attack and a minor tip loss. The proposed ML model is proven to successfully enable a rapid and accurate prediction of impeller performance.

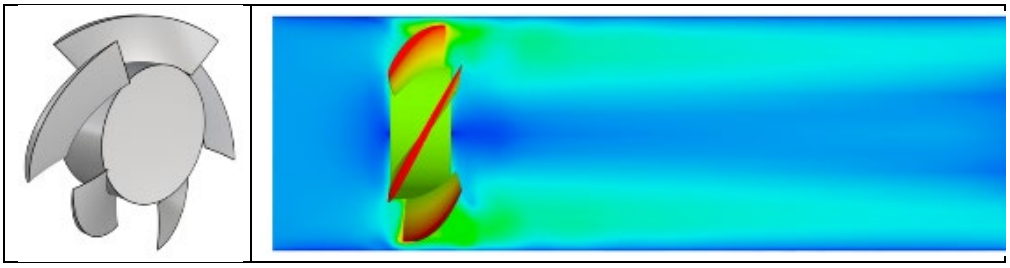

Figure 1. An impeller design and the prediction of its flow field distribution in operation

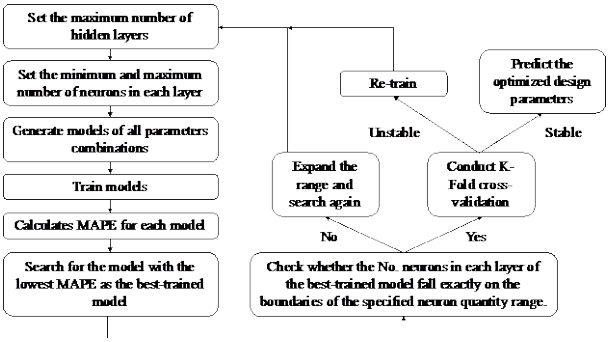

Figure 2. An iterative process to optimize the parameters defining the DNN model

Keywords: Impeller design, performance prediction, machine learning, CFD, DNN

Topology Optimization for Soft Pneumatic Actuators

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Soft actuators can produce large, compliant, and smooth deformations, enabling superior adaptability and interaction compliance. These actuators have been widely applied in fields such as aerial and aquatic locomotion, as well as biomedical devices, with common activation methods including light, electric, thermal, and mechanical stimuli. Soft pneumatic actuators (SPAs) utilize air pressure to achieve controlled deformations, offering relatively high force output in lightweight designs.

In the design of soft actuators, bionic methods [1] play an important role, while analytical methods have also been developed for some specific types, such as fiber-reinforced soft actuators [2]. Evidently, both methods are powerful, but they are not universal and may rely on researchers' experience and trial-and-error approaches. In contrast, topology optimization methods determine the optimal material distribution under given constraints, independent of prior experience or initial structural assumptions. Furthermore, in the design of soft actuators, researchers have found that the design problem can be regarded as a topology optimization problem of compliant mechanisms.

In our series of research works on topology optimization for soft actuators, we formulate the design problems of soft pneumatic actuators as compliant mechanisms. Topology optimization frameworks, methods, and algorithms have been developed for compliant mechanisms considering (1) design-dependent pressure loadings [3], (2) geometrical and material nonlinearities, (3) multi-objective and multi-constraint formulations, (4) concurrent optimization of structural topology and fiber orientation, and (5) machine learning-assisted topology optimization. The key contributions include the following: (1) for design-dependent pressure loading problems, we developed modeling schemes for the fluid-structure interface using an equivalent virtual work method (geometrically linear) and a substructure method (geometrically nonlinear), and proposed an element-based searching scheme for tracking multiple fluid-structure interfaces; (2) for compliant mechanisms under fixed loadings, we investigated multi-objective and multi-constraint design optimization considering geometrical and material nonlinearities and developed the relevant optimization method; (3) for fiber-reinforced compliant mechanisms, we introduced an analytical solution based on the variational method for orientation optimization, considering anisotropic materials and multi-input-multi-output compliant mechanisms; (4) we developed a novel higher-dimensional function online learning and prediction method to accelerate gradient-based (e.g., level-set method) and non-gradient-based topology optimization methods using machine learning; and (5) we explored the applications of the developed topology optimization methods in soft pneumatic actuator designs and achieved efficient soft bending and contraction actuators, soft grippers, and morphing wing rib designs.

Keywords: Topology optimization, Soft pneumatic actuator, Nonlinearity, Compliant mechanism, Design-dependent load, Machine learning

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Molecular dynamics simulation of the deformation of bicrystalline Al nanopillar under compression

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Molecular dynamics simulations were executed to clarify the deformation mechanism of crystalline materials. In this paper, the effect of the grain boundaries on the plastic deformation was especially focused, and bicrystalline nanopillar models were applied. The atomistic models were created by dividing an fcc rectangular parallelepiped pillar into two domains and applying different orientations to each domain. Two types of models were prepared; one is vertical boundary type, which has a grain boundary along the longitudinal direction, and the other is horizontal boundary type, in which the grain boundary is set perpendicular to the pillar axis. Symmetric and asymmetric boundaries were generated by varying the orientation of two grains, while only the tilt grain boundaries were considered. LAMMPS was used for simulation and an EAM potential for aluminum was applied. Assuming that the pillar was compressed by a rigid plate, the deformation process was observed using the change in configuration of atoms as well as common-neighbor analysis, centrosymmetric parameters, and dislocation analysis. Commonly, the dislocation and slip appeared first in one grain, followed by the slip expansion in the other grain. Then the role of the grain boundary as both the obstruction and origin of the slip behavior was investigated by collecting the data from various models. As a result, the effects of the grain boundaries were categorized by the types of the grain boundary and the relation between the slip orientation and Schmid factors of the corresponding crystals.

Figure 1 shows an example of the simulation result, corresponding to a vertical symmetric boundary model. Dislocations and slip planes are observed in symmetric orientations but discontinuous at the grain boundary. Therefore, it is indicated that the slips in a grain are obstructed at the grain boundary and do not pass through the other grain.

Keywords: Molecular dynamics, Bicrystal, Nanopillar, Dislocation, Grain boundary.

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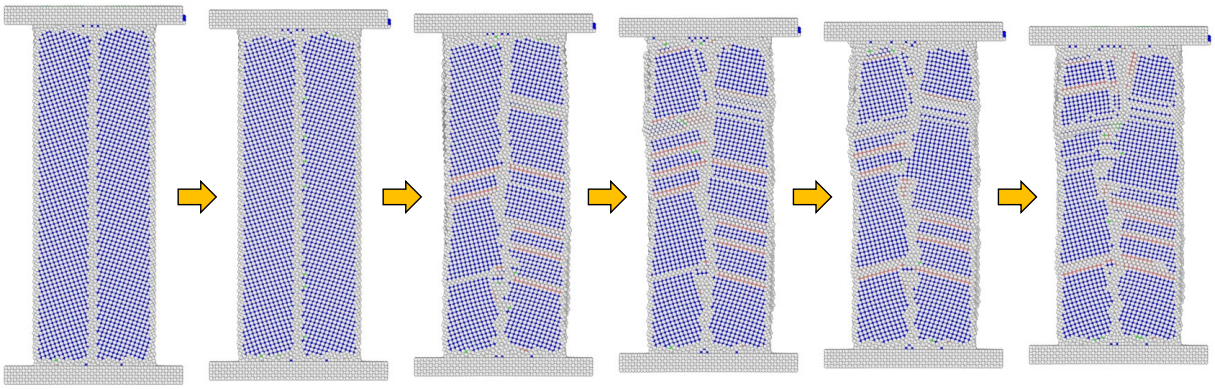

Figure 1.

An energy equivalent flow stress theory for plastic bending of fully clamped beams

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Fully clamped solid beams and thin-walled beams are extensively utilized in modern industrial products and engineering structures as energy absorption components. Existing large-deformation quasi-static plastic bending theories for fully clamped beams predominantly adopt the rigid-plastic material assumption, where the flow-stress of actual materials is typically determined through empirical formulas. These empirical formulas commonly include the arithmetic mean of yield stress and ultimate tensile stress, direct use of yield stress, and the geometric mean (square root of the product) of yield stress and ultimate tensile stress. The uncertainty of flow-stress introduces significant uncertainty into the theoretical predictions of structural deformation and force responses.

To overcome this limitation, we establish a flow-stress calculation method based on the energy equivalence principle. In this method, the flow stress of the material is no longer treated as a constant value, but is instead defined as a hardening-dependent stress value linked to the actual deformation history during bending. Furthermore, the method can further improve prediction accuracy by incorporating the local indentation effect of the indenter. Based on numerical method, parametric studies and sampling data analysis are conducted to verify the effectiveness and accuracy of the proposed method. Compared with empirical flow-stress formulas, the proposed method achieves significantly higher accuracy in predicting the large-deformation bending responses of fully clamped beams.

Keywords: Thin-walled beams, Large deformation, Fully clamped, Energy absorption, Crashworthiness

Level-set Topology Optimization of Electrode Pattern for Multi-Focusing and Acoustic Holography

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Conventional focusing methods via acoustic lenses have some limitations, such as a low transmittance and crosstalk, which degrade the imaging performance [1]. These issues originate from the complex structure and material properties of acoustic lenses, which absorb or scatter sound. To overcome these, this study introduces a new focusing concept based on a topology-optimized electrode pattern on a piezoelectric transducer without the acoustic lens for the ultrasonic focusing. To this end, a fully-coupled piezoelectric–acoustic interaction model is developed for the modeling of the piezoelectric transducer with air-backing conditions, and a systematic inverse design method to find optimal electrode patterns is proposed based on level-set topology optimization (LSTO) [2], in which the electrode pattern layouts are represented by the level-set function with a signed-distance property. The electric boundary condition is topologically parameterized using area fractions of design elements cut by the zero level-set contour. The electrode pattern layouts are evolved by solving the Hamilton-Jacobi equation with boundary point sensitivities calculated via a discrete adjoint method. The Kirchhoff–Helmholtz integral is used for efficient far-field evaluation during optimization. Numerical examples confirm that the optimized electrode pattern enables flexible multi-point focusing, with potential for applications such as multi-site stimulation and acoustic holography.

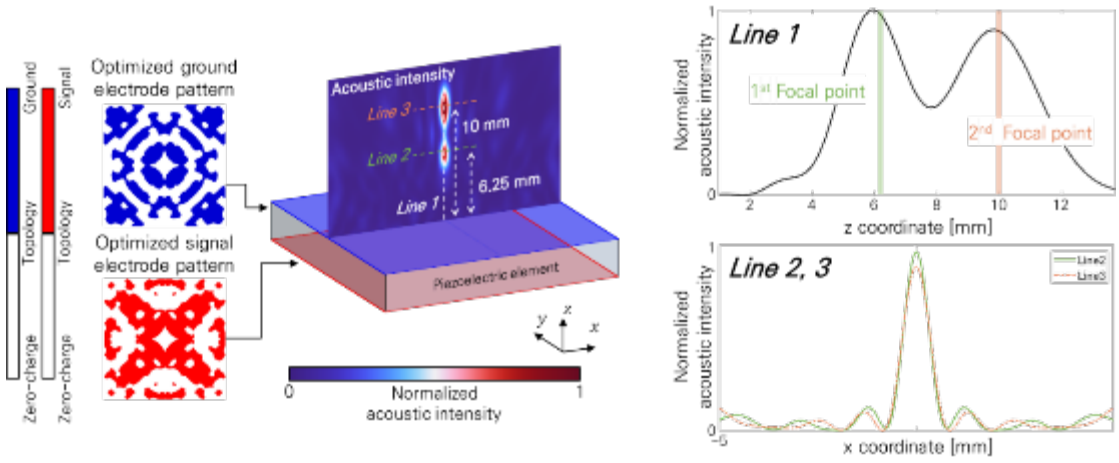

Figure 1.

Acknowledgement

This work was supported by the National Research Foundation (NRF), South Korea, under project BK21 FOUR (Smart Robot Convergence and Application Education Research Center)

Keywords: Ultrasonic focusing, Electrode pattern optimization, Level-set topology optimization, Piezoelectric-acoustic coupling, Acoustic holography

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A Multi-fidelity Data Fusion Method Combining Neighborhood Information and an Improved Multi-head Self-attention Mechanism

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Multi-fidelity data fusion is a critical challenge in scientific computing and engineering, aiming to integrate data of varying fidelities to enhance predictive accuracy while reducing computational cost. Traditional fusion approaches—such as co-kriging, deep neural networks, and convolutional neural networks—often suffer from low-fidelity data redundancy and underutilization of high-fidelity information. We propose K-MFA, a novel fusion framework that synergistically combines neighborhood search with an enhanced multi-head self-attention mechanism. First, a localized neighborhood search explicitly captures the relationships between each high-fidelity sample and its nearest neighbors. Next, a fidelity-aware transformer module dynamically fuses multi-fidelity information by assigning greater attention weight to high-fidelity data and suppressing low-fidelity redundancy. Extensive experiments on classic benchmark functions (Forrester, Jump-Forrester, Continuous) demonstrate that K-MFA consistently achieves scores above 0.97, markedly outperforming state-of-the-art methods. In aerodynamic prediction of a transonic supercritical RAE2822 airfoil, K-MFA reduces the root-mean-square errors of lift and drag coefficients relative to co-kriging, MFDNN, and MDACNN by 33% and 47%, respectively. These results validate K-MFA as a robust and generalizable solution for high-precision, cost-effective multi-fidelity modeling.

Keywords: Multi-Fidelity Data Fusion; Neighborhood Search; Self-Attention Mechanism; Aerodynamic Prediction

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A Scalable Meshfree Point Generation Approach for Efficient Filling and Optimization of Internal Particle Distribution

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Meshfree numerical methods offer significant advantages in simulating complex physical systems due to their flexibility in handling deformable domains and large displacements. However, their performance and accuracy heavily depend on the quality of the underlying point cloud used to represent the computational domain. Traditional techniques for point cloud generation, such as lattice-based arrangements or conversions from volumetric meshes, often struggle to achieve body-conforming, isotropic, and uniformly distributed particles, especially in complex geometries [1]. These limitations restrict the broader application of meshfree methods in high-resolution or industrial scenarios.

To address these challenges, we propose a physically inspired, scalable point cloud generation approach capable of efficiently filling and optimizing internal particle distributions. Unlike conventional point cloud generation methods, the proposed approach leverages a two-stage process. First, a robust initial filling algorithm distributes particles within the volume bounded by the geometry using a regular spacing strategy that respects local boundary curvature. Second, an iterative optimization procedure based on an improved Discrete Element Method (DEM) is proposed to refine the distribution by enforcing isotropy and local uniformity through physically motivated repulsive interactions. In this model, only normal elastic forces between particles within a defined interaction radius are considered, excluding tangential and damping forces to accelerate convergence toward a uniform configuration. The governing equation for particle adjustment is:

$$\boldsymbol{F}_{ii} = \sum_{jj \in N(ii)} \boldsymbol{F}_{\xi, jj \to ii} \tag{1}$$

where $\boldsymbol{F}_{\xi, jj \to ii}$ represents the normal elastic force applied by a neighboring particle jj within the interaction range of particle ii. Once the force is calculated, the particle is displaced accordingly, and its velocity is reset to zero, ensuring that each time step reflects only the local imbalance due to spatial inhomogeneity. We also explore proper parameters for the improved DEM calculation.

This approach is further enhanced by leveraging high-performance computing techniques, including single GPU and multi-GPU acceleration for large-scale computations. Extensive experiments demonstrate that the system produces high-quality, body-fitted, and isotropic point distributions that are well-suited for meshfree simulations applied to complex geometries. Validations include a 2D dam-break benchmark and a 3D dam-break scenario involving geometrically intricate obstacles, where the generated particles support stable and accurate fluid behavior.

Our results indicate that the proposed method not only improves particle quality but also ensures computational scalability, making it a robust pre-processing solution for large-scale meshfree applications in complex engineering domains.

Keywords: Meshfree method, pre-processing, graphics processing unit (GPU), discrete element method (DEM)

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A physics-based reduced-order modelling combined with the localization of microscopic problems for efficient nonlinear FE^2 multiscale analyses

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The computational homogenization-based multiscale analysis considering geometric and material nonlinearities is one of the challenging topics as they require huge amounts of computational resources[1]. In this study, we present a physics-based reduced-order modelling for efficient nonlinear multiscale analyses. In particular, the construction of multiple local reduced-order models combined with physics-based reduced-order basis is introduced to efficiently consider the nonlinearities of given multiscale models. There have been proposed various methods to relieve computational burdens occurred by repetitive procedures of FE^2 analyses focusing on surrogating microscopic problems to pre-constructed models. Among them, model order reduction methods combined with advanced neural networks are popularly investigated replacing microscopic boundary value problems of the representative volume element calculations during the spatial integration of the macroscopic problem[2]. On the other hand, the methods with physics-based linear reduced-order basis show efficient performance compared to those based on conventional auto-encoders in the viewpoint of recovery process to full order space. Considering those characteristics, we localized and constructed multiple local reduced-order models using linear reduced-order basis. Using several numerical examples, we evaluate the performance of the proposed method comparing with the methods reported in literature.

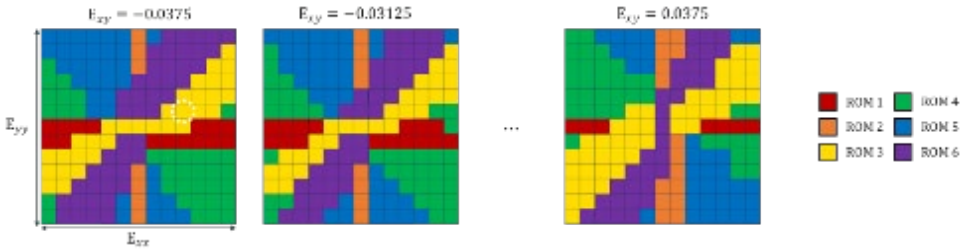

Figure 1. Construction and selection of multiple local reduced-order models with error minimization

Keywords: nonlinear reduced-order model, multiscale finite element method, physics-based, localization

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Vortex-induced vibration of a graphene origami-enabled metamaterial plate in laminar flow

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Vortex-induced vibration (VIV) is a significant research area in understanding the interaction between fluid and structures under various fluid conditions for engineering applications. This study conducts a comprehensive numerical investigation into the VIV behaviors of functionally graded (FG) graphene origami-enabled auxetic metamaterial (GOEAM) splitter plates attached to a circular cylinder, utilizing finite element analysis. The present work focuses on investigating the influence of negative Poisson's ratio (NPR) on the vibration behavior, the effect of plate length on wake patterns, and the influence of fluid loads on the cylinder–plate body and vortex pattern. Key findings include: 1. plates with an $H_{GR}X$-$W_{GR}X$ metamaterial distribution pattern and high elastic moduli in surface layers exhibit low deflection amplitude, 2. shorter plates intensify vortices, while longer plates reduce their prevalence, 3. the natural frequencies of both FG-GOEAM and pure metallic plates are significantly above the vortex shedding frequency, resulting in negligible effects of fluid loads on the cylinder–plate body and vortex patterns. These insights provide valuable guidance for the design and optimization of graphene-based metamaterial structures in engineering applications.

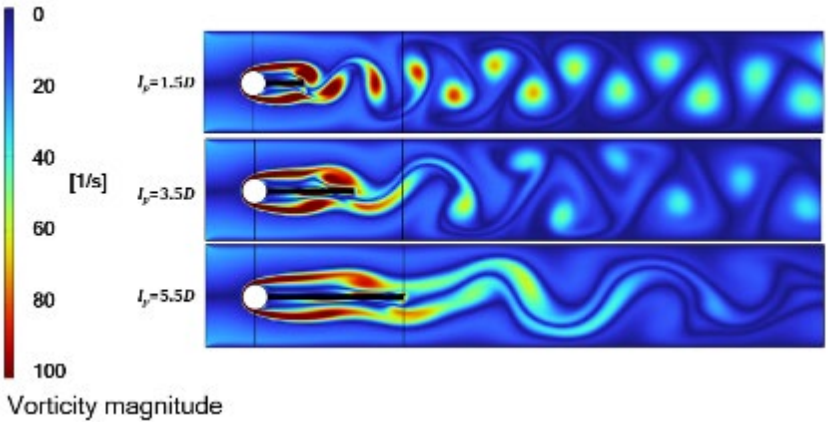

Figure 1 Effect of plate length on wake pattern

Keywords: Vortex-induced vibration, Functionally graded Plate, Graphene origami, Auxetic material

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A Combined Quadtree-Octree Partitioning Framework for Parallel FEM Model Generation and Analysis Applied to 3D Parametric Modeling of Shear Wall-Frame Structural Systems

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In structural design workflow, parametric modelling is performed before conducting detailed engineering design to first satisfy the architectural constraints and expected global structural safety and serviceability limits. For the design of shear wall-frame structures an efficient computation scheme for this stage is warranted because parameters, such as building drift and base shear distribution are sensitive to the layout of shear walls and columns. In practice where limited time is usually allotted for this stage, opting to the use of low fidelity numerical models that are not properly formulated may lead to unnecessary iterations and high computationally costs. However, available studies on shear wall-frame layouts are limited. In this study, a framework to automatically generate and analyze 3D high fidelity FE models is developed. The model generation utilizes a developed quadtree-octree partitioning to tailor the unstructured and structured elements to satisfy the geometrical requirements at the member (columns, beams, slabs, shear walls) level. This allows for simultaneous generation of models with different layouts through applying MPI parallelization, while for the analysis step, Eq. (1) is solved by conjugate gradient method implemented with Block-Compressed Row Storage and accelerated with OpenACC.

$$\left(\mathbf{K}+\frac{2}{\Delta t}\mathbf{C}+\frac{4}{\Delta t^2}\mathbf{M}\right)\mathbf{u}^{n+1}=\left(\frac{2}{\Delta t}\mathbf{C}+\frac{4}{\Delta t^2}\mathbf{M}\right)\mathbf{u}^{n}+\left(\mathbf{C}+\frac{4}{\Delta t}\mathbf{M}\right)\mathbf{v}^{n}+\mathbf{M}\mathbf{a}^{n}+\mathbf{f}^{n+1} \quad (1)$$

where **K**, **C**, **M**, **u**, **v, a, f,** n are the stiffness, damping, mass matrices, displacement, velocity, acceleration, external force vectors, and time step, respectively.

The developed framework was applied to a 10 storey structure model. From the digitized building plan, 40 shear wall-frame layouts were created and subjected to multiple checks: structural irregularity, base shear distribution, story drift in dynamic analysis, etc. Through these checks the optimal model can be selected. Figure 1 shows a sample shear wall-frame layout, generated model and discretization, and a result of subjecting the model to a three-direction earthquake time-history.

In terms of computation cost, the mesh generation time on average for a model with about 1.2 million elements (with roughly equal number of tetrahedron and hexahedron elements) is 4 minutes 30 seconds. This shows a significant reduction than in the case of conventional workflow which is partly manual and takes hours to complete (not including needed sequential iterations). In the solver, implementation of Block-CRS reduced the computation time by 40% compared to standard CRS. In using one GPU device, the computation time was reduced by 30% compared to serial implementation.

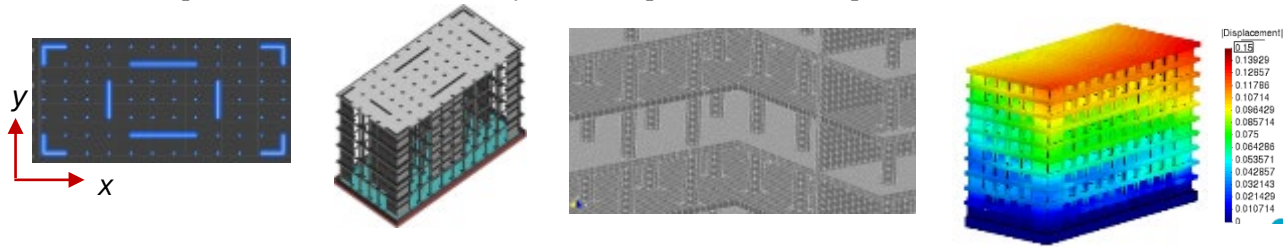

Figure 1. (L-R) Examples of: shear wall frame layout; the generated model; the distribution of elements in the model; displacement result in a time step (m)

Keywords: Shear wall-frame structural systems, automated model generation, finite element method, parallel computing

Concurrent optimization of continuous fiber-reinforced composites with integrated manufacturing and stress constraints

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Continuous fiber-reinforced composites (CFRCs) have attracted significant attention in aerospace and automotive industries due to their high strength-to-weight ratio, design flexibility, and potential for performance breakthroughs through curved fiber paths enabled by 3D printing. However, challenges persist in globally optimizing fiber path curvature constraints, stress criteria, and manufacturing limitations while enhancing structural performance. This study proposes a gradient-driven framework integrating additive manufacturing constraints and stress criteria for concurrent optimization of continuous fiber paths and structural topology. A unified optimization model is established by introducing spatially correlated random field functions, with expansion coefficients of the expansion optimal linear estimation (EOLE) method [1] serving as design variables. The contour lines of these random fields (shown in Figure 1) simultaneously characterize structural topology and fiber placement paths, effectively describing fiber orientation and local fiber content. To address manufacturing constraints, a mathematical formulation based on local curvature limitations is developed to prevent printing defects caused by small curvature radii. The Tsai-Wu failure criterion is integrated to quantify local stress risks, which are incorporated as optimization constraints. The proposed framework maximizes structural stiffness through an augmented Lagrangian (AL) method to handle large-scale local constraints and employs the method of moving asymptotes (MMA) to resolve highly nonlinear optimization challenges. Numerical results demonstrate that the proposed method outperforms conventional uniform fiber layouts, achieving 15–22% higher stiffness while satisfying manufacturing and stress constraints. This work advances the integration of manufacturing-aware optimization and multi-physics constraints in additive manufacturing of CFRCs.

$$\phi(\mathbf{r},\boldsymbol{\varphi}) = \sum_{i=1}^{g} \varphi_i \lambda_i^{-1/2} \psi_i^{\mathrm{T}} \mathbf{C}_Z(\mathbf{r}) \tag{1}$$

where $\boldsymbol{\varphi} = [\varphi_1, \ldots, \varphi_g]^{\mathrm{T}}$ denotes the uncorrelated random variables and $C_Z(\mathbf{r}) = [C(\mathbf{r},\mathbf{r}_1), \ldots, C(\mathbf{r},\mathbf{r}_n)]^{\mathrm{T}}$. λ_i and ψ_i are the eigenvalue and its corresponding eigenvector of spatial correlation matrix $\mathbf{C}$.

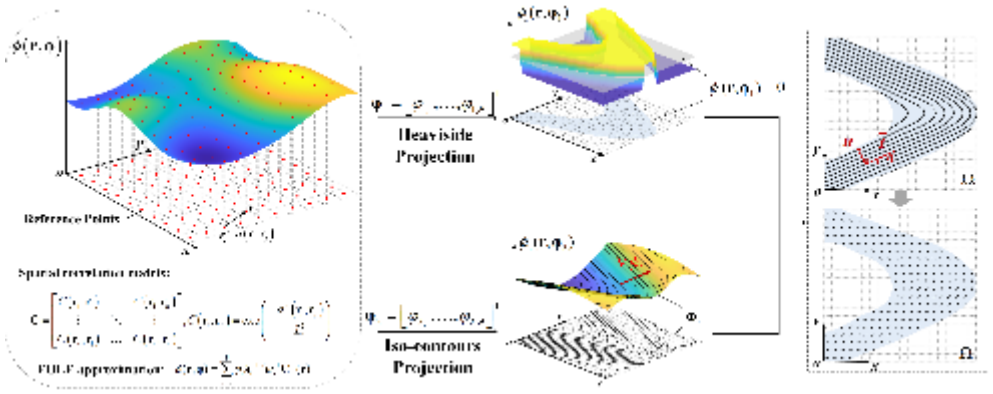

Figure 1.

Keywords: Continuous fiber-reinforced composites, concurrent optimization, random field function, additive manufacturing constraints, stress constraints

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An Enhanced Bi-directional Evolutionary Structural Optimization Method Considering Stress Constraints and Elastoplastic Materials

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This study introduces an enhanced Bi-directional Evolutionary Structural Optimization (BESO) method that incorporates both stress constraints and elastoplastic material behaviour. In traditional topology optimization, methods based on elastic materials face issues of topological instability and stress concentration when extended to elastoplastic materials [1][2]. To address this, the proposed method includes adaptive evolutionary parameters, stress-related sensitivity analysis, and an incremental finite element approach for elastoplastic modelling. The optimization is governed by the objective function defined as:

$$f^* = f(\boldsymbol{x}) + \lambda \cdot \sigma_{PN} \tag{1}$$

where $f(\boldsymbol{x})$ represents the selected objective function with design variable vector $\boldsymbol{x}$, λ is a Lagrange multiplier that iteratively determined on maximum von Mises stress $\sigma_{vm}^{\max}$ and critical von Mises stress σ^*, and σ_{PN} is the aggregated p-norm global stress measure.

Numerical results demonstrate that the proposed method yields stable, manufacturable topologies under both stress-constrained and elastoplastic conditions. **Figure 1** illustrates the topology obtained using the stress-based design method with elastic materials and the topology when elastoplastic materials are considered. Notably, the topologies from both designs are similar in certain cases, suggesting that the methods converge under specific loading and boundary conditions. Additionally, the study explores how different objective functions affect the performance and topology evolution when applied to elastoplastic materials, providing insights into the optimal selection of design goals.

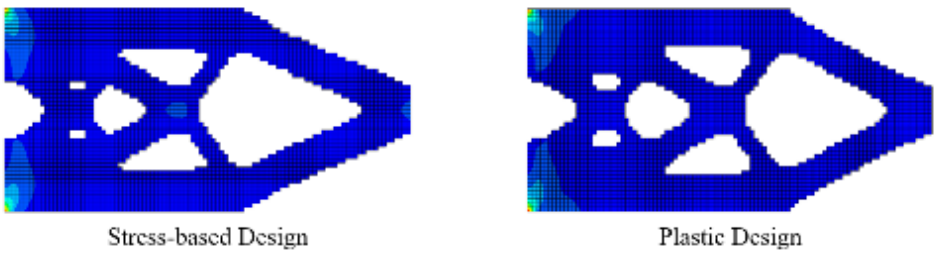

Figure 1.

Keywords: Topology Optimization, Bi-directional Evolutionary Structural Optimization, Stress Constraint, Elastoplastic Material

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Inverse design of non-axisymmetric aero-engine nacelles using denoising diffusion probabilistic models

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Inverse design methods provide significant benefits for aerodynamic applications by enabling performance and efficiency improvements. This study develops a framework using a denoising diffusion probabilistic model (DDPM) [1] to generate surface isentropic Mach number (M_{is}) flow field distributions for non-axisymmetric aero-engine nacelles. The DDPM approach employs forward noise addition and reverse denoising processes to produce varied M_{is} flow field samples from a standard normal distribution.

Algorithm 1 Training	**Algorithm 2** Sampling
1: **repeat**	1: $x_T \sim N(\mathbf{0}, \mathbf{I})$
2: $x_0 \sim q(x_0)$	2: **for** $t = T, \dots, 1$ **do**
3: $t \sim$ Uniform($\{1, \dots, T\}$)	3: $\mathbf{z} \sim N(\mathbf{0}, \mathbf{I})$ if t > 1, else $\mathbf{z} = \mathbf{0}$
4: $\epsilon \sim N(\mathbf{0}, \mathbf{I})$	4: $x_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right) + \sigma_t \mathbf{z}$
5: Take gradient descent step on $\nabla_\theta \left\|\epsilon - \epsilon_\theta\left(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t\right)\right\|^2$	5: **end for**
6: **until** converged	6: **return** x_0

The framework integrates two neural networks: a geometry predictor mapping flow fields to nacelle shapes, and a performance estimator predicting drag coefficients. The harris hawks optimizer (HHO) further refines geometries based on drag characteristics. Compared to a conditional GAN baseline, the DDPM-generated flow fields show superior agreement with CFD results, while the DDPM-HHO combination achieves better drag reduction, confirming its effectiveness for inverse aerodynamic design.

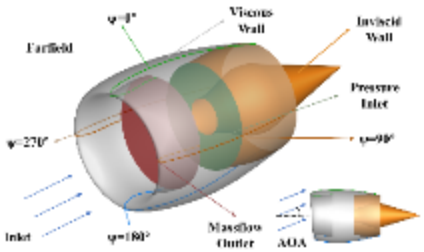

Figure 1.

Keywords: denoising diffusion probabilistic model, non-axisymmetric aero-engine nacelles, inverse aerodynamic design, harris hawks optimizer, machine learning

References

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Computational modelling on the dynamics of human eukaryotic cell in microchannel flows

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The motion of eukaryotic cells in a fluid medium, such as blood, lies at the heart of fundamental biological processes and underlies various pathologies, from infections to cancer metastasis. In the flow, cells experience stresses-induced deformations due to the fluid-structure interaction, and it heavily influences their behaviour and function. The accurate modelling of the associated dynamics of the human eukaryotic cell will underpin a wealth of fundamental and applied research. In most of the previous of research, the cell was considered as a membrane, leaving the effects of the underlying cortex, cytoplasm and nucleus not seriously considered. In this work, a highly efficient numerical solver is developed to study the dynamics of human eukaryotic cell in microchannel flows. In this solver, the lattice Boltzmann method and finite element method are respectively used to solve the microfluid dynamics and the human eukaryotic cell dynamics (governed by Eq. 1) independently and coupled by using an immersed-boundary method.

$$\rho \frac{D\boldsymbol{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}, \tag{1}$$

The solver is parallelized using Compute Unified Device Architecture (CUDA) -enabled Graphics Processing Units (GPUs) for accelerated computation. The numerical studies focuse on the comparison between the membrane-based and solid-based cell models to explain the effects of the underlying cortex, cytoplasm and nucleus on the cell dynamic behaviours in microchannel flows (a snapshot for the cell in microchannel flows is shown in Fig. 1).

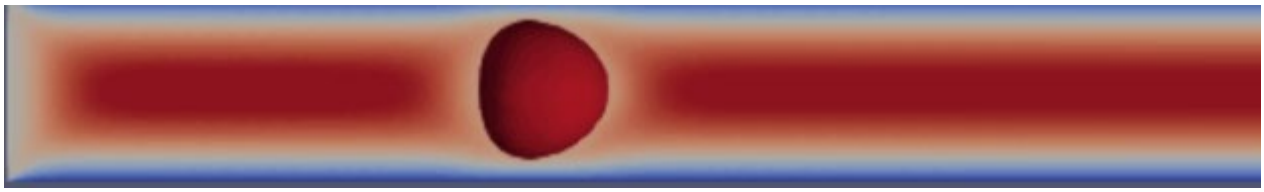

Figure 1.

Keywords: Biofluid mechanics, computational modelling, fluid-structure interaction, cell dynamics

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Laminar Vortex Dynamics in Pore-Scale MICP: A 3D LBM-FE-CA Numerical Model Analysis

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Despite the low flow velocities characteristic of Microbial Induced Calcite Precipitation (MICP), laminar vortices can form in response to the dynamic alterations and complexity of the pore structure. These vortices significantly influence the mixing of bacteria and substrates, thereby affecting calcite precipitation. Gaining insights into the vortex impact on MICP within the pore space is crucial for advancing geotechnical applications yet poses significant challenges for both experimental and numerical quantification. This study unveils our latest findings on laminar vortex dynamics within a 3D MICP numerical microfluidic model, an extension of our earlier 2D model. The enhanced 3D model enables a detailed quantitative analysis of vortex patterns and their correlation with the strength and distribution of vortices, as well as the mixing of substances.

Keywords: MICP, LBM, pore-scale, reactive mass transport, porous media

Numerical investigation of thermal transport in viscoelastic fluids using the Lattice Boltzmann method

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Many important industrial and technological applications, including microfluidic cooling, biomedical devices, and energy systems, involve the transport of non-Newtonian fluids such as viscoelastic fluids, which exhibit nonlinear stress-strain relationships due to their elastic and viscous nature. In particular, the elastic properties of such fluids have been shown to give rise to purely elastic instabilities, even in the absence of inertia, which can significantly influence heat transfer characteristics. In this study, we conduct numerical simulations of viscoelastic fluids using a lattice Boltzmann method to investigate their thermal convection behaviour in micro-scale geometries relevant to compact heat exchangers. LBM is used for both flow and heat transfer, with a D2Q9 lattice for hydrodynamics and a D2Q5 lattice for the thermal field. The polymer stress evolution is solved using a finite difference scheme, coupled to the flow to capture viscoelastic effects on convection. By systematically varying the Weissenberg number ($0 < Wi \leq 10$), which shows the relative importance of elastic to viscous effects, and the Rayleigh number ($10^3 \leq Ra \leq 10^6$), which shows the effect of buoyancy-driven flow due to temperature gradients, we explore the impact of fluid elasticity on mixed convection regimes. Results from benchmark configurations reveal a complex interplay between viscoelasticity and thermal gradients, leading to distinct flow regimes. As the system approaches a regime dominated by natural convection, increasing elasticity is found to enhance convective currents, depending on the Rayleigh number and geometric constraints, which in turn alters the heat transfer rate. When the forced convection becomes dominant over the natural convection, the alignment and stretching of polymer chains rise to elastic instability, characterised by improved thermal transfer. The transition between laminar and unstable flow states is closely linked to the elastic properties of the fluid and the flow configuration. Overall, the study provides insights into the role of elasticity in thermal convection processes and offers guidance for viscoelastic fluid systems for advanced heat exchanger design.

Digital twin for full-field structural strength assessment and prediction

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The digital twin modelling method is proposed for the strength assessment and performance prediction of complex structures. Firstly, a multi-source data fusion approach is introduced to integrate simulation data with sensor readings, enabling the construction of a high-accuracy and robust digital twin. Secondly, an optimal sensor placement strategy is established for complex curved structures, enhancing the monitoring efficiency of sparse sensors. Thirdly, a dynamic update method for the digital twin is developed based on a reduced order model, ensuring the accuracy and reliability of the digital twin used in practical strength assessment scenarios accounting for loading deviations. Finally, the effectiveness of the proposed method is validated through structural strength tests on open-hole panels, hierarchical stiffened plates, and cargo spacecraft cabins. The results demonstrate that the method can achieve real-time, high-accuracy, and full-field strength assessment and performance prediction of complex structures.

Keywords: Digital twin; data fusion; optimal sensor placement; structural strength; multi-fidelity model

Predicting Air Pollutant Concentration Using Deep Neural Network: Path towards a Physics-Informed Machine Learning Framework

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Air pollution poses significant impacts to both human health and the global climate, requiring robust predictive models for accurate simulation of pollutant dispersion. The concentration of air pollutants exhibits considerable variability across short spatial distances due to diverse emission sources, meteorological conditions, and chemical processes. Traditional models often struggle to capture these complex and nonlinear atmospheric scenarios, leading to inaccuracies in their predictions; to overcome these limitations Machine Learning-particularly Physics Informed Machine Learning offers a promising solution. The primary objective of this study is to develop a purely data driven deep neural network model to capture pollutant dispersion without incorporating explicit physical knowledge. In this study, two monitoring stations in South East Queensland were selected and a deep neural network model was trained selecting $PM_{2.5}$ as the pollutant. A preliminary data analysis is conducted to identify the key meteorological factors that directly influence $PM_{2.5}$ concentration. Through this analysis, seven meteorological parameters were identified, which were used as inputs for feedforward neural network to predict future $PM_{2.5}$ concentrations. The accuracy of the model is evaluated using performance metrics and the results reveal that the model is closely capturing underlying patterns. However, the study exhibits noticeable discrepancies in predicting rapid concentration changes. To overcome such limitations, Physics Informed Machine Learning has emerged as a significant research avenue, as it is capable of making accurate predictions even under noisy and sparse data conditions.

Keywords: Air pollution, Deep neural network, $PM_{2.5}$, Physics informed machine learning

A Random Pore Model (RPM) for Predicting Mechanical Properties of Sea Ice

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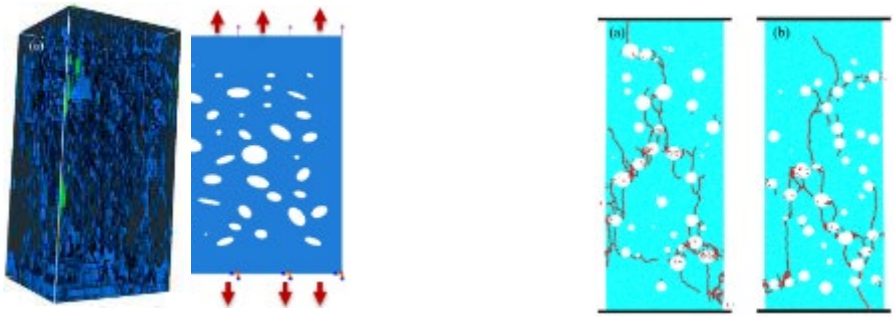
Sea ice contains gas and brine pockets arising from its special growth environments.The mechanical properties are strongly dependent on the meso-structure of sea ice, the most prominent of which is described by its porosity, see the scanned structure of a sea ice specimen in the left picture of Figure 1(a). In this paper a Random Pore Model (RPM) is proposed, the basic assumption of which is that sea ice is made of pure ice sheet embedded with a lot of randomly distributed pores of random sizes, see the right picture of Figure 1(a). Monte Carlo method is then employed to generate the random pore field. Simple numerical tests show that there exists upper limit value for porosity, which is close to 0.61. Simple numerical tests are then performed to find the dependence of tensile and compressive strengths of sea ice on porosity, see Figure 1(b). The results turn out to be in good agreement with experimental results, see Figure 1(c). This is followed by further studies on the effect of porosity on mechanical properties of sea ice, such as elastic modulus, Poisson's ratio, failure strains.



(a) Measured sea ice structure and RPM (b) RPM-based fracture (c) Comparison

Figure 1. Random Pore Model which reproduces mechanical properties of sea ice

More numerical simulations are performed to investigate scale effect of mechanical properties of sea ice and pore shapes influence on the results. The results reveal that scale effects arise from the fact that pore sizes are same for small and large sea ice samples. Pore shapes show influence on the scatters of mechanical properties vs porosity, but show much less influence on trends.

It is interesting to note that mechanical properties of sea ice and fresh ice (free of salts) are different. Both properties are measured separately, meaning that sea ice is treated as a separate material from fresh ice in terms of mechanical properties. The RPM proposed here bridges the gap between sea ice and fresh ice so that the mechanical properties of sea ice can be predicted from those of fresh ice once the latter is given. This provides an useful theoretical model and numerical methodology to study mechanical properties of sea ice.

Keywords: Mechanical property, sea ice, porosity, Random Pore Model (RPM), scale effect

Advanced Phase Field Modeling of Rising Bubble Dynamics in Viscoelastic-Newtonian Multiphase Flows

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A thorough understanding of multiphase flow systems is essential for the advancement of industrial processes, particularly when dealing with complex fluids exhibiting viscoelastic properties. The nonlinear interactions between viscoelastic and Newtonian fluids introduce significant challenges in numerical modeling. In this study, we investigate the dynamics of a rising bubble in a viscoelastic-Newtonian multiphase system through comprehensive numerical simulations using FEniCS, an open-source finite element platform.

To ensure both accuracy and efficiency, we introduce a robust phase field method based on the numerical Gibbs dividing surface. This approach effectively prevents the artificial diffusion of elasticity into the Newtonian phase and strictly enforces that material properties remain within the physical bounds of the two bulk phases, even when the phase field variable overshoots or undershoots. Additionally, we implement a rule-based Adaptive Mesh Refinement (AMR) strategy to optimize computational resources without compromising accuracy. By incorporating a flux correction into the Cahn-Hilliard phase field equation, we further reduce volume loss in all simulations to below 3% [1], [2].

We systematically explore the effects of key viscoelastic parameters—retardation parameter, relaxation time, and surface tension—on the rising dynamics and morphology of the bubble. Our results highlight the role of polymer stretching and relaxation in the viscoelastic medium, demonstrating that polymer relaxation below the bubble equator enhances rising velocity, promotes elongation, and leads to phenomena such as negative wake and velocity jumps. The observed bubble shapes are categorized into three types: (1) elongated tail without fragmentation, (2) fragmentation of the Newtonian bubble with an elongated tail, and (3) spherical shape without fragmentation. This study offers new insights into the complex interplay between viscoelastic properties and multiphase flow behavior.

Keywords: Computational fluid dynamics, finite element method, phase field method, viscoelasticity, bubble dynamics

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From linear elastic to finite strain elastoplastic fracture analysis using the Fragile Points Method (FPM)

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This paper describes the formulation and analytical results for fracture mechanics analyses, ranging from linear elastic to finite deformation elastoplasticity, using the Fragile Points Method (FPM) [1]. FPM is one of the meshless methods whose test and trial functions are constructed using randomly distribute points in the problem domain, as shown in Fig. 1(a). The problem domain is divided into the subdomains, as also depicted in Fig. 1(a). The test and trial functions are piecewise polynomials, constructed by the generalized finite difference (GFD) method using the distributed points, connecting neighboring points. They are defined at each distributed point. Consequently, a local Galerkin weak form is constructed in each subdomain. An exact numerical integration for the local weak form is performed by Gaussian quadrature. Then, a system of linear simultaneous equations for solving the boundary value problem is generated by summing-up the local weak forms. However, it is noted that the test and trial functions are discontinuous at the boundaries of the subdomains. Numerical flux corrections are introduced to suppress the discontinuity.

In order to introduce a crack in the analysis model, connections between points across the crack face are discarded. Model including a crack is shown in Fig. 1(b). This process is very tractable, making FPM well-suited for fracture mechanics analyses.

In the present investigation, we have performed linear elastic and finite strain elastoplastic fracture mechanics analyses by FPM. Necessary development for FPM, coupled with a finite strain elastoplasticic constitutive law were carried out. The framework of the finite strain model is based on the implicit updated Lagrangian scheme and the Hencky hyperelastic law, combined with isotropic and kinematic hardening law.

The results o echanics analyses performed demonstrate t ure the intensive deformation concentration neters accurately. The authors are now condu l at APCOM 2025.

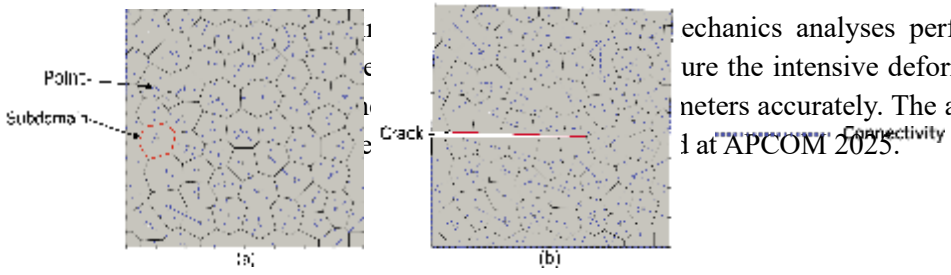

Figure 1.

Keywords: Fragile Points Method, Meshless Method, fracture mechanics analyses, linear elastic analyses, finite strain elastoplastic analyses

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An Experimental Calibration Method for Fatigue Life Prediction of Bonded Joints with Dissimilar Composites

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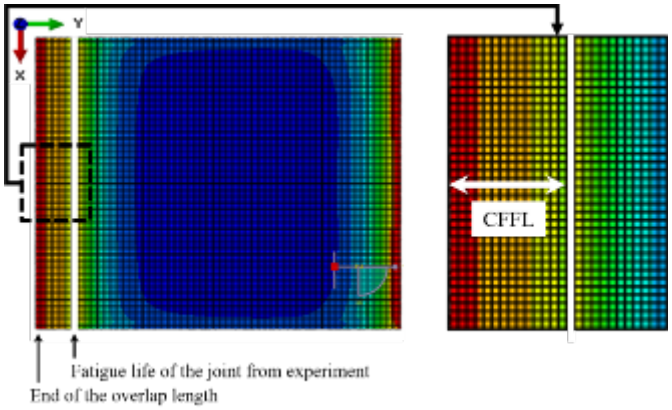
This study proposes a fatigue life prediction methodology for bonded joints with dissimilar composites. To account for the large scatter in fatigue life data of each material, probabilistic stress-life (P-S-N) curves were employed using the two-parameter Weibull distribution:

$$F(N) = 1 - exp\left[-\left(\frac{N}{\beta}\right)^{\alpha}\right] \quad (1)$$

where, N is the fatigue life, and α, β are shape and scale parameters, respectively. These curves were integrated into finite element analysis (FEA) and Monte Carlo simulations to derive the probabilistic force-life (P-F-N) curves of the joints. While FEA predicted immediate failure within less than one loading cycle due to localized stress concentrations at the adhesive edge, the experimental results exhibited a progressive accumulation of fatigue damage over many cycles. To bridge this gap, the critical fatigue failure length (CFFL) was proposed as a calibration method. CFFL represents the damage-accumulating region observed in experiments and is defined as the distance from the overlap edge to the location where the local fatigue stress from FEA equals the experimentally determined fatigue strength from the S-N curve of the joint. This allows FEA to better reflect the gradual failure behavior observed in real joints. CFFL was subsequently found to exhibit a linear relationship with both the overlap length and its corresponding load level, enabling its estimation at untested overlap lengths using fitted trendlines. The FEA results calibrated with CFFL showed good agreement with the P-F-N curve obtained from experiments, demonstrating the effectiveness of the proposed methodology. This approach enables accurate fatigue life predictions for dissimilar bonded joints while significantly reducing the need for extensive experiments.



Keywords: Fatigue life prediction, probabilistic stress-life (P-S-N) curve, Weibull distribution dissimilar bonded joint, finite element analysis (FEA)

Fourier Feature-Embedding for improving computational efficiency of Physics-Informed Neural Networks for complex applications

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This conference abstract presents a novel approach to improve efficiency of Physics-Informed Neural Networks (PINNs) through Fourier Feature-Embedding (FFE) techniques for solving physics-based models [1]. This specially demonstrates significant improvements in computational efficiency for complex engineering applications without loss weights [2] and weight initialisation [3]. Our research focuses on complex time-domain variation investigations as a case study, where we develop FFE based PINN computational framework for modelling coupled heat- and mass- transfer variations of a plant tissue drying.

Mass transfer is based on Fickian Diffusion model [4];

$$\frac{\partial c}{\partial t} + \nabla .(-D\nabla c + uc) = S, \tag{3}$$

where c denotes the moisture concentration, t denotes drying time, D denotes diffusivity, u denotes flow velocity, and S denotes source term.

Heat transfer is based on energy conservation equation;

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p u . \nabla T = \nabla .(k\nabla T) + Q_e, \tag{4}$$

where ρ denotes density, c_p denotes specific heat, T denotes temperature, k denotes thermal conductivity, and Q_e denotes heat generation.

These equations can be coupled within one PINN framework allowing to update instant temperature and moisture concentrations between models to capture their effects for computation. This complexity cannot be simply solved with traditional PINN modellings due to convergence issues. Those issues are mainly due to derivative computational errors. This is where FFE plays the major role, where this step involves transforming the input data with Fourier feature mapping, which enables the tuning of NTK's spectrum by modifying the frequency vector during the training process. Hence, it enables to solve physics for complex domains and/or coupling within PINN computations. Our results demonstrate that the FFE-PINN approach achieves comparable accuracy for computing heat and mass transfer for extended drying time up to 60 mins. The results will be presented in the conference presentation.

Keywords: Fourier Feature-Embedding, Physics Informed Neural Network, Computaional Efficiency, Mass Transfer, Heat Transfer, Food Drying.

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Structural Health Monitoring of Retrofitted Buildings Post-Earthquake

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The seismic resilience of urban high-rise residential buildings is crucial for public safety. In the Banqiao District of New Taipei City, a residential community comprising 30 reinforced concrete buildings, each approximately 22 stories high, underwent extensive structural retrofitting in 2016 after damage was detected in several buildings. To ensure long-term structural integrity, a routine monitoring program was established, employing ambient vibration monitoring to detect changes in dynamic properties.

On April 3, 2024, a magnitude (Mw) 7.2 earthquake struck offshore of Hualien. To ensure the structural safety of the residential community, a week-long full-scale monitoring campaign was conducted. The main objective was to assess the potential damage to structures caused by seismic. Three sensors were installed on the rooftops of each building to capture motion in the longitudinal and transverse directions. Each measurement lasted 10 minutes and was repeated twice per building at a sampling rate of 200 Hz. Two system identification methods were utilized: Frequency Domain Decomposition (FDD) [1] in the frequency domain and Stochastic Subspace Identification (SSI) [2] in the time domain, providing consistent and cross-validated estimates of natural frequencies. A comparison with a previous post-earthquake dataset from August 8, 2019, revealed that most buildings exhibited a slight reduction in natural frequencies across all modes, suggesting potential stiffness loss.

This study demonstrates that structural health monitoring combined with robust system identification methods can provide a rapid, non-invasive assessment of structural condition. Such data is valuable for prioritizing inspections, planning retrofits, and enhancing the seismic resilience of urban housing stock.

Keywords: structural health monitoring, system identification, stochastic subspace identification, frequency domain decomposition, building retrofitted

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A novel node-based smoothed polygonal finite element method with reconstructed strain fields for solving heat conduction problems

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This paper presents a novel node-based smoothed polygonal finite element method (NS-PFEM) with reconstructed strain fields for solving heat conduction problems. In order to approximate the thermal strain field in Wachspress coordinates, the high-order smoothed thermal strain field is constructed using pick-out theory. Two high-order S-FEM models have been developed: NS-PFEM-1 for linear thermal strain and NS-PFEM-2 for second-order thermal strain. By employing the gradient smoothing technique, the shape function values on the boundaries of node-based smoothing domains are required rather than the derivatives of the shape function, which reduces the continuity requirements for shape functions. It also eliminates the isoparametric mapping in polygonal finite element methods, which can significantly enhance computational efficiency. The performance of the high-order NS-PFEMs is rigorously examined against the standard NS-PFEM, PFEM, FEM-T3, ES-FEM-T3 and the finite element software COMSOL. Numerical examples demonstrate that our high-order NS-PFEMs produce super convergent and nearly exact solutions in both temperature and energy at low computational costs.

Keywords: High-order smoothed finite element method; polygonal finite element method; thermal strain field reconstruction; Wachspress shape function; heat conduction problem.

Theoretical Model for Predicting Jet Grouting Column Diameter

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Jet grouting is a ground improvement technique that forms soil-cement columns by eroding soil with high-pressure grout [1]. Existing methods for predicting column diameters rely heavily on empirical correlations [2-3], neglecting the fundamental energy exchange between submerged jets and soil. This study proposes an energy-based theoretical model to predict jet grouting column diameters by equating the average submerged jet energy to the soil's resistance energy at the limiting erosion distance. The model integrates hydrodynamic jet characteristics, soil shear strength, and breakage mechanics, and is applicable to both clay and sandy soils.

The initial velocity v_0 is calculated based on grouting flow rate, and the limiting erosion distance x_L, defining the column radius, is solved by balancing $E(x_L)=E_{Rs}$.

$$E(x_L)=\delta\frac{M\rho v_0^3 d_0^3}{x_L^3}=\frac{\varepsilon\left(\sigma_1-\sigma_3\right)_f}{R_f}=E_{Rs}, \tag{1}$$

where δ is jet energy coefficient, M is the number of nozzles, ρ is the slurry density, d_0 is the nozzle diameter, ε is the strain, $(\sigma_1-\sigma_3)_f$ is the compressive strength, R_f is the failure ration, which had been found to be between 0.75 and 1.00.

Case studies validated the model, covering single-, double-, and triple-fluid systems in diverse soils. Predictions showed average deviations of 7.0%–12.8%. The model reduces reliance on empirical databases, offering a mechanistic framework for optimizing jet grouting design.

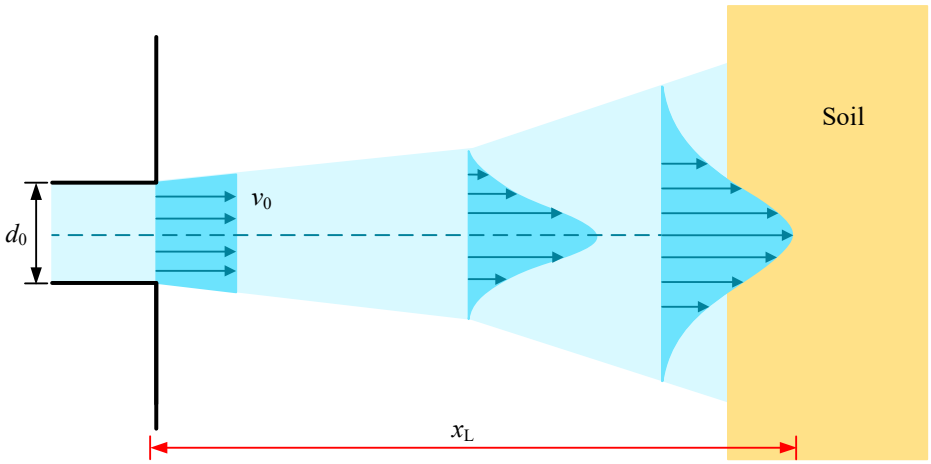

Figure 1.

Keywords: Jet grouting, column diameter prediction, energy balance; soil resistance

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Deep learning framework for accelerating the data-driven multiscale finite element analysis

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This study introduces an efficient deep learning framework for multiscale finite element analysis (FE^2) based on the data-driven mechanics and data augmentation [1]. To overcome classical FE^2 inefficiencies, we utilize a distance-minimizing data-driven computational mechanics approach. The key innovation lies in leveraging a deep neural network for adaptive sampling points without prior knowledge of the mechanical problem. Utilizing the distance-minimizing algorithm, macroscopic strain and stress solutions are derived, representing the closest dataset to mechanistic constraints (i.e., equilibrium and compatibility equations) using the NN constitutive datasets. The obtained macroscopic strain solutions at each integration point, denoted as $\{\mathbf{E}^{(m+1),1},\ldots,\mathbf{E}^{(m+1),\mathrm{Ngpt}}\}$, where the number of integration points is N_{gpt}. The newly added sampling points are exclusively those that do not overlap with the points sampled in the preceding iterations. To impose the tolerance for the intersection, we defined the function Cover as follows:

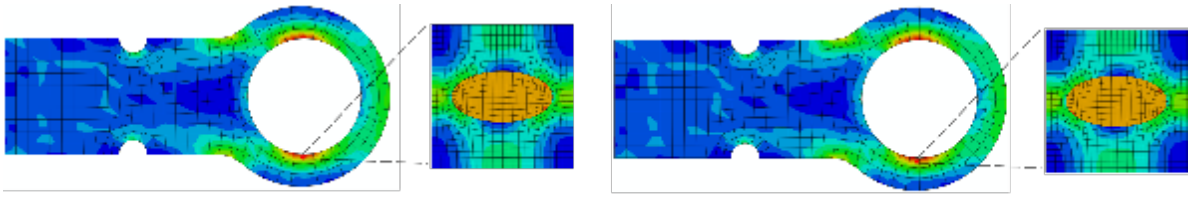
$$Cover(\mathscr{D}^{(m)},\ \mathrm{Tol}) \equiv \bigcup_{\mathbf{E}_p \in \mathscr{D}^{(m)}} N_{\mathrm{Tol}}(\mathbf{E}_p)\,. \tag{1}$$

Here, it is defined as the union of the Tol-neighborhood of a database at m-step. The Tol-neighborhood is defined:

$$N_{\mathrm{Tol}}(\mathbf{E}_p) = \left\{\mathbf{E}\middle|\, d_E(\mathbf{E},\ \mathbf{E}_p) < \mathrm{Tol}\right\}, \tag{2}$$

where the distance in the strain space is defined as follows:

$$d_E(\mathbf{E},\ \mathbf{E}_p) = \left\|\mathbf{E} - \mathbf{E}_p\right\|. \tag{3}$$



(a) Data-driven FE^2 based on reference data (b) Proposed data-augmentation

Figure 1.

The proposed deep learning framework plays a key role in identifying suitable solution points, guiding the data augmentation process to minimize constraints and perform RVE calculations selectively for those strains. Consequently, the iterative process discovers solution points beyond the initial data, facilitating improved prediction performance for specific mechanical problems.

Keywords: Data-driven mechanics, Nonlinear homogenization, Multiscale finite element, Neural network, Data augmentation

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Homogenization Analysis using s-version Isogeometric Analysis (s-IGA)

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The homogenization method has been applied to compute the effective mechanical properties for composite materials under the assumption of periodic micro structure [1], as shown in Fig. 1 (left). The finite element method is very popular analytical method, but it has two major drawbacks compared to the Isogeometric Analysis (IGA) [2]. The basis functions of the finite element method has only the C^0 continuity and are not capable of representing the geometries of objects exactly.

In the present investigation, the s-version IGA [3] is applied to the homogenization method. Higher order continuity can be realized within the problem domain. To insert inhomogeneities such as reinforcing particles, fibers, voids, etc., the use of the s-version Isogeometric Analysis (s-IGA) is proposed. The inhomogeneities represented by local IGA models can be superimposed on the global IGA model for the unit cell as whole, as depicted in Fig. 1 (right). The global IGA model is based on 2nd or 3rd order B-spline functions. Periodic boundary conditions are assigned by connecting the companion side by continuing B-splines, without placing any open knots at the outer surfaces of the unit cell, as also shown in Fig. 1 (right). The proposed homogenization method using the s-IGA has been found to be capable of computing the effective mechanical properties. The results of present homogenization analysis compare very well with those of Zhilin et al. [4]. Furter details will be discussed at APCOM 2025.

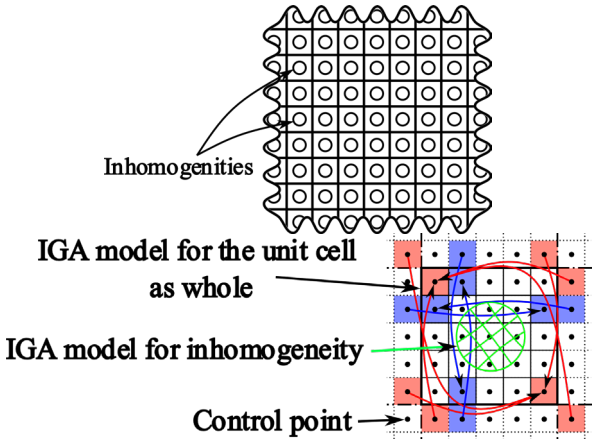

Figure 1.

Keywords: homogenized method, isogeometric analysis, s-version isogeometric analysis, periodic boundary condition

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Super-resolution of 2D Stress Tensor Fields Using physics Informed Neural Networks

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Accurate finite element analysis (FEA) often requires high-resolution meshes, resulting in substantial computational costs that are impractical for real-time simulation and iterative optimization. This study proposes a super-resolution framework that predicts high-resolution 2D stress tensor fields from low-resolution contour plots using a modified U-Net architecture, referred to as PI-UNet (Physics-Informed U-Net). Unlike existing deep learning models that treat physical field super-resolution as a purely image-based problem, our approach embeds equilibrium constraints directly into the training loss function, thereby improving the physical plausibility of the predicted stress tensor fields.

The model was trained on coarse and fine mesh data generated by standard FEM simulations of simple geometries (cantilever and L-shape beams) under various boundary and loading conditions. To evaluate generalizability, we applied the trained model to unseen geometries, such as a truss-like cantilever. The proposed PI-UNet achieved superior performance compared to traditional U-Net, U-Net++, and GAN-based models like ESRGAN, particularly in reducing the residuals of the equilibrium equation and maintaining smooth contour representations that obscure mesh artifacts.

Our results indicate that PI-UNet provides a promising and efficient surrogate model for high-resolution FEA results. It can be applied to topology optimization and real-time structural simulations, significantly reducing computational time while preserving essential physical fidelity. This work highlights the potential of integrating physics-informed loss functions with convolutional neural networks for advancing engineering applications in computational mechanics.

Keywords: Physics-informed neural network, super-resolution, finite element method, stress tensor, U-Net, equilibrium constraint, structural simulation.

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Topology optimization with worm-like highly deformable features

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The feature-driven method is an emerging topology optimization approach that has gained extensive attention in recent years [1]. Geometric features are treated as basic design primitives with their geometric parameters serving as the design variables. These features are mathematically expressed using implicit level-set functions (LSFs). Topology optimization is achieved through the size, shape, and layout optimization of these features.

Various geometric features with different design freedoms are proposed, including the superellipse [2], closed B-spline (CBS) [3], multi-section B-spline offset feature (MS-BSOF) [4,5] ect. Among these, the MS-BSOF is a worm-like highly deformable feature whose shape is determined by a directrix and several multi-sections. The MS-BSOF is used to solve both structural and compliant mechanism design problems, showing that complex structures can be optimized using only a small number of MS-BSOFs.

Besides, MS-BSOFs are employed for the design of fluid channels and integrated structure with internal fluid channels. The MS-BSOFs are used to model the fluid channels while the CBSs are utilized to represent voids for weight reduction. A multi-field interpolation model is developed to describe the material properties of fluid, void, and solid. A geometric constraint is developed to avoid the intersection between the fluid and void phases. The concurrent optimization problem is formulated to optimize simultaneously the load-bearing capacity and fluid dissipation energy. Numerical examples are tested to illustrate the effectiveness and advantages of the proposed method using MS-BSOFs.

Keywords: Topology optimization, Feature-driven method, Structure design, Fluid channel design, Multi-Section B-Spline Offset Feature (MS-BSOF)

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Mechanistic Insights into Monovalent Cation Selectivity in Modified Ion Selective Membranes: A Model-Based and Experimental Study

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Abstract

Surface modification techniques involving introducing charge-opposite thin layers on ion exchange membranes have proven highly effective for separating monovalent and divalent ions in various chemical and biochemical processes. Although monovalent cation selective membranes (MCSM) have been widely employed in various electrodialysis studies, the underlying separation mechanisms and the transport behavior of monovalent and multivalent cations under different modification layer charge densities and applied voltages are still not fully understood. This study establishes a nanochannel-based MCSM model grounded in the physical nature of porous media, providing a clear depiction of ion transport processes, micro-nanoscale flow fields, and ion energy distributions. The model is further validated through electrodialysis experiments. The results demonstrate that, compared to the traditional ideal homogeneous volume model based on Darcy's law, the nanochannel model more accurately captures the experimentally observed trends in perm-selectivity, particularly under conditions of high current density and high modification layer charge density. Near the limiting current density (LC regime), the solid–liquid structure of the modification layer in the nanochannel model induces a stronger local electric field, which more effectively suppresses the transmembrane transport of divalent cations. This results in a higher selectivity of 6.5, which closely matches the experimentally measured value of 6. Furthermore, in the overlimiting current (OLC) regime, the nanochannel model successfully reproduces the experimentally observed increase in current density, attributed to electrokinetic instabilities. More importantly, the nanochannel model reveals that the decline in perm-selectivity at high modification layer charge densities is primarily due to local divalent ion accumulation on the anodic side of the membrane leads to an increased diffusive flux. When the charge density of the modification layer is ten times that of the cation charge concentration in the solution, the MCSM system achieves its highest selectivity, with a value of 35. These results significantly contribute to our understanding of the mechanisms underpinning the selective transport of

monovalent cations and offer valuable guidance for their practical application in selective electrodialysis.

