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Abstract Book



Contents

PL-01	Characterization, Simulation and Design of Cross-Scale Mechanics Properties of Advanced Materials Yueguang Wei	1
PL-02	Blue Economy CRC Offshore Aquaculture Projects: SeaFisher and SubSCI Chien Ming Wang	2
PL-03	Computational Methods Based on Peridynamics and Nonlocal Operators Timon Rabczuk	3
PL-04	Numerical Methods for System Design of Aerospace Vehicles Yao Zheng	4
PL-05	Machine Learning Assisted Multiscale Modelling and Design of Flexoelectric Nanostructures Xiaoying Zhuang	5
PL-06	AI-assisted Engineering Our understanding and Typical Applications Weihong ZHANG	6
PL-07	Modelling Nonlinear Damping in Large-Amplitude Vibrations of Structures Marco Amabili	7
PL-08	Conquering Generalization Challenges—A Problem-Independent Machine Learning (PIML) Approach for AI enhanced Computational Mechanics Xu Guo	8
PL-09	Is Physics-Informed Machine Learning the Next Powerful Modelling Tool for Engineering and Science? Yuantong Gu	9
PL-10	On Mixed Mode Crack Propagation Analyses Using Fragile Points Method (FPM) Hiroshi Okada	10
PL-11	A Boundary-Based Machine Learning Approach for Elastic and Piezoelectric Crack Analysis Chuanzeng Zhang	11
SPL-01	Interval Field Model and Interval Finite Element Methods Chao Jiang	12
SPL-02	Vibration of Strain Gradient Nano Structures via a Mesh-free Moving Kriging Interpolation Method Lifeng WANG	13
SPL-03	Ghost Hammering Phenomena in Stochastically Driven Shells Francesco Pellicano	14
SPL-04	A Novel Approach for Deriving a State-Dependent Soil Constitutive Model Using Stress Probing Analysis Zhongxuan Yang	15
SPL-05	Computational Design of Multifunctional Lattice Structures Qing Li	16
SPL-06	Conservative Sharp Interface Methods for Interfacial Flows: Development and Simulations Hang Ding	17
SPL-07	Numerical Study of Droplet Impact on a Deep Pool by CLSVOF Method Decheng Wan	18
SPL-08	Wavelet Methods for Solving Hyperbolic Conservation Laws Jizeng Wang	19

SPL-09	Phase Field Modelling of Spinodal Decomposition and Nucleation in Ferritic Alloys Raj Das	20
SPL-10	Uncovering the Mystery of Floating Wind Turbine Modelling Wenhua Zhao	21
MS-00.01	Study on the Response of Elastic Wheel to Excitation Yu Cao	22
MS-00.02	Mechanism of Isolation Piles on Displacement Control of Adjacent Tunnels under Foundation Pit Unloading and Surcharge Loading Conditions Hongyi Chen	23
MS-00.03	Seismic Performance of Central Columns for a Multi-Story Subway Station under Vertical Earthquake Excitations Wei Chen	24
MS-00.04	Seismic Resilience Assessment Method of a Multi-Story Underground Structure Xiyue Du	25
MS-00.05	<i>GraphBRep</i> : Explicit Graph Diffusion of B-Rep Topology for Efficient CAD Generation Weilin Lai	26
MS-00.06	The State-Space FEM: Formulation and Analysis for Laminated Composite Plates Subjected to Body Forces Haifei Liao	27
MS-00.07	Diffusion-Induced Stress Analysis of Lithium-ion Battery Layered Electrode Based on the Boundary Element Method Jingwen Liu	28
MS-00.08	Development, Verification and Validation of a Dedicated FEM Code for Simulating Masonry Structures Maddegadara Lalith	29
MS-00.09	Semi-Analytical Evaluation for Nearly Singular Integrals in Isogeometric Thermoelasticity Boundary Element Method Feiyang Wang	30
MS-00.10	Mechanics of Multiphase Media Under Hypergravity Hongrui Yang	31
MS-00.11	Long-term Adhesion Durability Revealed through a Rheological Paradigm Rui Wu	32
MS-00.12	Multi-physics Coupled Solid-Liquid Phase Transition under Hypergravity Yinnan Zhang	33
MS-00.13	Comprehensive Performance Assessment of Isolation Piles on Existing Tunnel-deep Foundation Pit System under Construction Disturbance based on Projection Pursuit Model Yiqing Zhu	34
MS-00.14	Influence of Back Pressure on the Flow Characteristics of Hydrogen Supersonic Two-Phase Expander Aihong Zou	35
MS-00.15	Multiscale Constitutive Modeling of Cohesive Granular Materials Zeyong Liu	36
MS-01.01	A Novel Temporal Finite Element Method to Solve Static Viscoelastic Problems Fengling Chen	37
MS-01.02	Multi-Objective Optimization Method for Metro Wheel Reprofileing YuZhi Cheng	38

MS-01.03	A Fusion Topology Optimization Strategy of CutFEM and MMC for Improving Computational Efficiency and Geometric Accuracy Zhiqiang Guan	39
MS-01.04	A Computational Homogenization Method for Thin Composite Beams/Shells Qun Huang	40
MS-01.05	On Some Novel Analytic Methods in Mechanics of Plates and Shells and Their Applications Rui Li	41
MS-01.06	Suppressing Grayscale for Multiphysics Topology Optimization of Multiphase Smart Materials and Structures via a Dual Projection Cheng Liu	42
MS-01.07	Nonlinear Analysis of Steel Frames with Semi-rigid Joints under Thermal loading Joe Petrolito	43
MS-01.08	Analytical and Numerical Studies on Mode Selection in Proper Generalized Decomposition Methods Kang Wang	44
MS-01.09	Time-Frequency Signal Analysis Based on the Gauge Theory Zhihai Xiang	45
MS-01.10	Efficient Numerical Simulation and Design Method for Bidirectional Steel-Concrete Composite Floors Mingyue Zhou	46
MS-02.01	SPH Simulation of the Rock Cutting Process by a Conical Pick Xiangwei Dong	47
MS-02.02	Numerical Modeling of Bacterial Multi-physical Processes with SPH, LBM and Finite Element Methods Dianlei Feng	48
MS-02.03	Threshold of Sediment Particle in Turbulent Flow Ping Wang	49
MS-02.04	Numerical Analysis of Lunar 3D Printed Concrete Construction Based on Discrete Particulate Liquid Bridge Theory YuChing Wu	50
MS-02.05	An Efficient Collocation-type Meshfree Method for Nonlinear Problems Zhiyuan Xue	51
MS-02.06	Adaptive Phase-field Material Point Framework for Large-Deformation Fracture Modelling and Structural Optimization Yonggang Zheng	52
MS-02.07	Study on the SPH Method for Macro-Meso Mechanical Behavior of Porous Media by Considering Fluid-Solid Interaction Lisha He	53
MS-03.01	An Enhanced Numerical Wave Tank Based on DualSPHysics+ Guozhen Cai	54
MS-03.02	A GPU-accelerated SPH Framework for Patient-specific Simulations of Vascular Fluid-Structure interactions Yao Lu	55
MS-03.03	Lagrangian-Eulerian Stabilized Collocation Method and Its Applications in Fluid-Structure Interaction Problems Zhihao Qian	56
MS-03.04	S-PINN: Stabilized Physics-Informed Neural Networks for Alleviating Barriers between Multi-level Co-optimization Tengmao Yang	57

MS-03.05	Numerical study on debris flow-turbidity currents transformation process of submarine landslides Can Yi	58
MS-03.06	Rayleigh Bénard convection under the coupled effects of a side-heated wall and bottom charge injection Jiachen Zhao	59
MS-04.01	A Graph-Based Spatio-Temporal Operator Learning Method for Structural Dynamics Xinkai Du	60
MS-04.02	A Lightweight Mesh-Free Network for Strain Field Prediction under Small Geometric Perturbations Minxue Liu	61
MS-04.03	Machine Learning Surrogate Models of Many-body Dispersion Interactions in Soft Polymer Systems Zhaoxiang Shen	62
MS-04.04	A Generative Model Approach for Topological Design of Nonlinear Mechanical Metamaterials Huiyu Wang	63
MS-04.05	A Refined Higher-order Finite Strip Formulation Based on Carrera Unified Formulation for the Free Vibration Analysis of Axially Moving Laminated Composite Plates Yanzheng Wang	64
MS-04.06	Deep-Learning Based Prediction of Chemo-Mechanics and Damage in Battery Active Materials Zehou Wang	65
MS-04.07	Unusual Stretching–Twisting of Liquid Crystal Elastomer Bilayers Ya Wen	66
MS-04.08	A Gaussian Kernel Deep Operator Network for Efficient Full-Field Prediction of Dynamic Responses on Variable 3D Geometries Chi Zhang	67
MS-05.01	Optimization Design of Out-of-Plane Stability Bracing System for Double-Arch Structures Based on the Matrix Stiffness Method Yilei Ge	68
MS-05.02	Cut-Cell Cartesian Meshes for Incompressible Laminar and Turbulent Flows Based on n-sided Cell-based Smoothed FEM Chen Hong	69
MS-05.03	Development of the Coupled Smoothing Technique λ S-FEM for Mechanical Analysis of Twist Drills Qiuxia Fan	70
MS-05.04	A Novel Implementation of Efficient Inertia Relief Analysis Using Smoothed Finite Element Method for Unconstrained Structures Shuhao Huo	71
MS-05.05	Pressure Checkerboarding Suppression in the Next-gen Smoothed Finite Element Method: EC-SSE-SRI-T4 Yuki Onishi	72
MS-05.06	Polyhedral and Polygonal Smoothed Finite Element Method for Engineering Analysis Shijie Zhao	73
MS-06.01	XFEM based on VCCT for Composite Delamination Yong Jiang	74
MS-07.01	Scalable Molecular Dynamics with Deep Potential Long-range Framework Lijun Liu	75
MS-07.02	First-principles Study of Thermal Conductivity in Ti_2CT_2 and $\text{Ti}_3\text{C}_2\text{T}_2$ MXenes: Roles of Surface Terminations and Structural Features Yuki Nagao	76
MS-07.03	Verification of PDS-FEM for Simulation of 3D Dynamic Fault Rupture Using Consistent Fault Stress Induced by Far-Field Loading Elia Nicolin	77

MS-07.04	Simulations, Design and Experimental Validation of a High-Speed Electrically Powered Rocket Oxidizer Pump Ondrej Pavlik	78
MS-07.05	Machine Learning Techniques in the Three-omega Method to Predict Thermophysical Properties with Low Variation Yasuaki Ikeda	79
MS-08.01	Exact Second-order Dynamic Stiffness Matrix for Torsion and Warping of Axially Loaded Members Xiao Du	80
MS-08.02	Accurate Analysis of General Composite Structures Using Mixed Finite Element and DQM Jiaqing Jiang	81
MS-08.03	A Novel Unsymmetric Quadrilateral Plate Element Based on Reissner–Mindlin Theory Using Radial–Polynomial Interpolation Yan-Liang Ju	82
MS-08.04	An Efficient Isogeometric Collocation Method for Superconvergent Analysis of Sixth-Order Elastic Gradient Kirchhoff Plates Ao Shen	83
MS-09.01	Computational Analysis of Contact Wear with Pressure-Dependent Friction Coefficients Yan Li	84
MS-10.01	Crack Velocity, Oscillations, and Acoustic Emission in Rock Fracture: Insights from Numerical and Analytical Models Xu Li	85
MS-11.01	On-chip Surface Acoustic Wave Metasurfaces Yabin Jin	86
MS-11.02	Analytical Realization of Complex Thermal Meta-devices for Omnidirectional Heat Manipulation Weichen Li	87
MS-11.03	Optimization Design and Dynamic Control of Anisotropic Intelligent Elastic Wave Metasurface Exciter Zhenyu Lin	88
MS-11.04	Shear Localization in Gradient High-entropy Alloy at High Strain Rates: Crystal Plasticity Modeling Chuan-zhi Liu	89
MS-11.05	Multiplexing Same-order Acoustic Spiral Waves by Generalized Impedance Metasurfaces Yuze Tian	90
MS-11.06	Experimental Study on SHPB Impact Deformation of Metastable $V_{10}Cr_{10}Co_{30}Fe_{50-x}Ni_x$ High Entropy Alloy in Wide Temperature Range Zehui Wang	91
MS-12.01	Multi-patient Study for the Correlation between Carotid Artery Vascular Elasticity and Clinical Biomarkers Jian Cai	92
MS-12.02	Age-Related Changes in Dermal Elastin Fiber Architecture and Their Impact on Skin Firmness : A Finite Element Analysis Fei Jiang	93
MS-12.03	An Efficient Multiscale Computational Framework for Glycocalyx-Modulated Microvascular Blood Flow Xinhao Jin	94
MS-12.04	Wall Shear Stress Oscillation in Microvascular Network Arising from Red Blood Cell Motion Ken-ichi	95

MS-12.05	Lateral Migration Patterns of Deformable WBC and CTC in Microchannels: Effects of Geometry and Hematocrit Yonggang Li	96
MS-12.06	Motion of Capsules in Curved Tubes Deyun Liu	97
MS-12.07	Numerical Simulation and Lift Force Analysis for Cross-streamline Migration of Slip Particles in Viscoelastic Microchannel Flow Shuhao Ma	98
MS-12.08	Numerical Investigation of Fixation Plate Mechanics in Mandibular Reconstructive Surgery Boyang Wan	99
MS-12.09	Auxiliary Quantitative Methods for the Selection of Preoperative Surgical Plans for Aortopulmonary Septal Defect Qingyu Wang	100
MS-12.10	Cellular Blood Flow Modeling with Smoothed Dissipative Particle Dynamics Ting Ye	101
MS-13.01	Efficient Spectral Methods for Volume-Constrained Nonlocal Models Jiashu Lu	102
MS-13.02	Manifold Adaptive Method for Thermo-Mechanical Coupled Fatigue Phase-Field Model Yu'e Ma	103
MS-13.03	Re-derivation and Mathematical Analysis for Linear Peridynamics Model for Arbitrary Poisson Ratio's Material Yufeng Nie	104
MS-13.04	Phase-Field Modeling of Flexoelectricity and Dislocation Effects in Ferroelectrics Lihua Shao	105
MS-13.05	Computable Peridynamics: Enhancing Asymptotic Compatibility and Suppressing Zero-Energy Modes Hao Tian	106
MS-14.01	Enhanced Identification of the Parameters of a Jeffcott Rotor from Run-up Transients using Physics-informed Neural Networks with Sinusoidal Activations Cabaj Gabriel	107
MS-14.02	LP-PINN: A Locally Connected Physics-informed Neural Networks Based on Local Boundary Knot Method Le Liu	108
MS-14.03	Wind Turbine Wake Prediction by Deep Convolutional Neural Networks with Spatial-coordinate Embedding Decheng Wan	109
MS-14.04	A Machine Learning-Driven Decoupling Framework for Efficient Prediction of Cohesive Zone Model Parameters in Polymer Composites Li Zheng	110
MS-14.05	Structural Parameter Identification with Neural Ordinary Differential Equations Xinqun Zhu	111
MS-14.06	Physics-informed Neural Networks for Modeling Moving Boundaries and Capturing Fine-scale Flow Structures Xin Bian	112
MS-15.01	Development of High Reynolds Number Immersed Boundary Methods Shang-Gui Cai	113

MS-15.02	Evolution of Large-Scale Vortices and Its Influence on Flow and Flexible Vegetation Dynamics of a Finite-length Canopy in a 2-D Laminar Flow Chunning Ji	114
MS-15.03	Investigation on Wake Hydrodynamics under Multi-operating Conditions of a Marine Propeller Based on Immersed Boundary Method Haoyu Li	115
MS-15.04	Coupled Peridynamic and Lattice Boltzmann-immersed Boundary Method for Fluid Solid Interaction Weizhong Li	116
MS-15.05	Research Progress of Fluid-Solid Interaction about Hydroelectric Unit Wenquan Wang	117
MS-15.06	Analysis of Vibration Characteristics of a Pelton Turbine Based on Two-Way FSI Wenquan Wang, Xiu Wang	118
MS-16.01	Re-understanding and Application of Quasi-Coarse-Grained Dynamics DongDong Jiang	119
MS-16.02	Bending Behavior of Diamane and Twisted Bilayer Graphene: Insights from Four-point Bending Deformation Shangchun Jiang	120
MS-16.03	Molecular Dynamics Investigation of Hydrogen Diffusion in Polycrystalline α -Iron Under Multiaxial Stress States Changyou Li	121
MS-16.04	Sliding Behaviour of Carbon Nanothread within a Bundle Embedded in Polymer Matrix Chengkai Li	122
MS-16.05	Computational Simulations of Interfacial Heat Transfer and Crystallization in 3D-printed Continuous Fiber-reinforced Thermoplastic Composites Xin Yan	123
MS-16.06	Theoretical Prediction of Stress-tunable Optoelectronic and Thermal Properties of GaSeI: A Novel 1D Helical van der Waals Crystals Jian Zhang	124
MS-16.07	A Super-coarse-grained Simulation method for Cellulose Nanofiber Networks Shuze Zhu	125
MS-17.01	Numerical Sandbox Experiments with DEM: Frictional and Structural Controls on Prism Deformation Jian Chen	126
MS-17.02	Micromechanical Simulation of Liquefaction using 2D Solid-DEM and Liquid-FEM Coupling with Body-fitted Mesh Gamaliel Jeevan Dewanto	127
MS-17.03	Granular Simulation of Earthquakes in Geological-scale Structural Evolution Mikito Furuichi	128
MS-17.04	Multiphase Continuous-discrete Modelling of Geological Hazards with Particle Method Chong Peng	129
MS-17.05	A Coarse-grained Model for Gas Transport in Swelling Porous Media Luming Shen	130
MS-17.06	Pullout of a Plate Anchor from a Granular Medium beyond Material Failure Shun Nomura	131
MS-17.07	Unveiling Heat Transfer Pathways in Unsaturated Granular Materials via Network Modeling Wenbin Fei	132
MS-17.08	A Coupled 3D MPS–NOSB-PD Model for Fluid–Structure Interaction with Large Deformation Decheng Wan	133

MS-17.09	Three-dimensional Micromechanical Expression for the Average Strain Tensor of Granular Materials Chaofa Zhao	134
MS-18.01	Hybrid Deep Learning and Iterative Methods for Accelerated Solutions of Viscous Incompressible Flow Xin Bian	135
MS-18.02	A Novel Mesh-Based Data-Driven Approach for Optimization of Tidal Turbine Blades Longyan Wang	136
MS-19.01	Simulation of Bond Failure between FRP Bar and Concrete Based on a Full Mesoscale Model Shuwei Li	137
MS-19.02	Axial Compression Capacity Prediction Model of FRP-Steel-Concrete Composite Columns Based on Stacking Ensemble Learning Yi TAO	138
MS-19.03	Macroscale and Mesoscale Modelling of Interfacial Debonding Between FRP and Concrete Zihua Zhang	139
MS-20.01	Analysis of the Effect of an Electric Field on the Vibrational Properties of Hexagonal Boron Nitride and Boron Nitride Nanotubes Hongqiang Pang	140
MS-20.02	Advanced Hygrothermal Flexural Analysis of Functionally Graded Plates using Generalized Differential Quadrature and Higher-order Haar Wavelet Methods Mahaveer Sree Jayan Madasamy	141
MS-20.03	Hybrid Depth Physics-informed Neural Network for Solving Partial Differential Equation Xu Xu	142
MS-20.04	Vibrational Analysis of sp^3 Carbon Nanostructures via Atomistic Simulations and Continuum Mechanics Models Zhuoqun Zheng	143
MS-21.01	Numerical Simulation and Theoretical Prediction of Ultimate Tensile Capacity for Screw Piles Wenbin Fei	144
MS-21.02	GPU-accelerated MPM-LSDEM Approach for Particle-Continuum Interaction Ning Guo	145
MS-22.01	Self-consistent Clustering Analysis-Based Dual-scale Ablation Mechanism and Performance Prediction of Silica Fiber-Reinforced Phenolic Resin Composites (SiFPRCs) Shuo Cao	146
MS-22.02	Multi-scale Collaborative Optimization Design Method for Multi-layer Thermal Protection Structures Jie Hou	147
MS-22.03	Plant-inspired Crashworthiness Design for Composite Materials Shujuan Hou	148
MS-22.04	Programming Nonlinear Thermo-mechanical Intelligence via Topology Optimization Weichen Li	149
MS-22.05	Information Geometry Perspective on Constitutive Models and Its Inspired Dual-Space Model Optimization Wenyang Liu	150
MS-22.06	Optimization Design Method of Smart Hydrogel Double-Layer Structures and Programmable Metamaterials Yisong Qiu	151
MS-22.07	An Efficient Approach to Shape Optimization of Structures with Viscous Dampers for Strain Energy Minimization Zhiqiang Wu	152

MS-22.08	Robust Topology Optimization of FRP Composite Structures under Uncertain Dynamic Excitations Furong Xie	153
MS-22.09	Concurrent Topology–Path Optimization and Vacuum-Assisted Reprocessing for Continuous-Fiber 3D-Printed CFRP Yanan Xu	154
MS-22.10	High-Fidelity Process Modeling of Alumina Melt Pool Dynamics in Laser Powder Bed Fusion Zhilang Zhang	155
MS-22.11	Data-driven Thermo-mechanical Interfaces: Thermal Mismatch Induced Interface Debonding Lizhenhui Zhou	156
MS-23.01	Acceleration of Stiffness Matrix Numerical Integration Using a Finite Element Inspired Neural Network Amir Haderbache	157
MS-23.02	Several Novel Physics-informed Neural Networks for Solving Varied PDEs Zhuojia Fu	158
MS-23.03	A Profile Structure Model Based on Model Driven and Data-driven Coupling Approach Yanchuan Hui	159
MS-23.04	A Large Language Model-inspired Data-driven Mechanics Framework for Viscoelastic Soft Structures Yicheng Lu	160
MS-23.05	Rapid Prediction of Textile Forming Deformation via a Graph-Based Learning Approach Junjie Rong	161
MS-23.06	A Large Language Model-inspired Data-driven Mechanics Framework for Viscoelastic Soft Structures Shan Tang	162
MS-23.07	Improved Artificial Neural Network Algorithms and Its Engineering Applications Lihua Wang	163
MS-23.08	FEM-PIKFNN for Structural Vibration Induced Underwater Acoustic Propagation Qiang Xi	164
MS-23.09	Novel Actuator Lines Method Accounting for Structural Geometries Decheng Wan	165
MS-24.01	Unified Theory and Method for Computational Stochastic Mechanics Hui Li	166
MS-24.02	DPIM-based Neural Network Model for Stochastic Acoustic-vibration Response of Underwater Structure Hanshu Chen	167
MS-24.03	Structural Design and Intelligent Optimization of a Combined Seismic Metamaterial Yu Ding	168
MS-24.04	Rare Event Probability and Global Reliability Sensitivity Analysis for Engineering Structures Based on Direct Probability Integral Method Hui Li	169
MS-24.05	High-dimensional Reliability Analysis using Combined Dimensionality Reduction and Adaptive Sparse Polynomial Chaos Expansion Jian Zhang	170
MS-24.06	Research on Adaptive Loss Physics-Informed Neural Network Algorithm Based on KAN Network for Heat Conduction Equation Tao Zhang	171

MS-25.01	Mechanical Property Evaluation of Nuclear Fuel Assembly Spacer Grids under Extreme Service Conditions Junwei Kang	172
MS-25.02	Generalization Analysis of Direct Weights Inversion Method for Small datasets Yijun Lu	173
MS-25.03	Numerical Method for Irradiation Deformation of Rod-Bundle Fuel Assemblies Based on Beam Model Quanyao Ren	174
MS-25.04	Coupled Autoencoder for Joint Dimensionality Reduction and Inversion Zhijun Shen	175
MS-25.05	Optimized Bubble Suppression in Piezoelectric Jet Dispensing for Microelectronic Packaging Yunshu Zhang	176
PS-01	A High-order Accurate Wavelet Method for Two-dimensional Turbulence Peize Wan	177
PS-02	Wavelet Solution for Moving Point Heat Source Problems Jian Tao	178
PS-03	Study on Seismic Resilience Assessment Method of a Multi-Story Underground Structure for ICCM Xiyue Du	179
PS-04	Acetone Adsorption Behavior on Two-dimensional ZnO Regulated by Doping Engineering: A DFT Study Hongping Zhang	180
PS-05	From Molecule to Membrane: Integrating Molecular Dynamics and In Vitro Experiments for Tyrosinase Inhibition Mechanism Discovery Changji Yin	181
PS-06	The Optimized Runge-Kutta-Chebyshev Method for Semi-discretizations of Hyperbolic Conservation Equations Zihao Duan	182
PS-07	Surface Strengthening of Laser Additive Manufactured AlSi10Mg Alloy: A Multiscale Numerical Simulation Study Based on SPH-FEM Coupling YingPengHou	183
PS-08	SPH Simulation of Dual Roller Cutters Penetrating into Coal Seam with Hard Nodules Zhihao Guo	184
PS-09	Application of the Lattice Boltzmann Flux Solver in Large-Scale Hydrodynamic Numerical Problems Yunpeng Lu	185
PS-10	Effect of Particle Shape on Cohesion and Friction Angle in Clay Studied by DEM Biaxial Shear Simulations Zhipeng Yu	186
PS-11	Impact of Physical Constraints on Spatio-Temporal Neural Networks for Predicting Cylinder Water Entry Flow Fields Chongbin Shi	187
PS-12	A Multiscale Continuum Model for the Mechanics of Cross-linked Elastomer Composites Reinforced with Nanofibers Jianzheng Cui	188
PS-13	An Efficient Approach to Shape Optimization of Structures with Viscous Dampers for Strain Energy Minimization Zhiqiang Wu	189

PS-14	Layout Design of Complex Multi-connected Fluid Channel System with Multi-material Topology Optimization Method Qijin Zeng	190
PS-15	Feature-driven Topology Optimization of Complex Fluid Channel Network with Predefined Inlet-outlet Parings Ze Zheng	191
PS-16	Transformed Tensor Decomposition Method for Topology Optimization Jiayi Hua	192
PS-17	Mechanical Response of Protein-embedded Vesicles under Osmotic Pressure: A Monte Carlo Simulation Long Li	193
PS-18	A Robust E-CUSP Method for Compressible Fluid-Solid Multiphase Diffuse Interface Model Yi Cheng	194
PS-19	Machine-learning Enabled Atomic Insights into the Phase Diagram of Lead Zirconate Titanate Xiaohan Huang	195
PS-20	Density of States Engineering: A Physics-Inspired Framework for Efficient Topology Optimization of Phononic Bandgaps Zonghao Li	196
PS-21	Nonlinear Flutter Analysis of Orthotropic Laminated Thin Rectangular Plates Chao Ye	197
PS-22	Symplectic Contact Analysis of Inhomogeneous Media Lizichen Chen	198
PS-23	SPH Method with Self-contact Treatment for Simulation of Transient Deformation of Soft Structures Yihua Xiao	199
PS-24	Topology Optimization with Node Density Adaptation and Geometric Multigrid Solving Zhanbin Yuan	200

Characterization, simulation and design of cross-scale mechanics properties of advanced materials

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Abstract

The principle of "maximum strain energy density" is introduced, and one can find that there exists a normal-inverse Hall-Petch effect between the "maximum strain energy density" and grain size, but its turning point is in micron scale. Based on the principle of "maximum strain energy density", a special variational principle is developed, which can be used to simulate the mechanics properties of advanced materials. The representation theory and method of cross-scale mechanics behavior are established, and the "ghost force" of macro-micro correlation is eliminated. By establishing the theory of strain gradient viscoelasticity, the strengthening-softening behavior of nanostructured materials is effectively characterized.

Blue Economy CRC Offshore Aquaculture Projects: SeaFisher and SubSCI

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Abstract

As global demand for sustainable food and marine biomass intensifies, offshore aquaculture has become an increasingly vital contributor to food security and environmental resilience. This talk focuses on two Blue Economy Cooperative Research Centre's offshore aquaculture projects: the SeaFisher – a submersible offshore fish pen and the SubSCI – a submersible seaweed cultivation infrastructure that can perform depth cycling in deep offshore waters. The conceptual design, modeling, structural and hydroelastic analyses, and testing of these two offshore aquaculture systems will be presented.

Computational Methods Based on Peridynamics and Nonlocal Operators

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Abstract

Energy harvesters are an increasingly attractive alternative to conventional batteries. They capture minute amounts of energy from one or more of the surrounding energy sources where a remote application is deployed, and where such energy source is inexhaustible. One of the most common energy harvesters are based on piezoelectricity converting mechanical energy into electrical energy. While most computational studies focus on macro-scale energy harvesters, there are comparatively few studies on nano-scale energy harvesters which promise a significant improvement due to the presence of size effects at the nano-scale. Furthermore, there are only a few studies on flexoelectricity. Flexoelectricity can be considered as an extension of piezoelectricity and is a size dependent phenomenon even in the absence of surface effects.

However, modeling flexoelectricity is challenging due to the C1 requirement of the underlying discretization. This presentation will propose an efficient computational formulation for flexoelectric nano-structures which exploits the higher continuity of the underlying discretization and therefore avoids a complex mixed formulation. Furthermore, an efficient level-set based topology optimization will be presented. The formulation will subsequently be extended to multi-materials and it will be shown that adding soft materials can significantly enhance the energy conversion efficiency of a composite energy harvester.

Numerical Methods for System Design of Aerospace Vehicles

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Abstract

In the design and development process of aerospace vehicles, multidisciplinary integrated design plays a crucial role in enhancing the system performance of aerospace vehicles, shortening the development cycle, and improving flight reliability. To address the complex issues of multidisciplinary coupling design in aerospace vehicles, we have addressed key technologies such as overall design, integrated aerodynamic/structural design, and multi-system collaborative control, resulting in a multidisciplinary comprehensive design platform for aerospace vehicles.

For the multidisciplinary coupling overall collaborative design of complex aerospace vehicles, we have developed multidisciplinary design optimization software based on reinforcement learning, which solves mixed integer nonlinear programming problems, breaks through the traditional serial design paradigm, and achieves high-efficiency parallelization of the entire process from rapid generation to comprehensive evaluation to iterative optimization, significantly improving the design efficiency of aerospace vehicles.

For the integrated aerodynamic/structural design of aerospace vehicles, we have developed software for aerodynamic-structural coupled analysis. By establishing real-time data-efficient iteration between the fluid dynamics solver and the structural mechanics solver, the efficiency of bidirectional data transfer between aerodynamic and structural iterations has improved by more than 10 times compared to traditional methods.

For the multi-system collaborative control of aerospace vehicles, we have developed an integrated design and optimization platform for body-power-operation. We have integrated multiple key subsystems such as manipulation, energy, navigation, communication, and payload, into a collaborative control system, significantly enhancing the autonomous decision-making efficiency and flight performance of the aerospace vehicles.

Keywords: System Design of Aerospace Vehicles, Multidisciplinary Coupling Overall Collaborative Design, Integrated Aerodynamic/Structural Design, Multi-System Collaborative Control

Machine Learning Assisted Multiscale Modelling and Design of Flexoelectric Nanostructures

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Abstract

In this talk, I will present machine learning-assisted flexoelectric materials characterization and the use of topological optimization for single and multi-phase flexoelectric structures across atomistic to continuum scales. New formulations for nonlinear topological optimization of flexoelectric structures, accounting for nonlocal stress and large deformation processes considering the environmental medium, will be presented. Different from pure data-driven area, in Engineering and Science, AI is transforming research with domain specific physical and mathematical knowledge. Materials exploration and design could be accelerated by orders of magnitude, which cannot be conceived decades ago. I will give some interesting examples that I have carried out with my team for 2D flexoelectric materials exploration with various thermal, optical, mechanical and electrical properties.

AI-assisted Engineering

Our understanding and typical applications

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Abstract

Design and manufacturing of lightweight & high-performance structures are eternal goals in aeronautic and aerospace industries to meet the serious loading conditions. Nowadays, AI is an attractive topic and plays a more and more important role worldwide. How to combine AI with engineering scenarios in advanced design and manufacturing of aerospace structures is a motivating and challenging problem. This lecture aims to share some experience of our research team at Northwestern Polytechnical University.

First, some basic concepts related to Neural Network (NN) are introduced based on our understanding. The contents are then focused on additive manufacturing process, curing process of composite structures, metal cutting process including milling process with robots, design optimization of smart SMA structures. Typical industrial applications are presented. Perspective developments are discussed.

Modelling nonlinear damping in large-amplitude vibrations of structures

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Abstract

An increase in damping is relevant for the passive control of vibrations and noise; therefore, it is very relevant in design. Experimental data show a strong and nonlinear dependence of damping on the vibration amplitude for beams, plates (see Fig. 1), and shells of different sizes and made of different materials (metal, composite materials, silicone rubber, and graphene) [1, 2]. While the frequency shift of resonances due to stiffness nonlinearity is 10 to 25 % at most for common structural elements, a damping value up to several times larger than the linear one can be obtained for vibrations of thin plates when the vibration amplitude is about twice the thickness. This is a huge change in the damping value! Therefore, the nonlinear nature of damping affects structural vibrations much more than stiffness nonlinearity. Despite this experimental evidence, nonlinear damping has not been sufficiently studied yet. A model of nonlinear damping was derived from linear viscoelasticity for single-degree-of-freedom systems [3, 4] and rectangular plates [5] by taking into account geometric nonlinearity. The resulting damping model was nonlinear, and the model parameters were identified from experiments. Numerical results for forced vibration responses of different structural elements in large-amplitude (nonlinear) regimes were obtained and successfully compared to experimental results, validating the nonlinear damping model.

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Conquering Generalization Challenges—A Problem-Independent Machine Learning (PIML) Approach for AI enhanced Computational Mechanics

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Abstract

Artificial Intelligence (AI) for computational mechanics is one of the current research focuses in the field of solid mechanics. The field of computational mechanics involves complex physical phenomena and diverse engineering scenarios. Traditional end-to-end AI models often perform well on specific datasets but exhibit significant loss of generalization ability when facing new boundary conditions, material properties, or geometries. To address this challenge, a problem-independent machine learning (PIML) enhanced large-scale structural analysis and topology optimization framework is developed. The main idea is to focus on the origin of finite element analysis method—the shape function. This is achieved by using machine learning to establish an implicit mapping between the material distribution within coarse mesh elements and corresponding numerical Green's functions. The proposed PIML algorithm is truly independent of specific analysis and topology optimization problems. This is because the numerical shape functions of coarse mesh elements are uniquely determined by the material distribution inside, and do not depend on the external loads, boundary conditions, or shapes of design domain. Numerical examples demonstrate that this algorithm can achieve a two-order-of-magnitude improvement in optimization efficiency for million-scale three-dimensional topology optimization problems compared to mainstream commercial topology optimization software, under the same computational resources. In a 6750-core parallel environment, a 3D topology optimization problem with 10 billion degrees of freedom requires only 42 seconds per iteration. In the future, it is possible to develop a universal CAE software framework based on this technology by integrating AI with traditional numerical methods, enabling more efficient and intelligent engineering simulation and design.

Key Words: *AI enhanced computational mechanics; Generalization; Problem-Independent Machine Learning (PIML); Large-scale structural analysis and topology optimization*

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Is Physics-informed Machine Learning the next powerful modelling tool for engineering and science?

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Abstract

In recent years, Physics-informed Neural Networks (PINNs) have revolutionized the application of Machine Learning to solving Partial Differential Equations (PDEs). By integrating data-driven learning with physics-based modelling, PINNs combine the strengths of both approaches and demonstrate exceptional potential in tackling a wide range of complex problems—particularly those with strong nonlinearities. As a result, PINNs are rapidly emerging as game-changers in computational modelling and simulation for Engineering and Science. This talk will first review the latest advancements in applying PINNs to various mechanics problems, including solid mechanics, nonlinear mechanics, fracture analysis, structural optimization, and fluid mechanics. Recent research from the speaker's group will be presented, covering topics such as novel neural network architectures for PINNs, PINN-based structural topology optimization, food drying modelling, dynamic and nonlinear problem solving, and inverse problems. Finally, the discussion will then highlight key challenges in employing PINNs for mechanics.

On mixed mode crack propagation analyses using Fragile Points Method (FPM)

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Abstract

In the presentation, Fragile Points Method (FPM), its applications to fracture mechanics problems in linear elastic fracture mechanics problems are discussed. FPM is a new point base meshless analytical methodology based on a local weak formulation (Yang, Dong and Atluri [1], Wang et al. [2]) and the generalized finite difference method (Liszka and Orkisz [3]). The discretization in FPM is based on points distributed in the problem domain. Test and trial functions are established based on the distributed points and the generalized finite difference scheme. Connections between the points across the crack face are discarded for modeling the displacement discontinuity. A Local Galerkin symmetric weak form is established in each subdomain determined for each point. Then, pointwise stiffness matrix is constructed at each point. Subdomains cover the the problem domain. The integration of the local weak form can be achieved without any difficulty. Recently, FPM with an explicit formulation for dynamic fracture mechanics problem was presented by Li et al. [4].

The authors developed a strategy to perform mixed mode fracture mechanics. The most recent outcomes of the authors' research will be presented in the conference.

Acknowledgement: Research collaborations of Mr. Kaikou Yoshida, former graduate student of TUS is highly appreciated. The authors gratitude extends to Professor Yuto Ootoguro of Waseda University with whom the authors had valuable discontinuous in Galerkin method, etc.

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A boundary-based machine learning approach for elastic and piezoelectric crack analysis

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Abstract

A novel boundary-based machine learning (BBML) approach for two-dimensional (2D) crack analysis in linear elastic and piezoelectric materials will be presented. The proposed approach integrates the machine learning (ML) technique based on artificial neural networks (NNs) with the boundary integral equation (BIE) method, which enables an efficient and accurate evaluation of the characteristic fracture mechanics parameters. The local asymptotic behavior of the crack-tip field is properly captured by the developed novel special crack-tip elements based on NNs (CTNNs), which ensures the modelling accuracy of the displacement and stress fields near the crack-tips. In the developed special CTNNs, the local asymptotic characteristics of the crack-tip field are embedded into the NNs to guarantee the high accuracy for describing the inherent stress singularities and high deformation gradients near the crack-tips. In comparison to many conventional numerical methods in fracture mechanics, the proposed BBML approach exhibits several distinct advantages. Firstly, by embedding higher-order terms of the asymptotic crack-tip field into the NNs, the proposed approach can achieve a more accurate and reliable description of the crack-tip field, even by using relatively large crack-tip elements. Secondly, the proposed approach can be easily extended to other crack problems involving complex material properties and crack-tip geometries, because the CTNNs can incorporate important information about the variable singularity orders of the crack-tip field, and thus ensuring the versatility and robustness of the approach. In addition, in comparison to the domain-based ML (DBML) approach, the proposed novel BBML approach boasts an excellent computational efficiency due to the dimension-reduction and analytical/semi-analytical nature of the involving BIEs. Several numerical examples will be shown to demonstrate that the proposed novel BBML approach can offer certain significant advantages over many other conventional numerical methods, and hence provide a reliable, robust and accurate numerical simulation tool for solving 2D linear elastic and piezoelectric crack problems.

Interval field model and interval finite element methods

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Abstract

Uncertain parameters with inherent spatial or spatiotemporal variability are commonly encountered in engineering. These include material properties of the heterogeneous media, such as concrete or porous rock, external loads such as wind loads applied to structures, etc. This type of uncertain parameters are traditionally quantified by the random field model, while the large amount of information required in the construction of the precise probability distribution functions is often difficult to obtain for many practical engineering problems. For this reason, the authors proposed an interval field model to represent the spatial and spatiotemporal uncertainties with insufficient information, in which the variation of the parameter at any spatial or spatiotemporal location is quantified only by an interval with the upper and lower bounds. In the interval field model, the spatial and spatiotemporal dependency can be measured by a covariance function or a correlation coefficient function that is defined for the interval variables at different locations or space-time points. Based on the correlation information, an interval K-L expansion is formulated for the proposed interval field model, by which the continuous spatial uncertainty can be expressed through a series of deterministic functions with uncorrelated interval coefficients. Particularly, a spatiotemporal uncertain parameter could be decomposed into a series of interval processes firstly, which relates only to time and can be furtherly represented by time-independent interval variables. By introducing the interval field model into the finite element analysis, the interval finite element method (IFEM) is then formulated to predict the response bounds of structures with spatial or spatiotemporal uncertainties. The primary challenge of interval finite element analysis lies in solving a class of non-deterministic interval linear equilibrium equations. The solution of the interval equations formulates an NP-hard problem, which cannot be precisely obtained in most cases. To compute an interval vector that approximates the exact solution set, the authors proposed a series of IFEMs, including the sequential simulation method, interval iterative method, field optimization method, etc., which provide either an inner enclosure or outer enclosure for the structural response bounds. With both the outer and inner enclosures obtained, the exact solution as well as the prediction error can then be demarcated, which is very beneficial to the subsequent structural reliability analysis and design.

Keywords: Interval field, spatial uncertainty quantification, structural response bounds, interval finite element analysis

Vibration of Strain Gradient Nano Structures via a Mesh-free Moving Kriging Interpolation Method

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Abstract

Nanoscale structures, serving as core components in M/NEMS devices, exhibit outstanding dynamic behaviors such as ultra-high resonant frequencies, high quality factors, and exceptional sensitivity. It is of significant practical importance to establish appropriate dynamic research methodologies and achieve a comprehensive understanding of their size-dependent dynamic characteristics. Strain gradient theory is widely employed to account for size-dependent material behavior. In this work, the Moving Kriging Interpolation (MKI) method is utilized to systematically investigate the vibration characteristics of nanostructures, taking into account van der Waals forces, interlayer shear effects, and scale phenomena. The accuracy and stability of the conventional Moving Least Squares (MLS) approximation and the MKI method are compared through function fitting and their first three derivatives. The vibrational frequencies of nanoplates are computed using both MLS and MKI approaches. Dynamic models for nanoplates and nanoshells are established based on strain gradient theory. Furthermore, a meshfree method based on Moving Kriging Interpolation that satisfies C^2 continuity requirements is employed to study vibration problems in strain gradient-based nanoplates and nanoshells. Results indicate that the natural frequencies of nanoplates and nanoshells modeled via strain gradient theory are lower than those predicted by classical plate theory. Additionally, ultra-high-order mode shapes associated with lower frequencies are observed in the meshfree computational results. It is also demonstrated that the meshfree MKI method offers high accuracy and robust stability when solving higher-order partial differential equations.

Keywords: Size effect, Nano structure, Meshfree method, Moving Kriging interpolation.

Ghost hammering phenomena in stochastically driven shells

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Abstract

Random phenomena are widespread in disciplines such as Engineering, Physics, Geophysics, and Medicine, reflecting the inherent variability of natural and artificial systems. In Structural Mechanics, stochasticity arises from environmental loads like wind and seismic activity, as well as from manufacturing tolerances and operational uncertainties. These factors can induce vibrations with non-deterministic features that challenge predictability. Linear models, long employed to study vibrations, remain valuable but often fail to capture the rich spectrum of behaviours produced by nonlinear dynamics. The combination of stochastic forcing and nonlinear structural response can generate highly complex patterns beyond the reach of traditional theories.

This study examines the nonlinear dynamic response of a circular cylindrical shell subjected to strong, narrowband random excitation representative of seismic events. Laboratory experiments revealed striking phenomena: sporadic, large-amplitude spikes in the vibrational response, occurring irregularly in time and without any external impulses. Such bursts cannot be explained within a linear framework and instead reflect emergent dynamics rooted in the nonlinear character of the system.

The observed spikes bear strong resemblance to phenomena in other fields. They recall Extreme Events (EE) in oceanography and finance, Stochastic Resonance (SR) enhancing weak signals in physics and biology, and Bursting Behaviour (BB) reported in neuroscience. Yet, in Solid Mechanics, such phenomena are rarely documented, in this experimental work we observed a special type of EE that we called “Ghost Hammering (GH),” which appears as transient oscillations having a spectral content populated by the natural frequencies of the shell, creating the illusion of sudden impacts despite the absence of external hammer strikes.

The evidence suggests that GH is produced by nonlinear interactions activated under random excitation, driving the system into states where energy is suddenly released. Similar mechanisms are well described in models of nonlinear physics and neuroscience, such as the FitzHugh–Nagumo systems and stochastic Langevin formulations. These models provide conceptual and mathematical frameworks that could clarify the dynamics responsible for GH, highlighting the value of adopting cross-disciplinary approaches.

The work outlines the experimental setup and modal analysis of the tested shell, followed by a focused discussion of the GH. The findings emphasize the need to extend nonlinear stochastic modelling to structural systems, where randomness and nonlinearity can combine to produce rare but significant behaviours. This perspective offers new opportunities for understanding, predicting, and eventually controlling the unexpected dynamics of mechanical structures operating in uncertain environments.

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Keywords: Random vibration, Shells, Nonlinear dynamics, Stochastic resonance, Complexity

A novel approach for deriving a state-dependent soil constitutive model using stress probing analysis

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Abstract

Nonlinearity, irreversibility, and state-dependency are fundamental characteristics of soil mechanics. To develop a constitutive model that accurately captures these features, a comprehensive understanding of the incremental stress-strain response is crucial. In this study, a numerical stress probing technique is employed in conjunction with the discrete element method to investigate the strain response of soil under stress increments along different directions. The impact of density and stress state on the incremental behavior is systematically analyzed. Leveraging the strain response envelopes obtained from the probing tests, explicit formulations of key components of the constitutive model are derived, including the yield surface, plastic potential surface, plastic modulus, and dilatancy function. Subsequently, a state-dependent constitutive model is established within the critical state framework. The predictive capability of the model is demonstrated through simulations of soil behavior in both discrete element tests and laboratory experiments under varying loading conditions. This research contributes to the development of a robust constitutive model for soil, facilitating improved predictions of soil behavior in geotechnical engineering applications.

Computational Design of Multifunctional Lattice Structures

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Abstract

While additive manufacturing has offered substantially new opportunities and flexibility for fabricating 3D complex lattice structures, effective design of such sophisticated structures with desired multifunctional characteristics remains a demanding task. To tackle this challenge, we develop an inventive multiscale topology optimisation approach for additively manufactured lattices by leveraging a derivative-aware machine learning algorithm [1]. Our objective is to optimise non-uniform unit cells for achieving an as uniform strain pattern as possible. The proposed approach exhibits great potential for biomedical applications, such as implantable devices mitigating strain and stress shielding. To validate the effectiveness of our framework, we present two illustrative examples through the dedicated digital image correlation (DIC) tests on the optimised samples fabricated using a powder bed fusion (PBF) technique. Furthermore, we demonstrate a practical application of our approach through developing bone tissue scaffolds composed of optimised non-uniform iso-truss lattices for two typical musculoskeletal reconstruction cases [1,2]. These optimised lattice-based scaffolds present a more uniform strain field in complex anatomical and physiological condition, thereby creating a favourable biomechanical environment for maximising bone formation effectively. The proposed approach is anticipated to make a significant step forward in design for additively manufactured multiscale lattice structures with desirable mechanical characteristics for a broad range of applications [3].

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Conservative sharp interface methods for interfacial flows: development and simulations

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Abstract

Interfacial flows can be numerically considered as a class of deformable boundary problems, and interfaces between different phases have different jump conditions (or boundary conditions). These conditions, which define the coupling between phases such as transfer of mass, momentum, and energy, are fundamental in determining the resulting flow characteristics. Consequently, high-fidelity simulation of interfacial flows necessitates not only high-order numerical discretization of the governing equations but also a high-resolution representation of the interface geometry and an accurate approximation of its jump conditions. Cut cell method addresses these requirements by reconstructing the interface on a regular grid and generating dynamic meshes that realign with the interface. This approach provides a foundation for high-resolution interface tracking and high-order approximation of jump conditions at interfaces. Recently, we have developed a series of conservative sharp interface methods based on this cut-cell strategy. This report will introduce the core concepts and current developments of this conservative sharp interface method and demonstrate its application to several key problems in fluid dynamics.

Keywords: Computational fluid dynamics, interfacial flows, sharp interface method

Numerical Study of Droplet Impact on a Deep Pool by CLSVOF Method

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Abstract

A coupled Level-Set and Volume-of-Fluid (CLSVOF) method was implemented in the open-source multiphase flow solver Basilisk to investigate droplet impact on a deep water pool. The approach combines the geometric reconstruction capability of the PLIC-VOF method with the geometric accuracy of the Level-Set function, ensuring sharp interface representation and improved mass conservation. Validation against the single vortex benchmark confirmed the superiority of CLSVOF over the Level-Set method, particularly in maintaining interface integrity under severe deformation and reducing sensitivity to grid resolution. Numerical simulations for droplets with different aspect ratios revealed distinct impact behaviors: elongated droplets penetrated deeper, generated stronger vortex rings, and induced large bubble entrapment and vertical jets, while spherical and flattened droplets produced shallower cavities and smaller bubbles. Analysis of energy evolution further highlighted the role of droplet geometry in controlling turbulent kinetic energy and potential energy exchange. The results highlight CLSVOF as a robust and accurate tool for capturing complex multiphase free-surface flows.

Keywords: Free-surface flows, CLSVOF method, Droplet impact, Multiphase simulation.

Wavelet Methods for Solving Hyperbolic Conservation Laws

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Abstract

Compressible flow problems governed by hyperbolic conservation laws typically involve various strong discontinuities and multiscale structures. Over the years, a range of grid-based high-order numerical methods has been developed for such problems. However, these methods can truly achieve high-order accuracy only when high-order meshes are employed on regular domains. For problems defined on complex domains, it is very difficult to generate sparse high-order meshes; in practice, fine global meshes are often required to successfully capture discontinuities and localized small-scale features, leading to a challenging trade-off between computational accuracy and efficiency. Wavelet theory, developed in recent decades, offers closure under nonlinear approximation, as well as multiresolution analysis and time–frequency localization. Moreover, its rich families of basis functions provide potentially effective tools for efficiently solving problems with discontinuities and multiple scales. In this work, by constructing wavelet basis functions with specific symmetries, we develop a high-order, adaptive, multiresolution wavelet collocation upwind method within a meshless framework. A variety of classic one- and two-dimensional benchmark tests demonstrate the superior accuracy and efficiency of the proposed wavelet method.

Phase field modelling of spinodal decomposition and nucleation in ferritic alloys

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Abstract

Understanding and predicting phase separation in alloys enables evaluation of the resulting hardening and embrittlement under a range of processing or service conditions. Fe-Cr-based ferritic alloys are desirable structural materials for high-temperature, corrosive environments. However, Fe-Cr alloys are susceptible to thermal embrittlement by phase separation, which increases the tendency for brittle fractures, limiting the safe service life of these materials in pressure vessel structural applications. Numerical methods have been used to simulate microstructural evolution in alloy systems. The phase field method, a common numerical approach for microstructural evolution, is effective at describing phase separation at long timescales, as it can model diffusion and segregation in a continuum system. However, further study needs to be performed to integrate physically-based parameters of the free energy, mobility and interfacial width into phase field models, to facilitate accurate modelling of phase transformations. This paper employed the phase field method to model phase separation under elevated temperatures in the Fe-Cr alloy system. The phase field model integrated the essential physically-based parameters, including a CALPHAD free energy function, measurements of substitutional diffusion in Fe and Cr, measurements of the Fe-Cr single-crystal elastic properties, and a calibrated interfacial width. To implement nucleation in the phase field method, a discrete logical algorithm was used. The phase field method was then used to model α - α' nucleation, or α - α' continuous transformation, at 773 K. The simulated phase evolution has been quantified and critically compared to the applicable experimental measurements. It was shown that phase field modelling has the potential for quantitative, physically-based modelling of metallurgical phase transformations, especially in the Fe-Cr system. The use of physically-based parameters, particularly the CALPHAD free energy function, facilitates accurate modelling of phase transformations at high temperatures. Importantly, the implemented phase field model with carefully selected parameters demonstrates improved accuracy at modelling key features of spinodal decomposition compared to simplified phase field models. For example, the model elucidates the significant difference in kinetics of the Fe- and Cr-rich phases. Finally, the discrete nucleation algorithm was shown to facilitate non-classical nucleation characteristics of some Fe-Cr alloys exhibited in practice, including nuclei with intermediate compositions, without significantly penalising the computational cost of the model. In future, this work will investigate phase transformation induced by displacement damage from high energy radiation.

Keywords: Phase field modelling, CALPHAD method, Stainless steel, Fe-Cr alloy, Phase separation

Uncovering the Mystery of Floating Wind Turbine Modelling

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Abstract

Floating offshore wind energy is poised to be the next frontier in marine renewable energy, unlocking the immense potential of marine resources. It is essential to accurately predict the responses of floating wind turbines. Potential flow calculations seem to deviate from experimental studies, particularly under severe sea states where viscosity plays a significant role. Focusing on a semi-submersible type of floating wind turbine, a series of experiments in a wave basin have been re-analyzed using novel data analysis techniques. New phenomena have been observed through the analysis of the experiments. Viscosity is found to affect both the response amplitude (via damping) and the natural frequency (via extra added mass) – way beyond the damping effect in a damped spring system. This study will present how these insights have been integrated into improved numerical modelling.