Application of Quantum Machine Learning to Polymer Alloy Phase Separated Structures

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Composite materials, which possess excellent lightweight properties, strength, and rigidity, are being increasingly applied in various fields such as aircraft and spacecraft. Composite materials are composed of a matrix resin, which serves as the base material, and reinforcing fibers. The matrix resin is often made of polymer alloys. Polymer alloys are multi-component systems containing two or more types of polymers. By combining two or more polymers, benefits such as overcoming weaknesses and reducing costs can be achieved. Additionally, polymer alloys form microphase-separated structures with various degrees of order. Such phase-separated structures in polymer alloys influence the macroscopic mechanical properties of the material. However, developing polymer alloys with excellent properties requires extensive experimentation under various conditions, which is costly. To reduce these costs, numerical simulations are employed. For example, simulations using self-consistent field theory have been developed to predict the phase separation structures of polymer alloys. To manufacture polymer alloys with desired properties, it is crucial to characterize the phase separation structures.

Recently, quantum machine learning models utilizing quantum effects have attracted attention. Quantum extreme reservoir computing (QERC) developed by Sakurai et al. [1] has achieved success in MNIST classification. However, there is room for further investigation into the suitability of quantum machine learning such as QERC for various problems. Applying it to the materials field could contribute to efficient materials development. Therefore, this study aims to compare the results of classifying a dataset of two-dimensional phase-separated structures generated using simulations based on the self-consistent field theory, using both a linear separator and QERC.

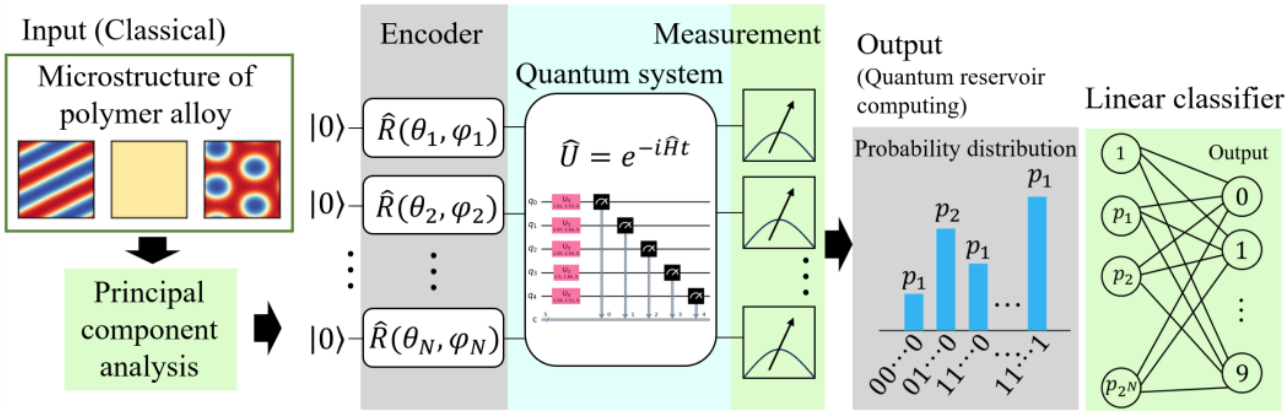

Figure 1.

Keywords: quantum extreme reservoir computing, polymer alloy, phase separated structure

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Numerical Simulation of Fluid-Structure Interaction in Blood-Vascular Systems Based on the Material Point Method

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The fluid-structure interaction algorithm are essential for uncovering mechanics underlying cardiovascular diseases. However, it is still significant that the lack of user-friendly software to simultaneously simulate the interaction between hemodynamic and vascular mechanics, due to dynamic states and complex material properties within the cardiovascular system.

The Material Point Method (MPM) achieves coupling through the interaction between material points and a background grid, eliminating the need for complex coupling equations or surface tracking mechanisms. Material points carry material information, and the background grid is fixed, allowing for natural handling of large deformation problems and avoiding mesh distortion. To date, there has been no application of the MPM in blood-vascular interaction. Therefore, this study aims to develop the MPM to address fluid-structure coupling problems in the blood-vascular system.

A toy model for the fully coupled blood-vascular interaction has been implemented in an monolithic program with the MPM. As shown in the Fig. 1, the large deformation of the vascular subject to the fluid dynamic and the counteraction of the solid structure on the blood flow, can be observed. This program is under development to achieve high-fidelity simulation by various strategies and will be used to improve understanding the mechanics in the cardiovascular system.

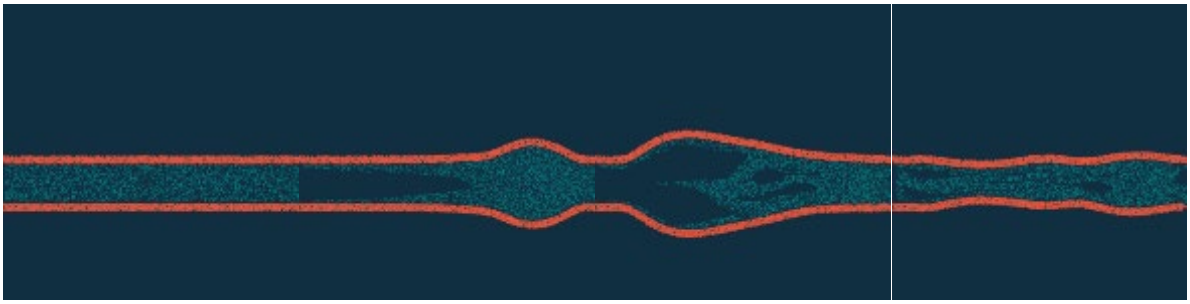

Figure 7: a toy model of the fully coupled blood-vascular interaction with the MPM

Keywords: Fluid-Structure Interaction, Blood-Vascular System, Numerical Simulation, Material Point Method

A Time-Domain Perfectly Matched Layer for Flexural Wave Simulation in Euler-Bernoulli Beams

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This study introduces a time-domain Perfectly Matched Layer (PML) approach tailored for simulating flexural wave propagation in infinite Euler-Bernoulli beams. To accurately model wave propagation within truncated computational domains, a complex coordinate stretching technique is implemented, transforming frequency-domain equations back to the time domain through inverse Fourier transforms. The developed Euler-Bernoulli PML (EB-PML) employs a mixed finite-element formulation, explicitly treating deflection, slope, moment, and shear as independent variables. For implicit time integration, a third-order Newmark-β method is employed to solve the semi-discrete equations of motion constructed using the finite element method. The performance of the EB-PML is assessed through numerical experiments involving unit-impulse and harmonic loading scenarios. Comparisons with analytical solutions indicate that the EB-PML effectively absorbs outgoing waves, significantly reducing reflections at domain boundaries. Detailed error analyses demonstrate numerical errors consistently below 0.02%, confirming the reliability and accuracy of the proposed method. The EB-PML formulation presented herein offers practical advantages for structural health monitoring applications and dynamic analysis of lifeline infrastructure systems, such as water and gas pipelines, by enabling precise wave simulations in truncated computational domains.

Keywords: perfectly matched layer (PML), flexural waves, Euler-Bernoulli beam, finite element method, structural health monitoring

Numerical Evaluation of Fire Suppression in Compartment Fires

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Firefighters employ three primary water application strategies to suppress compartment fires: direct attack on the fire's seat, gas cooling by spraying water into the hot gas layer to reduce flashover risk, and surface cooling by applying water to the compartment boundaries. Various compartment characteristics, such as fire size, compartment dimensions, and the number and size of openings, impact the effectiveness of the suppression strategies. However, the combined effects of these variables on effectiveness remain insufficiently explored and require further investigation. Therefore, the aim of this study is to compare the effectiveness of the suppression strategies under different conditions via numerical modelling. In this study, an existing experimental investigation involving a series of suppression tests using two nozzles with different characteristics was selected as a case study. The free-burning and suppression scenarios in the case study were modelled using the Fire Dynamics Simulator (FDS) and compared against experimental results. The simulation showed good agreement with the experimental data in terms of heat release rate, temperature, radiation, and oxygen concentration at various locations. Further studies are being conducted on the effectiveness of suppression strategies by varying the following parameters: fire sizes, compartment sizes, number of hoses employed, and their flow characteristics. The findings will assist firefighters in making quick decisions about which suppression strategy or strategies to use upon arriving at the fire scene, based on the compartment's characteristics.

Keywords: Compartment fires, Fire Dynamic Simulator, gas cooling, numerical modelling, surface cooling,

Numerical Modelling of Ornamental Vegetation and Safe Distances from Buildings in Bushfire-Prone Areas

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Ornamental plants represent a potential vulnerability to buildings during bushfires. The Australian Bushfire Construction Standard AS3959 does not specify safe separation distances between ornamental vegetation and buildings, despite historical evidence highlighting ornamental plants' role in building ignition during bushfire events. This study aims to fill this critical gap by developing and validating a numerical model using the Fire Dynamics Simulator (FDS). Initially, experimental investigations were conducted to characterise the flammability of Lilly Pilly (Syzygium smithii), a popular ornamental hedge species in Australian bushland-urban interface areas. Three laboratory-scale fire tests were performed, where complete hedge specimens were ignited using radiant heat panels. The geometrical representation of the plant for the simulator was generated from a point cloud produced via Gaussian splatting, using multiple photos of the plant taken from different angles. The Fire Dynamics Simulation model predictions of mass loss rate, temperature profiles, and radiant heat flux were validated against the experimental results, demonstrating strong agreement in magnitude and temporal evolution. Utilising this validated numerical model, a parametric study was conducted to determine safe separation distances for different hedge sizes and various cladding materials, including glass, timber, steel, and aluminium. This study provides valuable numerical tools and practical recommendations for improving fire safety planning and landscape management near structures in bushfire-prone environments.

Keywords: Ornamental plant, Bushfire, Numerical modelling, Safe distance, Fire Dynamics simulation.

Topology Optimization for Multi-Component Robotic Arms under Time-Varying Loads

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High structural performance of robotic arms is essential for positioning precision and energy efficiency in industrial applications. This study presents a design-dependent topology optimization framework for multi-component robotic arms, addressing dynamic multi-load scenarios during motion. Utilizing the Bi-directional Evolutionary Structural Optimization (BESO) method, the framework incorporates self-weight and inertia loads, and takes into account the time-varying acceleration of serial robotic arms in a forward manner. The objective is to minimize mean compliance under a transient context. Three numerical examples, namely a 2D single robotic arm, 3D two-arm in-plane rotation, and 3D three-arm spatial movement are presented to demonstrate the efficacy of the proposed framework. The optimization results highlight the necessity of considering design-dependent loads and different robotic configurations in topological evolution. Comparative studies on motion strategies and travel times further emphasize the importance of integrating structural performance with movement dynamics. This approach offers significant insights into the topological design of robotic arms, potentially improving their operational efficiency and precision in various industrial applications.

Keywords: Robot, topology optimization, evolutionary structural optimization, multi-load, inertia

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validated FINITE-ELEMENT predictions OF THE Stability of graft fixation for Latarjet Surgery

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Graft osteolysis and non-union are complications associated with the primary stability of the Latarjet-Bristow procedure. The primary stability of alternative fixation techniques is typically experimentally measured at a selected location at the bone-graft rim [1]. Finite element model (FEM) could complement experimental methods, enhancing efficiency and mapping micromotion across the entire graft–glenoid interface. This study aims to develop and validate an FE modelling procedure for predicting graft stability.

CT scans and experimental tests were obtained earlier [1]. Sixteen cadaveric scapulae (69.3 ± 8.6 years) [1] were obtained and CT scanned (Aquilion Lightning, Toshiba). The Latarjet-Bristow procedure was completed by fixing the graft using a screw–screw (SS) (n=5) and screw–button (SB) (n=11). The displacement of the graft was measured by applying a hundred cyclic load of 200 N on the graft by an indenter. Experimentally, micromotion was 0.13 ± 0.26 mm for SS and 0.27 ± 0.2 mm for SB. Bone geometry was segmented (Materialise, Belgium), and virtual Latarjet procedures were simulated (3-matic, Belgium). Screws were modelled with frictional contact (μ = 0.4), and inhomogeneous material properties were mapped from CT data. Mesh sensitivity analysis showed <5% force variation at element size ≤1.4 mm. Displacement was applied to replicate a 200 N experimental load, with full distal constraint. Graft motion was averaged across four superior-edge points and compared to experiments using linear regression (R^2) and root mean square error (RMSE). FEM estimated contact micromotion due to experimental limitations and it filled this gap.

The FE models showed good agreement with corresponding experimental SS (R^2 = 0.698; RMSE was 0.091 mm) and SB measurements (R^2 = 0.638; RMSE = 0.227 mm). FE results captured the experimental outputs, providing a cost- and time-efficient option

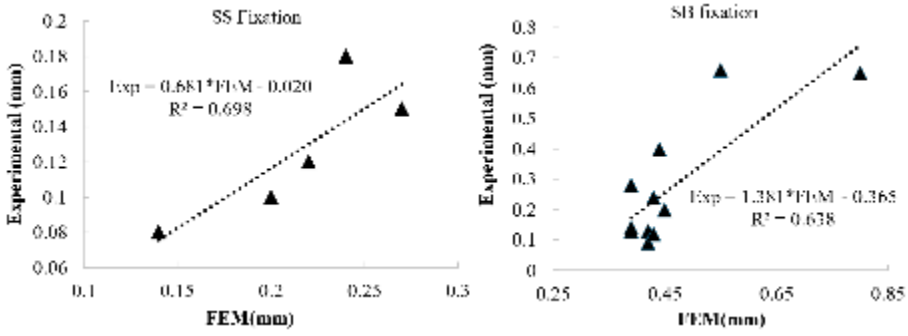

Figure 1. Linear regression between experimental and FE modelling

Keywords: Latarjet surgery, Graft stability, FE modelling, Validation study, Bone morphology.

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Evaluation of crack propagation criterion under extremely low cycle fatigue

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Predicting unstable structural failure in piping systems subjected to excessive cyclic loading induced by large-scale seismic events is of paramount importance. The J-integral is widely employed as a fracture mechanics parameter applicable to elastic–plastic deformation; however, its applicability becomes limited under cyclic loading conditions. In the regime of low-cycle fatigue, the fatigue crack growth rate is typically evaluated using ΔJ, defined based on the stress and strain ranges within a single load cycle. Nonetheless, the validity of ΔJ under extremely low-cycle loading has not been sufficiently established.

In analyses of the crack initiation phase, previous investigations have demonstrated the necessity of multiple experimental parameters obtained from the fracture behavior of compact tension (CT) specimens. Among these, the crack length and its front are of primary importance in evaluating the applied load and the corresponding load-line displacement, particularly from a local fracture mechanics perspective.

In the present study, the crack propagation criterion previously proposed by the authors is assessed under three distinct crack growth modes: (i) simultaneous propagation along the entire crack front, (ii) sequential propagation via nodal release along the crack front, and (iii) localized propagation near the mid-section of the specimen under plane strain conditions. Finite element models representing one-quarter of the actual CT specimen geometry with a 1-inch thickness are employed. While load-controlled conditions are adopted in experimental testing, displacement control is applied in the numerical simulation of the crack initiation phase. An approximation curve, established from experimental data to characterize the relationship between crack length and load-line displacement, is used to determine nodal release criteria for simulating crack propagation. Among the ΔJ-based evaluations, the generation phase analysis yielded the most accurate results, exhibiting the least deviation from experimental observations.

Under monotonic loading conditions, the critical crack tip opening displacement (CTOD) can be corrected by accounting for stress triaxiality [1]. Furthermore, in the context of fracture in cracked piping, an inverse relationship between stress triaxiality and equivalent plastic strain has been identified [2]. The interrelation between stress triaxiality and incremental equivalent plastic strain along the crack front has been examined in detail, revealing that the incremental equivalent plastic strain serves as an indicator of the critical condition for fracture onset. Based on these findings, the crack propagation criterion is redefined in terms of equivalent plastic strain and stress triaxiality, adopting a local fracture mechanics approach.

However, previous evaluations revealed significant retardation in surface-side crack propagation, indicating that the originally proposed criterion fails to accurately represent the local stress state along the entire crack front. To address this limitation, accumulated equivalent plastic strain is newly incorporated into the crack propagation criterion, and the model is re-evaluated accordingly. Future work will provide a comprehensive discussion on the validity and applicability of the extended three-parameter approach incorporating stress triaxiality, equivalent plastic strain, and accumulative equivalent plastic strain.

Keywords: Crack propagation criterion, local approach, stress triaxiality, equivalent plastic strain, accumulated plastic strain

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Atomic Study of the Vacancy Absorption near Grain Boundary in the Presence of Hydrogen in Alpha Iron

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Hydrogen embrittlement (HE) of high-strength steels often reveals an IG (inter granular) fracture. Even for the alpha iron, base metal of a steel, also shows the IG fracture with lower strain rate and higher hydrogen contents. Grain boundary (GB) have comparably large free volume so that interstitial hydrogen atoms stably exist at GB. Therefore, the locally accumulated hydrogen atoms are believed to weaken the GB cohesive energy and/or strength and yield in IG fracture. However, the detailed observation of the IG fracture surface of HE reported that the fracture surface exhibits some traces of plastic deformations rather than GB planes. In addition, contributions of vacancy or vacancy cluster during HE fracture process at GB, i.e. damage accumulation, is strongly supported for recent studies[1]. Those vacancies are considered to generate by dislocation motions such as dislocation cut-off and/or dislocation jog dragging. It indicates that vacancies are generated within a grain. On the other hand, the GB is reported to act as a sink of vacancies[2]. The vacancies generated within a grain are thought to diffuse to the GB and absorbed into the GB.

In this study, we performed molecular statics analyses to evaluate the effects of interstitial hydrogen atoms on vacancy absorption into GBs. The <110> symmetrical tilt GB are employed for calculations. The results show that increasing the introduced vacancies, the GB energy converged to almost constants, it indicates that damage accumulation to GB during fracture process of iron. It also results in the constant value of the cohesive energy in the absence of hydrogen. In contrast, the vacancy does not absorb into GB in the presence of hydrogen, and show the linear decrease of the cohesive energy in the presence of hydrogen atoms. It attributes not the vacancy diffusion rate but the pre-existing effects of hydrogen atom at GB.

Keywords: hydrogen, vacancy, grain boundary, iron, absorption, diffusion, molecular statics

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Linearly Implicit, High-Order Time Integration for Multi-physics Simulation

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Linearly implicit time integration methods suitable for multi-physics simulations have been developed up to fourth order. Order conditions are derived by applying the Lie-Trotter-Suzuki decomposition [1-2] to a combination of the exponential shift operator and the underlying Cauchy problem. The result is a sequence of commutator-free exponential factors that can approximate time varying flows. Padé approximants of the exponentials are chosen to ensure structure-preserving and unconditional linear stability properties. The number of linear solves per time step remains fixed for a given order of accuracy which is advantageous when computing on accelerators. Numerical experiments of two different nonlinear differential equations were conducted: (1) zero-dimensional ignition equation and (2) two-dimensional variable coefficient reaction-diffusion equation. The results demonstrate expected formal order of accuracy, and that numerical solutions remain stable with relatively large time steps even in the presence of strong nonlinearity and stiffness.

Keywords: Linear implicit, Lie algebra, GPU

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A numerical simulation of ferrofluid droplet emulsion in shear flow under magnetic field

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Applications of ferrofluid droplets have emerged due to their characteristic behaviours. In emulsions, rheological properties of the bulk fluid may vary in shear flow due to interactions between ferrofluid droplets. However, the effect of magnetic fields on the rheology of ferrofluid droplet emulsions has not been well understood. We simulate a ferrofluid droplet emulsion in shear flow under a magnetic field using a boundary integral method with adaptive mesh refinement [1].

Consider ferrofluid droplets in a triply-periodic domain subjected to shear flow $\boldsymbol{v}^{\infty}$. The Stokes and Maxwell's equations govern the incompressible two-phase flow of the ferrofluid droplets and the surrounding fluid:

$$\nabla \cdot \boldsymbol{v} = 0, \nabla \cdot \boldsymbol{T} = \boldsymbol{0}, \tag{1}$$

$$\nabla \cdot \boldsymbol{B} = 0, \nabla \times \boldsymbol{H} = \boldsymbol{0}, \tag{2}$$

where $\boldsymbol{v}$ is the velocity, $\boldsymbol{T}$ is the stress tensor, $\boldsymbol{B}$ is the magnetic flux density, and $\boldsymbol{H}$ is the magnetic field. An external magnetic field $\boldsymbol{H}^{\infty}$ was applied perpendicular to the shear flow. We solved Eqs. (1) and (2) employing the boundary integral method [1]. The Ewald summation was introduced to apply the periodic boundary condition [2]. The droplet surfaces were discretized into triangular elements with an adaptive mesh refinement technique. Multipole expansion and multi-GPU computation were implemented for the speed up of computation.

Figure 1 shows typical snapshots of numerical results, where the volume fraction is 0.1. The ferrofluid droplets were initially deployed at random. As time evolved, they formed chain-like structures owing to the interaction with each other by the magnetic force, and anisotropy appeared in droplet distribution.

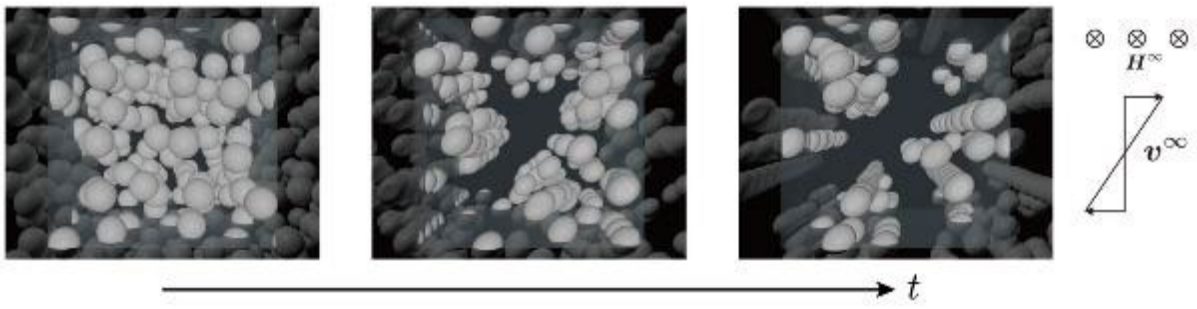

Figure 1.

Keywords: Ferrofluid, droplet, two-phase flow, computational fluid dynamics, boundary integral method

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Explicit Solvent Modeling in Protein Dynamics Using Mixed Overlapping Element

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The conformational dynamics of proteins are essential to their biological function and require accurate modeling of both the protein structure and its solvent environment. This study presents a finite element framework for continuum-based protein dynamics simulations that explicitly incorporates solvent effects [1]. Traditional approaches rely on high-order mixed finite elements to ensure stability in incompressible flow analysis, but these methods are computationally expensive. To overcome this limitation, we introduce a three-dimensional mixed overlapping element strategy for constructing solvent finite element models [2]. This technique maintains numerical stability while substantially reducing computational overhead, thereby enabling more efficient continuum-based simulations of protein dynamics.

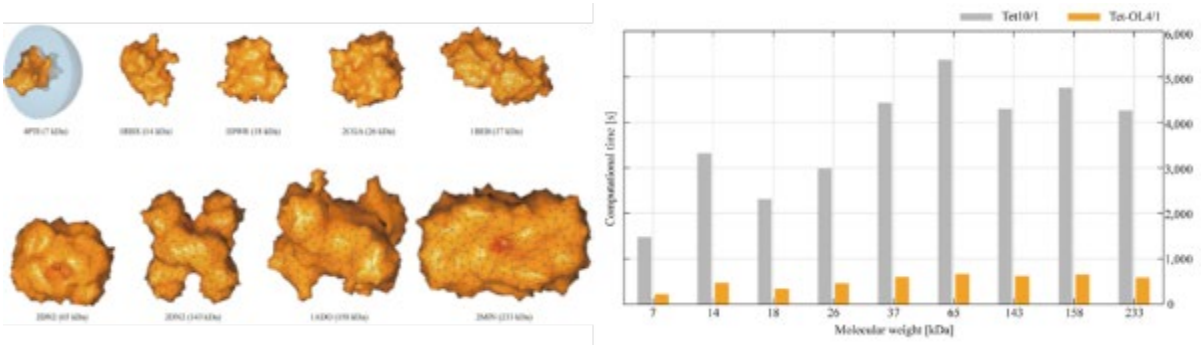

Figure 1.

PDB ID	Translational [10^{-2} Å^2/ps]			Rotational [10^{-6} ps^{-1}]		
	Tet-OL4/1	Tet10/1	Exp.	Tet-OL4/1	Tet10/1	Exp.
4PTI	1.45	1.46	1.29	4.65	4.87	4.17
1RBX	1.15	1.17	1.07	2.34	2.46	N.A.
193L	1.18	1.17	1.09	2.55	2.63	2.6
1DWR	1.06	1.08	1.02	1.85	1.97	1.72
2CGA	0.93	0.95	0.93	1.28	1.36	N.A.
1BEB	0.80	0.81	0.78	0.80	0.84	0.75
2DN2	0.72	0.72	0.69	0.60	0.61	0.44
2GPD	0.52	0.52	0.5	0.22	0.23	N.A.
1ADO	0.49	0.49	0.45	0.18	0.18	N.A.
2MIN	0.46	0.46	0.4	0.15	0.16	N.A.

Table 1.

Keywords: Finite element analysis, Mixed overlapping element, Incompressible analysis, Protein dynamics, Continuum modeling

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Heat Transfer in Energy-Efficient, Fire-Rated wall systems for Australian Construction: A numerical study

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The construction industry contributes 35 to 40 % of global CO_2 emissions. In response, the National Construction Code (NCC 2022) [1] raised the Nationwide House Energy Rating Scheme (NatHERS) benchmark from 6 to 7 stars and mandated thermal bridging mitigation, targeting a 25% reduction in residential operational energy use. In alignment with these objectives, this study investigates the energy performance, quantified in terms of thermal resistance (R-value, m²·K/W), of fire-rated steel framed wall systems using numerical simulation models under Australian climatic conditions. A load-bearing light steel frame (LSF) wall measuring 1.03 m in height and 1.06 m in width, previously tested using a mini hot box to determine its R-value [2], was adopted for numerical validation. Validated finite element models were subsequently employed to simulate and evaluate the thermal behaviour of steel wall assemblies under comparable boundary conditions. The primary focus of this study is the effect of web perforations, which have demonstrated considerable potential to disrupt conductive heat transfer pathways and enhance overall R-values. Computational simulations were performed using THERM for two-dimensional steady-state analysis and ABAQUS for three-dimensional transient thermal modelling. Key parameters assessed include section type, steel thickness, insulation detailing, thermal break application, and perforation geometry. The total thermal resistance (RT) was computed according to ISO 6946 [3]:

$$R_T = R_{si} + \sum_{x=1}^{n} Rx + R_{se} \quad (1)$$

where Rsi = 0.13 m²·K/W and Rse = 0.04 m²·K/W are the internal and external surface resistances, and Rx refers to the resistance of individual material layers. Given the widespread use of hot rolled steel (HRS) members in fire rated wall systems for medium to large span applications, a comparative case was incorporated to assess the influence of web perforations in both HRS and cold formed steel (CFS) configurations. To ensure consistent insulation cavity depth, a 100 PFC HRS section with 100 mm depth, 50 mm flange width, 6.0 mm thickness, and 8.64 kg/m mass, as per AS/NZS 3679.1:2016, was compared with a CFS lipped channel stud of 100 × 50 × 15 × 1.5 mm and 2.2 kg/m mass, in accordance with AS/NZS 4600. Although both materials exhibit high thermal conductivity, around 50 W/m·K, the CFS section showed significantly lower thermal bridging due to its reduced thickness. Moreover, the addition of web perforations resulted in a marked improvement in thermal resistance, increasing R values by 15 to 20 % across both systems. Modified equations are also proposed to analytically estimate R values of complex LSF wall systems with web perforations using NZ 4212:2006 for practical design applications.

Keywords: Light steel frame walls, Cold-formed steel, Hot-rolled steel, Web perforations, Thermal bridging, R-value, U-value, Thermal transmittance, Energy efficiency and Heat flux

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A Diffuse-Interface Method for Modeling Two-Phase Flow with a Boussinesq-Scriven Interface

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The diffuse-interface method is an interface capturing technique for multi-phase flow problems based on the Cahn-Hilliard model. In this study, the diffuse-interface method is employed to model a Boussinesq-Scriven interface, incorporating interfacial viscosity alongside classical interfacial tension.

In previous studies utilizing the sharp-interface method, interfacial stress was treated as a boundary condition [1]. This study, with the help of the diffuse-interface method, reformulates the interfacial boundary condition into the momentum conservation equation, localizing the interfacial stress at the interface [2, 3]. Assuming incompressible Newtonian fluids, the momentum conservation equation for the Stokes flow reads as follows:

$$-\nabla \cdot (2\eta \boldsymbol{D}) + \nabla p = \nabla \cdot \boldsymbol{\tau}_c + \delta_s \nabla_s \cdot \boldsymbol{\tau}_s, \tag{1}$$

where η is the viscosity, $\boldsymbol{D}$ is the rate-of-strain tensor, $\boldsymbol{\tau}_c$ is the capillary stress tensor, δ_s is the Dirac-delta function of the diffuse-interface, $\boldsymbol{\tau}_s$ is the interfacial viscous stress, and ∇_s is the surface gradient operator. Main advantage of the present formulation is that it allows the model to describe topological changes of the interface without encountering singularity issues. The Stokes-Cahn-Hilliard system is numerically solved using the finite element method. An adaptive mesh refinement is employed to improve the computational efficiency.

Convergence of the numerical solution is first tested, demonstrating optimal rates in both time and space. A two-dimensional drop deformation in shear flow is then studied using both the present formulation and a sharp-interface approach, confirming good agreement between the two results as the diffuse-interface thickness decreases (Fig. 1). Finally, two-dimensional drop coalescence is investigated, with particular focus on the effect of interfacial viscosity.

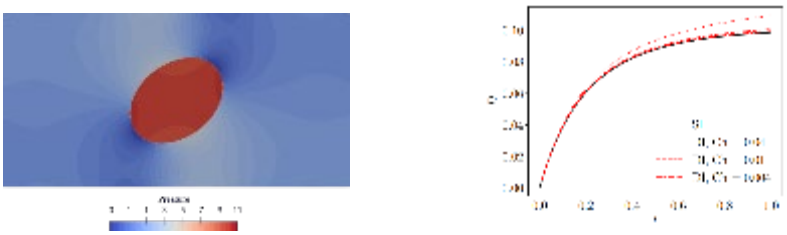

Figure 1.

Keywords: Diffuse-interface method, two-phase flow, Boussinesq-Scriven interface

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A data-driven probability uncertainty analysis method based on the B-spline theory and the maximum entropy method

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Abstract

Stochastic uncertainties of material properties, geometric dimensions, and applied loads result in the randomness of structural responses, which can be described by using the probability density function (PDF) of the responses. Recovering the PDF of the structural response accurately is pivotal in probability uncertainty analysis. Many parametric or non-parametric methods have been developed in recent decades. The maximum entropy method (MEM) is usually popular, and has achieved great success in probability uncertainty analysis. However, it is still confronted with some difficulties. For instance, when only limited statistical moment information is available, accurate prediction for complex multimodal PDFs is very challenging. To this end, this study develops a novel metaheuristic data-driven PDF reconstruction method for probability uncertainty analysis based on the B-spline theory and the MEM.

In fact, the estimation of a complex PDF can be seen as the problem of complex curve fitting to some extent. With the prior assumption that the complete B-spline basis space can represent a complex curve well, this study regards the PDF of interest as a response surface composed of the B-spline functions. Jaynes' maximum entropy principle indicates that MEM is a rational approach to obtain the most unbiased probability distribution amongst all possible candidates and the determined distribution is consistent with available data and contains minimum spurious information. Therefore, the MEM is a judicious choice to solve the corresponding coefficients of the B-spline response surface. Our method originates from the maximum entropy principle and is a purely data-driven approach for the PDF construction, integrating the advantages of the B-spline theory and the traditional MEM. The undetermined parameters are learned from the sample data directly using the MEM and the reasonable B-spline knot configuration is further determined via an advanced metaheuristic algorithm, Beluga whale optimization algorithm. Therefore, the results of our method are faithful to the raw data. Compared with the traditional MEM and other moment-based methods, our study uses the sample data directly but not in the form of statistical moments; thus, some tricky problems caused by statistical moments can be bypassed.

In summary, the proposed method provides a data-driven approach for constructing complex PDF, such as multimodal PDFs. Firstly, a B-spline proxy of the MEM PDF is used for probability uncertainty analysis. We derive the parameter calculation formulation based on the idea of the optimization criterion method and calculate the undetermined parameters via the raw data of structural responses. Then, to determine the knots of the B-spline functions, we propose a novel data-driven approach with the aid of a powerful metaheuristic algorithm and the response data information. Different from the traditional MEM, the proposed method is a complete data-driven solution approach and does not involve the statistical moment calculation and the nonlinear equations composed of statistical moments. Combining the advantages of the B-spline theory and the MEM, the proposed method can reconstruct the response PDF with a complex shape, such as the PDF with multiple peaks or heavy tails. For verification, three numerical examples and one engineering example are analysed, and compared with some classical PDF

modelling methods. The results show that the proposed method is superior to the compared methods in terms of computational accuracy, when the same sample data is used.

Keywords: Maximum entropy method, B-spline theory, Data-driven method, Probability density function, Uncertainty analysis, Metaheuristic algorithm

A RPIM-Based Extrinsic Enriched Finite Element Method for the Helmholtz Equation

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The conventional finite element method (FEM) provides accurate solutions to the Helmholtz equation only at low wave number, as numerical dispersion errors significantly degrade accuracy at higher wave number. To address this issue, this paper proposes an extrinsic enhanced FEM (EFEM) based on the Radial Point Interpolation Method (RPIM) to reduce the numerical dispersion errors In this method, the shape functions of discrete elements are constructed using RPIM, and the approximation space is enriched with polynomial functions to more effectively capture the highly oscillatory characteristics of the Helmholtz equation. Several numerical examples are considered to verify the performance of this RPIM-based extrinsic EFEM in solving the Helmholtz equation. It is shown that this method significantly outperforms the traditional FEM in suppressing dispersion errors and often yields more accurate numerical results for high-frequency Helmholtz problems. Thus, when solving high-frequency Helmholtz equations, the RPIM-based extrinsic EFEM may serve as an excellent alternative to the conventional finite element method.

$$\tilde{u}(\mathbf{x}) = \sum_{i \in n} \phi_i(\mathbf{x}) u_i + \sum_{i \in n} N_i^*(\mathbf{x}) \psi(\mathbf{x}) a_i \tag{1}$$

In this extrinsic EFEM, the interpolation form of the field function $u(\mathbf{x})$ is given in Equation (1), where $\phi_i(\mathbf{x})$ denotes the shape functions of the nodes constructed using RPIM, and $N_i^*(\mathbf{x})$ represents the additional shape functions introduced by enriching the nodal degrees of freedom. The coefficients u_i and a_i are the corresponding unknowns to be determined. The function $\psi(\mathbf{x})$ is a specially-designed enrichment function and it always plays a very important role in improving the numerical performance of this extrinsic EFEM.

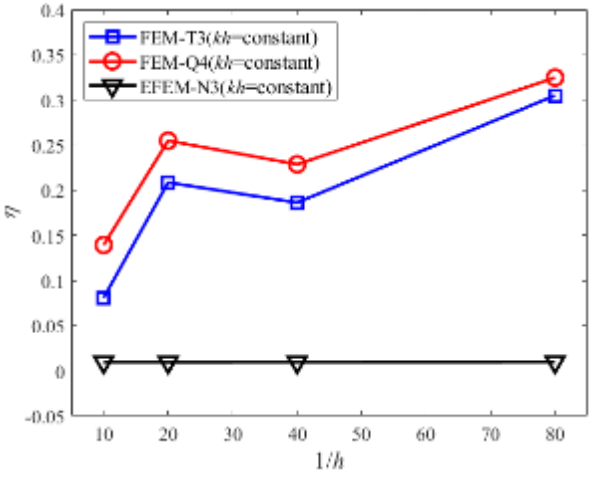

Figure 1.

Keywords: RPIM, EFEM, Helmholtz equation

Overlapping finite element modeling of hyperelastic materials

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Hyperelastic materials, such as rubbers, polyurethane elastomers, and some biological tissues, are extensively employed in vibration isolation, sealing systems, and biomedical engineering applications [1]. These materials exhibit a complicated nonlinear relationship between stress and strain, so advanced numerical schemes are needed for accurate prediction of mechanical behaviors of hyperelastic structures.

The overlapping finite element method demonstrates excellent performance in general analyses of linear elastic solids [2]. In this method, a group of well-designed basis functions is employed to improve the computational efficacy of overlapping finite elements. Moreover, virtual nodes (See Figure 1) are introduced to construct a novel interpolation function, which significantly suppresses the linear dependence issues arising from the use of basis functions [2]

$$\gamma_J = h_J + \beta \sum_K \left(h_K - h_J \right) \hat{h}_L \tag{1}$$

in which γ_J is the interpolation function in the overlapping elements (J = 1, 2, 3, 4), h_J and $\hat{h}_L$ represent the shape functions of 4-node and 8-node quadrilateral finite elements, respectively, here K stands for the field nodes directly connected to node J through the element edges, and L in $\hat{h}_L$ denotes the mid-side node between J and K; β is a coefficient that determines the numerical abilities of overlapping elements.

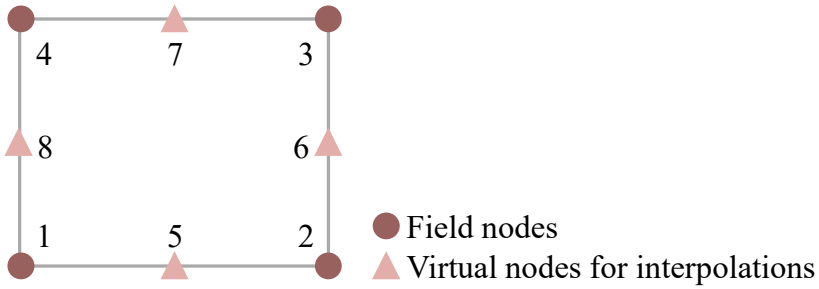

Figure 1.

In this work, the overlapping finite element method is employed for hyperelastic structure simulations owing to its numerical advantages. A numerical test is carried out to assess the performance of the overlapping finite element method, and standard finite element solutions are provided for comparison. From the test, it is observed that the overlapping finite element method is computationally accurate and efficient in the evaluation of the hyperelastic structures, demonstrating its superior capability in handling large deformation compared to the conventional finite element method.

Keywords: Overlapping finite elements, hyperelastic materials, nonlinear analysis, large deformation, computational solid mechanics

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Variational Quantum Topology Optimization

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In the recent decade, quantum scientific computing has emerged as a new paradigm to solve difficult engineering problems such as simulation [1] and optimization [2]. Topology optimization is an example of such problems. It requires to solve the constraint of partial differential equations and search for the optimal structural configurations together. High dimensionality of the search space is the main challenge.

In this work, a variational quantum topology optimization algorithm is proposed where a single-loop variational quantum algorithm is used to optimize the configuration and solve the constraint simultaneously [3]. The quantum circuit also encodes the volume and connectivity constraints. The compliance minimization problem is reformulated as

$$\min_{\boldsymbol{\theta}} \boldsymbol{u}^{\top}(\boldsymbol{\theta})[K(\boldsymbol{q}(\boldsymbol{\theta})) + \lambda L(\boldsymbol{q}(\boldsymbol{\theta}))]\boldsymbol{u}(\boldsymbol{\theta}), \tag{1}$$

where $\boldsymbol{\theta}$ is a vector of quantum circuit parameters, $\boldsymbol{u}$ is the estimated displacement vector, $\boldsymbol{q}$ is the configuration, K is the global stiffness matrix, λ is a Lagrange multiplier, and L is a Hamiltonian which encodes the residual of the linearized partial differential equations. The new algorithm is tested with truss structures and Messerschmitt-Bölkow-Blohm beams. For the truss structure in Figure 1(a), the success probability of 0.4 is achieved within 20 iterations of optimization, as shown in Figure 1(b).

(a) (b)

Figure 1. (a) an example of truss structures and (b) the distribution of optimal solutions, where four out of ten runs result in the true optimal configuration of "1001" within 20 iterations, subject to the volume constraint that no more than two optional elements are allowed.

Keywords: Topology optimization, Quantum computing, Variational quantum algorithm

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Multi-task Approach to Physics-informed Deep Operator Network for Electromagnetic Scattering Analysis

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Accurate prediction and efficient analysis of electromagnetic scattering phenomena are critical to the development and design optimization of advanced military platforms, including antenna systems for aircraft, weapon systems, and stealth technologies. Traditional design procedures involving physical prototype fabrication and experimentation incur significant economic and time costs. Numerical methods, notably the finite element method, have been widely employed for computational electromagnetic analyses; however, their applicability to large-scale problems or problems involving complex heterogeneous materials remains computationally demanding.

To overcome these limitations, surrogate modelling approaches have gained significant attention, incorporating strategies such as domain decomposition, reduced-order model, and deep learning-based approximations. Among recent advances, deep operator network [1,2], leveraging the universal approximation theorem for operators, have shown great promise in learning operator-level mappings between input function spaces and output solutions, providing a generalized framework capable of solving partial differential equations under diverse conditions.

In this research, we propose an enhanced physics-informed deep operator network with multi-task learning capabilities [3], capable of simultaneously addressing electromagnetic scattering problems involving multiple geometric heterogeneous domains. Our approach integrates prior physical knowledge from the Helmholtz equation directly into the training process, enhancing the generalization, accuracy, and computational efficiency of surrogate predictions across diverse scenarios. Through multi-task learning, it can be simultaneously predicted scattering characteristics for various domain configurations. The performance of the proposed framework is validated by demonstrating accuracy and efficiency in solving electromagnetic scattering problems with varying shapes, properties, and boundary conditions. Our results highlight the potential of the proposed framework to accelerate the design and optimization processes for complex electromagnetic applications.

Keywords: Electromagnetic scattering, Physics-informed, Deep operator network

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Level-set Topology Optimization of Vibroacoustic Systems Considering Harmonic Stress Concentration

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Topology optimization of acoustic-structural coupled systems has been emerged as a flexible and prominent design methodology for applications such as noise reduction, vibration control, and underwater stealth. These systems often rely on small-scale resonant structures to enhance low-frequency performance. However, such designs tend to cause significant local stress concentrations due to their high compliance and small length scales, which can degrade structural reliability. While some prior studies have introduced structural compliance-based criteria to preserve load-bearing capacity, they have not explicitly addressed stress in dynamic vibroacoustic contexts. To overcome this limitation, we propose a novel topology optimization framework that simultaneously accounts for both stress and transmitted acoustic power in the optimization formulation. The proposed design approach employs a level-set method for clear structural boundaries, and the mixed displacement-pressure finite element formulation is used to accurately track the interaction between the acoustic and structural domains [1]. Local von-Mises stresses are aggregated via *p*-norm, and sensitivities are efficiently computed using the discrete adjoint method. By managing both local stress and acoustic power transmission, this framework enables the design of structurally robust and acoustically efficient vibroacoustic systems.

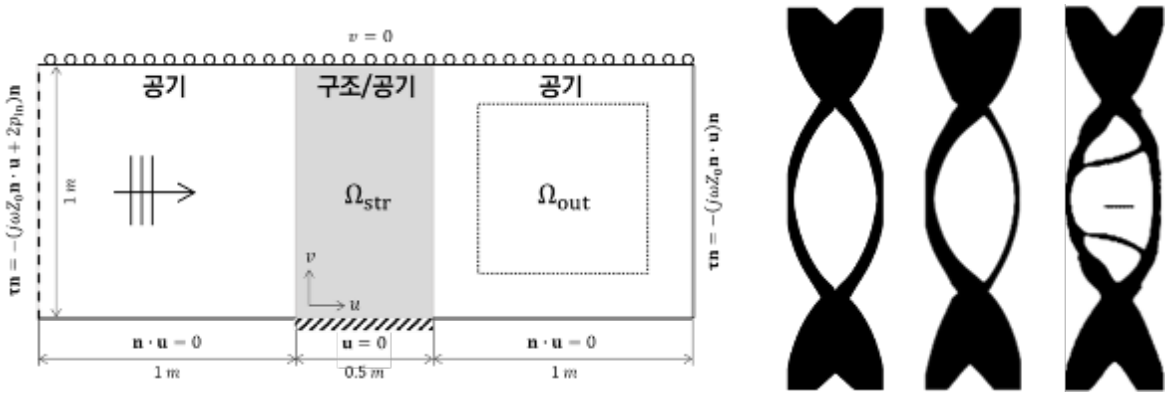

Figure 1.

Keywords: Topology optimization, level-set method, acoustic-structural interaction, von-Mises stress, *p*-norm aggregation, adjoint method

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Inverse Design of Phase Change Material-based Sandwich Panels for Thermally Tunable Acoustic Performance

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To address the increasing demand for multifunctional acoustic systems adaptable to dynamically varying environments, this study explores the inverse design of vibroacoustic systems integrated with phase change materials (PCMs). Conventional sandwich panel core designs, e.g., truss lattices, triply periodic minimal surface (TPMS) lattices, and acoustic black hole-inspired structures, etc. are typically optimized for a single functionality such as vibration or sound absorption, and lack the ability to adapt their behavior once manufactured [1]. In contrast, the integration of PCMs enables significant temperature-dependent variations in material properties, including shear modulus and wave speed, and thereby offering opportunities for non-mechanical stimulus-responsive control of acoustic performance [2]. Focusing on sandwich panel structures, we examined the feasibility of thermally-tunable PCM core designs through parametric optimization. Our findings demonstrate a distinct on/off behavior in acoustic performance driven solely by thermal stimuli, without requiring geometric modification. While the present work is focused on parametric optimization, it will be extended to more generic inverse design approach, i.e., topology optimization of PCM structures to achieve multifunctionality across thermal, vibrational, and acoustic domains.

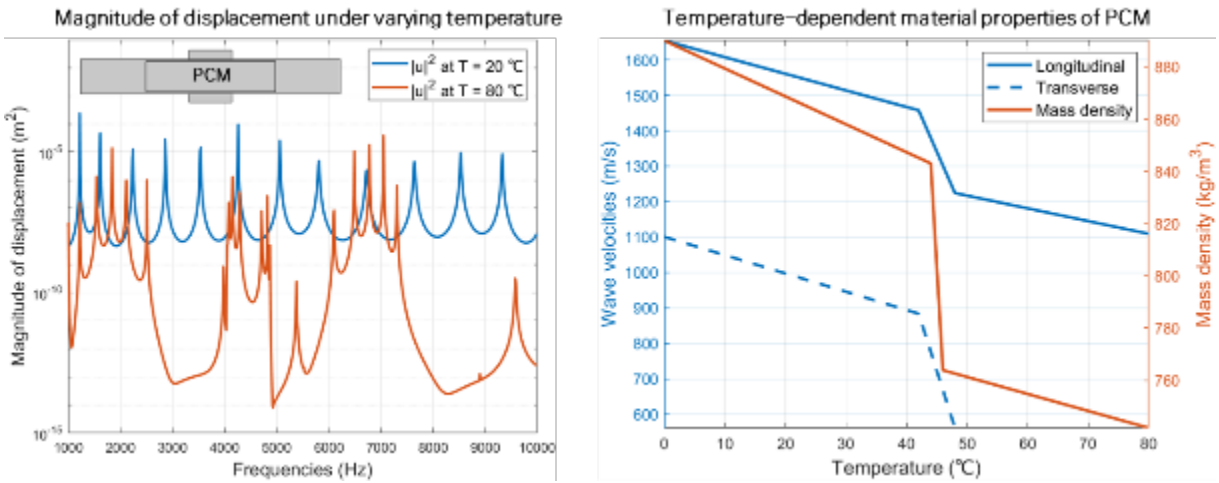

Figure 8.

Acknowledgement

This work was supported by the National Research Foundation (NRF), South Korea, under project BK21 FOUR (Smart Robot Convergence and Application Education Research Center)

Keywords: Inverse design, Phase change material, Sandwich panel, Acoustic-structure interaction, Thermal tunability

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Nanoscale Transport in Hydroxyapatite: The Impact of Pore Size and Ionic Concentration on Diffusivity

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The diffusion of particles in tooth enamel, which is made of 96% Hydroxyapatite (HAp), plays a crucial role in developing dental products, tissue scaffolds and implantable biomaterials [1]. However, the diffusion of mineral particles, such as calcium and fluoride, in HAp often involves a combination of various effects, including deposition, ion exchange, dissolution and precipitation [1]. To reduce the complexity and only consider the pure diffusion, this study investigates the diffusivity of sodium chloride in HAp nanopores using molecular dynamics. We deploy the TIP3P-PME water [2], hexagonal close-packed HAp with a chemical formula of $Ca_{10}(PO_4)_6OH$ [3, 4] and coefficients for sodium chloride from [5]. The simulation has a geometry shown as Fig. 1(a).

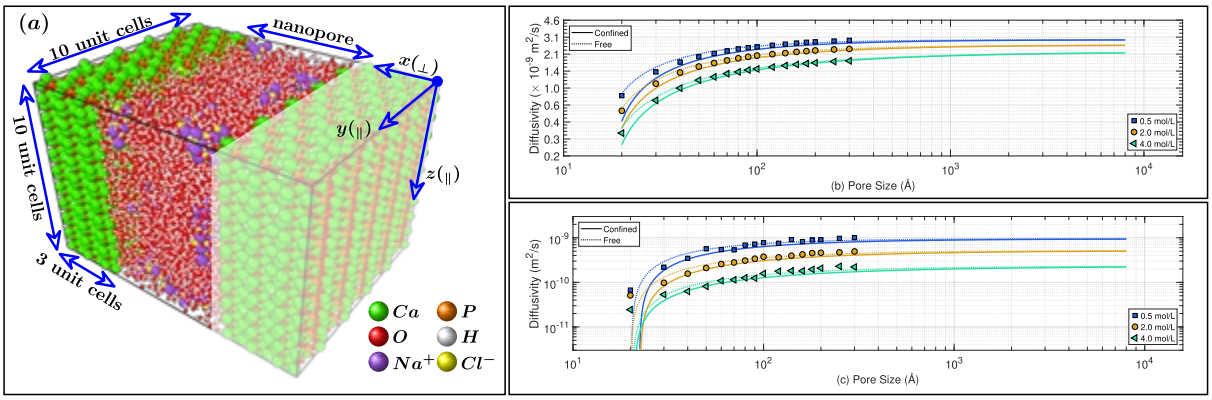

Figure 1. (a) diffusion of $2.00M$ saline in a 50Å nanopore; (b) diffusion coefficient of water in saline solutions in nanopores; (c) diffusion coefficient of ions in saline solutions in nanopores.

The self-diffusion of the sodium chloride model used in simulation matches measurements from Nuclear Magnetic Resonance, and this study uses an empirical function to fit the outputs. The results in Fig. 1(b) and 1(c) show a similar tendency between water and ions, where they both exhibit reduced and anisotropic diffusivity when the pore size is below 10^2Å, caused by induced hydrogen bonds and interactions with wall atoms. Also, with the increase of concentrations, the hydration shell formed around ion clusters increases the hydrodynamic radius disproportionately, resulting in a higher resistance to diffusion, making the wall effect extend to a micrometre scale in higher concentrations.

Keywords: Molecular Dynamics, Hydroxyapatite, Diffusivity, Nanopore

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Crystal-Inspired Multiscale Design of Additively Manufactured Titanium Lattice Structures

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While additive manufacturing (AM) offers exceptional freedom in tailoring topology and composition for architected titanium lattices, their mechanical performance remains limited by a disconnect between structural design and atomic-scale material behaviour. To address this, we present a crystal-inspired multiscale framework that bridges atomic principles—such as bonding symmetry, phase stability, and deformation mechanisms—with macroscopic architectural optimization. By integrating laser-based AM techniques with material innovation, we demonstrate how hierarchical control over lattice topology and composition can overcome traditional strength-ductility-energy absorption trade-offs. Key advances include: (1) Crystal-mimetic topology design, where atomic bonding concepts guide node and strut reinforcement strategies to enhance load transfer and energy dissipation; (2) Phase engineering through in-situ alloying to stabilize metastable phases and suppress detrimental microstructural transformations; (3) Synergistic material-structure optimization combining gradient architectures with nanoscale strengthening mechanisms to enable unprecedented deformation control. Experimental and computational results reveal how these strategies collectively transform failure modes from catastrophic collapse to progressive hardening, while maintaining lightweight characteristics. This work establishes a paradigm for designing high-performance titanium lattices, where AM acts not merely as a fabrication tool but as an enabler of multiscale material-structure synergy.

Keywords: Additive manufacturing, titanium alloys, lattice structures, crystal-inspired design, multiscale optimization, energy absorption

Metastructure with gradient zigzag beams and masses

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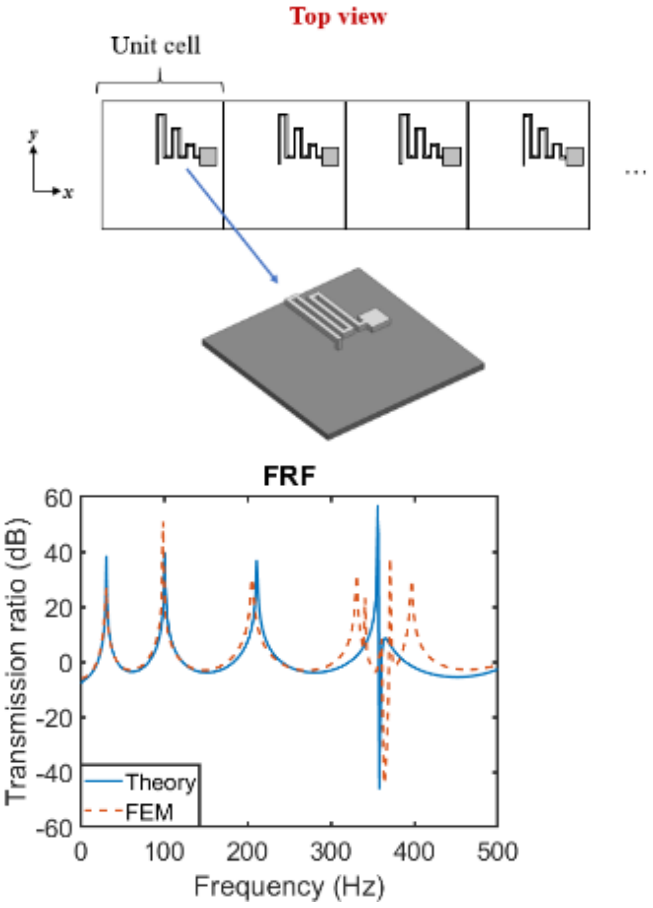
There has been growing interest in low-frequency vibration attenuation recently. Phononic crystals (PCs) with periodic constitutive properties have demonstrated their uniqueness in controlling elastic wave propagation. However, PCs are not effective in eliminating low-frequency elastic wave due to their structure size. Liu et al. [1] introduced locally resonant (LR) sonic crystals, which consist of an array of locally resonant units, offering a novel approach to attenuating low-frequency sounds. Following their work, elastic structures with locally resonating systems have been vigorously proposed [2, 3]. This study proposes a metastructure with a periodic gradient zigzag beam and mass system, as illustrated in Fig. 1. Using the transfer matrix method and Bloch's theorem, the characteristic equation can be obtained as:

$$\det\left|\mathbf{T}-e^{iqa}\mathbf{I}\right|=0\,, \tag{1}$$

The relationship between wave frequency ω and propagation constant *qa* can be readily obtained by using Eq. (1). Fig. 1 shows the FRF of the proposed metastructure, obtained by theoretical model and finite element simulation. It can be seen that the theoretical result matches perfectly with the FE result. The predicted and simulated bandgap ranges are 357Hz-360Hz and 362Hz-369Hz, respectively.



(a) (b)

Figure 1 (a) A metastructure with a periodic gradient zigzag-beam and mass system (b) The predicted and simulated FRFs.

Keywords: metastructure, gradient zigzag beam and mass system, wave propagation, bandgap

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Physics-Informed Neural Network for Predicting Grain Structure Evolution Governed by the Allen-Cahn Equation

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Simulating grain growth through the Allen-Cahn equation [1] enables predictive modelling of microstructural evolution in polycrystalline materials. While traditional numerical simulations based on this equation can provide accurate predictions, they are often computationally expensive, particularly when simulating long time intervals or exploring a wide range of physical conditions. As a result, it becomes impractical to simulate every possible condition and time frame to analyze grain structure evolutions. To address this challenge, data-driven machine learning approaches have been explored, but these methods often require large volumes of simulation data and tend to produce physically inconsistent results. To overcome these limitations, we propose a physics-informed neural network that incorporates not only simulation data but also the governing physical law, the Allen-Cahn equation, into the training process. Specifically, the neural network is trained to minimize both data loss and the residual of the Allen-Cahn equation, ensuring that the predicted phase evolution follows known physical principles. The equation used in this study is:

$$\partial\phi_n = -\partial t \times [M\,(-\phi_n - 2\phi_n^3 + 3\phi_n \textstyle\sum_{q=1}^{N} \phi_q^2 - 2K\nabla^2\phi_n)]. \quad (1)$$

Here, ϕ_n denotes the phase field of the nth component, t is time, M is the mobility coefficient, K is a constant related to interfacial energy, ∇^2 is the Laplacian operator describing spatial diffusion, and $\sum_{q=1}^{N} \phi_q^2$ accounts for interactions among N phase components. The neural network outputs the spatial and temporal evolution of grain order parameters, and these predictions are evaluated against the Allen-Cahn equation. This enforcement of physics is made possible by automatic differentiation that enables the network to analytically compute derivatives of its outputs with respect to spatial and temporal coordinates. These derivatives are used to evaluate the residuals of the Allen-Cahn equation at each input point, and the magnitude of these residuals is incorporated into the loss function. By minimizing this physics-based loss alongside the data loss, the network learns to produce physically consistent outputs, even in regions where no training data is provided. The proposed method accurately predicts the evolution of grain structures at future time steps beyond the training data, producing results that closely match conventional simulation outputs while requiring only a few seconds of inference time. This makes the approach an efficient surrogate model for grain growth simulations, enabling rapid mapping of grain coarsening behavior across varying thermal and kinetic conditions. By significantly reducing computational cost, it facilitates accelerated exploration and optimization of processing parameters, with only minimal reliance on full-scale simulations for final validation.

Keywords: Allen-Cahn equation, physics-informed neural network, phase-field model, machine learning, grain growth, grain structure evolution

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Diffusion-based Generative Topology Design under Uncertain Boundary Conditions

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In many structural design problems, boundary conditions such as loads, supports, and volume fraction constraints are not fully defined in the early stages. Conventional optimization-based methods typically require fully defined boundary conditions, which convert this uncertainty into repeated and expensive simulations when specifications evolve. To address this issue, we represent the design task as a conditional generative problem, in which the algorithm learns the distribution of admissible topologies that satisfy the given boundary conditions. Specifically, we adopt a conditional diffusion process [1] for the generative method. The model receives an incomplete condition vector that encodes known Dirichlet and Neumann boundaries, load magnitudes, and volume fraction targets; missing entries are masked during training to promote diversity and to train the network to operate under uncertainty in the data.

The training dataset is generated by randomly varying boundary conditions, loading configurations, and volume fraction constraints in a finite element solver. For each sample, the corresponding condition vector is intentionally masked during training to simulate uncertainty and to encourage the model to learn a broad distribution of admissible designs. This enables the model to generalize to ill-posed settings where some input conditions are missing. The denoising process in the reverse diffusion follows a standard variance-preserving formulation with conditioning:

$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon_\theta(x_t, t, c) \right) + \sigma_t z, \tag{1}$$

where α_t and β_t are the forward-process coefficients, ϵ_t is the learned score network, and σ_t is the posterior noise scale. Equation (1) explicitly couples the generative trajectory to the partial BC specification c, ensuring constraint satisfaction while still exploring the high-entropy manifold of admissible designs.

Preliminary results show that the proposed framework generates structurally sound layouts even when more than half of the boundary information is hidden at inference. In comparison with conditional generative adversarial networks and variational autoencoders trained on the same data, the diffusion model yields lower compliance variance across repeated samplings and avoids mode collapse. These findings indicate that conditional diffusion, combined with an efficient masking scheme, offers a practical route to diverse concept generation when design specifications are only partially known.

Keywords: Topology optimization, Generative design, Diffusion model, Tokenization, Structural optimization

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Nonlinear Wave Making Simulation Based on Second-Order Smoothed Particle Hydrodynamics

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Ship-generated waves will undergo a series of complex flow phenomena such as rolling up, breaking and air entrainment during the propagation. These phenomena significantly affect the hydrodynamic performance and flow noise characteristics of vessels. Consequently, the accurate capturing and simulation of such nonlinear flows have become one of the critical focuses in ocean engineering research.

Smoothed Particle Hydrodynamics is a meshfree method which developed in recent decades, and demonstrates unique advantages over traditional grid-based approaches when simulating nonlinear problems: Its meshfree nature eliminates grid distortion limitations, while the Lagrangian approach explicitly tracks fluid interfaces without requiring complex reconstruction procedures.

It is noteworthy that conventional discretization scheme is difficult to maintain sufficient accuracy under non-uniform particle distributions. This challenge becomes particularly pronounced when using adaptive refinement techniques, as inconsistent diameters between neighboring particles exacerbate numerical dissipation and accuracy degradation. In order to solve this problem, the present study proposes a correction method based on Taylor series expansion and the least squares method. Assuming the current particle is indexed as i and its neighboring particles as j, the continuous physical field $f(x)$ can be expanded as follows under one-dimensional conditions:

$$f(x_j) = f(x_i) + f'(x_i)\cdot(x_j - x_i) + \frac{1}{2}f''(x_i)\cdot(x_j - x_i)^2 + O\left((x_j - x_i)^3\right) \tag{1}$$

By performing Taylor series expansions for all neighboring particles within the support domain and assembling them into matrixes, with the kernel function W serving as the weighting function, the expressions for $f(x_i)$ and its derivatives under minimized error can be formulated as:

$$\begin{bmatrix} f(x_i) \\ f'(x_i) \\ f''(x_i) \end{bmatrix} = (\boldsymbol{P}^T\boldsymbol{W}\boldsymbol{P})^{-1}\boldsymbol{P}^T\boldsymbol{W}\begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{bmatrix} \tag{2}$$

$$\boldsymbol{P} = \begin{bmatrix} 1 & x_1 - x_i & \frac{1}{2}(x_1 - x_i)^2 \\ 1 & x_2 - x_i & \frac{1}{2}(x_2 - x_i)^2 \\ \vdots & & \\ 1 & x_n - x_i & \frac{1}{2}(x_n - x_i)^2 \end{bmatrix}, \quad \boldsymbol{W} = \begin{bmatrix} W_1 & & & \\ & W_2 & & \\ & & \ddots & \\ & & & W_n \end{bmatrix} \tag{3}$$

The aforementioned formulation can be extended to multidimensional problems. The improved method effectively improves numerical accuracy while reducing dissipation errors. Building upon this framework, the present study simulates a large cruise ship wave making by using 2D+t method, adaptive

particle refinement technique and multiphase model. The simulation primarily focuses on capturing the evolution of bow wave roll-up processes and local nonlinear flow features. The results will provide researchers with deeper insights of the nonlinear characteristics of ship waves and the interaction mechanisms between structures and flow filed.

Keywords: Smoothed Particle Hydrodynamics, nonlinear wave-making, 2D+t method

Stabilized DeepSDF with Local Feature Weighting for Robust Thin-Plate Generation

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Recent progress in deep learning has significantly propelled the field of generative AI, with neural field-based models emerging as powerful tools for high-fidelity 3D shape representation, interpolation, and completion. Among these, DeepSDF has demonstrated remarkable capabilities in generating smooth and continuous shapes. However, the application of such generative models in engineering domains, particularly for structural design involving thin-plate structures, faces persistent challenges. Existing methods often struggle to capture the intricate geometric features and meet the specific mechanical requirements crucial for these structures, leading to issues like geometric distortions and the loss of critical local details.

Addressing these limitations, this research introduces a novel approach that integrates Curriculum DeepSDF to stabilize the representation of thin-plate geometries and enhance learning efficiency. Furthermore, we incorporate a point cloud feature extraction technique, based on Principal Component Analysis, to emphasize the importance of local geometric features, such as indentations and protrusions, which significantly influence the mechanical behavior of thin-plate structures. This allows our model to achieve high-fidelity reconstruction and accurate Parameter-to-3D generation. The proposed model takes dimensional parameters as conditional inputs, enabling the generation of shapes that adhere to specific size constraints.

The efficacy of our approach is validated through comprehensive experiments. Quantitative evaluations using the Chamfer-L1 Distance demonstrate a significant improvement in reconstruction accuracy compared to existing state-of-the-art methods, particularly in capturing the fine details of thin-plate structures. Moreover, in the shape generation task conditioned on dimensional parameters, our model exhibits high accuracy in producing shapes with the desired dimensions, even for values not explicitly present in the training data, indicating robust generalization capabilities.