Study on the response of elastic wheel to excitation

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Abstract

This paper compares the responses of elastic wheel and standard wheel at different positions under excitation. Within the frequency range of 500 Hz to 3750 Hz, the radial modes of elastic wheel are relatively concentrated. Additionally, the mobility of elastic wheel is higher than that of standard wheel, which can easily lead to increased rim vibration. Above 3750 Hz, the vibration levels of two types of elastic wheel are several orders of magnitude lower than those of standard wheel. This is primarily due to the dissipation of vibration energy in the rubber layer, which reduces the vibration level of the elastic wheel tread.

Keywords: Elastic wheel, velocity response, vibration

Mechanism of Isolation Piles on Displacement Control of Adjacent Tunnels under Foundation Pit Unloading and Surcharge Loading Conditions

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Abstract

Existing studies on the mechanism of isolation piles in controlling displacement of adjacent tunnels have predominantly concentrated on the foundation pit excavation stage, with inadequate systematic investigation into the entire construction process. Taking a deep foundation pit project adjacent to a tunnel in Shanghai as a case study, this paper establishes a coupled analysis model of "foundation pit-isolation pile-tunnel" by means of Plaxis2D finite element software. It further systematically explores the control mechanisms and influence regularities of tunnel displacement induced by three key parameters of isolation piles—namely pile length, pile diameter, and pile top embedment depth—throughout the entire construction process. Research findings indicate that during the whole foundation pit construction process, the tunnel presents a deformation pattern characterized by "horizontal stretching and vertical compression". Based on the distribution characteristics of pile shaft bending moment, isolation piles can be divided into upper and lower segments with the inflection point serving as the boundary, and their action mechanisms exhibit significant differences. Under excavation conditions, the soil on the sidewall of the foundation pit tends to incline toward the pit interior; the upper isolation piles block the soil to restrain this inclination, whereas the lower isolation piles induce soil displacement toward the pit interior via a traction effect. Under surcharge conditions, the soil at the foundation pit bottom, upon compression, extrudes outward in all directions, leading to heaving of the soil around the pit; the lower isolation piles block the soil to prevent it from moving away from the foundation pit, while the upper isolation piles induce soil movement away from the foundation pit through a traction effect. The control efficiency reaches its optimum when the length of isolation piles is 2.0 times the foundation pit depth; the application of embedded isolation piles can significantly enhance the control effect on tunnel horizontal displacement.

Keywords: Isolation piles, surcharge conditions, control mechanism, tunnels outside the pit

Seismic performance of central columns for a multi-story subway station under vertical earthquake excitations

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Abstract

A series of shaking table tests were carried out to investigate effects of vertical earthquake on central columns of a multi-story subway station. Dynamic responses of central column induced by vertical earthquake were focused, especially the variation of axial force, story drift, and the relationship between responses and bearing capacity. Results from tests show that vertical earthquake causes significant amplification in axial force demand of central columns. The axial force of central column increases with the vertical peak acceleration. For example, when the horizontal peak acceleration (a_H) was 0.2 g and the vertical peak acceleration (a_V) increased from 0 to 0.4 g, the axial force increased 26.4%. When a_H was small, it showed a good linear relationship with the maximum dynamic axial force and a_V/a_H . With the increase of a_H , although the maximum axial force increased, it grew slower compared to small earthquakes. With the same a_H , the distribution of vertical axial force on the central column (compared with the side wall) increased with a_V . The maximum axial force distribution can reach 23.5%. Then shear and drift capacities of the central column under different axial compression ratios were evaluated by numerical simulation. And the results show that under high axial compression ratio, shear capacity and ductility decrease sharply.

Keywords: vertical motion; shaking table test; multi-story subway station; central column; seismic performance.

Seismic resilience assessment method of a multi-story underground structure

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Abstract

Unlike traditional seismic design methods, the seismic design method based on resilience focuses on both personnel safety and post-earthquake recovery. With the national strategy of Building Safe and Resilient Cities, seismic resilience has also become one of the research hotspots in the current seismic design of underground structures. However, there is still a lack of research on seismic resilience assessment of underground structures. This article starts with seismic resilience, sorts out the methods for seismic resilience assessment, and uses the method provided in China's current *Standard for seismic resilience assessment of buildings* to evaluate the seismic resilience of an underground structure. Based on the resulting repair cost, repair time, and casualty indicators, the seismic resilience rating of the underground structure is evaluated, and the applicability and limitations of the method provided in the *Standard for seismic resilience assessment of buildings* are analyzed. The results show that the method provided in the *Standard for Evaluation of Seismic Resilience of Buildings* is applicable to this underground structure and can provide a reference for the seismic resilience assessment of other underground structures.

Keywords: Underground structures, seismic resilience, Monte Carlo, resilience assessment

GraphBRep: Explicit Graph Diffusion of B-Rep Topology for Efficient CAD Generation

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Abstract

Direct B-Rep generation is increasingly important in CAD workflows, eliminating costly modeling sequence data and supporting complex features. A key challenge is modeling joint distribution of the misaligned geometry and topology. Existing methods tend to implicitly embed topology into the geometric features of edges. Although this integration ensures feature alignment, it also causes edge geometry to carry more redundant structural information compared to the original B-Rep, leading to significantly higher computational cost. For efficient generation, GraphBrep, a B-Rep generation model that explicitly represents and learns compact topology is proposed. Based on the original B-Rep structure, an undirected weighted graph is constructed to represent the surface topology. A graph diffusion model is employed to learn topology conditioned on surface features, serving as the basis for determining connectivity between primitive surfaces. The explicit representation ensures a compact data structure, effectively reducing computational cost during both training and inference. Experiments on two large-scale unconditional datasets and one category-conditional dataset demonstrate the proposed method significantly reduces training and inference times (up to 31.3% and 56.3% for given datasets, respectively) while maintaining high-quality CAD generation compared with SOTA.

Keywords: B-Rep Generation, Graph Diffusion, Generative CAD

The State-Space FEM: Formulation and Analysis for Laminated Composite Plates Subjected to Body Forces

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Abstract

The state equations governing laminated plates under the influence of body forces are derived employing a mixed variational principle. A state-space finite element method is proposed to solve these non-homogeneous state equations. In laminated plate analysis, planar domain discretization follows finite element principles, while thickness-direction computations employ exact integration methods. Owing to the fact that discretization is implemented only on the in-plane level, a notably smaller number of elements is required relative to the conventional finite element method, thereby effectively increasing computational efficiency. This investigation explores the impact of diverse material properties, boundary conditions, and load configurations on the suitability and robustness of the developed methodology. Unlike conventional finite element solutions, which are characterized by an approximate fulfillment of stress boundary conditions, the present approach ensures strict adherence to them. Furthermore, the present method ensures a continuous distribution of transverse stresses across the layer interfaces through the thickness, in contrast to conventional FEM, which often fails to provide interfacial continuity of these stresses.

Keywords: Laminated plate, Mixed variation, Finite element, State equation, Transverse stresses

Diffusion-induced stress analysis of lithium-ion battery layered electrode based on the boundary element method

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Abstract

The diffusion-induced stress generated during the charging and discharging process of layered electrodes of lithium-ion batteries is a key factor affecting the performance and lifetime of the lithium-ion batteries. In this paper, a computational method based on the boundary element method and the radial integration method is proposed for the efficient and accurate calculation of the diffusion-induced stress of the layered electrode. The method is predicated on the simplification of the electrode into a layered structure, the solution of the elastic equilibrium equation by means of the boundary element method, and the combination of the radial integration method to deal with the domain integrals containing the lithium ion concentration field. The effect of changes in the partial molar volume of the active layer on diffusion-induced stress was investigated. The results suggest that the partial molar volume is a key parameter that influences the distribution and size of diffusion-induced stress. In addition, the mechanical responses under constant-current charging and constant-voltage charging conditions were compared, and it was found that the constant-current condition at the beginning of charging produced less deformation as well as smaller diffusion-induced stress than the results under constant-voltage conditions. A charging strategy of constant current followed by constant voltage is recommended to effectively reduce the diffusion-induced stress and improve the cycle life and safety of the battery.

Keywords: lithium ion battery; boundary element method; diffusion-induced stress; Chemical-mechanical coupling

Development, Verification and Validation of a Dedicated FEM Code for Simulating Masonry Structures

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Abstract

With the aim of quantitatively estimating the effectiveness of various retrofitting techniques of masonry buildings, we are developing a FEM code dedicated for simulating 3D full scale brick buildings. Evaluating the seismic resistance of masonry buildings using solid FEM elements is computationally expensive due to the large difference between the thickness of mortar layers and brick dimensions. In this study, following Lourenco et al.[1], we used elastic solid elements and zero-thickness elasto-plastic interface elements to model the bricks and mortar layers, thereby reducing computational cost. Nonlinear behavior of mortar is modeled using a rate-independent plasticity model by Nitin *et al.*[2] that consists of two composite yield surfaces. Closest Point Projection Method (CPPM) is used to obtain the remapped state when the elastic predictor violates one of the yield criteria. A one-step integration method[3] based on Koiter's rule[4] is used to handle the singularity at the intersection of the two independent yield surfaces. We used arc-length method to simulate nonlinear response at structural level, and arc-length is adaptively controlled to reduce computational cost. The plasticity model was verified and validated against the experimental observations from an in-plane loading test of a single-layer brick wall. The validation test successfully reproduced key structural behaviors such as the load-displacement relation, crack patterns, and failure modes. We applied the validated model to study the behaviour of a double-layer brick wall under in-plane and out-of-plane loading.

Keywords: Brick-masonry walls, micro modeling, nonlinear deformation, validation, composite yield functions

Semi-analytical evaluation for nearly singular integrals in isogeometric thermoelasticity boundary element method

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Abstract

The isogeometric boundary element method has been preliminarily developed and applied in the field of thermoelasticity in recent years, demonstrating its unique advantages in geometric modeling and numerical computation. However, in practical applications of this method, the efficient and accurate calculation of nearly singular integrals remains a significant and persistent technical challenge. The present paper proposes a near-singular integral calculation method applicable within the isogeometric boundary element method framework for thermoelasticity. Firstly, the nearly singular integrals in the isogeometric boundary element method of thermoelasticity are separated to non-singular parts and singular parts through the subtraction method. The integral kernel function of the singular part is represented by a polynomial approximation form obtained through the Taylor series expansion, while the non-uniform rational B-spline interpolation is used to accurately approximate the derivatives of each order. On this basis, through multiple integration by parts operations, the analytical expression of the singular integral part containing the approximate kernel function is derived, thereby achieving its semi-analytical calculation. The present method combines the advantages of analytical derivation and numerical integration, not only improving the accuracy of integral calculation but also significantly enhancing the overall computational efficiency. Compared with the traditional isogeometric boundary element method, this method can provide more accurate displacement and stress field solutions for internal points much closer to the boundary. By leveraging NURBS basis functions for precise boundary geometry representation and requiring only boundary discretization, the proposed method significantly reduces discrete elements compared to finite element method at equivalent accuracy levels, further improving computational efficiency and resource utilization.

Keywords: Nearly singular integral, isogeometric boundary element method, thermal stress analysis, semi-analytical computation

Mechanics of Multiphase Media Under Hypergravity

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Abstract

Rayleigh–Taylor instability (RTI) is a gravity-driven phenomenon classically observed in fluids, but recent studies have demonstrated its emergence in soft solids. Li and Lv revealed the gradual surface evolution of soft materials under varied gravity intensities, while Liang and Cai showed that gravity can induce creasing and folding instabilities in compliant substrates. Building on these insights, we introduce hypergravity as a novel route to regulate the structural and surface instabilities of tunable soft materials. Through combined centrifuge experiments and simulations, we identify the critical parameters governing RTI onset in hydrogels and soft composites. Specifically, we find that the threshold acceleration for instability decreases with increasing thickness, whereas external shape has minimal influence. By contrast, enlarging the contact area raises the required acceleration for RTI, underscoring the interplay between geometry and gravitational effects.

The relevance of such phenomena extends beyond soft matter physics to aerospace and aviation applications, where living tissues and engineered biomaterials may undergo severe deformation or instability under hypergravity conditions. To address these challenges, we further establish theoretical and numerical frameworks for large deformations and multiphase flows subjected to extreme gravity. Moreover, we explore the use of fiber- and particle-reinforced soft composites, where microscale parameters such as dimension, orientation, and interfacial tension are tailored to enhance stability. This integrated approach provides new physical insights into the mechanics of multiphase media under hypergravity and offers guiding principles for the design of advanced biomaterials relevant to astronaut health and aerospace technologies.

Long-term Adhesion Durability Revealed through a Rheological Paradigm

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ABSTRACT

The question of how long an object can adhere to a surface has intrigued scientists for centuries. Traditional studies focus on rapid crack-propagation detachment and account only for short-term adhesion governed by interfacial-viscoelastic dissipation, failing to explain long-term phenomena like sudden detachment after prolonged adherence and to predict corresponding adhesion lifetimes. Here, we investigate the long-term adhesion through a rheological paradigm using both theory and experiment. By considering both the bulk rheology and interfacial viscoelasticity mechanisms, we show that long-term adhesion durability is governed by the competition between them. This understanding leads to accurate lifetime predictions, which we validate through experiments. Additionally, our study reveals a previously undocumented, counterintuitive phenomenon unique to long-term adhesion: the expansion of the contact area under tensile forces, in contrast to short-term adhesion in which the contact area always shrinks during detachment. This research fills a critical gap in adhesion physics.

Keywords: Adhesion durability; viscoelasticity; long-term adhesion; debonding

Multi-physics coupled solid-liquid phase transition under hypergravity

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Abstract

Hypergravity—gravity levels greater than Earth’s gravity—can significantly impact the solid-liquid phase transition by enhancing heat/mass transfer, inducing component separation, and altering solid deformation. Leveraging these effects, hypergravity techniques are widely employed laboratory experiments and industrial processes, including space-time scaling studies, high-performance material manufacturing and substance extraction processes. While previous studies have demonstrated that gravity level and direction notably affect solid-phase morphology, the quantitative relationship between solidification characteristics and hypergravity magnitude, as well as the underlying mechanisms of these hypergravity effects, have not yet been fully revealed.

This study systematically investigates the hypergravity effects on the dendritic growth. A quantitative phase field model is adopted to describe the solidification process. Based on a hybrid lattice Boltzmann method, the solidification characteristics, including the solidification rate and dendritic morphology, are quantitatively analyzed. Our results demonstrate that, as gravity increases, the solidification rate first decreases and then increases. This nonlinear behavior arises from the competition between a suppression effect on dendritic growth in the downstream region and a promotion effect in the upstream region. In contrast, the specific surface area (SSA, surface area per unit volume) increases monotonically with gravity. A linear relation between the logarithmic function of gravity and SSA is established. The interaction between neighboring seeds restricts dendritic growth and induces vortex formation between them. Furthermore, the effect of seed number with depth, a distinct phenomenon under hypergravity, is examined by simulating a multiple-seed solidification process, where the seed number increases with depth. Flow channels gradually form between dendritic arms, beginning at the lower boundary and spreading throughout the domain as solidification progresses. Within these channels, the fluid flow redistributes concentration and enhances solidification. As a result, dendritic growth at the bottom is initially faster but gradually surpassed by the upper regions, which have more space for dendritic growth. This work provides theoretical insights for the application of hypergravity in material manufacturing, supporting the design of materials under hypergravity conditions.

Keywords: Hypergravity, Phase transition, Lattice Boltzmann method

Comprehensive performance Assessment of Isolation Piles on Existing Tunnel-deep Foundation Pit System under Construction Disturbance based on Projection Pursuit Model

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Abstract

With the saturation of above-ground spatial resources, megacities are increasingly shifting their development focus to underground space. However, new underground construction inevitably disturbs adjacent structures. To ensure underground engineering safety, isolation piles are often employed in practice to mitigate such disturbances. It is therefore necessary to conduct a full-lifecycle evaluation of construction disturbances and the performance enhancement effects of isolation piles, so as to reveal the overall response of the existing tunnel-deep foundation pit system. This study proposes a comprehensive evaluation method for assessing the construction performance and improvement effects of existing tunnel-deep foundation pit system. Refined spatiotemporal coupled numerical simulations under scenarios with and without isolation piles are conducted using Plaxis 2D. A system performance evaluation indicator framework for the existing tunnel-deep foundation pit system is established according to the relevant codes. Furthermore, projection pursuit model is introduced to construct a multi-indicator weighting framework, and adaptive genetic algorithm with elitist strategy is employed for optimization, yielding weighted comprehensive performance evolution curves. The results indicate that the installation of isolation piles significantly enhances the overall performance of existing tunnel-deep excavation systems throughout the full lifecycle of construction disturbances. The proposed method innovatively integrates AI-driven optimization with exploratory data analysis and performance evaluation, provides a data-driven decision-making tool for construction safety optimization.

Keywords: Comprehensive performance, projection pursuit model, existing tunnel-deep foundation pit system, isolation piles, numerical simulation

Influence of Back Pressure on the Flow Characteristics of Hydrogen Supersonic Two-Phase Expander

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ABSTRACT

Efficient, low-cost hydrogen liquefaction is key for its large-scale use. Addressing stability issues with high-speed turbines in current systems, this work innovatively employs a liquid-hydrogen-temperature supersonic two-phase expander. This device integrates expansion refrigeration, condensation, phase separation, and pressure recovery within a compact space, offering advantage like direct liquefaction. This paper focuses on the impact of back pressure on the flow characteristics within the hydrogen supersonic two-phase expander, holding significant value for advancing clean energy goals.

Multiscale Constitutive Modeling of Cohesive Granular Materials

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Abstract

Cohesive granular materials play an important role in both natural and engineered structures, as they are able to resist against traction forces. However, modeling the mechanical behavior of such materials is still challenging, and most of the constitutive models are based on phenomenological approaches that unavoidably disregard the microstructural mechanisms taking place on the bonded grains scale. This paper presents a multiscale approach applicable to any kind of granular materials, including solid bonds between particles. Inspired from the *H*-model, this approach allows simulating the behavior of cemented materials along various loading paths, by describing the elementary mechanisms taking place between bonded grains. In particular, it can be investigated how the local bond failure process can affect the macroscopic response of the whole specimen, according to the bond strength characteristics.

Key words: Cohesive granular materials, bonded contact model, H-model, meso- structure, multiscale approach, homogenization

A novel temporal finite element method to solve static viscoelastic problems

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Abstract

A novel temporal finite element (TFE) method is presented to solve static viscoelastic problems, which is more flexible and appropriate to describe temporal variation of displacement than conventional finite difference or numerical integral methods. By using principle of virtual work, a finite element based governing equation is derived in terms of displacement and its derivatives. Two TFE models are developed using Gurtin variational principle and weighted residual technique. A kind of hybrid shape functions with polynomial basis and trigonometric basis is stressed to give more flexible description of time varying variables. A criterion of stability analysis is derived, which can numerically be conducted when the constitution of shape functions and step size are prescribed. A recursive algorithm is developed by which the displacement solution at a specific time can be obtained only via a matrix power product with the initial condition.

The proposed approach is available for the viscoelastic model described by linear differential equations with order $N \leq 2$, and can conveniently be combined with well-developed numerical algorithms for the boundary value problem, such as FEM, SBFEM etc.

Various numerical examples, including those with static/harmonic loads, creep, stress singularity and heterogeneous structures, etc. are provided to illustrate the efficiency of the proposed approaches, and impacts of the TFE model, constitution of shape functions, and step size, etc. are taken into account. Satisfactory results are achieved in comparison with analytical or ABAQUS solutions.

Keywords: Viscoelasticity, Temporal finite element, Variational principle, Hybrid shape functions, Stability analysis

Multi-Objective Optimization Method for Metro Wheel Reprofilng

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Abstract

To enhance the economic efficiency of wheel reprofiling and extend the service life of wheelsets, a multi-objective optimized wheel reprofiling strategy is proposed that integrates a solution method for circumferential wear in this paper. Compared to traditional fixed reprofiling strategies, the multi-objective optimized scheme significantly reduces wheel diameter reprofiling losses while prolonging the wheel life. Data indicates that wheel diameter reprofiling losses are decreased by approximately 54%, and the service life of wheels is extended by over 15%. The research and application verification presented in this paper are closely related to metro wheel overhauls, providing valuable optimization recommendations for existing overhaul strategies.

Keywords: wheel reprofiling; wear; multi-objective optimization; metro wheels

A Fusion Topology Optimization Strategy of CutFEM and MMC for Improving Computational Efficiency and Geometric Accuracy

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Abstract

Topology optimization has emerged as a crucial approach in engineering design, as it enables effective material allocation to optimize structural performance. However, existing methods still face challenges such as strong mesh dependence, time-consuming mesh reconstruction, and ambiguous boundary treatments—limitations that restrict their applicability in complex scenarios.

In this work, we propose an innovative method that integrates the Cut Finite Element Method (CutFEM) and the Moving Morphable Component (MMC) method, enhanced by Nitsche's method, to address these aforementioned challenges effectively. Our approach improves computational efficiency by eliminating the need for repeated regeneration of the background grid, while also significantly enhancing geometric accuracy through high-precision interface processing. To validate the effectiveness of the proposed method, we conducted numerical experiments on a series of benchmark problems, including cantilever beams, fluidic pressure-loaded structures, and multi-material topology optimization. Additionally, we extended this method to three-dimensional (3D) applications. The results demonstrate that our method outperforms traditional topology optimization techniques in both computational efficiency and accuracy.

Overall, this study provides a robust and efficient strategy for tackling complex structural design challenges, particularly in addressing boundary-related issues. Notably, a key advantage of our approach—independent of boundary problem considerations—is that it can generate optimized configurations of comparable quality with only half the number of meshes required by traditional methods.

Keywords: CutFEM, MMC, topology optimization, multi-material, Nitsche's method, dynamic boundary

A computational homogenization method for thin composite beams/shells

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Abstract

This paper proposes a novel computational homogenization framework for the analysis of large rotations and finite strains in thin composite beams/shells. The macroscopic beam/shell is modeled as a continuum beam/shell described by the Kirchhoff shell kinematics (or Euler beam kinematics) within the updated Lagrangian formulation. At the microscale, through-thickness representative volume elements (RVEs) are considered and embedded at each integration point of the macroscopic beam/shell via a local co-rotational Cartesian coordinate system, thereby effectively decoupling the microscopic problem from the influence of macroscopic rotations. The RVEs are subjected to in-plane boundary conditions and zero out-of-plane tractions, representing the free top and bottom surfaces. Several numerical examples (e.g., large rotation, finite strain and buckling of thin composite beams and plates) are performed with comparison to the referenced direct numerical simulation. The results demonstrate that the proposed homogenized beam/shell models can accurately and efficiently predict both the macroscopic large deformations and the microscopic stress distributions.

Keywords: Computational homogenization, composite beams/shells, large deformation

On some novel analytic methods in mechanics of plates and shells and their applications

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Abstract

Although various numerical methods can undoubtedly provide engineering-oriented acceptable solutions for buckling, vibration, and bending of plates and shells, analytic methods as well as analytic solutions still deserve exploration, which can accurately reflect the correlation between key parameters toward rapid parametric analysis and optimization, and can serve as the benchmarks for testing various numerical methods. However, most available analytic studies found for plates and shells are semi-inverse or based on the semi-inverse methods, in which the pre-determination of solution forms is necessary. This shortcoming limits the scope of application of the semi-inverse methods. Accordingly, rational analytic solution methods, without the pre-determination of solution forms, are extremely useful. For the past decade, we have been dedicated to the study on novel analytic solution methods in mechanics of plates and shells, including the symplectic superposition method, the finite integral transform method, the quasilinearization-precise integral method, etc. This talk summarizes the recent progress on these novel methods and associated new analytic solutions, and introduces the applications of the relevant results in the analysis and design of some important engineering structures, such as the panels of an aircraft and the underwater pressure shells of a submarine.

Keywords: plate, shell, buckling, vibration, bending, analytic method.

Suppressing Grayscale for Multiphysics Topology Optimization of Multiphase Smart Materials and Structures via a dual projection

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Abstract

Topology optimization (TO) of smart materials and structures (SMSs) enhances mechanical-to-physical energy conversion efficiency. However, special grayscale issues induced by multi-material TO with nonmonotonic objective functions distort optimized configurations, constrain the design domain and compromise manufacturability. This study elucidates how nonmonotonic objective functions cause this grayscale issue and the design domain constraint in multi-material TO of SMSs and develops an effective grayscale suppression strategy into a SIMP-based TO framework through a sequential projection of elastic/piezoelectric densities, demonstrated via a piezoelectric energy harvester (PHE) for electrical energy conversion efficiency (EECE) optimization. Heaviside projection as the first projection converts elastic density to physical density, followed by piezoelectric density projection as a penalty function of elastic physical density for the second projection. Numerical examples demonstrate that this dual-projection approach can effectively eliminate grayscale issues, lead to a larger design domain with strategic piezoelectric material distribution near loading zones and prevent grayscale-induced EECE overestimation. Compared with multi-material TO using ordered SIMP reported in literature, our method achieves superior constraints over material volume fractions.

Keywords: Smart Materials and Structures; Multi-material; Topology Optimization; Grayscale Issue; Projection Function

Nonlinear analysis of steel frames with semi-rigid joints under thermal loading

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Abstract

The analysis of building frames under elevated temperatures, such as fire conditions, is an important task in structural engineering, particular for predicting the failure conditions. This type of analysis is complicated because the material properties cannot be considered constant. In particular, steel loses both rigidity and strength at high temperatures, and any analysis under these conditions must take these effects into account. In addition, joints in building frames are usually modelled as pinned or rigid. However, no joint is either perfectly pinned or rigid, and a semi-rigid joint model is generally more appropriate, as it can deal with real joints using an empirical model that is calibrated for a particular joint design.

Linear analysis is generally inadequate for predicting failure conditions at high temperatures, and nonlinear analysis is essential to correctly model the behaviour of the structure. Various nonlinear models are used in practice and these models usually involve some form of approximation of the nonlinear effects. Hence, it is important to study the effects of the approximations on the analysis since significant differences in results are possible using different approximations.

Therefore, this paper details a general approach for the nonlinear analysis of two-dimensional steel frames with semi-rigid joint under thermal loading. We start with a fully nonlinear model for the member behaviour and then systematically consider the effects of simplifying approximations on the results of the analysis. The nonlinear and simplified models are combined with the changes in the material properties to calculate the failure condition of the structure.

Several examples are given in the paper that demonstrate the various effects of the simplifying approximations on the results, and recommendations are provided to accurately deal with this class of problems.

Analytical and Numerical Studies on Mode Selection in Proper Generalized Decomposition Methods

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Abstract

Proper Generalized Decomposition (PGD) represents an important class of reduced order modeling approach for solving partial differential equations (PDEs) in terms of residual minimization among a selected number of modes, each in a variable-separated form. We explore mode selection within the PGD framework, contrasting it with the Singular Value Decomposition (SVD). They yield optimal rank-one series of the solution for residual minimization and error reduction respectively. Taking the elliptic equation in two-space dimensions with a two-mode source term under certain constraint as an example, we analytically study the residual minimization and prove that the mode ordering in the optimal PGD rank-one series differs from that in SVD. For more general source terms, the elliptic equation and heat equation, numerical simulations verify and extend the theoretical results. In this way we reveal that the PGD algorithm does not provide optimal numerical convergence in general. We further discuss the preconditioning of PGD, which rectifies the residual functional and better aligns with SVD.

Time-frequency signal analysis based on the gauge theory

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Abstract

Classical spectral theory presumes strict stationarity, interpreting a signal as a superposition of sinusoids with constant amplitude and phase. For non-stationary signals, such as seismic wavelets, radar backscatter, musical transients, this premise collapses, and one seeks instead the Instantaneous Frequency (IF) [1] denoted by $f(t)$, which is usually calculated as the time derivative of phase $\phi(t)$. However, IF remains conceptually controversial [2, 3] because any estimate at time t necessarily integrates data over an interval $[t - \Delta t, t + \Delta t]$, i.e., local characterization is extracted from non-local information.

State-of-the-art Time-Frequency Analysis (TFA) predominantly relies on windowed Fourier transforms rooted in Gabor's Gaussian kernel [4] and subsequently refined via wavelets [5] and other adaptive windows [6]. These methods introduce locality through the window function, yet the underlying Fourier transform is inherently global. Consequently, all window-based techniques are constrained by the Heisenberg-Gabor uncertainty principle, whose lower bound fixes $\Delta t \cdot \Delta f \geq 1 / (4\pi)$.

Besides windowed Fourier transforms, TFA can be reframed as an inverse problem, which identifies the parameters of a generative signal model from measured data [7]. In the standard signal model $s(t) = A(t) \cdot \cos(\phi(t))$, amplitude $A(t)$ and phase $\phi(t)$ are treated as independent variables, rendering the inversion severely ill-posed.

Actually, non-stationarity originates in local, time-varying system interactions, which can be understood in the framework of gauge theory [8]. Such interactions manifest as a damping effect that modifies the instantaneous dispersion relation. Embedding this physics into the signal model yields a damped oscillator equation whose phase $\phi(t)$ is explicitly coupled with the amplitude $A(t)$ through the damping coefficient $\zeta(t)$. Thus, one can obtain the signal model $s(t) = A(\zeta(t)) \cdot \cos(\phi(\zeta(t)))$, which results in a more stable and accurate inverse problem. Numerical examples demonstrate that the effective uncertainty product $\Delta t \cdot \Delta f$ can be driven significantly below the classical $1 / (4\pi)$ limit, corroborating the theoretical framework.

Keywords: Time-frequency analysis, gauge theory, inverse analysis, nonstationary signal

Efficient numerical simulation and design method for bidirectional steel-concrete composite floors

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Abstract

With the increasing diversification of building functions and the growing demand for multi-story, large spaces, the application of long-span structures in engineering is becoming increasingly widespread. Steel-concrete composite structures have been widely used in long-span buildings due to their advantages such as reduced sectional height, high stiffness, efficient space utilization, strong spanning capacity, and convenience in construction. Among these, bidirectional steel-concrete composite floor slabs have seen expanding application in long-span structures owing to their excellent integrity, stiffness, and load-bearing capacity. However, their spatial mechanical behavior is complex, and achieving efficient yet accurate numerical simulation and design methods remains a research challenge. Current calculation methods for bidirectional composite floors exhibit significant gaps, and the lack of reliable computational basis in practical engineering considerably restricts their broader application.

This paper aims to develop an efficient numerical simulation techniques and practical design methods for bidirectional steel-concrete composite floors. First, a beam-shell hybrid finite element model suitable for the compression-bending analysis of composite floors was systematically developed. The selection of fiber beam elements and layered shell elements, as well as the material constitutive model, was detailed. Numerical fitting of a series of classical experiments (clamped concrete beams, simply supported composite beams, and simply supported two-way composite slabs) verified the accuracy of the proposed finite element model in simulating the entire structural process from elasticity to elastoplasticity and ultimately to failure. Furthermore, for the commonly used 3×3 and 4×4 grid arrangements in engineering, the spatial force transmission mechanism and bearing capacity performance of symmetric and asymmetric bidirectional composite floors under vertically uniformly distributed loads were systematically analyzed. A simplified calculation formula centered on the bearing capacity amplification factor was proposed. Parametric analysis showed that the stiffness and bearing capacity advantages of bidirectional composite floors decrease with increasing aspect ratio. Finally, based on a comprehensive consideration of mechanical properties and economic efficiency, this paper proposes a practical design process and recommendations for symmetric and asymmetric two-way composite floors, providing a theoretical basis and technical support for engineering design.

Keywords: Two-way steel-concrete composite floor; finite element analysis; beam-shell hybrid model; parameter analysis; design method

SPH simulation of the rock cutting process by a conical pick

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Abstract

Rock fragmentation mechanisms during linear cutting are governed by complex interactions between tool parameters, material properties, and stress environments. To address the insufficient understanding of confining stress effects, this study develops a novel SPH (Smoothed Particle Hydrodynamics) model to simulate the dynamic rock-cutting process with conical picks. The SPH framework explicitly incorporates elastoplastic constitutive laws with damage failure criteria, enabling natural modeling of large deformation and fracture propagation under multi-axial stress states. Results reveal that confining stress significantly modifies stress field symmetry and fracture initiation thresholds. High confining pressure promotes shear-dominated failure with 23% denser microcrack networks near the tool tip compared to tensile-dominated fractures under low confinement. Notably, the SPH simulations capture the transition from brittle spalling to ductile flow regimes, evidenced by 40% reduction in particle ejection velocity and 18% increase in subsurface plastic zone depth under elevated stresses. The proposed SPH approach provides new insights for optimizing pick geometry and cutting parameters in deep mining scenarios, particularly highlighting the advantage of controlled confining stress to direct fracture paths and reduce tool wear. This work establishes a computational paradigm bridging continuum damage mechanics and discrete fragmentation processes in stressed rock cutting systems.

Keywords: SPH; Confining stress; Rock breakage; Conical pick; Linear cutting

Numerical Modeling of Bacterial Multi-physical Processes with SPH, LBM and Finite Element Methods

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Abstract

Bacterial microorganisms play a crucial role in human production and daily life. Quantitatively predicting the mechanical behavior of microbial biochemical reactions is essential for developing new biotechnologies. During the microbial life cycle, the growth and detachment of bio-porous materials are key physical processes governing microbial systems. Constructing mathematical and mechanical models to describe these processes is critical for advancing biotechnological developments, particularly in promoting microbial-induced calcium carbonate precipitation (MICP). MICP is an innovative, environmentally friendly self-healing geotechnical technique, representing the forefront of "green" engineering solutions.

Modeling the microbial life cycle requires accounting for reactive mass transport and fluid-structure interactions. The challenge lies not only in developing validated mathematical models for these complex processes but also in numerically solving the resulting coupled models, which demands high-precision computational methods. In this study, we present several recently developed bacterial models and their corresponding numerical simulation approaches. The focus is on advanced numerical methods, including the space-time finite element method (STFE), smoothed particle hydrodynamics (SPH), and the lattice Boltzmann method (LBM). Additionally, we demonstrate an engineering application case of pore-scale modeling for MICP technology.

Keywords: Bacterial microorganisms; Microbial-induced calcium carbonate precipitation (MICP); Smoothed particle hydrodynamics (SPH); Lattice Boltzmann method (LBM); Finite element method (FEM)

Threshold of sediment particle in turbulent flow

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Abstract

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. 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-resolved 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-resolved particle, Four-way couple, Entrainment threshold

Numerical analysis of lunar 3D printed concrete construction based on discrete particulate liquid bridge theory

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Abstract

This study addresses the challenges of 3D printed concrete construction in the complex lunar environment by developing a numerical analysis method grounded in discrete particulate liquid bridge theory. The research investigates the influence of multi-scale and multi-physics lunar conditions on the microstructural properties of cementitious materials, while elucidating the interactions between lunar in-situ regolith and cement mortar. Through systematic analysis, the hydration evolution of concrete materials incorporating lunar soil is quantitatively characterized.

Key findings contribute to advancing the fundamental understanding of 3D printed concrete construction mechanisms in extraterrestrial environments, as well as the material science theory of lunar soil-enhanced concrete. The results provide critical theoretical support for achieving sustainable lunar base construction, offering valuable insights for future extraterrestrial infrastructure development.

This work establishes a novel framework for analyzing lunar construction materials under extreme conditions, bridging the gap between terrestrial concrete technology and extraterrestrial engineering applications. The proposed methodology demonstrates significant potential for optimizing material formulations and construction processes for off-world habitats.

Keywords: Numerical analysis, lunar 3D printed concrete construction, discrete particulate liquid bridge theory

An efficient collocation-type meshfree method for nonlinear problems

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Abstract

Nonlinearity is common in engineering applications. Accurately simulating nonlinear behavior is crucial for evaluating the performance of critical components and optimizing manufacturing and durability design. It also helps reduce testing cycles, costs, and variability. The rapid development of computer technology and high-performance processors has greatly supported efficient numerical simulation methods. These methods have become a core tool in engineering research. However, structures often display geometric nonlinearity behavior under large loads. Changing configuration states make simulating nonlinear mechanical responses even more complex.

Traditional mesh-based methods require high-quality meshes. Large deformations may cause mesh distortion, which can affect simulation accuracy. In contrast, meshfree methods do not rely on discrete grids, making them more suitable for highly nonlinear problems. Meshfree methods are generally classified into Galerkin-type and collocation-type approaches. Galerkin-based methods offer high accuracy but are computationally complex and less efficient. Collocation-based methods are simpler and require no integration. Collocation-type methods are more efficient, though they may suffer from accuracy and stability issues in complex nonlinear problems when only one collocation point is used to represent the local property. This research aims to develop a stable and efficient collocation-type meshfree algorithm to solve mechanical problems involving geometric nonlinearity, and to validate its effectiveness through numerical simulations.

Keywords: nonlinear, large deformation, collocation method, stability, accuracy, efficiency

Adaptive Phase-field Material Point Framework for Large-Deformation Fracture Modelling and Structural Optimization

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Abstract

Accurate analysis of structural fracture behavior and efficient topology optimization are critical to the reliability and performance of engineering systems. Yet strong nonlinearities—such as large deformations, evolving cracks, and contact—pose major challenges for numerical simulation and limit the applicability of conventional methods. To overcome these limitations, we develop an adaptive phase-field total Lagrangian material point method (TLMPM) that efficiently simulates thermo-mechanical fracture, large-deformation fracture, and contact-induced failure within a unified framework. For nearly incompressible soft materials, volumetric locking is alleviated through a multi-physics variational formulation coupled with a hybrid F-bar technique. In addition, a volumetric decomposition technique resolves the inconsistency between incompressibility constraints and the diffusive crack representation in phase-field models. Building on this foundation, we further introduce a dynamic topology optimization formulation under large deformation within the TLMPM framework. The objective minimizes compliance to enhance impact resistance, sensitivities are computed via an adjoint method, and evolving boundaries are captured with high fidelity using adaptive mesh refinement. The proposed framework delivers an efficient and robust toolset for multi-mode fracture simulation and large-deformation topology optimization, advancing structural design under extreme loading and failure scenarios.

Keywords: Total Lagrangian material point method, soft material, adaptive mesh refinement, dynamic fracture, topology optimization

Study on the SPH method for macro-meso mechanical behavior of porous media by considering Fluid-Solid Interaction

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Abstract

Porous media typically exhibit geometrically nonlinear characteristics, with interactions between multiphase media occurring inside pores and at interfaces. These structural features and the discontinuous nature of the media result in significant differences between macroscopic mechanical behavior and that of continuous media. A fundamental challenge remains in understanding the multi-scale mechanical response mechanisms of porous media—particularly the relationship between pore-scale fluid – solid interactions and macroscopic seepage behavior—which requires further in-depth investigation. To address this, the present study employs the Smoothed Particle Hydrodynamics (SPH) method to simulate fluid flow within pores at the mesoscopic scale. By analyzing variations in pressure and velocity distributions throughout the flow field, a macroscopic seepage model grounded in mesoscopic characteristics is developed. In addition, a classical Darcy’ s law-based seepage model is used to simulate the flow through porous media with isotropic and anisotropic permeability coefficients at the macroscopic level, thereby providing validation for the proposed model. The simulation results indicate that fluid – solid interactions in porous media manifest as viscous shear effects between the pore fluid and the solid phase at the mesoscopic scale. The intensity of this interaction depends on fluid viscosity and solid surface area. At the macroscopic scale, these effects are reflected in the anisotropy of the permeability coefficient. These findings are consistent with established seepage theory and confirm that the developed numerical model exhibits both high accuracy and stability.

Keywords: porous media, SPH, fluid-solid interaction, seepage

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An enhanced numerical wave tank based on DualSPHysics+

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Abstract

Wave–structure interaction (WSI) remains a fundamental challenge in ocean and coastal engineering. In this study, an enhanced numerical wave tank is established on the basis of the improved open-source SPH solver DualSPHysics+. For the fluid, the δ -SPH density diffusion term is combined with a Riemann dissipation term (δ R-SPH) to mitigate spurious energy dissipation. To suppress spurious pressure oscillations, the Velocity-divergence Error Mitigation (VEM) and Hyperbolic/Parabolic Divergence Clearing (HPDC) are incorporated. Long-distance propagation accuracy is further improved by a Volume Conservation Shifting (VCS), while particle distribution near the free surface is regularized through an Optimized Particle Shifting (OPS). For structural response, the framework employs a second-order momentum discretization together with a dynamic hourglass stabilization scheme to prevent zero-energy deformation. A series of two- and three-dimensional benchmarks are carried out to assess the model. The results demonstrate that, compared with the standard DualSPHysics formulation, the δ R-SPH approach markedly reduces artificial energy dissipation and wave attenuation. Moreover, the combined use of VEM and HPDC effectively minimizes pressure noise without introducing excessive damping, and the VCS scheme ensures improved volume conservation. Overall, the enhanced numerical wave tank is capable of reliably reproducing wave generation, long-distance propagation, and complex interactions with floating or flexible structures.

Key words: DualSPHysics+; Numerical wave tank; Smoothed Particle Hydrodynamics

A GPU-accelerated SPH framework for patient-specific simulations of vascular fluid-structure interactions

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ABSTRACT

Patient-specific simulations of fluid-structure interaction (FSI) problems in vascular systems are crucial for both fundamental research and clinical applications. However, these simulations present significant challenges due to large structural deformations, morphing flow domains, and complex FSI interfaces. In this study, we develop a smoothed particle hydrodynamics (SPH) framework that is well-adapted to vascular FSI simulations. The matrix-free iterative incompressible SPH (ISPH) method is employed to simulate blood flow dynamics, while the stabilized total Lagrangian SPH (TLSPH) method is used to capture the dynamics of blood vessels. We then introduce a novel FSI coupling strategy that integrates ISPH with TLSPH, ensuring strict interface matching conditions between the blood and vessel wall. Additionally, lumped parameter (0D) models are incorporated into the 3D SPH framework, allowing for accurate simulation of the physiological effects in downstream vascular beds. To enhance computational efficiency, we implement graphics processing unit (GPU) parallelization techniques. Leveraging the particle-based nature of SPH and the matrix-free property of our framework, the parallelized computations can be performed efficiently, ensuring optimal utilization of GPU resources. The developed framework is first validated through several benchmark tests of pulsatile flows in straight vessels. Subsequently, we apply the framework to simulate the FSI processes in patient-specific blood vessels, including the cerebral aneurysm and the aorta. The simulation results show that our framework is both effective and efficient, providing a promising tool for patient-specific vascular simulations.

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Lagrangian-Eulerian Stabilized Collocation Method and Its Applications in Fluid-Structure Interaction Problems

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Abstract

This presentation introduces the Lagrangian–Eulerian Stabilized Collocation Method (LESCM), a hybrid computational framework combining Lagrangian particle tracking with Eulerian collocation on fixed nodes. LESCM can be used in fluid dynamics, including fluid-structure interaction (FSI), water wave dynamics, and Lagrangian coherent structure analysis of fluid. The method circumvents computationally intensive neighboring-particle searches while maintaining numerical consistency via high order reproducing kernel (RK) approximations. For FSI problems, the method efficiently simulates free surface flows interacting with rigid bodies while preserving mass and momentum conservation. In ocean engineering, LESCM is implemented in a novel numerical wave tank (NWT) to simulate wave generation, propagation, and absorption, providing a reliable tool for offshore wave-structure interaction studies. Beyond flow simulation, LESCM’s Eulerian framework enables precise LCS extraction via finite-time Lyapunov exponents calculated directly on fixed nodes, avoiding errors from particle shifting techniques and accurately resolving critical flow features like vortices. Validated across diverse benchmarks, LESCM demonstrates exceptional efficiency, as it can handle 16 million particles in MATLAB without parallelization, and bridges high-fidelity simulations with real-world engineering demands. By unifying accuracy, efficiency, and adaptability, LESCM emerges as a powerful tool for advancing fluid dynamics simulation and industrial applications

Keywords: Particle method, Lagrangian–Eulerian Stabilized Collocation Method, fluid-structure interaction, fluid dynamics, Lagrangian coherent structures.

S-PINN: Stabilized Physics-Informed Neural Networks for alleviating barriers between multi-level co-optimization

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Abstract

Physics-informed neural networks (PINNs) have shown significant potential in integrating physical laws with data-driven models for complex dynamical systems. However, conventional PINNs suffer from stability issues and lack conservation properties due to conflicts between data and physics constraints. To alleviate these limitations, we propose a stabilized physics-informed neural network (S-PINN) framework that incorporates local subdomain integration and minimizes the cumulative residuals of conserved quantities, significantly enhancing stability and conservation. The proposed S-PINN is evaluated on a range of benchmarks, including the Burgers equation, Poisson equation, three-dimensional heat conduction, and two- and three-dimensional lid-driven cavity flows. The results demonstrate that S-PINN achieves superior accuracy, stability, and conservation compared to conventional PINNs. Furthermore, to address the optimization conflicts in inverse wave propagation problems where simultaneous wavefield prediction and parameter identification are required, we introduce a dual-network architecture and annealed physics weighting strategy within the S-PINN framework, which enhances convergence and stability in ill-posed inverse problems. The approach is validated on inverse wave propagation problems in one, two, and three dimensions, demonstrating accurate and robust performance under sparse and noisy measurement conditions. These results indicate that the proposed stabilized physics-informed neural network framework provides an efficient, reliable, and interpretable computational tool for solving forward and inverse problems governed by partial differential equations, advancing data-driven scientific computing in computational mechanics and engineering applications.

Keywords: Physics informed neural networks, multi-level co-optimization, enhanced conservation, neural networks, interpretability, incompressible flows.

Numerical study on debris flow-turbidity currents transformation process of submarine landslides

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Abstract

The transition from debris flow to turbidity currents represents a critical phenomenon in the evolution of submarine landslides. In this study, we present an innovative particle splitting technique implemented through a GPU-accelerated parallel computing framework within the Smoothed Particle Hydrodynamics (SPH) method, specifically designed to model this complex transition process. The distinctive feature of our model lies in its capability to perform large-scale parallel particle splitting through an advanced spatial expansion algorithm coupled with particle mapping and labeling mechanisms. To validate the proposed transition model, we conducted comprehensive numerical investigations focusing on the submerged slides problem. The simulation results demonstrate that our model not only achieves efficient parallel computation of particle splitting processes but also provides accurate simulation of the debris flow to turbidity currents transition dynamics. This methodological advancement offers significant potential for large-scale numerical simulations of debris flow-turbidity current conversions in submarine landslide scenarios.

Keywords: Smoothed Particle Hydrodynamics (SPH); Particle splitting technique; GPU parallelization; Debris flow; Turbidity currents

Rayleigh Bénard convection under the coupled effects of a side-heated wall and bottom charge injection

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Abstract

This work investigates the combined effects of a side-heated wall and bottom-wall charge injection on heat transfer and flow structure in Rayleigh–Bénard convection (RBC). The results show that a side-heated wall, in the absence of charge injection, enhances the heat transfer rate. When electric charge is injected from the bottom wall, the thermal boundary layer thickness decreases, leading to a further enhancement of heat transfer. However, systematic simulations over a wide range of Rayleigh numbers Ra and electric field strengths T reveal that the Coulomb force delays the onset of convection, with the transitional Rayleigh number Ra_T increasing as the Coulomb force strengthens. This transition is accurately predicted by a dimensionless parameter defined as the ratio of buoyancy to Coulomb forces. In addition, by analysing the flow structure using the Fourier mode decomposition, a phase diagram describing the dominant flow modes is proposed. The results further reveal that the Ra_T line is also capable of precisely characterising the transition of the flow structure when the electric field T strength exceeds the critical value. Our findings offer new insights into the complex interaction between buoyancy and Coulomb forces and their influence on heat transfer and the onset of convection in classical RBC, with potential implications for the design of heat exchangers aimed at actively and efficiently controlling heat transfer.

Keywords: Lattice Boltzmann method, heat transfer, charge injection

A Graph-Based Spatio-Temporal Operator Learning Method for Structural Dynamics

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Abstract

Accurate spatio-temporal prediction of structural fields is essential for time-resolved simulations in damage assessment (e.g., impact and heat transfer). Pronounced nonlinearities, however, hinder traditional solvers from balancing accuracy and efficiency, especially for impact. We propose Graph-DeepONet, a graph-structured deep operator network for field evolution on unstructured domains. Extending DeepONet with graph neural components, it handles irregular topologies and captures both local interactions and long-range propagation [1]. A structure-aware encoder-decoder couples a graph MLP encoder with a gated TCN + PointNetConv decoder for joint temporal-spatial modeling [2]. Fusion of graph and temporal convolutions enables fine-scale variation capture and global response pathways without requiring analytical solutions or explicit PDE forms. Trained end-to-end, Graph-DeepONet learns nonlinear operator mappings from input fields to node-level responses, exhibiting strong approximation capacity and structural transferability. Experiments across structural-dynamics tasks show effectiveness for irregular geometries, multi-scale loads, and time-varying boundaries, achieving stable training, high accuracy, and robustness. Owing to its modeling flexibility and expressive graph learning, Graph-DeepONet suits high-dimensional response prediction in large-scale applications such as structural health monitoring, dynamic simulation, and data-driven modeling.

Keywords: Data-driven modeling, Graph Neural Network, Deep operator networks, Spatiotemporal physical-field prediction

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A Lightweight Mesh-Free Network for Strain Field Prediction under Small Geometric Perturbations

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Abstract

Accurate prediction of local strain distributions under subtle geometric perturbations is vital for structural safety evaluation and design optimization. We present a lightweight mesh-free neural network that directly processes unstructured point clouds and predicts nodal strain responses without relying on parametric geometry descriptors or mesh connectivity. Node features are formed by combining raw coordinates, relative positional encodings, and frequency-based components to improve adaptation across different structural forms. A structure-aware feature fusion module aggregates local geometric context and maintains tractable compute and stable training on high-resolution point clouds, without graph construction or graph convolutions; the model further employs channel-wise squeeze-and-excitation (SE) and spatial attention (SAM) to refine responses in physically relevant regions. To enhance sensitivity to sparse yet critical high-strain areas, we use gamma-weighted fusion together with a top-k weighted loss to emphasize learning on peak-strain nodes. Experiments on perturbed steering-wheel components demonstrate reliable accuracy in both global prediction and hotspot localization, with robustness in tracking strain variations under relatively small geometric deformations. Overall, this model serves as an efficient, mesh-free surrogate for data-driven prediction of stress and strain fields on unstructured point clouds.

Keywords: Point clouds, Mesh-free learning, Strain field prediction, Attention mechanisms (SE/SAM), Structure-aware fusion

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Machine learning surrogate models of many-body dispersion interactions in soft polymer systems

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Abstract

Accurate prediction of many-body dispersion (MBD) interactions [1] is essential for understanding the van der Waals forces that govern the behavior of many complex soft materials [2]. However, the high computational cost of MBD calculations limits their direct application in large-scale simulations. To address this, we introduce a machine learning surrogate model specifically designed to predict MBD forces in polymer melts, a soft system that demands accurate MBD description and offers structural advantages for machine learning approaches. Our model is based on a trimmed SchNet architecture [3] that selectively retains the most relevant atomic connections and incorporates trainable radial basis functions for geometric encoding. We validate our surrogate model on datasets from polyethylene, polypropylene, and polyvinyl chloride melts, demonstrating high predictive accuracy and robust generalization across diverse polymer systems. In addition, the model captures key physical features, such as the characteristic decay behavior of MBD interactions, providing valuable insights for optimizing cutoff strategies. Characterized by high computational efficiency, our surrogate model enables practical incorporation of MBD effects into large-scale molecular simulations.

Keywords: Many-body dispersion, van der Waals interaction, machine learning force field, surrogate modeling, polymer melts, deep neural network

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A Generative Model Approach for Topological Design of Nonlinear Mechanical Metamaterials

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The topological design of advanced materials with extraordinary complex, nonlinear mechanical properties has exhibited promising applications in soft robotics, biomedical implants, and energy absorbers. Recent studies have demonstrated the potential of generative model (GM) to predict and tune the nonlinear deformation and stress response of periodic stochastic cellular structures under large strain conditions. However, their reliance on periodic boundary conditions restricts their applicability and reliability to real-world, non-periodic structures.

This study extends the generative modelling framework beyond periodic boundary conditions by introducing a latent diffusion model that optimize topological layouts of cellular structures with tailored nonlinear mechanical responses. By integrating advanced data-driven techniques with full-field mechanical analysis via nonlinear finite element (FE) analysis, our approach enables to capture complex deformation behaviours, including localized buckling and contact, in irregular unit-cell structures. FE simulations validate the accuracy of the predicted stress-strain responses, showing strong agreement with the GM predictions.