Keywords: Thin-Plate Structures, Generative AI, DeepSDF, Curriculum Learning

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Sliding Behaviour of Carbon Nanothread within a Bundle Embedded in Polymer Matrix

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Carbon nanothread (NTH) has been widely used as reinforcement for polymer nanocomposites. Through molecular dynamics (MD) simulation, this work systematically assessed the pull-out behaviours of carbon nanothread bundle embedded in poly(methyl methacrylate) (PMMA) matrix compared to uniform dispersion patterns. Pull-out tests reveal that the loaded NTH exhibits a significantly enhanced interface load transfer after functionalization, corresponding to an order of magnitude higher than the pristine case in terms of the interfacial shear strength. It is also found that functionalized NTH exhibit weaker effects in enhancement under bundle distribution scenario due to the deteriorated entanglement compared to dispersed samples wrapped by PMMA chains. More importantly, inter-thread cross-linking is created in the sp^3 bundle structure, which provides much stronger interface load transfer efficiency. The reason is that the cross-linked NTH fillers in the bundle can be pulled out of the PMMA matrix together with the loaded NTH. Further work also reveals that NTH in the bundle structure exhibits stable interfacial interaction and mechanical interlocking with a rising temperature. These intriguing features suggest that diamond nanothread could be an excellent candidate for constructing next-generation carbon fibres and reinforcements for the polymer matrix.

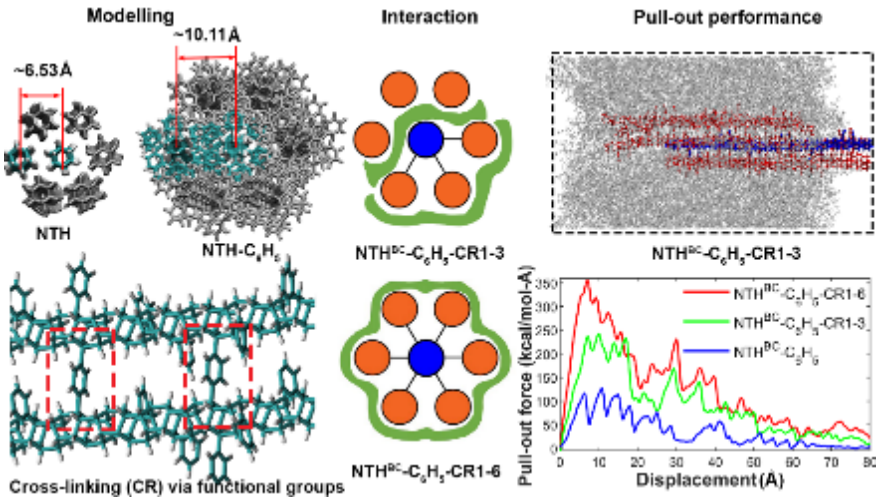

Figure 1. The Pull-out Behaviours of NTH from Bundle in Polymer Nanocomposite

Keywords: Carbon nanothread, Bundle, Polymer, Pull-out test, Molecular dynamic simulation

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Design and numerical assessment of shock absorbing flooring for the elderly using mechanical metamaterials

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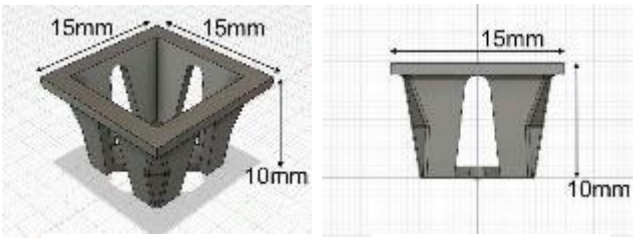
In recent years, falls and related fractures among the elderly have emerged as a significant social issue, making fracture prevention an important area of concern. However, conventional impact-absorbing structures often reduce stiffness to enhance shock absorption, which paradoxically increases the risk of falling. As a result, impact-absorbing structures utilizing mechanical metamaterials have attracted growing attention.

Mechanical metamaterials are artificial materials with engineered unit structures arranged periodically to overcome the limitations of conventional mechanical properties. Leveraging these unique properties, flooring materials have been developed that maintain high stiffness during walking while becoming flexible and absorbing impact only in the event of a fall.

Takeuchi et al. [1] proposed a numerical analysis method for impact-absorbing structures using viscoelastic materials and validated their approach through numerical simulations. However, the complex performance requirements of mechanical metamaterials and their mechanical behavior have not yet been sufficiently investigated.

This study aims to evaluate the mechanical performance of flooring materials designed with mechanical metamaterial characteristics that provide both walking stability and shock absorption during falls, using Eulerian structural analysis. In addition, several new structural designs are proposed and examined through comprehensive comparative analysis.



a) Overall view b) Front view

Figure1. Image of mechanical metamateria

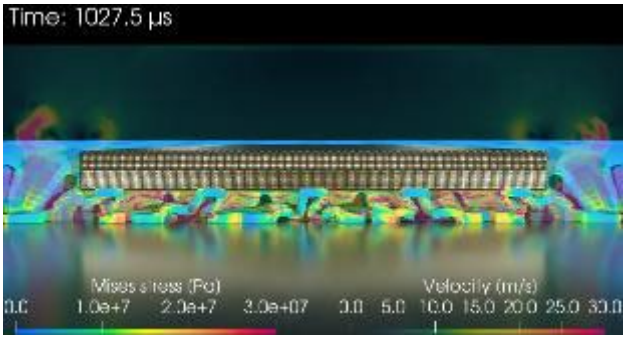


Figure2. Deformation and velocity distribution

Keywords: mechanical metamaterials, walking stability, shock absorption, fall prevention

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High-order explicit time integration with controllable numerical damping

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This work presents novel explicit high-order time-integration schemes using a polynomial approximation of the matrix exponential in the solutions of the equations of motion. The proposed schemes allow for controllable numerical dissipation, allowing the user to suppress high-frequency oscillatory modes whilst preserving accuracy in low-frequency responses.

In previous works (see [1-4]) high-order *implicit* schemes with controllable numerical dissipation were developed based on rational approximations of the matrix exponential; and shown to have excellent performance in a range of linear and nonlinear problems in wave propagation and structural dynamics. The rational approximations of the matrix exponential used in previous works is modified here to produce explicit methods.

The divisor matrix polynomial is approximated using a Neumann series expansion, which naturally has a limited radius of convergence:

$$\boldsymbol{T} = \frac{\boldsymbol{P}(\boldsymbol{A})}{\boldsymbol{Q}(\boldsymbol{A})} \approx \boldsymbol{P}(\boldsymbol{A}) \cdot \sum_{k=0}^{M} \big(\boldsymbol{I} - \boldsymbol{Q}(\boldsymbol{A})\big)^k, \quad \|\boldsymbol{I} - \boldsymbol{Q}\| < 1, \tag{1}$$

where **A** is the system coefficient matrix, **P, Q** are the matrix polynomials from the rational approximation, and **T** is the resulting amplification matrix used in this work. This approach eliminates the need to solve a system of equations at a given sub-step, though at the expense of unconditional stability – the same as other common explicit methods.

This research demonstrates the spectral properties of the proposed explicit time-integration methods for second-, third-, and fourth-order accurate models with and without numerical dissipation and assesses the performance of the model against a range of wave propagation and problems in structural dynamics. Preliminary findings show the approach to be competitive with conventional and alternative modern approaches regarding both efficiency and accuracy. The proposed approach for controllable numerical dissipation is shown to effectively suppresses spurious high-frequency oscillations in the well-studied one-dimensional wave propagation problem.

Keywords: High-order **t**ime-integration, structural dynamics, wave propagation, controllable numerical damping

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Efficient Homogenization Based on Sub-Cell Meshes for Microstructure Topology Optimization

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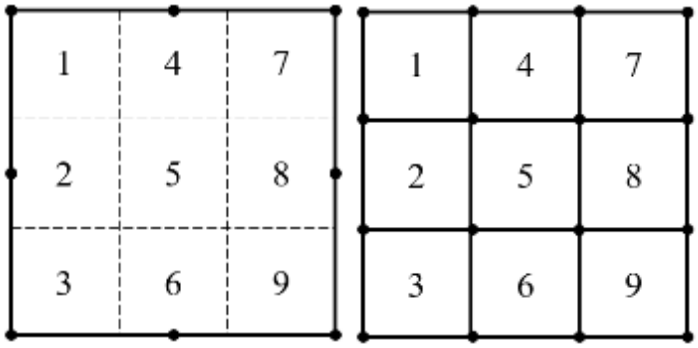
Homogenization plays a crucial role in microstructure topology optimization by enabling the computation of effective material properties that bridge microscopic design and macroscopic behaviour. However, for three-dimensional (3D) problems, conventional homogenization approaches often involve a large number of degrees of freedom (DOFs), resulting in high computational cost and limited scalability.

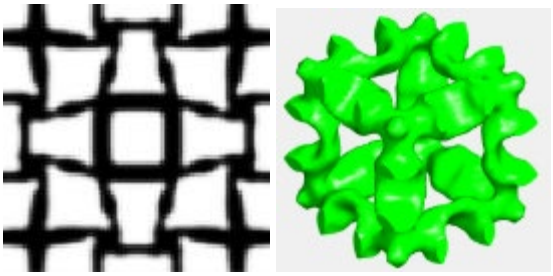
In this study, we propose a novel homogenization and sensitivity analysis framework based on sub-cell meshes for efficient microstructure topology optimization. The method utilizes high-order finite elements, within which a set of sub-cells is embedded, as shown in Fig. 1(a). These sub-cells serve as the design variables, enabling fine resolution in the material distribution. The number of DOFs is 16, which is much lower than the mesh shown in Fig. 1(b). By decoupling the design resolution from the number of DOFs required for finite element analysis, the proposed method significantly reduces computational complexity while maintaining high design fidelity.



(a) (b)

Fig. 1 (a) High order element with sub-cells (b) Low order elements

We demonstrate the effectiveness of the proposed approach through a series of two-dimensional (2D) and 3D numerical examples, targeting microstructures with maximum shear modulus, maximum tensile modulus, and negative Poisson's ratio. Fig. 2 shows the 2D and 3D result for designing microstructure with negative Poisson's ratio by the proposed method. Compared with conventional finite element-based methods, the proposed framework achieves comparable results with significantly improved computational efficiency.



(a) (b)
Fig. 2 (a) 2D result (b) 3D result

Keywords: Topology optimization, efficiency, material design, homogenization, sub-cell

Meta-materials for acoustic analogue computing

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The growing demand for real-time, energy-efficient computing has renewed interest in physical, wave-based analogue computing platforms. Unlike traditional digital processors, which are constrained by finite clock speeds, high energy consumption, heat generation, and diminishing returns from transistor miniaturization, wave-based analogue computing offers a scalable, low-power alternative driven by continuous physical dynamics. These systems are particularly suited for solving classes of partial differential equations and signal processing tasks, without the overhead of digitization.

In this work, we develop acoustic computing architectures based on meta-materials—periodic assemblies of unit cells whose geometry is carefully designed to perform specific computational tasks. The design process employs the isogeometric boundary element method (IGABEM) for the Helmholtz boundary value problem, paired with a shape optimisation algorithm. Our approach enables precise geometric control over the boundary of the computational domain, eliminates domain discretisation error, and significantly reduces pollution error, resulting in high-accuracy solutions.

We demonstrate performance of the approach in several benchmark examples for such operations as matrix-vector multiplication and solving differential equations. These results contribute to the foundation for future hardware platforms that harness wave physics to perform real-time and low-energy computations.

Keywords: wave-based analogue computing, acoustic, shape optimisation, isogeometric boundary element method

Finite Element Modelling for Additively Manufactured Metal Microlattice Structures Under Low-Velocity Impact

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Microlattice structures consist of struts with diameters ranging from 100 to 2000 μm, connected at nodes to form unit cells typically measuring 1–5 mm [1]. Additive manufacturing enables the fabrication of complex metallic microlattices [2] that are used in various engineering applications. Understanding the influence of design parameters on the dynamic performance of metallic microlattices under low-velocity impact is crucial for enhancing their mechanical properties for crashworthiness applications. This study investigates the impact behaviour of Ti-6Al-4V body-centred cubic (BCC) and BCC with vertical strut (BCCZ) that were designed following two approaches: varying the unit cell size and aspect ratio (the ratio of unit cell length or width to its height). Microlattice samples were 3D printed using electron beam powder bed fusion. The analytical approach [3] was used to make estimates of their mechanical properties. Drop tower testing and finite element (FE) simulations with ANSYS/LS-DYNA were conducted to analyse and predict the dynamic performance of microlattices with different unit cell sizes and aspect ratios. Three-dimensional FE models were validated by comparing their results with experimental and analytical ones. Then, numerical simulations were used to predict the dynamic performance of different microlattices. The finite element results showed good agreement with both experimental and analytical findings. Furthermore, the numerical simulations enabled the evaluation of microlattice crushing behavior under increased initial velocities. Varying the aspect ratio outperformed adjusting the unit cell size in improving the strength and Young's modulus. However, when comparing microlattices with comparable relative densities between the two designs, adjusting the unit cell size resulted in greater energy absorption prior to failure than modifying the aspect ratio. Vertical struts within structures played a significant role in enhancing impact resistance, however, body centre cubic structures showed better ductility than structures with vertical struts.
Keywords: Microlattice structures, low velocity impact, finite element simulations, design parameters.

Acknowledgements. The authors acknowledge the UNSW Resource Allocation Scheme at National Computational Infrastructure [project mz70].

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Numerical analysis of axial compression performance of CFRP reinforced square aluminum-wood composite columns

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Engineered timber has gained attention as a sustainable construction material due to its renewability, carbon storage capacity, and good mechanical properties. However, its low fire resistance, biological degradation, and durability concerns limit its broader application, especially in harsh environments. To address these issues, encasing timber cores with thin-walled aluminum alloy tubes is one promising approach, leveraging aluminum's high strength-to-weight ratio, corrosion resistance, and recyclability to improve durability and structural capacity. Although aluminum–wood composites can enhance axial strength and stiffness, the local buckling susceptibility of thin aluminum tubes often weakens their confinement effect, limiting the full interaction between aluminum and timber.

In response to this critical limitation, this study introduces an innovative aluminum–wood composite column, which incorporates a timber core enclosed by an aluminum alloy square tube and is externally reinforced with carbon fiber reinforced polymer (CFRP) sheets. CFRP materials, known for their high tensile strength, excellent fatigue resistance, and lightweight properties, are expected to enhance the local buckling resistance of the aluminum tube and improve the overall confinement of the timber core. A finite element model was developed(as shown in Figure 1), and a comprehensive parametric study was conducted to investigate the effects of key design variables, including timber core ratio, aluminum tube thickness, and CFRP layer number, on axial load-bearing capacity and failure modes. The numerical results demonstrate that CFRP strengthening significantly improves buckling resistance and confinement effect(as shown in Figure 2), while optimizing the core ratio and tube thickness further enhances structural capacity. These findings provide valuable design guidelines and highlight the potential application of the proposed composite columns in sustainable and high-performance structural systems.

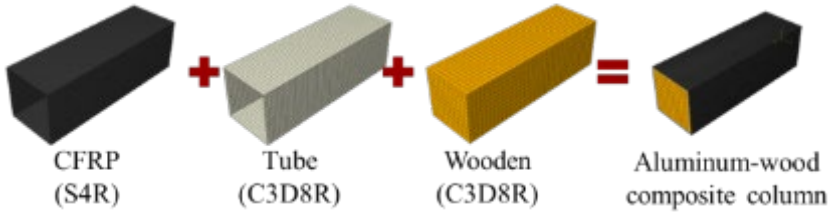

Figure 1. Finite element model of aluminum-wood composite column

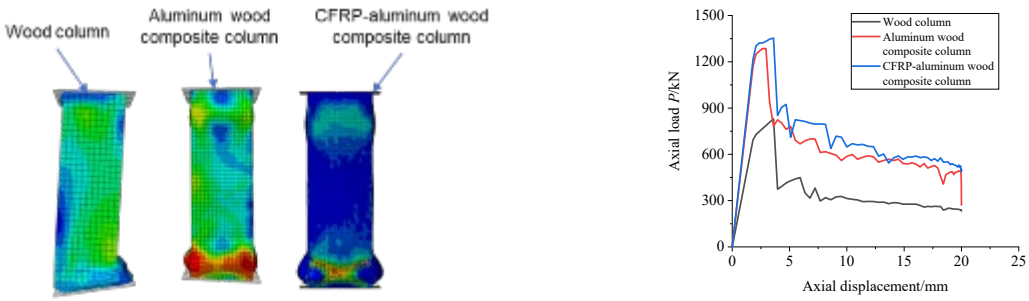

Figure 2. Axial compression failure mode and load-displacement curve of the composite columns

Keywords: Aluminum-wood composite column; CFRP; Axial compression performance; Numerical analysis;

Hydrogen absorption in Fe-Cr-Ni austenitic systems: Effect of major elements (Cr, Ni)

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Although solute hydrogen has been considered a detrimental metal element for a long decade, recently, a novel improvement in the strength-ductility balance of Fe-Cr-Ni-based austenitic was demonstrated [1]. The improvement depends on the chemical composition of these alloys through the solute hydrogen content. The authors revealed that the Cr and Ni atoms reduced the hydrogen absorption energy (H-absorption energy) required to solidify the hydrogen into alloys and increased the hydrogen content of these alloys [2]. Unlike the independent effects of Cr and Ni atoms, the interaction between these atoms hasn't yet been investigated. In the present study, the systematic calculation of the H-absorption energy was performed to examine the interactive effect in Fe-Cr-Ni systems using first-principles calculations.

In the Fe-Cr and Fe-Ni systems, the H-absorption energy decreased with the number of Cr and Ni atoms increasing, respectively. These effects were mutually inhibited in the Fe-Cr-Ni ternary system. From the result, the H-absorption energy, E_{ab} at Octahedral sites (O-site) in the Fe-Cr-Ni system was defined as follows;

$$E_{\mathrm{ab}} = 0.186 - (0.0646 - 0.0103 n_{\mathrm{Ni}}) n_{\mathrm{Cr}} - (0.0178 - 0.0049 n_{\mathrm{Cr}}) n_{\mathrm{Ni}}$$

n_{Cr} and n_{Ni} denotes the number of Cr and Ni atoms consisting of the O-site, respectively. Hydrogen occupancies (H-occupancy) of several practical Fe-Cr-Ni-based austenitic alloys were calculated using the equation, and these are well-consistent with the experimental results. The result indicates that the predominant factor in the hydrogen content of these alloys is the change in the H-absorption energy by Cr and Ni atoms. Additionally, the origins of the Cr and Ni effects were considered, and it was indicated that each effect stemmed from the austenitic phase stability and local magnetic state.

Keywords: Hydrogen absorption energy, Hydrogen solubility, Austenitic alloys, First-principles calculation

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A Modal-Based Topology Optimization Approach for Acoustic Metamaterials

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Acoustic metamaterials are periodical artificial materials which unnaturally control the propagation of sound waves through meticulously designed microstructures. In recent decades, systematic design of targeted acoustic metamaterials using various topology optimization methods has made substantial progress. However, these methods have focused on direct band gaps while overlooking the vibrational characteristics—mode shapes—of acoustic metamaterials, which can sometimes lead to ambiguities in optimization conditions or directions. This study proposes a modal-based topology optimization method. Our approach tracks the modes of acoustic metamaterials during wave vector scanning and classifies them in the band diagram. This classification enables topology optimization to be precisely designed for different modes, specifically vibration patterns. Consequently, this leads to new discoveries and novel vibrational acoustic unit cell geometries. Numerical results demonstrate that the proposed optimization algorithm is effective, enabling design optimization from the modes of acoustic metamaterial vibrations and yielding new acoustic metamaterial topological structures.

The governing equation for vibration and wave propagation:

$$\rho(\boldsymbol{r})\ddot{\boldsymbol{u}} = \nabla[\lambda(\boldsymbol{r}) + 2\mu(\boldsymbol{r})](\nabla \cdot \boldsymbol{u}) - \nabla \times [\mu(\boldsymbol{r})\nabla \times \boldsymbol{u}], \tag{1}$$

where $\boldsymbol{u} = \{\boldsymbol{u_x}, \boldsymbol{u_y}, \boldsymbol{u_z}\}^{\mathrm{T}}$ represents the displacement vector. $\rho(\boldsymbol{r})$ is the material density at position $\boldsymbol{r}$, and $\lambda(\boldsymbol{r})$ and $\mu(\boldsymbol{r})$ are the Lamé constants at position $\boldsymbol{r}$.

Modal assurance criterion for mode tracking:

$$M(i,j) = \frac{|\int u_i \cdot u_j^* \, dV|}{(\int u_i \cdot u_i^* \, dV)(\int u_j \cdot u_j^* \, dV)}, \tag{2}$$

where u_i represents the eigenvectors of the i^{th} band. The matrix $M(i,j)$ is utilized to compare and track the similarity between the eigenvectors of the i^{th} band and the j^{th} band.

Keywords: Acoustic metamaterials, Topology optimization, Mode shapes, Band diagram, Sound wave propagation

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Effect of the Density Gradient on the Mechanical Behaviour of an Architectured Material Under Dynamic Loading

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Architectured cellular structures are usually manufactured by additive manufacturing [1] due to their small sample size. This work aims to develop a new type of architectured structure using a conventional foundry process. Very few cellular materials, such as foams [2] and periodic cellular materials [3], have been successfully fabricated by casting. Thus, there remains a significant gap in understanding the mechanical behaviour of such cast structures, especially under dynamic loading conditions [4]. Maximizing the energy absorption capacity of these structures is the primary goal of this study which is guided by the formula

$$EA = \int_0^{\delta} F dx \quad (1)$$

where EA is the total energy absorbed up to densification displacement δ, and Fdx is the force-displacement relationship.

Quasi-static compression and dynamic tests are performed on cylindrical samples made of AlSi7Mg0.6 and pure aluminium made up of kelvin unit cells. The specimens measure 100 mm in diameter and 90 mm in height. Finite Element simulations were conducted using explicit and implicit solvers, calibrated with experimental data to model the nonlinear response, including material plasticity, large deformations, and geometric instabilities. The computational results exhibited good agreement with experimental force-displacement curves, stress-strain behaviour, and energy absorption capacities. Specific Energy Absorption and Energy Absorbed at Densification were computed for performance comparison across materials and geometries.

Initial results indicate that cast aluminium Kelvin structures deform via a progressive collapse mechanism: beginning with elastic buckling, followed by local plastic deformation, and culminating in densification. The simulations accurately capture strain-rate-sensitive behaviour and align closely with experimental observations. This integrated computational–experimental approach offers new insights into the behaviour of cast cellular metals and provides a pathway for designing next-generation energy absorbers with density gradients for impact-critical applications.

Keywords: Architectured cellular structures, aluminium, energy absorption, sand casting, strain-rate sensitivity, density-graded cellular materials, finite element modelling.

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Distortion Control of 3D-Printed Ceramic Scaffolds with TPMS Architectures

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Bone is the second most transplanted tissue globally, with over 2 million grafting procedures performed annually [1]. This increasing clinical demand has driven the development of porous biomaterials that replicate the complex architecture and mechanical behaviour of natural bone. Among these, 3D-printed ceramic scaffolds have shown great promise due to their excellent thermal stability, mechanical strength, and chemical resistance. In particular, triply periodic minimal surface (TPMS) structures such as Schwarz P, Schwarz D, and Gyroid offer variable porosity and load-adaptive mechanical behaviour.

This study integrates computational modelling, additive manufacturing, and experimental validation to design and optimise ceramic bone scaffolds. Several scaffold structures were first modelled in nTopology and analysed in Abaqus via finite element analysis (FEA) under compression to evaluate stress distribution and structural stiffness. The selected designs were then fabricated using Stereolithography (SLA) with alumina ceramic slurry, producing scaffolds of 12×12×12 mm^3 with unit cells of 1.5 mm^3. Four porosity levels were set per structure by adjusting strut width, and three samples per design were printed, totalling 48 specimens.

One key challenge addressed in this study is the printing distortion observed in SLA-manufactured scaffolds, which can significantly deviate from the CAD geometry and compromise performance. To quantify this, initial specimens were scanned via micro-CT (μCT) to assess deviations in pore geometry and strut dimensions. Mechanical testing was performed to evaluate elastic modulus, yield strength, and permeability, and compared with FEA predictions. Based on the distortion patterns, optimised models were proposed to compensate for deformation and reprinted under the same conditions.

Preliminary results show that Gyroid and Schwarz-based structures provided more uniform stress distribution and higher stiffness-to-weight ratios. The distortion-controlled designs exhibited noticeable improvements in geometric accuracy and mechanical performance, confirming the value of design compensation strategies in ceramic AM. These findings demonstrate the potential of combining computational tools, high-resolution printing, and in-process error correction to fabricate reliable, high-performance scaffolds for biomedical applications.

Keywords: Bone scaffold, Tissue Engineering, Additive manufacturing, Stereolithography (SLA), TPMS, Distortion control

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Machine learning enhanced multiscale topology optimization with structural genome database

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Multiscale topology optimization (MTO) offers a larger design space and enables the concurrent design of macroscopic "structure" and microscale "material". Even adopting the asymptotic homogenization analysis, the solution process could still be time-consuming, especially for multiscale topology optimization with multiple microstructures. To alleviate such issue, a released structural genome database (SGD) in reference[1] is incorporated into the multiscale topology optimization process to replace the asymptotic homogenization analysis. The effectiveness, accuracy and efficiency of the SGD-MTO algorithm are validated by the various benchmark MTO examples, including optimization design cellular structures with uniform and multiple microstructures, and concurrent multiscale design of uniform and multiple microstructures with connectivity constraint. It is validated that, comparing with the traditional MTO algorithm with asymptotic homogenization analysis, the SGD-MTO algorithm can accelerate the solution efficiency by more than 30 times. Even for general MTO problems with optimized design desiring asymmetric microstructures, the proposed algorithm can still efficiently supply a reasonable initial design, which can re-optimized in a few iterations using the explicit topology optimization method.

Keywords: Multiscale topology optimization, Moving morphable component, Machine learning, structural genome databases, Connectivity

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Multiphase transport through a porous packed bed of solid electrolyte

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Modelling multiphase transport through high-surface area, porous structures is critical in various electrochemical devices to enhance reaction rates and facilitate commercial performance. Often balancing the rates of flow or restricting the location of different phases is performed by experienced operators to ensure efficient transport of various reactants to reaction sites. This presentation provides details on a simulation workflow to assess the liquid-gas interaction within complex porous materials, with a target application of hydrogen peroxide generation.

The presentation will introduce the numerical simulation code, TCLB, before describing several benchmark cases for the phase-field Lattice Boltzmann Model [1,2] implemented here. Following on from these idealised cases, a packed bed is generated using the LIGGGHTS discrete element software to provide a realistic flow domain for a solid electrolyte layer within an electrochemical cell. The analysis of varying flow rates and the influence this has on gas penetration into the bed will be discussed.

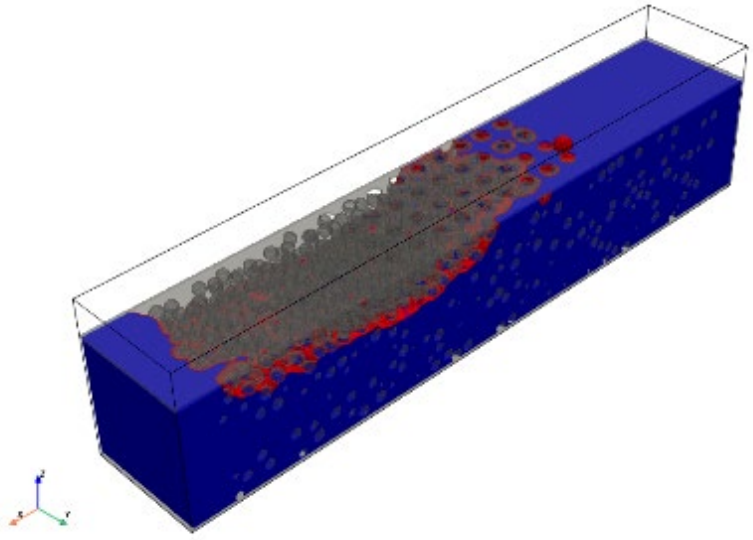

Figure 1. Gas penetration into saturated packed bed.

Keywords: Multiphase flow, Lattice Boltzmann Methods, Porous media flow

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A Study on the Development of a Crack Propagation Analysis Using s-version Isogeometric Analysis (s-IGA)

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In the present investigation, a three-dimensional crack propagation analysis system based on Isogeometric Analysis (IGA) [1] has been developed. IGA is known for its high accuracy as an analytical methodology. IGA utilizes B-spline or Nonuniform Rational B-Spline (NURBS) functions for its basis functions. However, building an IGA model for three-dimensional crack analysis is not an easy task because arranging the so-called B-spline or NURBS volume to represent a crack in a complex-shaped solid is very troublesome.

The present authors have been developing an IGA based crack propagation system that combines the s-version IGA (s-IGA) [2] and the singular patch method [3]. s-IGA is based on the superposition of IGA models to add features to the analysis model, such as cracks, holes, reinforcing fibers, etc. In the present development, s-IGA scheme is used to "insert" a crack into an existing IGA model for some structure. The s-IGA model for the crack adopts the singular patch method, which can reproduce the so-called square root-r singularity in the stresses. The stress intensity factors can be computed using the three-dimensional J-integral or interaction integral method for the singular patch method [4]. The stress intensity factors can be computed very accurately even though very coarse IGA patch discretization along the crack front, as also presented in [4]. The three-dimensional s-IGA crack analysis scheme is schematically presented in Fig. 1.

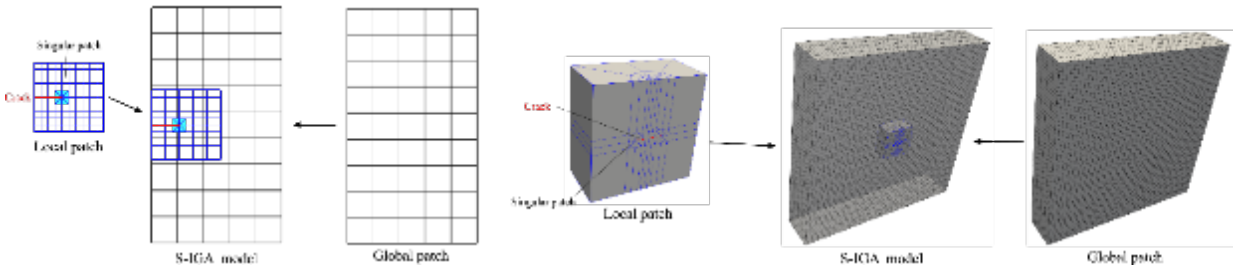

Figure 1.

Keywords: Isogeometric Analysis, S-version Isogeometric Analysis, Crack propagation

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Development of polymer micromachined insect-mimetic wings using fluid-structure interaction analysis

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Insect flapping flight is governed by complex aerodynamic forces that induce cambering and pitching, making it crucial to understand their locomotion dynamics. This study employs fluid-structure interaction (FSI) analysis to develop a polymer micromachined insect-mimetic wing based on the FSI design concept. The design solution is determined through design window search using static analysis and then fabricated via polymer micromachining, incorporating actual insect and polyimide material properties. Further, a pixel model is employed for the FSI analysis, which transforms an unstructured mesh into a structured one, reducing the computational cost [1].

The monolithic equation system for the FSI can be written as:

$$_{\mathrm{L}}\mathbf{Ma} + \mathbf{Cv} + \mathbf{N} + \mathbf{q}(\mathbf{u}) - \mathbf{Gp} = \mathbf{g}, \;\; _{\tau}\mathbf{Gv} = \mathbf{0}, \qquad (1a, b)$$

where $\mathbf{M}$, $\mathbf{C}$, $\mathbf{G}$, and $\mathbf{N}$ are the mass, diffusive, divergence operator matrices, and convective term vector, respectively, $\mathbf{q}$, $\mathbf{g}$, $\mathbf{a}$, $\mathbf{v}$, $\mathbf{u}$, and $\mathbf{p}$ are the internal force, external force, acceleration, velocity, displacement, and pressure vectors, respectively. Eq. (1) is solved using a parallelized projection method based on iterative algebraic splitting, stable for large elastic deformation [1].

The fluid and structural meshes are composed of P1P1 and MITC4 elements, respectively. Table 1 shows the parameters, while Fig. 1 (a) shows the insect-mimetic wing employed in this setup.

Parameters	Ref. [1]	Present
Flapping freq. [Hz]	148	148
Stroke angle [deg.]	71.4	71.4
Poisson's ratio [ν]	0.49	0.289
Membrane [Pa]	7.0×10^{9}	3.5×10^{9}
Center vein [Pa]	2.8×10^{12}	1.3×10^{9}
Leading edge [Pa]	3.5×10^{16}	2.5×10^{9}
Root vein [Pa]	5.1×10^{15}	2.3×10^{9}
Mass [kg]	0.49×10^{-6}	0.23×10^{-5}

Table 1.

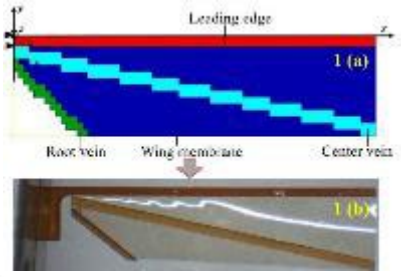

Figure 1 (a), (b).

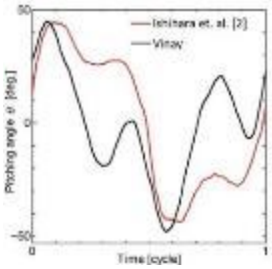

Figure 2.

Fig. 1 (b) shows the wing fabricated using polymer machining, and its flight performance is evaluated using FSI analysis. The result in Fig. 2 shows a rapid decrease in pitch angle after reaching the maximum,

with lift and camber synchronized to pitching. The average lift C_L required for insect hovering is 1.19, while the present model achieved 1.0, indicating insufficient lift. Comparison with actual insects shows the model to be 4 to 5 times stiffer. Despite the model's roughness, vibration theory aligns with the numerical results, indicating further adjustments to mass and stiffness are needed. Then, modifying the membrane stiffness and flapping frequency using FSI analysis improves the aerodynamic performance to exceed the required lift, leading to the successful development of the polymer micromachined insect-mimetic wing.

Keywords: fluid-structure interaction analysis, polymer micromachining, insect-mimetic wings

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Interfacial Dislocation Networks in Nickel-based Superalloys via Atomistic Simulations

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Ni-based single crystal superalloys are indispensable in aerospace industry, enduring extreme temperatures exceeding 1,100 °C. Their outstanding mechanical characteristics stem from a unique two-phase microstructure comprising L12 ordered Ni3Al precipitates (γ′ phase) embedded in a ductile disordered face-centered cubic Ni matrix (γ phase). The interface between these two phases hosts interfacial dislocation networks (IDNs), crucial for enhancing their mechanical performance. Despite extensive works on IDNs, existing studies, particularly atomistic simulations, have largely overlooked the dynamic changes of lattice parameters occurring during service, such as alloying elemental diffusion, temperature variation, and extreme centrifugal forces. Such variation of lattice parameters for a given γ′ phase size is anticipated to profoundly influence the IDNs, a crucial aspect that has been rarely discussed. In the current work, we unveil the size-dependent patterns of IDNs for the first time. We reveal that these patterns are governed by moiré patterns at the interface, dictated by the lattice misfit. Particularly, the compatibility between the moiré superlattice parameter and the γ′ phase size profoundly impacts the integrity of the dislocation networks. Additionally, we demonstrate how these initial IDNs contribute to pseudo-elastic behaviour and influence subsequent dislocation activities during plastic deformation.

Keywords: superalloys, interfacial dislocation networks, molecular dynamics simulation, lattice misfit

Computational Design and Optimisation of 3D-Printed Ceramic Lattices

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The integration of computational design with additive manufacturing (AM) has driven significant progress in the development of high-performance materials and complex structures. Among these, three-dimensional printed advanced ceramics have emerged as highly promising materials due to their excellent thermal stability, mechanical strength, and chemical resistance. Various AM techniques have been explored for fabricating ceramic components, such as direct ink writing, selective laser sintering, and stereolithography [1].

The VAT photopolymerisation process, in particular, enables the fabrication of geometrically complex parts that are otherwise difficult or impossible to produce via conventional manufacturing methods. Materials such as alumina, zirconia, hydroxyapatite, aluminium nitride, silicon nitride, and tricalcium phosphate can be printed with high precision and surface quality using this technique [2].

In this study, several ceramic-inspired scaffold structures were designed using nTopology, leveraging its implicit modelling capabilities to create complex, bioinspired architectures. These geometries were then exported and analysed in ANSYS to simulate mechanical behaviour under realistic loading conditions using finite element analysis (FEA). The simulations focused on evaluating stress distribution, stiffness, and structural integrity under compression.

Computational tools such as finite element analysis (FEA) and topology optimization support the enhancement of mechanical, structural, and thermal performance, enabling the design of custom ceramic components tailored for specific loading conditions. These techniques are particularly valuable in applications across biomedical, energy, aerospace, automotive, semiconductor, and electronics industries, where functionality and sustainability are critical. Preliminary results from this study demonstrated that Gyroid and Schwarz-based structures provided favourable stress distribution and superior stiffness-to-weight ratios, highlighting their potential for lightweight, load-bearing applications.

Keywords: Additive Manufacturing, Advanced Ceramics, Bio-manufacturing, Computational modelling, Optimisation, Mechanical Strength.

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Numerical Investigation of Solid Particle Erosion in U-Bend Geometries: Influence of Rotation and Surface Roughness

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The occurrence of erosion in pipelines constitutes a common failure source with potential environmental and economic impacts. A deeper understanding and improved prediction of this phenomenon enable the development of effective mitigation strategies, such as optimized geometric design and preventive maintenance. However, studies focusing on U-bend geometries remain limited and often overlook the effect of particles rotation and wall roughness. This study evaluates erosion behaviour in a U-bend pipe by incorporating rotation and roughness effects into an Eulerian-Lagrange model. Experimental results from elbow configuration investigated by Solnordal et al. [1] and then extended to simulate a U-bend configuration. Preliminary results indicate a significant influence of particle rotation and surface roughness on impact location and erosion depth. Additionally, the effects of varying injection conditions and bend curvature radius are analysed to understand their impact on erosion patterns and severity. In order to model the influence of rotation, the Magnus lift force was implemented based on Oesterle-Bui-Dinh formulation, demonstrating a notable impact on erosion distribution. The force is defined as:

$$\boldsymbol{F}_{ML} = \frac{1}{2} A_p \, C_{LR} \, \rho_f \frac{|\boldsymbol{v}|}{|\boldsymbol{\Omega}|} \, (\boldsymbol{v} \times \boldsymbol{\Omega})$$

where A_p is the projected particle surface area, C_{LR} the rotational lift coefficient, ρ_f the fluid density, $\boldsymbol{v}$ the relative fluid-particle velocity, and $\boldsymbol{\Omega}$ the relative fluid-particle angular velocity. Figure 1 shows strong agreement between the predicted and experimental erosion depth, both in magnitude and angular position of peak.

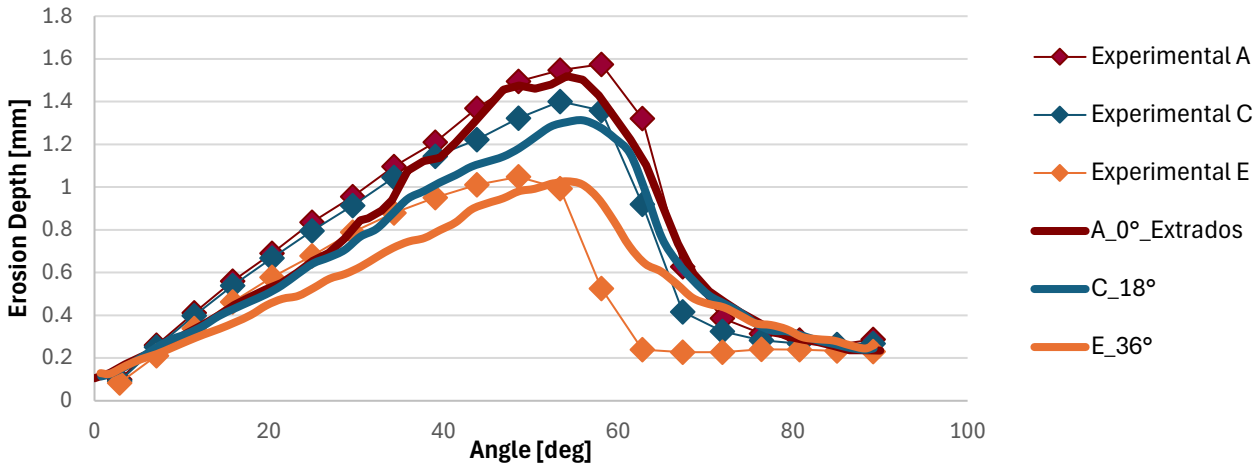

Figure 1.

Keywords: Erosion modelling, U-bend pipe flow, particle rotation, roughness effect.

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Numerical modelling of microbially-induced calcium carbonate precipitation for crack-healing in concrete

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Microbially induced calcium carbonate precipitation employs naturally occurring microorganisms and their metabolic activities to precipitate calcium carbonate, eliminating the need for high-energy inputs or toxic chemicals. This approach significantly reduces carbon emissions and environmental pollution, offering a sustainable and eco-friendly solution for healing cracks in cementitious materials such as concrete. However, a key research gap lies in the fundamental understanding of the healing mechanisms. This gap persists largely because most existing studies rely on trial-and-error experimental methods, while the limited numerical models available fail to capture the full multiscale coupling of mechanical deformation, transport processes, and chemical precipitation inherent to the self-healing process. Furthermore, most models are limited to one-dimensional simulation and lack a detailed biochemical coupling framework essential to solute diffusion and carbonate precipitation.

Based on Fick's second law, a modified time- and location-dependent diffusion law with bacteria-induced calcium carbonate precipitation is first proposed in this research. The governing equation takes the following form:

$$\frac{\partial C(\mathbf{x},t)}{\partial t} - D\frac{\partial^2 C(\mathbf{x},t)}{\partial \mathbf{x}^2} + \xi(T,\alpha,pH)C(\mathbf{x},t) = 0$$

where C is the concentration of urea, $\mathbf{x}$ is the spatial vector, t is the reaction time, and D is the diffusion coefficient. The term ξ denotes the precipitation rate of carbonate, formulated as a function of temperature, T, bacterial cell concentration, α, and pH value.

After that, the finite difference method with an implicit time integration scheme was applied to implement the above governing function in a two-dimensional domain. Unlike the explicit method, the implicit approach is unconditionally stable, allowing for larger time steps without sacrificing numerical stability. Neumann boundary conditions were imposed at both ends of the domain to simulate a closed system within the crack, and an initial concentration domain was prescribed. As presented in Figure 1, the preliminary simulation results captured the expected diffusion behaviour of urea. The results indicate that urea was nearly depleted, and the region with the highest healing ratio exceeded 80%, suggesting that the crack was effectively sealed.

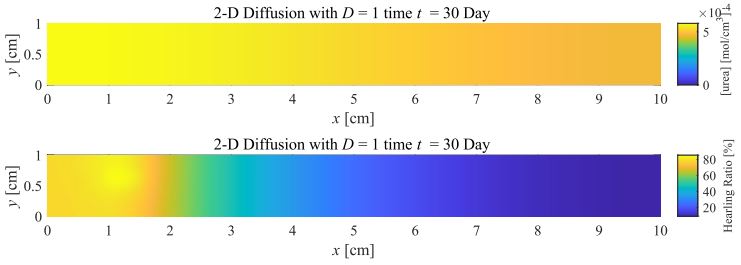

Figure 1.

These early-stage findings provide a computational foundation for future studies on bacteria-based self-healing materials, contributing to the development of more sustainable and intelligent infrastructure solutions.

Keywords: Self-healing concrete, Microbially-induced calcium carbonate precipitation, Finite difference method, Diffusion law

Multiscale Topology Optimization for Reducing Dynamic instability

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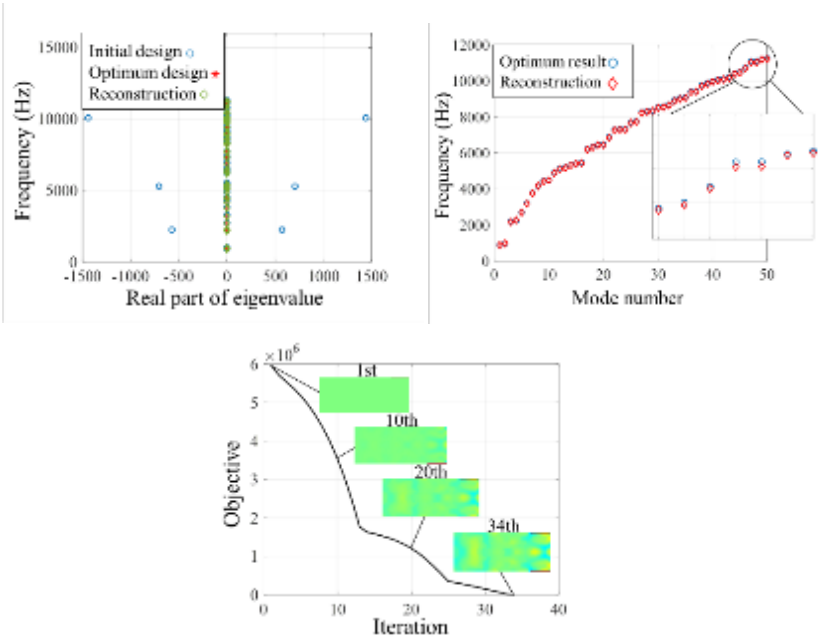
This study aims to reduce dynamic instability in multiscale structures, which is caused by the real part of complex eigenvalues and can cause structural divergence. Conventional structural optimization produces non-physical grey elements for reducing this dynamic instability. Moreover, there is no attempt to solve dynamic instability in multiscale systems. To address these limitations, we propose a cellular structure optimization method commonly used in additive manufacturing [1], which effectively reduces dynamic instability while ensuring physically meaningful designs.

$$\begin{aligned} &\underset{\gamma_e}{\text{Min}} \sum_{i=1}^{n} \text{real}\left(\lambda_i\right)^2 \\ &\text{Subject to} \quad \sum_{e=1}^{N} V_0 \gamma_e \le V_{\text{limit}} \quad , \\ &\qquad\qquad 0 \le \gamma_{\min} \le \gamma_e \le \gamma_{\max} \le 1 \end{aligned} \tag{1}$$

The process of optimizing cellular structures includes homogenization, design optimization, and structural reconstruction. The equation above is the optimization formulation.



(a) **(b)** **(c)**

Figure 1: (a) complex eigenvalues, (b) eigenvalues between optimum and reconstruction and (c) Optimization history.

The proposed approach significantly reduces dynamic instability and offers a practical solution for advanced structural design (Figure 1). Furthermore, the eigenvalues of optimum and reconstruction design closely match, indicating that the homogenized FE model accurately approximates the reconstructed system.

Keywords: Multiscale, cellular structure optimization, topology optimization, dynamic instability

Acknowledge

This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MSIT) (RS-2024-00351611).

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A mesh refinement method for isogeometric analysis based on the T-image and Bézier extraction

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T-splines are widely used in isogeometric analysis with local mesh refinement [1]. However, in conventional mesh refinement methods, each time the mesh is refined and new control points are introduced, we must adhere to complex rules to maintain analysis-suitable meshes. This constraint increases computational cost, especially when extensive mesh refinement is required or high degree T-splines are used. In this study, we propose a new mesh refinement method that separates the analysis-suitability verification process from the computation of the new control points. Furthermore, this method facilitates adaption to isogeometric analysis and parallel computation.

We construct a T-spline mesh (T-mesh) based on a T-image that expresses the parametric domain of the T-mesh. Using the T-image, we can efficiently assess whether a given T-mesh is analysis-suitability or not for any degree. Initially, we set up the T-image of analysis suitable T-mesh, for example, B-spline. we refine the initial T-image arbitrarily and modify the mesh to satisfy the analysis suitability (Fig. 1 (left)). We determine the Bézier extraction operator of each element for initial T-image and modified T-image independently (Fig. 1 (center)). Bézier extraction operator is generally used to determine the basis function for each element from Bernstein basis functions. We can obtain the positions of the new control points in each element using the following equation:

$$\tilde{\boldsymbol{x}}_{\boldsymbol{i}} = \sum_{j=0}^{n-1} \left[\left(\tilde{\boldsymbol{C}}\right)^{-T} (\boldsymbol{C})^{T} \right]_{ij} \boldsymbol{x}_{\boldsymbol{j}} , \tag{1}$$

where $\boldsymbol{x}$ are the positions of control points, $\boldsymbol{C}$ is the Bézier extraction operator, n is the number of control points involved in an element, and $\widetilde{(\cdot)}$ represents after refinement (Fig. 1 (right)). Finally, using obtained the positions of control points, Bézier extraction operator, and the tensor product of p-th and q-th degree Bernstein basis functions $\boldsymbol{B}^p \otimes \boldsymbol{B}^q$, the refined T-spline surface $\tilde{T}(t,s)$ can be obtained as

$$\tilde{T}(t,s) = \sum_{i=0}^{n-1} \left[\tilde{\boldsymbol{C}} \boldsymbol{B}^p \otimes \boldsymbol{B}^q(t,s) \right]_i \tilde{\boldsymbol{x}}_{\boldsymbol{i}} . \tag{2}$$

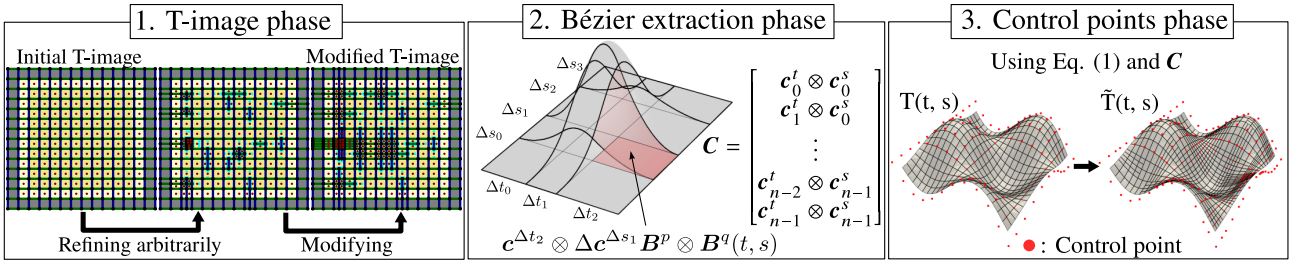

Figure 1.

Keywords: Isogeometric analysis, adaptivity, T-spline, Bézier extraction, parallel computation,

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Physics-Informed Neural Networks for Forward and Inverse VBI Problems with Applications to Structural Damage Detection

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Physics-Informed Neural Networks (PINNs) are an emerging class of machine learning models that embed physical laws—typically expressed as partial differential equations (PDEs)—directly into the training process. By incorporating these governing equations into the loss function, PINNs enable robust and physically consistent learning from sparse and noisy data [1]. In addition to solving forward problems, PINNs are particularly well-suited for inverse problems, where unknown system parameters or inputs are inferred from indirect measurements. This framework has shown strong potential across various engineering domains, including structural dynamics, where real-world systems often exhibit coupling effects that challenge traditional modelling approaches. This work presents a PINN-based methodology for inferring structural damage in coupled vehicle–bridge interaction (VBI) systems by identifying the unknown constant flexural stiffness EI of the bridge. Unlike simplified moving load models, the VBI formulation captures the mutual interaction between a moving vehicle (modeled as a sprung mass system) and the dynamic response of the bridge. The coupled system of partial and ordinary differential equations is embedded into the neural network architecture to solve the inverse problem of parameter identification. To facilitate the treatment of dynamic signals and improve numerical conditioning, the governing equations and input acceleration data are transformed into the frequency domain using the continuous Fourier transform [2]. This frequency-domain formulation enables the PINN to operate directly on spectral representations of the system dynamics, offering enhanced robustness in the presence of limited or noisy measurements. Numerical results demonstrate that the proposed framework accurately estimates the global stiffness parameter, enabling effective damage quantification in coupled VBI systems.

Keywords: Physics-Informed Neural Networks, vehicle–bridge interaction, inverse problems, structural damage identification, Fourier transform

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Radial Pulse Waveform Harmonics as Non-Invasive Biomarkers of Musculoskeletal Pain Severity

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Accurately assessing pain remains a clinical challenge, as self-reported measures may not fully capture underlying physiological states—particularly in patients with chronic comorbidities. This study investigated the utility of radial pulse waveform harmonics as non-invasive biomarkers for pain intensity, with a specific focus on sex differences.

A total of 341 adults aged 45–85 with musculoskeletal pain were recruited from a rehabilitation clinic. Pain intensity was measured using the Numeric Rating Scale (NRS) and categorized as mild (<5) or moderate to severe (≥5). Simultaneously, radial pulse waveforms were recorded using a wearable monitoring device, and harmonic features were extracted using Fast Fourier Transform. To evaluate relationships between waveform harmonics and pain severity, sex-stratified logistic regression models were applied, incorporating clinical covariates.

Higher pain intensity was associated with increased BMI and lower Barthel Index scores, particularly among females (p = 0.03). Notably, pain severity correlated with elevated eleventh harmonic phase (P11) and reduced second harmonic amplitude (H02), with stronger effects observed in female participants (p = 0.04 and 0.02, respectively). The presence of chronic liver disease further amplified these associations. Models incorporating harmonic and clinical variables achieved strong discriminative performance (area under the receiver operating characteristic curve > 0.84, Figure 1).

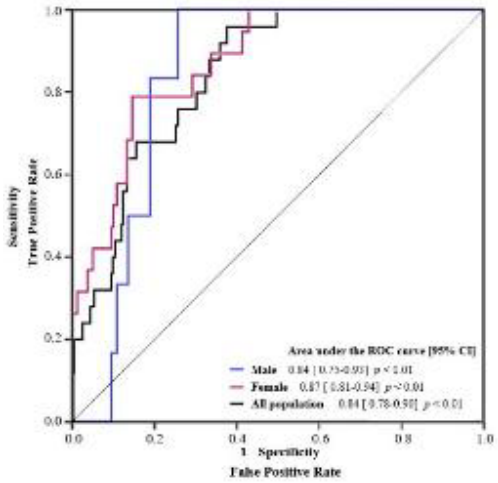

Figure 1.

Pulse waveform harmonics, particularly H02 and P11, show promise as non-invasive physiological biomarkers for assessing pain intensity and capturing sex-specific autonomic responses. These findings highlight the potential of wearable monitoring technologies for developing personalized pain assessment tools, especially in patients with musculoskeletal pain and systemic comorbidities.

Keywords: Pulse waveform harmonics, Pain intensity, Non-invasive biomarker, Sex differences, Wearable monitoring, Musculoskeletal pain

A material point method approach to modelling cave propagation

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Understanding the mechanisms of cave propagation is critical for block and sub-level caving design to avoid unplanned downtime and manage safety hazards such as rock bursts and air blasts. Numerical modelling is useful for simulating and predicting the caving process in rock masses with complex geological environments and mining conditions. The traditional continuum modelling methods for cave mining, such as the finite element method and the finite difference method, can suffer severe mesh distortions under large deformation of rock masses, which often occur in underground cave mining [1]. Hence, a material point method (MPM) modelling framework for cave propagation is developed in this work.

The MPM approach represents rock masses as Lagrangian material points by carrying physical quantities such as stress, strain, and damage variables. At each time step, MPM uses the background grid to solve the governing equation of momentum in the Eulerian configuration by calculating the nodal quantities at the grid from the material point quantities. The equation of momentum balance is given as [2]:

$$\rho \mathbf{a} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b}, \tag{5}$$

where ρ is the mass density of the material, $\mathbf{a}$ is the acceleration, $\boldsymbol{\sigma}$ is the stress tensor, and $\mathbf{b}$ is the specific body force. The physical quantities of material points are then calculated from the updated nodal quantities, followed by resetting the background grid to its initial configuration. Therefore, MPM allows for the explicit simulation of the large deformation and fracture of solid materials without the issues of mesh distortion, providing realistic modelling of large deformation and post-failure behaviour of rock masses. To simulate the elastoplastic behaviour of the rock mass, a strain-softening Mohr-Coulomb failure criterion with a tension cut-off is implemented in the MPM modelling framework. The bulking factor of rock masses is also incorporated into the modelling to account for dilatancy during caving.

The MPM modelling framework is verified by comparing the simulation results with the results of physical modelling [3]. The preliminary results show that the model captures the discontinuous damage profile above the cave back, which was also observed in the experiment and mine sites [3, 4]. The developed model will be applied to simulate large-scale caving operations in Australia, enabling engineers to optimise mine designs and risk-mitigation strategies.

Keywords: Cave propagation, rock mass behaviour, material point method, block cave mining.

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Effect of cryogenic temperature and freeze-thaw cycles on the dynamic behaviour of ultra-high performance concrete

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Abstract

Concrete infrastructure in polar regions and liquefied gas storage facilities is exposed to extreme low temperatures and freeze-thaw cycles, and these critical infrastructures are calling for proper safety designs against dynamic mechanical loads The combined environmental and dynamic loading conditions pose a unique and critical challenge to conventional construction materials which lead to extended interests in advanced materials such as ultra-high performance concrete. So far, the behaviour of this high-strength, fibre-reinforced material under combined cryogenic temperature and dynamic loading remains insufficiently understood.

To address this, a comprehensive experimental study was conducted to evaluate the dynamic compressive and splitting tensile behaviour of ultra-high performance concrete under temperatures of 20 , −70 and −160 °C, and across a range of strain rates from 40 to 160/s in compression and 20 to 80/s in splitting tension. The results demonstrated a strong rate-dependent. Interestingly, while the compressive strength declined at lower temperatures for the same strain rate, the tensile strength displayed a contrasting trend, increasing as the temperature decreased. This indicates that ultra-high performance concrete exhibits distinct temperature sensitivity under different loading modes.

In addition, the influence of cryogenic freeze-thaw cycling on the dynamic compressive behaviour of ultra-high performance concrete was examined. Specimens went through 2~8 freeze-thaw cycles at −160 °C before dynamic testing at strain rates of 80, 130, and 180/s. The findings revealed that dynamic compressive strength increased with both strain rate and the number of freeze-thaw cycles. Furthermore, the rate sensitivity of the material became more pronounced after freeze-thaw cycles. The increased porosity and water content following freeze-thaw cycling may contribute to this enhanced rate sensitivity.

Keywords: Ultra-High performance concrete; Dynamic loading; Cryogenic temperature; Freeze-thaw cycles

Exploration of C−N Coupling for Electrocatalytic Urea Synthesis

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Electrocatalytic coupling of N_2 and CO_2 into urea under mild conditions is a promising approach to reducing energy consumption and environmental pollution associated with the conventional Haber-Bosch process. However, the existing method suffers from the extremely low reaction efficiency due to the sluggish C–N coupling and the low selectivity for urea formation. Here, two novel mechanisms for high-efficiency urea production from N_2 and CO are proposed based on density functional theory (DFT) calculations. In the first mechanism, we proposed a potential pathway involving the N−N bond breakage to facilitate the subsequent C−N coupling. Interestingly, the inert N≡N bond of the adsorbed $*N_2$ can be gradually weakened and eventually broken through two protonation steps, leading to the facile CO adsorption on the dissociated *NH and the effortless C−N coupling to form the urea precursor *NHCONH. The second mechanism suggests a promising route for urea production from N_2 and CO, where C−N coupling can be achieved without breaking the N−N bond. Additionally, a simple descriptor, namely, effective d electron number, which merely consists of intrinsic properties of the catalysts, is constructed to quantitatively describe and predict the electrocatalytic urea activity of dual-atoms catalysts. Our work offers new opportunities to advance the rapid discovery of novel mechanisms and efficient catalysts for electrochemical synthesis of urea.

Keywords: Urea electrosynthesis, C−N coupling, density functional theory, activity and selectivity

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Full-Waveform Inversion for Simultaneous Reconstruction of Material Profiles in a Prestressed Beam-Soil System

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This study proposes a full-waveform inversion (FWI) method for reconstructing the material properties of underground prestressed Euler-Bernoulli beams based on dynamically measured beam deflections. The forward problem is formulated as an initial-boundary-value problem, incorporating the prestressed Euler-Bernoulli beam equation and a Winkler foundation model in the time domain. A PDE-constrained optimization framework is employed to solve the inverse problem, aiming to minimize the misfit between measured and computed deflections, with regularization terms for control variables. The material profiles include the beam's elastic modulus and prestressing force, as well as the soil stiffness of the Winkler foundation. The optimization process transforms the objective functional into a Lagrangian functional, enforcing its stationarity conditions to iteratively solve the state, adjoint, and control problems. Numerical examples explore four reconstruction scenarios: (1) simultaneous reconstruction of the beam's elastic modulus and soil stiffness with known prestressing force, (2) simultaneous reconstruction of the beam's elastic modulus and prestressing force with known soil stiffness, (3) simultaneous reconstruction of the soil stiffness and prestressing force with known beam modulus, and (4) simultaneous reconstruction of all properties. Results show that three profiles can be accurately reconstructed simultaneously using a single set of measured deflections, without subjective intervention. The proposed FWI method shows promising applicability in the nondestructive evaluation and health monitoring of lifeline structures, such as underground pipelines and pavements, by enabling the quantitative reconstruction of material properties in prestressed beam-soil systems.

Keywords: Euler-Bernoulli beam, Winkler foundation model, flexural waves, finite element method, Full-waveform inversion

Static Analysis of Braided Colonic Stent Deployment: Effects of Normalization Method for Initial Inter-Wire Contact

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In recent years, the use of self-expanding braided colorectal stents has seen increasing application in palliative treatment and as a Bridge to Surgery (BTS) for obstructive colorectal cancer. Compared to conventional treatment methods, colorectal stenting improves quality of life (QOL). However, a significant challenge is the increased risk of complications such as perforation, migration, and re-obstruction, which can arise from mechanical stress exerted on the colorectal cancer tissue during stent placement.

To prevent such complications, it is essential to quantitatively evaluate the mechanical stress exerted on the colorectal cancer tissue during stent deployment. However, directly measuring this mechanical stress on colorectal cancer tissue remains challenging, underscoring the need to establish evaluation methods based on numerical analysis. The first step towards evaluating this mechanical stress on the colorectal cancer tissue using numerical methods is to accurately reproduce stent deployment behavior through numerical simulation.

Simulating the deployment behavior of colorectal stents requires addressing strong nonlinearities and complex contact interactions. Traditionally, dynamic explicit methods, which can avoid convergence issues, have been widely used for stent deployment analysis. However, since stent deployment is an inherently static phenomenon, solving it using static analysis is considered preferable.

The objective of this study is to accurately reproduce stent deployment behavior using static analysis. In this presentation, we report on a fundamental investigation of a normalization method for the initial contact conditions between the wires constituting the stent, and its effectiveness.

Keywords: Braided Colonic Stent, Static Analysis, Contact, Finite Element Method

Underwater Acoustic Source Localization Based on Deep Learning

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Passive underwater acoustic source localization is a critical technology in underwater acoustics. Matched field processing, a commonly used approach for passive underwater acoustic source localization, has garnered extensive research and practical applications. However, traditional matched field processing suffers from a significant limitation: its localization accuracy degrades rapidly under conditions of environmental parameter mismatch and low signal-to-noise ratio. At the same time, deep learning, through hierarchical feature extraction enabled by multi-layer neural networks, demonstrates exceptional capabilities in learning and predicting complex patterns.

Assuming a acoustic source emits a narrowband signal with center frequency f, the signal received by an array of N hydrophones after propagating through the underwater acoustic channel can be expressed in the frequency domain as:

$$\boldsymbol{y}(\theta_0) = \boldsymbol{h}(\theta_0)s + \boldsymbol{n} \tag{1}$$

In the equation, $\boldsymbol{h}$ represents the transfer function from the acoustic source to the target position, where θ_0 denotes the actual location of the acoustic source that needs to be found; s is the source strength at frequency f in the frequency spectrum; $\boldsymbol{n}$ is a vector composed of the noise at each hydrophone; $\boldsymbol{y}$, $\boldsymbol{h}$, and $\boldsymbol{n}$ are all $N \times 1$ dimensional vectors. The covariance matrix can be expressed in the following form:

$$\mathbf{C}(\theta_0) = E\left[\boldsymbol{y}(\theta_0)\boldsymbol{y}^H(\theta_0)\right] \tag{2}$$

In the equation, E denotes the mathematical expectation, and $\mathbf{C}(\theta_0)$ is also referred to as the cross-spectral density matrix.

In traditional matched field processing, it is necessary to simulate the acoustic field vectors generated at the receiving hydrophone array for each assumed acoustic source location point through an underwater acoustic channel model, forming a "copy field". The actual signals received by the hydrophones are then matched against each vector in the copy field, and the location with the highest correlation is identified as the desired actual acoustic source position.

Within the framework of deep learning, neural networks possess the capability to match matrix features with previously learned matrix features. That means a model can be constructed by taking the cross-spectral density matrix of the copy field as input and the corresponding acoustic source location as output for training [1]. Using this trained model, the acoustic source location can be obtained from the cross-spectral density matrix derived from observed data, thereby accomplishing the underwater localization task. Comparisons using the SwellEX-96 ocean experiment test data reveal that the accuracy of matched field processing substantially degrades under conditions of environmental parameter mismatch, whereas deep learning approaches maintain a high level of localization accuracy.

Keywords: passive underwater localization, deep learning, matched field processing.

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Transfer learning-based efficient structural topology optimization of complex design domains

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Topology optimization requires dozens or even hundreds of iterations, each requiring a complete finite element analysis (FEA). Significant computation cost limits the application of topology optimization in engineering, especially for high-resolution problems containing complex design domains. To address the issue, a Problem-Independent Machine Learning (PIML) model based on isoparametric elements is proposed [1]. Effectively reducing the computational time of FEA, the proposed model enables efficient topology optimization and extends the solvable problem range to complex design domains. The essential idea is leveraging the substructure method and establishing a mapping from element shapes and material distribution within the substructure to its numerical shape functions through machine learning models.

However, In the context of three-dimensional (3D) cases, several challenges arise: first, the scale of substructure numerical shape functions increases drastically, necessitating a corresponding increase in the number of output neurons in the neural network, which makes it difficult to guarantee the accuracy of the machine learning model; secondly, complex design domains contain isoparametric elements of diverse morphologies. How to generate samples efficiently and construct a reasonable dataset remains challenging. In many practical applications, collecting the required training data is very expensive or even impossible; thirdly, for different topology optimization problems, such as non-self-adjoint problems and stress optimization problems, the generalization capability of the machine learning model requires further investigation; finally, how to efficiently train machine learning models and reduce training costs remains to be explored.