Our work significantly broadens the scope of inverse topological design for nonlinear mechanical metamaterials, offering a new strategy to efficiently optimize cellular metastructures without limitations imposed by periodic boundary conditions in a nonlinear context. The proposed method enhances design flexibility and accelerates the discovery of novel metamaterials with highly customized nonlinear mechanical performance for practical applications.

Key Words: *Metamaterial, Finite Element Analysis, VQ-VAE, VQ-Diffusion, Stress-Strain Response*

A refined higher-order finite strip formulation based on Carrera unified formulation for the free vibration analysis of axially moving laminated composite plates

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Abstract

Investigating axially moving laminated composite structures is of critical importance in engineering applications, such as high-speed aircraft, as high-speed axial motion can significantly alter their dynamic characteristics and may even induce divergence-type dynamic instability. However, accurate and efficient prediction of their dynamic behaviors remains challenging. This paper presents a refined higher-order finite strip method, developed within the Carrera Unified Formulation (CUF), for free vibration analysis of axially moving laminated composite plates, with the corresponding formulation rigorously derived and detailed. This approach enables a hierarchical methodology that allows for efficient refinement of the model by simply increasing the order of the expansion, rather than refining the mesh excessively. Owing to its quasi-3D nature and higher-order formulation, the proposed approach can accurately capture through-thickness deformation effects, making it a general and robust tool for analyzing structures without restriction on thickness. The governing equations are derived in a compact form using the principle of virtual work. Therefore, the stiffness, mass, and gyroscopic matrices are explicitly derived and formulated in terms of fundamental nuclei (FN), which are independent of the order of the expansions adopted. The accuracy of the proposed formulation is validated through comparison with results reported in the literature. Numerical examples are then conducted to examine the effects of strip number, model expansion order, and boundary conditions on the computational results. Furthermore, the interplay between ply angles, traveling speed, and in-plane tension on the natural frequencies and stability of the plates is thoroughly investigated. This work thus provides a robust analytical tool and valuable insights for the design and performance assessment of axially moving laminated composite structures, supporting their safe and reliable operation in engineering applications.

Keywords: Axially moving plate, laminated composite plate, finite strip method, refined plate theory

Deep-learning based prediction of chemo-mechanics and damage in battery active materials

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Abstract

Layer-structured cathode active materials of Li-ion batteries such as $\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$ (NMC) provide benefits including high specific capacity and energy density. However, NMC secondary particles consist of randomly oriented primary particles with internal anisotropic lattice chemical strain and weak intergranular bonding. This causes high interfacial stresses and particle disconnections during Li^+ insertion into and extraction from the active material. Therefore, material microstructure characteristics such as grain orientation and morphology play a critical role in determining cycling performance of the active material. However, resolving particle microstructures with different characteristics remains challenging due to high computational costs and limited statistical generalizability. This work uses ConvLSTM to predict the dynamic evolution of critical physical fields (Li^+ concentration, stresses and damage) within secondary particles with diverse microstructures. First, the microstructure of active particles are generated with a certain number of primary particles, whose sizes and orientations can strictly follow given statistical distributions with binning method, even with limited particle numbers. Second, images carrying essential characteristics of microstructure evolution are incorporated into the model. A hybrid loss combining Mean Squared Error (MSE) and Structural Similarity Index (SSIM) is employed, along with a scheduled sampling training strategy, to enhance prediction accuracy. The model's out-of-sample predictive performance has also been evaluated. Additionally, a microcrack density-based damage model is also used to assess microstructure damage evolution. The proposed approach demonstrates high prediction accuracy, offering valuable insights into microstructure behavior.

Keywords: Li-ion battery, Microstructure, ConvLSTM, Chemo-mechanical coupling, Damage evolution



Unusual stretching–twisting of liquid crystal elastomer bilayers

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ABSTRACT

Liquid crystal elastomers (LCEs), as a unique class of smart soft materials combining the properties of liquid crystals and hyperelasticity, are capable of rapid, anisotropic, and reversible deformations in response to mechanical, thermal or optical stimuli. Here, we report a hitherto unknown stretching-induced twisting behavior of LCE bilayer strips. Under uniaxial stretching, we reveal that due to the spontaneous mismatch strain arising from interlayer anisotropy, the bilayer strips exhibit notable twisting deformations. We develop an LCE bilayer strip model based on semi-soft elasticity to quantitatively understand and predict such intriguing tension-twisting response. Based on our experiments and theoretical analyses, we systematically explore how the liquid crystal director orientation, geometric dimensions and material parameters of the strips would affect the twisting behavior. We find that when the alignment of directors of bilayer are symmetric about the stretching direction, a larger deviation angle of the initial directors results in a more significant twisting deformation. Additionally, a longer, narrower and thicker strip has a more pronounced twisting effect. Furthermore, the material anisotropy encourages the twisting, while the feature of semi-soft elasticity discourages it. The findings not only reveal the tension-twisting coupling behavior of LCE bilayer strips, but also offer new insights into the design of LCE actuators, intelligent structures and soft robots.

A Gaussian Kernel Deep Operator Network for Efficient Full-Field Prediction of Dynamic Responses on Variable 3D Geometries

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Abstract

Accurate and efficient prediction of structural responses with dynamic loading and geometric variations is crucial for design automation and real-time decision-making. While finite element methods (FEM) offer high accuracy, their computational cost limits use in iterative workflows. Data-driven surrogates like the deep operator network (DeepONet) have emerged as promising alternatives. Geom-DeepONet extends DeepONet by encoding parameterized 3D geometries and predicting full-field solutions on an arbitrary number of nodes, supporting flexible solution prediction across varying mesh resolutions. However, it relies on linear feature fusion (e.g., element-wise multiplication), limiting its ability to capture strong nonlinearities. Moreover, it is primarily suited for static problems and performs poorly under dynamic loading. To address these limitations, we propose the Gaussian Kernel DeepONet (GK-DeepONet), which introduces a nonlinear feature fusion mechanism via a Gaussian kernel in a reproducing kernel Hilbert space (RKHS). By adaptively modeling similarity between geometric and spatial features using a learnable bandwidth, GK-DeepONet enhances expressive power and modeling accuracy. To efficiently handle time-dependent loads, we integrate the equivalent static load (ESL) method, transforming transient dynamics into a set of static sub-problems. Each sub-problem is solved independently with a time identifier, enabling parallel prediction without recurrent networks. Numerical experiments on structures with complex geometries and dynamic excitations show that GK-DeepONet outperforms DeepONet and Geom-DeepONet in accuracy and generalization. The method provides a scalable, efficient framework for surrogate modeling in nonlinear, time-varying engineering systems.

Keywords: Deep operator network (DeepONet), Gaussian kernel method, Equivalent Static Load Method (ESL), Data-driven modeling, Dynamic response prediction

Acknowledgments

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Optimization Design of Out-of-Plane Stability Bracing System for Double-Arch Structures Based on the Matrix Stiffness Method

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Abstract

This study addresses the out-of-plane stability of funicular twin arch systems and proposes an efficient approach for bracing design. An exact matrix stiffness method (MSM) was employed to obtain the out-of-plane buckling load, and a dataset incorporating sectional parameters and bracing positions was established. An artificial neural network (ANN) with attention mechanisms and residual connections was trained to predict the buckling capacity with high accuracy ($R^2 > 0.99$). SHAP analysis demonstrated that transverse flexural rigidity and bracing location are the most influential factors. A two-stage optimization framework combining global differential evolution and local SLSQP was further applied under a material volume constraint. Results show that the ANN-based optimization is stable and reliable. With five symmetric braces, the optimal configuration occurs near 0.166S and 0.318S along the arch span, with an optimal cross-sectional area ratio of $k=0.785$. This work provides an effective analysis and optimization strategy for enhancing the out-of-plane stability of twin arch structures.

Keywords: Funicular twin arch systems; Out-of-plane stability; Matrix structural analysis; Artificial neural network; Optimal bracing positions; Buckling capacity

Cut-Cell Cartesian Meshes for Incompressible Laminar and Turbulent Flows based on n-sided Cell-based Smoothed FEM

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Abstract

The cut-cell Cartesian mesh is widely favored in Computational Fluid Dynamics (CFD) due to its ease of generation, body fitting and high quality. However, the presence of hanging nodes and irregular body-fitted polygonal elements makes it challenging to construct shape functions in traditional Finite Element Methods (FEM). In this work, the n-sided Cell-based Smoothed Finite Element Method (nCS-FEM) is developed, introducing detailed construction techniques of smoothed domains in various cut-cell Cartesian meshes and solving incompressible laminar and turbulent flows. The Streamline-Upwind/Petrov–Galerkin stabilization, combined with the Stabilized Pressure Gradient Projection (SUPG/SPGP) method, is employed to mitigate convection and pressure oscillations in nCS-FEM when solving the Unsteady Reynolds–Averaged Navier–Stokes (URANS) equations. Several numerical examples—including analytical solutions for laminar flows and benchmark results from aerospace applications—are presented to validate the applicability and accuracy of the nCS-FEM in solving problems with cut-cell Cartesian meshes (nCS-FEM-Cart). The results demonstrate excellent performance in predicting flow characteristics. Compared to Q4 elements, cut-cell elements facilitate the generation of variable-density meshes, thereby enabling faster computations. Furthermore, a complex structure, i.e. multistage Tesla valves, is employed to evaluate the capability of the realizable k- ϵ model in simulating the flow separation and forced convection, highlighting its significant potential in complex engineering problems.

Keywords: N-sided CS-FEM; Cut-cell Cartesian meshes; Laminar/turbulent flow; Incompressible; URANS; Streamline-Upwind/Petrov-Galerkin stabilization (SUPG); Stabilized Pressure Gradient Projection (SPGP).

Development of the Coupled Smoothing Technique λ S-FEM for Mechanical Analysis of Twist Drills

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Abstract

A coupled smoothing technique, λ S-FEM, is introduced to improve the accuracy of numerical simulations in the mechanical analysis of twist drills. This method combines the edge-based smoothing finite element method (ES-FEM) with the node-based smoothing finite element method (NS-FEM). The λ S-FEM model is designed to evaluate the mechanical properties of twist drills made from tungsten carbide (WC), titanium nitride (TiN) coatings, and high-speed steel (M35), providing a theoretical basis for lifespan estimation and wear prediction. Linear tetrahedral elements construct the smoothing domain, and optimized weighting parameters balance and combine the smoothed strains from ES-FEM and NS-FEM. This integration enhances the accuracy of solutions for displacements, stresses, and strain energies, constructing stiffness matrices with optimal precision. The method's feasibility is demonstrated through numerical case studies involving flange and shell extractor components. Analyses of straight shank twist drills compare displacement and stress magnitudes across FEM, S-FEM, and λ S-FEM under various degrees of freedom (DOF). Results show λ S-FEM significantly reduces errors, particularly with coarse meshes, validating its practical application in solving engineering challenges.

Keywords: S-FEM, Scale factor, Gradient smoothing technique, Coupled, Twist drill, Solid mechanics

A Novel Implementation of Efficient Inertia Relief Analysis Using Smoothed Finite Element Method for Unconstrained Structures

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Abstract

Inertia relief analysis is crucial for simulating unconstrained structures subjected to external loads, such as aerospace and automotive systems, where traditional displacement boundary conditions are absent. This study presents an innovative framework that integrates the Smoothed Finite Element Method (S-FEM) with the Pardiso direct solver to address the computational challenges of inertia relief problems. The S-FEM enhances solution accuracy and mesh adaptability by smoothing strain fields at element boundaries, effectively mitigating issues of low stress accuracy in conventional FEM under complex loading scenarios. The Pardiso solver is employed to efficiently resolve the resulting indefinite linear systems, leveraging its capabilities in parallel sparse matrix handling and memory optimization to achieve scalability for large-scale models. Key contributions include the development of a stabilized formulation for inertia relief within the S-FEM framework, as well as a systematic comparison of computational performance with classical FEM approaches. Numerical experiments on 3D structural benchmarks demonstrate that this method improves stress accuracy and reduces solver time, being particularly suitable for large-scale models. The proposed methodology not only extends the applicability of S-FEM to free-floating systems but also provides a robust template for integrating advanced finite element techniques with high-performance solvers. Results underscore the framework's potential for industrial applications, meeting the needs for rapid analysis of mobile structures without artificial constraints.

Keywords: Inertia Relief Analysis; Smoothed Finite Element Method; Computational Solid Mechanics; Unconstrained Structural Systems; Gradient Smoothing Technique

Pressure checkerboarding suppression in the next-gen smoothed finite element method: EC-SSE-SRI-T4

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Abstract

The smoothed finite element method (S-FEM) [1], which has long been called the “next-gen finite element method”, has been already moved into the practical phase and is being implemented in commercial or general-purpose software [2, 3]. On the other hand, research on improvements to S-FEM itself has also progressed further in recent years. The edge center-based strain smoothing element using 4-node tetrahedral mesh (EC-SSE-T4) [4] is especially a revolutionary formulation in the field of solid mechanics. EC-SSE-T4 achieves a high-accuracy in strain/stress solutions even using T4 meshes, which have conventionally been known as a low-accuracy mesh. Besides, EC-SSE-SRI-T4, which combines EC-SSE-T4 with selective reduced integration (SRI), avoids not only shear locking but also volumetric locking; therefore, it is applicable to various types of nearly incompressible analyses (hyperelastic, thermo-viscoelastic, plastic, etc.).

However, EC-SSE-SRI-T4 has only one weakness, that is, pressure checkerboarding. In nearly incompressible analysis, many finite elements are known to have issues in volumetric strain and pressure accuracy, resulting in unnatural pressure distribution in a checkerboard pattern. EC-SSE-SRI-T4 also has this issue and exhibits pressure checkerboarding in nearly incompressible analyses. The accuracy of displacement, load, and deviatoric strain/stress is excellent with EC-SSE-SRI-T4, but only the accuracy of volumetric (hydrostatic) strain/stress is still insufficient.

One of the known methods for suppressing pressure checkerboarding is the multiple strain smoothing method. Our study on F-barES-FEM-T4(c) [5], a conventional S-FEM for large deformation nearly incompressible analyses, showed that multiple volumetric strain smoothing was effective to suppress pressure checkerboarding in T4 meshes. By increasing the number of volumetric strain smoothing iterations (c), pressure checkerboarding can be suppressed even when the Poisson’s ratio approaches 0.5, like 0.49, 0.499, 0.4999, $\dots$. However, since the computational cost increases in proportion to c^3 , a formulation with a large c (too many times strain smoothings) is not practical. Therefore, employing as few iterations as possible is essential for the assumed Poisson’s ratio, such as 0.49.

In this study, we propose a new method to suppress pressure checkerboarding in nearly incompressible large deformation analysis by introducing multiple volumetric strain smoothing to EC-SSE-SRI-T4. The new method is formulated to suppress pressure checkerboarding to a practically acceptable level for solids with a Poisson’s ratio up to 0.49. The number of volumetric strain smoothing is limited to two so that the computational cost remains the same as that of EC-SSE-T4. Some incompressible large deformation analyses confirm that the new formulation sufficiently suppresses the checkerboarding level.

Keywords: Smoothed finite element method, Strain smoothing element, Large deformation, Nearly incompressible, 4-node tetrahedral mesh, Complex geometry, Pressure checkerboarding.

Polyhedral and Polygonal Smoothed Finite Element Method for Engineering Analysis

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Abstract

In the polyhedral or polygonal smoothed finite element method, we propose a discretization strategy that constructs cell-based and node-based smoothing domains on polyhedral or polygonal background elements. This strategy converts the volume integral over each element into an equivalent surface integral defined on its associated smoothing domains. Because gradient smoothing requires only shape-function values along domain edges, derivatives of shape functions are no longer needed. Consequently, the formulation avoids the coordinate-mapping complexities of conventional finite element methods and circumvents the challenge of constructing shape functions for arbitrary polyhedra. The method also satisfies the positivity condition in a normed G space without any additional stabilization. Numerical experiments demonstrate that the proposed approach delivers high-accuracy solutions and remains robust in the presence of heterogeneous materials and severe stress concentrations.

Keywords: S-FEM; Linear elasticity; Non-conforming meshes

XFEM based on VCCT for composite delamination

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Abstract

Delamination is the most popular failure mode in composite material. Cohesive element method, which is most widely used for delamination simulation, suffers from rigorous element size requirement. In this work, extended finite element method (XFEM) and virtual crack closure technology (VCCT) are combined together to develop XFEM based on VCCT (XFEM-VCCT) for delamination analysis. In this method, delamination is represented by XFEM, and VCCT is used as delamination initiation and propagation criterion. The strain energy release rate for XFEM is obtained based on Irwin's integration. The XFEM-VCCT is applied to three examples to validate. Through the three examples, the newly developed XFEM-VCCT can simulate arbitrary crack geometry and propagation without remeshing, thus simplifying mesh work. Also the XFEM-VCCT does not require such fine mesh as cohesive element method, alleviating element size requirement. Ignorant of material property degradation, iterations are not needed for XFEM-VCCT and greatly improves the computational efficiency. Finally, the newly proposed method XFEM-VCCT is easy for mesh and can provide highly efficient and accurate solution for composite delamination.

Keywords: Composite material, delamination, XFEM-VCCT, cohesive element method

Scalable molecular dynamics with deep potential long-range framework

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Abstract

Molecular dynamics (MD) simulations play a pivotal role in exploring atomic- and molecular-scale dynamics in materials and life sciences. While ab initio MD based on density functional theory (DFT) provides high accuracy by explicitly considering electronic states, its cubic-scaling computational cost severely limits accessible system sizes and time scales. To overcome this bottleneck, neural network potentials (NNPs) have emerged as a promising alternative, retaining ab initio accuracy with near-classical efficiency.

In this study, we focus on the Deep Potential Long-Range (DPLR) [1] framework, which integrates (i) short-range interactions modeled by the Deep Potential (DP) [2], (ii) long-range electrostatics via the particle–particle particle–mesh (PPPM) method [3], and (iii) dynamic polarization effects captured by the Deep Wannier (DW) model. This combination enables accurate and scalable simulations of complex molecular systems. However, large-scale applications face performance challenges, including 3D FFT communication overhead, neural network inference cost, and load imbalance across MPI ranks.

To address these issues, we developed three architecture-aware optimizations on the supercomputer Fugaku: (1) utofu-FFT, a high-performance communication scheme leveraging the Barrier Gate hardware and quantized data exchange to accelerate 3D FFTs; (2) on-node overlapping of PPPM electrostatics and neural network inference to reduce idle CPU time; and (3) a ring-based load-balancing algorithm to dynamically redistribute atoms among MPI ranks.

Performance evaluation demonstrated excellent weak scaling up to 8,400 nodes for a 403,200-atom water system, achieving a throughput of 32.5 nanoseconds/day while maintaining first-principles accuracy. These results highlight the feasibility of DPLR with our optimizations for ultra-large, long-time MD simulations, paving the way for practical applications in materials design and biomolecular science.

Keywords: Neural network potential, molecular dynamics, high performance computing

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First-principles study of thermal conductivity in Ti_2CT_2 and $\text{Ti}_3\text{C}_2\text{T}_2$ MXenes: roles of surface terminations and structural features

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Abstract

MXenes, a family of two-dimensional transition metal carbides and nitrides, can be expressed by the general formula $\text{M}_{n+1}\text{X}_n\text{T}_x$ (M: transition metal, X: carbon or nitrogen, T: surface terminations such as O, OH, and F). They possess structural stability, high surface area, and excellent electrical conductivity, while exhibiting diverse physical properties owing to the combination of transition metals and surface functional groups. This unique versatility enables a wide range of applications, including energy conversion materials, next-generation electronics, thermoelectric devices, and catalysis [1]. In these applications, understanding and controlling thermal transport properties are indispensable. However, accurate experimental measurement of the thermal conductivity of two-dimensional materials, including MXenes, remains challenging. Therefore, theoretical analysis based on first-principles calculations and phonon transport theory is essential.

In this study, we systematically evaluated the lattice thermal conductivity of Ti_2CT_2 and $\text{Ti}_3\text{C}_2\text{T}_2$ MXenes using density functional theory (DFT) combined with the phonon Boltzmann transport equation. Phonon dispersion relations were calculated with high accuracy, and fundamental transport parameters such as specific heat, group velocity, and relaxation time were extracted. Our analysis clarified the dominant roles of surface functionalization. The results indicate that O termination suppresses thermal conductivity by eliminating phonon band gaps and increasing scattering channels, which significantly shorten phonon relaxation times. In contrast, OH termination induces nearly free electron states [2], enhances the structural stability of the lattice, suppresses phonon scattering, and extends relaxation times, thereby leading to a marked enhancement of thermal conductivity. Furthermore, structural comparison revealed that Ti_3C_2 exhibits a thermal conductivity nearly 30 times higher than Ti_2C , primarily due to the substantial extension of phonon relaxation times.

These findings demonstrate that controlling phonon relaxation times serves as a crucial strategy for modulating thermal conductivity in MXenes. By selecting appropriate surface terminations and designing structural features, thermal transport can be either enhanced or suppressed, offering promising pathways toward efficient thermal management in thermoelectric devices and advanced electronic systems.

Keywords: MXene, thermal conductivity, first-principles calculation, two-dimensional materials, surface modification

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Verification of PDS-FEM for simulation of 3D dynamic fault rupture using consistent fault stress induced by far-field loading

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Abstract

The characteristics of fault rupture are significantly influenced by geometric complexities such as curvature, regions of overlapping segments, as well as material heterogeneity, non-linearity, and frictional behaviour. Together with the tectonic setting, these factors characterise the stress on the fault system, whose initial distribution significantly affects the nature of the rupture. Given the coupling between the fault stress, its geometry and the surrounding medium, it is necessary to determine fault stress that is mechanically consistent with the surrounding material properties, frictional behaviour, and loading configuration. This is a challenging task if making use of commonly used empirical methods. To obtain a fault stress distribution compatible with aforementioned factors, we take the approach of inducing fault stress via the far-field loading conditions. We use Particle Discretisation Scheme FEM (PDS-FEM) in our rupture model, as it facilitates simple and light weight modeling of fracture phenomena. A Hamiltonian framework is used for the governing equations due to flexibility it provides when using non-linear material models and due to the availability of a wide range of symplectic integrators. We verify and validate the ability of PDS-FEM to numerically capture stress intensity factors and the global stress fields for static frictional problems, before performing a numerical verification of dynamic rupture using TPV10 from the SCEC/USGS Spontaneous Rupture Code Verification Project. To demonstrate the use of far-field loading induced stress in rupture simulations, we reproduced the observed supershear rupture of the 2018 Palu earthquake.

Keywords: Fault rupture, Physics-based, Consistent fault stress, Far-field loading, PDS-FEM, Verification

Simulations, Design and Experimental Validation of a High-Speed Electrically Powered Rocket Oxidizer Pump

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Abstract

Seal-less e-powered (canned-motor) centrifugal pumps are attractive for rocket propellants, in this case liquid-oxygen (LOX) transfer because they eliminate dynamic seals and potential leakage paths, but they impose tightly coupled constraints across hydraulics, rotordynamics, electromagnetics and thermal management. This contribution reports a design and validation methodology for a high-speed pump targeted at LOX, together with lessons learned from an instrumented water-surrogate test campaign.

In the design, the following methods were incorporated: (i) Steady RANS CFD ($k-\omega$ SST) of a semi-open impeller and volute with near-wall refinement provided head-flow characteristics, slip correction and incidence losses; (ii) a beam-FE rotordynamic model with temperature-dependent material properties was coupled to thermo-hydrodynamic bearing film solutions (tilting-pad radial and spiral-grooved thrust) to obtain stiffness/damping matrices and stability margins; (iii) an electromagnetic model of the permanent-magnet synchronous motor (PMSM) with a conductive can yielded a loss map (copper, iron, stray/eddy) and torque ripple inputs; (iv) a thermal network predicted stator/rotor temperatures and heat paths compatible with oxygen cleanliness; and (v) similitude-based extrapolation from water to LOX used specific speed, cavitation number and Reynolds-number effects, with a sensitivity analysis to propagate measurement and model uncertainties.

Experimental validation on a water rig at ambient conditions employed pressure-flow metrology, shaft-displacement probes and inverter telemetry. Start-up control combined a frequency ramp with field-oriented control and sensor-less back-EMF estimation to interrogate critical transients. Model-test agreement captured the curvature of the head-flow curve and onset of cavitation proxies; eigenvalue trends and probe data were consistent with predicted stability margins during synchronization and ramp-down.

Keywords: Cryogenic Centrifugal Pump; Liquid Oxygen (LOX); Hydrodynamic Bearings; PMSM drive

Machine learning techniques in the three-omega method to predict thermophysical properties with low variation

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Abstract

Increasing heat generation density in semiconductor devices is critical for the stable operation of integrated circuits and power devices. In such devices, thermal management and thermal measurement also play an increasingly important role, and it is desirable to obtain multiple thermophysical properties, such as volumetric heat capacity and thermal conductivity, to evaluate the thermal phenomena.

The three-omega method offers a simple and precise technique for measuring the thermophysical properties of a wide range of materials. The three-omega method measures the frequency response of the third harmonic voltage and fits an analytical solution to the results. For accurate measurements of micro- and nanoscale materials, nonlinear fitting-based analysis is indispensable in higher frequency regions. Moreover, simultaneous determination of multiple thermophysical properties, including thermal conductivity, heat capacity, and thermal boundary conductance, also necessitates the application of nonlinear fitting techniques. However, the nonlinear fitting process is unstable due to its dependency on initial guess and convergence to a local minimum. Moreover, when thermal conductivity profiles in the depth direction are required, the nonlinear fitting process is even more complicated, and it is difficult to apply to the analysis using the heat conduction model.

In this work, we introduce a machine learning-based prediction method for materials with uniform or nonuniform thermal conductivity in three-omega measurements. We assumed a thermal model of the three-omega method, and accumulated calculation results from analytical models assuming various parameters and created training datasets. By training a neural network using these datasets, we have developed machine learning models capable of predicting thermal conductivity and volumetric heat capacity and models capable of predicting the thermal conductivity profile in the depth direction from three-omega measurements. First, we confirmed the superior stability of the machine learning model in predicting thermophysical properties by the comparative simulation between machine learning-based and conventional fitting methods. We further validated the machine learning model using an experimental data of water, IPA, and their mixture, confirming that the predictions were in good agreement with the literature or theoretical values. In addition, for the case of nonuniform thermal conductivity, the prediction was conducted for an analytical test set, confirming the machine learning model can predict thermal conductivity profiles in the depth direction.