To address the above issues, we propose a mechanical information-embedded transfer learning model that improves the efficiency of FEA during the topology optimization process, enabling efficient solutions to 3D topology optimization problems of complex design domains. Based on the well-trained machine learning model [2], we use transfer learning to predict numerical shape functions of isoparametric substructures. The training process is accelerated while the same loss function value is achieved. When constructing the transfer learning model, a mechanical information-embedded neural network is employed to enhance accuracy. Moreover, the proposed machine learning model is problem-independent: it requires no modifications when optimization problems, design domains, boundary conditions, or loads change. A compliance minimization problem demonstrates that the method improves topology optimization efficiency by over two orders of magnitude without parallel computing. A compliant mechanism problem and a stress minimization problem verify the reliability and generalizability of the proposed model.

Keywords: Machine learning, topology optimization, transfer learning, complex design domain

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Structure-to-Stress: cGAN-Based Direct Modeling of Composite Material Stress-Strain Curves

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Designing high-performance composites requires a deep understanding of material behavior and failure mechanisms under large deformations. Traditionally, predicting composite material behavior relies on complex simulations that demand significant computational resources. This makes the process inefficient and time-consuming, often limiting its practicality for rapid design iterations or large-scale applications.

To overcome the issue, our study presents a deep learning model based on conditional generative adversarial networks (cGANs) to directly predict stress–strain curves from composite structures. The model uses a U-Net generator enhanced with fully connected layers to translate composite structural images into stress–strain curves, while a PatchGAN discriminator assesses the realism of generated data. This end-to-end approach eliminates the need for computationally expensive simulations and post-processing traditionally required to derive stress–strain behavior. Trained on phase-field simulation data covering diverse composite designs, the model achieves accurate predictions, significantly accelerating composite material design by bypassing labor-intensive mechanical analyses.

The study uses a diverse dataset of soft-hard binary composites-including random, layered, chessboard-like, soft-scaffold, and hard-scaffold structures to enhance design variety beyond random sampling limitations. Phase-field simulations generate stress–strain curves up to 15% strain and extract mechanical properties like Young's modulus, strength, and toughness.

Despite training on a limited dataset with only about 1.5% bio-mimetic and very few random structures, the surrogate model achieves excellent accuracy. After 2 million iterations, mean absolute error (MAE) converges to ~0.01 for training (6402 samples) and ~0.05 for testing (1600 samples), accurately predicting key mechanical behaviors across all composite types. Moreover, the study finds a strong correlation between strength and toughness. Direct correlation between Young's modulus and the volume fraction of hard material, especially in random and layered composites. However, strength and toughness show complex relationships influenced by microstructure, not simply by volume fraction. A 3D scatter plot of Young's modulus, strength, and toughness summarizes these findings, guiding the identification of optimal composite designs that balance mechanical properties to meet specific performance goals.

Overall, this approach significantly reduces computational cost and offers a promising framework for inverse design of composites using machine learning.

Keywords: composite design, deep learning, cGAN, phase-field method, stress–strain curves

Luxury Cruise Ship Vibration and Noise Analysis of Modular Cabin Systems

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Luxury cruise ships are acclaimed as the "crown jewel" of global shipbuilding, representing unparalleled complexity in large-scale manufacturing with exceptionally high requirements for onboard comfort and habitability. Unlike conventional merchant vessels, these floating resorts contain over a thousand passenger cabins, making vibroacoustic analysis particularly critical. This study investigates China's first domestically-built luxury cruise ship's modular cabin system through numerical simulation. The governing finite element equations for the fluid-structure interaction system are formulated as follows:

$$\begin{bmatrix} M_{\mathrm{s}} & 0 \\ -Q^{T} & M_{\mathrm{f}} \end{bmatrix} \begin{pmatrix} \ddot{a} \\ \ddot{p} \end{pmatrix} + \begin{bmatrix} K_{s} & \frac{1}{\rho_{f}} Q \\ 0 & K_{f} \end{bmatrix} \begin{pmatrix} a \\ p \end{pmatrix} = \begin{pmatrix} F_{s} \\ 0 \end{pmatrix}, \tag{6}$$

where p is the nodal acoustic pressure vector (fluid domain), a is the nodal displacement vector (structural domain), Q is the fluid-structure interaction (FSI) coupling matrix, M_{f} and K_{f} are the fluid mass matrix and fluid stiffness matrix, respectively, M_{s} and K_{s} are the structural mass matrix and structural stiffness matrix, respectively, F_{s} is the external load vector acting on the structure.

The main research content of this article includes:

(1) Modal Analysis: Conducted modal analysis on prefabricated cabin modules, with simulated acoustic cavity modes informing optimal noise source/speaker placement to enhance acoustic comfort and entertainment performance.

(2) Structure-Acoustic Coupling: Revealed cluster coupling characteristics between structural vibration and acoustic cavities. Findings demonstrate that structural modes, cavity resonances, and their interactions collectively influence vibration response peaks under acoustic excitation.

(3) Partitioning Optimization: Treating non-rigid inter-cabin walls as rigid partitions in combined cavities, results show partition configuration significantly affects radiated noise. Tailored partitioning can effectively mitigate high-amplitude peaks by modifying either cavity modes or coupling conditions.

Keywords: Acoustic cavity modes, cluster coupling, vibroacoustic radiation, rigid partitioning

Computational models for the dynamic stability analysis of composite cylinders

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With the progress of advanced composite material technology, composite wall-cylinder-shell structure with its excellent specific strength, specific modulus and corrosion-resistant properties gradually replace the traditional single metal materials in modern engineering equipment applications to show unique advantages.

However, its performance stability and reliability in complex working conditions and extreme environments are still facing many challenges, which has become a key bottleneck restricting its large-scale engineering applications. Especially in the long time, high stress, cyclic loading and unloading and other typical service conditions, there are composite nonlinear and thin-walled structure nonlinear double impact, to the composite cylindrical shell dynamics behavior of the study has caused great difficulties, but also to the safe and stable operation of the equipment has brought a huge hidden danger. On the one hand, it is due to the complex coupling between the anisotropy of composite materials, multi-scale damage failure behavior, and the mechanical properties of heterogeneous material interfaces and structural dynamic instability behavior under service conditions.

In addition, the dual support of material and structural nonlinearities makes the composite cylindrical shells extremely prone to unbalanced vibration and dynamic instability under complex service conditions, which results in the rapid accumulation of high-period fatigue damage and triggers sustained material damage failure.

Therefore, the study on the dynamic instability mechanism of composite thin-walled cylindrical tube under extreme loading is expected to provide guidance for the dynamic design of key structural components of major engineering systems and improve the service performance of actual engineering equipment.

Keywords: Composite structure, Anisotropy; Nonlinear vibration, Dynamic instability

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Flow Field Design of Redox Flow Batteries via homogenization-based topology optimization

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Redox flow batteries are attracting attention as promising energy storage systems for renewable energy applications, but their inherently low energy density remains a major obstacle to widespread adoption. Yaji et al. [1] demonstrated that topology optimization can improve flow channel design and outperform conventional geometric approaches in terms of the electrochemical reaction rate. However, the high design freedom of topology optimization often leads to limited solution quality due to the complexity of the design space. To address these challenges, we propose a homogenization-based topology optimization method, aiming to efficiently generate complex structures beyond the capability of conventional mono-scale topology optimization methods.

The method proposed in this study designs a flow channel geometry through a three-step process, which is illustrated in Figure 1. In the first step, the effective permeability of the Representative Volume Element (RVE) is determined through the homogenization approach. In the second step, two design variables, d and θ, are optimized for each unit cell on a coarse mesh, where d represents the height of the electrode region, and θ denotes the rotation angle. The physical model used for the optimization is based on [1]. In the final step, the optimized distributions of d and θ are dehomogenized to reconstruct a high-resolution channel geometry. In this process, a smooth flow channel structure is derived from the design variables through a wave function, based on [2].

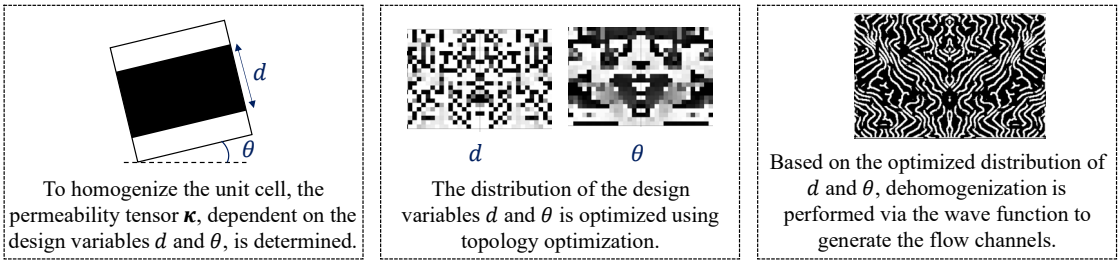

Figure 1.

Using the proposed method, we successfully generated complex flow channel geometries. When the flow rate is fixed, the electrochemical reaction rate is approximately 2.5 times higher than that of the conventional approach. This improvement entails increased pressure loss, illustrating a trade-off between reaction efficiency and flow resistance.

Keywords: Topology Optimization, Redox flow battery, Flow field, Homogenization, Dehomogenization

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A Scaled Boundary Finite Element Method for Coupled Soil-Structure Interaction Analysis Using Non-Matching Meshes

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Soil-structure interaction simulations are essential for evaluating the safety and performance of geotechnical and structural systems. However, a major challenge lies in handling incompatible meshes between solid domains and structural components (e.g., columns, slabs, walls or pile foundations). Traditional approaches typically require matching meshes at interfaces, significantly increasing difficulties in mesh generation for complex geometries. Alternatively, constraint-based techniques can be used but may introduce instability or inaccuracies, particularly when rotational degrees of freedom are involved.

The scaled boundary finite element method is a semi-analytical method which offers a potential solution to these challenges [1]. This method solves an eigenvalue problem (see Eq. 1), enabling the construction of polyhedral elements with arbitrary numbers of nodes, edges, and faces, reducing the mesh burden. A coupling method for non-matching meshes has been developed through interface reconstruction—inserting non-matching nodes into opposing surfaces without modifying elements away from the interface [2]. However, extending this technique to solid-shell coupling, which requires handling rotational degrees of freedom, remains unresolved.

$$\boldsymbol{E}_0\xi^2\boldsymbol{u}(\xi)_{,\xi\xi} + \left(2\boldsymbol{E}_0 + \boldsymbol{E}_1{}^{\mathrm{T}} - \boldsymbol{E}_1\right)\xi\boldsymbol{u}(\xi)_{,\xi} + \left(\boldsymbol{E}_1{}^{\mathrm{T}} - \boldsymbol{E}_2\right)\boldsymbol{u}(\xi) = \boldsymbol{0}. \tag{1}$$

In this work, we present a coupling method for soil-structure interaction analysis using polyhedral elements based on the scaled boundary finite element method. The soil domain is discretised using an octree mesh, trimmed to conform to the structural boundary. The structure is independently meshed with triangular and quadrilateral shell elements, while pile foundations are modelled as beam elements. The coupling process begins by merging interfaces between solid and shell to ensure node compatibility. Pile foundations are embedded into solid elements, with only the boundary of the solid elements subdivided. Translational degrees of freedom are merged directly at overlapping nodes, while rotational degrees of freedom in shell and beam elements are constrained via multi-point constraints tied to neighbouring solid mesh nodes.

The proposed method is validated through benchmark problems and practical case studies, demonstrating its accuracy, robustness, and scalability. Results highlight its effectiveness in handling complex geometries and non-matching meshes, offering a reliable tool for soil-structure interaction analysis.

Keywords: Soil-structure interaction, Scaled boundary finite element method, Non-matching meshes, Polyhedral elements, Solid-shell coupling

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AI-enhanced fluid-structure interaction analysis of turbine blades

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A precise and cost-effective prediction tool for fluid-structure interaction (FSI) analysis is crucial for optimizing the structural design of tidal turbine blades. However, the high computational costs associated with fluid dynamic analysis pose a significant challenge, as the current lack of efficient FSI prediction methods hinders the advancement of cutting-edge tidal turbine designs. To address this issue, this paper proposes a novel consolidated framework that integrates deep learning convolutional neural networks (CNN) with blade element momentum (BEM) theory and finite element method (FEM) to perform deformation analysis of turbine blade structures. The proposed CNN-BEM-FEM integrated framework efficiently identifies the geometric features and predicts the hydrodynamic parameters of turbine blades and thus, achieving accurate assessments of the structural behavior of tidal turbines. The study applies two-step verification procedures to validate the prediction accuracy of the CNN-BEM-FEM framework and the result demonstrates excellent agreement with experimental tests for hydrodynamic performance and blade deformation. When compared with the static one-way FSI calculated by Ansys Workbench software, the computational efficiency of CNN-BEM-FEM framework increases by more than 18 times, with discrepancies in blade deformation and equivalent stress calculations generally less than 5 %. By applying the proposed method to predict the FSI performance of tidal turbine blades with various shear web structures, the practical applicability for composite turbine blade design is successfully demonstrated. The results underscore the potential of the CNN-BEM-FEM framework as an efficient and accurate prediction tool for optimizing the structural design of tidal turbine blades.

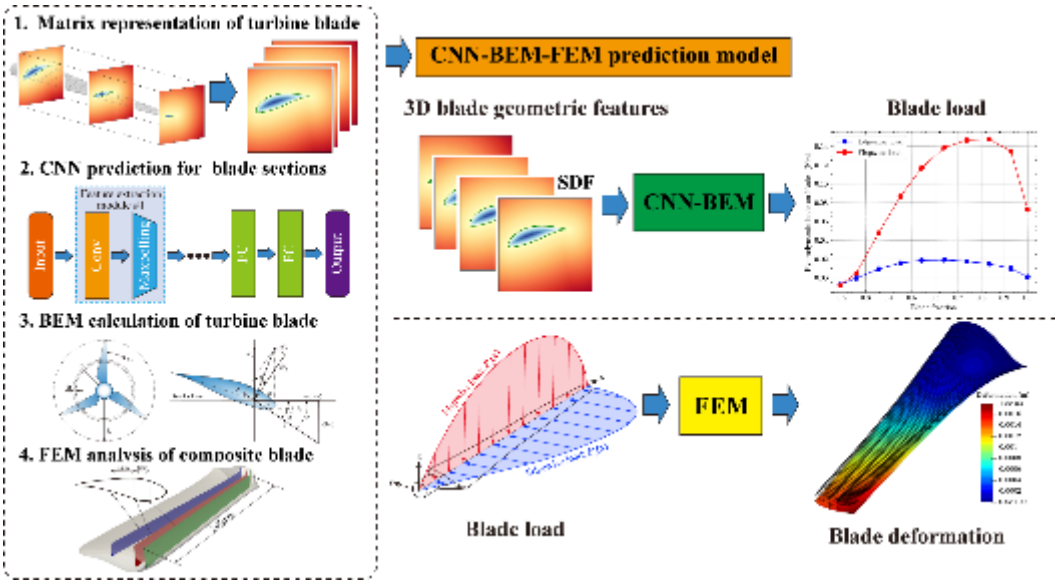

Figure 9 Schematic of the integrated CNN-BEM-FEM framework for predicting turbine blade.

Keywords: Horizontal axis tidal turbines (HATT), Convolutional neural networks (CNN), Blade element momentum (BEM), Finite element method (FEM), Fluid-structure interaction (FSI), Deep learning

Parametric Molecular Dynamics Model for Block Copolymers

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Controlling the orientation of block copolymer (BCP) morphologies in thin films is essential for their use as nanostructured coatings, yet remains a significant challenge across diverse block chemistries. In this work, we develop a parametric, coarse-grained molecular dynamics (MD) model and use it to systematically investigate the ordering of di-block copolymers in thin films, examining the roles of chain composition, substrate surface energy, and surface tension differences between blocks.

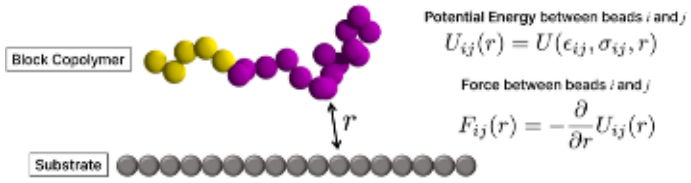

Figure 1. Schematic of an MD model of block copolymer thin films and the interactions

To efficiently map the complex parameter space associated with parameters of the model, we integrate a machine-learning framework based on a Gaussian process (GP) control algorithm, which autonomously identifies and prioritizes simulations of greatest value. The GP kernel is specifically designed to encode relevant physical symmetries, enabling the trained model to serve both as a comprehensive system response map and a tool for extracting key material insights.

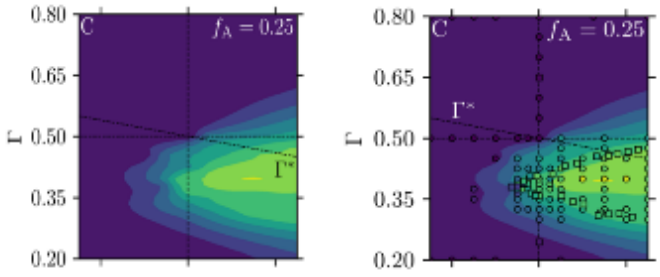

Figure 2. Phase map of the block copolymer thin films; (left) posterior mean and (right) posterior mean and observation points

Our results reveal that achieving vertical orientation of BCP domains is governed by a balance of competing energetic factors, including entropic and enthalpic enrichment at interfaces, morphological distortions through the film thickness, and interfacial energies. Notably, lamellar BCP phases exhibit greater resilience to these competing effects, consistently forming vertically oriented structures across a wide range of conditions. In contrast, cylindrical BCP morphologies are highly sensitive to surface tension disparities, leading to less robust vertical alignment. These findings provide new guidance for the design and processing of BCP thin films with targeted orientations.

Keywords: molecular dynamics, autonomous experimentation, kernel, block copolymers

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Generalization Analysis of Direct Weights Inversion Method for Small datasets

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This study presents a theoretical and numerical investigation of the generalization performance of the direct weights inversion method for solving inverse problems with limited data. The direct weights inversion method is a novel approach that directly maps the weights and biases of a well-trained forward neural network into explicit expressions for the inverse neural network. Previous studies have demonstrated that this method offers significant computational efficiency advantages over directly training inverse neural networks. The key formula is as follows:

$$\underbrace{\vec{\mathbf{a}}^{l-1}}_{\overleftarrow{\mathbf{a}}^{l'+1}} \approx \underbrace{\left[\left(\overrightarrow{\mathbf{W}}^{l}\right)^{\mathrm{T}}\overrightarrow{\mathbf{W}}^{l}+\alpha^{2}\mathbf{I}\right]^{-1}\left(\overrightarrow{\mathbf{W}}^{l}\right)^{\mathrm{T}}}_{\overleftarrow{\mathbf{W}}^{l'+1}}\underbrace{(\boldsymbol{\psi}^{l})^{-1}(\vec{\mathbf{a}}^{l})}_{\overleftarrow{\mathbf{a}}^{l'}}+\underbrace{\left(-\overleftarrow{\mathbf{W}}^{l'+1}\vec{\mathbf{b}}^{l}\right)}_{\overleftarrow{\mathbf{b}}^{l'+1}}, \tag{1}$$

Here, the "□" notation represents the forward neural network's propagation process, where $\vec{\mathbf{a}}^{l-1}$ and $\vec{\mathbf{a}}^{l}$ denote the activation values of the $(l-1)$-th and l-th layers, respectively, and $\overrightarrow{\mathbf{W}}^{l}$ and $\vec{\mathbf{b}}^{l}$ are the weights and biases of the l-th layer. The "□" notation indicates the inverse neural network's propagation process, with $\overleftarrow{\mathbf{a}}^{l'+1}$ and $\overleftarrow{\mathbf{a}}^{l'}$ representing the activation values of the $(l'+1)$-th and l'-th layers, respectively, and $\overleftarrow{\mathbf{W}}^{l'+1}$ and $\overleftarrow{\mathbf{b}}^{l'+1}$ denoting the weights and biases of the $(l'+1)$-th layer. The term $\left(\Psi^{l}\right)^{-1}(\,)$ is the inverse function of the activation function for the l-th layer.

Through comprehensive theoretical analysis and extensive numerical experiments, we demonstrate that the direct weights inversion method maintains exceptional generalization capabilities even with small datasets. The method's unique inverse-problem-solving mechanism and favorable convergence properties enable it to achieve high accuracy in data-scarce scenarios. Multiple case studies validate the effectiveness of our approach, showing consistent performance across different problem domains.

This research advances computational inverse techniques by providing an efficient solution for small-sample learning scenarios, with significant potential for practical engineering applications where data acquisition is challenging.

Keywords: Computational inverse problem, surrogate model, direct weights inversion method, small-sample learning, generalization

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Model updating of numerical models based on image measurement in experiments

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Understanding and predicting the behavior of structural systems under various conditions is a critical challenge in structural engineering. While experimental tests are commonly conducted to observe failure modes and investigate material or structural properties, the full potential of these tests can be realized when they are used to update and validate numerical models. However, discrepancies often exist between experimental data and initial numerical assumptions, leading to a need for efficient model updating techniques that can integrate experimental observations directly into the numerical framework.

In this study, we prototyped a model updating method that combines finite element analysis with image-based measurement. A shake table test of a structure under seismic excitation serves as the experimental case. Initial estimates of key parameters—such as vertical and horizontal stiffness—are iteratively adjusted to minimize the difference between the numerical responses computed by OpenSeesPy and the experimental displacements obtained through image tracking using ImProMeasure, a Python-based tool built on OpenCV. By leveraging Python scripting, the entire optimization process is integrated and automated, enabling near real-time model updating during the experiment. This framework allows researchers to estimate key structural parameters more effectively and gain a deeper understanding of the experimental specimen's behavior as testing progresses.

Density-Based Topology Optimization Using Subloading Surface Model of Elastoplasticity

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The present study proposes a elastoplastic topology optimization method considering subloading surface model to stabilize the convergence of optimization caused by the material nonlinearity. Conventional methods often face difficulties in convergence performance due to the discontinuity of the gradient at the yield point in the stress-strain relationship of traditional elastoplastic models. Conventional topology optimization methods, despite relying on gradient-based optimization techniques that require C^1 continuity, have historically tolerated such discontinuities, leading to suboptimal results. To overcome this limitation, the proposed approach incorporates the subloading surface model, an elastoplastic material model introduced by Hashiguchi [1]. This model enables a smooth transition from the elastic to plastic state, thereby resolving the discontinuity issue and enhancing convergence stability. By integrating this model into topology optimization, the proposed method aims to achieve reliable and efficient optimization for elastoplastic materials. The objective of optimization is to maximize the energy absorption capacity of a structure under prescribed loading conditions. The sensitivity analysis for the optimization process is derived analytically, building upon the framework established by Kato et al. [2]. Numerical examples are presented to validate the proposed method. These examples demonstrate that the proposed approach improves the convergence performance compared to conventional methods. The findings suggest that the proposed approach with subloading surface model has significant potential to advance the field of topology optimization for not only elastoplastic materials but also other nonlinear behavior.

Keywords: Topology optimization, subloading surface model, elastoplasticity

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CFD-Based Investigation of Primary Droplet Breakup from an Impaction-pin nozzle: Towards Predictive Models for Spray-Induced Plume Formation

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Accurate estimation of multiphase spray dynamics is critical in case of complex geometric designs for application of large-scale plume behaviour in environmental engineering areas such as artificial marine cooling and coral reef conservation. CFD-based studies focus on both primary and secondary breakup of droplets from different types of nozzles in spray systems, but literature shows very few evidence of modelling primary and secondary breakup of droplets from an impaction-pin nozzle. This study proposes a detailed CFD investigation of primary droplet breakup from an impaction-pin nozzle, playing a key role in initiating the atomisation process under high-pressure operating conditions. Using the interface resolving Volume of Fluid (VOF) methods, the major primary breakup stages sheet formation, ligament dynamics, and initial droplet formation will be simulated. The main equations involved in VOF method and its coupling with the Navier-Stokes equations is given by:

$$\frac{1\alpha}{\rho_q}\left(\frac{\partial}{\partial t}\left(\alpha_q\rho_q\right)+\nabla.\left(\alpha_q\rho_q\vec{v}_q\right)=S_{\alpha_q}+\sum_{p=1}^{n}(\dot{m}_{pq}-\dot{m}_{qp})\right) \quad (1)$$

$$\frac{\partial}{\partial t}(\rho\vec{v})+\nabla.(\alpha\vec{v}\vec{v})=-\nabla p+\nabla.[\mu(\vec{v}\vec{v}+\vec{v}\vec{v}^{T})]+\rho\vec{g}+\vec{F} \quad (2)$$

The planned numerical analysis will build on prior validated secondary breakup of droplets from impaction-pin using Discrete Phase method (DPM) by authors. During the simulation process, special attention will be paid to the pin geometry and alignment to analyse the influence of these on breakup behaviour and initial droplet size distribution. The objective is to develop a physics-informed understanding of the primary atomisation process that enhances predictive capabilities in multi-scale CFD models. This work contributes to the broader goal of integrating detailed nozzle-scale breakup phenomena with environmental-scale flow predictions within computational mechanics frameworks.

Keywords: Primary breakup, volume of fluid, flow optimisation, multiphase flow, interface tracking, environmental CFD applications

Thermo-mechanical analysis of electronic packaging using FEM and virtual element method (VEM) coupling

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Electronic packaging trends toward miniaturization and higher integration, with 3D ICs facing increased thermal and mechanical stresses that reduce device lifespan. Traditional FEM struggles with multi-scale packaging analysis due to excessive mesh requirements. We propose a coupled FEM-VEM approach for efficient thermo-mechanical analysis of multi-scale electronic packaging structures.

The fundamental concept of the VEM involves constructing a projection operator Π_k^∇ for both displacement and temperature fields, and performing calculations on the computational domain through the mapping $\Pi_k^\nabla u$. The projection operator Π_k^∇ can be calculated using the definition of degrees of freedom and the orthogonality condition:

$$a(u^h - \Pi_k^\nabla u^h, p) = 0, \quad \forall p \in P_k(E) \tag{1}$$

For $u^h, \upsilon^h \in V^h$ the bilinear form within an element decomposes into:

$$\begin{aligned} a(u^h, \upsilon^h) &= a(u^h - \Pi_k^\nabla u^h + \Pi_k^\nabla u^h, \upsilon^h - \Pi_k^\nabla \upsilon^h + \Pi_k^\nabla \upsilon^h) \\ &= a(\Pi_k^\nabla u^h, \Pi_k^\nabla \upsilon^h) + a(u^h - \Pi_k^\nabla u^h, \upsilon^h - \Pi_k^\nabla \upsilon^h) \end{aligned} \tag{2}$$

This decomposition yields the stiffness matrix with two components:

$$\mathrm{K}_E = \mathrm{K}_E^{\mathrm{c}} + \mathrm{K}_E^{s} \tag{3}$$

where $\mathrm{K}_E^{\mathrm{c}}$ is the consistency matrix and K_E^{s} is the stabilization matrix.

VEM accommodates arbitrary polygonal elements with flexible meshing that enables local modifications without disrupting the global mesh structure—a critical advantage for analyzing complex, multi-scale electronic packaging reliability issues. The method employs a non-matching mesh strategy that combines polygonal meshes for intricate small-scale regions with regular quadrilaterals for larger areas, while eliminating the need for explicit basis functions.

The FEM-VEM coupling further enhances analysis of electronic packaging structures by combining the strengths of both methods while mitigating their individual limitations. This hybrid approach enables appropriate method selection for different regions, delivering more accurate simulations of thermo-mechanical behavior with improved computational efficiency. Our analysis of actual electronic packaging structures confirms the feasibility and accuracy of both the standalone VEM and coupled FEM-VEM approaches for thermo-mechanical coupling problems, offering effective solutions for complex multi-scale electronic packaging structures.

Keywords: Virtual Element Method, FEM-VEM Coupling, Non-matching Mesh, Thermo-mechanical Coupling, Electronic Packaging

Image-Based 3D Time-Series Analysis of Suspended Ceiling Deformations for Shake Table Tests Utilizing Consumer-Grade Cameras.

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Recent developments in image processing and video capture technologies have led to the introduction of vision-based motion tracking and measurements. Vision-based measurements are believed to be effective in capturing the motion of structures during seismic excitations, such as shake table tests. The market offers industrial-level, high-speed cameras specifically designed for motion capture. However, these industrial-level camera systems are expensive and complex to operate. Using consumer-level cameras for motion tracking and three-dimensional measurements offers a cost-effective and practical solution compared to industrial-grade systems, particularly for suspended ceiling experiments. These cameras provide a reliable level of precision suitable for our needs. This study proposes a two-step camera calibration method along with a novel camera synchronization method that computes the time lag by minimizing triangulation projection errors and optimizes using polynomial interpolation to achieve subframe accuracy. Additionally, the study developed simplified application software for video synchronization and three-dimensional time series displacement measurement using the Python programming language. The software has a simple graphical user interface that enables users to define the video source folder, the range of cameras, the number of tracking points, the number of frames required for tracking, the number of frames needed for synchronization and stereo triangulation, and plot the time series displacement of target points. This study used three camera configurations to capture the shake table ceiling motion: a parallel camera setup, an opposite camera setup, and a 90-degree camera setup, and it employed a motion capture system to verify the accuracy of the proposed method. Demonstrations successfully achieved video synchronization with subframe precision. The maximum time series displacement error of the proposed approach was less than one millimeter across all experiments involving three degrees of freedom motion.

Keywords: Vision based measurement, calibration, image tracking, stereo triangulation, synchronization.

Overcoming Time Discontinuity in Finite-Discrete Element Method using a Node Binding Scheme

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The combined finite-discrete element method [1] has been widely used to simulate the progressive fracturing process in brittle rocks. Most simulators developed in this field utilize the intrinsic cohesive zone model to simulate crack initiation and propagation. Although it is easy to implement, it introduces the artificial compliance problem. Accordingly, the extrinsic cohesive zone model is proposed to address this problem. Nevertheless, it introduces the "time discontinuity" problem, i.e., inconsistent local nodal forces before and after cohesive element insertion due to essentially different constitutive models. This study builds upon our previous node binding scheme [2] to eliminate the time discontinuity problem. We propose an implementation that considers the dynamic equilibrium of nodal forces, calculating internal forces acting on adjacent finite element pairs during elastic deformation. When inserting a cohesive element, we achieve a smooth transition of local nodal forces by equating internal forces with cohesive tractions. The momentum conservation governing equation is expressed as:

$$\mathbf{f}_i + \sum_{j=0}^{N_i} \mathbf{f}_{ij} = m_i \mathbf{a}\,, \tag{4}$$

where $\mathbf{f}_i$, m_i, and $\mathbf{a}$ represent the node force, mass, and acceleration of node i, respectively, and N_i is the number of nodes connected to node i. The internal force $\mathbf{f}_{ij}$ applied by node j to node i can be expressed as:

$$\mathbf{f}_{ij} = \frac{k}{2} a_{ij} (\boldsymbol{\delta}_j - \boldsymbol{\delta}_i)\,, \tag{5}$$

where k is the stiffness of cohesive elements, $\boldsymbol{\delta}_i$ and $\boldsymbol{\delta}_j$ are the relative displacements of slave nodes i and j with respect to the master node, a_{ij} is the length/area of the edge/face between the finite elements i and j.

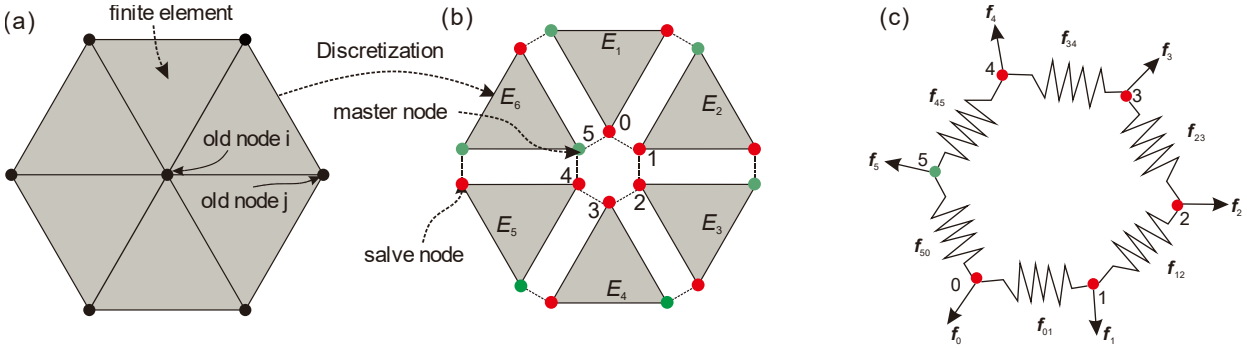

Figure 1.

The proposed node-binding approach has been verified by benchmarking a series of numerical cases. Results demonstrate that our approach effectively resolves both the artificial compliance issue in the intrinsic cohesive zone model and the time discontinuity problem in the extrinsic cohesive zone model. This approach significantly improves simulation stability and accuracy, and may promote further

applications of the finite-discrete element method in rock fracture simulations associated with various geotechnical and mining engineering problems.

Keywords: finite-discrete element method, time discontinuity, extrinsic cohesive zone model

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Sizing Optimization of Truss Structures Using an Improved Differential Evolution Algorithm

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Structural optimization has attracted the attention of the research community over recent years because of its close relationship with practical engineering design. However, optimization problems associated with structural optimization are generally multivariate, nonlinear, and the design space is highly constrained, making them difficult to solve. Hence, there is demand for a robust global optimization algorithm which can reliably identify the optimal feasible design in an efficient manner.

Throughout the years, metaheuristic algorithms have emerged as a branch of global optimization algorithms, taking inspiration from nature to build their optimization framework. Some of the renowned examples include genetic algorithms, differential evolution, particle swarm optimization. Whilst they have demonstrated their capability in solving a wide range of optimization problems, the algorithms may be subject to premature convergence issues. Also, massive information of the design space is generated from the iterative optimization process, however, lacking efficient use. Candidate solutions with medium-level objective function values tend to be eliminated quickly by those with superior function values and hence contributing little to the optimization process.

In this study, we propose a novel multi datasets differential evolution algorithm (DE-MDS). Instead of relying on only one set of candidate solutions to carry out optimization, we manage three memory sets A, B, and C, corresponding to the population, population's best records, and an external archive, each serving different purposes. Candidate solutions with medium-level objective function values are preserved as the population, driving the exploration of the design space, whilst their best records are utilized to trigger intensive exploitation. The external archive preserves historical information of the design space and assists with both exploration and exploitation phases of the optimization process.

To validate the DE-MDS algorithm, we apply it to solve truss sizing optimization problems of the form in equation (1). We would like to identify the design variables $\boldsymbol{A}$, which represent the cross-sectional area of truss members, such that the overall weight of the truss structure $W(\boldsymbol{A})$ is minimized, subject to constraints on element stresses σ_i and nodal displacements Q_j.

$$\begin{aligned} &\min: W(\boldsymbol{A}) = \sum_{i=1}^{N_T} \rho_i A_i L_i \\ &\text{s.t.: } \sigma_{i,\min} \le \sigma_i \le \sigma_{i,\max}, \qquad i = 1, 2, \dots, N_T \\ &\quad Q_{j,\min} \le Q_j \le Q_{j,\max}, \qquad j = 1, 2, \dots, N_{\mathrm{DOF}} \\ &\quad A_{i,\min} \le A_i \le A_{i,\max} \end{aligned} \tag{1}$$

We implement the DE-MDS algorithm on 4 illustrative examples, involving the sizing optimization of 10, 25, 72, and 200-bar trusses. Results obtained from the method are either equal to or better than the best feasible designs recorded in literature. On the 200-bar planar truss sizing problem, despite the high volume of constraints and existence of multiple local minimal solutions within proximity, we have achieved the lightest, feasible structure to our best knowledge.

Keywords: Structural optimization, evolutionary computation, truss structures

Interfacial Thermal Transport in PEEK/Graphene Nanocomposites: Unravelling the Impact of Polymer Crystallinity and Graphene Functionalization

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Polyetheretherketone (PEEK) is a high-performance semicrystalline polymer known for its excellent thermal, mechanical, and chemical properties. However, the thermal conductivity of PEEK is relatively low, which limits its application in high-performance thermal management systems. The addition of graphene has emerged as a promising solution. However, the interfacial thermal resistance often diminishes the great thermal conductivity of graphene. Phonon scattering at disordered or weakly bonded interfaces significantly hampers energy transfer efficiency, reducing the overall thermal performance of the composite. Improving interfacial thermal transport is further complicated by two interdependent factors: the semicrystalline nature of PEEK, and the surface chemistry of graphene, where functionalization affects dispersion, bonding, and phonon coupling. Despite their significance, the synergistic effects of polymer crystallization and nanofiller functionalization on interfacial thermal transport are still not well understood.

In this study, molecular dynamics simulations are employed to investigate the crystallization process of PEEK chains on graphene surface. The results reveal that PEEK chains tend to crystallize in a direction that aligns with phonon frequencies similar to those of graphene. As a result, in the crystallized interfacial region, weak interchain interactions facilitate thermal transport in the out-of-plane direction. To calculate the thermal conductivity, semicrystalline interface models are constructed using a chain-by-chain deposition algorithm. In the out-of-plane direction, the semicrystalline model exhibits lower thermal conductivity compared to the amorphous interface. Functionalization of graphene alters the phonon frequencies and crystallization direction of PEEK, thereby improving interfacial thermal conductivity. This work elucidates the synergistic effects of crystallization and functionalization at the PEEK/graphene interface, providing valuable insights for engineering nanocomposites with tailored thermal properties.

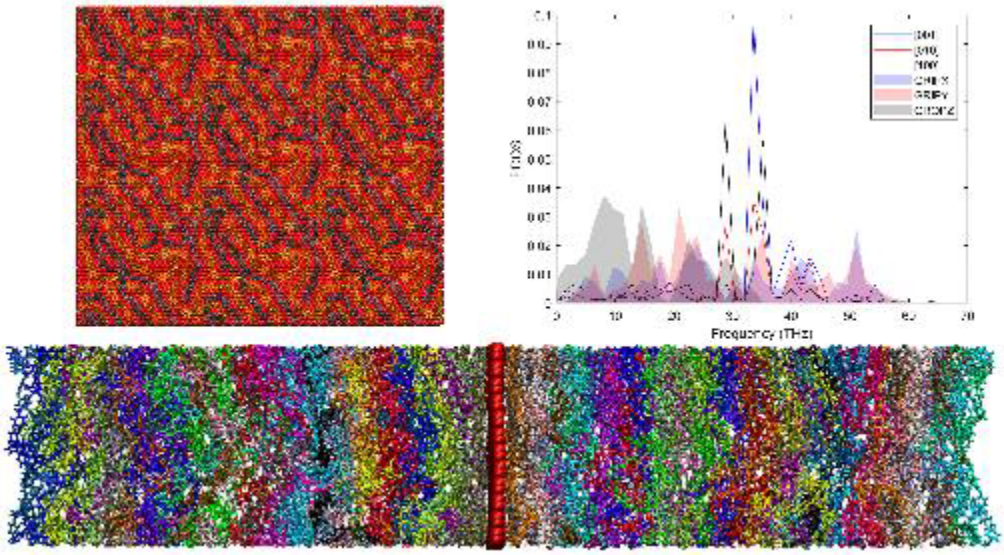

Figure 1.

Keywords: Polymer Nanocomposite, Interfacial Thermal Transport, Semicrystalline Polymer, Functionalized Graphene, Molecular Dynamics.

Enhancing Accuracy of Statistical Shape Models for Predicting Tooth Root Morphology

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This study demonstrates that tooth root morphology can be accurately predicted from crown shape, which can be obtained non-invasively, using a model constructed from CBCT slice images. The proposed approach contributes to the realization of safer and more effective orthodontic treatment by enabling detailed anatomical assessment without the use of X-ray.

Accurate assessment of tooth root morphology is essential for the success of orthodontic treatment [1][2]. Although panoramic radiography is minimally invasive, it provides only 2D information with limited accuracy. Cone-beam computed tomography (CBCT) offers high-resolution 3D data but poses higher radiation exposure. In this context, approaches using Statistical Shape Model (SSM) have been proposed to predict root morphology without relying on X-ray data from patients during treatment. However, some existing methods suffer from low generalization performance due to suboptimal selection of the number and positions of anatomical landmarks. In this study, we aim to enhance the generalization capability of the model by optimizing both the number and placement of these corresponding landmarks.

The method consists of the following steps:

(1) Creating 3D tooth models by manually segmenting the target teeth on CBCT slice images and stacking the segmented regions. The resulting models are then processed using Laplacian smoothing to remove surface noise and ensure geometrically clean and consistent meshes for subsequent analysis.

(2) Constructing a SSM with high generalization performance by optimizing both the number and positions of corresponding landmarks using Particle-Based Modeling (PBM), which enables accurate representation of diverse tooth morphologies using a small number of principal components.

(3) Estimating the root morphology by identifying shape parameters that best reproduce the crown morphology.

For the numerical experiments, we used 49 3D models of mandibular first premolars. Among them, 40 models were used to construct the SSM, and the remaining 9 models were used for testing. The proposed method achieved a 30.1% improvement in prediction accuracy compared to a conventional SSM. In particular, the angular error in root angulation and inclination was reduced by 73.4% and 60.7%, respectively.

Keywords: Image-based modelling, Orthodontics, Tooth Root, Statistical Shape Model

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Topology optimization considering anisotropy in all-solid-state battery design

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All-solid-state batteries (ASSBs) are regarded as a promising next-generation energy storage device that can potentially replace conventional lithium-ion batteries employing liquid electrolytes. However, the use of solid electrolytes introduces several challenges. In particular, ensuring sufficient interfacial contact between active materials and electrolytes, as well as forming continuous electron and ion conduction pathways, is more difficult than in conventional systems, which can lead to a significant decrease in charge–discharge efficiency. While many studies have focused on improving the intrinsic properties of battery materials, an alternative and equally important approach is to enhance battery performance through optimizing the spatial configuration and distribution of the constituent materials.

In this study, we develop a topology optimization (TO) framework to determine the mathematically and physically optimal material distribution within the composite electrode of an ASSB. The proposed method incorporates material anisotropy and derives not only the optimal volume fraction of active material, solid electrolyte, and conductive additive, but also their preferred orientation directions. The optimization problem is formulated as follows:

$$\min_{\varepsilon_a,\varepsilon_c,\theta_a,\theta_c,\theta_e} J = \frac{\int_0^{t_{max}} (U_p(\tilde{c}_p) - \tilde{\phi}_s) dt}{t_{max}\, I}\ , \tag{1}$$

where ε_a and ε_c are the volume fractions of active material and conductive additive material in composite cathode, respectively, and θ_a, θ_c and θ_e are the orientation distribution of active material, conductive additive and electrolyte material in composite cathode, respectively. $\tilde{c}_p$ and $\tilde{\phi}_s$ are the average lithium concentration and electric potential in the composite cathode. Moreover, U_p is the standard electrode potential, and t_{max} is the time taken for the discharge process, and I is the current applied during discharge. In other words, the optimization problem is formulated by setting the volume fractions and orientations as design variables, while minimizing the ratio of overvoltage to current during the discharge process under constraints on the total volume of each material. A sensitivity analysis is performed using the adjoint variable method, and the design variables are iteratively updated based on the Method of Moving Asymptotes (MMA). Numerical examples are presented to demonstrate the effectiveness and validity of the proposed approach.

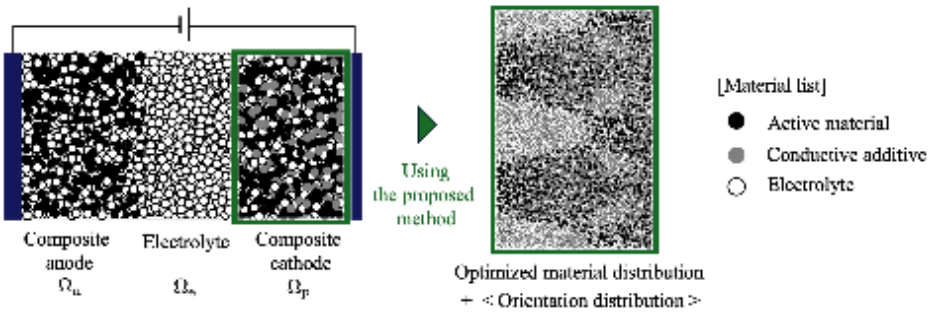

Figure 1.

Keywords: Topology Optimization, Butler–Volmer Equation, Time-Dependent Analysis, Sensitivity Analysis, Data-Driven Methods, Material Anisotropy

Development on B-spline MPM-SPH coupling algorithm for fluid-solid coupling problems

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The Material Point Method (MPM)[1] and Smoothed Particle Hydrodynamics (SPH)[2][3], as two representative meshless algorithms, exhibit significant advantages in simulating large deformation problems under extremely loading. In fluid-structure interaction (FSI) problems, the MPM algorithm can directly apply boundary forces on grid nodes and act on material points through mapping process, which makes boundary treatment extremely convenient. However, this algorithm also faces challenges of pressure oscillation and low accuracy of the free surface when simulating fluids[4]. On the other hand, the SPH method has great advantages in simulating free surfaces. Nevertheless, it requires the use of ghost particles and repulsive particles to prevent fluid particles from penetrating the fluid-solid interface. Moreover, it also suffers from tensile instability problem when simulating large deformations of solids[5]. To combine the advantages of both algorithms, this paper establishes a coupled algorithm between MPM with B-spline shape function (BSMPM)[6] and SPH. The coupled algorithm can not only solve the particle penetration problem of MPM, but also ensure the consistency of the interpolation or mapping values of two algorithms at the same point, due to the consistency of the shape functions. At the interface between the two types of particles in the coupled algorithm, SPH particles are regarded as material points and mapped to the background nodes of BSMPM by the B-spline function. Meanwhile, material points which exist in the support domain of SPH particles are treated as neighboring particles and interact with the SPH particles. In this way, the interaction between the two types of particles can be directly calculated, achieving deep coupled of the two algorithms. The proposed B-spline MPM-SPH coupled algorithm in this paper can inherit the advantages of both algorithms and show strong capabilities in FSI problems. It can not only use the SPH method to simulate the fluid flow with free surfaces but also utilize the BSMPM algorithm to simulate the large deformation process of solids under fluid pressure. Moreover, there is no need to use ghost particles and repulsive particles at the fluid-solid interface. The interaction at the fluid-solid interface can be directly calculated using the B-spline MPM-SPH coupled method. In this work, the accuracy and stability of the proposed B-spline MPM-SPH coupled algorithm are first demonstrated by two benchmark problems of solid in one- and two-dimensional space. Then two classical FSI problems are modeled by the proposed method. The simulation results demonstrate that the coupled algorithm can prevent fluid particles from crossing the fluid-solid interface, accurately capture the free surface of the fluid and simulate the large deformation process of solids caused by fluid impact. This indicates that the coupled algorithm can integrate the advantages of both algorithms, featuring high accuracy and stability.

Keywords: MPM, SPH, Coupled algorithm, B-Spline function, Fluid-solid interaction

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Physics-Informed Chebyshev Polynomial Neural Operator for Parametric Partial Differential Equations

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Existing neural operators for solving parametric partial differential equations (PDEs) rely on multilayer perceptron (MLP) with fixed activation functions. This design creates a fundamental limitation: the network's nonlinear mapping is confined to a single, predefined form. It cannot adapt to different solution regimes or effectively represent multiscale phenomena. This inherent inflexibility leads to insufficient robustness, particularly in physics-informed training. Current mitigation strategies, such as advanced loss functions or sampling techniques, only apply post-hoc corrections at the training level without fixing the core issue of the weak functional basis.

We propose a fundamental solution by constructing a polynomial neural operator. To overcome the severe numerical instability (Runge phenomenon) of standard monomials, we use a Chebyshev polynomial basis. This provides a numerically stable, high-degree basis that is optimal for approximating smooth functions and handling boundary conditions. By embedding this mathematically sound foundation directly into the network architecture, the model learns in a more appropriate function space from the start. This proactive, architectural enhancement systematically reduces large residuals in difficult regions, diminishing the need for complex training remedies. We thus introduce the Physics-Informed Chebyshev Polynomial Neural Operator (CPNO), a robust model whose capabilities are built-in rather than patched during training.

The network comprises m hierarchical levels, progressively generating the solution through feature interactions. The solution can be written as

$$u(x,t;\theta) - \mathbf{W}_q\left[\sigma\left(\mathbf{f}_m^\theta\left[\sigma\left(\cdots\sigma\left(\mathbf{f}_m^\theta[\Phi(x,t)]\right)\cdots\right)\right]\right)\right],$$

where the nested application of $\sigma \circ \mathbf{f}_m^\theta$ occurs q times, starting from the Chebyshev-encoded input $\Phi(x,t)$. The encoding then employs the three-term recurrence relation of the first-kind Chebyshev polynomials $T_k(z)$:

$$T_0(x) = 1, \qquad T_1(x) = x, \qquad T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x), k \geq 1,$$

$$\Phi(\mathbf{x}) - [T_0(x_1'), \dots, T_P(x_1'), \dots, T_0(x_d'), \dots, T_P(x_d')]^T \in \mathbb{R}^{d\times(P+1)}.$$

A joint weight magnitude-phase modulation strategy is designed in order to decompose the parameter space of the super-network into a magnitude modulation matrix and phase coding vectors. The modulation is performed using an amplitude vector $\boldsymbol{\omega_l(\theta)} \in \mathbf{R}^{\boldsymbol{d_h}}$ and a phase vector $\boldsymbol{\varphi_l(\theta)} \in \mathbb{R}^{\boldsymbol{d_h}}$, which are generated by the parameter-mapping network, followed by a nonlinear activation $\boldsymbol{\sigma}$:

$$\mathbf{h}^{(j)}(\mathbf{x};\theta) - \sigma\big(\omega_l(\theta) \odot \mathbf{h}^{(j)}(\mathbf{x}) + \varphi_j(\theta)\big)$$

In order to verify the effectiveness of the method, three PDEs are selected as test benchmarks. A comparison of the experiments with the traditional meshless neural operator reveals that the new method enhances the prediction accuracy and robustness.

Keywords: Partial Differential Equations, Neural Operators, Chebyshev Encoding, Modulations, Physics Informed

Simulation-Driven Design of Additively Manufactured Ceramic Structures

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The integration of manufacturing-integrated simulation with ceramic additive manufacturing (AM) offers a powerful strategy for designing complex, high-performance components in biomedical engineering. This study presents a unified simulation framework that couples structural design, process parameter modelling, and mechanical evaluation across three representative domains: bone scaffolds, dental restorations, and porous cylindrical components.

In each domain, finite element simulations were employed not only to evaluate mechanical performance but also to investigate how AM process parameters influence residual stress development, shape distortion, and material response. Scaffold structures featuring triply periodic minimal surfaces (TPMS) were analysed under compression and fluid flow conditions, revealing sensitivity to pore morphology and print-induced geometric deviation. Dental ceramic components were assessed using extended finite element methods (XFEM) to simulate crack initiation and propagation under occlusal loads, showing that residual stress patterns significantly affect fracture behaviour and fatigue resistance.

The third domain focused on additively manufactured alumina cylinders with varied open porosity, where layer-wise shrinkage, thermal gradients, and phase-related volumetric changes were simulated and validated against experimental results. Direction-dependent mechanical responses were observed, with out-of-plane compressive strength exceeding in-plane strength due to anisotropic microstructural evolution. Residual stresses were found to correlate with porosity gradients and influence failure mechanisms under compressive and bending loads.

This integrated simulation framework highlights the importance of coupling manufacturing process effects with structural design for ceramic AM. By embedding residual stress analysis into the early design phase, this framework enables more reliable, application-specific performance in both orthopaedic and dental ceramic structures.

Keywords: Additive Manufacturing (AM), Manufacturing-Integrated Simulation, Residual Stress, Finite Element Analysis (FEA), Ceramic Scaffolds, Dental Ceramics

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A stochastic gradient online learning and prediction method for accelerating structural topology optimization

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Topology and shape optimization are typically constrained optimization problems, which can be defined as: finding the optimum solution for design variable $\boldsymbol{x}$ that

$$1. \qquad \begin{aligned} &\min/\max: \quad f(\boldsymbol{x}) \approx f(\bar{\boldsymbol{x}}) + \nabla f(\bar{\boldsymbol{x}})(\boldsymbol{x}-\bar{\boldsymbol{x}}) + \frac{1}{2}(\boldsymbol{x}-\bar{\boldsymbol{x}})^T \nabla^2 f(\bar{\boldsymbol{x}})(\boldsymbol{x}-\bar{\boldsymbol{x}}) \\ &\text{subject to:} \begin{cases} g_i(\boldsymbol{x}) = 0 & (i = 1,2,\dots,I) \\ q_j(\boldsymbol{x}) \le 0 & (j = 1,2,\dots,II) \end{cases} \end{aligned} \tag{7}$$

where $\boldsymbol{x}$ is a vector of N_e design variables; $f(\boldsymbol{x})$ is an objective function of design variable $\boldsymbol{x}$, and it can be approximated using a quadratic function with $\nabla f(\bar{\boldsymbol{x}})$ and $\nabla^2 f(\bar{\boldsymbol{x}})$ representing the first and the Hessian matrix of the objective function at point $\bar{\boldsymbol{x}}$; $g_i(\boldsymbol{x})$ and $q_j(\boldsymbol{x})$ are the equality and inequality constraints; I and II are the total numbers of equality and inequality constraints. The solution of Eq. (1) can be iteratively solved via repeatedly performing finite element analysis (FEA), sensitivity analysis, and design updates. These iterative processes can be computationally intensive, especially when large-size and complex physical problems are involved. In this presentation, we present a new stochastic gradient online learning and prediction (SGoLap) method for accelerating topology optimization. In the SGoLap method, a one-hidden-layer recurrent neural network (RNN) is used to learn and predict the first and second-order derivative information by performing online learning and prediction in routine and prediction iterations, respectively. Specifically, in routine iterations, a novel stochastic sampling scheme is applied to randomly select a subset of training samples from the first and second-order derivatives of the objective function calculated or predicted in previous and current iterations, enabling a reduction in the size of the training datasets and the number of trainable parameters in the RNN. In selected prediction iterations, the full first and second-order derivatives can be predicted by running forward calculations of the RNN, skipping time-consuming FEA runs and sensitivity analysis, and thus reducing total computational time. The activation of routine and prediction iterations depends on the learning and prediction scheme used. The SGoLap method is implemented to accelerate both the Solid Isotropic Material with Penalization (SIMP) and level set method (LSM) methods. By implementing SGoLap into the SIMP method, two RNNs can be established to learn the first-order derivative and the approximated and diagonalized Hessian matrix of the objective function, allowing the design variables to be updated using both exact first- and approximated second-order derivatives calculated or predicted in routine and prediction iterations. For the implementation of SGoLap in LSM, one RNN can be built to learn and predict the topological derivatives online. The advantages of the SGoLap method, in terms of prediction accuracy of the final objective functional value and the total computationally timesaving, are numerically demonstrated using minimum compliance topology optimization problems. By incorporating SGoLap, the numerical results demonstrate that fewer FEA runs and sensitivity analyses are needed to reach convergence, significantly reducing the total computational time required as compared to the SIMP and LSM methods considered. This reduction of total computational time can be significant for complex problems, such as a design problem with fine mesh and/or nonlinearities.

Keywords: Machine learning, topology optimization, Recurrent neural network, quadratic programming

On the Merits of a Lifting Line Model for Simulating Hydrofoils

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In the last decade, the popularity of hydrofoils on marine craft has increased significantly, particularly in the yachting industry and on recreational products. With a widespread push for more efficient, low-emission transport, commercial applications for fast ferrying of passengers and cargo are also being explored. Hydrofoil design poses a significant challenge to naval architects, due to complex hydrodynamics and operating regimes which are challenging to analyse (Faltinsen, 2005). Marine engineers employ a range of tools to study hydrofoil hydrodynamics, ranging from experimental methods in water tunnels and tow tanks; to simulation-based approaches such as computational fluid dynamics (CFD) and other numerical models. To reduce cost, much of the preliminary design is done using the latter (Newman, 2018). Accurate and validated methods for simulating hydrofoils are therefore crucial for engineers seeking to develop efficient and performant designs.

In this study, we showcase validation and application of a numerical lifting-line (LL) model, developed originally by Goates and Hunsaker (2022), for simulating hydrofoil hydrodynamics. This model was adapted to simulate free surface and wave-making effects by employing a Green's function for a source in steady motion under a free surface, originally derived by Newman (1987). High-fidelity steady Reynolds-Averaged Navier Stokes (RANS) simulations were used as a benchmark to verify the LL model's accuracy. This was done by first validating the RANS model against experimental datasets, and then using it to simulate a rectangular NACA4412 hydrofoil submerged one chord-length beneath the free surface at Reynolds numbers between 2.57×105 and 2.06×106 (Froude numbers between 0.5 and 4) and comparing the results with the LL model.

Overall reasonable agreement between LL and RANS was seen when comparing the lift, drag and moment coefficients across all simulated Froude numbers. The LL model also simulated the downstream induced velocities behind the hydrofoil with fidelity that was on par with RANS. This increased our confidence that the LL model can be relied upon for dictating design choices and direction at the preliminary stage of design. Its key advantage over RANS was its efficiency with compute resources, permitting extensive parametric design studies (e.g. exploring how different taper/twist combinations affect the resistance) and optimisation. However, great care should be taken when interpreting the LL results as the theoretical models employed, especially for the free surface effects, were difficult to validate and still showed considerable discrepancies with RANS, particularly when simulating regimes with intermediate Froude numbers.

Keywords: hydrofoil; computational fluid dynamics; waves; lifting line

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Physics guided training of neural network regression models for simulation results

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In mechanical design, the goal is to create shapes that satisfy specific performance requirements. This task, known as an inverse design problem, typically involves running numerous simulations and manually adjusting the design through trial and error. Such a process is not only time-consuming but also heavily dependent on the experience and intuition of the designer.

To address this issue, machine learning approaches have gained increasing attention in recent years.

Physics-Informed Neural Networks (PINNs) [1] are one such method that embeds the governing equations of mechanics into the learning process, thereby improving inference accuracy. However, when applying PINNs, the governing equations of mechanics must be incorporated as part of the neural network in a form that allows for error backpropagation. As a result, it is difficult to use external software, such as general-purpose CAE tools.

To overcome these limitations, Yonekura [2] and Wada et al. [3] introduced the Physics-Guided Generative Adversarial Network (PG-GAN). In this framework, the physical validity of each generated shape is classified as either desirable or undesirable. These classifications are then used as real and fake labels for training, enabling learning without requiring backpropagation through the physical model. However, in this approach, the binary classifications (0 or 1) are imposed even in cases where the results deviate significantly from the equations or lie just near the threshold, despite the presence of a gradient in the degree of deviation.

In this study, we propose a method to enhance the PG-GAN framework by incorporating the residuals of the governing equations as continuous physical guidance. This allows the model to better account for the degree of deviation from the physical laws, leading to more accurate and physically plausible design generation. We demonstrate the effectiveness of our approach through illustrative examples in the context of mechanical inverse design

Keywords: Inverse problem, Physics-Informed Neural Networks, Physics-Guided Generative Adversarial Networks, Deep Generative Models, Airfoil design

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Electrical conductivity changes in early-age concrete during the hydration process using electrical impedance tomography

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This study presents an electrical impedance tomography (EIT) method to reconstruct cross-sectional distributions of electrical conductivity in mortar specimens, focusing on the temporal evolution of conductivity in early-age concrete. EIT is a nondestructive testing (NDT) method that estimates internal electrical properties, such as conductivity and resistivity, by injecting currents through surface-mounted electrodes and measuring the resulting electric potentials. The forward problem of EIT is formulated using the complete electrode model, which involves solving the Laplace equation for electric potential along with boundary conditions that account for electrode contact impedance and surface current flow. The inverse problem employs a Lagrange multiplier method, converting the constrained optimization problem into an unconstrained form by augmenting an objective functional with the governing equation and boundary conditions as constraints. The electrical conductivity distribution is iteratively updated from an initial estimate until the first-order optimality conditions of the Lagrangian functional are satisfied. To verify the method experimentally, electric potentials were measured at the surface electrodes of mortar specimens, and these measurements were inverted to reconstruct conductivity distributions. The results demonstrated that the cross-sectional electrical conductivity profiles were effectively reconstructed, showing a consistent decrease in conductivity with increasing curing age. Specifically, conductivity at 28 days was reduced to approximately one-tenth of its value at 7 days, attributable to reduced internal moisture content and increased porosity associated with hydration. Consequently, the proposed EIT method enables real-time monitoring of the hydration process and offers potential as an NDT-based approach for evaluating the hydration state of early-age concrete through electrical property analysis.

Keywords: electrical impedance tomography (EIT), electrical conductivity, early-age concrete, nondestructive testing (NDT), complete electrode model

Using a strength criterion based on a cohesive frictional model to predict the onset of localisation

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An important failure mechanism that influences the behaviour of geomaterials such as sand, rock etc. is strain localisation. The complication involving predicting the onset and orientation of localisation zones has been a challenge in the field of geomechanics. Accurate identification of the onset and orientation of localisation bands aids in understanding the bifurcation behaviour and failure mechanisms of geomaterial. In this study, the strain localisation behaviour of an representative volume element (RVE) is analysed using the two-scale framework for modelling localisation behaviour [1] incorporating a cohesive-frictional model [2]. Triaxial compression tests with various confining pressures are employed for the calibration and validation of the model parameters. The onset of localisation along with orientation of localisation band are determined based on the activation of yielding in the cohesive-frictional model. This approach differs from the classical approach based on the loss of positiveness of the acoustic (localisation) tensor. It establishes a strong link between the experimental observations and the constitutive model parameters that defining both onset and evolution of the localisation band, thereby contributing to a more comprehensive understanding of the bifurcation response.

Keywords: Bifurcation analysis, Geomaterials, Localised failure, Cohesive-frictional models, Two scale model

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Continuum–Discrete Coupled Modelling of Triaxial Hopkinson Bar (Tri-HB) for Dynamic Fracturing in Geomaterials

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Deep underground rock engineering frequently involves high in-situ stresses and dynamic disturbances such as seismic and blasting events. These factors lead to complex coupling effects between confining pressure and strain rate, which significantly influence the dynamic behaviour of rocks. To investigate this complex interaction, this study develops a three-dimensional numerical model of the Triaxial Hopkinson Bar (Tri-HB) system using the continuum–discrete coupled method. In the model, the bars system is modelled using continuum zones with elastic model to accurately simulate wave propagation process, while the rock specimen is represented by a bonded particle assembly with both parallel bond and soft bond models, accounting for internal geometric and strength heterogeneity. By transmitting contact forces within wall facets and nodal forces within zones, the coupled wall interface facilitates accurate stress wave transfer between the continuum bars and the discrete specimen. The numerical framework focuses on key physical aspects of dynamic loading, and it is calibrated and validated in terms of multi-directional wave propagation and attenuation, dynamic stress equilibrium, and energy transmission. The method of applying confining pressure is assessed by boundary friction and loading uniformity. Model performance is validated through comparison with experimental observations, confirming its capability to accurately reproduce waveforms and stress histories within the Tri-HB system. The microstructure of rock specimen is generated by statistically calibrating particle size distribution and bond strength against laboratory data, ensuring realistic heterogeneity. Fracture of cohesive bond between particles enables explicit simulation of crack initiation, propagation, and coalescence, reflecting realistic rock failure under static and dynamic conditions. Based on the validated model, dynamic responses of rock specimens under various confining pressures and high strain rates can be further investigated. This study provides a validated numerical framework for Tri-HB design and interpretation, and offers valuable insights into dynamic mechanical behaviour of rocks under complex loading conditions.

Keywords: Tri-HB; Simulation and validation; Continuum-discrete coupled method; Dynamic and static loading.

Desiccation cracking in reactive soils

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Desiccation cracking in soils, particularly for reactive soil with high degree of saturation is a significant phenomenon. The occurrence of soil desiccation cracking has a significant effect on the engineering properties of soils as it can considerably increase the hydraulic conductivity and decreases the shear strength of a soil. Thus, it can pose a significant threat to the hydraulic and structural integrity of earthworks, dykes, embankments, engineered barriers and can increase the erosion potential of surface soils [1]. The traditional methods in studying desiccation cracking are based on laboratory testing, analytical methods and numerical modelling. This study will investigate the available computational methods in studying soil desiccation cracking, particularly the approaches involving multiphysics coupling associated with desiccation cracking.

Keywords: desiccation cracking, reactive soil, numerical simulation

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DeepSDF-Powered 3D Generative AI: Training and Validation using 21,998 Eulerian Elastoplastic Simulations

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Existing 3D generative Artificial Intelligence methods often lack mechanical relevance for engineering design due to dataset limitations. We address this by proposing a "Parameter-to-3D" generative model using Deep Signed Distance Functions (DeepSDF) capable of generating 3D shapes conditioned directly on specified mechanical parameters. This study develops and validates such a model using a novel, large-scale simulation dataset.

We constructed a dataset of 21,998 automotive crash box shapes generated via linear topology optimization [1]. Each shape was annotated with its dimensions (height, depth, width) and impact energy absorption values (at varying crush distances), obtained from computationally expensive Eulerian elastoplastic analyses [2] performed using the Supercomputer “Fugaku”. Using this dataset (20,000 for training, 1,998 for testing), we trained a DeepSDF-based auto-decoder model [3]. This neural network model learns to predict the Signed Distance Function (SDF) value, which implicitly represents the 3D shape, based on inputs including a latent vector identifying the specific shape, the target mechanical parameters (dimensions, energy), and positional encoded spatial coordinates [4] for high-resolution detail. Training minimized SDF reconstruction error alongside latent vector and network regularization terms. The model training utilized distributed parallel processing on GPU nodes (NVIDIA Tesla V100) of the Nagoya University Supercomputer “Flow” Type II.

The trained model demonstrated high fidelity in reconstructing shapes from the test set (average Chamfer Distance approx. 0.021m), confirming good generalization. In the generative task, the model accurately produced diverse shapes satisfying specified parameter combinations within the training data range (interpolation), achieving high accuracy for both dimensions (>99%) and impact energy (>92.5% for 10.0mm crush). As expected, generation accuracy decreased for parameter values outside the training range (extrapolation), particularly for the non-linear energy absorption metric (53.0% for 10.0mm crush).

In conclusion, we successfully developed a DeepSDF-based generative model conditioned on mechanical parameters and validated it using a large-scale dataset derived from physics-based simulations on “Fugaku”. The model, trained efficiently using “Flow” Type II, effectively generates shapes meeting specified mechanical criteria within the learned distribution, highlighting its potential for accelerating mechanically-informed engineering design exploration.