Keywords: Machine learning, nonlinear fitting, three-omega method, thermophysical property

Exact second-order dynamic stiffness matrix for torsion and warping of axially loaded members

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Abstract

In order to establish three-dimensional dynamic stability analysis of beam-column systems, this paper presents an exact second-order dynamic stiffness matrix of axially loaded members considering the natural frequency and axial compression effect. First, dynamic equilibrium analysis is developed for torsion and warping of an axially loaded member. A fourth-order differential equation governing twist angle is derived, where a dimensionless quantity λ_ω associated with the natural frequency is defined for the dynamic effect, and another dimensionless quantity λ_c indicates the Saint Venant torsion and axial load effect. Then, the exact element dynamic stiffness matrix defining the correlation between the element-end torsional stress resultants (torques and bimoments) and the associated deformations (angles and rates of twist) is obtained. Exact element dynamic torsional stiffness matrices for three configurations of warping restraints at ends of element are then developed via the matrix structural analysis. Moreover, for structural three-dimensional analysis, a 14-order exact element second-order dynamic stiffness matrix is derived through analogies between dynamic axial-torsional and axial-flexural problems.

Keywords: Matrix structural analysis; Element dynamic stiffness matrix; Torsion; Warping; Dynamic axial-torsional problem

Accurate analysis of general composite structures using mixed finite element and DQM

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Abstract

A comprehensive mixed finite element method with differential quadrature method (MFE-DQM) is presented for accurate analysis of general composite structures. The method was initially developed for static analysis of composite beams through equivalent transformation of cross sections and mixed variational principles, where nodal displacements and their energy-conjugated stresses are treated as fundamental variables. A two-dimensional analysis method was established using the differential quadrature method to solve the state equations without requiring assumptions of displacement and stress distributions along the thickness direction. Subsequently, the approach was extended to dynamic analysis for vibration and buckling behavior of general composite beams consisting of transversely layered and axially jointed materials. The governing equations were derived using Hamilton's principle, where both displacements and stresses were treated as fundamental variables. The developed finite element model ensures continuity of both displacements and stresses across material interfaces, thereby resolving interfacial stress singularity issues and offering more reliable simulations of boundary conditions at both ends. The method was formulated and validated for free vibration and buckling analysis of transversely multi-layered and axially jointed composite beams. Analysis of periodically distributed and bi-directional composite beams demonstrated the versatility of this method in handling different combination forms, with material properties such as Young's modulus, density, and interface stiffness showing significant effects on structural responses.

Furthermore, the method was extended to solve wave propagation problems and calculate band structures of periodic composite structures. The approach demonstrates exceptional computational efficiency, particularly for longitudinal wave analysis where traditional transfer matrix methods fail to provide efficient and accurate solutions for multilayered composite structures. For transverse wave solutions, the number of transverse DQM points can be selected as needed to form large matrix systems for solving complex eigenvalue problems. The proposed MFE-DQM method serves as a valuable reference for obtaining accurate static, dynamic, and wave propagation results while ensuring stress-compatibility for composite structures in practical engineering applications.

Keywords: Composite structures, Mixed finite element method, Differential quadrature method, free vibration, wave propagation.

A novel unsymmetric quadrilateral plate element based on Reissner–Mindlin theory using radial–polynomial interpolation

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Abstract

Traditional Reissner-Mindlin plate elements face significant challenges, particularly their sensitivity to mesh distortion and limitations in stress prediction accuracy. This study develops a novel unsymmetric quadrilateral plate element formulation and extends its application to doubly-curved shells and geometric nonlinear analysis. The element employs distinct test and trial functions to construct virtual and real displacement fields respectively. The virtual displacement field utilizes standard isoparametric interpolation combined with the Mixed Interpolation Tensorial Components (MITC) method to suppress shear locking, while maintaining inter-element displacement continuity and inheriting the advantages of isoparametric elements in boundary condition enforcement and nodal force computation. The real displacement field adopts a radial-polynomial interpolation strategy through the construction of element support domains, which significantly improves interelement stress continuity. Numerical examples demonstrate that the new element eliminates shear locking, exhibits high resistance to mesh distortion, achieves high stress accuracy, and maintains excellent inter-element stress continuity.

Keywords: Reissner–Mindlin plate, Unsymmetric finite element, Geometrically nonlinear analysis, Mesh distortion, Radial–polynomial interpolation

An Efficient Isogeometric Collocation Method for Superconvergent Analysis of Sixth-Order Elastic Gradient Kirchhoff Plates

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Abstract

A superconvergent isogeometric collocation method is proposed to analyze the sixth-order elastic gradient Kirchhoff plate problems. This method employs the conventional Greville abscissae as collocation points and introduces a basis transformation that preserves the exact geometry representation inherent to isogeometric analysis. More specifically, the geometry is exactly represented by the transformed isogeometric basis functions and the Greville points functioning as control points. The proposed transformed basis functions allow a straightforward formulation of the consistency conditions and span the same solution space as the standard isogeometric basis functions [1]. Subsequently, with the help of these consistency conditions, a theoretical accuracy measure is developed for the isogeometric collocation formulation for the sixth-order elastic gradient Kirchhoff plate problems. It is shown that the collocation solution accuracy is governed by the highest even degree in the basis functions. Thus, despite that the governing equations of elastic gradient Kirchhoff plates contain both fourth-order and sixth-order differential operators, and the sixth-order differential operator essentially dominates the accuracy order of the isogeometric collocation method. For a basis function of order p , it is proven that the accuracy is only of order $(p-4)$ for even p and $(p-5)$ for odd p . This basis discrepancy issue is further overcome by introducing a recursive gradient formulation [2] for the transformed basis functions, and the recursive gradients actually satisfy extra higher-order consistency conditions. This recursive construction of high-order gradients required by the collocation computation significantly enhancing the computational efficiency. An employment of these recursive gradients leads to an efficient and superconvergent isogeometric collocation method for the sixth-order elastic gradient Kirchhoff plate problems. Numerical examples comprehensively demonstrate the accuracy, convergence, and efficiency of the proposed approach regarding solving the sixth-order elastic gradient Kirchhoff plate equations.

Keywords: Isogeometric collocation method; Elastic gradient Kirchhoff plate; Basis transformation; Six-order recursive gradient; Superconvergence.

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Computational Analysis of Contact Wear with Pressure-Dependent Friction Coefficients

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Abstract

Contact and wear phenomena are prevalent in mechanical systems, and their precise modeling plays a critical role in preventing wear-induced failures. This study proposes a comprehensive numerical simulation framework for contact and wear analysis, capable of simultaneously addressing geometric, material, and boundary nonlinearities. The framework integrates the penalty function contact algorithm with Archard's wear theory, incorporating Coulomb friction models featuring three distinct pressure-dependent characteristics: constant, linear variation, and exponential variation. To overcome convergence challenges introduced by variable friction coefficient models, we developed an adaptive penalty factor algorithm. Its effectiveness was validated through contact wear simulations involving both linear elastic and Mooney-Rivlin hyperelastic materials.

Numerical experiments revealed that under large-slip conditions, the adaptive algorithm significantly improves computational convergence while reducing normal penetration and adhesive slip compared to conventional methods. Furthermore, the selection of the friction model demonstrably alters all measured parameters, with contact pressure differences progressively amplifying under increasing cyclic loading. These findings underscore pronounced material-dependent characteristics.

Keywords: Contact wear, Pressure-dependent variable friction coefficients, Mooney-Rivlin hyperelastic material, Large-sliding contact problems

Crack Velocity, Oscillations, and Acoustic Emission in Rock Fracture: Insights from Numerical and Analytical Models

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Abstract

The acoustic emission (AE) generated at crack tips during crack propagation accounts for a portion of the overall energy budget. Previous studies have shown that the proportion of AE energy increases with both crack velocity and the grain size of rock materials. However, the role of crack velocity oscillations in AE generation during rock fracturing remains unclear. Some studies suggest that AE at crack tips may be governed either by the absolute crack velocity or by fluctuations in crack velocity. In addition, a quantitative description of AE energy on crack velocity or its oscillations is still lacking. Moreover, the identification of AE waveforms and their corresponding frequency ranges remains unclear in numerical models.

In this study, we combine laboratory experiments, numerical simulations, and analytical modelling to investigate AE behaviour during rock fracturing. Preliminary results indicate that AE from numerical simulations can be calibrated against laboratory measurements. The effects of crack speed, crack speed oscillations, and grain size are further evaluated using numerical models. Finally, two analytical approaches are used to analyze the relationship between crack velocity, velocity oscillations, and AE in fracture propagation. Overall, this study provides new insights into the grain-size dependence of AE characteristics in rock fracturing.

Keywords: rock fracturing; acoustic emission; peridynamics; fracture mechanics

On-chip surface acoustic wave metasurfaces

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Abstract

Metasurfaces, consisting of subwavelength-thickness units with different wave responses, provide an innovative possible method to manipulate elastic and acoustic waves efficiently. Unlike traditional metamaterials and phononic crystals, metasurfaces' compactness aligns with modern chip integration, reducing power consumption and cross-talk. However, most elastic metasurface research focuses on macro-scale structures, limiting their application in small chips and communication technology. To solve this, we propose an on-chip surface acoustic wave (SAW) metasurface, consisting of gradient submicron niobium (Nb) rectangular pillars positioned on a 128 °Y-cut lithium niobate (LiNbO₃) substrate that operate at hundreds of megahertz. Leveraging the pillar platform's microfabrication advantages, we design the metasurface unit consisting of a series of identical pillar to enhance resonant modes, enabling efficient phase shifts and high-amplitude transmitted SAWs. Such metasurface is also validated through simulations and optical probe experiments, confirming broadband focusing performance. This study opens a door for realizing on-chip SAW metasurfaces for diverse industrial fields, such as nanoelectromechanical systems, sensing, communications, microfluid control and quantum processing.

Keywords: Surface acoustic wave, metasurface, resonant pillars

Analytical realization of complex thermal meta-devices for omnidirectional heat manipulation

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Abstract

Fourier's law dictates that heat flows from warm to cold. Nevertheless, devices can be tailored to cloak obstacles or even reverse the heat flow. Mathematical transformation yields closed-form equations for graded, highly anisotropic thermal metamaterial distributions needed for obtaining such functionalities. For simple geometries, devices can be realized by regular conductor distributions; however, for complex geometries, physical realizations have so far been challenging, and sub-optimal solutions have been obtained by expensive numerical approaches. Here we suggest a straightforward and highly efficient analytical de-homogenization approach that uses optimal multi-rank laminates to provide closed-form solutions for any imaginable thermal manipulation device. We create thermal cloaks, rotators, and concentrators in complex domains with close-to-optimal performance and esthetic elegance. The devices are fabricated using metal 3D printing, and their omnidirectional thermal functionalities are investigated numerically and validated experimentally. The analytical approach enables next-generation free-form thermal meta-devices with efficient synthesis, near-optimal performance, and concise patterns.

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Optimization Design and Dynamic Control of Anisotropic Intelligent Elastic Wave Metasurface Exciter

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Abstract:

Currently, ultrasonic testing primarily employs piezoelectric materials to generate longitudinal waves for ultrasonic imaging. However, due to the relatively large wavelength of longitudinal waves, detection of finer defects remains challenging. The wavelength ratio between longitudinal and shear waves is related to the Poisson's ratio. In medical ultrasound applications, human tissues exhibit a high Poisson's ratio, leading to a significantly shorter calculated wavelength for shear waves compared to longitudinal waves. The relatively longer wavelength of longitudinal waves limits their sensitivity to minute defects, thereby complicating detection. Additionally, longitudinal waves introduce artifacts at tissue boundaries, making them unsuitable for complex and deformable tissues.

Therefore, this study aims to design a metasurface-based exciter capable of generating shear waves, which possess much shorter wavelengths and can detect finer defects. Although many existing studies have effectively excited shear waves through shear deformation mechanisms, such excitation requires exceptionally high driving voltages—far exceeding those used in conventional ultrasonic imaging—and suffers from rapid energy attenuation and low signal-to-noise ratio. As a result, the practical application of currently generated shear waves remains limited.

Given the rapid attenuation of shear waves generated by tangential excitation, we draw inspiration from Lamb's problem and propose applying a vertical excitation on the surface of an elastic half-space to generate surface waves, shear waves, and longitudinal waves. The interference of elastic waves produced by point-source excitations can yield various intriguing phenomena, particularly enabling the generation of desired shear waves.

Keywords: Shear wave, piezoelectric, nondestructive testing

Shear Localization in Gradient High-entropy Alloy at High Strain Rates: Crystal Plasticity Modeling

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Abstract

Gradient-structured metals have attracted considerable attention due to their good strength–ductility synergy, whether it can be used as a candidate to effectively hinder shear localization failure under high strain rate deformation is still an open question. Corresponding to the particular mechanisms of dynamic recrystallization and twinning at high strain rates, a physically based crystal plasticity constitutive model containing a new equation of dislocation-density evolution and the twinning model is developed to investigate the detailed process of shear localization of gradient-structured CoCrFeMnNi high-entropy alloy under dynamic shear simulations. A physically based strain gradient theory is considered to capture the hardening effect of gradient structures. The agreement of the predicted stress-strain curves and the evolution of shear localization of the HEAs with the corresponding experimental data validates the developed constitutive model. The competition between microstructural softening and strengthening effects from the continuous dynamic recrystallization and twinning as well as the gradient structure effect is quantified to disclose the effects of grain size and gradient structure on the mechanical response and shear localization of gradient-structured HEAs. The results show shear localization in gradient-structured HEA can be significantly delayed and gradient structures have significant effects on the evolution of shear localization, the corresponding mechanisms are analyzed. This study contributes to understanding the influence of gradient structure on shear localization and provides insights for further optimization of the mechanical behavior of gradient structures at high strain rates to develop strong and ductile metals and alloys for dynamic applications.

Keywords: Gradient Structure; High Strain Rate; Shear Localization; Crystal Plasticity

Multiplexing same-order acoustic spiral waves by generalized impedance metasurfaces

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Abstract

Waves with spiral wavefront have demonstrated exceptional potential in electromagnetic multiplexed communication systems due to their inherent orthogonality. However, their implementation in acoustic communication faces significant challenges. Generation of acoustic spiral waves typically requires extensive speaker arrays, but the purity of the signal may not be ideal. The intrinsic absence of spin degree of freedom in acoustic waves further limits channel capacity. In this work, generalized impedance theory for the design of metasurfaces with perfect wave manipulation is developed to generate high-capacity acoustic spiral signal. It is argued that arbitrary sound fields can be connected perfectly and passively as long as global power flow conservation is guaranteed. Perfect capability can be detected for simultaneous modulation of phase and amplitude, which is exactly the signature required by spiral waves. Meanwhile, by fully exploring the propagating waves of acoustic waveguides, multiple modes can be observed to have strict orthogonality but the same order. They are named as complex Bessel modes (CBMs), which could substantially enhance information capacity. Numerical simulations are given, showing perfect CBM conversion via generalized impedance metasurfaces. Notably, adaptability of the generalized impedance metasurface allows deployment between waveguides of contrasted cross-sections. Single-speaker CBM generation can be therefore supported and experimental verified, which eliminates dependency on bulky arrays. This work is expected to expand the design of acoustic metasurfaces and their applications in acoustic communication.

Keywords: Metasurface, impedance theory, acoustic spiral wave, multiplex communication

Experimental study on SHPB impact deformation of metastable $V_{10}Cr_{10}Co_{30}Fe_{50-x}Ni_x$ high entropy alloy in wide temperature range

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Abstract

High-entropy alloys exhibit significant advantages over traditional materials in terms of strength, toughness, etc. In recent years, remarkable progress has been made in the research of high-entropy alloys. However, the research on high-entropy alloys in extreme environments remains relatively limited. In particular, the understanding of the microstructural evolution, deformation mechanisms, and influencing factors of high-entropy alloys under impact loading in a wide temperature range is insufficient. Therefore, studying the dynamic mechanical properties of novel high-entropy alloys and establishing the relationship between macroscopic mechanical properties and microstructural evolution is of great scientific significance and engineering application value.

This paper focuses on metastable $V_{10}Cr_{10}Co_{30}Fe_{50-x}Ni_x$ ($x = 1, 2$) high-entropy alloys. At room temperature, for both high-entropy alloys, the stress gradually increases with the increase of strain after yielding, demonstrating significant strain hardening ability. The materials exhibit a strong strain rate effect, and the strain rate sensitivity increases significantly with the increase of the strain rate. When deformed at low temperature (77 K), the yield stress and ultimate stress of the two high-entropy alloys are significantly higher than those at room temperature, indicating a strong temperature effect. In addition, the temperature sensitivity of the two materials under impact deformation was calculated. When adiabatic temperature rise is considered, the temperature sensitivity of the two materials gradually increases with the increase of strain. However, when adiabatic temperature rise is not considered, the temperature sensitivity changes little with temperature, indicating that the influence of adiabatic temperature rise on the material properties cannot be ignored during high-strain-rate deformation. The plastic deformation under dynamic impact is affected by the coupled action of dislocation slip and martensitic transformation. With the increase of Fe content and the decrease of deformation temperature, the stacking fault energy of the material decreases, thus promoting the occurrence of martensitic transformation. The martensitic transformation follows a specific transformation path and forms a typical K-S orientation relationship with the parent phase. However, due to the symmetry of the crystal structure, different transformation variants exist, leading to significant refinement of the transformation region.

Keywords: High strain rate, High entropy alloy, Martensitic transformation, Temperature effect

Multi-patient study for the correlation between carotid artery vascular elasticity and clinical biomarkers

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Abstract

Ultrasound imaging is one of the most important clinical screening and evaluation method. However, the images provided by static ultrasound are difficult to help doctors make an effective diagnosis of patients with moderate to low stenosis. The dynamic imaging method based on elastic ultrasound imaging can effectively obtain the plaque deformation characteristics, which is helpful for the quantification and classification of the vascular elasticity level of patient. For analyzing carotid artery biomechanical properties in 48 diabetic patients, we computed axial and radial vascular change rate. The results demonstrated significant correlations between vascular elasticity and metabolic, inflammatory, and autoimmune biomarkers. Key findings include strong positive correlations between maximum axial vascular change rate and HbA1c ($\rho=0.435$, $p=0.002$), as well as negative associations of mean axial vascular change rate with serum creatinine ($\rho=-0.416$, $p=0.003$). The maximum radial vascular change rate showed a strong positive correlation with urinary NAG levels ($\rho=0.432$, $p=0.002$), suggesting renal tubular injury may influence radial vascular dynamics. Thyroid peroxidase antibody demonstrated consistent negative correlations with both maximum radial vascular change rate ($\rho=-0.424$, $p=0.003$) and mean radial vascular change rate ($\rho=-0.382$, $p=0.007$), potentially linking autoimmune activity to impaired radial vascular adaptation. Notably, cytokeratin 19 fragment (CYFRA21-1) was inversely associated with maximum radial vascular change rate ($\rho=-0.349$, $p=0.015$) and mean radial vascular change rate ($\rho=-0.407$, $p=0.004$), indicating epithelial damage markers may reflect vascular remodeling processes. Age-related reductions in mean radial vascular change rate ($\rho=-0.347$, $p=0.016$) aligned with expected arterial aging trajectories. These findings underscore the potential of biomechanical-clinical biomarker integration for early vascular dysfunction detection. The study proposes a paradigm shift toward precision vascular medicine, advocating for multi-modal elasticity indices in personalized cardiovascular risk assessment.

Keywords: vascular elasticity, ultrasound elastography, clinical biomarkers, carotid

Age-Related Changes in Dermal Elastin Fiber Architecture and Their Impact on Skin Firmness : A Finite Element Analysis

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Abstract

Skin firmness and elasticity are governed by the dermal extracellular matrix, especially the elastin fiber network, yet the quantitative link between elastin microarchitecture and macroscopic firmness has been unclear. We develop an image-based finite element (FE) framework that embeds realistic 3D elastin geometries—segmented from confocal stacks of human abdominal skin from Caucasian females aged 38–78—directly into a continuum dermal matrix to mechanistically relate fiber architecture to firmness. Elastin networks are represented as beam elements and the dermis is modeled as a near-incompressible Saint Venant–Kirchhoff material; unconfined compression is applied until the model height reaches 80% of its original value (20% compression), with standard constraints and MPC planarity conditions; fiber and matrix moduli are set to 0.5 MPa and 80 kPa, respectively, and simulations are run in MSC Marc. The computed firmness metric shows a clear age-dependent decline that tracks specific geometric degradations: thinning and loss of fibers, reduced volume fraction, greater fragmentation with smaller maximum cluster size, and a lower proportion of vertically oriented fibers エラー! 参照元が見つかりません。 . Among all descriptors, fiber count and maximum cluster size emerge as the strongest predictors of firmness, highlighting that load-bearing capacity depends on both network density and continuity rather than quantity alone. Mechanistic readouts explain these trends: dense, vertically connected hubs co-localize with low-strain regions under compression, vertical fibers predominantly carry compressive loads, and aged networks exhibit narrowed force distributions with far fewer fibers in high compression, indicating diminished load sharing. This framework isolates elastin geometry as the variable of interest and provides quantitative, mechanistic evidence that preserving network integrity—especially maintaining connectivity and vertical pathways—is central to maintaining skin firmness; it thereby motivates therapeutic and cosmetic strategies aimed at protecting, rebuilding, or mimicking the elastin framework. The study’s scope intentionally excludes age-related collagen remodeling and adopts a simplified dermal constitutive law to focus on elastin; future extensions could incorporate viscoelastic or more complex hyperelastic matrices and coupled collagen–elastin remodeling.

Keywords: Elastin fiber, Skin firmness, Finite element modeling

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An Efficient Multiscale Computational Framework for Glycocalyx-Modulated Microvascular Blood Flow

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Abstract

The simulation of microvascular blood flow remains as a significant computational challenge, primarily due to the inherent multiscale discrepancy between cellular-scale blood components (e.g., red blood cells) and molecular-scale endothelial surface structures — a gap that renders conventional single-scale approaches incapable of reconciling physical fidelity with computational feasibility. To address this issue, we propose a novel multiscale computational framework based on domain decomposition, which integrates a coarse-scale model for bulk blood flow with a fine-scale model for the near-wall region. The hybrid framework is validated quantitatively against analytical solutions for Couette and Poiseuille flows, achieving good agreement with theoretical predictions while offering a substantial reduction in computational cost compared to full-domain fine-scale simulations. To demonstrate its practical utility in biomechanical studies, we apply the framework to a microvessel featuring the endothelial glycocalyx layer (EGL). Simulations successfully capture physical phenomena that are inaccessible to coarse-scale-only models, including flow-induced deformation of the EGL and EGL-induced resistance of flow at the endothelial surface. This work establishes a validated, computationally efficient multiscale platform that bridges cellular and molecular scales in microvascular flow, addressing a longstanding gap in vascular biomechanics modeling and enabling high-fidelity investigations of complex wall-blood interactions relevant to physiological and pathological processes.

Keywords: microvascular blood flow, domain decomposition, multiscale modeling, concurrent coupling, endothelial glycocalyx layer

Wall shear stress oscillation in microvascular network arising from red blood cell motion

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Abstract

The wall shear stress (WSS) acting on endothelial cells in microvessels influences physiological phenomena such as vasoconstriction, vasodilation, and thrombus formation. WSS is likely to be affected by red blood cells (RBCs) because the size of an RBC is close to microvessels. In this study, we performed 2D simulations of the blood flow in a microvascular network using the particle method to investigate the spatio-temporal dynamics of wall shear stress under the influence of RBC motions.

The microvascular network model was created using the published images of micro vessels in a rabbit omentum [1]. In making the vascular model, control points were extracted from the vessel wall surfaces in the images, and spline interpolation was applied to smooth the wall surface geometries. The modeled RBC was composed of an elastic membrane and internal fluid, and involved in the modeled blood with blood plasma [2]. Fluid dynamics simulations were performed using the LSMPS method [3]. At the inlet, a constant flow rate was given, the Reynolds number was as small as 0.35, and the hematocrit (i.e., volume fraction of RBCs in whole blood) was varied at 0–30 %.

In blood flow simulations, WSS increased significantly when RBCs moved near the vessel wall. An RBC cluster was formed if RBCs stagnated at a vascular bifurcation, and this caused the substantial increase and oscillation of WSS. The frequency of this oscillation due to RBC clusters was 20–300 Hz, which is lower than approximately 600 Hz regarding WSS caused by individual RBC motion near the wall. The low frequency oscillation decayed as the inlet hematocrit decreased. Thus, the RBC clusters according to the inflow hematocrit are suggested to play important roles in WSS oscillation at a low frequency, which might be related to physiological responses of endothelial cells.

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Lateral Migration Patterns of Deformable WBC and CTC in Microchannels: Effects of Geometry and Hematocrit

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Abstract

Cell migration dynamics in confined microenvironments critically influence physiological processes such as immune surveillance and cancer metastasis. This study investigates motion patterns of deformable cells—white blood cell (WBC, 8 μm) and circulating tumor cell (CTC, 12 μm)—in microchannels using the immersed boundary method. We analyze how channel size, axial initial positions, and hematocrit (Ht) influence migration. For single cells, CTC exhibit slower translational velocity than WBC in small channels, but this reverses in larger channels. In small channels with WBC upstream and CTC downstream, fluctuations in the lateral migration trajectories and axial distance can be observed when the two cells are close to each other. WBC exhibits larger axial velocity fluctuations than CTC, ultimately forming stable cell pairs that maintain a fixed separation distance along the flow direction. Simulations of the migration of cell pairs in the presence of red blood cells (RBCs) consistently demonstrated that the axial spacing between cells decreases to zero due to blockage effects induced by CTC. In large channels, no channel size constraints result in upstream CTC overtaking downstream WBC. At 10% Ht, CTC reach equilibrium positions while RBCs shielding confines WBC near walls. These results elucidate how vessel size and Ht jointly regulate competitive cell trafficking. The geometry-dependent overtaking mechanisms suggest CTC exploit large vessels to bypass immune interception, while RBCs enhance WBC margination—behavioral patterns mirroring in vivo metastatic evasion and inflammation responses.

Keywords: cell migration, channel size, axial distances, microfluidics

Motion of Capsules in Curved Tubes

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Abstract

The migration of capsules in curved tubes constitutes a fundamental multiphase flow in which the membrane tension extensively interacting with the secondary flow due to the centrifugal effect. And it is closely related to microfluidic applications.