Keywords: 3D Shape Generation, Deep Implicit Representation, Eulerian Analysis, Computational Mechanics, Generative AI, Parameter-to-3D

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Development of degree of freedom-based reduction for broadband frequency response analysis in local damped systems

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Reduced order models have been widely used to save the computational resources in large scale structural analysis. Most of the methods generate a single reduced model that captures the essential physical behavior of the original system. However, these single models are mostly composed of low-order mode, which makes them inaccurate in high frequency response or especially in nonlinear damping systems. In this study, we propose a degrees of freedom (DOFs)-based reduction method applicable to local nonlinear damping systems covering a wide frequency range by generating multiple reduced models suitable for each frequency. The motion of equation with local damping are given by rearranging the DOFs:

$$\left(\begin{bmatrix} \boldsymbol{K}_{pp} & \boldsymbol{K}_{ps} \\ \boldsymbol{K}_{ps}^{T} & \boldsymbol{K}_{ss} \end{bmatrix} + jw_i \begin{bmatrix} \boldsymbol{C}_{pp} & \\ & \end{bmatrix} - \lambda_i \begin{bmatrix} \boldsymbol{M}_{pp} & \boldsymbol{M}_{ps} \\ \boldsymbol{M}_{ps}^{T} & \boldsymbol{M}_{ss} \end{bmatrix}\right) \begin{Bmatrix} \boldsymbol{u}_p \\ \boldsymbol{u}_s \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{F}_p \\ \boldsymbol{F}_s \end{Bmatrix}, \tag{1}$$

where $\boldsymbol{K}$ and $\boldsymbol{M}$ represent the stiffness and mass matrices, respectively. $\boldsymbol{u}$ and $\boldsymbol{F}$ are displacement and force vectors. 'w_i' stands for i-th angular frequency, and λ_i is the square of the angular frequency. Under subscripts *p* and *s* denote primary DOFs to be reduced and secondary DOFs to be removed, respectively. When all damping DOFs are selected as primary DOFs, the transformation matrix does not include any damping elements. The transformation matrix used for model reduction can be obtained by expanding the second row of Equation 1:

$$\boldsymbol{t}(\lambda_i) = (\boldsymbol{K}_{ss} - \lambda_i \boldsymbol{M}_{ss})^{-1}\left(\boldsymbol{K}_{ps}^{T} - \lambda_i \boldsymbol{M}_{ps}^{T}\right). \tag{2}$$

To implement an efficient transformation matrix, we use Taylor series in Equation 2 so that the transformation matrix generated at the expansion point is reused and interpolated according to frequency. The proposed transformation matrix form is as follows:

$$\boldsymbol{t}(\lambda_i) = \boldsymbol{t_1}(\lambda_0) + \Delta\lambda_i \boldsymbol{t}_2(\lambda_0) \sum_{n=3}^{\infty} \Delta\lambda_i^{n-1} (\boldsymbol{K}_{ss} - \lambda_0 \boldsymbol{M}_{ss})^{-1} \boldsymbol{M}_{ss} \boldsymbol{t}_{n-1}(\lambda_0), \tag{3}$$

where λ_0 is an expansion point and $\Delta\lambda_i$is the difference between λ_0 and λ_i. All matrix operations are performed at the expansion point, and the transformation matrix at a new frequency is simply generated by multiplying the pre-calculated matrix by the frequency information. The detailed explanation of the methodology can be found in our previous work [1] on undamped systems.

To verify the proposed method, frequency response was performed using a computational model of wingbox. The number of total DOFs of the model is 4030 and about 1% of the primary DOFs were selected. The local damper with a damping effect that changes nonlinearly with frequency was attached to the tip of the wingbox. In the numerical example, it was confirmed that the proposed method well represents the response of the full order model even in the high frequency range, and the calculation time of the proposed method was approximately six times faster than full order model.

Keywords: Model order reduction, Nonlinear damping, Frequency response, Finite element analysis

Acknowledgment: This work was supported by the National Research Foundation of Korea (NRF) funded by the Korea government (MSIT) (RS-2023-00278230).

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A Novel Meshless Free Element Collocation Method for Solving Kirchhoff Plate Bending Problems

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The bending problem of Kirchhoff thin plates is governed by a set of higher-order partial differential equations. The traditional finite element method faces challenges in requiring C^1 continuity at element interfaces, where constructing elements with complete compatibility conditions becomes highly cumbersome. At the same time, the development of the mesh-free approximations has been hindered by computationally intensive shape function construction and inefficient derivative calculations. In this work, an innovative Free Element Collocation Method (FECM) that integrates the meshless approximation concept with domain-specific element-type polynomial interpolation, is proposed to solve the bending problems of the thin plate. This method employs the mesh of nodes and the elements are created appropriately around nodes according to its location. Firstly, the Galerkin weak-form formulation of plate governing equations is established using the virtual work principle. Secondly, a strong-form collocation scheme is developed, where interior nodes strictly satisfy governing equations while boundary nodes enforce prescribed conditions. Finally, this method also uses the recursive technique and equation decomposition strategy to improve the computational efficiency of the derivatives of higher order shape functions.

The equilibrium equations for the Galerkin weak-form FECM is:

$$\int_{\Omega} \sum_{I=1}^{n} \sum_{J=1}^{n} \frac{\partial^2 N_I}{\partial x_i x_k} \boldsymbol{D}_{ijkl} \frac{\partial^2 N_J}{\partial x_l x_j} \boldsymbol{\omega}^{\alpha} d\Omega = \int_{\Omega} \sum_{I=1}^{n} N_I \bar{q} d\Omega - \int_{\Gamma_2} \sum_{I=1}^{n} N_I \bar{V}_n d\Gamma + \int_{\Gamma_2+\Gamma_3} \sum_{I=1}^{n} \frac{\partial N_I}{\partial x_i} \bar{M}_n d\Gamma, \quad (1)$$

where I and J represent the computational nodes within the interpolation element, and n is the number of nodes in the interpolation element, Ω and Γ represent the computational domain, and boundary respectively, N is the shape function, D denotes the bending stiffness, ω is the deflection, $\bar{q}$ represents the transverse load, $\bar{V}_n$ and $\bar{M}_n$ represent prescribed equivalent shear, and bending moments respectively.

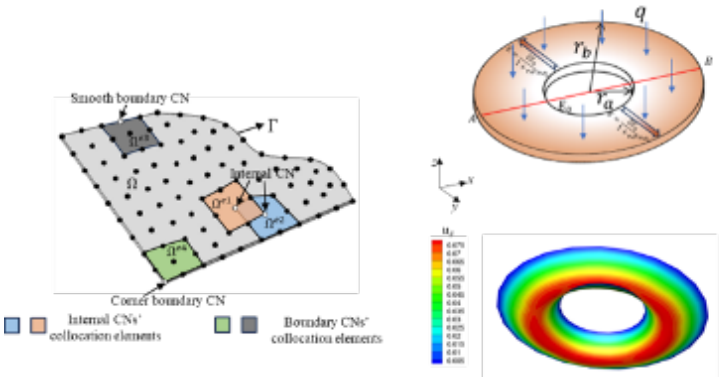

Figure 1.

Keywords: Kirchhoff plate, weak-form meshless method, strong-form collocation method, free element collocation method

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Assessment of LES Accuracy for Indoor Airflow Prediction: A Comparison with PIV Measurements in a Partitioned Ventilation Setup

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This study presents a comparative analysis of indoor airflow characteristics using experimental Particle Image Velocimetry (PIV) measurements and Large Eddy Simulation (LES) results. The investigation focuses on a simplified room configuration featuring a central vertical partition, designed to replicate a ventilated indoor environment. Both streamwise and spanwise mean velocity fields were evaluated to assess the accuracy and predictive capability of LES in capturing complex three-dimensional flow behavior. The results demonstrate strong qualitative agreement between the experimental and numerical data, particularly in capturing the primary recirculation regions and jet impingement dynamics. However, discrepancies are observed near boundary layers and in secondary flow zones, emphasizing the influence of resolution and subgrid-scale modelling (results will be presented later). The spanwise velocity analysis further confirms the presence of significant cross-plane motions, highlighting the need for fully three-dimensional modeling in ventilation studies. This comparison provides a valuable benchmark for validating LES models and supports their applications in indoor air distribution design and optimization.

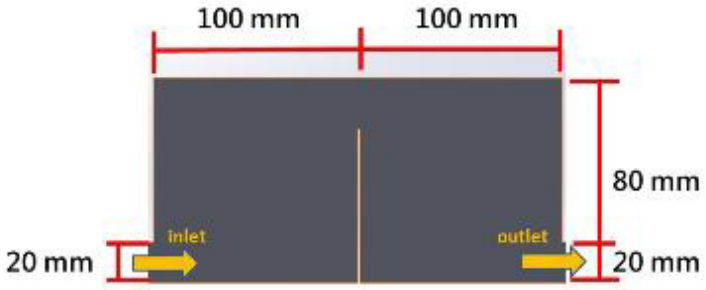

Figure 1. Schematics of the studied indoor ventilation domain

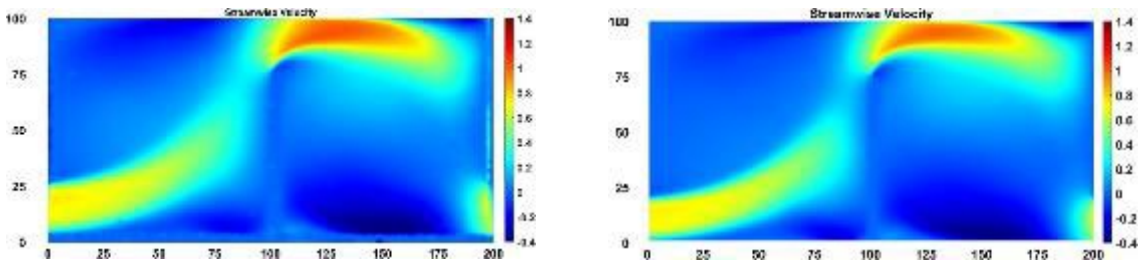

Figure 2. Contours of streamwise mean velocity obtained from PIV measurements (left) and LES results (right)

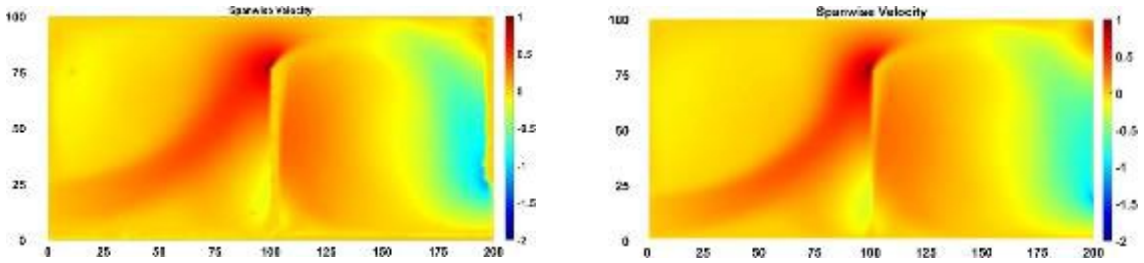

Figure 3. Contours of vertical mean velocity obtained from PIV measurements (left) and LES results (right)

Keywords: Particle Image Velocimetry, Large Eddy Simulation, Indoor Airflow Ventilation

Physics-guided Surrogate Model using Deterministic Latent Mapping for Composite Microstructures

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Recent years have witnessed rapid growth in the application of deep learning to multiscale modeling of heterogeneous materials [1]. Numerous approaches have leveraged neural networks for tasks such as homogenization, parameter identification, and surrogate modeling in both linear and nonlinear regimes. In this study, we present a physics-guided approach for accurate and efficient prediction of full-field stress distributions in composite microstructures. The proposed model combines three key components: an autoencoder for dimensionality reduction of stress fields, a deterministic latent transformation based on normalizing flows to regularize the latent space, and a deep neural network that maps material and loading parameters to latent representations. To improve spatial regularity and enhance learning consistency, same-size clustering is applied to preprocess the microstructural domain prior to encoding [2]. This modular structure enables the surrogate to generalize across a wide range of geometries and nonlinear loading conditions without requiring repeated full-field simulations.

Numerical evaluations on 2D and 3D RVEs under both monotonic and cyclic loading demonstrate that the model achieves high predictive accuracy, with relative errors typically below 3.5%, while offering significant reductions in computational cost. These results highlight the potential of integrating latent generative modeling with physics-guided learning for scalable multiscale analysis of heterogeneous materials.

Keywords: Surrogate modeling, Latent space, Composite microstructures, Normalizing flow, Autoencoder, Full-field stress prediction

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Study on Two-Dimensional Functional Materials via Deep-Learning Molecular Dynamics

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Understanding how complex strain affects ferroelectricity remains challenging due to limited simulation tools. Here, we combine density functional theory (DFT) and deep learning molecular dynamics (DLMD) to study domain formation in 2D ferroelectric materials. In In_2Se_3, bending, rippling, or bubbling induces strain gradients that modulate switching barriers, enabling spontaneous polarization reversal and size-tunable domains. The switching dynamics follow Arrhenius behavior, governed by curvature and temperature. In bilayer $CuInP_2S_6$, twist-induced stacking variations (AA/AB) give rise to interfacial ferroelectric or antiferroelectric coupling, with distinct switching barriers and domain stability. These domains differ from topological structures $(PbTiO_3)_n/(SrTiO_3)_n$ [1, 2] in superlattices and sliding bilayers of BN and MoS_2 [3, 4] and arise from stacking-dependent kinetics. Domain lifetimes are strongly twist and temperature sensitive, and tunable via electric fields or strain.

This work offers a cross-scale simulation framework to explore strain and rotation driven ferroelectricity, enabling precise control of polarization for nanoelectronic applications.

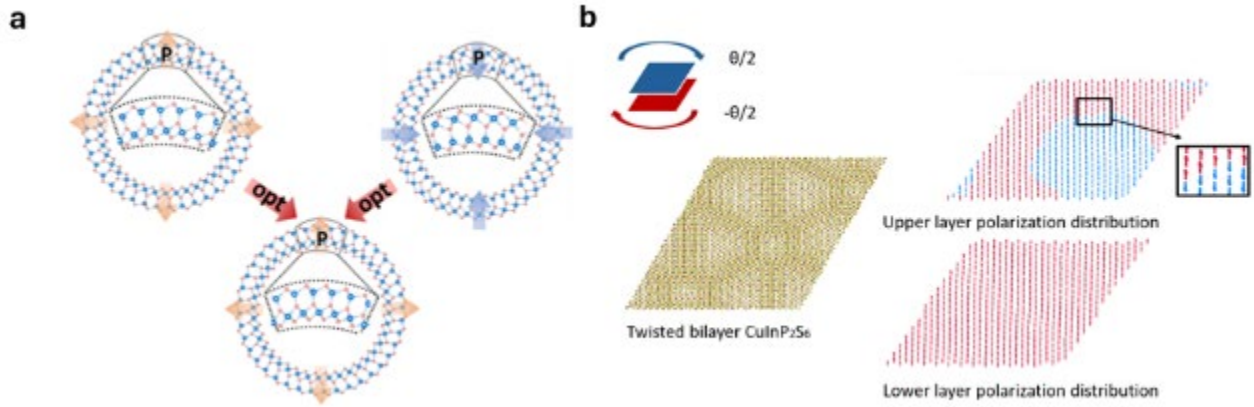

Figure 1. (a) The initial and optimized partial structure of In_2Se_3 nanotube from P↑ and P↓ states. (b) The structure of twisted bilayer CIPS and its polarization distribution under static conditions

Keywords: Polar domain, Deep learning, Domain dynamics, Twist bilayer, Strain engineering

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Development of Coupling Scheme of Grid- and Particle-Based Methods for Numerical Prediction of Supercooled Large Droplet Icing on NACA0012 Airfoil Using Parcel Assumption

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The icing on aircraft induces serious accidents. Moreover, glaze icings by supercooled large droplets (SLD) have still been challenging to reproduce numerically because the ice shape becomes complicated due to the droplet behavior before the solidification [1]. Recently, a coupling scheme of the grid- and particle-based methods has been developed using the Parcel assumption [2]. The grid-based method simulates the surrounding airflow by RANS and the droplet trajectory apart from the solid surface by the simplified Basset–Boussinesq–Oseen equation. On the other hand, the particle-based method simulates the droplet behavior, including the solidification, in the vicinity of the solid surface. The Parcel assumption, which enlarges the droplet size when the droplet is installed into the particle-based method, is employed to reduce the computational cost in the simulation by the particle-based method [2]. Here, the heat release of the water droplet was considered for the heat transfer to the airflow and heat conduction to the airfoil surface. The heat transfer to the airflow was estimated by the empirical equation of heat transfer coefficient h_c considering the surface roughness on the flat plate [4]. Consequently, the ice shape was reasonably reproduced in terms of ice thickness near the leading edge and the icing limit location. However, the reproduction of horn and feather shapes has not been satisfactory. Then, we modify the heat transfer Q_{ht} by the coefficient c_{Parcel} because of the Parcel assumption which delays the droplet solidification by enlarging the diameter.

$$Q_{ht} = c_{\mathrm{Parcel}}\, h_c (T - T_{\mathrm{air}}) \tag{1}$$

Where T and T_{air} denote the temperature of a computational particle at the water surface and the surrounding air, respectively. Figure 1 shows the ice shape using the modified heat transfer model with $c_{\mathrm{Parcel}} = 5$. The uneven shape representing the horn ice was obtained near the leading edge. Therefore, heat transfer estimation plays an important role in predicting the shape of SLD icing.

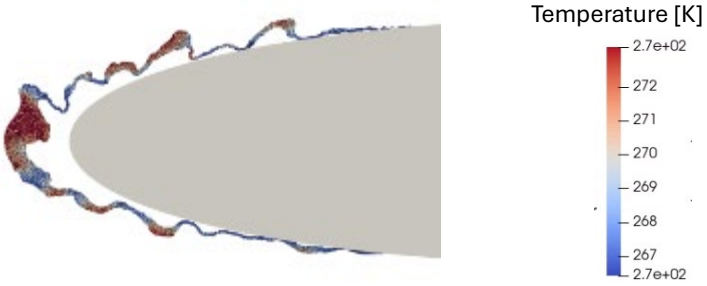

Figure 1. SLD icing simulation by coupling scheme with Parcel model for $c_{\mathrm{Parcel}} = 5$.

Keywords: Aircraft Icing, SLD Icing, Grid- and Particle-based methods, RANS, Parcel Model

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Study on the in-plane compression performance of bionic honeycomb structures with stepped energy absorption effect

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Abstract

Drawing inspiration from nature's evolutionary optimization of complex architecture, innovative bionic units that play a significant role in load-bearing and energy-absorbing in biological structures were constructed. These innovative bionic units were strategically integrated into conventional honeycomb structures to enhance their load-bearing and energy absorption capabilities. This new bio-honeycomb structures design strategy was defined as the bionic unit reinforcement (BUR) strategy. The bio-inspired honeycomb specimens for in-plane compression testing were fabricated using additive manufacturing technology, and corresponding mechanical compression experiments were systematically conducted. The experimental results confirmed that the bio-inspired honeycomb structures exhibited dual energy absorption plateaus, demonstrating the enhanced mechanical reinforcement effect achieved through bionic unit integration. Based on the experimental data, the finite element (FE) models of the bio-inspired honeycomb structure were developed. The computational model accurately captured both the deformation patterns and load-displacement responses observed experimentally, with discrepancies in average compressive load between experimental and numerical results ranging from 0.52% to 6.31%, thereby validating the simulation's predictive fidelity. The experimental and numerical analyses revealed that the performance enhancement mechanism originates from sequential collapse behaviors: bio-inspired units undergo controlled collapse initiation, followed by progressive failure of honeycomb cell walls. This hierarchical collapse sequence establishes stepwise deformation patterns, corresponding to dual energy dissipation stages with distinct stress plateau characteristics on the compressive stress-strain curve. The optimized bio-inspired honeycomb structure exhibits a 124.74% enhancement in MCF relative to conventional hexagonal counterparts, demonstrating significant performance superiority through BUR strategy. The findings demonstrate that this strategic innovation establishes a novel

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design paradigm for engineering high-performance honeycomb architectures with tunable energy absorption capabilities.

Keywords: Honeycomb structures; Bionic strategy; Theoretical model; Experimental research.

A probabilistic Atlas of Hemodynamics in the Major Cerebral Arteries through Statistical Geometric Analysis and Blood Flow Simulation

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Cerebral aneurysms are known to be initiated in regions with high wall shear stress Hemodynamic factors such as wall shear stress and oscillatory shear index are associated with flow, which are primarily determined by vascular geometry [1] and boundary conditions. This study aims to investigate the relationship between geometrical characteristics of the major cerebral arteries and wall shear stress.

The major cerebral artery consists of the internal carotid and middle cerebral arteries. In this study, the major cerebral arteries in the BraVa dataset are analysed using principal component analysis (PCA) and also categorized into geometric types - U, V, C, and S - based on their spatial complexity and bending angles as well as geometric parameters such as curvature and torsion. Through these two analytical approaches of PCA and geometric parameters, vascular geometry is classified to find its relationship with wall shear stress (WSS). It was found the maximal value of individual principal component in the PCA significantly affects curvature, which leads to an association between curvature and WSS peaks. The results demonstrate a positive correlation between WSS peak values and each principal component identified by PCA. As illustrated in Figure 1, when the principal components have similar values, the corresponding curvature and torsion, which represent the geometric features exhibit the similar distributions. Consequently, the blood flow simulations in two different patient-specific cases with similar geometry result in similar WSS distributions as shown in Figure 1.

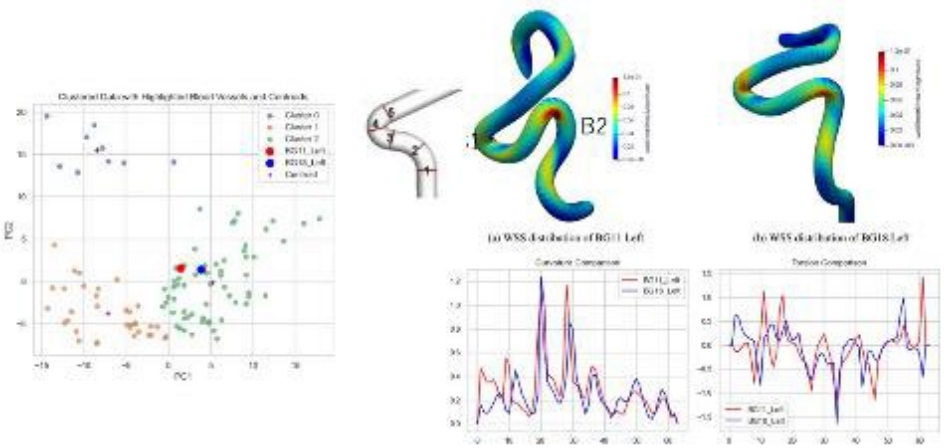

Figure 1 Wall shear distributions in two different cases of similar geometry categorized by PCA

Keywords: principal component analysis, blood flow simulation, cerebral artery, cerebral aneurysm、statistical geometric analysis

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Simulation of the Hydrodynamics of Flapping Wings under High Reynolds Numbers using the Immersed Boundary Method

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By combining the implicit force method-immersed boundary method[1] with large eddy simulation (LES), a new simulation framework is proposed, which successfully addresses the simulation challenges encountered under high Reynolds number flows, complex geometries, and dynamic boundary conditions as shown in Figure 1. Algorithm improvements include: multi-linear interpolation and virtual flow wall model.

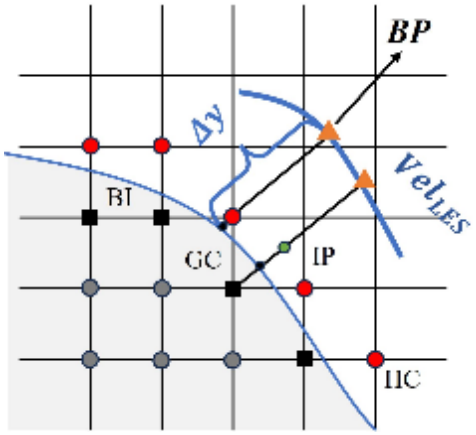

Figure 1 Schematic diagram of grid classification and wall model application of the immersed boundary method

The IBM is used to study the penguin flapping as shown in Figure 2. It shows that under high Reynolds numbers, the improved boundary layer attachment enhances fluid adhesion, resulting in more uniform thrust output with reduced fluctuations, while demonstrating significant optimization in both overall thrust and energy efficiency.

Keywords: Navier-Stokes equations, Immersed boundary method, Large Eddy Simulation, flapping wing

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Acknowledgements

The research was partially supported by the National Natural Science Foundation of China (No. 12272383)

Advanced structural material design based on computational simulation and data-driven method

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Advanced structural materials have received extensive attention in the field of materials and structural design in recent years. These materials generally achieve excellent performances via structural design at multiple length-scales. In the early material design, some researchers created reasonable mathematical and mechanical models from the natural topologies; some researchers established bionic mechanical models based on the structural and functional characteristics of biological systems. Nevertheless, it isn't easy to obtain the optimal designs only based on ingenious design. To traverse the design space to search for the optimal design by trial and error is also not practical. Data-driven methods can establish complex relationships of multi-dimensional variables, and they can reveal mechanical mechanisms and laws that are difficult to be discovered by traditional methods. Hence, this talk reviews the development of advanced structural material design methods. Various mainstream design methods are compared and illustrated. The status of intelligent design of advanced structural materials based on data-driven methods is introduced. The prospect of this research area is discussed.

Keywords: Data-driven, computational mechanics, structural material, material design

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Numerical Analysis of Reduced Basis Methods for Steady Thermal-Convection Problems

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We consider steady thermal convection problems to find temperature distributions and flow fields in the environments:

$$\begin{cases} -\nabla \cdot \big(v\, D(u)\big) + \nabla p - \beta\theta = f, \\ \nabla \cdot u = 0, \\ -\nabla \cdot (k \nabla \theta) = g. \end{cases}$$

Here, u denotes the velocity, p the pressure, θ the temperature, f an external force, g an external heat source, v a viscosity, k a thermal conductivity, β a thermal expansion coefficient. To create more comfortable environments, we are required to optimize temperature distributions and flow fields. Because we need to touch some iterative procedures in the optimization, we are required to reduce computational costs of finite element computations appearing in every iterative steps. Therefore, we introduced reduced basis methods for steady thermal convection problems in the environments; for example, see Quarteroni, et al. [1].

First, we have obtained the error estimate of reduced basis methods for steady thermal convection problems by following the same analogy in Quarteroni, et al. [1], Girault-Raviart [2], and Tabata-Tagami [3]. Second, we have shown some numerical examples on manufactured solution problems to confirm theoretical results and to verify efficiency and accuracy of the proposed methods. Finally, we have shown some numerical results of applications of the proposed methods into practical problems; for example, optimizations of temperature distributions and flow fields in the simple-shape room. Figure 1. shows sample results; the snapshot of the temperature, the pod basis, and the reduced basis temperature from the left to the right.

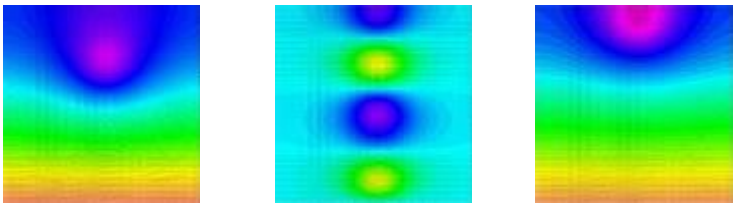

Figure 1.

Keywords: reduced basis method, finite element method, error estimate, Stokes equations, thermal convection problems

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Analysis the Free Vibration of Kirchhoff Thin Plates by Plate Free Element Collocation Method

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In this study, an efficient strong form collocation method called the Plate Free Element Collocation Method (PFECM) is proposed to analyze the free vibration of Kirchhoff thin plates. In PFECM, a novel collocation technology that combines the Lagrange isoparametric element to interpolate the physical variables is used to generate the system equations node by node, which maintains stability and ease of use in solving higher-order equations. The method enhances computational efficiency by creating independent isoparametric elements at each collocation node with freely chosen surrounding nodes, which reduces the bandwidth of the coefficient matrix and improves the application of boundary conditions due to the Kronecker property of the shape functions. A recursive computational technique and a physical decomposition strategy are used to improve the efficiency of shape function derivative calculations. Moreover, the mass term exists only in the internal nodes, which can accelerate the assembly of the final system equations. Building upon this foundation, the present study developed the Krylov reduced dimensional iterative method, which approximates the solution of the equation system by constructing a lower-dimensional subspace. This approach avoids the complex equation transformations involved in traditional algorithms for solving eigenvalue problems, thereby further enhancing computational efficiency.

The equilibrium equations after reduced order decomposition of the plate eigenvalue problem are:

$$D\nabla^2 h + \rho t\ddot{w} = q, \tag{1}$$

$$\nabla^2 w = h, \tag{2}$$

where D denotes the bending stiffness, h is the auxiliary variable, w is the deflection, ρ is the density, t is the thicknesses and q represents the transverse load.

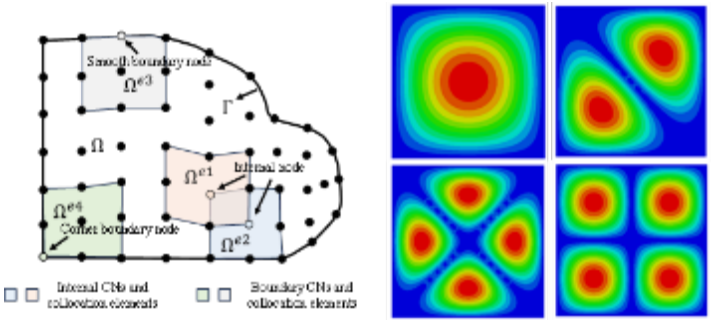

Figure 1.

Keywords: Kirchhoff plate, strong-form collocation method, free element collocation method, free vibration

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Prediction of Microscopic Stress in Composite Materials Using Graph Neural Networks

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Accurate prediction of microscopic stress distribution is crucial for evaluating the mechanical performance and long-term reliability of composite materials. The microscopic stress field within a composite is strongly governed by both the macroscopic loading conditions and the detailed configuration of its microstructure, including the spatial distribution, orientation, and properties of reinforcement phases. In practical applications, reliability assessments often require a large number of simulations to account for microstructural variability and uncertainty, which leads to prohibitively high computational costs when relying on conventional finite element analysis (FEA).

In recent years, data-driven approaches have emerged as promising alternatives. Convolutional neural networks (CNNs)[1] have been applied to microstructure images, while multilayer perceptrons (MLPs)[2] have used predefined features such as inclusion positions or volume fractions. However, CNN-based models typically require large training datasets and exhibit high computational overhead, and MLPs often lack the expressive power needed to generalize across diverse or irregular microstructures.

In this study, we investigate the use of graph neural network (GNN) architectures specifically designed to capture the topological and spatial characteristics of composite microstructures. By representing the microstructure as a graph—where nodes correspond to material points and edges encode spatial relationships—we enable flexible and efficient modeling of a wide range of configurations. GNN architecture is evaluated for their ability to predict microscopic stress distributions under given macroscopic loading conditions. Their performance is assessed against ground-truth stress fields computed using FEA.

Our method demonstrates high predictive accuracy across various microstructural patterns while reducing computational cost. These findings highlight the potential of GNNs as scalable, generalizable surrogate models for multiscale analysis in composite materials, facilitating efficient reliability evaluation and materials design.

Keywords: Machine learning, graph neural network, fiber reinforced composite, microscopic stress

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Multidirectional Wave Propagation and Higher-Order Topological States in 3D Acoustic Metamaterials

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Achieving high-quality wave concentration and manipulation is a longstanding goal in integrated photonics and phononics, yet energy loss due to backscattering and structural imperfections remains a significant challenge. The emergence of topological insulators—materials that support robust, nontrivial edge states while maintaining insulating behavior in the bulk—offers a promising strategy to overcome these limitations. However, most existing designs are constrained to two-dimensional (2D) systems, limiting waveguiding capabilities to specific hinges or planar directions. In this work, we propose a three-dimensional (3D) acoustic topological insulator with full spatial degrees of freedom to enable lossless and robust multidirectional wave transport. The system's dispersion relations are theoretically analyzed using an equivalent electrical circuit model, allowing the characterization of topological states at various orders. By carefully tuning intra- and inter-cell couplings, we realize a hierarchy of topological modes, including third-order point-like corner states, second-order one-dimensional hinge states, and first-order two-dimensional surface states. These distinct topological phases enable spatially confined wave propagation at increasing levels of geometric localization. Notably, we demonstrate a twisted 3D waveguiding path that channels acoustic energy along complex trajectories without significant leakage into the surrounding bulk or surfaces. This result illustrates the potential for higher-order topological insulators to achieve unprecedented control over acoustic wave transport in 3D structures. Our findings provide a new framework for designing advanced acoustic metamaterials and may open new avenues for robust, compact, and multifunctional acoustic devices in future integrated systems.

Keywords: directional bandgap, robust 3D waveguiding, topological hinge state, topological corner state

Real-time Response Estimation of Time-Dependent PDEs via Causality-Aware Physics-Informed Machine Learning: Robustness to Unmodeled Effects

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In this study, we propose a causality-aware Physics-Informed Machine Learning (PIML) framework for real-time inference of full-field transient responses in time-dependent Partial Differential Equations (PDEs) using sparse sensor measurements. As shown in Fig 1, the framework incorporates temporal causality to address limitations of naive PIML approaches, such as slow convergence and convergence to trivial solutions. Two representative model architectures are considered: (1) a PIML-based surrogate model (PBSM), which takes sensor data as input and modifies the loss function for multiple-instance settings, and (2) a PI-DeepONet, which employs a branch network for sensor-based instances and a trunk network for spatiotemporal coordinates to learn solution operators. Both models are designed to solve time-dependent PDEs with strong extrapolation capability.

To validate their effectiveness, we apply the proposed methods to benchmark PDEs, including cases with unmodeled effects such as structural damping. Results show that both causal PBSM and PI-DeepONet accurately capture complex behaviors using only a few sensors and significantly outperform naive models in relative L2 error. Trade-off studies on key hyperparameters further confirm the stability and robustness of the framework. These findings demonstrate that the causality-aware PIML framework provides a reliable and efficient solution for real-time full-field inference of time-dependent PDEs under unmodeled conditions and limited sensor data.

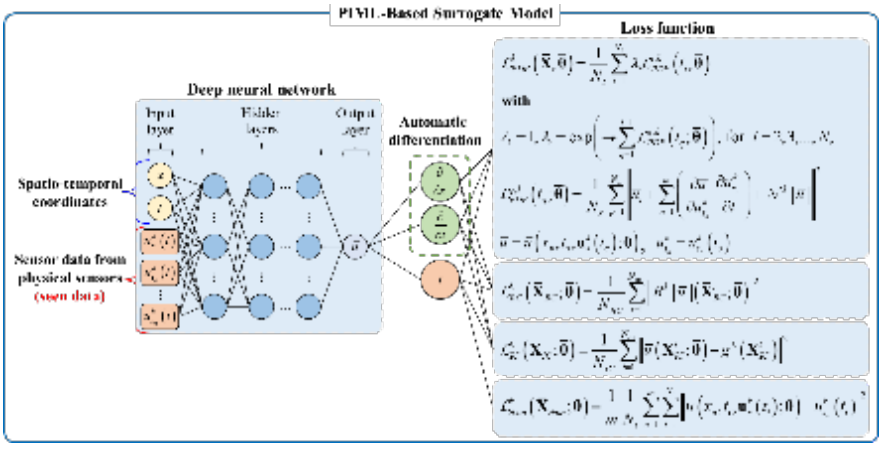

Figure 1.

Keywords: physics-informed machine learning, temporal causality, long-time integration, surrogate model, real-time simulation, unmodeled effect

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Real-time dynamic response estimation of beam/plate system using a physics-informed machine learning considering temporal causality

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In this study, we propose a method for real-time inference of the global response of time-dependent partial differential equations (PDEs) using a spatial measurement data obtained from physical sensors. This method is applied to beam and plate systems to infer their dynamic responses in real time. To achieve this, we introduce two surrogate modeling approaches: a PINN-based surrogate model (PBSM) [1], which combines conventional physics-informed neural networks (naïve PINN) with temporal causality integration via Causal PINN [2] for accurate initialization and sequential learning over time; and a physics-informed operator learning framework based on PI-DeepONet, designed for efficient inference under high-dimensional inputs and multi-response prediction in time-dependent PDE problems. To validate their performance, we applied them to Euler-Bernoulli and Timoshenko beam system problems and inferred their dynamic responses over time. The results demonstrate that even with a limited amount of measurement data, the proposed models can achieve highly accurate real-time inference in both interpolation and extrapolation scenarios. Finally, we aim to extend the proposed surrogate models to two-dimensional problems, such as Mindlin and Kirchhoff plates, and perform dynamic response inference for these systems.

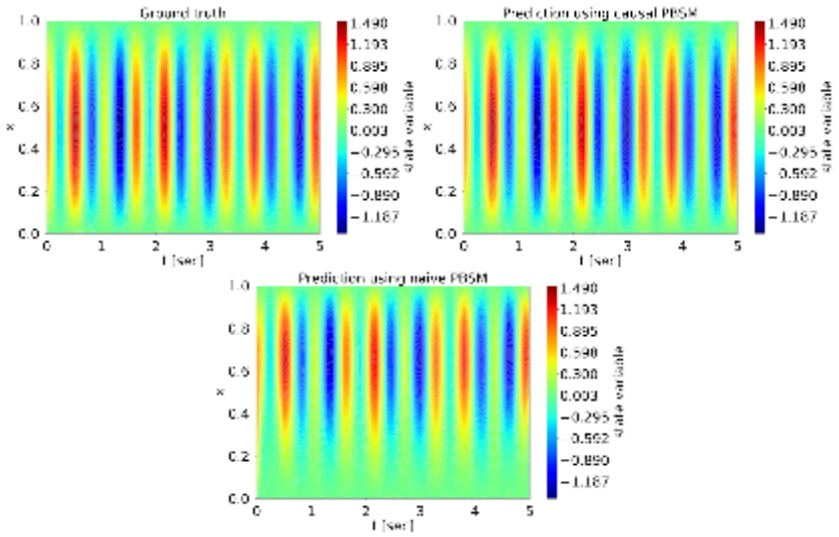

Figure 1.

Keywords: Physics-informed machine learning; Temporal causality; Euler-Bernoulli/Timoshenko beam system; Mindlin/Kirchhoff plate system; Dynamic response.

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The pressure-based flux reconstruction method for flow in elastocaloric cooling pipes

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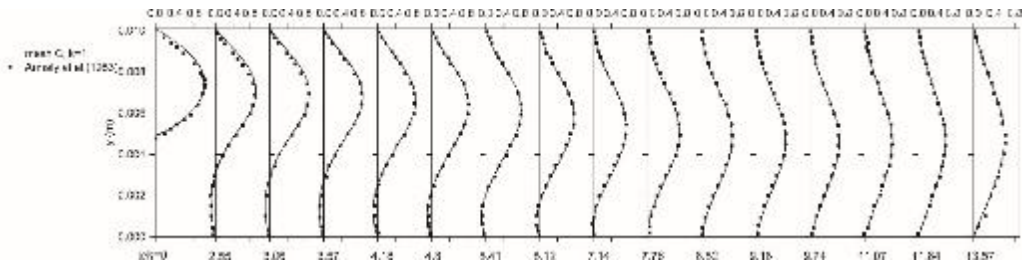
Abstract The flux reconstruction method can improve precision by increasing the number of nodes in elements. Even though there is no integration, it can be equivalently equivalent to the discontinuous Galerkin method by using special correction functions. In this paper, we propose a pressure-based flux reconstruction method to improve the convergence for incompressible flow, so that one can simulate the flow in complex cooling pipes both accurately and efficiently. The proposed method employs the generalized momentum interpolation method to avoid non-physical oscillations in pressure caused by the lack of an equation for pressure, where the mass flux can be computed using

$$
\begin{aligned}
m_j^C(\xi_i) &= N_\alpha(\xi_i)\left[\rho\left(\overline{v}_j - \overline{v}_{jp} + v_{jp}\right)\right]^\alpha \\
&+ g^L(\xi_i)\left[\left[\rho\left(\overline{v}_j - \overline{v}_{jp} + v_{jp}\right)\right]^{(F)}_{(\xi_i=-1)} - \left[\rho\left(\overline{v}_j - \overline{v}_{jp} + v_{jp}\right)\right]^{(e)}_{(\xi_i=-1)}\right] \\
&+ g^R(\xi_i)\left[\left[\rho\left(\overline{v}_j - \overline{v}_{jp} + v_{jp}\right)\right]^{(F)}_{(\xi_i=1)} - \left[\rho\left(\overline{v}_j - \overline{v}_{jp} + v_{jp}\right)\right]^{(e)}_{(\xi_i=1)}\right].
\end{aligned}
$$

Different from the artificial compression method, mass conservation is ensured in each iteration step in the proposed pressure-based method. The proposed method is verified using the backward-facing step flow and the velocity profiles agree well with that in literature as in the following figure



In this paper, we use turbulent equations in logarithmic form to avoid negative interpolated turbulent variables in the boundary layer. The classical benchmark cases are computed using the proposed method, and the results show better accuracy compared with the second-order finite volume solver. Then, the proposed method is used to study the conjugate heat transfer between fluids and elastocaloric cooling pipes.

Key words: the flux reconstruction method, the generalized momentum interpolation, incompressible flow, conjugate heat transfer, elastocaloric cooling

Advances of AI-enabled material multiscale modeling in LS-DYNA

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Modern manufacturing techniques produce advanced materials with heterogeneous microstructures, which are challenging to model using phenomenological constitutive laws and calibrated by mechanical tests. To resolve the issue, concurrent micro-macro mechanical simulation is accurate but computationally infeasible. Hence, it is essential to develop AI-enabled material multiscale analysis to fill the gap and accelerate virtual product development for industrial digitalization.

In this talk, we will present an AI-enabled material multiscale simulation workflow for industrial-level applications. This AI-enabled workflow is driven by the physics-based deep material network (DMN) which was proposed and developed by LS-DYNA in 2019 for short fiber-reinforced composite materials [1]. The key feature that distinguishes DMN from other neural networks is that it recognizes heterogeneous microstructure patterns in linear elastic training data to make efficient online prediction of nonlinear material behaviours in macroscale. First industrial application of DMN was released in 2022 Ansys LS-DYNA for multiscale structural analysis of injection moulded short fiber-reinforced bumper cover [2]. Recent version of Ansys/LS-DYNA DMN introduces a micro-damage model in DMN for short fiber composite failure prediction [3], thereby offering a useful AI-enable multiscale modeling approach for material design and virtual mechanical tests for injection-molded fiber composites. This talk will be concluded by discussing opportunities and challenges beyond DMN short fiber composites analysis.

Keywords: Deep material network, machine learning, multiscale and material modeling, short fiber-reinforced composites, multiscale structural failure analysis, Ansys LS-DYNA.

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39th Annual Technical Conference, US-Japan Joint Symposium, D30 Meeting, October 21-23, 2024, San Diego, California, USA

Flow Field Prediction for High-Speed Trains Using Vortex Generators Based on Deep Learning

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The increased speed of high-speed trains results in higher aerodynamic drag, which causes a significant wasted energy. The flow field at the rear of the train can be adjusted by deploying vortex generators in the tail car, thereby improving the train drag. Traditional methods require extensive computational fluid dynamics simulations, resulting in high computational and time costs. In this study, a deep neural network (DNN) model is developed to establish the relationship between the geometric parameters of the train tail vortex generator and the aerodynamic characteristics of the tail of a high-speed train. The design space was explored using a Latin hypercube sampling methodology based on sample data derived from Reynolds-averaged Navier-Stokes simulation post-processing results. The simplified mathematical expression of the middle is as follows:

$$C_d^j = f\left(c_k^j; w, b\right) \tag{1}$$

where c_k represents the shape of the vortex generators; w and b represents the parameters of DNN respectively; C_d represents the prediction results of drag coefficient. Cross-validation results show that the DNN has a higher prediction accuracy than conventional agent models and a higher degree of interpretability for the prediction process. The results demonstrate that the proposed DNN model provides a computationally efficient method for the design of eddy current generators for high-speed trains.

Keywords: Deep learning, High speed train, Vortex generator, Flow prediction

References

Machine Learning-Driven Exploration of the Mechanical Properties of Non-Equiatomic FeCoNiCrTi High-Entropy Alloys

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High-entropy alloys (HEAs) are emerging as promising candidates for structural applications due to their unique multi-elemental compositions and exceptional mechanical properties. Among these, FeCoNiCr-based HEAs have drawn significant attention; however, their mechanical performance at room temperature remains suboptimal. In this study, we investigate a non-equiatomic variant of FeCoNiCrTi HEAs, incorporating Ti as a strengthening element, to assess the compositional influence on mechanical behavior.

In the present study, first-principles calculations based on Density Functional Theory (DFT) using VASP were performed to generate potential energy datasets for face-centered cubic FeCoNiCrTi alloys with varying atomic ratios. These data were used to train Deep Potential models via the DeePMD-kit framework, enabling efficient and accurate large-scale molecular dynamics simulations with LAMMPS. Mechanical properties, including elastic moduli and Poisson's ratio, were computed using the stress-strain method. Finally, multivariate regression analysis was applied to elucidate the correlation between atomic composition and mechanical response.

The integrated approach demonstrates that machine learning interatomic potentials can effectively bridge the accuracy of DFT with the scalability of classical MD, offering an efficient route to explore the vast compositional space of HEAs. The results provide theoretical guidance for the rational design of non-equiatomic HEAs with tailored mechanical properties.

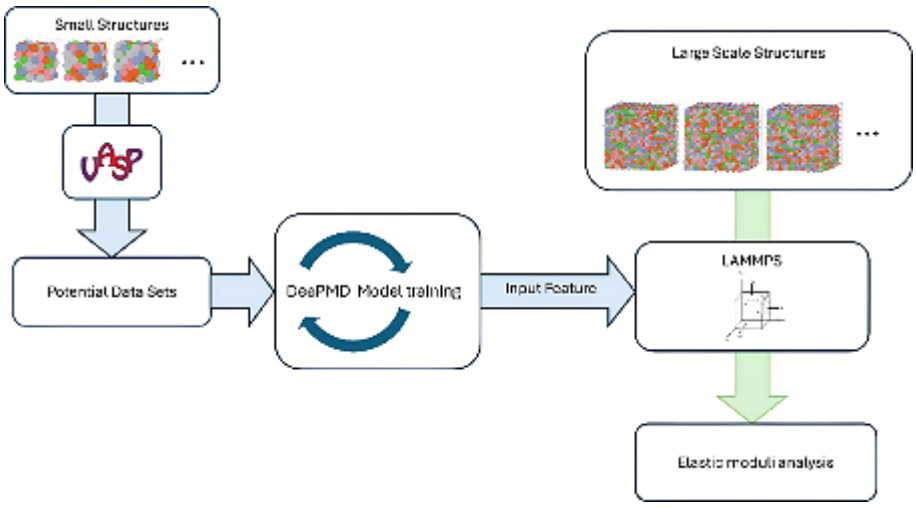

Figure 1. Computational workflow of DFT data generation (VASP), potential training (DeePMD-kit), and mechanical property prediction (LAMMPS) for FeCoNiCrTi HEAs.

Keywords: high-entropy alloys (HEAs), FeCoNiCrTi, machine learning, interatomic potential, mechanical property

Three-Dimensional Topological Derivatives in Anisotropic Elasticity: Theory and Applications

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The concept of topological derivatives has emerged as a powerful tool in structural optimization, enabling the systematic identification of regions where material addition or removal improves performance. This paper presents a rigorous derivation and application of three-dimensional topological derivatives within general elasticity theory, building upon Eshelby's solution for inhomogeneities in elastic media. Eshelby's tensor, originally formulated to describe elastic field perturbations due to embedded inclusions, forms the foundation for the asymptotic expansion used in topological sensitivity analysis.

We first revisit Eshelby's classical solution and its role in modeling inhomogeneous materials. The polarization tensor's fundamental role in capturing perturbations caused by small inclusions is examined in detail. We then extend this framework to develop a general formulation for the three-dimensional topological derivative, which quantifies the sensitivity of a given objective function to infinitesimal material modifications. The derivation uses an asymptotic expansion, with the leading-order term capturing the first-order influence of a vanishingly small inclusion on structural response.

The theoretical framework is validated through numerical implementations based on the finite element method (FEM), with the evaluation of polarization tensors conducted using FreeFem++ and Octave. Numerical results for isotropic and anisotropic elastic materials show excellent agreement with analytical predictions, confirming the robustness of the proposed approach.

A key contribution of this study is the explicit formulation of topological derivatives for three-dimensional anisotropic elasticity, significantly extending previous work primarily limited to isotropic materials. The results provide new insights into how material anisotropy affects sensitivity fields and offer new possibilities for optimizing advanced composite materials and metamaterials.

Finally, we discuss practical engineering applications, including structural optimization, damage detection, and computational material design. This work establishes a unified bridge between classical Eshelby theory and modern three-dimensional topological optimization techniques. Future research will expand this framework to nonlinear elasticity and multiphysics problems, broadening its relevance across engineering and applied sciences.

Keywords: Three-dimensional topological derivative, Eshelby tensor, polarization tensor, structural optimization, anisotropic elasticity, finite element method, FreeFem

Keywords: Three-dimensional topological derivative, Eshelby tensor, polarization tensor, structural optimization, anisotropic elasticity, finite element method, FreeFem

Local RBF Based Meshfree Scheme to Simulate Mixed Convection in a Square Cavity with Moving Walls and Elastic Heat Sources

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Abstract

This study investigates the numerical behavior of mixed convection flow in a square lid- driven cavity with the top and left walls in motion and an elastic, heat-generating porous elliptical cylinder centrally positioned. The flow within the enclosure is driven by both the motion of the walls and buoyancy forces, and the porous medium is modeled using the Brinkman–Forchheimer–extended Darcy formulation. The dimensionless governing equa- tions for an incompressible, laminar, Newtonian fluid in two dimensions, incorporating the Boussinesq approximation, are given by:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0,$$

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\mathbf{u}}{\xi}\frac{\partial \mathbf{u}}{\partial x} + \frac{\mathbf{v}}{\xi}\frac{\partial \mathbf{u}}{\partial y} = -\frac{\xi}{\partial x}\frac{\partial \mathbf{p}}{} + \frac{1}{Re}\nabla^2\mathbf{u} - \frac{\xi}{DaRe}\mathbf{u} - \frac{\xi F_\xi}{\xi F_\xi}\sqrt{\mathbf{u}^2 + \mathbf{v}^2},$$

$$\frac{\partial v}{\partial t} + \frac{u}{\xi}\frac{\partial v}{\partial x} + \xi\frac{\partial p}{\partial y} = -\xi\frac{\partial^2 v}{\partial y^2} + \frac{1}{Re}\nabla^2 v - \frac{\sqrt{Da}}{Re}v - \sqrt{Da}\,v^2$$

$$\frac{\partial \theta}{\partial t} + u\frac{\partial \theta}{\partial x} + v\frac{\partial \theta}{\partial y} = \frac{1}{\quad}\nabla^2\theta,$$

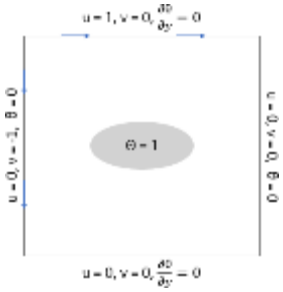
$$d^2\mathbf{d_s} - \rho E\nabla\sigma = \rho E\mathbf{F};$$

$u + v$

$+ \xi Ri\theta,$

$$\frac{\partial t}{\partial x} \quad \frac{\partial y}{PrRe}$$

$$\frac{}{dt^2}$$



where, $\mathbf{d_s}$ is solid displacement vector, E is modulus of elasticity, σ is stress tensor and $\mathbf{F}$ is applied body force. The porous medium is assumed to be isotropic and homogeneous, with constant perme- ability $\kappa(= Da.L^2)$ and porosity ξ and identical thermal diffusivity is assumed for both the solid and fluid phases. To simulate fluid flow in the absence of a porous medium, the system (1). The cou- pled nonlinear equations are discretized using a local radial basis function (RBF)-based meshfree method, and the resulting algebraic system is solved iteratively using techniques such as successive over- relaxation or the bi-conjugate gradient stabilized method. is em-

ployed to solve the resulting algebraic system. The computed results are presented in the form of streamlines, isotherms, entropy generation due to viscous dissipation and heat trans- fer, velocity profiles, average Nusselt number plots (Nu) and Bejan number (Be) plots with variations depending on parameters such as Richardson number ($0.01 \leq Ri \leq 100$), Prandtl number ($Pr = 0.71, 6.946$) and Darcy number ($10^{-6} \leq Da \leq 10^{-2}$).

Keywords: Porous elastic heat sources; Brinkman and Forchheimer-corrected Darcy model; Radial basis function; Local RBF scheme; Modulus of elasticity.

Enhanced thermo-hydro-mechanical coupling for anisotropic geomaterials and its smoothed-FEM simulation

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In submarine engineering, pipelines buried in soil or laid on the seabed for oil and gas transportation are vulnerable to thermally induced buckling under unfavorable conditions, potentially resulting in catastrophic failure. Despite the significance of thermal effects, existing studies on submarine pipelines often overlook the influence of temperature on the surrounding soil, highlighting the need for a comprehensive understanding of thermo-hydro-mechanical coupling in porous geomaterials.

This study first revisits the established poromechanics theory and advances it by (1) deriving a generalized fluid flow equation that accounts for both mechanical and thermal strain anisotropy, expressed as:

$$\boldsymbol{b}:\frac{d\boldsymbol{\varepsilon}}{dt}+(\mathbf{1}-\boldsymbol{b}):\frac{d\boldsymbol{\varepsilon}^{p}}{dt}-\beta_{\text{ave}}\frac{d\Theta}{dt}+\frac{1}{M}\frac{dp}{dt}+\frac{\nabla\rho_f}{\rho_f}\cdot\boldsymbol{q}_f+\nabla\cdot\boldsymbol{q}_f=0 \tag{1}$$

where, $\boldsymbol{\varepsilon}$ is the total strain, $\boldsymbol{\varepsilon}^{p}$ is the plastic strain, $\boldsymbol{b}$ is the Biot coefficient, $\mathbf{1}$ is the second-order identity tensor, β_{ave} is the generalized bulk average volumetric thermal expansion coefficient, Θ represents the single temperature field, M is the generalized Biot modulus, ρ_f is the intrinsic density of fluid, p is the fluid pressure, $\boldsymbol{q}_f$ is the Darcy velocity, and (2) proposing a poro-elasto-plastic structural heating/cooling term that bridges not only the phenomenological porothermoelasticity but also the uncoupled standard thermal equation. To capture the enhanced coupling effects numerically, the stabilized node-based smoothed finite element method is enriched to incorporate thermo-hydro-mechanical coupling through the development of smoothed nodal thermal strain and thermal strain gradient.

The proposed numerical framework is validated through three benchmark tests that assess the implementation of heat convection, thermo-hydro-mechanical contact behavior, and consistency with conventional finite element solutions. Finally, two hypothetical case studies are presented: one examining the influence of mechanical anisotropy and cross-coupling in a biaxial test, and the other investigating temperature effects on pipeline penetration, demonstrating the framework's applicability to complex geomechanical problems.

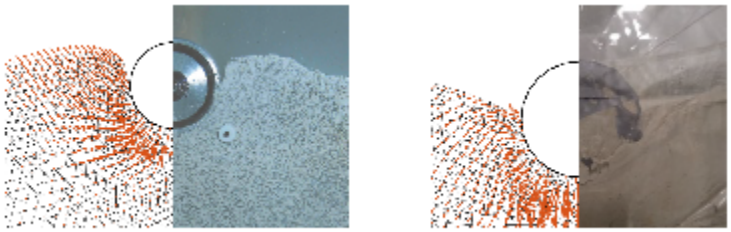

Figure 1.

Keywords: Poromechanics, Thermo-hydro-mechanical coupling, S-FEM, Anisotorpy, Submarine pipeline

3-D Tetrahedral Mesh Generation Based on Advancing Front Method and Its Application to Fracture Mechanics

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A huge scale parallel structural analysis using the finite element method on various kinds of massively parallel supercomputers, such as K Computer and Fugaku, enables fracture analysis of a real world highly complicated model. Through the whole simulation task including its pre- and post-processing, however, now the mesh generation step becomes the clear bottleneck. Handling crack geometry for fracture analysis is a tough work, especially if crack propagation process is involved.

Currently, we are developing a fast and robust tetrahedral mesh generation technique based on the advancing front method. Here with this method, assuming a tetrahedral mesh model without crack geometry has already been available, a crack of arbitrary shape and at arbitrary location can be inserted into the existing mesh using the advancing front method.

Detail of the mesh generation algorithm will be explained and some examples of huge scale mesh generation will be demonstrated in the presentation.

Keywords: finite element method, mesh generation, tetrahedral element, large scale analysis, advancing front method

3D Numerical Simulation of Intermittent microwave- convective Drying(IMCD) using Dehumidified Air: Multi-sample configuration on food material

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The increasing demand for energy-efficient and quality-preserving drying methods has accelerated research into hybrid drying systems. Among these, IMCD using dehumidified air has shown promising results due to its enhanced moisture removal, reduced drying time, and improved product uniformity. However, existing models often fail to consider the spatial variations in airflow and energy distribution, especially in multi-sample drying setups, leading to inaccurate predictions of drying behavior.

This study presents a **3D numerical simulation** of IMCD applied to multiple **cylindrical apple samples,** incorporating **computational fluid dynamics (CFD)** and **volumetric microwave heating** using Maxwell's law. The model solves coupled heat and mass transfer equations. Heat transfer (HT)is governed by:

$$\rho C_p \frac{\partial T}{\partial \mathrm{t}} = \nabla.(k_{eff} \nabla T) + Q_{mw}, \quad (1)$$

Where ρ is the density, C_p is specific heat capacity, k_{eff} is the effective thermal conductivity, T is temperature and Q_{mw} Maxwell's equations to resolve the microwave heating.

Moisture transport (MT) is described using Fick's law:

$$\frac{\partial c}{\partial \mathrm{t}} + .(-D_{eff} \nabla c) = 0 \quad (2)$$

Where c **moisture concentration** within food material, D_{eff} **effective moisture diffusivity.**

The results show notable spatial variability in heat and mass transfer coefficients (HTC and MTC) due to uneven airflow and microwave absorption across the sample surface. The model closely matches experimental drying kinetics, while models without airflow coupling tend to overestimate moisture loss and temperature. Temporal and spatial surface variations significantly influence heat and moisture transport, especially in later drying stages. This integrated modeling framework offers a reliable tool for predicting drying behavior and provides practical insights for scaling up hybrid dryers, improving energy efficiency, and ensuring product quality in industrial-scale IMCD applications.

Keywords: Heat and mass transfer, hybrid drying, dehumidified air, apple drying, spatial and temporal distribution.

Study on the application of generative models to 3D turbine blade design.

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In general product design, there is a need in the conceptual design phase to generate and compare various shapes rather than optimise them. On the other hand, due to the high dimensionality of the design variables and the high cost of analysis, skilled skills, know-how and long calculation times are required to create shapes that satisfy the required conditions. The design of turbine blade geometries in jet engines is a prime example.

Recently, it has been shown that conditional diffusion models are effective in 2D airfoil shape generation [1] and that shapes can be generated conditional on prescribed aerodynamic performances such as lift and drag coefficients [2,3,4]. However, applications to 3D turbine blades are scarce and no examples have been reported where performance metrics have been directly incorporated into the training.

This study aims to provide the systematic validation of the application of diffusion models to 3D blade optimisation of 3D turbine blade geometries, and to propose a method that can shorten the design process of turbine development and enable a wide range of geometries to be considered.

An open-source CFD platform, SU2, developed by the Computational Aerodynamics Group at Stanford University, was used for the numerical fluid dynamics calculations to solve Reynolds averaged Navier—Stokes equations written as

$$\rho\bar{u}_j\frac{\partial\bar{u}_i}{\partial x_j}=\rho\bar{f}_i+\frac{\partial}{\partial x_j}\left[-\bar{p}\delta_{ij}+\mu\left(\frac{\partial\bar{u}_i}{\partial x_j}+\frac{\partial\bar{u}_j}{\partial x_i}\right)-\rho\overline{u'_i u'_j}\right]$$

Keywords: Reynolds-averaged Navier–Stokes equations, turbo machine, conservation laws, machine learning, diffusion model

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Adaptive isogeometric analysis–based phase-field modeling of fracture in bidirectional functionally graded materials

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Functionally graded materials (FGMs) are advanced materials with spatially varying composition. This smooth gradation alleviates sharp bi-material interfaces, which are common crack initiation sites. As a result, FGMs exhibit enhanced resistance to thermal stresses and fracture, and smoother material transitions that suppress stress discontinuities. In this study, we aim to investigate the fracture behaviour of FGMs by employing phase-field modelling (PFM) in conjunction with isogeometric analysis (IGA).

A bi-directional functionally graded plate having a length L and a width W is considered. Material 1 is placed along the bottom and left edges. The volume fractions of Materials 1 and 2 at any position in the x- and y-directions obey the power law, respectively, in the form of

$$V_2 = \left(\frac{x}{L}\right)^n \left(\frac{y}{W}\right)^m$$

$$V_1 = 1 - V_2$$

where n and m are the gradient indices in the x and y-directions. The effective material property $P(x, y)$ is given by the rule of mixtures:

$$P(x, y) = P_1 V_1 + P_2 V_2$$

Figure 1 shows the material gradation for m=0.2, n=1.

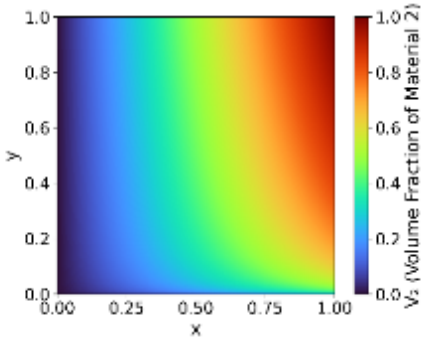

Figure 1

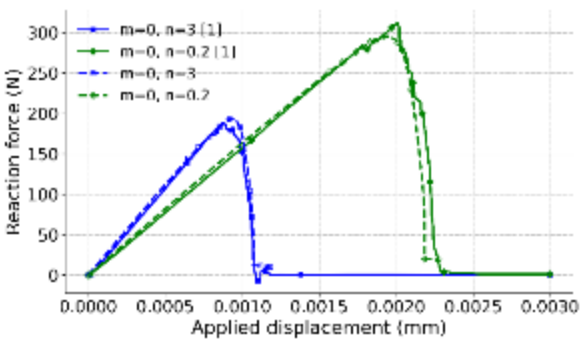

Figure 2[1]

Simulations are performed for both Mode I (opening) and Mode II (shearing) fracture scenarios. The Mode I response is validated against the literature; the simulated load–displacement and crack-growth behaviour show close agreement with reference data (refer to Figure 2). This validation confirms the accuracy of the current model in capturing fracture behaviour in FGMs.

Keywords: Functionally graded materials; Phase-field modelling; isogeometric analysis.

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Prediction of Material Properties from Cross-sectional Dendritic Microstructure Images via Machine Learning Trained on Systematic Phase-field Simulations

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Prediction and control of the solidification microstructure are crucial for improving the quality of solidified products. The solidification microstructure is formed through dendrite growth [1], which is very challenging to observe under high-temperature and opaque conditions. Therefore, it is essential to evaluate the solidification microstructure through simulation. The phase-field (PF) method [2] is known to be the only approach that can reproduce dendrite growth with high accuracy, but the lack of material properties required remain a major issue. Since traditional experimental methods to obtain the material properties have limitations in measurement accuracy, a new method for acquiring these values is required.

In this study, we focused on machine learning [3] to extract material properties from cross-sectional dendritic microstructure images, which can be relatively easily obtained through quench experiments. Since obtaining a large number of dendritic microstructure images with known material properties is impractical, we generated training data by performing phase-field simulations of dendrite growth with systematically varying the material properties. We employed a convolutional neural network (CNN) for machine learning, which has been shown to be highly effective in the field of image analysis. The developed CNN model was validated using test data.

Keywords: phase-field method, machine learning, material property, dendrite

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On the interlocking profile of nacre-like materials: design, optimization and fabrication

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Synthetic materials exhibit a wide range of mechanical properties. Ceramics and glass, for example, are known for their excellent strength and stiffness but are brittle and lack significant toughness. In contrast, metals and polymers offer good toughness but fall short in hardness compared to ceramics. Generally, pure synthetic materials do not simultaneously achieve high levels of toughness, strength, and stiffness. However, natural materials, such as bone and mollusc shells, exhibit a remarkable combination of these properties. Inspired by nature, researchers have developed strategies to create bio-inspired materials that integrate strength, stiffness, and toughness. One such approach involves interlocking structures, composed of multiple stiff material plates tessellated with an interlocking angle and separated by a bio-polymer layer. For instance, the abalone shell features a nacreous layer with numerous stacked plates. This structure is composed of 95% Aragonite, a stiff material, and 5% bio-polymer between the layers. Therefore, it can be concluded that this structure exhibits significant stiffness. Notably, it also demonstrates substantial toughness due to two primary factors. First, the presence of a bio-polymer layer between the plates enhances toughness. Second, the plates can slide slightly on top of each other, which contributes to the overall toughness of the structure. Researchers have explored these interlocking structures by mimicking bio-inspired geometry. Most studies have focused on bow-tie geometry plates, which interlock with adjacent plates. Despite researchers efforts, it remains uncertain whether the bow-tie geometry is truly optimal. This research aims to address this gap by designing a more general shape that includes the bow-tie as a subset. We aim to investigate nacreous structures' mechanical properties and geometrical optimization through finite element analysis (FEA) and experimental study.

Finite Element Analysis of Stress Distribution in Anterior Cervical Fusion According to Implant Type

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To evaluate the biomechanical behavior of different cervical implants in anterior cervical discectomy and fusion (ACDF), a validated three-dimensional finite element model (FEM) of the cervical spine (C3–T1) was constructed. Four models were compared: (1) Reference model without surgery, (2) CCP (conventional cage-plate implant) model, (3) ZPSC (zero-profile stand-alone cage) model, and (4) FPCS (flexible plate cage system) model.

The anatomical components included cortical and cancellous bones, intervertebral discs (annulus fibrosus and nucleus pulposus), upper and lower endplates, and posterior elements (pedicles, laminae, and facet joints). The implants were positioned at the C5–C6 level. The material properties were assumed isotropic and homogeneous, with titanium used for screws and plates, and polyetheretherketone (PEEK) for cages. Quadratic tetrahedral meshes were used with local refinement (0.7 mm for cage, 1 mm for other regions).

Loading conditions consisted of a vertical compressive force of 73.6 N and a flexion moment of 1.0 Nm applied to the superior end of C3. The inferior end of T1 was fully fixed. All implant–bone contact surfaces were modeled as fully bonded due to anatomical complexity.

The von Mises stress was evaluated as the average of the top 5% highest nodal values in each structure to avoid overestimation due to singularities. The CCP and ZPSC models showed elevated stress concentrations at the endplates and cortical bones, while the FPCS model demonstrated a more distributed stress profile, particularly at the cage–endplate interface. Among the models, the ZPSC model exhibited the highest stress in the screw region, while the reference model consistently exhibited the lowest stresses.

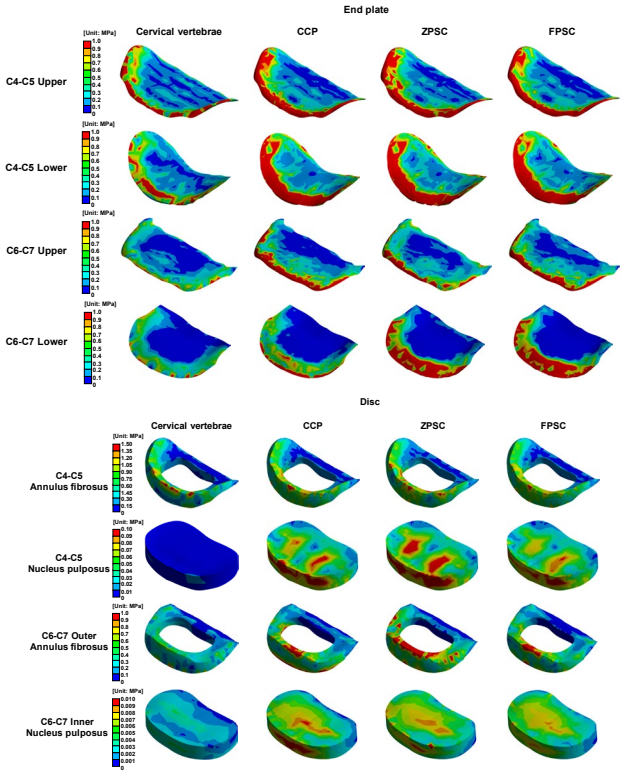

Figure 1. von Mises stress results at each structure in four different models

These findings suggest that implant design significantly influences local stress distribution and may affect long-term stability and subsidence risk. The FPCS model may offer a biomechanical advantage by reducing peak stresses without the drawbacks associated with plate removal or anterior prominence.

Keywords: anterior cervical fusion, finite element method, cervical implant, stress distribution, cage subsidence, spinal biomechanics

A quantitative understanding of glymphatic transport and amyloid deposition using image-based subject-specific modelling

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The glymphatic system is a brain-wide network of perivascular pathways that facilitates waste clearance by enabling solute exchange between cerebrospinal fluid (CSF) and interstitial fluid (ISF). Dysfunction in this system can lead to the accumulation of amyloid beta (Aβ) and tau proteins—key hallmarks of Alzheimer's and other neurodegenerative diseases. A mechanistic understanding of glymphatic transport and deposition of these biomarkers is essential for developing strategies to prevent or slow disease progression. However, characterization of the glymphatic system in pre-clinical models remains limited. In this work, we developed an image-based, subject-specific computational framework—tightly integrated with experimental data—to enable a quantitative analysis of glymphatic transport and protein deposition throughout the brain.

Amyloid transport and deposition are modelled through an unsteady advection–diffusion equation of soluble amyloid, c (nM), coupled with an irreversible amyloid plaque deposition model [1]:

$$\frac{\partial c}{\partial t} = \boldsymbol{\nabla} \cdot (D\, \boldsymbol{\nabla} c) - \boldsymbol{\nabla} \cdot (c\, \boldsymbol{u}) + S^{+} - \frac{\partial P}{\partial t} \tag{1}$$

Here, D is the diffusivity of soluble amyloid molecules (mm^2/min), $\boldsymbol{u}$ is the CSF velocity vector in mm/min, and S^{+} represents soluble amyloid production due to neural activity (nM/min). The last term in Eq.(1) models plaque accumulation, P (nM), by allowing for soluble amyloid to agglomerate and convert to fibrilized plaque. We use immersed isogeometric analysis, stabilized using the streamline upwind Petrov-Galerkin (SUPG) method, where the transport model is constructed using parameters inferred directly from brain imaging data resulting in a subject-specific model accounting for anatomical geometry and heterogeneous material properties. The diffusive field and the subject-specific brain geometry are extracted from diffusion-weighted magnetic resonance imaging (DW-MRI) data of a mouse brain. The advective field is reconstructed by solving the inverse problem of velocity estimation, informed by contrast-enhanced MRI (CE-MRI) data acquired through tracer injection into the CSF via the cisterna magna. The CE-MRI is performed over a two-hour period at discrete time points to capture the dynamics of tracer transport. Finally, plaque deposition model parameters are calibrated against CE-MRI-based estimation of amyloid plaque burden in 2-month- and 7-month-old subjects through an inverse problem approach. The model predictions are then compared against plaque deposition data from 12-month-old subjects. By integrating imaging, image processing, computational simulations, parameter tuning, and model validation, the framework offers a robust pipeline for predicting brain-wide glymphatic transport and Aβ deposition. It provides a valuable tool for studying

the role of glymphatic dysfunction in the progression of neurodegenerative diseases, thereby paving the way for subject-specific prevention and treatment strategies.

Keywords: isogeometric analysis, immersed methods, THB-splines, neurodegenerative diseases

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Multiscale models and computational strategies for linking process, structure, and performance in AM parts

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Understanding and predicting the mechanical properties and performance of additively manufactured (AM) components across different length scales remains a major challenge. To address this, we have developed a suite of multiscale integrated models tailored for AM parts, capturing key features from melt pool formation through to grain structure and component-scale mechanical response.

The computational framework includes melt-pool-scale thermal simulations using the finite difference method, microstructure evolution modelling via cellular automata [1], and micromechanical simulations using crystal plasticity finite elements. An analytical method based on the Voigt–Reuss–Hill (VRH) averaging scheme is also incorporated to estimate anisotropic elastic properties over larger volumes, supporting efficient and predictive modelling. All models have been validated experimentally for laser powder bed fusion alloys, with some extension to directed energy deposition.

A key outcome of this work is the ability to link process conditions to mechanical performance taking into account microstructure features. By optimising our in-house cellular automata and finite difference code with OpenMP parallelisation, we achieved the simulation of grain structure evolution in a printed part exceeding 1,000 mm³ in volume using a single workstation [2]. The predicted microstructures exhibit strong agreement with experimental data. These capabilities enable the design and optimisation of AM processes with part-scale performance in mind.

Looking forward, this scalable simulation framework offers a pathway to bridging local microstructural predictions with part-scale mechanical behaviour through segmentation and homogenisation techniques. By partitioning the component domain into microstructure-informed regions and applying effective property models, it becomes possible to incorporate grain-level features into larger-scale simulations. This approach supports the digital design and optimisation of AM parts with spatially varying properties, advancing integrated computational materials engineering for additive manufacturing.

The authors acknowledge the UNSW Resource Allocation Scheme at National Computational Infrastructure [project mz70].

Keywords: Metall additive manufacturing, Multiscale modelling, Mechanical performance, Process–structure–property relationships, Finite elements

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Calibration of Discrete Element Method contact law parameters on multiple soil mechanics element tests

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Calibration of Discrete Element Method (DEM) models consists of determining a relatively small number of micromechanical parameters to describe the contact forces that develop between numerical particles. These micromechanical parameters, which depend on the adopted contact law, are not physically related to any specific soil mechanics tests and this renders their calibration for geotechnical engineering applications cumbersome: Contact law parameters are interdependent, and there may exist multiple parameter combinations that result in similar macromechanical predictions. To streamline the use of DEM in practical geotechnical engineering applications, we have developed a method for the systematic calibration of contact law parameters, informed by measurements obtained during multiple soil mechanics element tests. Our aim to offer analysts a rigorous procedure to obtain a single set of contact law parameters to describe the macromechanical behaviour of coarse-grained soils at different densities, subjected to different stress paths under varying stress levels. Details about the method, which is based on the Bayesian calibration framework "GrainLearning" of Hartmann *et al.* [1], are provided in Li *et al.* [2, 3]. The method consists of performing first a series of soil mechanics tests (e.g., isotropically-consolidated triaxial compression tests, Constant-Rate-of-Strain one-dimensional compression tests or Direct Shear tests) on specimens prepared at different densities, subjected to varying confining stresses. Of pivotal importance is to use element tests involving stress paths relevant to the analysed problem. Numerical DEM models are then prepared to replicate the selected experiments, using spherical particles that feature particle size distribution similar to that of the real material, while scaling their mean diameter. The calibration algorithm requires providing as input an initial range of contact law parameters, to sample parameter values from. Calibration of the parameters is iterative: During each iteration we sample N_p parameter sets and we perform N_p sets of soil mechanics test simulations. Each simulation set may involve multiple tests, including tests imposing different stress paths. From each simulation set we collect predictions of micromechanical response (e.g., stress-strain curves) and we compare these predictions with the test measurements. Accordingly, we update the probability distribution of each contact law parameter, to inform resampling of parameters from the input range for the next iteration. The process is repeated until we find an "optimal" parameter set, that minimises the error between DEM predictions and measurements. Comparisons of predictions obtained with DEM models incorporating the described calibration procedure against experimental measurements are provided in Li *et al.* [2, 3]. There we show that the method provides excellent blind predictions of the response observed in physical model tests of boundary value problems, without having to resort to "back-analysis".

Keywords: Discrete Element Method; Contact law; Calibration

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Nanoscale Elasticity and Adhesion of Solid-state Electrolyte

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Solid-state lithium-ion batteries have attracted much attention in recent years for their high energy density, high safety, and high flexibility, and thus are regarded as the next-generation lithium batteries. Solid-state batteries that are based on polymer solid-state electrolytes (SSEs) are of good choice for their low price and high flexibility. The mechanical properties of polymer SSEs on a nano-scale are still unclear especially considering the effectiveness of lithium-salt concentration inside. Increasing lithium salt benefits the ionic conductivity increment of SSEs, but sacrifices the softness and flexibility of SSEs. Optimizing the composition to pursue a balance between mechanical robustness and ionic conductivity in SSEs is a precondition for the application of polymer SSEs. Given the heterogeneous nature of these solid-state electrolytes (SSEs), gaining a deep understanding of their complex mechanical behavior at the nanoscale is both fundamentally significant and highly challenging. In this study, the nanomechanical properties of polymer-based SSEs, such as elasticity and adhesion, were investigated using advanced Scanning Probe Microscopy (SPM) techniques. The elasticity of these SSEs exhibited a strong correlation with the morphological characteristics of the different microconstituents within the electrolytes, while adhesion was less influenced by compositional distribution. Additionally, it was demonstrated that both high elasticity and adhesion can be achieved in these polymer-based SSEs, attributed to the enhanced dissolution of lithium salt at elevated temperatures. Notably, the nanomechanical analysis revealed that the interface region of the polymer-based composite SSEs displayed unique characteristics, featuring moderate elasticity alongside exceptionally high adhesion. This study offers valuable insights into the nanomechanical properties of polymer-based SSEs, contributing to a deeper understanding of the underlying mechanisms. These findings can serve as a guide for future microstructure and compositional design strategies for SSEs.

Keywords: Mechanical properties; battery; solid-state electrolyte; SPM

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Simulation of heavy mining vehicle impacts on safety barriers

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Safety barriers such as standard safety berms (also called windrows or edge protectors) are critical for preventing fatal vehicle accidents in open-cut mining operations. Traditional design guidelines rely on simple rules of thumb, which fail to address the complex dynamics of vehicle-structure interactions. In addition, such guidelines do not take into account non-standard safety barriers such as gabions and Jersey-type barriers. Hence, there is a need to develop a dynamic simulation framework that allows the accurate representation of such vehicle-structure interactions.

The study integrates full-scale experimental testing with advanced numerical modelling to simulate various collision scenarios. The discrete element method (DEM) is used to represent the granular material whereas the structures that are either filled or placed in front of the granular material are represented using the finite element method (FEM). The heavy mining vehicle (i.e. dump truck) is modelled using rigid multi-body dynamics. The coupled model is calibrated based on data from full-scale tests, ensuring accurate reflection of real-world behaviour. The calibrated model is then used for parametric studies, exploring various factors such as approach conditions and different types of safety barriers.

The study demonstrates that advanced numerical modelling, combined with full-scale testing, offers a robust framework for designing effective safety barriers for heavy mining equipment. This approach moves beyond simplistic guidelines, providing evidence-based design standards that enhance safety in mining operations. By leveraging computational modelling, this research provides a comprehensive understanding of vehicle-structure interactions, leading to safer and more effective safety barrier designs tailored to specific site conditions.

Figure 1. Example of an articulated dump truck impacting on a standard edge protector: impact angle 30 degrees, impact speed 25 km/h.

Keywords: Dynamic impact, soil-structure interaction, discrete element method (DEM), finite element method (FEM), multi-body dynamics (MBD), coupling.

Initial Damage Prediction under Diverse Impact Conditions: The insights from Peridynamics surrogate artificial neural network

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Accurate understanding of initial damage is critical to safety and maintenance of materials and structures in real engineering applications. However, due to the limitations of conventional continuum-based models and high computational costs of newer mesh-free methods, it is challenging to efficiently and accurately simulate the initial damage under diverse impact conditions. With the emergence of the 4th paradigm——data driven methods, machine learning (ML) offers transformative opportunities for this problem. High-fidelity data of initial damage are first generated using a peridynamics (PD)-based surrogate solver, ensuring accurate capture of the initial contact between impactor and objects. Furthermore, an artificial neural network (ANN) model is trained to build the mapping relationship between varying impact conditions and corresponding initial damage. Our results demonstrate that the proposed PD-ANN model significantly outperforms traditional PD-based methods, reducing computational cost to mere tens of seconds while capturing initial damage with considerable generation capacity. This study pave the avenue for fast and accurate engineering guidance of initial damage.

Keywords: Machine learning; Neural Networks; Peridynamics; Damage

The equation of motion of OSBPD is expressed as:

$$\rho(x)\ddot{\boldsymbol{u}}(\boldsymbol{x},t)=\int_{\Omega_x}[\boldsymbol{T}(\boldsymbol{x},t)<\boldsymbol{x}'-\boldsymbol{x}>-\boldsymbol{T}(\boldsymbol{x}',t)<\boldsymbol{x}-\boldsymbol{x}'>]dV_{x'}+\boldsymbol{b}(x,t) \tag{2}$$

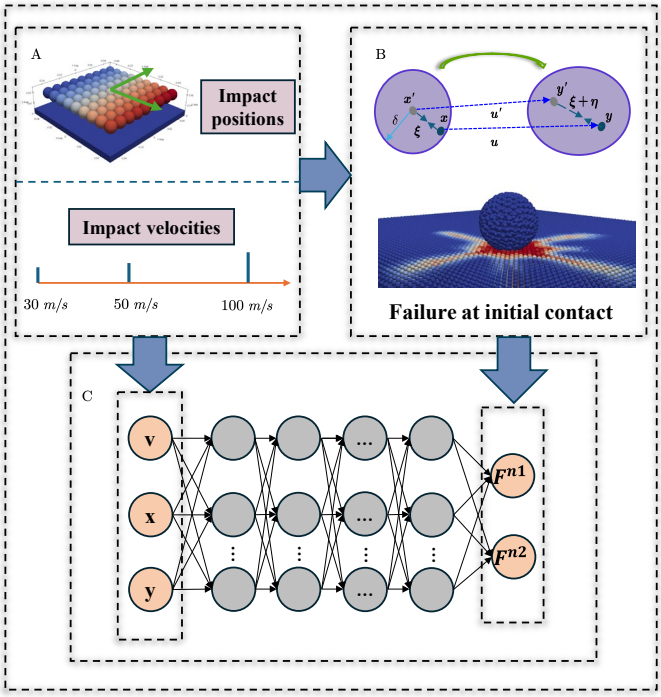

Fig. 2 The proposed framework for using a PD-based surrogate data-enriching artificial neural network (PD-ANN)

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Quantifying irregular pulsation of intracranial aneurysms using 4D-CTA

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Recent studies have suggested that irregular pulsation of intracranial aneurysms during the cardiac cycle may be potentially associated with aneurysm rupture risk. However, there is a lack of quantification method for irregular pulsations. This study aims to quantify irregular pulsations by the displacement and strain distribution of the intracranial aneurysm surface during the cardiac cycle using four-dimensional CT angiographic image data. Four-dimensional CT angiography was performed in 8 patients. The image data of a cardiac cycle was divided into approximately 20 phases, and irregular pulsations were detected in four intracranial aneurysms by visual observation. Then, the displacement and strain of the intracranial aneurysm were quantified using coherent point drift and the finite element method, as shown in Figure 1. The displacement and strain were compared between aneurysms with irregular and normal pulsations in two different ways (total and stepwise). The stepwise first principal strain was significantly higher in aneurysms with irregular than normal pulsations (0.20±0.01 vs 0.16±0.02, p=0.033), as shown in Table 1. It was found that the irregular pulsations in intracranial aneurysms usually occur during the consecutive ascending or descending phase of volume changes during the cardiac cycle. In addition, no statistically significant difference was found in the aneurysm volume changes over the cardiac cycle between the two groups [1]. Our method can successfully quantify the displacement and strain changes in the intracranial aneurysm during the cardiac cycle, which may be proven to be a useful tool to quantify intracranial aneurysm deformability and aid in aneurysm rupture risk assessment.

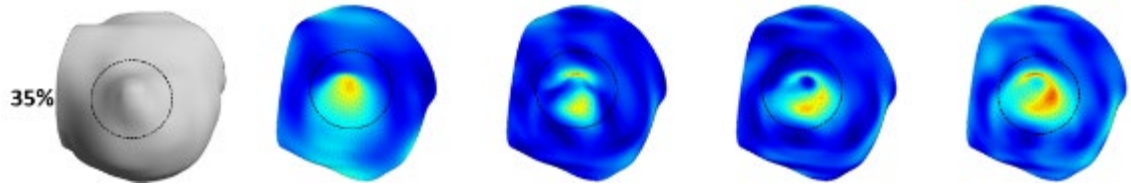

Figure 1.

	IAs with irregular pulsation	IAs without irregular pulsation	*P*
Stepwise space displacement	0.26 ± 0.04	0.25 ± 0.05	0.841
Stepwise space strain	0.20 ± 0.04	0.17 ± 0.02	0.372
Stepwise first principal strain	0.20 ± 0.01	0.16 ± 0.02	0.033
Stepwise Von Mises strain	0.24 ± 0.04	0.19 ± 0.02	0.087

Table 1.

Keywords: 4D-CTA, intracranial aneurysm, irregular pulsation, strain.

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In-vivo Blood Flow Simulation with Moving Wall Boundary for Patients with Atrial Fibrillation

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Atrial Fibrillation (AF) is the most common cardiac rhythm disorder which is characterized by irregular and often rapid heartbeats, leading to ineffective atrial contraction and consequently causing irregular atrial motion and deformation. The changes in atrial motion can further increase the risk of adverse cardiovascular events, such as stroke and heart failure. Clinically, the CHA_2DS_2-VASc score is widely accepted for assessing stroke risk in patients with atrial fibrillation. Since it solely relies on demographic and clinical factors, important information embedded in heart deformation and blood flow is often ignored. Our object is to explore effective stroke risk stratification parameters. A mesh regularized sub-volume tracking method was proposed to calculate atrial wall displacements and strain and via 4D-CTA images [1]. Subsequently, patient-specific computational fluid dynamics models simulating blood flow in the left atrium were developed. Boundary conditions at pulmonary veins (pressure) and mitral valve ring (flow rate) were computed via heart morphology data derived from 4D-CTA. Results from our blood Flow analysis were compared with those measured with Doppler echocardiography and a good agreement was found (Figure 1). Our proposed work has great potential in stroke event prevention and optimizing treatment procedures for atrial fibrillation patients.

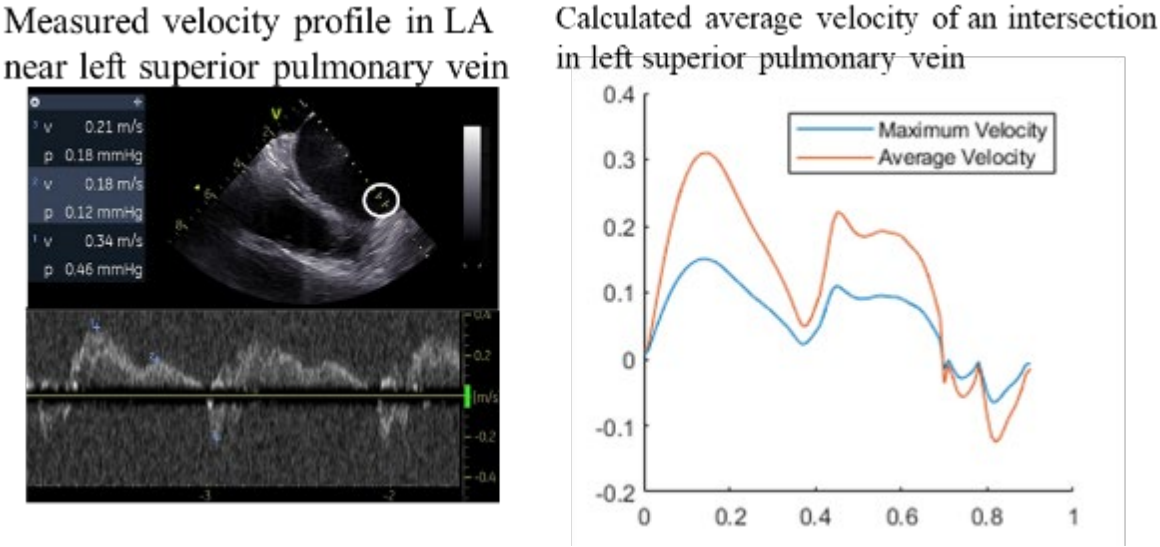

Figure 1.

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Effects of Tibial Fracture-Induced Gait Alterations on Healing Outcomes: Implications for Patient-Specific Rehabilitation Strategies

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Partial weight-bearing (PWB) exercise is critical in fracture rehabilitation. However, the effects of tibial fracture-induced gait alterations on musculoskeletal loading conditions, particularly regarding body weights and walking speeds, remain unclear. These patient-specific gait deviations can substantially modify mechanical stimuli at the fracture site, thereby affecting healing trajectories. This study aims to evaluate how fracture-altered gait mechanics influence loading conditions during rehabilitation to inform patient-specific strategies. A gait-based biomechanical model was developed to simulate PWB walking in patients with tibial fractures, based on changes in ground reaction forces (GRFs) compared to the uninjured limb. Fracture-induced effects on joint and muscle loading rates were quantified and integrated into the fracture healing model, simulating mesenchymal stem cell (MSC)-mediated tissue differentiation under various walking speeds and body weights. Tibial fracture-induced gait changes increased peak loading rates at knee and ankle joints by 0.9–1.3 BW/s and 0.8–1.2 BW/s (BW = body weight), respectively, as speed rises from 0.6 to 1.0 v_0 (v_0 = 5 km/h). The tibialis posterior and rectus femoris exhibited the largest increase in peak loading rates, by 92% and 220%, respectively. Ignoring fracture effect could underestimate the mechanical stimulation and risk of fracture non-union. There exists an optimal walking speed for patient-specific body weight to promote endochondral ossification, while controlling fibrous tissue formation (*e.g.,* walking at 0.6 v_0 for a 65 kg patient).

$$t_{\mathrm{fr}} = \frac{S_{\mathrm{fr}}}{S_0} \cdot \min\left(t_0, T_{\mathrm{end}} \cdot S_0\right) + \frac{1-S_{\mathrm{fr}}}{1-S_0} \cdot \max\left(t_0 - T_{\mathrm{end}} \cdot S_0, 0\right) \quad (1)$$

where t_{fr} represents the timestamp with consideration of fracture effect using gait-based biomechanical model; S_{fr} and S_0 represent the stance phase percentage at the maximum tibial muscle activity with and without consideration of fracture effect, respectively; t_0 is the timestamp without consideration of the fracture effect; T_{end} is the total duration of the stance phase.

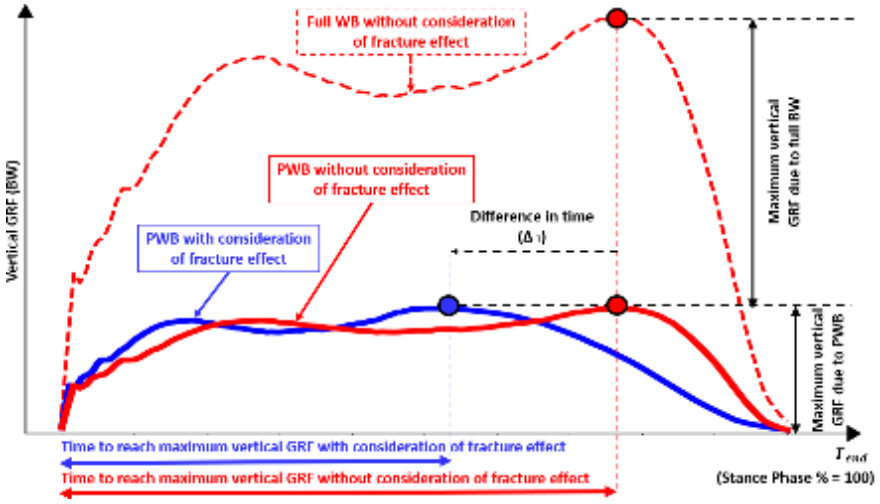

Figure 1. Details of gait-based biomechanical model for patients with tibia fracture.

Keywords: Partial weight-bearing rehabilitation; Tibial fracture; Gait alteration; Musculoskeletal loading; Fracture healing simulation

Sensing and Security Analysis in Hybrid VLC/RF Aided Cognitive Radio-based Internet of Things Networks

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Abstract: The Internet of things (IoT) is a network of interconnected objects that connect and control autonomous machines in the world. However, the main challenges of the hybrid visible light communication (VLC)/radio frequency (RF) aided cognitive radio-based IoT (CR-IoT) networks for fifth generation (5G) faced by researchers are the sensing performance and security issues. The main contribution of this paper: Firstly, we analysis cooperative spectrum sensing gain and security issue in hybrid VLC/RF aided CR-IoT networks; Secondly, we analysis the security issues based on the machine learning (ML) algorithms i.e., support vector machine (SVM), k-nearest neighbours (kNN), and decision tree (DT); Thirdly, this proposed scheme enhances security by excluding unauthorized (malicious) CR-IoT users from CR-IoT networks; Fourthly, as a proof-of-concept, the performance of this propose scheme is evaluated through experiment via MATLAB; and Finally, the simulation results show that the proposed scheme achieved a better performance than the conventional systems in terms of sensing gain, and security issue.

Keywords: Cognitive radio, Internet of things, Visible light communication, Radio frequency, Machine learning

Physics-informed reduced-order surrogate for cardiovascular flow extrapolation in multiple irregular geometries

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Various machine learning-based surrogate models have been developed to map cardiovascular geometries to corresponding flow field distributions, enabling fast and accurate predictions [1]. However, these data-driven approaches often struggle to generalize beyond the range of training geometries, leading to poor performance on unseen cases, a challenge known as the extrapolation problem. To address this problem, we propose a Transductive Proper Orthogonal Decomposition-Physics Informed Neural Network (T-POD-PINN) surrogate model. The proposed method maps multiple irregular vascular flow fields onto a uniform Cartesian grid and employs POD to extract low-dimensional representations. A neural network is then trained to learn the mapping from geometries to flow fields in the reduced-dimensional space, incorporating prior physical constraints from fluid dynamics governed by the following equations:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \tag{1}$$

$$\rho\left(u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right)=-\frac{\partial p}{\partial x}+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right) \tag{2}$$

$$\rho\left(u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right)=-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right) \tag{3}$$

where u and v are the velocity components in the x and y directions (m/s), respectively; p is the pressure field (Pa); μ is the dynamic viscosity (Pa·s).

Our T-POD-PINN demonstrates superior extrapolation performance on synthetic stenotic vessel flow problems compared to common data-driven neural network surrogates as shown in Table 1. Our model holds particular promise for cardiovascular flow predictions in clinical settings, where patient morphologies often extend beyond the range of collected data.

Quantity	Samples	POD	T-POD-PINN
Velocity	Training	2.11%	0.86%
	Testing	15.96%	9.59%
Pressure	Training	2.75%	1.77%

	Testing	33.81%	21.76%

Table 1. Comparison of relative errors

Keywords: Physics-informed, reduced-order model, transductive machine learning, extrapolation, cardiovascular flow, Navier-Stokes

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Modelling on Electrical Properties of Cement-Based Composites

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The conductive graphene/cement composites are currently under extensive investigation due to their potential applications in structural health monitoring. The electrical conductivity of these composites is closely tied to porosity and pore-contained fluid. We have established constitutive equations for electron tunnelling and interface resistance to determine the electrical conductivity of graphene nanoplatelet-reinforced cement composites (GNPRCC). Additionally, a hybrid micromechanical model (HMM) has been developed to simulate the effects of pores and saturation, showing excellent agreement with experimental data. In the HMM-FGEDL model, it is essential to consider enhancing GNPs before incorporating pores for dry samples, and for saturated samples, pores should be considered first.

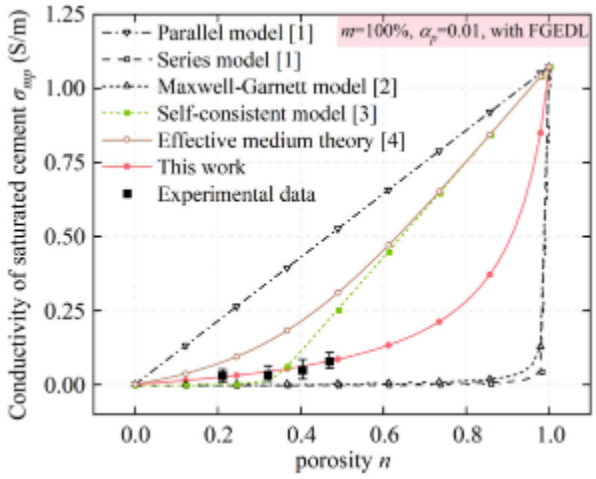

Figure 1. Electrical conductivity of plain cement pastes with FGEDL.

Keywords: Cement composites, micromechanics, electrical conductivity

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Advancements on the Coupled DEM-BEM for Multiscale Geomechanics

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Numerical modelling of geomechanical problems poses unique challenges due to the coexistence of discrete and continuum behaviours across scales. Discrete Element Method (DEM) is well-suited for capturing complex material behaviours, whereas Boundary Element Method (BEM) offers efficient solutions for wave propagation on infinite continuum domains. This work presents recent developments in the coupling of DEM and BEM, enabling a unified framework to simulate complex geomechanical problems. The motion of DE particles and continuum are governed by Newton's second law and the boundary integral equation, respectively:

$$m_p \ddot{\boldsymbol{u}}_p = f_p^{\text{ext}} + \sum_{q \in I_p} f_{pq}^{\text{contact}}, \qquad c u_i + \int_\Gamma T_{ij} u_j \mathrm{d}\Gamma = \int_\Gamma U_{ij} t_j \mathrm{d}\Gamma, \tag{1}$$

in which m_p and $\ddot{\boldsymbol{u}}_p$ are the mass and acceleration vector of particle p, while f_p^{ext} and f_{pq}^{contact} are external and contact vector forces acting on p. Contact forces arise between p and all particles q in the set I_p of particles in contact with p. In addition, which $\boldsymbol{u}$ and $\boldsymbol{t}$ are displacements and tractions along the boundary of the continuum, $\boldsymbol{U}$ and $\boldsymbol{T}$ are fundamental solutions for displacement and traction that allow for the eliminate domain integrals, and c is a local geometry-dependent coefficient. In the coupled framework, the interfacing DE particles forces are transferred onto the BEM domain, which updates the displacement and apply it back to the particles, updating their motion [1,2]. A staggered time integration scheme is adopted to allow for different time steps on each method. Figure 1 shows a benchmark validation in 3D. The application of the new method will be shown on 2D and 3D examples.

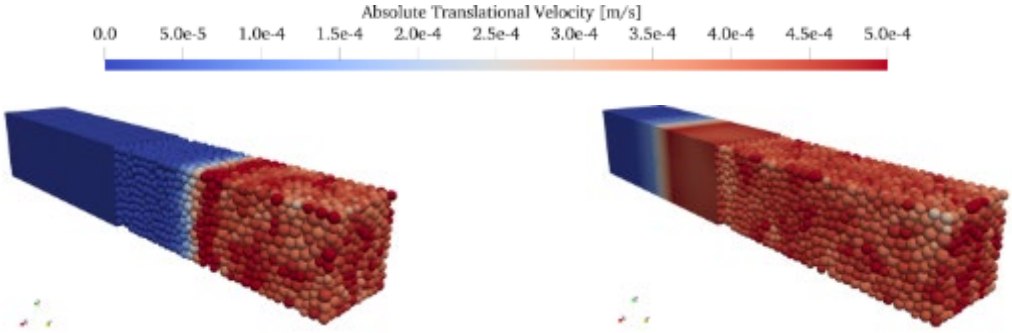

Figure 1. Validation benchmark of finite rod under tension in 3D.

Keywords: Discrete Elements, Boundary Elements, wave propagation, infinite domains

References

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Coupled Finite Element-Crystal Plasticity Modeling of High Cycle Fatigue behaviour and Life Prediction of 42CrMo4V Steel

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Abstract

High-cycle fatigue (HCF) remains a critical mode of failure in high-strength structural steels subjected to prolonged cyclic loading. The present study combines advanced numerical modelling with in-depth experimentation and characterisation to provide a thorough multiscale analysis of the HCF behaviour of 42CrMo4V steel. The macroscale Finite element (FE) based HCF model developed here works with the input data derived from the experimental tensile test results. Initially, the Quality Index (QI) is computed based on experimental tensile results. Subsequently, the key material parameters such as the fatigue strength coefficient (σ_f') and fatigue strength exponent (b)—are determined from the QI. These parameters serve as inputs for the FE-based fatigue simulation. Thereafter, a mesoscale crystal plasticity model is coupled with the macroscale FE model to analyze the fatigue damage of the said material at microstructural length scale. Finally, experimental fatigue tests are performed on the test specimens for model validation purpose. Moreover, the HCF tested specimens are rigorously analysed by Optical microscopy (Olympus BX53M), to identify the surface fatigue features and crack initiation sites, Field Emission Scanning Electron Microscopy (FESEM), and Electron Backscatter Diffraction (EBSD) techniques. The present study also delves into the detailed analysis of grain orientation, slip localization, and texture evolution under cyclic loading, and in turn contributes to the understanding of fatigue crack nucleation and propagation in the HCF regime, in case of 42CrMo4V steel. The findings advance predictive modeling capabilities and contribute to the design of fatigue-resistant components in engineering applications where durability and performance are critical.

Keywords: High-cycle fatigue (HCF), Microstructural Characterization, Quality Index (QI), Crystal Plasticity, Finite Element Method

Some advances in AI enabled mesh generation approaches

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AI enabled mesh generation represents a new branch of mesh generation, which is traditionally enabled by the studies on computational geometry theories and algorithms. In this talk, we will discuss recent advances achieved by our group in this new research branch. Our first focus is on the AI enabled model feature recognition algorithm. Our preliminary studies in this direction show that AI enabled algorithms can be used to identify a wide range of features, such as film cooling holes inside the turbine vane, fillets of mechanical parts, features specified to automotive body panels, and so on. Meshing examples are presented to show that these new developments can improve the resulting mesh quality evidently. Our second efforts are devoted to the issue on how to create an appropriate sizing function for unstructured mesh generation, which is key to create a cost-effective mesh for numerical simulations. We propose an AI enabled algorithm to simplify the mesh structure representing the sizing function. After simplification, the mesh size can be reduced significantly while the loss of the sizing function quality is limited. As a result, the timing costs associated with the sizing function can thus be reduced a lot. Moreover, we will attempt to extend such AI enabled algorithms to mesh adaptation. Combining with other AI enabled techniques, we hope to develop an efficient, accurate and robust computing cycle.

Keywords: Grid Generation, Machine Learning, Feature Recognition, Sizing Function

Deep Learning-based Automatic Recognition and Mesh Optimization for Film Cooling Holes

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In the coupled thermal-flow analysis of gas turbine blades with film cooling holes, the physical field along the hole channel direction exhibits relatively small gradient changes. This characteristic makes it possible to apply anisotropic meshes at film cooling hole locations. Anisotropic meshes can reduce the number of grid elements while maintaining computational accuracy, thereby improving computational efficiency. However, actual turbine blades contain a large number of film cooling holes (typically hundreds or even thousands), making manual identification of these feature structures extremely inefficient. The researchers have attempted to detect cooling holes using geometric feature recognition algorithms[1], but when applied to complex geometric models of actual engine blades, the recognition accuracy is often low and fails to meet engineering requirements. To address this issue, we propose an automated recognition method based on deep learning. We have constructed a training dataset specifically targeting the features of turbine blade film cooling holes, covering various cooling hole configurations commonly found in practical engineering applications. We designed a novel neural network architecture capable of effectively encoding and extracting features from CAD surfaces. Experimental results show that our method achieves recognition accuracy exceeding 95% in complex geometric models from industrial scenarios. Furthermore, after our framework automatically identifies film cooling hole regions, it can generate appropriate anisotropic meshes and perform mesh refinement in the hole outlet areas to accurately capture steep temperature gradients. This approach significantly reduces manual operations and improves both the efficiency and accuracy of thermal-flow coupled analysis for turbine blades.

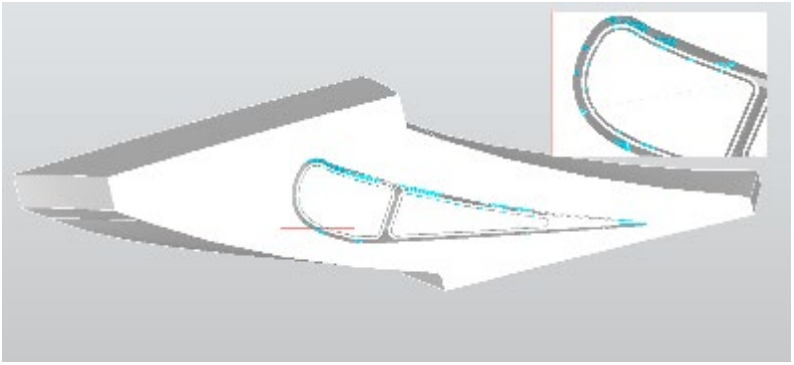

Figure 1. Film Cooling Holes

Keywords: mesh generation, Navier-Stokes equations, boundary-layer, machine learning, feature detection

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Efficient Background Mesh Refinement with Graph Convolutional Networks for Sizing Field

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In unstructured mesh generation, element sizing is typically governed by a background size field that enables local control of mesh resolution. Such size fields are often defined on background meshes—e.g., octrees or STL triangle meshes—with sizing values prescribed at mesh vertices and interpolated throughout the domain. However, when the background mesh is defined by an STL triangulation, "banding" artifacts (see Figure 1) can arise along triangle edges, leading to locally inappropriate refinement. A naïve global refinement strategy alleviates banding only at the cost of excessive background mesh density and degraded query performance. To address this challenge, we propose a novel GCN-based size-field adjustment framework: a graph convolutional network is trained to detect banding edges within the STL mesh, and a targeted remeshing algorithm is then applied in the vicinity of these edges. This approach achieves a balanced trade–off between background mesh complexity and the elimination of banding artifacts.

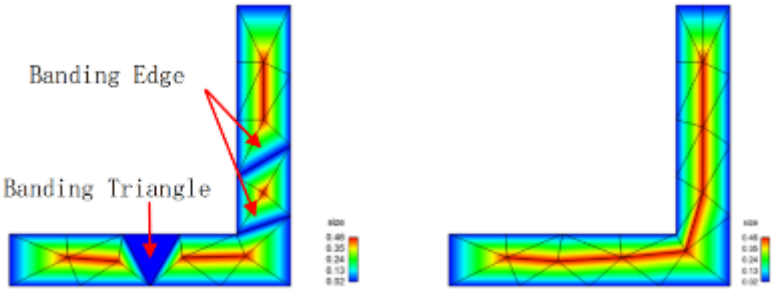

Figure 1. Comparison of size fields with and without banding artifacts(Left: With banding edges and triangles.Right: Normal size field.).

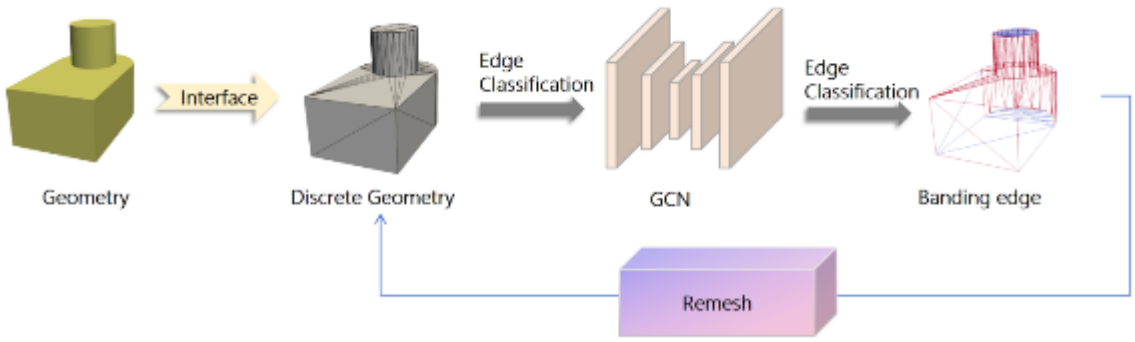

Figure 2.

The overall framework is illustrated in Figure 2. Initially, we load the geometry file and use a geometry engine to generate the STL mesh. The mesh edges are treated as graph nodes, and the adjacency relationships between edges are represented as graph edges to construct a graph neural network (GNN). Mesh dihedral angles, vertex geometric curvatures, and other relevant features are then input into the network. The graph convolutional network (GCN) is trained to predict which edges exhibit banding behavior. Once the banding edges are identified, we introduce a remeshing algorithm to locally reconstruct the mesh, aiming to remove banding by adding only a few additional nodes. After 2-3 iterations of optimization, we can effectively reconstruct the background mesh and eliminate the banding artifacts, while minimally increasing the number of mesh points.

Keywords: GCN, mesh generation，sizing field

A fully adaptive modelling of damage process based on the scaled boundary finite element method

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Cracks inevitably occur in quasi-brittle materials like concrete when subjected to excessive tensile loading. In damage theory, cracks are treated as a damage process zone with a high gradience of strains. These localized strains, together with elastic strains in un-damaged regions, are effectively captured by a scaled boundary finite element approach in this work. The scaled boundary finite element method (SBFEM) naturally allows the presence of hanging nodes between neighbouring cells, and thus permits a high level of mesh flexibility in modelling localized damage. On top of that, an adaptive meshing approach is proposed to model the progressive damage growth with a sequence of updated meshes. This avoids unnecessarily fine meshes in elastic regions, and thus significantly reduces amounts of nodes involved in analysis. The performance and advantages of this presented approach are illustrated by numerical examples of predicting the damage evolution.

Keywords: Scaled boundary finite element method; Damage analysis; Quasi-brittle materials.

Early-age creep and relaxation in alkali-activated slag concrete: Quantification via repeated short-term creep tests

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Alkali-activated slag concrete, a low-carbon alternative to Portland cement-based concrete, offers excellent mechanical and durability properties but faces practical limitations due to autogenous shrinkage and early-age cracking. The quantitative link between shrinkage and cracking susceptibility remains unclear, and experimental data on its early-age viscoelasticity, particularly creep and relaxation, remains scarce. This knowledge gap hinders accurate predictions of deformation and internal stress, forcing researchers to rely on empirical models to assess creep behaviour and long-term performance. Therefore, this study employed repeated short-term creep tests to quantify the early-age viscoelastic properties of alkali-activated slag concrete. By integrating a double power law (Equation 1) and the Boltzmann superposition principle (Equation 2), a creep model was developed.

$$J(t,t') = \frac{1}{E(t')} + a \times (\frac{1}{t'})^b \times (t-t')^c \quad (1)$$

$$J(t,t')R(t,t') + \int_{t'}^{t} J(t,\hat{t}) \frac{dR(t\prime,\hat{t})}{d\hat{t}} d\hat{t} = 1 \quad (2)$$

The results indicate that repeated short-term creep tests effectively quantified the early-age creep compliance of alkali-activated slag concrete during hardening, as shown in Figure 1. Creep and relaxation must be considered by models when predict early-age stress development in alkali-activated slag concrete. The double power law closely aligns with experimental data, highlighting its applicability for predicting short-term creep and relaxation of alkali-activated slag concrete. Converting creep compliance into relaxation modulus is essential for simulating stress dissipation in alkali-activated slag concrete. This study compared two conversion methods, numerical solution and explicit exponential method, finding that the latter enhanced accuracy in long-term predictions.

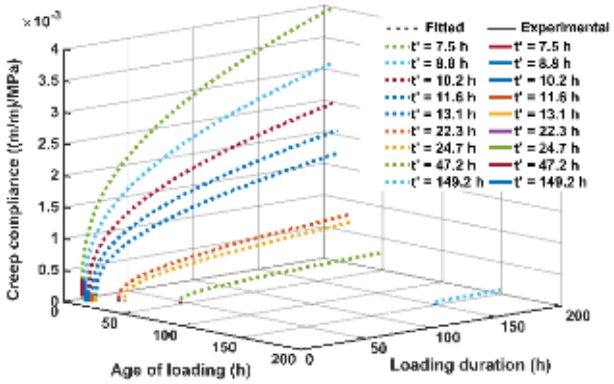

Figure 1. Creep compliance evolution from modelling and repeated short-term creep tests. Note that each dashed line begins with experimental data segments.

Keywords: Alkali-activated slag, viscoelasticity, creep, relaxation, modelling

Parallel topology optimization for continuous fibre reinforced composites

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Abstract. The diverse and complex failure modes of continuous fibre rein-forced composites (CFRC) impose a significant challenge on the optimization of both structural topology and fibre path. This study proposes a novel strength-based parallel optimization of topological layout and fibre path for CFRC structures, named SPOTF. The method combines level-set function for topology optimization and stream function for fibre path optimization. Both functions are represented as sums of radial basis functions with weights, where these weights are treated as design variables to update the topological layout and fibre path. In this study, the optimization aims to enhance mechanical strength with the Tsai-Wu strength criterion. As compared with the most popular methods, i.e., maximum principal stress direction (MPSD) and the stiffness-based design, the effectiveness of SPOTF has been validated through two classical examples. The results show that SPOTF reduces the Tsai-Wu maximum failure index of the cantilever and L-bracket structures by 38.5% and 59.3%, respectively when compared to MPSD. Compared with the stiffness-based design, the failure index was reduced by 42.9% and 61.4% respectively, e.g., as shown in Figure 1. This proves that SPOTF can generate more effective topological layouts with smooth and continuous fibre paths, appreciably alleviating the concentration of failure index and lowering damage and failure of CFRC structures. The proposed method is anticipated to provide a new and effective approach for design of CFRC structures considering structural strength for a wide range of engineering applications.

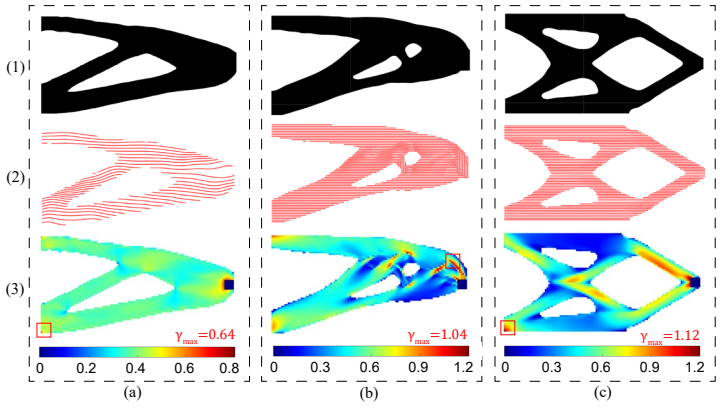

Figure 1. The comparison of the optimized cantilever beam structures: (1) topological layout; (2) fibre orientation of each element or path; (3) failure index distribution; (a) SPOTF, (b) MPSD-based, (c) Stiffness-based.

Keywords: Topology optimization; continuous fibre-reinforced composite, parallel optimization, Strength, composite structures.

Reference. Li GX, Chen Y*, Li Q. Strength-based collaborative topology optimization for continuous fiber reinforced composites. Comput Meth Appl Mech Eng 2024; 430: 117206.

A cohesion-enhanced granular kinetic multiphase CFD model for cemented paste backfill flow

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Cemented paste backfill (CPB) is widely adopted in underground mining to stabilise excavated voids and manage tailings sustainably, but its pipeline transport is challenged by complex rheological behaviour and solid sedimentation. Conventional single-phase CFD models treat CPB as a homogeneous non-Newtonian fluid, which fails to capture particle settling and localised yield-stress effects. To overcome these limitations, a two-phase Euler–Euler CFD model based on kinetic theory of granular flow (KTGF) is developed to incorporate interparticle cohesion arising from hydration bonding and van der Waals attractions. Cohesive interactions are incorporated into the solid-phase momentum and granular energy equations by introducing two physically meaningful parameters representing maximum bond strength and microstructural evolution. These cohesive parameters are calibrated against slump-cone tests, and the model is validated through closed-loop pipe-flow simulations. Compared to the standard KTGF, the cohesion-enhanced model improves pressure-drop prediction and captures the particle sedimentation profiles. Parametric studies show that higher flow velocities and larger pipe diameters improve suspension homogeneity, and that stronger interparticle cohesion enhances uniform particle distribution. The proposed approach offers improved practical guidance for optimising CPB pipeline design, preventing blockage, and mitigating wear in deep-mine backfilling operations.

Keywords: cemented paste backfill, granular flow , multiphase flow, particle cohesion, particle sedimentation

Advancing Predictive Accuracy: Integrating Mechanics into Machine Learning for Elastoplastic Behavior Modeling in Fiber-Reinforced Composites

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The fiber-reinforced composites are widely used in aerospace, automotive industries and medical area due to its distinguished properties, and its complex three-dimensional elastoplastic behavior can be modeled by machine learning (ML). However, the significantly reliance on substantial training databases hinders progress in ML modeling. To overcome this challenge, our research introduces an innovative mechanics-informed ML approach, aiming to advance the predictive accuracy of the elastoplastic behaviors of unidirectional FRC with a limited database. Incorporating a stress and strain decomposition method rooted in mechanical invariant theory, we establish two parallel Artificial Neural Networks (ANNs) to articulate deviatoric behaviors and the coupling of volumetric and fiber-directional behaviors respectively. The mechanics-informed approach streamlines the architecture of the ANNs, requiring only two inputs and two outputs for each ANN, in contrast to the conventional six-dimensional strain and stress tensors. This reduction in input dimensions significantly enhances predictive accuracy, even with a limited database. Additionally, a tensor transformation link for the output stress of ANNs is incorporated, ultimately deriving tensor-valued stress. Furthermore, our ML approach is refined to predict the impact of the loading path, ensuring a more comprehensive elastoplastic behavior modeling. To validate our proposed ML-based constitutive model, we conduct direct numerical simulations (DNSs) based on a representative volume element, generating datasets for model training and validation. Comparative analysis of results obtained through DNS and ML showcases the exceptional predictive accuracy of our proposed model, even with a small training database.

Optimization of CFRP Structures Tailored for Additive Manufacturing Performance

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Additive manufacturing (AM) has emerged as a powerful method for fabricating carbon fibre reinforced polymer (CFRP) composite structures, particularly due to its ability to realize complex, topologically optimized geometries. Nonetheless, CFRP components produced via AM often face inherent drawbacks, including low fibre volume fractions and high porosity, which compromise their mechanical performance. To overcome these limitations, this study presents an integrated framework aimed at enhancing the mechanical properties of 3D-printed CFRP structures through design optimization and vacuum-assisted thermal post-processing. A level-set-based concurrent optimization method is first proposed to simultaneously determine the structural topology and filament deposition paths, explicitly considering manufacturing constraints. The optimized designs are experimentally validated by fabricating both optimized and conventionally designed specimens using continuous fibre 3D printing. To further improve structural quality, a novel post-processing method—vacuum-assisted heating at one atmosphere—is applied, effectively reducing internal defects and improving overall integrity. Additionally, high-resolution micro-computed tomography (μCT) is utilized to reconstruct the printed geometries for refined numerical simulations. The results show strong agreement between simulations and experimental tests, with errors remaining below 10%. The proposed design strategy achieves a 47.0–52.1% increase in stiffness-to-mass ratio, while the post-processing reduces structural deformation by 10.8–26.8%. These outcomes highlight the potential of combining optimization-driven design with targeted reprocessing to significantly enhance the performance of AM-produced CFRP structures without incurring additional material costs.

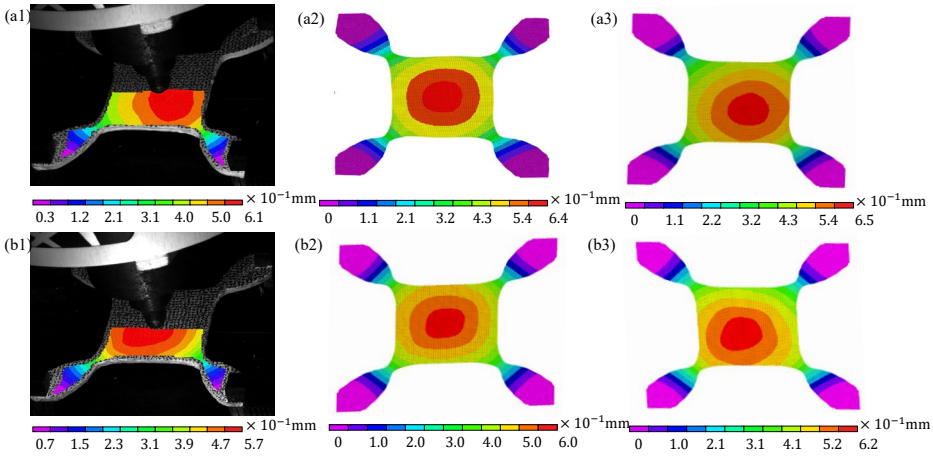

Figure 1.

Keywords: CFRP, Topology optimization, Filament path optimization, Additive manufacturing, Vacuum-assisted thermal post-processing

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Multiphysics Coupling Simulation of Underground Heat Dissipation from Fixed-Point Heat Sources Using Physics-Informed Machine Learning Method

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Abstract: Prediction of underground heat dissipation for fixed-point heat sources such as geothermal energy storage, energy pile, burried pipe and cable etc. necessitates efficient multiphysics numerical simulations, but traditional finite element methods (FEM) incur prohibitive computational costs in iterative parameter optimization and large singlar matrix inversion due to mesh dependency and high-dimensional solving. This study introduces a physics-informed machine learning (PIML) algorithm to build a surrogate model to transcend these limitations, explicitly embedding governing equations of heat transfer coupled porous fluid flow as soft constraints within neural networks. Unlike FEM, which requires costly remeshing and large matrix inversion solving for each optimization step, the surrogate model trained by PIML enables real-time sensitivity analysis and gradient-based optimization by unifying simulation and optimization into a single differentiable model. Validations show a high reduction in runtime versus finite element model while maintaining relatively accessible accuracy in prediction. This approach offers a transformative tool for sustainable geoenergy design and operation, minimizing computational cost while ensuring generalization with physical interpretability.

Multi-objective topology optimization of piezo-embedded compliant structures subject to external harmonic excitation

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Compliant mechanisms integrated with embedded piezoelectric actuators have been extensively employed in high-vibration environments, necessitating the avoidance of eigen-frequency resonance with the disturbance frequencies. Although topology optimization methods for compliant mechanisms have been extensively developed, very few studies have considered the dynamic properties of compliant mechanisms [1-3]. This work presents a concurrent optimization method of compliant structures embedded with movable piezoelectric actuators considering both the output stroke and dynamic response. A density-based material interpolation scheme is developed to represent material properties in different sub-domains occupied by compliant mechanisms or actuators, and the topology of host compliant mechanisms and position of actuators are optimized simultaneously through designing the density field and geometric variables. A multi-objective formulation is proposed for topology optimization of piezo-embedded compliant structures, in which the maximization of output stroke and the minimization of mean dynamic compliance subject to external harmonic excitation are considered simultaneously. With using the adjoint method, the sensitivities of the objective function and constraints with respect to design variables are derived for the gradient-based optimizer. Several numerical examples are investigated to verify the effectiveness of the proposed optimization method. The topological results illustrate that the proposed method can attain a reasonable design, which the output stroke is maximized, and the mean dynamic compliance is minimized.

Keywords: Topology optimization, Compliant mechanism, Piezoelectric actuators, Multiple objective, Frequency response function

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A shape optimization-based method for designing the cellular honeycomb cores with in-plane large morphing

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The sandwich-flexible-skin with cellular honeycomb cores is one of the most promising kinds of configuration for continuous morphing structures. The key problem is to find good configurations to ensure that the honeycomb core have enough large morphing before the strain exceeds the allowable limit[1]. The traditional honeycomb core is mostly designed according to experience or observational summaries, and an effective method for design the honeycomb core need to be developed. In this paper, a design method of honeycomb cores is proposed based on the shape optimization. The shape of the unit-cell is portrayed using Bezier curves and tailored through adjusting the coordinates of the control points. The optimization model is established through taking the coordinates of control points as the design variables, maximizing the displacement in the morphing direction as the objective and the maximum strain of the structure being less than the allowable one as the constraint. Taking the U-shaped honeycomb core as a typical initial design, a novel Ω-shaped honeycomb core is obtained though the proposed method. The detailed analysis through a combination of experiment and finite element validations, in terms of morphing capability (in-plane tension and shear) and load-bearing performance (out-of-plane bending and torsion resistance), shows that the in-plane morphing performance of the Ω-shaped honeycomb is far superior to that of the initial U-shaped honeycomb, but has weaker out-of-plane load-bearing capability[2, 3]. However, the out-of-plane load-bearing capability can be reinforced by adjusting the geometric parameters of the unit-cell.

Keywords: Sandwich-Flexible-Skin, Shape Optimization, Bezier Curve, Morphing Structures, Ω-Shaped Honeycomb

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Modelling of Competitive Failure Behaviour of CFRP Stepped-lap Repairs under Various Design Parameters

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Stepped-lap bonding is widely used for repairing damaged CFRP structures in aerospace applications, yet its design is challenged by complex competitive failure mechanisms involving adhesive debonding, delamination, and composite damage [1-3]. This study combines experimental and numerical methods to investigate the effects of step numbers and slope combinations on the tensile performance of CFRP stepped-lap repairs. Quasi-static tensile tests were conducted on specimens fabricated from CFRP prepreg and bonded with epoxy adhesive. A novel finite element (FE) model was developed, incorporating two cohesive zone model (CZM) configurations: cohesive contact for the adhesive interface and zero-thickness elements for interlayer delamination simulation, coupled with 3D Hashin criteria for composite damage prediction.

Key findings reveal:

1. Step numbers: Tensile strength increases with step count but plateaus beyond 3 steps (peak load: 27.03 kN experimentally, 25.76 kN numerically). The transition from 1 to 2 steps yields a 55% strength increase, while 2 to 3 steps offers 12%, indicating diminishing returns.

2. Slope combinations: The symmetric slope configuration 1/20-1/20-1/20 achieves optimal load-bearing capacity (23.09% higher than the weakest design), attributed to uniform stress distribution.

3. Failure mechanisms: Single-lap repairs exhibit cohesive failure, while stepped repairs show competitive failures (debonding, matrix cracking, and delamination). Damage initiates at step edges and propagates symmetrically, with adhesive failure preceding ply delamination (see Figure 1).

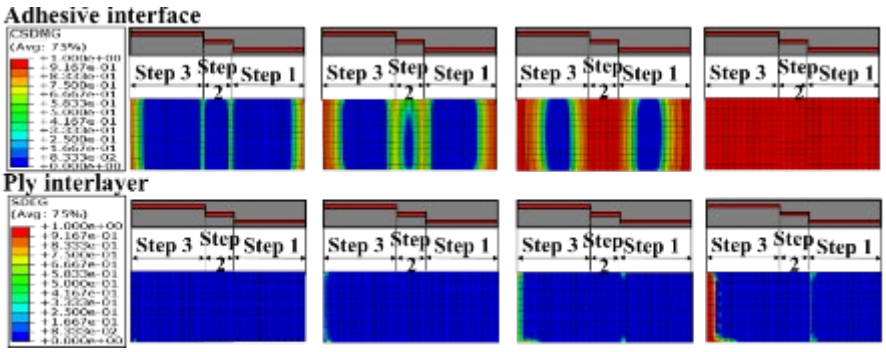

Figure 1.

This work provides validated design guidelines for stepped-lap repairs and a robust FE framework for predicting multi-mode failure in aerospace composites.

Keywords: Composite repair, Stepped-lap bonding, Cohesive Zone Model, Competitive failure

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Multi-level Numerical Simulation of 3D Concrete Printing: from Filaments to Structures

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Three-dimensional concrete printing (3DCP) has emerged as a promising manufacturing technology in the construction industry. A key challenge lies in achieving high geometric accuracy of 3D printed concrete structures, particularly in controlling the height and width of each printed layer. It is primarily attributed to the complex early-age behaviours of cementitious materials and the influences of critical process parameters, such as nozzle speed, nozzle height, and material outlet velocity on the final 3D printed concrete structures need to be determined for high-quality 3D printing. Along with experimental work, numerical modelling and simulations offer a powerful numerical analysis approach for simulating the layer-by-layer 3DCP process—from individual filaments to full-scale structures and they can be utilised to explore the effects of key 3DCP process parameters on the printing quality of final products.

To address this challenge, in this study, Smooth Particle Hydrodynamics (SPH) and Finite Element (FE) models are both developed to simulate the 3DCP process at both the filament and structural levels and investigate the effects of those above-mentioned key 3DCP process parameters on geometry and cross-sectional shape of extruded filaments. The SPH model incorporates the Bingham rheological model to capture the flow behaviours of fresh concrete and predict the geometry and cross-sectional shape of extruded filaments under varying process parameters and is validated against experimental results from this study. Meanwhile, the FE model, based on the tracing element method and employing the Mohr-Coulomb failure criterion to describe material behaviours, is validated through comparison with results reported in the literature, demonstrating the effectiveness of the model in capturing the key physical phenomena of 3DCP.

Keywords: 3D concrete printing (3DCP); Smooth Particle Hydrodynamics (SPH); Finite Element (FE) model; Layer geometry; Structural failure

Setting time prediction of metakaolin or fly ash-based geopolymer binders using machine learning

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Geopolymer binders, a type of low-carbon construction material, has been considered as a promising alternative to traditional portland cement-based cementitious material. However, it is still challenging to predict some properties of geopolymers such as setting time due to large variations in the chemical compositions of fly ash and many other influential factors. This conference paper aims at predicting the setting time of metakaolin and/or fly ash-based geopolymer binders by considering a series of detailed factors such as amorphous phase content, different quantities of oxides, and particle size of precursors, water usage, temperature, etc., based on machine learning methods. Several typical models were used and the corresponding prediction results were compared. Besides, the preciseness of predication was evaluated by comparing the predicted results and real values using loss function. Moreover, the positive and negative degree of different factors were obtained in order to showcase the correlation degree of each factor and the corresponding setting time. This conference paper demonstrates the feasibility and potential of using machine learning for predicting the setting time of geopolymer binders to promote their applications.

Keywords: Geopolymer, metakaolin, fly ash, machine learning, setting time

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A GPU Accelerated Multiphysics Solver based on Operator-splitting Galerkin Finite Element Method

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The ARPA-E HITEMMP TOPOLOGY (High Intensity Thermal Exchange through Materials and Manufacturing Processes) program is dedicated to advancing the design and manufacturing of high-temperature, high-pressure heat exchangers, which are pivotal for efficient thermal energy transfer across a range of industrial applications, including electricity generation, transportation, and waste heat recovery. HITEMMP initiatives aim to create a new class of heat exchangers that significantly enhance efficiency and performance leading to substantial improvements in power conversion efficiency, reduced fuel consumption, minimized system footprints, and lower emissions of CO2. [1]

Topology optimization (TO) is one of popular methods to design an efficient heat exchanger. However, the application of TO could be hindered by the requirement of solving a large-scale Multiphysics problem many times. This raises an immediate need to develop an efficient Multiphysics solver.

This study will show a GPU accelerated Multiphysics solver named Fast Linear Algebra Solver for Heat Exchangers (FLASHx). FLASHx is based on operator-splitting Galerkin Finite Element Method [2] and targeted to solve a coupled incompressible fluid, turbulent, unsteady heat and structure problem. Benchmark results show a good agreement between FLASHx and other solvers such as OpenFOAM or Abaqus. Furthermore, the results also show that the GPU based FLASHx can be significant faster than the CPU based solver.

Keywords: GPU, Multiphysics, Operator-splitting Galerkin Finite Element

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Atomic reconstruction and interfacial mechanics at the confined solid-liquid interface

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Under nanoconfinement, materials are often restricted to narrow spaces and complex interactions, this is especially important for liquid or gas because their structures will be largely influenced and the transport characteristics will be tuned, which is key to many applications. In this report, we will present molecular dynamics simulation results of structural variation under confined nanochannels, abnormal structural transition of water phases are identified and size effects are uncovered. Furthermore, for a two phase flow composed of water and supercritical carbon dioxide ($scCO_2$), we find that surface wettability strongly modifies of the structures of the phases at varied water saturation ratio (S_w), as shown in Fig. 1. In hydrophilic nanochannels, water preferentially adsorb onto channel walls, forming thin films that coalesce into a water bridge at higher S_w. This water bridge drastically impedes $scCO_2$ transport, reducing flow capacity by up to 95%. Conversely, hydrophobic nanochannels exhibit water clustering at the channel center, which facilitates higher $scCO_2$ mobility. At elevated S_w, the flow pattern transits from Poiseuille to Couette flow, further mitigating the decline in $scCO_2$ transport capacity. Analytical models accurately predict these behaviors, highlighting the interplay between channel wettability, S_w, and nanoscale confinement in dictating $scCO_2$ transports. We expect our results to offer new insights into mass transport and heat management in confined channels.