Previous studies have focused on curved tubes with a relatively small radius range, which does not exceed 10 times the radius of a cell due to the limitations of cartesian coordinate. In this research, we numerically studied the motion of a single spherical capsule in curved tubes with a large radius by solving the Navier-Stokes equations in cylindrical coordinate. And the fluid-membrane interactions are modeled by adopting the Immersed boundary method. The capsule is modeled as a viscous drop encapsulated by a hyper-elastic membrane that satisfies the Skalak model.

We find that the final steady state of capsules is independent of the initial released position. For relatively stiff capsules, under small Reynolds numbers, they finally equilibrate at a position near outer wall. With Reynolds number increasing, this balance position changes to near the inner wall. For sufficiently large Reynolds numbers, capsules do not have an equilibrium position in the cross-section, instead, they move periodically with Dean vortices. For soft capsules, they always equilibrate at a position near the outer wall of the cross-section.

In future work, we will explore the dynamics of the fluid surrounding the capsules and the membrane-fluid interactions more detailly to provide a more comprehensive understanding of this problem.

Key words: Immersed boundary method, curved tube, capsule motion, Dean vortex, Secondary flow

Numerical simulation and lift force analysis for cross-streamline migration of slip particles in viscoelastic microchannel flow

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Abstract

Precise manipulation of particle migration in microfluidic systems is fundamental to biomedical diagnostics, and lab-on-a-chip technologies. A key phenomenon that has attracted attention in microfluidic systems recently is slip-induced migration. We employ a hybrid simulation approach, combining the lattice Boltzmann method (LBM) with coarse-grained molecular dynamics (CGMD) to elucidate the underlying mechanisms. Our simulations reveal that an additional slip velocity aligned with the flow direction induces an elastic transverse force directing particles towards the channel centerline and an inertial transverse force towards the walls. Conversely, an anti-parallel slip velocity inverts the direction of these forces. Crucially, the additional elastic transverse force scales linearly with both particle size and slip velocity, and exhibits a power-law dependence on polymer chain length. These findings provide a fundamental understanding of the enhanced particle focusing observed experimentally, offering design principles for improved microfluidic devices for nanoscale manipulation.

Keywords: Particle migration, Microchannel, Viscoelastic fluids, Coarse-grained molecular dynamics, Lattice Boltzmann method, Slip velocity

Numerical Investigation of Fixation Plate Mechanics in Mandibular Reconstructive Surgery

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Abstract

Large bone loss and defects caused by trauma, tumor or osteoradionecrosis signify a common issue in the maxillofacial clinic. The reconstruction plate plays an important role in maintaining stability and load-sharing while a grafted fibula bone unites with adjacent bone in the course of healing and bone remodeling. Clinical experience and specialized literature show that titanium reconstruction plates used for mandibular defects are often subjected to excessive mechanical stress, conceivably leading to fatigue fracture. The study on fatigue characteristics for the design of medical devices is of fundamental importance, particularly for load-bearing prosthetic devices. However, failure of these devices due to fatigue under cyclic loading has been recognized as a primary concern on therapeutic longevity. In this study, we develop a computational approach for modelling fatigue process in the reconstruction plate based upon the eXtended Finite Element Method (XFEM). The mechanical stresses introduced by plate pre-bending and screw tightening were first modeled computationally and the residual stress data induced by the surgical procedure was incorporated to the deformed reconstruction plate for the subsequent bio-mechanical evaluation. The finding is of important clinical implications for surgeons who are commonly involved in selecting and preparing different forms of fixation plates for mandibular reconstruction. The simulation results demonstrate that the pre-stresses induced by screw tightening are more substantial than that from plate bending during the surgical procedure. This study helps elucidate the key factors contributing to the failure of reconstruction plates and guide the development of more robust and durable mandibular reconstruction systems.

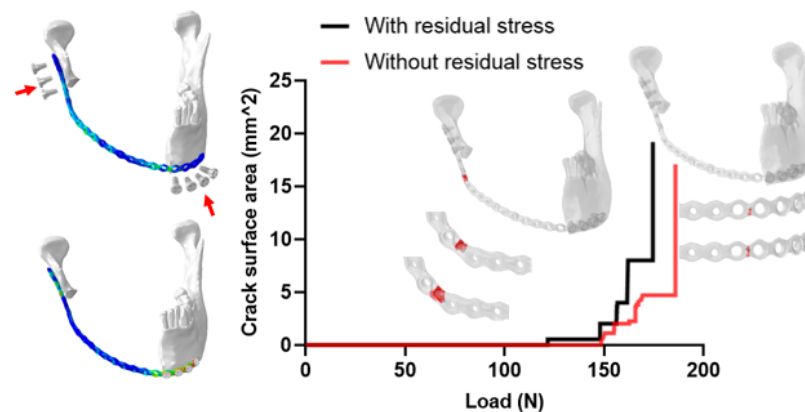


Fig. 1: Simulation of the screw tightening pre-stress. Crack propagation in the reconstruction plate and representative fracture patterns.

Keywords: XFEM, Bone remodeling, Fracture, Residual Stress, Mandibular reconstruction

Auxiliary quantitative methods for the selection of preoperative surgical plans for aortopulmonary septal defect

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Abstract

Cardiovascular diseases seriously threaten human life and health, among which congenital heart disease is a common congenital defect. Aortopulmonary septal defect (APSD), as a rare congenital cardiac vascular malformation, has a low incidence but serious clinical consequences. Surgery is an important treatment for this disease. At present, surgical methods such as direct ligation method, patch method, cut patch method and catheter occlusion method have been formed. At present, the surgical mortality of this disease is still high, and how to reduce the surgical mortality has become an urgent problem to be solved.

Based on the CT image data of the patients, this article uses numerical simulation methods to simulate the vascular structure of the patients under different surgical plans after the operation and quantify the postoperative aortic and pulmonary artery vascular parameters under the four surgical plans. In the first surgical procedure, both aorta and pulmonary arteries were ligated directly. The second method is to ligate the aorta directly and repair the pulmonary artery with artificial patch. In the third method, the aorta was repaired with the pulmonary artery wall and the pulmonary artery was sutured directly. In the last option, the aorta is repaired with the pulmonary artery wall and the pulmonary artery is repaired with an artificial patch.

The results showed that the postoperative results of different surgical procedures were significantly different. The maximum change of pulmonary artery volume after the four surgical procedures ranged from 59.9% to 106.67%.

The simulated postoperative vascular structure method provided in this paper can quantitatively evaluate different surgical plans for aortopulmonary septal defect before surgery. It provides a quantitative contrast approach for doctors to select the appropriate surgical plan before operation.

Keywords: Aortopulmonary septal defect, preoperative assessment, numerical simulation

Cellular blood flow modeling with smoothed dissipative particle dynamics

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Abstract

Computational modeling and simulation of cellular blood flow is highly desirable for understanding blood microcirculation and blood-related diseases, such as anemia, thrombosis and tumor, but it remains a challenge because the blood requires to be described as a dense suspension of different types of cells and the microvessels continually bifurcate or merge into a complex network. A smoothed dissipative particle dynamics-immersed boundary method (SDPD-IBM) has been developed, integrating the fluid flow and cell behavior to simulate physiological and pathological phenomena involved in blood flow. The SDPD is used to model the fluid flow, the IBM is used to model the interactions between the fluid and cells, and three phenomena are taken into account, cell deformation, aggregation and adhesion. The simulations in this talk consist of two parts: validation studies for the fidelity of the SDPD-IBM, and case studies for its potential and usefulness. The validation studies consider the flow of pure fluid, the mechanical behavior of cells, and the multi-outlet cellular flow, while the case studies include cells passing through simple vessels, successive bifurcations, and even a complex microvascular network. These studies concern the formation of a thrombus, the partitioning of red blood cells, and the metastasis of tumor cells.

Keywords: Cell deformation, Cell aggregation, Cell adhesion, Dissipative particle dynamics, Immersed boundary method.

Efficient Spectral Methods for Volume-Constrained Nonlocal Models

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Abstract:

This talk considers efficient spectral solutions for weakly singular nonlocal models with Dirichlet-type volume constraints. The equation contains an integral operator that typically has a singularity at the center of the integral domain, and the approximation of the integral operator is one of the essential difficulties in solving nonlocal equations. To overcome this problem, two-sided Jacobi spectral quadrature rules are proposed to develop a Jacobi spectral collocation method for one-dimensional nonlocal diffusion equations, and a nonlocal quadrature rule is constructed to develop Jacobi spectral method for multi-dimensional nonlocal diffusion and peridynamics equations. A rigorous convergence analysis of the proposed methods with the L^∞ norm is presented and numerical examples are given to verify the theoretical results.

Manifold adaptive method for thermo-mechanical coupled fatigue phase-field model

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Abstract

Phase-field method can automatically capture the nucleation, propagation, and coalescence of cracks by tracking the evolution of an order parameter. This makes itself a powerful tool for simulating fatigue fracture in structures. However, the highly nonlinear nature of the phase-field model, combined with the high number of loading cycles required for fatigue analysis, results in a significant computational cost. This challenge is further exacerbated when considering coupled thermo-mechanical effects. It makes numerical simulations of such problems particularly difficult.

To address this challenge, we proposed an efficient acceleration method based on manifold-adaptive finite elements. First, we rigorously derive the governing equations for coupled thermo-mechanical phase-field fatigue analysis from thermodynamic principles. We then introduce the constant load accumulation method to efficiently handle damage evolution under cyclic loading. To validate our proposed model and algorithm, we developed a manifold-adaptive mesh program in C++ for accelerated thermo-fatigue phase-field simulations. We used this program to perform numerical simulations of thermo-mechanical fatigue on three typical structures: a dog-bone specimen, a plate with a central hole, and a microstructure with a spherical void.

It is shown that the manifold-adaptive method can maintain the geometric shape of curved surfaces with high precision during mesh refinement, effectively avoiding errors that can be introduced by geometric discretization in traditional finite element methods. In terms of computational efficiency, this algorithm significantly speeds up the solution of coupled thermo-mechanical fatigue problems, thus reducing computational costs. By comparing with experimental data, we show that the coupled thermo-mechanical phase-field fatigue model can reproduce the S-N curve of material by selecting appropriate parameters. And its life prediction errors are within a factor of two scatter band, demonstrating good life prediction accuracy.

Keywords: Phase-field model; thermo-mechanical fatigue; manifold; adaptive

Re-derivation and Mathematical Analysis for Linear Peridynamics Model for Arbitrary Poisson Ratio's Material

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Abstract:

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This talk is concerned with the modeling and mathematical analysis of linear Peridynamics model for arbitrary Poisson ratio's material. Based on the fundamental laws of dynamics, we re-derive the bond-based Peridynamics model for anisotropic materials by relaxing certain assumptions. Through this process, we draw several significant conclusions, such as the relationship between the equivalent strain energy density hypothesis and the convergence of the Peridynamics operator to the classical Navier operator. Additionally, the well-posedness of time-dependent Peridynamics equations of motion is established. Finally, some necessary conditions for the material stability of anisotropic material are given.

Phase-Field Modeling of Flexoelectricity and Dislocation Effects in Ferroelectrics

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Abstract:

The phase field model is a thermodynamics-based approach widely employed to simulate phase separation processes. It is characterized by the Cahn-Hilliard diffusion equation, which captures complex pattern evolution during phase inversion through a diffuse interface representation between distinct phases. This method has found extensive applications in mechanics and materials science, including studies of grain evolution, martensitic transformations, fracture propagation, and ferroelectric domain switching.

In this study, we first demonstrate its application in modeling flexoelectric effects in ferroelectric materials.[1] The ferroelectric domain structure is represented using an independent order parameter governed by the Allen-Cahn equation. Modeling flexoelectricity presents computational challenges due to the high-order displacement derivatives involved. To address this, we develop a unified phase-field framework incorporating both flexoelectricity and dislocations. A four-node quadrilateral element with 20 degrees of freedom is formulated, which captures strain gradients for flexoelectricity without requiring high-order shape functions. This is achieved by interpolating nodal strains from Gaussian points in isoparametric space. The model successfully reproduces classic flexoelectric solutions in dielectric materials and demonstrates its capability by simulating phenomena in non-trivial geometries such as cylindrical tubes and truncated pyramids.

In the second case study, we model the effect of dislocations on ferroelectric thin films. Dislocations are efficiently introduced via eigenstrains applied at interfaces and surfaces.[2] Phase-field simulations quantify how dislocations pin domain wall motion and influence hysteresis loops. The pinning strength is shown to depend on the competition between external loading conditions and the magnitude of the dislocation's Burgers vector.

These studies illustrate that the phase-field model serves as an efficient microstructure simulation tool. It significantly contributes to the understanding of domain dynamics and provides valuable insights for the design of advanced ferroelectric devices.

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Computable Peridynamics: Enhancing Asymptotic Compatibility and Suppressing Zero-Energy Modes

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Abstract

Peridynamics, an emerging nonlocal theory, has progressed rapidly in recent years and is now widely used for modeling material fracture and the dynamics of complex media. Nevertheless, numerical simulation in peridynamics still faces substantial challenges. On the one hand, many formulations struggle to maintain asymptotic compatibility with classical local models, failing to recover the correct local behavior in limiting cases. On the other hand, simulations of anisotropic materials are often plagued by zero-energy modes, which trigger numerical instabilities and undermine accuracy and reliability. While refinements to standard discretizations can mitigate these issues to some extent, they have not addressed them at their root. This talk targets these core difficulties and proposes a class of **computable peridynamic models**. Rather than relying solely on algorithmic optimization, the approach modifies the theoretical model itself to fundamentally resolve the numerical pathologies. By **reformulating the nonlocal interaction mechanism**, we strengthen the model's **asymptotic compatibility** with local theory; simultaneously, we introduce a **new mechanism to suppress zero-energy modes**, thereby improving stability in simulations of anisotropic materials. Preliminary numerical experiments indicate that the proposed model preserves the nonlocal advantages of peridynamics while markedly improving accuracy and robustness. The talk will detail the model's theoretical underpinnings, the proposed design strategies, and numerical verification, offering new perspectives and tools for the continued development of peridynamics.

Enhanced Identification of the Parameters of a Jeffcott Rotor from Run-up Transients using Physics-informed Neural Networks with Sinusoidal Activations

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Abstract

Accurate identification of rotor-dynamic parameters is essential for the health monitoring of rotating machinery. Classical methods such as FRF fitting and Kalman filtering often require long stationary datasets and perform poorly under noisy transient conditions, such as during run-up tests. Physics-informed neural networks (PINNs) have emerged as a data-efficient alternative; however, standard tanh/ReLU architectures are susceptible to spectral bias, which limits their ability to capture rapidly varying responses. In this study, we employ a PINN with sinusoidal representation networks (SIREN) to estimate the stiffness, damping and eccentricity of a Jeffcott rotor undergoing constant angular acceleration directly from non-stationary run-up data. Sinusoidal activations mitigate spectral bias and improve the representation of the chirp-like dynamics near resonance. Using synthetic displacement signals with controlled noise, we demonstrate that the SIREN-based PINN outperforms a tanh-activated baseline in terms of both accuracy and training efficiency. Beyond full-signal runs, feasibility studies are discussed using only short run-up windows, showing that reliable parameter identification is possible from sub-second transients. The results suggest that using sinusoidal representations in PINNs is a good way to estimate parameters from data where the system is only temporarily operating. This is in addition to steady-state approaches and could lead to online health monitoring systems that work in practice.

Keywords: PINN, parameter estimation, sinusoidal activation, rotor dynamics, time-domain analysis

LP-PINN: A Locally Connected physics-informed neural networks based on local boundary knot method.

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Abstract

We propose a novel neural network architecture named Local-Connect physics-informed neural networks (LpPINN), which integrates the framework of physics-informed neural networks (PINNs) with the local boundary knot method. Compared to traditional PINNs, LpPINN introduces a filtering mechanism that utilizes only a subset of the collocation nodes instead of all computational nodes, significantly reducing computational cost. By incorporating the ghost point technique, the model achieves superior accuracy. In conventional methods, the free parameter known as the ghost radius is typically selected based on empirical testing or leave-one-out cross-validation (LOOCV) within a bounded interval. In contrast, our method allows this parameter to be optimized directly through the training process. Numerical experiments demonstrate that the proposed network not only achieves higher accuracy but is also robust to different initializations of the model parameters.

Wind turbine wake prediction by deep convolutional neural networks with spatial-coordinate embedding

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Abstract

Accurate prediction of wind turbine wake fields presents a persistent challenge in wind energy optimization. Current data-driven approaches typically generate mean-flow predictions solely at hub-height, limiting their application for high-resolution wind farm layout design. To overcome this limitation, we propose a novel deep learning framework incorporating spatial-coordinate embedding within a CBAM-enhanced U-Net architecture. This approach explicitly encodes continuous downstream positions as mathematical embeddings, enabling the model to dynamically adapt predictions to any coordinate at downstream distances between 3D and 10D. High-fidelity Large Eddy Simulations (LES) using the Actuator Line Method (ALM) simulating the NREL 5MW reference turbine under neutral atmospheric boundary layer conditions provide the foundational dataset. Our framework processes flow-field inputs from three consecutive upstream cross-sections while integrating trainable embedding vectors representing target downstream positions. Comprehensive evaluations benchmark the spatial-embedding model against: (1) baseline CBAM-Unet predictions trained exclusively on discrete locations (nD downstream, where n is an integer), (2) conventional linear and spline interpolation techniques applied to these nD predictions, and (3) ground-truth CFD results. The spatial-embedding approach consistently demonstrates enhanced capability in resolving complex turbulent structures and velocity deficit gradients at non-integer positions compared to interpolation methods. This innovative embedding paradigm establishes a continuous prediction capability beyond discrete sectional sampling, significantly advancing high-fidelity wake modeling for wind farm optimization. Validation confirms the framework's robustness across diverse positions downstream while maintaining physical consistency with fundamental fluid dynamics principles.

Keywords: Wind turbine wake, wake prediction, neural networks, positional embedding

A Machine Learning-Driven Decoupling Framework for Efficient Prediction of Cohesive Zone Model Parameters in Polymer Composites

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Abstract

In multiscale composite modeling, cohesive zone models (CZMs) derived from molecular dynamics (MD) are vital for capturing microscale interface behavior. However, obtaining CZM parameters from direct MD simulations is computationally expensive and not easily scalable, limiting their practical use. We present a novel machine learning (ML) framework that dramatically accelerates the prediction of interface CZM parameters by learning from a limited set of MD analyses. The core innovation is a decoupled simulation strategy that decomposes complex multi-atom interfacial interactions into fundamental single-atom interaction units. This simplification enables the systematic identification of key factors governing interfacial cohesion, notably non-bonded van der Waals (VDW) and hydrogen-bond interactions and the overall system density. Using these critical features, we trained an artificial neural network (ANN) to efficiently predict CZM parameters for diverse fiber–matrix systems. The model’s predictions were validated against experimental data and literature benchmarks. Among the identified factors, VDW interactions showed the highest correlation (>80%) with interface strength, whereas hydrogen bonding contributed only about 5–10%. The ANN accurately reproduced cohesive zone parameters for a variety of common polymer composite systems. It also correctly predicted the ranking of interfacial shear strength (IFSS) across 13 different fiber/matrix systems, with 85% of the predictions falling within 20% of measured values. Furthermore, the ML-predicted CZM parameters were directly applied in macroscale finite element simulations of fiber pull-out tests, demonstrating excellent agreement with observed interface debonding behavior. This ML-driven approach provides a scalable, practical tool for interface characterization in composites, significantly reducing reliance on time-consuming MD simulations and enhancing the efficiency of multiscale modeling in materials science.

Keywords: Cohesive Zone Model; Composites Interfaces; Machine Learning; Molecular Dynamics; Multiscale

Structural parameter identification with neural ordinary differential equations

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Abstract

Data-driven-based methods extract high dimensional features to identify structural damage from structural dynamic responses. Most existing data-driven-based methods are based on black-box models that cannot be interpreted and explained. In this study, a new method based on the neural ordinary differential equations (NODEs) is developed for structural damage identification from dynamic responses. The proposed method integrates the state-space based physical model with neural network. The state-space express equations of dynamic structural system are the physical constraints of prior knowledge, and a feed-forward neural network is to capture the discrepancy from the feed data comparing with the prior knowledge. Utilising the discrepancy term, a novel approach by exploring the closed-form expression from the neural network is proposed for structural system parameters reconstruction, which is to interpret and transparent the trained network model. Numerical results from building structures under various operational conditions are used to verify the performance of the proposed method. The results show that the proposed method is accurate and efficient to identify the local parameters and structural damage.

Physics-informed neural networks for modeling moving boundaries and capturing fine-scale flow structures

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Abstract

The integration of physics-based constraints with data-driven machine learning has emerged as a transformative paradigm in intelligent fluid mechanics. This work advances physics-informed neural networks (PINNs) with three key contributions: (1) forward modeling of moving-boundary problems, (2) inverse inference for hidden boundaries, and (3) hybrid PINNs-CFD frameworks for adaptive mesh refinement.

First, we address a fundamental limitation of conventional PINNs—their inability to handle time-varying boundaries—by reformulating moving spatial boundaries as static interfaces in an extended space-time domain. This dimension-lifting approach transforms transient problems into steady-state formulations compatible with PINNs.

Second, we propose HIDE-PINNs, an extended framework for inverse problems involving unknown stationary or moving boundaries. By incorporating a phase-specific volume fraction field into the governing equations, the model rigorously enforces mass/momentum conservation in fluid regions while satisfying no-slip/no-penetration conditions at implicit solid boundaries.

Third, we develop a hybrid strategy that synergizes PINNs with traditional CFD solvers. Recognizing the limitations of conventional adaptive mesh refinement (AMR)—particularly unreliable error indicators—we introduce a PINNs-enhanced AMR framework. The method leverages PINNs to compute physics-informed residuals via automatic differentiation of coarse-mesh solutions, providing robust error estimation for guiding Delaunay-based mesh refinement. This solver-agnostic approach demonstrably improves the resolution of fine-scale flow features while maintaining computational efficiency.

Collectively, these innovations expand the applicability of PINNs to complex fluid-structure systems while establishing new pathways for augmenting conventional CFD with machine learning.

Keywords: physics-informed neural networks, flow construction, boundary detection, adaptive mesh refinement

Development of high Reynolds number immersed boundary methods

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Abstract

The immersed boundary method is widely used for simulating complex geometries in fluid flow and fluid-structure interactions. However, its major application is restricted to low and medium Reynolds numbers, as resolving thin turbulent boundary layers requires impractical isotropic grid refinement for high Reynolds number flows. To overcome this issue, the immersed boundary method has been coupled with turbulence wall models. A significant challenge in this coupling arises from the non-smooth distribution of boundary grids relative to the wall surface, causing spurious oscillations that pollute wall surface quantities (skin friction, pressure) and lead to erroneous drag and lift force predictions. Recent developments focus on reducing these oscillations to improve aerodynamic force estimation. Additionally, traditional algebraic wall models present challenges. They are computationally expensive to invert, particularly for industrial flows, and can diverge due to poor initial guesses in Newton iterations. Addressing this, a series of explicit algebraic wall models has been developed, offering ease of inversion and adaptability to different turbulence models. Crucially, these wall models and immersed boundary enhancements are integrated into a highly efficient fluid solver and investigated with RANS, LES, and hybrid RANS-LES approaches. Numerous benchmarks are considered to demonstrate the strength of the proposed method.

Keywords: Immersed boundary method, high Reynolds number, turbulent flow

Evolution of large-scale vortices and its influence on flow and flexible vegetation dynamics of a finite-length canopy in a 2-D laminar flow

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Abstract

Submerged flexible aquatic vegetation exists widely in nature and achieves multiple functions mainly through fluid–structure interactions (FSIs). In this paper, the evolution of large-scale vortices above the vegetation canopy and its effect on flow and vegetation dynamics in a two-dimensional (2-D) laminar flow are investigated using numerical simulations under different bending rigidity γ and gap distance d . According to the variation of large-scale vortex size and intensity, the evolution process is divided into four distinct zones in the streamwise direction, namely the ‘developing’ zone, ‘transition’ zone, ‘dissipation’ zone and ‘interaction’ zone, and different evolution sequences are further classified. In the ‘developing’ zone, the size and intensity of the large-scale vortex gradually increase along the array, while they decrease in the ‘dissipation’ zone. The supplement of vegetation oscillating vortices to large-scale vortices is the key to the enhancement of the latter. The most obvious dissipation of large-scale vortices occurs in the ‘transition’ zone, where the position of the large-scale vortex is significantly uplifted. The effects of γ and d on the evolution of the large-scale vortex are discussed. In general, the features of vegetation swaying vary synchronously with those of large-scale vortices. The flow above the canopy is dominated by large-scale vortices, and the development of flow characteristics such as time-averaged velocity profile and Reynolds stress are closely related to the evolution of large-scale vortices. The flow inside the canopy, however, is mainly affected by the vortex shed by the vegetation oscillation, which leads to the emergence of negative time-averaged velocity and negative Reynolds stress.

Investigation on Wake Hydrodynamics under Multi-operating Conditions of a Marine Propeller Based on Immersed Boundary Method

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Abstract

The wake flow generated by a marine propeller represents a highly complex turbulent motion in both temporal and spatial dimensions, which exhibits a significant correlation with the macroscopic performance of the propeller. Consequently, the study of wake fluid dynamics during the operation of marine propellers remains a focal point of ongoing research.

In this study, a self-developed solver based on Cartesian grids for spatial discretization was employed to investigate the wake flow of a three-bladed propeller. The immersed boundary (IB) method was applied to capture the effects of large-scale boundary motion caused by propeller rotation on the fluid. A ray-casting algorithm was introduced to characterize complex spatial geometric topologies, and a spatial coordinate matrix equation coupling propeller rotation dynamics with background orthogonal grids was established to dynamically update complex geometric descriptions. Under the premise of ensuring grid orthogonality and computational accuracy, high-fidelity large eddy simulations (LES) of both single-phase and multi-phase unsteady flows around the marine propeller were achieved at a scale of hundreds of millions of grid cells.

Based on the numerical simulation results, an investigation was conducted on the hydrodynamic statistical characteristics of the propeller wake under open-water conditions at different loading operations, as well as the nonlinear interactions between the wake and free surface of propeller operating near the free surface along with the corresponding turbulent wake features. Under open-water conditions, as the load increases, the stable positions of the quasi-periodically distributed wake along the circumferential direction shift radially outward from the hub-region, while the peak of total kinetic energy (KE) moves upstream of the propeller disk, and the interaction between tip vortices is enhanced, which leads to the early collapse of tip vortices accompanied by the increase of turbulent kinetic energy (TKE). When the propeller operates near the free surface, flow instability increases due to interactions between the wake and the free surface. Under heavy loading condition, free surface breakup and air intake occur, leading to further significant disruption of wake symmetry and consequently enhancing the dissipation of the wake flow.