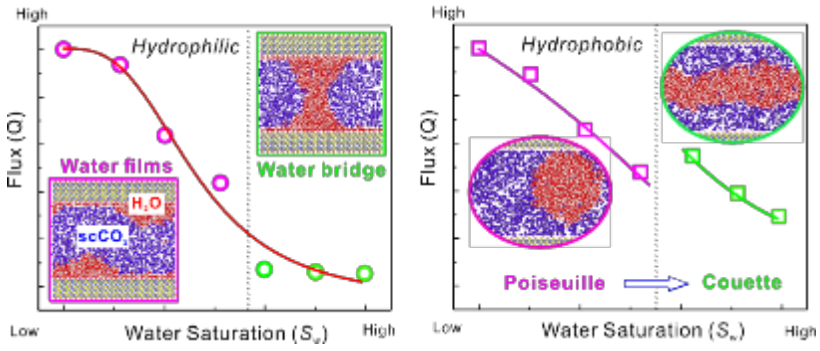

Figure 1.

Keywords: nanoconfinement, solid-liquid interface, structural reconstruction, mass transport, molecular dynamics, wettability.

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A novel multi-material topology optimization method for acoustic-structure interaction system based on a multi-resolution approach

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Noise pollution has emerged as a severe issue confronted by modern society. Consequently, the vibration reduction, noise suppression, and acoustic performance optimization of structures have become significant topics in the engineering community. For the analysis of exterior acoustic-structure interaction systems, the FEM-BEM coupling method is an effective numerical tool[1]. Eq (1) presents the discretized form of the governing equation for acoustic-structure interaction systems. However, it faces high computational costs in the analysis of large-scale acoustic-structure interaction systems.

$$\begin{bmatrix} \mathbf{K}_d & -\mathbf{C}_{sf} \\ -\omega^2 \rho_f \mathbf{G} \boldsymbol{\Theta}^{-1} \mathbf{C}_{fs} & \mathbf{H} \end{bmatrix} \begin{Bmatrix} \mathbf{u} \\ \mathbf{p} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_s \\ \mathbf{0} \end{Bmatrix} \tag{1}$$

A multi-material and multi-resolution topology optimization method is proposed for exterior acoustic-structure interaction system in this study. This study adopts a FEM-BEM coupling method for the response analysis of acoustic-structure interaction system. By employing a multi-resolution modelling strategy[2] and an ordered SIMP approach[3], a novel multi-material, multi-resolution topology optimization framework for acoustic-structure interaction system is developed. Eq (2) formulates the element matrix under this approach.

$$\begin{aligned} \mathbf{K}_e &= \sum_{i=1}^{N_{ed}} \left[\left(A_E (d_{ei})^p + B_E \right) \int_{\Omega_{ei}} \left(\left(\nabla \mathbf{N}_s^e \right)^{\mathrm{T}} \mathbf{D}_0 \nabla \mathbf{N}_s^e \right) \mathrm{d}\Omega_{ei} \right] \\ \mathbf{M}_e &= \sum_{i=1}^{N_{ed}} \left[\left(A_\rho (d_{ei})^p + B_\rho \right) \int_{\Omega_{ei}} \left(\rho_0 \left(\nabla \mathbf{N}_s^e \right)^{\mathrm{T}} \nabla \mathbf{N}_s^e \right) \mathrm{d}\Omega_{ei} \right] \end{aligned} \tag{2}$$

This framework enables the attainment of high-resolution designs with reduced computational costs. Numerical examples substantiate the effectiveness and dependability of the proposed approach, offering novel strategies for the design of vibration and noise reduction in engineering structures.

Keywords: Acoustic-structure interaction system, boundary element method, finite element method, topology optimization, multi material design, multi resolution design

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Phase-Field Modeling of Ductile Fracture: Insights from Solid and Shell Element Implementations

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The accurate prediction of ductile fracture is critical for the structural integrity assessment of modern engineering components. Phase-field models have emerged as a powerful tool to capture crack initiation and propagation without the need for explicit tracking of crack surfaces. However, the choice of finite element formulation—solid vs. shell - can significantly influence the computational efficiency and accuracy of these models. This research presents a comprehensive study comparing phase-field implementations for ductile fracture using both solid and shell elements. The formulations have been rigorously verified against analytical solutions to ensure their theoretical soundness. Beyond this, a series of numerical examples are conducted to validate the models under practical conditions. These include representative material-level specimens, benchmark crack propagation problems, and complex topologies such as triply periodic minimal surface (TPMS) structures. The comparison reveals distinct advantages and limitations of each approach. Solid elements provide more detailed stress resolution and are suitable for bulk materials, but they incur higher computational costs. Shell elements, on the other hand, offer reduced computational demand and are advantageous for thin-walled structures, though they may struggle to capture three-dimensional stress states accurately. Furthermore, the fracture mechanisms predicted by the two formulations are critically analysed, revealing differences in crack patterns, energy dissipation behaviour, and damage localisation. These insights help guide the appropriate selection of element type based on structural characteristics and computational constraints for phase field fracture problems.

Keywords: Phase field fracture model, shell element, additive manufacturing, stress state, triply periodic minimal surface structures

A new gradation equation for coarse-grained subgrade fillers and its applicability based on the fractal theory

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Abstract: Quantitatively descripting the gradation using equation has a great significance on the investigating of the optimal gradation and multi-scale effects for coarse-grained subgrade fillers. A new gradation equation for coarse-grained subgrade filler (CSF) was proposed according to the traditional fractal theory. Relationship between the shape of gradation curve and model parameters was analyzed, the curve shows sigmoid when $-\sqrt{-2\alpha} < \beta < \sqrt{-2\alpha}$, and the curve respects hyperbolic when $\beta > \sqrt{-2\alpha}$. The values of model parameters when CSF is well-graded range were captured, i.e., $\beta 2<2.590\alpha 2+5.627\alpha+1.239$ and $\alpha<0$. Applications of the new gradation equation in the scale effect and particle breakage were investigated and verified. Based on the traditional scaled methods, i.e., exclusion method (EM), similar gradation method (SGM), equivalent substitution method (ESM) and hybrid method (HM), a new unified form of gradation scale formula was proposed. In addition, the new expressions for calculating breakage rate and disintegration ratio were established. Specifically, the particle breakage experiment for CSF using the large-scale triaxial test and the disintegration breakage experiment for red-bed soft rock under different dry-wet cycles were carried out to use and verify the correctness of these new expressions. Findings provides theoretical support for the study of gradation effects and multi-scale effects.

Keywords: coarse-grained subgrade filler, new gradation equation, multi-scale effect, gradation scale method, particle breakage

A general-purpose meshfree Kirchhoff-Love shell formulation

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A thin shell formulation is developed for the approximation by a meshfree Reproducing Kernel Particle Method (RKPM)[1]. The formulation is derived from a degenerated shell approach where the structure is treated as a 3D solid subjected to kinematic constraints of the Kirchhoff–Love (KL) shell theory. To address the challenge of surface geometry representation in a meshfree method, a local parameterization using principal component analysis (PCA) is employed. Taylor-series expansion adapted to the shell formulation is developed to address the accuracy and stability issues of nodal quadrature. The weakly coupled strategy is proposed to address the rotational continuity conditions in KL shells. Several approaches that address membrane locking are also considered. The effectiveness of the proposed RKPM KL shell formulation is demonstrated using an extensive set of linear-elastic and finite-deformation inelastic test cases.

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Nonlinear dynamic and stability analysis of piezoelectric smart plates and shells considering piezoelectric nonlinearity

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The existing research on the mechanical analysis of piezoelectric smart plates and shells mainly focuses on linear piezoelectric constitutive models and small rotations under the von Kármán assumption. However, these studies often overlook the inherent nonlinearity of piezoelectric materials and significant geometric nonlinearities arising from large displacements and rotations, which are commonly encountered in practical engineering applications. To address this gap, this study introduces a numerical model for piezoelectric smart plates and shells (PLS), which integrates both geometric and piezoelectric nonlinearities. This is achieved through the Mixed Interpolation of Tensorial Components (MITC) technique, which provides a robust solution for nonlinear analyses of post-buckling behavior, nonlinear dynamic responses, frequency-amplitude responses, and dynamic control of piezoelectric smart structures. The model is based on the Reissner-Mindlin theory, and the MITC elements effectively resolve the common shear-locking issues in numerical simulations. The large displacements and rotations of the PLS are described using the piezoelectric nonlinear constitutive relations and the covariant Green-Lagrange strain field. The complete nonlinear governing equations of the structure are derived using Hamilton's principle and the total increment formulation. The frequency-amplitude response is computed using an efficient Galerkin averaging-incremental harmonic balance method combined with arc-length continuation facilitated by tensor contraction and FFT techniques. Post-buckling analysis is conducted using a generalized displacement control method, and nonlinear dynamic responses are solved with the Newmark-β method. This study explores the influence of piezoelectric nonlinear parameters on the frequency-amplitude response, post-buckling behavior, nonlinear dynamic behavior, and active control performance of piezoelectric smart structures. The results show that piezoelectric nonlinearity significantly affects the amplitude-frequency response and instability characteristics of the structure, leading to more complex nonlinear phenomena and improved active control performance. This study provides valuable theoretical insights for the stability design and control of structures in engineering practice and offers a comprehensive approach to addressing the challenges posed by nonlinearity in smart structures.

The piezoelectric nonlinear constitutive equation is given as

$$\boldsymbol{\sigma} = \boldsymbol{Q}\boldsymbol{\varepsilon} - \boldsymbol{e}^{\mathrm{T}}\boldsymbol{E} - \frac{1}{2}\boldsymbol{b}\left|E_z\right|E_z, \boldsymbol{D} = \boldsymbol{e}\boldsymbol{\varepsilon} + \boldsymbol{g}\boldsymbol{E} + \frac{1}{2}\boldsymbol{h}\left|E_z\right|E_z \tag{1}$$

Keywords: MITC, Piezoelectric smart structures, Piezoelectric nonlinearity, Large rotations, Frequency-amplitude response, Post-buckling analysis, Nonlinear dynamics and control

HIGH ORDER AND SHAPE-PRESERVING ADVECTION SCHEME ON HEXAGONAL GRID

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A global advection transport model with non-negativity property is developed by implementing the high order multi-moment constrained finite volume (MCV) method [1] on icosahedral-hexagonal grid. Our previous studies conducted show that the transport model on icosahedral-hexagonal grid has rigorous numerical conservation and third-order accuracy, however, the positivity definiteness of the numerical solution is not guaranteed and nonphysical undershoots are existed in the numerical results, which violates the physical principle.

Considering advection Equation:

$$\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} = 0 \tag{1}$$

where q is the transported field and $f(q) = uq$ is the flux function with u being the advection speed. Two kinds of moments, including the volume-integrated average (VIA) and the point values (PV), are adopted in the MCV scheme and the focus of this study is to assure the non-negativity of the VIA moment. As the spatial discretization of the VIA is accomplished by the numerical fluxes, for the positive definiteness of the numerical results, an upper limits on the fluxes leaving the cell edges, which following the basic idea of the Flux-Corrected-Transport (FCT) method[2] proposed by Smolarkiewicz in 1989 , is adopted to impose restriction on the numerical fluxes. Since the transport fluxes are evaluated by the PVs defined along the cell boundaries, to adjust the flux limiter, the PVs are modified by using the approximation fluxes leaving the cells. To remove the overshoots and undershoots of the PVs, a minimum-maximum bound modification is used to the determination of PVs.

The proposed non-negativity numerical scheme on icosahedral-hexagonal grid is validated by widely used benchmark tests and the numerical results reveal that the non-negativity of the numerical solutions is guaranteed while the high-order accuracy is preserved. The present numerical framework provides a promising and practical base for further development of atmospheric general circulation models on unstructured grids.

Keywords: Multi-moment method, Shape-preserving scheme, Smoothness indicator, Hexagonal grid, Advection equation

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Resistance reduction quantification of RAC structural member and suggestion for compensatory section adjustment

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This paper presents a detailed numerical analysis to evaluate the structural resistance and performance degradation of Recycled Aggregate Concrete (RAC) compared to Natural Aggregate Concrete (NAC). Using recycled aggregates (RA) provides environmental benefits by reducing waste, but they generally show reduced mechanical properties due to inherent microcracks and previous damage. This degradation is quantified by the water absorption (Wa) of RA, which strongly correlates with adhered mortar and directly affects RAC performance.
The stress-strain relationship for RAC is adapted from the Xiao model with modifications to capture the effects of varying Wa. The adjusted model improves predictions of RAC resistance in reinforced members under different loads. The mechanical properties of RAC, especially compressive strength, show significant variability, which is analyzed probabilistically to classify RAC quality and quantify resistance loss. Results show that for RAC beams with Wa up to 10%, structural resistance drops by less than 5% compared to NAC, avoiding the need for larger sections. However, RAC columns display greater performance variability, influenced by axial force and bending. The paper proposes design correction factors and sectional adjustments to ensure RAC columns reach up to 95% of the resistance of NAC columns with the same dimensions. (Fig. 1)
This research improves RAC's practical use by analyzing its structural limits and suggesting solutions to address them, supporting wider adoption of sustainable materials and waste reduction goals.

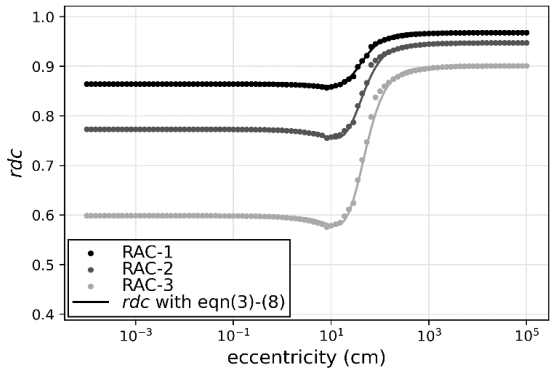

Figure 1. resistance reduction rate(rdc) with eccentricity in RAC column

Acknowledgement

This work was supported by the Korea Government as the National Research Foundation of Korea (NRF) grant (No.RS-2023-00220921) and the Ministry of Land, Infrastructure and Transport (MOLIT) as "Innovative Talent Education Program for Smart City".

Keywords: Structural Reliability, Recycled Aggregate Concrete, Stochastic FEM

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A Highly Scalable Parallel Algorithm for Non-Newtonian Blood Flow in Intracranial Aneurysm

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Numerical simulations of blood flow offer valuable insights into hemodynamic behavior in both healthy and diseased vascular systems. Although blood exhibits non-Newtonian property, most image-based models simplify the problem by assuming Newtonian behaviour. While this assumption is commonly acceptable for large, healthy arteries, its accuracy under pathological conditions has not been thoroughly studied.

The non-Newtonian effect is characterized by shear-dependent viscosity, as described by models like the Carreau–Yasuda model formulation in this study, which inherently involves strong nonlinearities and increases computational complexity. By utilizing a supercomputer platform and patient-specific blood flow parameters, the present work applies a fully implicit overlapping domain decomposition method to solve the three-dimensional non-Newtonian Navier-Stokes equations in a cerebral artery with an intracranial aneurysm. To enhance numerical convergence, an analytically derived Jacobian matrix is implemented. The algorithm is validated through a benchmark test and a series of mesh convergence studies. Numerical results confirm its scalability to thousands of processor cores and its robustness against variations in model parameters.

Keywords: Blood Flow Simulations, non-Newtonian, Finite element method, Parallel Computing, Incompressible Navier-Stokes Equations

Numerical Simulation of Fluid-Structure Interaction in Soft Cylindrical Actuators

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This study presents a computational analysis of fluid-structure interactions between fluid and a soft membrane in an axisymmetric 2D domain, using the continuous forcing Immersed Boundary Method (IBM). The flexible membrane undergoes significant deformations and is modeled using both linear and nonlinear constitutive relationships. The governing equations for the homogeneous isotropic axisymmetric membrane are derived using the variational asymptotic method, as prior implemented by Steigmann [1] and Ali et al. [2].

The fluid is treated as a Newtonian fluid under laminar flow conditions, governed by the 2D axisymmetric Navier-Stokes equations. The incompressible Navier-Stokes equations are solved numerically using Chorin's Projection method. The IBM employs continuous forcing to handle the interaction between the fluid and the membrane, enabling the structural geometry to remain independent of the fluid's Cartesian grid. Two-way coupling is achieved between the Eulerian grid and the Lagrangian nodes through a smoothing function. The membrane exerts forces on the fluid, while the fluid's velocity is interpolated onto the membrane nodes at the interface. Various smoothing functions [3, 4] can be used depending on the application.

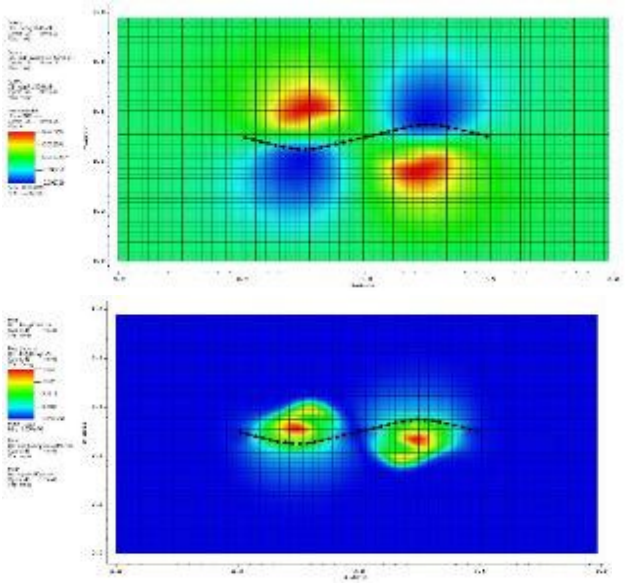

Figure 1.

The stability of the IBM algorithm is significantly influenced by factors such as geometry, discretization, material properties, flow conditions, and smoothing kernel parameters. A Python-based solver has been developed to simulate several cases like transverse fluid impact on the membrane, deformation of a perturbed membrane in a static fluid and axisymmetric actuator (where the fluid flows inside a

cylindrical tube). The resulting solutions effectively capture velocity profiles, pressure distributions, and boundary layer dynamics at the interface. The framework can be used to simulate various biomechanics and soft robotics simulations.

Keywords: Fluid structure interaction, immersed boundary method, hyper-elastic membrane modelling.

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Clinical and Computational Study of the Impact of Pressure Wire on Blood Flow and Pressure-Derived Indices

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Fractional flow in intracranial arteries and fractional flow reserve in coronary arteries are invasive indices used to assess the functional severity of arterial stenoses. They are calculated as the ratio of mean distal to proximal pressure, typically measured using pressure wires during catheter-based procedures. Recently, noninvasive numerical methods have advanced rapidly, offering patient-specific flow evaluation without procedural risk. However, validation of these methods often uses invasive FF/FFR as a reference, without accounting for the fact that the catheter and wire themselves can alter blood flow and pressure. This may affect both the invasive measurements and the accuracy of noninvasive techniques calibrated against them.

To address this issue, we conducted a combined clinical and numerical investigation to quantify the hemodynamic disturbance caused by pressure wire and catheter insertion in both cerebral and coronary arteries. Patient-specific three-dimensional vascular geometries were reconstructed from clinical imaging in six coronary artery disease cases and five intracranial atherosclerotic stenosis cases. Pulsatile blood flow was simulated by solving the unsteady incompressible Navier–Stokes equations,

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \boldsymbol{\sigma} = -\mathbf{f} \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{2}$$

where u is the velocity vector, p is pressure, ρ is fluid density, $\sigma = -pI + \mu\left(\nabla u + (\nabla u)^T\right)$ is the Cauchy stress tensor and μ is dynamic viscosity, $\mathbf{I}$ is a 3×3 identity matrix. $\mathbf{f}$ is the external force. The equations are discretized using an unstructured finite element method with fully implicit time integration. A domain decomposition-based parallel algorithm was implemented to efficiently solve the resulting nonlinear systems on high-performance computing platforms. For each case, we simulated configurations including a baseline 'in vivo' state without instrumentation and catheter and pressure wire insertion with sensor positions distal to the lesion.

Our results revealed that instrumentation can significantly alter local hemodynamics, especially in severe stenoses. In intracranial atherosclerotic stenosis models with ≥70% narrowing, fractional flow was reduced by up to 88%, while in coronary models, fractional flow reserve decreased by as much as

16.8%. Flow rate through the lesion also declined, and the magnitude of indices disturbance was strongly correlated with the minimum lumen diameter. These findings demonstrate that invasive measurement itself may overestimate stenosis severity due to device-induced artifacts, and that clinical validation of noninvasive methods should account for such effects.

Keywords: intracranial stenosis, coronary flow, computational fluid dynamics, fractional flow reserve, pressure wire, patient-specific simulation

Effects of Structural Details on Brittle Crack Arrestability in Thick Cross-joint Components Under Different Propagation Scenarios

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Brittle fracture poses significant risks in large container ships; therefore, enhancing brittle crack arrestability is essential for structural integrity. While structural design offers a promising solution, its effects under different crack propagation scenarios remain unclear.

This study investigates these effects in thick cross-joint components—critical features in ship construction—under three realistic scenarios: Scenario Zero (S0), without discontinuities, simulating full penetration welding; Scenario One (S1), with discontinuities, crack propagation from hatch coaming to deck; Scenario Two (S2), also with discontinuities but in the reverse direction. Specimens were designed for crack arrest tests to simulate these scenarios using PMMA capable of capturing high-speed crack propagation/arrest behaviour, similar to that observed in steel, in situ. Experimental results demonstrated that discontinuities significantly improved crack arrestability in S1 but had negligible effect in S2. To analyse these effects, we employed the s-version-finite-element-based framework for simulating high-speed crack propagation/arrest behaviour [1]. As illustrated in Fig. 1, Fig. 1(a) shows the global and local meshes and a representative simulated stress field for an S1 test, while Fig. 1(b) presents the histories of the dynamic stress intensity factor (DSIF) across the three scenarios.

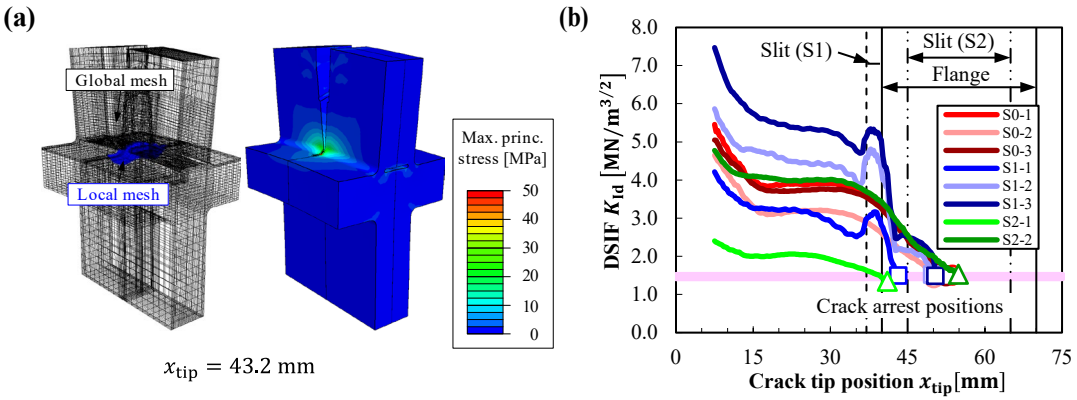

Fig. 1. Simulation results: (a) meshes and simulated stress filed for an S1 test; (b) histories of the DSIF across the three scenarios.

Numerical results revealed that, compared to S0, discontinuities significantly reduced the dynamic stress intensity factor in S1, while showing negligible effect in S2. These findings highlight the substantial potential of structural design to ensure the safety of ship structures.

Keywords: s-version of the finite element method; brittle fracture; crack arrestability; dynamic analysis; PMMA

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High-Order Mesh *r*-Adaptivity with Tangential Relaxation and Guaranteed Mesh Validity

Ketan Mittal [1*], Veselin Dobrev [1] , Patrick Knupp [2], Tzanio Kolev [1], and Vladimir Tomov [1]

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High-order meshes are crucial for achieving optimal convergence rates in curvilinear domains, preserving symmetry, and aligning with key flow features in moving mesh simulations [1] but their quality is challenging to control. In prior work, we have developed techniques based on Target-Matrix Optimization Paradigm (TMOP) to adapt a given high-order mesh to the geometry and solution of the partial differential equation (PDE) [2.3]. Here, we extend this framework to address two key gaps in the literature for high-order mesh *r*-adaptivity. First, we introduce tangential relaxation on curved surfaces using solely the discrete mesh representation, eliminating the need for access to underlying geometry (e.g., CAD model). Second, we ensure positivity of the Jacobian determinant throughout the domain and not just at a discrete set of quadrature points. This determinant positivity is essential for using the high-order mesh resulting from the proposed method with arbitrary quadrature schemes. The proposed approach is demonstrated to be robust using a variety of cases with different element types in two- and three-dimensions.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-2005078.

Keywords: high-order meshes, mesh adaptation, tangential relaxation, FEM.

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A highly parallel simulation for Navier-Stokes/Darcy equations and its application in human liver

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In this presentation, I will present a highly parallel method for the incompressible Navier-Stokes and Darcy equations for the simulation of the blood flows in the full three-dimensional patient-specific human liver, which include hepatic artery, portal vein, hepatic vein and hepatic tissue (see Fig. 1). To compute the blood flows, a scalable parallel method is used to implicitly solve the unsteady incompressible Navier-Stokes and Darcy equations discretised with a stabilized finite element method on fully unstructured meshes. The parallel algebraic solver includes a Newton method, a Krylov subspace method (GMRES) and an overlapping Schwarz preconditioner. As applications, I also simulate the flow in a patient with hepatectomy and calculate the Portal Pressure Gradient (PPG), where PPG is a gold standard value to assess the portal hypertension. Moreover, the robustness and scalability of the algorithm are also investigated (see Table 1). At last, some extensions about nonlocal fluid model will also be introduced.

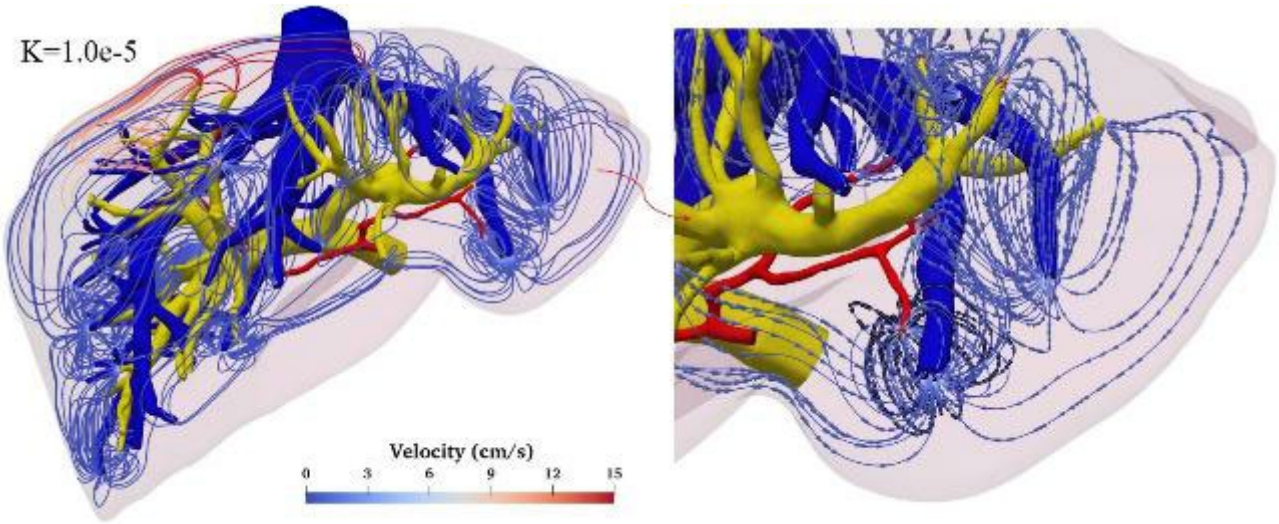

Figure 1.

Mesh	No. of cells	C_D	C_L'	St
M1	16,192	1.538	1.034	0.245
M2	64,792	1.546	1.053	0.241
M3	261,600	1.547	1.064	0.239

Table 1.

np	Time (s)	Speedup	Efficiency
1200	19.75	1	100%
2400	13.64	1.45	72%
3600	11.23	1.76	60%
4800	8.51	2.32	58%

Keywords: Darcy equations, porous media, Navier-Stokes equations, Parallel scalability

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Thermal Control and Amplification of Viscoelastic Secondary Flows in Microfluidic Devices

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Viscoelastic fluids in microfluidic channels exhibit complex secondary flows, i.e. cross-stream movements superimposed on the primary flow, that are crucial for particle manipulation and mixing applications. While these elasticity-driven flows offer significant potential, their effective control remains challenging.

This study presents a novel thermal control strategy that exploits temperature-dependent rheological properties to dramatically reconfigure and amplify secondary flow patterns. Relying on the temperature dependence of key rheological parameters, such as viscosity and relaxation time, we demonstrate via numerical simulations that moderate thermal contrasts can induce significant changes in the flow structure, even in regimes where inertial and buoyant forces are negligible.

Using a representative channel geometry and a viscoelastic fluid described by a Giesekus constitutive model, we show that thermal variations across the domain can alter the flow topology and impact the intensity of secondary motion. These effects are interpreted as the result of a spatially heterogeneous elasticity distribution, which reorganizes the internal stress field and associated vortical patterns

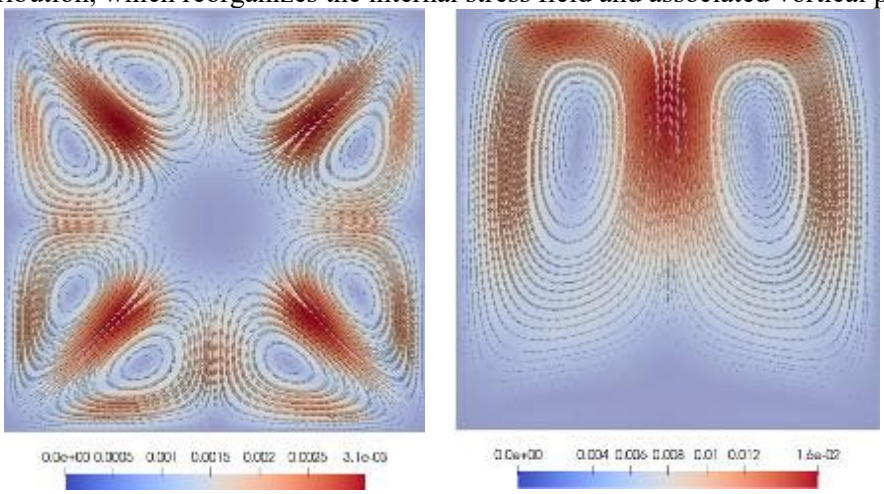

Figure 1. Secondary flow streamlines in a square duct for different thermal configurations (Re = 1, Wi = 1). **(Left)** Isothermal case: classical eight-vortex structure. **(Right) Horizontal thermal gradient: restructuration in a two-vortex structure and amplification of the flow.**

Our findings suggest that thermal gradients offer a promising, non-invasive lever to tune flow behavior in viscoelastic systems. This approach opens up new possibilities for adaptive microfluidic operations, including enhanced mixing, flow reconfiguration, and soft control of transport phenomena.

Keywords: Viscoelastic microfluidics, Secondary flow control, Thermal rheology, Flow amplification, Computational fluid dynamics

Scientific Machine Learning and Uncertainty Quantification for Aortic Hemodynamics and Wall Mechanics

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Scientific Machine Learning (SciML) is gaining interest in the broader mechanics field, notably also biomechanics. SciML offers a particular promise for Uncertainty Quantification (UQ), which concerns the estimation of uncertainties of a computational model's output due to the uncertainty of a computational model's input. To achieve such statistical estimates, a large number of computer simulations for different model inputs is necessary. In biomechanics, due to the computation time, such a large number is typically infeasible. As a work-around, one may learn a so-called surrogate model from a limited dataset of simulations, and use this surrogate to make fast, approximate predictions instead. Therein, SciML offers a compelling approach for surrogate modelling. In this talk, we will discuss a selection of real problems with ML-inspired surrogates for UQ of computational biomechanics models. The first example are Gaussian process (GP) or Polynomial Chaos surrogates for CFD simulations of non-Newtonian aortic hemodynamics [1], where the input uncertainty is first learned from experimental shear-rheometer data measured for human blood. The second example concerns Bayesian neural networks (BNN) for learning aortic wall mechanics with a stochastic, inhomogeneous tissue [2]. Therein, a fiber degradation parameter in an extended Gasser-Ogden-Holzapfel model is modelled via so-called β-random fields such that they respect physical-physiological constraints. The BNN is then trained to predict the Cauchy stress. Notably, the Bayesian approach offers a straight-forward handling of missing data and outliers, a frequent challenge in biological and medical data. Third, we will discuss the geometric uncertainty of the boundary resulting from uncertainty in imaging, segmentation, geometry- and mesh reconstruction [3] using CT-images of the thoracic aorta. We conclude with its impact on the resulting wall shear stress and pressure fields.

Keywords: scientific machine learning, uncertainty quantification, biomechanics, aortic hemodynamics, aortic wall mechanics

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A general phase-field model for electrical degradation and breakdown under electro-thermo-mechanical loading

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We present a general continuum-based thermodynamically consistent "meta"-model that couples electromagnetic fields via Maxwell's equations along with the usual conservation laws, and includes phase-field variables representing the damage caused by the electromagnetic and thermomechanical fields capable of causing electrical breakdown/failure in solid materials. We show how this metamodel includes as special cases a series of recent models proposed in the literature to attempt to model time-domain phenomena associated to electrical degradation and breakdown in polymers, such as treeing. The models are fundamental in capturing degradation in electrically insulating materials under complex loading conditions and general geometries, such as those found in modern batteries and form-wound stator coils. In this context, we elucidate how particular choices of constitutive models result naturally in Allen-Cahn equations describing the evolution of the phase-field variable, and the connection with Ginzburg-Landau theory that allows this metamodel, when the phase-field is interpreted in a specific way, to represent ferroelectric materials.

Keywords: Electrical breakdown, electrical degradation, phase-field model, electromagnetic damage in polymers, ferroelectric materials

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Adaptive phase-field cohesive zone model for simulation of mixed-mode interfacial and bulk fracture in heterogeneous materials with directional energy decomposition

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Interfacial debonding, a critical failure mechanism in heterogeneous materials, is often characterized by mixed-mode fracture. This study develops a numerical framework to simulate bulk and interfacial fractures in composite materials. A phase-field cohesive zone model, incorporating a directional energy decomposition scheme and a modified toughness method, is employed to capture complex fracture behaviors. A level-set method explicitly defines interface positions, while an adaptive mesh refinement strategy enhances computational efficiency. Numerical examples validate the model's accuracy and efficiency in predicting mixed-mode crack propagation and interfacial debonding. This work provides a robust and efficient approach to simulate complex fracture phenomena in heterogeneous materials, especially for the mixed-mode fracture.

Keywords: Phase-field method, Interfacial debonding, mixed-mode fracture, cohesive zone model, finite element method, adaptive mesh refinement

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Machine-learning enabled atomic insights into the phase diagram of Lead zirconate titanate

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Lead zirconate titanate ($PbZr_{1-x}Ti_xO_3$, PZT) exhibits exceptional electromechanical coupling properties, making it indispensable for applications in sensors, actuators, and energy harvesting. While Jaffe et al.[1] established the widely accepted PZT phase diagram, the low-temperature phase structures in the Zr-rich region near the morphotropic phase boundary remain controversial. The discovery of the monoclinic phase by Noheda et al.[2] further highlighted the complexity of this issue. Additionally, quantitative structure-property relationships in doped PZT and domain-engineered systems are poorly understood.

Recent advances in machine learning potentials have enabled breakthroughs in ferroelectrics. For instance, He et al.[3] developed a deep potential for $SrTiO_3$, successfully reproducing its temperature- and strain-driven phase transition. Similarly, Shi et al.[4] revealed the mechanism of high piezoelectric response of PZT in the morphotropic phase boundary, based on deep-potential-assited atomic simulations. Fan et al.[5] proposed the ***neuroevolution potential framework***, achieving ab initio accuracy while maintaining computational efficiency comparable to classical potentials.

Here, we combine the ***neuroevolution potential with active learning*** to develop a machine learning potential of PZT using first-principles calculation data. The potential is validated by predicting atomic forces, energies, phonon dispersions and reproducing the temperature-composition phase diagram, all of which are in good agreement with the experiments. Despite not explicitly modeling charge degrees of freedom, we observe long-range order of polarization and oxygen octahedral tilting in low-temperature phases. We further use this potential to clarify the proportion of the monoclinic phase across the whole rhombohedal range. This potential provides a fundamental tool for investigating ***domain dynamics, defect effects***, with relevant structures incorporated into the training.

Keywords: Lead zirconate titanate, phase diagram, machine learning potential, morphotropic phase boundary, monoclinic phase, neuroevolution potential

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Concurrent macro–micro topology optimization using neural networks

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Designing engineering structures that exploit material and geometric complexity across multiple scales remains a significant challenge in structural optimization. Traditional approaches often treat macrostructural layout and microstructural architecture as separate problems, limiting the potential for optimal performance. Recent studies have demonstrated the potential of neural networks in parameterizing complex microstructures and linking them with macro-scale design, yet most frameworks lack computational efficiency and compatibility of unit cells [1,2]. In this work, we propose a concurrent macro–micro topology optimization framework that integrates neural networks for both structural and microstructural design. At the macro scale, the topology of the structure is optimized for global performance objectives such as stiffness or compliance, while neural networks design the internal architecture of each microstructural unit cell to achieve specific material properties. The interaction between scales is established through computational homogenization, allowing local microstructural innovations to directly inform macroscopic behavior. Automatic differentiation is used to efficiently compute sensitivities required for optimization. Numerical experiments on benchmark examples illustrate the workflow and resulting designs, which display continuous material gradation and connectivity between microstructural cells. The framework can be adapted to various engineering applications and design requirements.

Keywords: Physics-informed neural network, topology optimization, multi-scale, mechanical metamaterials, machine learning

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An Efficient Analysis Method for Interlocking Bricks Using Representative Volume Element

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Dry-stacking interlocking brick systems present an efficient and sustainable construction method with enhanced structural integrity and resilience. However, existing numerical models for such systems are computationally expensive due to the complex brick geometry and contact interactions. This study proposes an efficient analysis method employing a Representative Volume Element (RVE) approach, enabling accurate yet efficient analysis under both static and dynamic loads. The developed model leverages the periodic construction pattern of interlocking brickwork by identifying a basic RVE composed of full, half, and quarter bricks. Detailed finite element simulations are conducted on the RVE under various loading conditions—including uniaxial, biaxial, and triaxial compression, shear, and strain rate-sensitive loading. Equivalent elastic constants, yield surface, plastic flow rules, hardening/softening behavior, and a damage evolution law are then derived in continuum damage mechanics. The results indicate the equivalent elastic moduli and Poisson's ratios are nearly isotropic, justifying a simplification of the material model. Strain rate effect is also incorporated via empirical formulations of Dynamic Increase Factors (DIFs) in tension, compression, and shear, enhancing its applicability to impulsive loading such as blast and impact. The equivalent strength envelope is constructed in both plane stress and meridional stress spaces, capturing the anisotropic failure behavior of the RVE under different stress paths. A rate-sensitive damage model is implemented to account for the progression of micro-cracking under high-rate loading, further aligning the homogenized behavior with physical responses. The homogenized model is validated against detailed finite element simulations and experimental data under different dynamic loading scenarios including both blast loading and impact loading. The RVE model is found to accurately capture failure modes and dynamic responses while reducing computational time by over 98% compared to the detailed models. The study demonstrates that the proposed RVE-based homogenized constitutive model provides a highly efficient and accurate means for simulating interlocking brick walls under dynamic loads. It facilitates performance-based design and optimization of such systems without the prohibitive computational

burden of detailed brick-level modeling. This work lays a robust foundation for extending homogenization techniques to other modular construction systems with complex interfaces.

Keywords: Interlocking brick; Dry-stacking; RVE; Homogenization; Resilience

Exploration of the application of physics to inform machine learning to drive structural optimisation in the biomedical space.

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Biomedical engineering faces significant challenges in translating complex anatomical geometries and physiological loading conditions into accurate mechanical models for structural analysis. Traditional finite element methods often struggle to fully accommodate nonlinear loading and heterogeneous material behaviour without introducing simplifications. Recent developments in physics-informed machine learning offer a compelling alternative, leveraging energy conservation principles to solve governing equations in a mesh-free, differentiable framework.

In this work, we propose an energy-driven, topology-optimisation framework composed of two coupled neural networks. The **Displacement-Enforcing Mechanics Neural Network** learns the mechanical displacement field by minimising the residual between internal strain energy and external work, while simultaneously penalising deviations from prescribed boundary conditions. The **Spatial Prediction and Interpolation Neural Network** predicts the distribution of material density across the domain by minimising structural compliance, enforcing a global volume constraint, and promoting connectivity through geometric regularisation. Together, these networks form a closed-loop system that links physics-based response and design generation through shared loss functions.

The framework is demonstrated through the optimisation of a femoral plate, a clinically relevant application that often suffers from simplification in computational models due to the difficulty of modelling full anatomical loading. Prior approaches typically impose symmetry or reduce the boundary conditions to enable tractable simulations. In contrast, our method handles physiologically realistic loading scenarios without requiring such simplifications. While the training incurs a higher computational cost per cycle, it enables structurally robust and manufacturable designs for biological loading conditions.

This study highlights the potential of physics-informed optimisation as a practical tool for biomedical structural design, offering improved connectivity, accuracy, and anatomical realism compared to conventional methods.

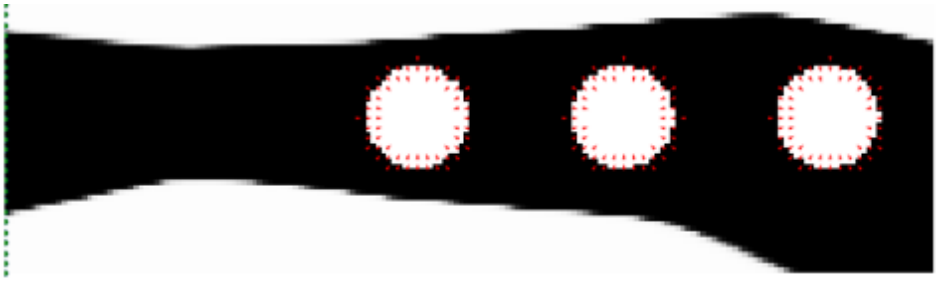

Figure 1. Sample Plate modelled using symmetry with radial compressive forces supported along left edge.

Keywords: Physics-informed machined learning, Topological Optimisation, Biomedical Structural analysis, conservation laws, machine learning, femur plate, **Displacement-Enforcing Mechanics Neural Network, Spatial Prediction and Interpolation Neural Network,**

Insights into impact damage and compression-after-impact strength of innovative composite architectures

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This talk addresses recent advancements in the experimental testing and modelling of composite structures subjected to low-velocity impact (LVI) and subsequent compression-after-impact (CAI) loading, focusing on two innovative composite architectures: 3D woven structures and 'Double-Double' (DD) laminates. Both studies leverage high-fidelity finite element analysis (FEA) to predict damage mechanisms and residual strength, offering valuable insights into optimising lightweight, damage-tolerant composite designs for aerospace and other demanding applications.

The first part of the talk highlights the role of 3D woven composites in addressing the limitations of traditional unidirectional and 2D woven composites, particularly their susceptibility to delamination. Different approaches to modelling the binder reinforcement are assessed. It is shown that modelling the binder reinforcement with an elliptical yarn cross-section, and accounting for compaction, closely replicates experimental outcomes, establishing a benchmark for accurately predicting damage and residual strength for such fibre architectures.

The second part explores 'Double-Double' (DD) laminates as replacements for traditional legacy quad laminates (LQL). DD laminates are constituted from sub-laminates of unidirectional plies where only two angles are used. The same high-fidelity finite element analysis as used to model 3D wovens is used to assess their response to low velocity impact (LVI) and compression-after-impact (CAI) strength. It is shown that DD laminates are effective replacements for LQL laminates where higher residual strengths were observed in the cases examined in this work.

Keywords: impact damage, compression-after-impact strength, double-double laminates, woven composites.

Applications of numerical methods in computation acoustics, a brief review

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Abstract: Finite element and boundary element analysis in acoustical analysis have been well developed for over 50 years, which have been broadly applied in many aspects of acoustics. This talk summarizes and discusses some of successful applications of numerical simulation techniques in disclosing complex vibro-acoustics coupling and unique sound absorption and insulation phenomena, particularly on the recent advancement of acoustical metamaterials. Applications of these numerical analysis tools on the transformation of computation acoustic analysis approaches and their profound effects on the evolution of modern industrial technologies will be discussed with supporting application cases.

Dissimilar control by streamwise traveling waves with long wavelength in turbulent plane Couette flows

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Simultaneous achievement of drag reduction and heat transfer enhancement, which is the so-called dissimilar control, is a challenging issue due to the Reynolds analogy between the momentum and heat transfer. In some previous studies, e.g., Kaithakkal et al.[1] and Uchino et al.[2], the dissimilar control has been achieved in the turbulent plane Poiseuille flow by using the streamwise traveling waves. However, despite the similarity of flow configuration between Poiseuille and Couette flows, the dissimilarity in a turbulent plane Couette flow has been hardly investigated.

In this study, a direct numerical simulation of a fully developed turbulent plane Couette flow under constant velocity difference and constant temperature difference conditions is performed to achieve dissimilar control using two different types of streamwise traveling waves: blowing/suction and wall oscillation. In the case of blowing/suction, the amount of the contribution in the turbulent heat flux is approximately double that in the Reynolds shear stress, leading to the achievement of dissimilar control: the maximum analogy factor is $A = 1.91$. Additionally, as shown in Fig. 1, in the case where the analogy factor is large, we simultaneously observe the regions where the quasi-streamwise vortices are drastically enhanced and those where they almost vanish, which means the formation of intermittent structures. In contrast, we observe that the similarity between momentum and heat transfer strongly holds in the case of wall oscillation, so that the analogy factor is $A \approx 1$ in all cases.

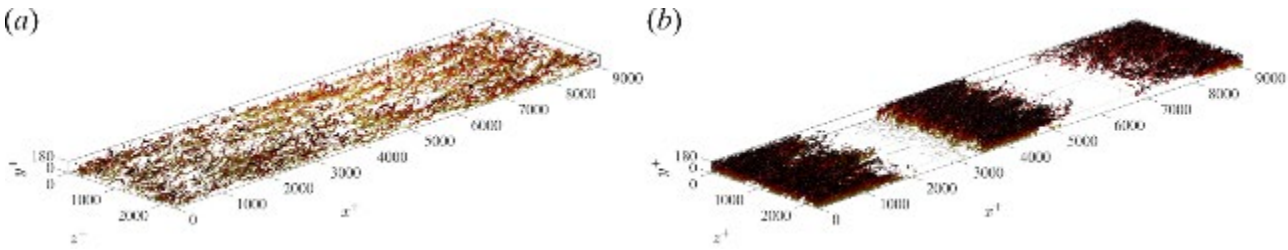

Figure 1. Instantaneous vortical structures in (*a*) the uncontrolled case and (b) the blowing/suction case with the maximum analogy factor.

Keywords: Dissimilar control, Streamwise traveling wave, Turbulent plane Couette flow, Direct numerical simulation

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Crystal-plasticity phase-field fracture model: on plastic crack driving force

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Coupled crystal-plasticity phase-field (CPPF) fracture models could potentially forecast short crack propagation, but there is no consensus on the crack driving force (CDF) from the plastic contribution among existing CPPF fracture models. Herein, we systematically investigate CPPF fracture models with four types of plastic CDFs and identify these models' capability in simulating crack propagation in single crystal. These models comprehensively account for various CDFs arising from plastic dissipated energy ($\Psi^{p,diss}$), plastic locking energy ($\Psi^{p,lock}$), defect energy ($\Psi^{p,defect}$), and $\Psi^{p,diss}$ combined with critical energy release rate (G_c) reduction. The objective is to assess the rationality and distinctions among different CPPF fracture models in simulating the fracture of single crystal and analyze the change of plastic strain and plastic energy during crack propagation. It is found that in a single-edge notched face-centered cubic single-crystal copper subjected to tension along [001] direction, the CPPF fracture models with CDF from $\Psi^{p,diss}$ and $\Psi^{p,defect}$ can only reproduce the brittle-like type-I cracking with crack path perpendicular to [001] axis. This is attributed to that both $\Psi^{p,diss}$ and $\Psi^{p,defect}$ are much lower than elastic energy (Ψ^{e}) and thusΨ^{e} dominates the cracking behavior. In contrast, CPPF fracture models with CDF from $\Psi^{p,lock}$ and $\Psi^{p,diss}$ with G_c reduction can replicate the ductile cracking with crack path along the slip direction (45◦ to [001] axis), agreeing with experimental observations. The model with ??p,lock is further demonstrated rational in predicting both brittle and ductile fracture. In addition, the model is utilized to simulate the crack propagation in polycrystalline copper, further validating its potential applicability in polycrystalline materials. Our work has clarified the role of different types of plastic CDFs in CPPF fracture model and could shed light on the CPPF modeling of short crack propagation in metals.

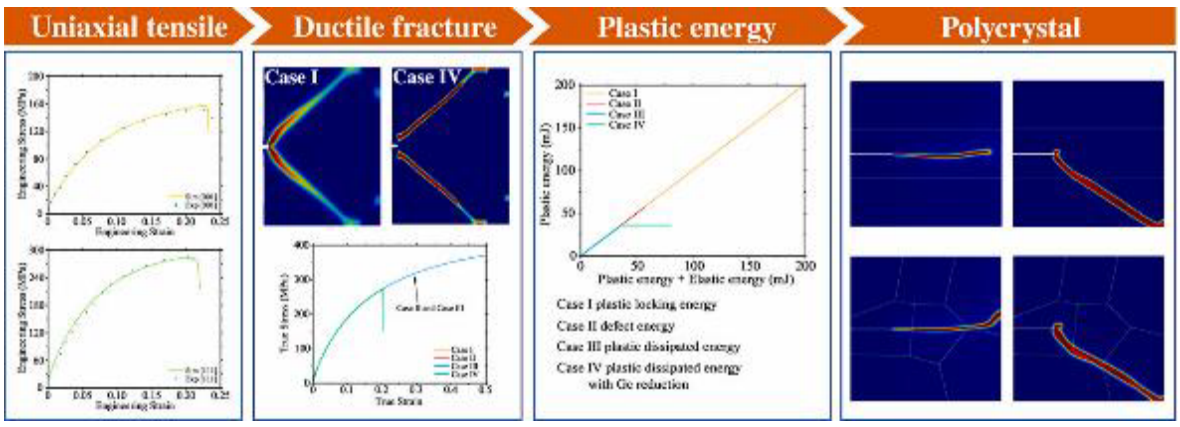

Figure 1.

Keywords: Phase-field model, Crack propagation, Crystal plasticity, Ductile fracture, Crack driving force

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SH-wave scattering in the orthotropic half-plane containing a hill using the boundary integral quadrature method

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The boundary integral quadrature method (BIQM) is a meshless method based on the boundary integral equation (BIE). By introducing the adaptive exact solution, this novel regularization technique was employed to deal with the singular integral. Furthermore, after using the Gaussian quadrature and parametric representation, the simultaneous equations can be obtained by only collocating boundary points. The BIQM has been successfully applied to steady-state heat transfer in heat exchanger tubes [2-3] and torsional bars with edge cracks [4]. In this paper, the BIQM is extended to simulate the SH-wave scattering problem in the orthotropic half-plane containing a hill. To deal with this problem conveniently, the techniques of the domain decomposition and the image method are adopted to obtain six constraint equations. Finally, the impact of the parameter study on dimensionless frequency, incident angle, and geometric parameters for the distribution of surface displacement amplitude is considered.

The anti-plane displacement field with the time-harmonic motion satisfies the following equation

$$G_{xz}\frac{\partial^2 u(\mathbf{x})}{\partial x^2}+G_{yz}\frac{\partial^2 u(\mathbf{x})}{\partial y^2}+\rho\omega^2 u(\mathbf{x})=0,\ \mathbf{x}=(x,y)\in D, \tag{1}$$

where $u(\mathbf{x})$ is the total displacement field, D is the domain, ω is the angular frequency, ρ is the density of the soil, G_{xz} and G_{yz} are the shear modulus.

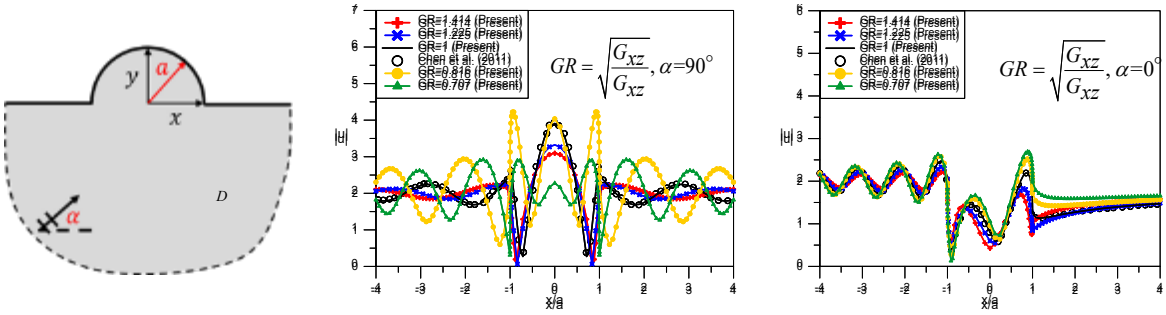

Figure 1. Surface displacement amplitudes for the semi-circular hill

Keywords: SH-wave scattering problem, adaptive exact solution, boundary integral quadrature method, Gaussian quadrature, orthotropic

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Diamond Nanothread's Morphology of Length-Dependent Torsion and Chirality Enlightened by Machine Learning Potential

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Carbon Nanothreads, one-dimensional chains of sp^3 hydrocarbon, are expected for advancing high-performance devices, if they could stretch to centimeters-scale length without curl and spiral.[1] However, up-to-date synthesis tend to introduce defects.[2] And enumeration of all topology-possible saturated configurations shows that aperiodic torsion distribution may induce spirals along diamond nanothreads, especially chiral ones. The morphology of diamond nanothreads still remains unknown, since prevailing empirical potentials have failed to give unified answers.

Here, we present a state-of-the-art neuron evolution potential [4], trained against van der waals force corrected density functional theory calculations under rounds of configuration space exploration. The potential, called NEP-DNT, is examined to predict mechanical and thermal properties in close accuracy to first principle calculation results. Afterwards, it is utilized to explore the length-dependent morphology of diamond nanothreads. We deduce a theoretical model to quantify variation of aperiodic helical formation according to torsion distribution. And the molecular dynamics simulation results show torsion become unchanged when lengths of diamond nanothread increase. We find that both achiral and chiral nanothreads could have helicals along axial direction, and their morphology matches results of macroscopic mechanics experiments. These discoveries may help to efficiently design synthesis by classifying preferrable diamond nanothreads without helical.

Keywords: carbon nanothread, chirality, local torsion distribution, atomic structure morphology, neuroevolution machine learning potential

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Large-eddy simulation of wind interaction with direct air capture systems in the atmospheric boundary layer

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Direct air capture (DAC) is a promising technology for removing atmospheric CO_2 via physical or chemical absorption, with this study focusing on liquid-based systems. Although still in early stages of development and encountering scaling challenges, DAC systems can benefit from computational fluid dynamics (CFD) for design optimization. While past studies focused on internal processes, this work employs Large-Eddy Simulation (LES) to investigate how atmospheric boundary layer (ABL) winds influence airflow around and within a DAC unit.

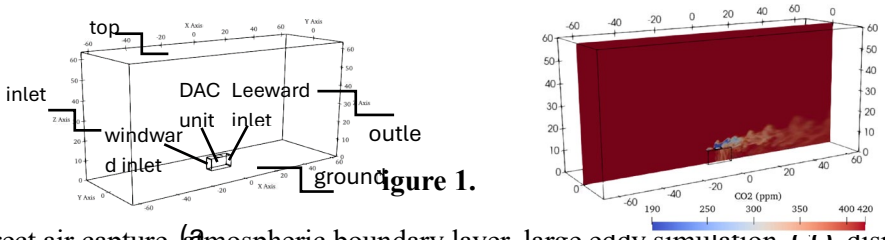
An in-house LES solver based on sprayFoam of OpenFOAM platform was used to model the flow interaction and non-reacting gas-phase CO_2 dispersion. For example, the continuity and momentum equations solved using the LES approach were [1].

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j} = 0, \tag{1}$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}^{sgs}}{\partial x_j} + \bar{\rho}g_i + \tilde{S}_p, \tag{2}$$

where u_i is the flow velocity at the i-direction, g , ρ and p are the gravitational acceleration, flow density and pressure, respectively. τ_{ij} is resolved viscous stress tensor and S_p is the (negative) source term porous media pressure drop associated with Darcy Fochheimer model.

A representative DAC geometry was considered and modelled as a rectangular crossflow cooling tower with a top-mounted fan and two vertical porous fills at the inlets on the windward and leeward sides, positioned in the surrounding environment (Figure 1 (a)). The LES model was validated using our experimental measurements as well as analytical, and numerical data available in the literature [1]. Several scenarios of no-wind and ABL wind speeds with different reference velocities were simulated to study the impacts of wind on the performance of the DAC unit. Results showed that at moderate to high wind speeds, recirculation can occur, with CO_2-depleted air plume re-entering the DAC unit through the leeward inlet (Figure 1 (b)). It was also found that the presence of wind significantly affects flow velocity behaviour at both windward and leeward inlets with greater flow entrainment through the windward inlet due to wake forming behind the unit.



(a) (b)

Figure 1.

Keywords: Direct air capture, atmospheric boundary layer, large eddy simulation, CO_2 dispersion

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Stabilized Reproducing Kernel Enhanced Material Point Method for Air Flow and Air-Structure Interaction with Shocks

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Mesh-based methods, such as the finite element method within a Lagrangian framework, face significant challenges in modeling air flows and air-structure interaction (ASI) problems involving shock waves, primarily due to excessive mesh entanglement and distortion. In contrast, meshfree methods such as the Reproducing Kernel Particle Method (RKPM) and the Material Point Method (MPM) have proven effective, as their particle-based descriptions naturally avoid singularities caused by mesh distortion. However, these meshfree methods still suffer from various numerical artifacts to differing degrees. Additionally, when modeling air flows with shocks, appropriate numerical stabilization is crucial. To address these limitations, we propose a Reproducing Kernel Enhanced Material Point Method (RK-MPM) for simulating inviscid compressible flows with ASI. In this framework, a mixed MPM formulation is employed to solve the Lagrangian momentum and energy conservation equations, while the Reproducing Kernel (RK) approximation [1,2] is used to alleviate cell-crossing instabilities within MPM. To further suppress shock-induced oscillations, we enhance the classical artificial viscosity by introducing tensorial formulations of the diffusion and divergence operators, guided by the vorticity modulus. This approach blends numerical dissipation between the dilatational and deviatoric components to achieve improved stabilization [3]. Finally, we incorporate a point-to-structure contact algorithm to model the ASI system. The proposed method is validated through a series of benchmark problems, including shock waves, vortical flows, and air-structure interaction scenarios.

Keywords: inviscid compressible flow, reproducing kernel approximation, material point method, artificial viscosity, air-structure interaction

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A probabilistic geometric imperfection model for uncertainty quantification of inflatable beams with local structure instability

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Abstract

Experimental data of inflatable beams present strong randomness that is caused by a locally post-buckling behavior, sensitive to boundary condition and initial geometric imperfection. It is so difficult for finite element analysis (FEA) to predict the post-buckling nonlinear behavior and collapse load accurately, and uncertainty quantification (UQ) still remains an open problem for inflatable beams. The paper proposes a new probabilistic geometric imperfection model that is used for post-buckling FEA and completes the uncertainty quantification of inflatable beams using Gaussian process regression (GPR). Differing from an empirical selection of buckling eigenmodes, the proposed imperfection model introduces two random variables describing uncertainties of material and structural coefficients. With scarce experimental data, the model is validated, and then the given confidence interval (CI) of load-deflection curves obtained by FEA and GPR can cover disperse experimental data. The cost of experiments for uncertainty quantification is thus saved greatly. The study shows that amplitude and location of wrinkles are two key factors influencing the collapse load of inflatable beams. The predicted CI can be used in structural design based on its lower bound and structural health monitoring (SHM). It suggests that usage of the proposed geometric imperfection model could be enhanced by popular machine learning or artificial intelligence technologies, such as Convolutional Neural Networks (CNN) and Generative Adversarial Networks (GAN), for real-time SHM in future.

The main equations for the problem or method of analysis are followed:

$$\boldsymbol{u}_0(\mathbf{X}_i) = c\sum_{j=1}^{n} k_j \boldsymbol{\omega}_j(\mathbf{X}_i), \tag{1}$$

in which $\boldsymbol{u}_0(\mathbf{X}_i)$ is the initial displacement of the initial coordinate $\mathbf{X}_i$. c is random variable following uniform distribution, used for tuning the amplitude of initial imperfection. k_j is random variable following uniform distribution, used to change the morphology of initial imperfection. $\boldsymbol{\omega}_j$ is the j-th buckling eigenmode.

Keywords: inflatable beams, locally wrinkling, initial geometric imperfection, collapse load, uncertainty quantification

Multi-scale analysis of structure damage behaviour using isogeometry analysis and generative adversarial network

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Structural damage analysis presents notable challenges due to localized nonlinear and anisotropic behavior induced by microcracks. Conventional single-scale methods, such as XFEM and phase-field models, often fail to capture microscale anisotropy and exhibit mesh dependency in failure prediction. Multiscale modeling offers a more robust and consistent framework by linking micro- and macro-scale behaviors. However, traditional FEM-based macroscale simulations require fine meshes for complex geometries, leading to high computational cost. At the microscale, conventional models either rely on overly simplified assumptions for efficiency or involve complex formulations that hinder computational performance. Recent efforts have introduced neural networks (NNs) to accelerate microscale simulations, yet selecting and training suitable NNs remains challenging.

This study proposes a hybrid multiscale damage analysis framework incorporating the meshfree method, Isogeometric Analysis (IGA) at the macroscale and Generative Adversarial Networks (GANs) at the microscale to improve computational efficiency. To address mesh dependency, an implicit failure description is employed, where microscale stress predictions are used to degrade integration points, inducing localized plasticity. GANs are trained to predict stress fields in cracked microscale plates under tension–compression loading. During explicit dynamic analysis, the updated stress fields are converted into resultant forces and integrated into the global stiffness matrix, enabling localized damage evolution. The matrix $\mathbf{K}$ represents the stiffness matrix and the $\mathbf{u}^{k+1}$ vector is the displacement vector at $k+1$ step. The $\mathbf{B}^m$, $\mathbf{B}^b$ and $\mathbf{B}^s$ are represent the differential approximate matrix related to membrane, bending and shear term from Mindlin plate theory. The N, M and Q are resultant force, moment and shear force. The N with AI represent the resultant force degraded by the micro-scale stress field. The w_G and J_G are Gauss integration weight and Jacobian matrix. The convergence of the IGA implementation was first verified through natural frequency analysis. For preliminary microscale validation, uniaxial and biaxial tension tests were conducted and compared with XFEM results. results show stress errors below 3% and crack propagation angle differences within 1°. Preliminary multiscale simulation shows the trends of stress concentration and material degradation.

$$\mathbf{K}\mathbf{u}^{k+1}_{(5\mathrm{x}1)} = \int_{\Omega}\left(\left(\mathbf{B}_I^m\right)^T_{(5\mathrm{x}3)} \begin{bmatrix} N_{11}^{AI} \\ N_{22}^{AI} \\ N_{12}^{AI} \end{bmatrix}_{(3\mathrm{x}1)} + \left(\mathbf{B}_I^b\right)^T_{(5\mathrm{x}3)} \begin{bmatrix} M_{11} \\ M_{22} \\ M_{12} \end{bmatrix}_{(3\mathrm{x}1)} + \left(\mathbf{B}_I^s\right)^T_{(5\mathrm{x}2)} \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}_{(2\mathrm{x}1)} \right) w_G \mathrm{J}_G \mathrm{d}\Omega \tag{1}$$

Keywords: Damage analysis, meshfree method, multi-scale analysis, Isogeometirc Analysis (IGA), Generative Adversarial Networks (GAN)

Gaussian Process Regression Model for Efficient Prediction of Pressure Capacity in Nuclear Structural Components

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The International Atomic Energy Agency Safety Standards [1] recommend the use of both deterministic and probabilistic analyses to ensure nuclear structural reliability and plant safety. The latter are typically based on finite element analyses owing to the limitations of experiments [2]. Although more efficient than experiments, they still incur high computational costs. To address the issue, approaches such as design of experiments and artificial intelligence have gained increasing attention. In particular, artificial intelligence has shown promising performance in improving the efficiency of structural safety assessment.

In the present study, a Gaussian process regression model is applied to reduce the number of required simulations for probabilistic analyses of containment vessel while maintaining accurate predictions of structural response. The model is trained with 20 cases generated by Latin Hypercube Sampling. After training, it is employed to predict structural response and estimate fragility curves of a containment vessel. The regression function, represented as a joint Gaussian distribution, is defined as follows:

$$\boldsymbol{P(f|X)} = \boldsymbol{N(f|\mu, K)} \tag{1}$$

where $X = [x_1, \cdots, x_n]$ represents the observed data points, $f = [f(x_1), \cdots, f(x_n)]$ the function values, $\mu = [m(x_1), \cdots, m(x_n)]$ the mean function, and $K_{ij} = k(x_i, x_j)$ the kernel function, which is a positive definite [3].

Using this model, fragility curves were estimated with substantially fewer simulations compared to conventional approaches. The results show that fragility curves derived from a small number of Latin Hypercube Sampling cases are consistent with those obtained from larger-scale simulation datasets, thereby confirming both efficiency and accuracy. These findings suggest that the Gaussian process regression model provides an effective tool for probabilistic safety assessment of nuclear structural components.

Keywords: Computational efficiency, containment vessel, Gaussian process regression, probabilistic analysis, structural reliability

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Development of a Stress Intensity Factor Solution for Cracks in a Small Modular Reactor Vessel

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The reactor vessel in a nuclear power plant is required to operate for more than 40 years without replacement, while maintaining structural integrity to prevent the release of reactor coolant and radioactive materials. Accordingly, the vessel material should retain sufficient strength and high fracture toughness throughout its service life. The integrity of the reactor vessel is generally assessed following the procedures specified in the American Society of Mechanical Engineers Boiler and Pressure Vessel Code [1], which is based on linear elastic fracture mechanics. One of small modular reactors currently under development in the Republic of Korea has adopted an integral design, introducing a new geometric discontinuity known as the transition region. A previous study reported that stress and stress intensity factor at this region may exceed those at the beltline [2]. However, the Boiler and Pressure Vessel Code provides stress intensity factor solutions only for the beltline and nozzle. In this study, finite element analyses were performed to derive stress intensity factor solution applicable to the transition region of a small modular reactor vessel. To reduce the effort associated with mesh refinement near crack-tip, the extended finite element method [3] was employed. The displacement vector function used in fracture mechanics analyses is described in equation (1).

$$u = \sum_I^N N_I(x)[u_I + H(x)a_I + \sum_{\alpha=1}^4 F_\alpha(x)b_I^\alpha] \quad (1)$$

where $N_I(x)$ represents the nodal shape function, u_I is the nodal degree of freedom, $H(x)$ is the discontinuous jump functions while a_I denotes nodal enriched degree of freedom. Similarly, $F_\alpha(x)$ and b_I^α denote the crack tip term and associated nodal enriched degree of freedom, respectively.

Finite element models were constructed by modifying geometric parameters such as wall thickness, inner radius, and angle between the beltline and transition region. Postulated cracks were introduced at the transition region, and the corresponding stress intensity factors were calculated. Based on the analyses results, a stress intensity factor solution for the transition region was derived and verified through an appropriate procedure. The developed solution enables efficient evaluation of stress intensity factors at the transition region, providing a practical tool for the design and assessment of small modular reactor vessels.

Keywords: Extended finite element method, small modular reactor vessel, stress intensity factor solution, transition region

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Integrity Assessment of SNF Cladding with PCI Effects Using a Machine-Learning Surrogate Model

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Spent nuclear fuel contains substantial inventories of fission products, posing inherent risks during post-irradiation management. Ensuring structural integrity throughout storage and transportation is therefore essential. The cladding, which functions both as an engineered barrier against radionuclide release and as a critical indicator of fuel condition, plays a central role in maintaining spent nuclear fuel. Under high burnup conditions, pellet-cladding interactions - including internal zirconia layer formation, pellet swelling, and cladding contraction - significantly affect cladding performance.

Previous studies have investigated the aforementioned effects individually, such as the influence of zirconia layers and pellet swelling [1]. Building upon this work, the present study considers three parameters collectively - internal zirconia layer, pellet swelling, and drop height - as input variables for a machine-learning surrogate model. Finite element analyses were performed for each parameter combination, with von Mises stress and maximum principal strain defined as the output responses to train the surrogate model. Figure 1 depicts a representative drop analysis result, which was included in the training dataset. The surrogate model accurately predicted output responses across a broad parameter space, and results were benchmarked against the 1% strain-based failure criterion [2].

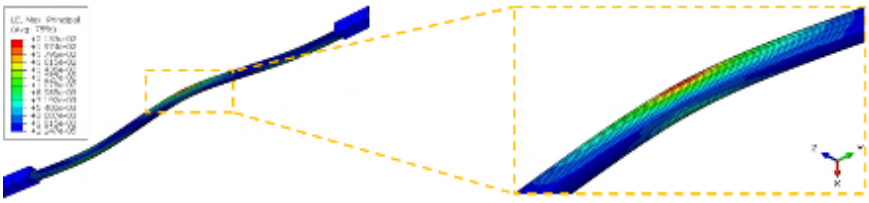

Figure 1.

This study proposes a comprehensive framework for assessing the structural integrity of spent nuclear fuel cladding considering pellet-cladding interaction effects. The framework enables reliable prediction of cladding behavior under postulated drop scenarios and facilitates the clear identification of conditions that exceed the failure threshold.

Keywords: Drop analysis, finite element method, machine learning, pellet-cladding interaction, spent nuclear fuel

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Strain based Formulation for Bayesian Model Updating Using Strain Modal Data

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Bayesian model updating provides a comprehensive framework for system identification and uncertainty quantification by utilizing the prior knowledge with measured data (Beck, 2010). Within this framework, the posterior probability density function (PDF) of the model parameters is estimated. There are two main approaches for model updating using modal data, namely mode matching (Goller et al., 2012; Yin, 2022) and eigenvalue equation–based methods (Bansal, 2020; Ching et al., 2006). The mode matching approach is based on the measure of difference between model predictions and data. The eigenvalue equation–based methods utilize the eigenvalue equation to formulate the model prediction error. In this paper, a methodology for Bayesian model updating of non-classically damped structures using strain modal data is presented. The dynamic strain-based equation of the motion, obtained by minimizing the energy functional of the structural system, is expressed as follows:

$$\mathbf{M}_{\Phi}\ddot{\mathbf{q}} + \mathbf{C}_{\Phi}\dot{\mathbf{q}} + \mathbf{K}_{\Phi}\mathbf{q} = \mathbf{f}_{\Phi}, \tag{1}$$

where $\mathbf{q}$ is vector of state variables consisting of independent elemental strains; $\boldsymbol{\Phi}$ is transformation matrix from state variables to nodal displacement vector; $\mathbf{f}_{\Phi}$ is strain-based force vector; $\mathbf{M}_{\Phi}$, $\mathbf{K}_{\Phi}$, and $\mathbf{C}_{\Phi}$ are strain-based mass, stiffness and damping matrices, respectively. Based on the two stage Bayesian model updating (Zhang & Au, 2016), the posterior PDF of uncertain parameters is expressed as:

$$p(\boldsymbol{\theta}_s, \boldsymbol{\kappa}, \mathbf{v} \mid D) \propto p(\boldsymbol{\theta}_s) \prod_r p(\boldsymbol{\kappa}_r) p_o(\mathbf{v}_r \mid D) p(\mathbf{v}_r \mid \boldsymbol{\theta}_s, \boldsymbol{\kappa}_r), \tag{2}$$

where $p(\boldsymbol{\theta}_s)$ and $p(\boldsymbol{\kappa}_r)$ are prior PDFs for structural parameters, $\boldsymbol{\theta}_s$, and r^{th} mode prediction error variance, $\boldsymbol{\kappa}_r$. $p_o(\mathbf{v}_r \mid D)$ is hypothetical posterior PDF for r^{th} mode modal parameters, $\mathbf{v}_r$, from modal identification, D represents measured data, $p(\mathbf{v}_r \mid \boldsymbol{\theta}_s, \kappa_r)$ represents PDF of model prediction error, $\boldsymbol{\kappa} = [\boldsymbol{\kappa}_1 \cdots \boldsymbol{\kappa}_m]$, $\mathbf{v} = [\mathbf{v}_1 \cdots \mathbf{v}_m]$, and m is number of modes. MWG sampling (Kiran & Bansal, 2024) is utilized to draw samples from the posterior PDF of the uncertain parameters. The effectiveness of the proposed approach is demonstrated through a numerical study on a cantilever aluminium beam, as shown in Figure 1. Among the bending strains, S1to S12, modal data corresponding to strains S1 S5 and S9 are considered for five modes. The stiffness scaling parameters of elements are treated as the structural parameters to be updated. The results show that the posterior sample mean values of structural parameters are close to their nominal values, and the posterior coefficients of variation (COV) are significantly reduced compared to the prior COV.

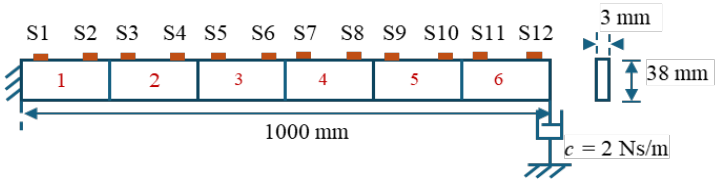

Figure 1.

Keywords: Bayesian model updating, non-classically damping, MWG sampling, Structural analysis, Strain modal data

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AI reinforcement on untrained compound damage detection and scour detection in offshore wind turbine

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Structural Health Monitoring (SHM) is crucial in the early stages of damage formation for life-cycle service of engineering structures. In scenarios involving compound damage detection and pile scouring, where different damages occur in different parts of a structure, identification of the minor damage becomes a big challenge.

This study first proposes a novel method for end-to-end damage detection solely based on vibration responses, employing Wavelet Transform (WT) and a Deep Convolutional Neural Network with Multiple Interference (MIDCNN). The main idea involves training the MIDCNN on time-frequency data from healthy and single damage states, without incorporating time-frequency data from compound damage during training. The proposed approach is verified by measured data from a laboratory-scale offshore jacket structure. The findings illustrate the superior precision of the method in extracting features and classifying various states, including healthy, single and compound damage. Furthermore, A digital twin is proposed as a solution for condition monitoring of scour detections in offshore wind turbine. The core foundation of the digital twin is finite element modeling, which is used to simulate and obtain dynamic responses. In this process, modeling a damage-sensitive model is prioritized. To achieve this, the model parameters are updated using the proposed optimization method and the results of experimental modal analysis. Based on the proposed graph neural network (GAT_GATv2), damage-sensitive features are learned in the simulation data under different scouring depths to train the model, and the data obtained from the experimental models are used for testing to achieve the classification of different damage scenarios.

Keywords: damage detection, graph neural network, finite element, offshore wind turbine, pile-soil interaction

Rate and Creep Effect on the Pull-out Performance of Suction Anchors in Clay

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Monotonic loading tests are commonly used to determine the pull-out capacity of suction anchors, yet the influence of loading rate is rarely examined. Research on creep effects under long-term sustained loads is also limited. This study addresses both issues by numerically investigating the short-term rate effect and the long-term creep effect on the pull-out performance of suction anchors in clay. The advanced ANICREEP soil model is employed to capture the time-dependent behavior of clay with respect to rate and creep. For the short-term response, the study examines load–displacement behavior and excess pore pressure considering the pull-out rate influences in displacement-control cases and loading rate influences in load-control cases, respectively. For the long-term response, it explores excess pore pressure evolution and variations in padeye trajectories for different $C_{\alpha e}$ (secondary compression coefficient) and loading angles. The results provide practical insights for incorporating rate and creep effects into the design and assessment of suction anchors in offshore engineering.

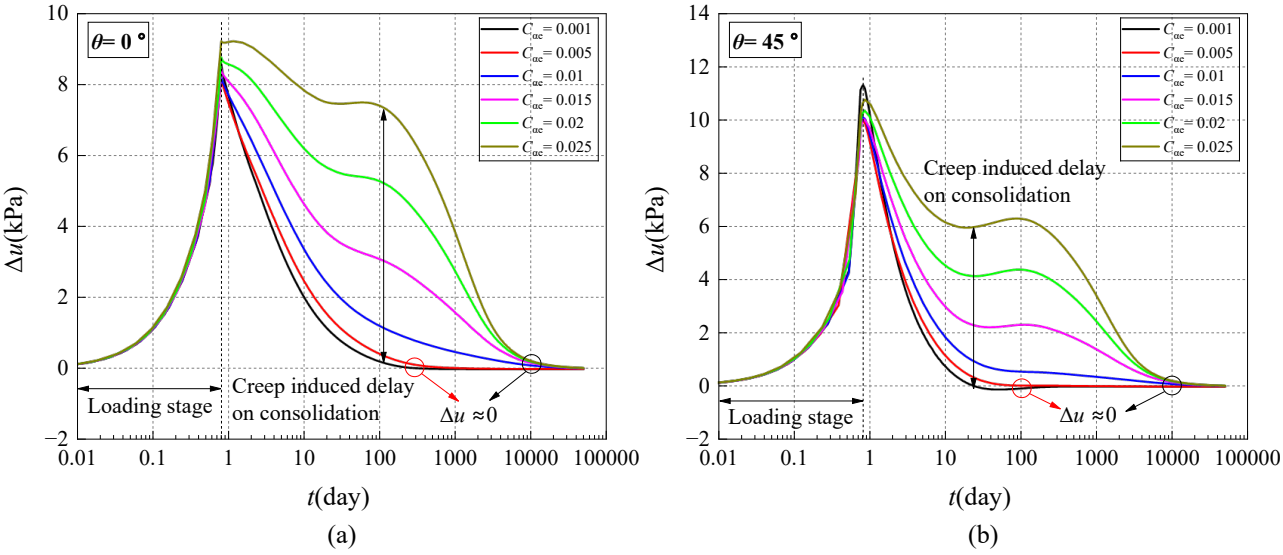

Figure 1. Creep effect on the excess pore pressure development for various $C_{\alpha e}$ and loading angles

Keywords: suction anchor, rate effect, creep effect, finite element analysis, clay

APCOM-ACCM 2025
Brisbane, Australia
7-10 December 2025

Computational Mechanics and Nanomaterial-Informed Modelling of Ship Collision Impact on Bridge Piers

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The resilience of bridge piers under extreme impact loading, such as ship collisions, is a critical aspect of modern infrastructure safety. This study integrates computational mechanics with advanced material modeling to analyze the behavior of nanomaterial-reinforced bridge piers subjected to high-energy impacts. A high-fidelity finite element (FE) model is developed using LS-DYNA to simulate a collision scenario in which a 16,000-ton vessel impacts a reinforced concrete pier at a velocity of 5 m/s.

The pier is modeled using the Johnson-Holmquist Concrete (JHC) model to accurately capture brittle failure and dynamic cracking, while steel reinforcement is defined with the Plastic Kinematic model to reflect strain hardening behavior. The impacting ship is treated as a Rigid body to isolate the structural response of the pier. Dynamic response parameters such as stress wave propagation, effective plastic strain, and crack evolution are analyzed using explicit time integration.

To enhance impact resilience, nanocomposite-reinforced concrete is introduced, accounting for nanoscale effects on fracture energy and ductility. Additionally, a Physics-Informed Machine Learning (PIML) framework employing a Multilayer Perceptron (MLP) is developed. The model is trained on FE simulation datasets to predict damage indices, crack distribution, and energy absorption levels across various collision scenarios. The MLP achieved high predictive accuracy ($R^2 \approx 0.96$), enabling rapid assessment of structural performance under diverse conditions.

This research advances the integration of computational mechanics and nanomaterial-enhanced design, providing a robust framework for improving the impact safety of bridge piers in maritime environments. The combination of material-specific FE modeling and AI-driven prediction offers a valuable pathway for future resilient infrastructure development.

Keywords: Computational mechanics, nanomaterials, finite element analysis, ship collision, machine learning, impact resilience, structural safety.

Optimal Design of Orthodontic Appliances for Malocclusion in Young Children Based on Explicit Topology Optimization

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Changes in living environments, dietary structures, and food processing methods have led to an unbalanced degeneration of human masticatory organs. This has resulted in the increasing incidence of malocclusions such as jaw hypoplasia, dental crowding, and crossbite. In young children, malocclusion can severely impact chewing function, leading to digestive system disorders and hindering normal physical growth and development, affect speech and overall facial aesthetics, and even cause psychological disorders. Statistics show that China currently has 150 million children in the mixed dentition period, with a malocclusion prevalence rate of 60.16%, meaning approximately 90 million children require timely occlusal guidance treatment. The types and severity of malocclusion vary among children due to individual biological differences. However, traditional orthodontic appliances are generally designed based on the subjective experience of clinicians. These appliances have similar shapes, lack personalization, and furthermore, do not employ rational mechanical analysis and optimization techniques based on the force distribution and efficient transmission. Consequently, traditional designs result in prolonged treatment durations, high costs, and uncertain therapeutic effects, often causing children to miss the optimal intervention period.

To achieve comfortable, convenient, and personalized occlusal guidance treatment, this study introduces explicit topology optimization into the structural design of orthodontic appliances. By employing the mathematically rigorous and geometrically explicit Moving Morphable Components (MMC) method, we integrate a personalized craniofacial complex model constructed from CBCT (Cone Beam Computed Tomography) imaging of the craniofacial region and dentition, finite element mechanical analysis, and topology optimization techniques for orthodontic appliance design. Based on the preliminary optimization results, we propose a novel orthodontic appliance for young children with malocclusion. Given the complexity of biological morphological structures and the short replacement cycle of pediatric orthodontic appliances, further improvements in optimization efficiency are essential. In the future, we plan to incorporate Problem-Independent Machine Learning (PIML) method [1-2] and voxel-based modeling techniques to achieve efficient topology optimization of orthodontic appliances. Preliminary explorations have been made in this direction, and some innovative optimization results obtained by AI-enhanced fast design algorithm will be reported.

Keywords: Orthodontic Appliances; Malocclusion; Explicit Topology Optimization; Moving Morphable Components (MMC) method; Problem-Independent Machine Learning (PIML) method

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Strongly-nonlinear Long-crested Rogue Wave within Monochromatic and Bichromatic Wave Systems

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Rogue waves (RWs) can cause severe damage to both offshore and nearshore human activities and infrastructures. While in deep water, the well-known nonlinear focusing as modelled by Nonlinear Schrödinger equation (NLSE), and linear dispersive mechanisms can explain and predict RWs at intermediate level of nonlinearity, the dynamics of strongly-nonlinear RWs on the other hand still remains unexplored due to its theoretical complexity and experimental difficulties, often associated with wave breaking and induced turbulence. In the current work, the strongly nonlinear RW focusing dynamic and mechanism are investigated both experimentally and numerically (fully-nonlinear Euler's equations) within monochromatic and bichromatic wave systems. Surprisingly, it is uncovered that by initiating from either a localized Peregrine-breather perturbation or a step change of carrier wave frequencies on a highly nonlinear background with wave steepness $ak \approx 0.1$, the generated RWs are focused far beyond the prediction of NLSE frameworks, and can reach **four times** the background wave amplitude. Meanwhile, its development remains coherent and non-breaking. In summary, the current investigation has identified a novel type of strongly nonlinear RW with significant practical danger and may help improve rogue wave prediction models once its mechanism is further clarified.

Keywords: Nonlinear waves, Rogue Waves.

Reinforcement Learning for Complex Flows Modelling

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In order to save energy, recovering industrial heat losses is necessary. One way to do this is by using non-ideal gases as working fluids in dedicated thermodynamic cycles. However, current closure models for Reynolds-averaged Navier-Stokes fail to capture all the aspects of the turbulent behaviour of non-ideal gases (see [1] for example), due to their complex thermo-physical properties. The present work aims at providing a proof-of-concept for the use of Reinforcement Learning for the enhancement of Reynolds-averaged Navier-Stokes (RANS) closure models. The Soft Actor-Critic algorithm [2] is employed with the aim of determining the relevant values of model constants. Initially, the algorithm is implemented and verified using a couple of test cases. The verified framework is used next to train an agent to reproduce the behaviour of the k-ω turbulence model as a first step in a verification case selected from the NASA database [3]: the 2D flow over a bump in a channel (Figure 1). The model is made up of two partial differential equations:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial \rho u_j k}{\partial x_j} = P - \beta^* \rho \omega k + \frac{\partial}{\partial x_j}\left[(\mu + \sigma_k \mu_t)\frac{\partial k}{\partial x_j}\right]$$
$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial \rho u_j \omega}{\partial x_j} = \frac{\gamma}{\nu_t} P - \beta \rho \omega^2 + \frac{\partial}{\partial x_j}\left[(\mu + \sigma_\omega \mu_t)\frac{\partial \omega}{\partial x_j}\right] \quad (1)$$

where k is the turbulent kinetic energy, ω the specific turbulent dissipation rate, ρ the density, u the velocity, t time, x the spatial coordinate, μ the dynamic viscosity, ν_t the kinematic turbulent viscosity, μ_t the dynamic turbulent viscosity, P the production term, and σ_k ,σ_ω ,β ,β^*,γ are the model constants. The k-ω SST turbulence model is eventually recreated using the Multi-Agent Reinforcement Learning paradigm, where two agents are needed to learn the two different sets of values of the model constants (close to and away from the wall).

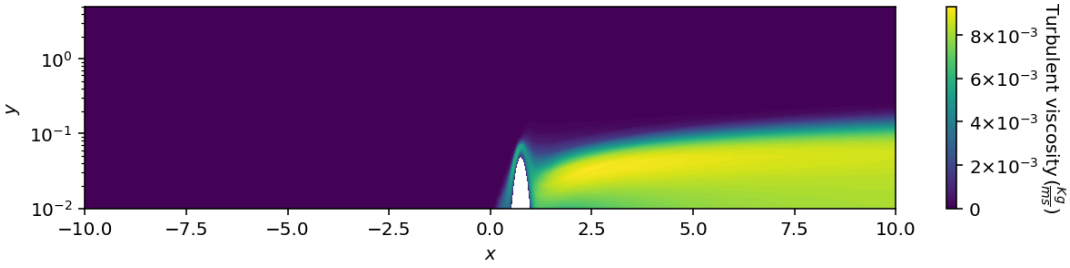

Figure 1.

Keywords: Turbulence modelling, machine learning.

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Probabilistic Digital Twin for Misspecified Structural Dynamical Systems via Latent Force Modeling and Bayesian Neural Networks

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Digital twins are rapidly emerging as powerful tools for monitoring and prediction in engineering systems, yet their reliability is often limited by misspecified or incomplete physics. This work proposes a probabilistic digital twin framework that systematically accounts for such model discrepancies while ensuring trustworthy prediction under uncertainty.

The framework combines Gaussian Process Latent Force Models (GPLFMs) with Bayesian Neural Networks (BNNs) to create an end-to-end pipeline linking diagnosis and prognosis. In the diagnostic stage, model-form errors (MFEs) — representing unmodeled nonlinearities and deviations from nominal physics — are treated as latent forces and jointly estimated with system states using GPLFM from sensor data. These posterior estimates are then used to train a BNN, which learns a flexible probabilistic mapping from system states to MFEs, thereby capturing diagnostic uncertainties.

For prognosis, the trained BNN generates pseudo-measurements of MFEs that are assimilated through Kalman filtering, enabling accurate and uncertainty-aware state predictions. This design ensures that uncertainty is consistently propagated from diagnosis to prediction — a key capability for building robust and trustworthy digital twins.

The proposed framework is validated on four nonlinear case studies: a single-degree-of-freedom oscillator, a multi-degree-of-freedom system, and two established benchmarks — the Bouc–Wen hysteretic system and the Silverbox experimental dataset. Across all cases, the framework demonstrates high predictive accuracy, adaptability to nonlinear behaviors, and robustness to physics misspecification, highlighting its potential for advancing next-generation digital twin technologies.

Keywords: Digital Twins, Machine learning, Gaussian process, Latent force models, Bayesian neural network, Bayesian filtering

A NOVEL SELF-CENTERING FRICTION DAMPER WITH ELASTIC POST-BUCKLING PLATES TO RETROFIT BRIDGE BENT

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Abstract:

The self-centering energy dissipation dampers (SCEDs) have been demonstrated in mitigating the residual deformation of structures under strong ground motions. However, existing researches show that the damping force demand of SCEDs is higher than conventional dampers such as viscous dampers, BRBs or friction dampers for same design displacement of self-centering retrofitted structures, which could lead to higher base shear and acceleration responses of structures. In order to alleviate the problem, a novel self-centering damper composed of elastic post-buckling plates and adjustable friction devices (PBSCFD) was proposed. Compared with conventional SCEDs, the proposed PBSCFD has low secondary stiffness and adjustable energy dissipation capacity, which is beneficial to control the additional internal force of members adjacent to the damper in self-centering retrofitted structures. Based on the configuration and working principle of the PBSCFD, the theoretical force-displacement relationship of the damper was derived. Subsequently, a scaled PBSCFD was manufactured and tested under quasi-static loading to investigate its mechanical properties and to verify the theoretical constitutive model. In order to demonstrate the seismic performance of PBSCFDs, the double-column bridge bent retrofitted with PBSCFDs was designed by direct displacement-based seismic design method (DDBD), and its seismic performance was examined by elastic-plastic time-history analysis. Finally, effects of secondary stiffness ratio of self-centering dampers on seismic mitigation of self-centering retrofitted bridge bent were investigated. The results show that PBSCFDs have certain advantages in controlling the base shear and acceleration of the retrofitted bridge bent compared to conventional SCEDs with significant secondary stiffness.

Keywords: self-centering damper; friction; post-buckling plate; bridge bent.

Notes:

- The deadline for abstract submissions is 15 May 2025.
- Abstract should not contain more than 250 words
- Please name your file as “Surname of the presenting author_Initials of the given names of the presenting author”. For example, “Shi_S.docx”.

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DEVELOPMENT AND DESIGN OF THE SMA-BASED RESILIENT SEISMIC MITIGATION DEVICES FOR BUILDING

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Abstract:

To advance the post-earthquake functional recovery of engineering structures and address inherent limitations of conventional energy dissipation devices—such as excessive residual deformation, inadequate initial stiffness, and limited performance designability—this study presents the development and evaluation of a novel family of self-centering dampers. A self-centering buckling-restrained brace (SC-BRB) utilizing shape memory alloy (SMA)wires was developed to mitigate residual deformations in conventional BRBs, enabling significant energy dissipation through metallic yielding coupled with reliable recentering. To overcome the drawbacks of viscoelastic dampers, a self-centering hybrid viscoelastic damper (SC-VED) was proposed, which leverages the moderate elastic modulus of SMA to enhance initial stiffness and exploits its superelasticity to minimize residual strains. In addition, a new self-centering friction damper incorporating SMA bolts and high-damping viscoelastic rubber was developed to enhance performance under minor earthquakes and reduce residual displacements. The research methodology integrated theoretical modeling, refined finite element simulations, and experimental testing to establish accurate mechanical models for each damper. Systematic parametric optimization and seismic performance assessments were conducted. Results demonstrate that all proposed devices exhibit stable flag-shaped hysteretic responses, excellent self-centering capabilities (with negligible residual deformation), and robust energy dissipation, successfully balancing high hysteretic damping with post-earthquake realignment. This work establishes a comprehensive framework covering core component development, integrated device design, theoretical advances, and engineering applications, offering advanced solutions and critical technologies for the realization of recoverable seismic-resistant structures.

Keywords:SMA; seismic mitigation; self-centering damper; building.

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APCOM-ACCM 2025
Brisbane, Australia
7-10 December 2025

Predictive Multiscale Modeling of Microstructural Defect Evolution in Metallic Materials under Harsh Environments

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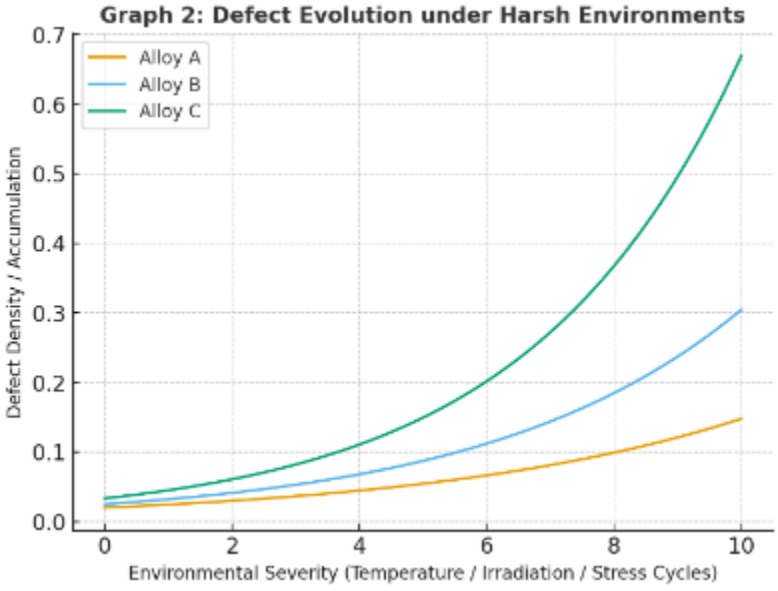
Abstract

Metallic materials deployed in aerospace, nuclear, and energy systems are frequently subjected to harsh environments characterized by elevated temperatures, irradiation, and cyclic mechanical loads. These conditions accelerate the formation and evolution of microstructural defects, ultimately governing material degradation, strength reduction, and failure. To address these challenges, this research develops a predictive multiscale modeling framework that captures defect evolution across atomic, mesoscopic, and continuum scales.

At the atomic scale, density functional theory and molecular dynamics simulations quantify defect energetics, migration, and clustering. The mesoscale domain integrates phase-field and dislocation dynamics to model defect interactions, grain boundary evolution, and void growth. At the continuum level, finite element modeling links defect-induced microstructural changes to macroscopic properties such as stress distribution, creep, and fatigue resistance. By bridging these scales, the framework provides robust predictions of defect progression and damage accumulation under extreme conditions.

Case studies on irradiated metallic alloys and thermomechanical cycling demonstrate the model's predictive power in correlating microstructural defect behavior with mechanical degradation. The results highlight pathways to design alloys with improved defect tolerance and service reliability. This work provides a vital contribution to predictive materials science, offering a foundation for engineering next-generation metallic systems optimized for durability in harsh operational environments.

Keywords: Multiscale Modeling, Defect Evolution, Metallic Materials, Harsh Environments, Molecular Dynamics, Phase-Field Modeling, Finite Element Analysis, Irradiation Damage, Fatigue



A Large Language Model-inspired Data-driven Mechanics Framework for Viscoelastic Soft Structures

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Soft fluidic actuators (SFAs), as a typical class of soft structures, have emerged as the principal actuation components in soft robotics due to their superior compliance, scalability, and biocompatibility. Nevertheless, current research remains predominantly confined to time-independent hyperelastic constitutive models, resulting in insufficient predictive accuracy for viscoelastic responses under large deformation conditions. This work proposes a mechanics-informed data-driven viscoelastic constitutive framework capable of accurately characterizing the time-dependent behavior of hydraulically/pneumatically actuated SFAs. The central innovation involves the tailored development of a finite-strain memory decay network (fMND), which incorporates two mechanics-informed constraints - the viscoelastic memory decay property and thermodynamic consistency - directly into the training process. Our data-driven approach only requires a small amount of experimental data while being integrated into the finite element method framework. The success of this approach highlights its ability to enhance generalization capabilities based on diverse experimental results, while also showcasing its potential to predict the viscoelastic behavior of other soft structures beyond SFAs. These inherent capabilities align well with the underlying principles of large language models.

Keywords: Large language model, Data-driven, Constitutive law, viscoelastic soft structures, Mechanics-informed

Latent Diffusion Model for Inverse Design of Nonlinear Mechanical Metamaterials

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The inverse design of materials with complex, nonlinear mechanical properties has broad applications in fields such as soft robotics, biomedical implants, and impact mitigation. Previous works have shown the great potential of generative model to predict and tune the nonlinear deformation and stress response of periodic stochastic cellular structures under large strain compression [1]. However, these works are inherently limited by its reliance on periodic boundary conditions, restricting its applicability and reliability to real-world, non-periodic applications.

In this study, we extend the generative modelling framework beyond periodic boundary conditions by introducing latent diffusion model that enables the design of 5*5 cellular structures with tailored mechanical responses [2]. By integrating advanced data-driven techniques with full-field mechanical analysis through Finite Element Analysis (FEA), our approach captures complex deformation behaviours, including localized buckling and contact, across irregular structures. Finite element simulations validate the accuracy of the predicted stress-strain responses, demonstrating strong agreement with the generative model's prediction.

This work significantly broadens the applicability of inverse design for mechanical metamaterials, offering a strategy to efficiently optimize structures without the limitations imposed by periodic boundary conditions. The proposed method enhances design flexibility and accelerates the discovery of materials with highly customized mechanical performance for practical engineering applications.

Key Words: *Metamaterial, Finite Element Analysis, Latent Diffusion Model, Stress-Strain Response*

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Robust Topology Optimization of FRP Composite Structures under Dynamic Load Uncertainties

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This study addresses the uncertainties associated with design of fibre reinforced plastic (FRP) composite structures under dynamic loads, particularly those related to excitation amplitude and direction, which can lead to excessive deformation and significantly degraded structural performance [1]. To tackle this challenge, a robust design framework is proposed for the topology optimization of fibre-reinforced plastic composite structures, which takes into account the stochastic nature of excitation amplitude and direction. The study employs the Discrete Material and Thickness Optimization (DMTO) method, which addresses the optimization of both topology and morphological variables through parametrization. The optimization objective is to minimize the mean and standard deviation of the structural dynamic compliance response, which can be rewritten as,

$$\text{Min} \quad J(\chi, \rho_e, x_{ec}) = \mu\left(\left|\mathbf{F}^{\mathrm{T}}(\chi)\mathbf{U}(\chi)\right|\right) + \kappa\sigma\left(\left|\mathbf{F}^{\mathrm{T}}(\chi)\mathbf{U}(\chi)\right|\right), \tag{1}$$

As shown in Fig.1, through the 2D cases study, the impact of dynamic load uncertainties on optimization results is explored, and further robust optimization of a composite beam under multiple loading conditions is investigated. Additionally, the study evaluates the potential application of the proposed method in complex structural components by conducting robust optimization of the dynamic performance of a 3D laminated plate.

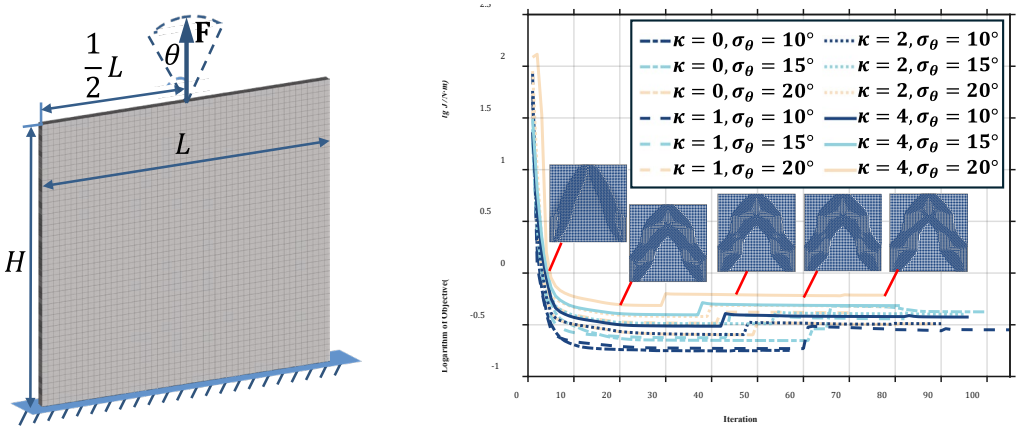

Figure 1.

Keywords: Robust optimization, Fiber-reinforced plastic composites, Discrete material and thickness optimization (DMTO), Dynamic response, Excitation forces uncertainty.

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Dissimilar Control of Momentum and Heat Transport in Turbulent Channel Flow using Deep Reinforcement Learning

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The simultaneous reduction of skin-friction drag and enhancement of heat transfer in turbulent flows is a highly desirable yet challenging objective in fluid engineering. This difficulty arises from the intrinsic similarity between momentum and heat transport, which causes most conventional control strategies to influence both in a similar manner. Although approaches such as optimal and adjoint-based control have demonstrated promising, problem-specific successes, their computational expense, horizon-length limitations, and restricted generality mean that the simultaneous achievement of drag reduction and heat-transfer enhancement remains an open challenge.

This study explores the feasibility of a dissimilar control law that manipulates momentum and heat transport independently, in contrast to the similarity constraint typically encountered in conventional methods. The flow is computed by direct numerical simulation of a turbulent channel, governed by the incompressible Navier–Stokes, continuity, and energy equations. Wall blowing and suction serve as the control input.

The control problem is formulated within a deep reinforcement learning framework. The agent observes near-wall distributions of shear stress and heat flux as the state and determines the spatial distribution of wall blowing and suction as the action. The reward to be maximized is defined as

$$r_t = 2St/C_f - w\,E_c \tag{1}$$

where St is the Stanton number, C_f the skin-friction coefficient, E_c the spatially averaged control-energy expenditure, and $w > 0$ a weighting factor. The first term promotes dissimilarity between heat and momentum transport, while the second penalizes actuation cost.

Using this framework, the agent acquired a control law that increased both heat transfer and friction drag, but with different rates of increase, thereby demonstrating dissimilar behaviour. Figure 1 illustrates iso-surfaces of the second invariant of the velocity-gradient tensor (Q^+ = 0.02), together with wall blowing and suction at the wall. Detailed analyses of turbulent statistics and thermal-transport pathways will be presented to elucidate the physical mechanisms underlying this dissimilarity.

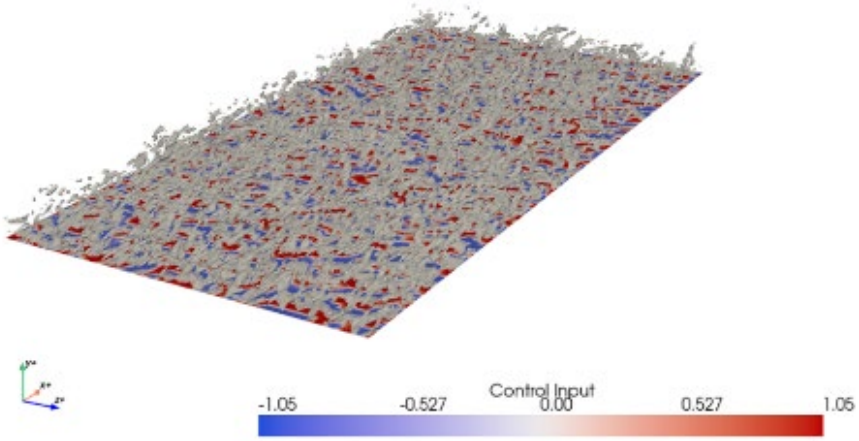

Figure 1.

Keywords: Turbulent channel flow, heat-transfer enhancement, deep reinforcement learning, direct numerical simulation, dissimilar control

Physics-informed machine learning for forward and inverse soil consolidation analysis

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Physics-informed machine learning has shown strong potential for modeling spatio-temporal soil consolidation. Traditional data-driven surrogates fit observations but may break basic consolidation laws, reducing interpretability, hindering parameter identification, and limiting generalization to unseen conditions. In contrast, self-supervised PIDL formulated enforces the governing PDE, but often struggles over long time evolution and scales poorly to high-dimensional or heterogeneous domains because of high computational cost and sensitivity to the choice of collocation points. Therefore, we present a physics-informed machine learning (PIML) framework for forward and inverse analysis of soil consolidation. The method embeds Terzaghi consolidation equations, and initial-boundary conditions directly into the learning loss, enabling data-efficient training from sparse and noisy measurements while preserving physical consistency. Flexible machine learning mdoels, neural networks or Gaussian processes, are supported, together with continuous- and discrete-time formulations (e.g., Runge-Kutta, backward-Euler) to improve stability over long time horizons. In the forward setting, the model predicts excess pore pressure dissipation and settlement across one- to multi-dimensional domains with heterogeneous layers and time-varying drainage. In the inverse setting, it identifies spatially varying parameters such as the coefficient of consolidation, permeability, and compressibility, and can include uncertainty quantification and multi-fidelity data fusion (laboratory and field). Numerical studies against analytic benchmarks and high-resolution simulations show that the discrete-time PIML variants offer superior stability and accuracy relative to purely data-driven surrogates and standard continuous-time formulations, while requiring fewer prior assumptions. The proposed framework provides a robust, interpretable, and extensible surrogate for geotechnical modeling, parameter estimation, and decision support in consolidation problems.

Keywords: Soil consolidation, machine learning, neural networks, gaussian process, forward modelling, inverse analysis

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High-fidelity Multiphysics Modeling of Metal Additive Manufacturing Process

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Additive manufacturing, as a transformative technology, demonstrates significant potential in the customized fabrication of complex structures, with Laser Powder Bed Fusion (LPBF) emerging as a research hotspot in the field of high-end manufacturing. High-fidelity process simulation techniques have substantially enhanced the understanding of melt pool behavior during LPBF. However, constructing high-precision models that effectively complement experimental observations remains a considerable challenge, particularly in simulations involving coupled particle motion and multi-component materials. To address this, this study first developed a multi-physics CFD-DEM model coupled with particle motion [1] and ray tracing [2], effectively simulating challenging additive manufacturing issues such as direct energy deposition. In response to the complex thermophysical characteristics of multi-material systems, a multi-medium, multi-physics coupled computational framework was further established to systematically investigate the melt pool dynamics of multiple materials during the LPBF process [3]. Additionally, this research integrates synchronous high-speed X-ray in-situ observation and high-fidelity numerical simulation to enable cross-scale observation and simulation of multi-material melt pool behavior. Results indicate that multi-material melt pools exhibit morphological characteristics significantly distinct from those of single materials, primarily attributable to the combined effects of component mixing, limited thermal penetration depth, Marangoni convection, and surface vortex effects. By systematically analyzing the influence of scanning parameters and light source characteristics on melt pool features, an AI surrogate model for process prediction and optimization of multi-material stable forming was established, providing a quantitative basis for research on the forming mechanisms and process optimization in additive manufacturing.

Keywords: Additive manufacturing, laser powder bed fusion, multiphysics modeling, CFD-DEM, surrogate model

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APCOM-ACCM 2025
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Revolutionizing Design and Analysis: Unleashing the Power of Data-driven Approaches in Predictive Maintenance Systems

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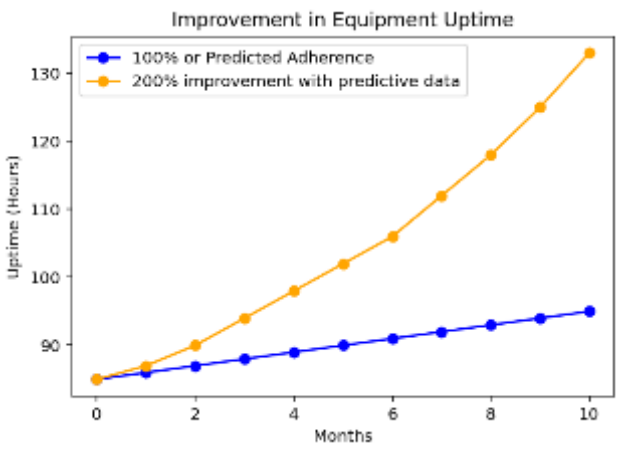
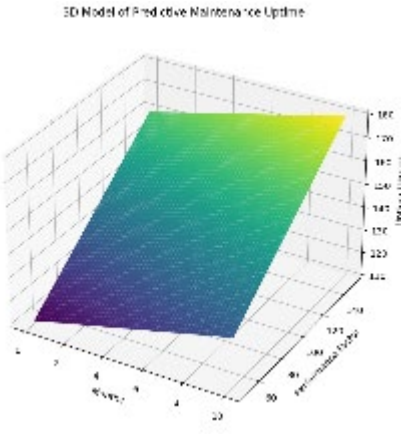
Abstract

Predictive maintenance has emerged as a cornerstone of modern industrial systems, revolutionizing the way organizations approach equipment longevity, performance optimization, and cost reduction. This research investigates the integration of advanced data-driven approaches into predictive maintenance systems, offering insights into their transformative capabilities. By leveraging historical data, sensor readings, and machine learning algorithms, this study explores how predictive models can forecast potential failures before they occur, thus enabling proactive interventions.

The findings demonstrate that by applying a diverse range of data-driven methodologies including regression analysis, neural networks, and anomaly detection techniques predictive maintenance systems can be optimized for real-time decision-making. Through a comprehensive analysis of case studies from manufacturing and energy sectors, the study highlights the improvement in operational efficiency and cost management. Furthermore, challenges such as data quality, model interpretability, and system integration are discussed, providing a balanced view of the practical considerations when implementing these approaches. The research concludes with recommendations for future advancements, emphasizing the potential of artificial intelligence and machine learning to further refine predictive maintenance strategies and set new industry standards.

Keywords: Predictive Maintenance, Data-driven Approaches, Machine Learning, Industrial Optimization





Machine-learning Facilitated Development of Silk-based Materials for Applications of on-Skin Devices

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Biomaterials such as silk fibroin possesses superior biophysical properties, including high strength, stretchability, biocompatibility, and biodegradability, attributed to its hierarchical structures like keratin [1]. Silk fibroin can be processed into various morphologies, such as hydrogels[2], films[3], sponges[4], etc., to facilitate its wide applications as surgical sutures, medical textiles, tissue engineering scaffolds, drug carriers, biosensors[5]. In addition, silk fibroin-based materials show great potential for flexible devices. Their excellent mechanical flexibility and biocompatibility make them ideal candidates for the development of wearable electronics, flexible sensors, and bioelectronic interfaces. In this study, we conducted AI-guided largescale molecular dynamics (MD) simulations to integrate natural plant compounds, such as aromatic turmerone, with silk fibroin for developing novel skin-whitening biomedical materials. Three potential topical agents were screened from a set of 36 aromatic turmerone derivatives using machine learning. Molecular docking and MD simulations were conducted to elucidate the molecular mechanisms underlying their skin-whitening potential and interaction mechanisms, revealing that methoxy-modified derivatives exhibited superior binding free energy and tyrosinase inhibition, as well as the influence of defects. The dipalmitoylphosphatidylcholine (DPPC) lipid bilayer model was further employed to evaluate the permeability of these compounds across the skin barrier, predicting their potential for dermal topical applications. These findings highlight the potential of silk fibroin-aromatic turmerone materials in developing next-generation skincare products and provide a guideline for the future design of bioinspired materials for various applications including wearable devices, energy storage.

Keywords: Biomaterials; Silk protein; Molecular dynamics; Biomedical; Machine learning algorithm.

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Analysis of floating platform-mooring system-pile-soil interactions under extreme wave loadings by using MPM-FEM approach

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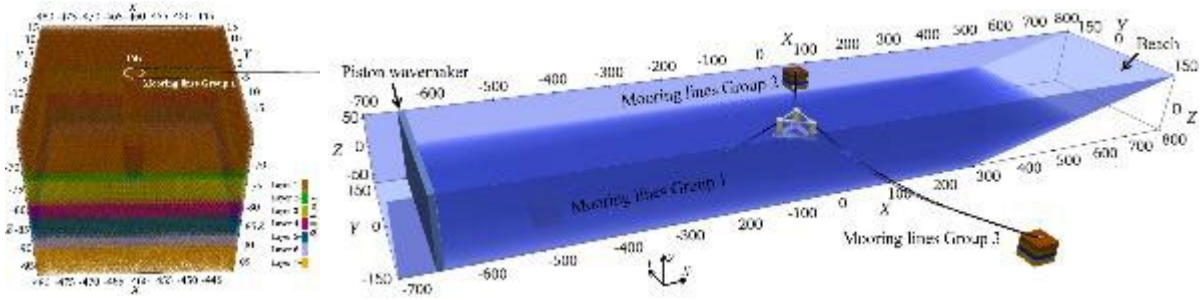
The ffoating platform-mooring system-pile-soil interactions under wave loadings represent a complex yet understudied aspect of ffoating offshore wind turbines (FOWTs). This paper presents the development and application of an Incompressible Material Point Method-Finite Element Method-Material Point Method (IMPMFEM-MPM) model to simulate these interactions for a triangle-shaped semi-submersible platform (Tri-SSP), which serves as the foundation of China's ffrst deep-sea FOWT, named 'Fuyao.' The proposed model is validated by studying the hydrodynamic responses of the OC4-DeepCwind platform. Under regular waves, increasing wave

heights lead to heightened motion amplitudes, with the Tri-SSP exhibiting distinct phase differences between surge, pitch, and heave motions. Anchor Group 1 experiences signiffcant peak tensions, ranging from 2.26 MN to 4.47 MN, which inffuence soil displacement, shear forces and bending moments along the pile shaft, emphasizing the impact of wave loading on pile-soil interactions. Under 1-h irregular waves, tension in Anchor Group 1 reaches extreme levels, with tensions up to 8 MN observed, underscoring the critical role of mooring systems in mitigating wave-induced forces. The calculated maximum stress within the pile indicates the structural integrity of the DH36 steel pile under these conditions. Comparisons of hydrodynamic responses, both with and without pile-soil interactions, show minimal discrepancies in motion amplitudes, indicating a minor inffuence on the dynamics of the platform and mooring system. These ffndings contribute to the understanding of complex interactions in deep-sea FOWTs, informing design and operational strategies for enhanced stability and performance. .



(a) (b)

Figure 1: Configuration of: (a) mooring lines Group 1-pile-soil interactions; and (b) the computational domain of the Tri-SSP (units in m).

Keywords: Wellbore strengthening; lost circulation materials; particle bridging; hydraulic fracturing

On the Effective Bounds of Semi-auxetic Laminates

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Semi-auxetic laminates are layered structural members composed of auxetic and non-auxetic layers. In the literature, the violation of Hill's bounds has been reported for such structures which is quite an anomaly in the composites' literature. Herein, it was aimed to investigate the extent of this discrepancy through numerical and experimental approaches for a semi-auxetic sandwich structure. Using fused-filament fabrication, a re-entrant honeycomb core combined with symmetrical solid face sheets were additively manufactured and then analysed using the finite element (FE) method. Tensile test results were used to validate the FE model, and a parametric study was carried out to identify the factors with the most significant impact on the effective in-plane stiffness of the laminate and the effective Poisson's ratio. It was found that the highest effective stiffness is obtained when the Young's moduli of all layers are identical and the Poisson ratios in the loaded direction are the furthest apart.

Keywords: semi-auxetic laminate, in-plane stiffness, effective stiffness, re-entrant honeycomb

Heat Transfer Enhancement by Traveling Wave Control in Turbulent Channel Flow

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The miniaturization of heat exchangers is demanded for efficiency. However, the narrow passages lead to low Reynolds numbers and laminarization, which significantly reduces heat transfer. Active flow control to sustain turbulence in these flows is therefore essential and various control methods has been examined. Aoki *et al.*[1] promoted the heat transfer at low Reynolds number flows by using feedback-controlled blowing and suction. The traveling wave control is also promising. Yamamoto *et al.*[2] reported that downstream traveling waves increase the heat transfer in a fully developed turbulent flow. Higashi *et al.*[3] demonstrated simultaneous heat transfer augmentation and friction reduction with this method.

This study performs direct numerical simulations to investigate the effect of the traveling wave control in turbulent channel flows at a low Reynolds number. The turbulent heat transfer naturally decays without any controls. We conduct a parametric study to evaluate the range of the turbulent heat transfer enhancement.

Figure shows the sample results of the control effect by the downstream traveling wave. The turbulent vortical structures decreases as time advance, while some of them survive. The remarkable heat transfer enhancement is obtained, i.e., the Stanton number increases up to 6.0 times compared to the uncontrolled laminar flow. In the presentation, we discuss the mechanism of the heat transfer enhancement.

Keywords: turbulent channel flow, turbulent vortical structures, traveling wave control, direct numerical simulation, enhancement of heat transfer

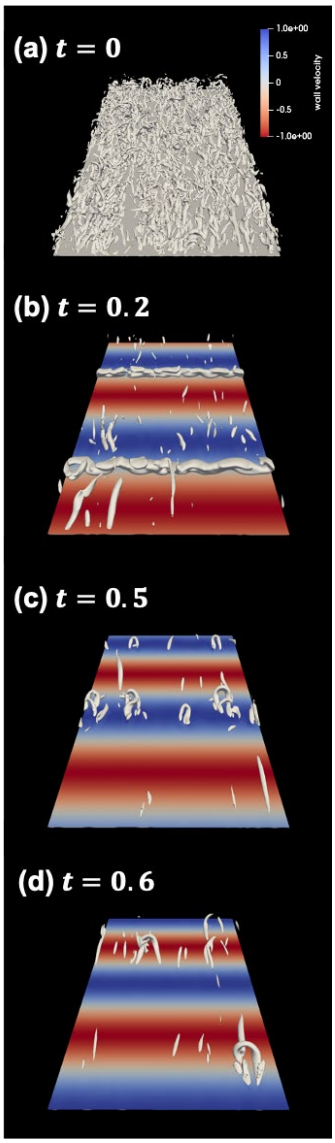

Figure. Instantaneous flow field: white isosurface, vortical

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The Numerical Manifold Method for Babuska's Paradox

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Thin plates represent a common structural form, and the thin plate model based on Kirchhoff's hypothesis was once an elegant reduced-dimensional model of three-dimensional elasticity. Even today, with highly advanced computational power, attempts to solve thin plate bending problems using three-dimensional solid elements still face significant challenges due to ill-conditioned issues. However, in 1962, Babuska discovered that for a simply supported circular plate under uniformly distributed load, approximating it with regular polygons leads to increasing solution error as the number of polygon sides grows, eventually converging to the solution of a non-simply-supported circular plate. For instance, the limiting centroidal deflection of a simply supported regular polygon is less than one-third of the central deflection of a simply supported circular plate. This phenomenon is known as the Babuska paradox. Despite intensive research over the years, no consensus has been reached regarding its underlying cause, nor has a convincing solution been found.

The direct consequences of the Babuska paradox are threefold: (1) all thin plate elements developed to date fail when analyzing non-polygonal simply supported plates; (2) some classic works by renowned scholars no longer teach Kirchhoff plate theory; and (3) almost all departments of engineering mechanics have discontinued courses on classical plate and shell theory. In this report, we will prove that this paradox can be satisfactorily resolved by adopting conformal approximation for boundaries. Among current mainstream numerical methods, only the Numerical Manifold Method (NMM), invented by Professor Genshua Shi, appears to possess this capability. After presenting NMM's fundamental framework, this report focuses on how the Moving Least Squares (MLS) approximation based on NMM can exactly satisfy the zeroth- and first-order essential boundary conditions of the biharmonic operator, while also introducing NMM solutions for several other classic problems in computational mechanics.

Keywords: numerical manifold method; moving least squares method; Babuska's paradox; Kirchhof's plate bending model

AI for PDEs in computational mechanics

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ABSTRACT

In recent years, deep learning has become ubiquitous and is empowering various fields. In particular, the combination of artificial intelligence and traditional science (AI for science, AI4Science) has attracted widespread attention. In the field of AI4Science, the use of artificial intelligence algorithms to solve partial differential equations (AI4PDEs) has become the focus of computational mechanics research. The core of AI4PDEs is to fuse data with equations and can solve almost any PDEs. Due to the advantages of AI4PDEs in data fusion, computational efficiency using AI4PDEs is usually increased by tens of thousands of times compared to traditional algorithms. Therefore, we comprehensively review the research on AI4PDEs, summarize the existing AI4PDEs algorithms and theories, discuss its application in solid mechanics, including forward and inverse problems, and outline future research directions, especially the foundation model of computational mechanics. Existing algorithms of AI4PDEs include physics-informed neural networks (PINNs), deep energy methods (DEM), operator learning, and (physics-informed neural operator, PINO). AI4PDEs has numerous applications in scientific computing, and this paper focuses on the application of AI4PDEs in the forward and inverse problems of solid mechanics. The forward problems include linear elasticity, elasto-plasticity, hyperelasticity, and fracture mechanics; while the inverse problems encompass the identification of material parameters, constitutive laws, defect recognition, and topology optimization. AI4PDEs represents a novel method of scientific simulation, which offers approximate solutions for specific problems by leveraging large datasets and then fine-tunes according to the specific physical equations, avoiding the need to start calculations from scratch as traditional algorithms do. Thus, AI4PDEs is a prototype for the foundation model of computational mechanics in the future, capable of significantly accelerating traditional numerical methods. We believe that utilizing artificial intelligence to empower scientific computing is not only a vital direction for the future of computation but also a dawn of humanity in scientific research, laying the foundation for mankind to reach new heights in scientific development.

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Keywords: PINNs, Operator Learning, Physics-Informed Neural Operator, Computational Mechanics, AI for PDEs, AI for Science

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Pore-Scale Investigation of Wettability-Controlled Capillary Barrier Effects under Gravity

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The capillary barrier effect (CBE) is widely utilised in geotechnical and geoenvironmental engineering to reduce deep percolation in landfill sites and enhance gas trapping in underground gas storage applications. In practise, field conditions are often complex, involving wettability alterations caused by post-fire or chemical contamination, and gravity-driven effects is associated with structural geometry or fault zones. Despite its practical importance, the pore-scale mechanisms governing the CBE under such coupled conditions remain poorly understood, hindering the scientific design and optimisation of capillary barrier systems. In this study, a pore-resolved interface-tracking algorithm is employed to explore the underlying mechanisms. The numerical model is first validated against previously published experimental results, demonstrating its ability to well capture the dynamic invasion behaviours. Building upon this validation, the algorithm is applied to double-layer configurations (transitioning from fine to coarse porous media) with varying pore topologies and sizes, incorporating both wettability and gravity effects. The analysis focuses on quantitative indicators for evaluating CBE performance, namely the normalised interfacial length and front width. By systematically varying the wettability and tilt angles, the results show that under hydrophilic conditions, smaller gravitational forces and larger pore sizes in the coarse layer reduce the driving pressure provided by the coarse medium, thereby enhancing the effectiveness of the CBE. In contrast, under hydrophobic conditions, this trend is reversed, leading to an earlier breakthrough and diminished barrier performance. These findings provide a mechanistic basis for optimizing the design of capillary barrier systems in practical applications such as landfill covers, slope protection layers, and subsurface gas migration control.

Keywords: capillary barrier effect, interface tracking algorithm, wettability, gravity, pore characteristics

Deformation Toolbox: A MATLAB-Based Program to Morph the Geometry of the Models while Preserving Mesh Quality

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We present a MATLAB-based mesh deformation toolbox designed to morph finite element (FE) models at the node level while preserving mesh quality, material properties, and boundary conditions. Applied to femoral bone models, the tool enables rapid generation of anatomically altered variants, significantly reducing the time and effort required for remodelling. This approach facilitates efficient sensitivity analyses by enabling high-fidelity and rapid simulations of morphological changes.

Introduction: In computational mechanics, particularly in FE analysis of biological structures, remeshing and material mapping are among the most labour-intensive and time-consuming steps. This is especially true for bone modelling, where anatomical complexity and heterogeneous material properties demand high fidelity [2]. Creating and validating a single subject-specific femur model can take several weeks, involving segmentation, mesh generation, assignment of material properties, and boundary condition setup. Even small changes in bone morphology, such as a few degrees of torsion or angulation, may appear trivial but often necessitate repeating the entire modelling pipeline from scratch.

This inefficiency raises a critical question: can we morph existing FE meshes at a fine-grained, node-level resolution to reflect subtle geometric changes while preserving all other model attributes, such as mesh quality, material distribution, and boundary conditions? If feasible, such an approach would enable rapid generation of variant models for comparative studies, surgical planning, and sensitivity analyses, without the need for full remeshing or revalidation.

Methods: The femur bone was selected for this study due to its anatomical variability, which can be systematically represented through controlled geometric morphing. Most of the femur's structural characteristics can be captured by adjusting two principal alignments, one along the shaft and one along the neck, without needing to reference specific anatomical terminology.
For proof of concept, we applied our proposed mesh morphing process to a representative femur model [1]. The goal was to generate deformed variants that reflect clinically observed pathological geometries. These deformations were introduced directly at the mesh node level, allowing for precise control over shape changes while preserving mesh integrity, material distribution, and boundary conditions. This approach enables rapid creation of anatomically altered models without the need for remeshing or reassigning material properties (Figure 1a).

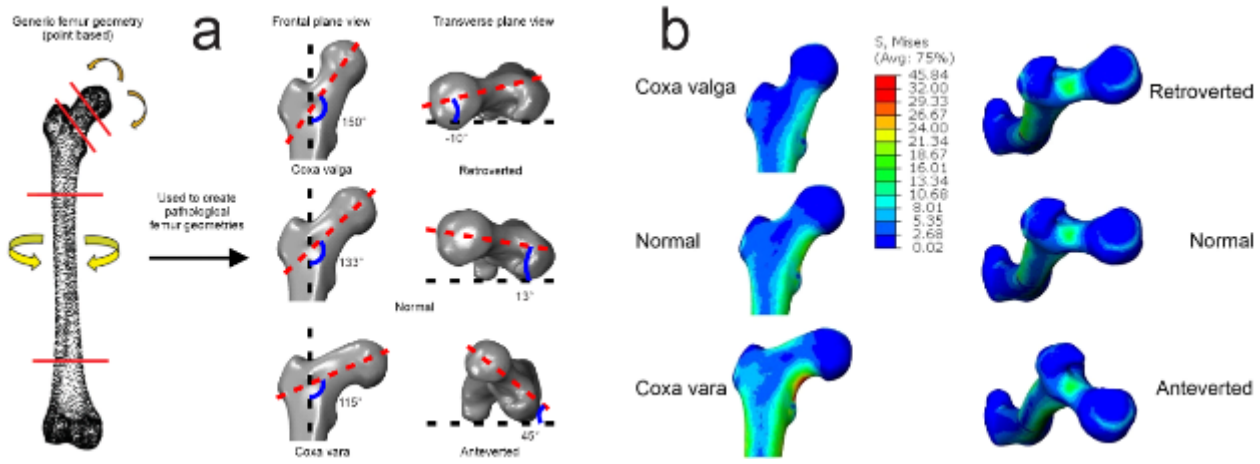

Figure 1: (a) femoral deformities produced by the deformation toolbox. (b) Von Mises stress distribution of a normal femur compared to deformed femurs under physiological boundary conditions across the stance phase of gait.

Results and Discussion: Femoral geometrical modifications were achieved within 30 seconds with mean error of ±2°. The FE of deformed femur models resulted in expected changes in stress and strain distributions predominantly in femoral neck region (Figure 1b). This fast and user-friendly toolbox can be used for predictive purposes in various fields to investigate changes in stresses and strains due to morphologic changes in an orphan mesh.

Keywords:

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Modelling the water retention and hydraulic conductivity curves of deformable unsaturated soils

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The water retention curve and hydraulic conductivity curve of unsaturated soils are critical hydraulic parameters for analysing water and gas flow in unsaturated soils. Experimental results in the literature generally indicate that, with increasing soil density, both the air-entry value and the adsorption/desorption rate of the water retention curve increase, while the relative hydraulic conductivity at a given degree of saturation changes. Except for the density-dependent air-entry value, these phenomena have not been considered in existing models. To address these gaps, this study developed new hydraulic models based on experimental evidence from microscopic analysis. First, a new equation was proposed to describe the evolution of pore size distribution with soil density. For a given pore, the ratio of its initial to final size is greater when the initial size is larger and when the increase in density is greater. Based on this equation, a new and simple water retention model was derived. This model can predict not only the increase in air-entry value (resulting from a reduction in pore size) but also the adsorption/desorption rate (due to a more uniform pore-size distribution) as density increases. Building on the water retention model, a new function for relative hydraulic conductivity was developed by incorporating the evolution of pore size distribution and tortuosity during soil deformation. Consequently, the new hydraulic conductivity model can capture changes in relative hydraulic conductivity as density increases. Finally, to validate these equations, a new stress-controlled soil column was developed that can monitor suction and water-saturation distributions, from which gas saturation can be deduced. Soil deformation during the hydro-mechanical process can be monitored. Using this new apparatus, six multi-phase flow (with water and CO_2 flow) tests were conducted for model validation. The measured and computed results showed good agreement.

Keywords: Multi-phase flow, Unsaturated soil, Constitutive modelling, Laboratory testing

Transportation of Silver Diamine Fluoride in Hydroxyapatite Nanostructure: A Molecular Dynamics Study

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Silver diamine fluoride (SDF) is widely used in dentistry to arrest dental caries and promote remineralisation [1], yet the mechanism of its transport behaviour within the Hydroxyapatite (HAp) nanostructure of enamel remains unclear. This study uses molecular dynamics (MD) simulation to investigate the diffusion of SDF solutions, evaporation, nanoparticle formation and the deposition within confined HAp nanostructure. We deploy ab initio-based force fields [2] to describe the $Ag(NH_3)_n$ and $Ag(H_2O)_n$ complexes and TIP3P water [3] as solvent. The simulation involves a $3ns$ diffusion followed by a $1ns$ evaporation, and has a geometry shown as Fig. 1(a).

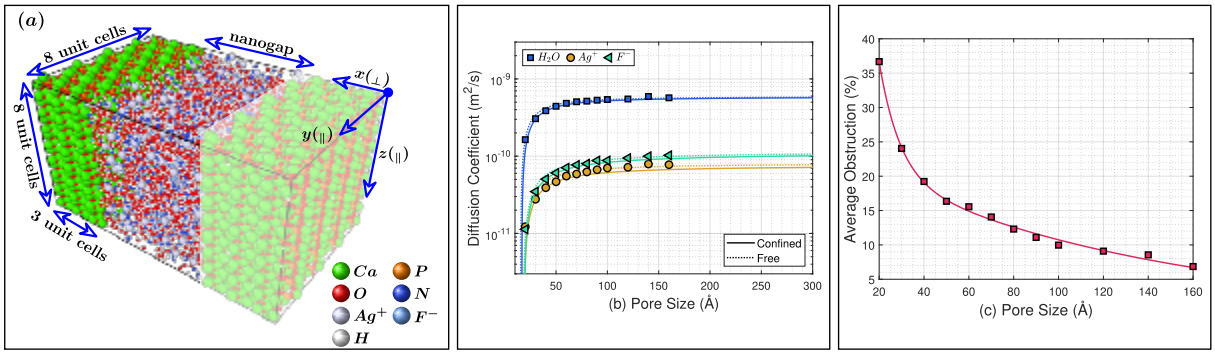

Figure 1. (a) diffusion of $32500ppm$ SDF in a 50Å nanogap; (b) diffusion coefficient of SDF in HAp nanostructure; (c) average obstruction in HAp nanostructure.

The diffusion coefficients in Fig. 1(b) show that silver particles, which are the main active component that inhibits the growth of bacteria [1], drop rapidly as the nanogap decreases below 50Å. Snapshots during the evaporation show that aggregated silver nanoparticles exhibit minimal mobility once ammonia has completely volatilised, not only because ammonia complexes play a crucial role in stabilising silver ions in the SDF solution, but also due to the rich PO_4 and OH group on the HAp surface offering favourable adsorption sites for nanoparticles. Fig. 1(c) shows the average reduction of different nanogaps due to the blockage of silver nanoparticles. These findings provide a molecular level of insight into the transportation of SDF in HAp nanostructure.

Keywords: Molecular Dynamics, Hydroxyapatite, Silver Diamine Fluoride, Diffusivity, Nanopore

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