Keywords: Marine propeller, immersed boundary method, large eddy simulation, wake hydrodynamics

Coupled peridynamic and lattice Boltzmann-immersed boundary method for fluid solid interaction

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Abstract: A coupling model between the peridynamic and lattice Boltzmann-immersed boundary method is established, to compute the dynamics of structural deformation and fracture caused by fluid solid interaction. First, the multiple-relaxation-time (MRT) lattice Boltzmann Method (LBM) serves as the flow solver, and the immersed boundary method (IBM) acts as the fluid-solid interface solver. Then using the peridynamic model to predict structural deformation and fracture. The strong coupling is achieved by adding velocity corrections for the fluid and solid phases simultaneously at each time step, which are calculated by solving a linear system of equations derived from an implicit force correction immersed boundary scheme. Meanwhile, the simulated immersed boundary force can be directly used as the hydrodynamic boundary conditions of peridynamic model. The proposed method is rigorously validated considering the cross-flow over a flexible beam, and the flow-induced deformation of an elastic beam attached to a rigid cylinder.

Keywords: peridynamic; immersed boundary method; lattice Boltzmann-immersed boundary method; fluid solid interaction; Hydraulic fracturing

Research Progress of Fluid-Solid Interaction about Hydroelectric Unit

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Abstract

In order to achieve complementary among wind, solar and hydropower, the function of hydropower will shift from "providing electricity" to "flexible regulation". The demand for "flexibility" has put forward an urgent need for hydropower units to have a wide range of regulation, fast regulation speed, and excellent regulation stability. However, due to insufficient operational flexibility, traditional hydroelectric units have significantly decreased efficiency, unstable operation even structural failure. Therefore, there is an urgent need for new design concepts to support the design of the new generation of ultra wide power stable regulation units. To this end, a system design concept based on dynamic loads is required. Through fluid-solid coupling synchronous computation, the dynamic loads of the unit under all operating conditions and transient conditions are identified, and structural response analysis is carried out synchronously.

Keywords: Hydroelectric unit; Flexible regulation; fluid-solid interaction; Dynamic load; Structural response

Analysis of Vibration Characteristics of a Pelton turbine Based on Two-Way FSI

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Abstract

The Pelton turbine is the preferred choice for utilizing hydropower with high head and low flow rate. Pelton turbines transfer the immense energy of water through high-velocity jets, concentrating energy exchange within an extremely confined area. This high-intensity, transient, and periodic load impact can easily induce severe vibrations, crack formation, and other issues in the turbine unit, ultimately compromising unit's safe operation. In order to reveal the internal flow characteristics, hydraulic performance, and structural response laws of an Pelton turbine under different operating conditions, this study conducts a full three-dimensional unsteady numerical investigation on a prototype Pelton turbine. Utilizing a two-way fluid-structure interaction approach, the research analyzes the vibration characteristics and explores the evolution of blade deformation and stress under varying load conditions.

Keywords: Pelton turbine, Vibration, Two-way FSI, Numerical simulation

Re-understanding and Application of Quasi-Coarse-Grained Dynamics

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Abstract

In recent years, mesoscale simulation approaches that leverage the scaling of atomic potential functions—with quasi-coarse-grained dynamics (QCGD) being a prominent example—have shown considerable utility in modeling crystalline systems, offering a computational bridge between atomic and mesoscopic scales. This study undertakes a systematic analysis to clarify the relationship between QCGD and molecular dynamics (MD) simulations, revealing that the spatiotemporal trajectories of QCGD systems exhibit a homothetic transformation relative to those of corresponding MD simulations, establishing a strict conjugacy between the two methodologies. Such conjugacy indicates that current QCGD implementations effectively amplify MD results across spatial and temporal dimensions while preserving key atomic-level structural features and thermodynamic properties (e.g., temperature, pressure, and stacking fault energy), which underpins its reliability for replicating atomistic-scale dynamics at extended scales.

While this inherent correspondence suggests that QCGD alone may not capture intrinsic scale-dependent effects that are absent in MD, it also highlights its strengths as a computationally efficient tool for extending the reach of atomistic simulations. Importantly, building on this established conjugacy, we propose a novel strategy to directly couple QCGD with MD simulations, enabling straightforward and efficient multiscale modeling. In this coupled framework, MD is employed to resolve fine-grained, atomistic-level details in regions where high precision is critical (e.g., defect nucleation and evolution), while QCGD is used to model larger, mesoscale domains with reduced computational cost. The strict spatiotemporal correspondence between QCGD and MD ensures seamless information transfer (e.g., momentum and energy exchange) across the coupled interface, avoiding artificial inconsistencies.

This work not only provides a nuanced understanding of QCGD's capabilities and limitations but also expands its application scope through the proposed MD-QCGD coupling strategy. It emphasizes that validating mesoscale methods against atomistic models remains essential, and that strategic coupling of complementary simulation tools offers a promising path to address multiscale challenges in materials science—particularly for crystalline systems where capturing both atomic-level defects and mesoscale structural evolution is critical.

Keywords: Mesoscale modelling, Quasi-coarse-grained dynamics, Molecular dynamics

Bending behavior of Diamane and Twisted Bilayer Graphene: Insights from Four-point Bending Deformation

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Abstract

The intriguing physical properties of two-dimensional (2D) nanomaterials make them promising building blocks for flexible electronics. Using a four-point bending approach, this work establishes a comprehensive understanding of the bending behavior of diamane – a 2D diamond nanostructure, from elastic deformation to structural failure through atomistic simulations. The four-point bending method accurately reproduces the pure bending of the sample, and the obtained force-displacement curve fit well with the classical Euler beam theory. Structural failure is observed from diamane under bending when its thickness or the number of layers increases. Atomic insights reveal that the crack initiates from the tension side of the sample, resulting in a tension-induced bending failure. Specifically, the bending limit is found to be slightly larger than the fracture strain under tensile deformation. Additionally, the bending behaviour of the diamane analogous – twisted bilayer graphene with interlayer-bonding (TBG^{IB}), has been investigated. Different from diamane, TBG^{IB} bends elastically at the initial stage and then experiences structural failures with increasing bending strain. Higher interlayer bonding density is observed to result in a higher bending stiffness. Meanwhile, significant interlayer shear strain is detected during bending, which leads to interlayer bond breakage, rippling, and buckling of the graphene layer. This work provides a full description of the pure bending behavior of diamane and its analogous structure, which could be beneficial for their applications in flexible electronics.

Keywords: Diamane; Twisted bilayer graphene; four-point bending; Molecular dynamics simulation

Molecular Dynamics Investigation of Hydrogen Diffusion in Polycrystalline α -Iron Under Multiaxial Stress States

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Abstract

Hydrogen diffusion is closely related to hydrogen embrittlement, which significantly affects material performance and structural integrity. Given that real-world engineering materials exhibit polycrystalline microstructures and typically operate under multiaxial loading conditions, this study employs molecular dynamics simulations to examine hydrogen diffusion coefficients in polycrystalline α -iron across various stress states. The study focused on both triaxial and uniaxial stress conditions to understand hydrogen diffusion behavior in complex stress environments. Under uniaxial stress states, hydrogen atoms exhibit enhanced diffusion coefficients under tensile stress conditions and reduced diffusion coefficients under compressive stress conditions, with the diffusion process demonstrating pronounced anisotropy under uniaxial tension or compression. Under triaxial stress states, the variation of diffusion coefficients with stress follows an Arrhenius-type relationship. This molecular dynamics simulation study provides valuable insights into the effects of stress states on hydrogen diffusion, which are critical factors for controlling hydrogen embrittlement phenomena in practical applications.

Keywords: Hydrogen diffusion; Triaxial stress state; Uniaxial stress state; Molecular dynamics

Sliding Behaviour of Carbon Nanothread within a Bundle Embedded in Polymer Matrix

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Abstract

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.

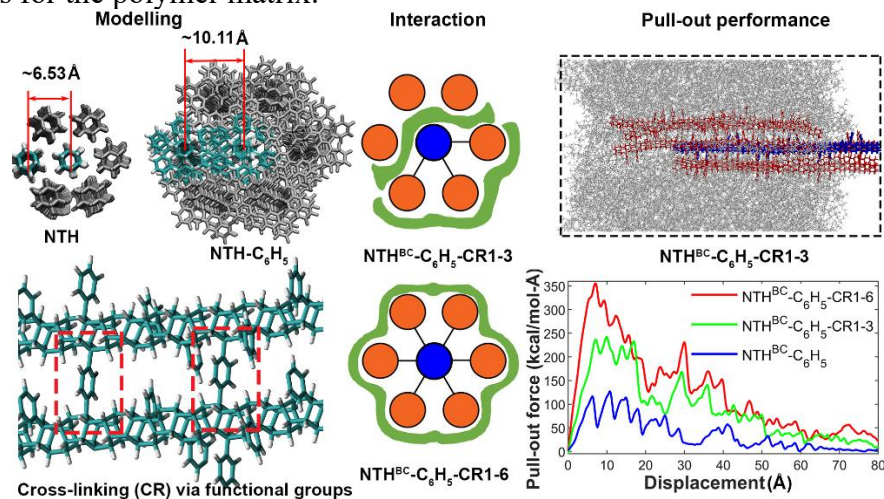


Figure 1. The Pull-out Behaviours of NTH from Bundle in Polymer Nanocomposite

Keywords: Carbon nanothread, Bundle, Polymer, Pull-out test, Molecular dynamic simulation

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Computational simulations of interfacial heat transfer and crystallization in 3D-printed continuous fiber-reinforced thermoplastic composites

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Abstract

The combination of continuous fiber-reinforced thermoplastic composites (CFRTPCs) and the 3D printing technique enables the rapid production of complex structural composites. Achieving the optimal performance of 3D-printed CFRTPCs necessitates a comprehension of their thermal transport and thermally-driven crystallization behaviors, which are strongly influenced by the fiber/matrix interfacial characteristics. However, experimental methods remain insufficient in resolving the molecular-level interactions and microstructural evolution during processing, leaving the governing mechanisms unclear. While computational simulations provide a powerful means to address this issue, such studies for 3D-printed CFRTPCs are still scarce in the literature.

In this study, we first investigated the interfacial thermal properties of thermoplastic composites with various filler materials using molecular dynamics (MD) simulations and theoretical model. We found that thermal resistance at interfaces exerts a notable effect on the effective heat conductivity of composites with high-volume fractions of nanofillers, whereas its influence is negligible in continuous fiber-reinforced composites. Second, we develop a non-isothermal phase-field model (PFM) for mesoscale simulating the crystallization process during the 3D printing of thermoplastic composites. We found that crystalline evolution is governed by the interplay of thermal history, fiber–matrix interfacial characteristics, and the spatial distribution of reinforcing fibers.

Our research illustrates a multiscale modeling approach to evaluate the interfacial thermal properties and thermally-driven crystallization process of thermoplastic composite, which could be extended to other composite systems. The findings could benefit the multiscale modeling of composite manufacturing and the micro-structure design of composites.

Keywords: thermoplastic composite, molecular dynamics, phase-field, interfacial, thermal properties, crystallization

Theoretical Prediction of stress-tunable Optoelectronic and Thermal Properties of GaSeI: A Novel 1D Helical van der Waals Crystals

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Abstract

One-dimensional (1D) van der Waals materials demonstrate exceptional potential for applications due to their unique electronic and mechanical properties. Among them, the recently synthesized 1D GaSeI nanochain features a non-centrosymmetric helical structure with individual helical chains interconnected by weak van der Waals interactions. Remarkably, these nanochains can be readily isolated from the bulk crystal using a straightforward micromechanical exfoliation method. Using first-principles calculations, we predicted the dynamic stability as well as the mechanical, electronic and optical properties of 1D GaSeI nanochains. 1D GaSeI exhibits an indirect band gap of 2.44 eV, with hole carrier mobility ($20.23 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$) approximately five times higher than that of the electron mobility ($4.06 \text{ cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$). Furthermore, 1D GaSeI can withstand a tensile strain of 22.5% along the chain direction, with a Young's modulus of ~ 25.6 GPa. Such mechanical flexibility endows the nanochains with exceptional stress tunability, motivating further investigation into the effects of strain on their electronic structures. Notably, under a compressive strain of 7.5%, 1D GaSeI nanochain undergoes a band gap transition from indirect to direct. The electronic localization function and optical properties of 1D GaSeI under various deformations are further analyzed. The nanochain exhibits a high absorption coefficient of $\sim 105 \text{ cm}^{-1}$ in the ultraviolet range along the chain direction. In addition, we developed a machine learning potential (NEP) based on a training set constructed using ab initio molecular dynamics (AIMD) simulations. Using this potential, we obtained stress-strain responses at various temperatures, which revealed that elevated temperatures increase the propensity for fracture. Finally, nonequilibrium molecular dynamics (NEMD) simulations were employed to evaluate the thermal conductivity under different applied stress, demonstrating that thermal conductivity decreases with increasing stress. These remarkable properties of 1D GaSeI nanochain highlight the potential of helical nanostructures in nonlinear optics and electronic device applications.

Keywords: 1D GaSeI nanochain, stress-tuned optoelectronic properties, stress-tuned thermal properties, first-principles calculation, molecular dynamics

A super-coarse-grained simulation method for cellulose nanofiber networks

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Abstract

Cellulose nanofiber networks are a class of widely investigated advanced material systems that can be both strong and tough systems. Currently, there are rare general computational models of nanofiber networks that can quantitatively produce stress-strain curves that resemble those of macroscopic measurements (e.g., failure strain), which poses significant challenges for understanding and designing cellulose-based materials with exceptional mechanical properties. This talk presents a scale-bridging approach to address multiscale modeling challenges. Recognizing that the macroscopic mechanical properties of cellulose nanofiber networks are governed by inter-fiber interface interactions, we develop a super-coarse-grained (SCG) computational concept that emphasizes on directly capturing these interactions. Individual nanofiber with diameter exceeding 100 nm and length of over 1.5 μm can be easily modeled. The nature of scale-bridging manifests in the accomplishment that although SCG parameters are systematically derived from atomistic molecular simulations, they can be rationalized by physical reasoning, and the resulting stress-strain curves agree well with experimental data.

Numerical Sandbox Experiments with DEM: Frictional and Structural Controls on Prism Deformation

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Abstract

Discrete Element Method (DEM) simulations [1] provide a versatile framework for investigating rock deformation processes in general [2], and for examining the structural evolution of faults in tectonic settings in particular [3, 4]. Our numerical sandbox experiments involve representing brittle upper-plate materials as assemblies of discrete particles [3, 4]. Unlike approaches that often rely on constitutive weakening laws to trigger localization [5], DEM generates fault-like structures as an emergent property of grain-scale interactions. This enables us to capture the nucleation, linkage, and evolution of fault networks under tectonic loading. By systematically varying the basal friction coefficients and geometry of the horst–graben domains, we can quantify the sensitivity of the emergent fault patterns to mechanical and structural parameters.

The simulations reproduce key features observed in natural subduction zones, such as thrust stacking, vergence asymmetry, and fault bifurcation. We then compare these features to geological evidence from the Japan Trench. Crucially, our results demonstrate how DEM can resolve deformation localisation driven by upper-plate heterogeneity. While continuum models reproduce localization by prescribing weakening through complex constitutive laws such as visco-plasticity or strain-softening [5], DEM generates weakening and subsequent fault development as natural outcomes of particle-scale interactions.

Keywords: Discrete Element Method, numerical sandbox, subduction zones, accretionary prism, graben structures, tectonic deformation

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Micromechanical Simulation of Liquefaction using 2D Solid-DEM and Liquid-FEM Coupling with Body-fitted Mesh

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Abstract

Liquefaction of saturated granular materials is often discussed in broad, intuitive terms, with limited reference to micro-mechanics or computations based on the governing equations of motion. In this research, we present two-dimensional fully micromechanical, in which each grain is individually resolved and particle-scale interactions are explicitly modeled, simulations of a saturated granular matrix in fluid subjected to vibration. The solid phase is modeled using the discrete element method (DEM) with polygonal particles, while the surrounding fluid is resolved using the finite element method (FEM) for incompressible viscous flow on a body-fitted triangular mesh. The DEM computes particle motion based on Newton's equations, while the FEM solves the incompressible Navier–Stokes equations. This fully resolved coupling enables accurate computation of the flow's features—such as boundary layers and vortices—through the complex pore spaces formed by the polygonal particles, which act as moving boundaries for the fluid. We emphasize the importance of capturing flow behavior along particle surfaces to accurately compute fluid–solid interactions, particularly the form drag and friction drag forces acting on the particles. To maintain mesh quality during deformation, we implement an adaptive mesh “relaxation” procedure. The results illustrate the onset and progression of liquefaction, including particle escape through gaps on the surface of the system. We discuss the micromechanics of the liquefaction based on the evolution of the force network in the granular matrix.

Keywords: Liquefaction, Granular materials, Discrete Element Method, Finite Element Method, Incompressible flow, Adaptive mesh.

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Granular simulation of earthquakes in geological-scale structural evolution

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Abstract

We present virtual earthquake simulation and its energy balance analysis using a numerical granular rock box experiment based on the Discrete Element Method (DEM). The rock box simulation is performed using the code named DEPTH (DEM based Parallel mulTi-pHysics simulator), which utilizes hybrid parallelization for shared and distributed memory systems with dynamic load balancing [1]. The DEPTH was used for real scale numerical sandbox simulation utilizing 1.9 billions of DEM element [2]. The rock box experiment is an extension of the numerical sandbox test with cohesive contact force to mimic the failure behavior of rocks. Horizontal shortening of a granular rock layer, comprising over 6 million elements within a thin 3D geometry, produced sequential thrust formation reminiscent of an accretionary wedge across a 100 km domain [3]. Intermittent, fast millimeter-scale motions of elements along faults, which generate seismic waves, were observed during a slow convergence test [4]. This indicates that the granular rock box simulation provides a new seamless model bridging seismological and geological-scale phenomena. The hypocenter, which was not predefined by the model, emerged within the active fault damage zone and shifted as the geological structures evolved. The seismic event occurred with the shear motion of the fault, characterized by the 3D elementwise rotation and the double-couple behavior, and followed the Gutenberg–Richter law. We also analyze energy budget over 150 earthquake events with a total shortening of 15 m [5]. One of the interesting aspects of the energy balance analysis of the granular rock simulation is that it includes the energy of the structural changes during the earthquake event. Our analysis revealed changes in energy balance with the local fault potential/stress drop generated the main shock, regional potential/stress release triggered by wave propagation, and the gravitational energy change with uplift of the popup as an early post seismic event.

Keywords: DEM, HPC, Seismology, Geology, Granularity

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Multiphase continuous-discrete modelling of geological hazards with particle method

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Abstract

Geological hazards become increasingly frequent and disastrous due to climate change. Accurate modelling is crucial for hazard identification, risk assessment, mitigation and prevention. Geological hazards include many different types such as landslides, debris flows, rock avalanches, rockfalls, and snow avalanches, among others. They can also trigger hazard chains such as landslide tsunamis, landslide dams and dam break floods. These phenomena involve different materials and different mechanisms and pose extremely high requirements to numerical methods. For example, landslides and mud flows can be considered as single-phase continuous material, but landslide tsunamis should be considered as a dynamic water-soil coupled problem, whereas debris flows and their interactions should be modeled as continuous-discrete system due to the existence of large boulders.

A unified numerical method for geological hazards and hazard chains should be able to model the following items: (1) free-surface flows for the fluid phase; (2) large deformation for the solid phase; (3) dynamic water soil coupling; (4) various material constitutive models for varying materials; (5) discrete method to model boulders and objects with arbitrary shape; (6) coupled continuous-discrete problems; (7) high-performance computing for realistic 3D simulations.

A multiphase continuous-discrete SPH-DEM method is developed for the simulation of geological hazards and hazard chains. It fulfills all the requirements above. By utilizing single and overlapping SPH particle layers, it can model problems with single phase fluid/solid, as well as coupled soil-water dynamic problems. By coupling with a newly developed surface mesh represented DEM, it has the full capability to simulate continuous and continuous-discrete geological processes. Furthermore, the SPH-DEM method is accelerated using GPU high-performance computing, making it applicable to large-scale engineering applications.

Keywords: Geological hazards, hazard chains, multiphase SPH, continuous-discrete SPH-DEM coupling, GPU acceleration.

A coarse-grained model for gas transport in swelling porous media

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Abstract

Many porous materials—such as soils, organic matters, and gels—exhibit significant deformation upon fluid absorption. This fluid-induced swelling behavior is critical in a range of applications. In petroleum engineering, for example, understanding fluid flow through swelling porous rocks is essential for optimizing oil and gas recovery, as rock deformation alters reservoir porosity and permeability [1, 2]. Similarly, in carbon geo-sequestration, injected CO₂ adsorbs into the rock matrix, inducing internal stress that reduces permeability and gas injectivity [3, 4].

Despite its importance, the coupled interaction between fluid flow and solid deformation in porous media remains incompletely understood, largely due to the complexity of capturing dynamic fluid-solid interactions at moving interfaces. To address this, we propose a novel coarse-grained molecular dynamics (CGMD) model that explicitly incorporates gas-gas, solid-solid, and gas-solid interactions to simulate the coupling between gas transport and solid deformation at the microscale.

The CGMD framework accurately reproduces key material properties—including gas viscosity, solid density, and Young's modulus—and enables the generation of a wide range of swelling ratios relevant to nanostructured systems via innovative bead-spring chain networks. We compare gas transport through deformable and non-deformable nanochannels of varying sizes, benchmarking the results against the macroscopic Hagen–Poiseuille equation. The model is further applied to a simplified nanoporous medium composed of randomly distributed spherical solids. While the Kozeny–Carman equation generally captures the permeability–porosity relationship, deviations are observed in the presence of swelling.

Our findings demonstrate that swelling significantly reduces gas permeability and highlight the potential of the CGMD approach for modeling gas transport in deformable porous media. This framework offers new insights for applications in nanofluidics, energy storage, and environmental nanotechnology.

Keywords: Coarse-grained molecular dynamics; Swelling porous media; Gas transport; Bead-spring chain networks; Fluid-solid interaction.

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Pullout of a plate anchor from a granular medium beyond material failure

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Abstract

Plate anchors are a common method to stabilize geotechnical structures. While they have been extensively studied numerically by means of continuum methods, most studies have been limited to small displacement due to numerical issues pertaining the deformation of the soil during pullout. In this work we study the pullout process of a plate anchor by means of a Discrete Element Method beyond the point of immediate failure. We show that the evolution of the mobilized material is directly related to the evolution of the resistance-displacement curve. The formation of hopper-like structures at the anchor boundaries then provides material transport from above to below the plate. Despite using a two-dimensional simulation, our results are in good agreement with results obtained from three dimensional laboratory experiments.

Keywords: Intruder pullout, Pullout resistance, Micro-mechanics, Avalanching, Discrete Element Method.

Unveiling Heat Transfer Pathways in Unsaturated Granular Materials via Network Modeling

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Abstract

Understanding heat transfer mechanisms in unsaturated granular media is crucial for geo-engineering applications. However, the specific pathways through which heat is transmitted between particles have not been quantitatively characterized. This study identifies six distinct pathways of heat transfer within granular assemblies under varying saturation levels: (a) direct particle contact accompanied by air bridges, (b) direct contact with both air and water bridges, (c) direct contact with water bridges only, (d) non-contact particles linked via air bridges, (e) non-contact particles linked through both air and water bridges, and (f) non-contact particles connected solely by water bridges.

To evaluate the thermal contribution of each pathway, a thermal conductance network model was constructed. In this framework, particles are represented as nodes, and the connections—whether physical or mediated by air/water bridges—are modeled as edges. Each edge is assigned a thermal conductance value, which serves as its weight in calculating the overall effective thermal conductivity of the system. The model's predictions showed strong agreement with experimental measurements. Notably, under unsaturated conditions, heat transfer is predominantly governed by edge types (b), (e), and (f), highlighting the significant role of water-mediated and mixed-phase connections in thermal transport.

Keywords: Heat transfer path, unsaturated, network model, thermal conductivity

A coupled 3D MPS–NOSB-PD model for fluid–structure interaction with large deformation

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Abstract

This study focuses on achieving the coupling of the three - dimensional Moving Particle Semi - implicit (MPS) method and Non - Ordinary State - Based Peridynamics (NOSB - PD) method, wherein the MPS method is used to handle the fluid flow, while the peridynamics method deals with the solid deformation of the elastic plate. First, the accuracy of the peridynamics solver is validated through the vibrating beam and the Kalthoff–Winkler experiment. Then, two numerical examples of dam - break flow interacting with an elastic plate and dam - break flow through an elastic plate are simulated to verify the accuracy of the three - dimensional fluid–structure interaction (FSI) solver. Finally, the developed FSI solver is applied to simulate a fluid–structure interaction problem considering structural fracture. This research provides an effective numerical tool for studying complex FSI phenomena, which is of great significance for understanding the dynamic response of structures under fluid impact.

Three-dimensional micromechanical expression for the average strain tensor of granular materials

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Abstract

In investigations of the behaviour of granular materials, the conversion of discrete contact information, specifically the force and displacement data, into macroscopic quantities such as stress and strain is a fundamental approach. The expression for the average stress tensor, a well-established formulation, involves the summation over all interparticle contacts while considering both the contact force and geometric parameters such as the branch vector. However, for the three-dimensional case, a general micromechanical expression for the average strain tensor is still missing.

In this study, a three-dimensional micromechanical expression is derived for the average strain tensor of granular materials. The new expression for the strain tensor involves only particle positions and relative displacements between particles, and does not depend on the tessellation method applied to the space occupied by the particles and interparticle voids. To validate the accuracy of the strain tensor, displacement data of granular assemblies were generated through Discrete Element Method simulations, and the strains of granular assemblies calculated by the derived strain tensor were compared with those calculated from the macroscopic deformation of granular assemblies. The results demonstrate that the proposed strain tensor is consistent with the macroscopic strain tensor, either in triaxial compression or in simple shear tests. This research conclusively addresses the fundamental question for the three-dimensional micromechanical strain tensor of granular materials and contributes to the development of accurate micromechanics-based constitutive models for granular materials.

Hybrid deep learning and iterative methods for accelerated solutions of viscous incompressible flow

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Abstract

The pressure Poisson equation, central to the fractional step method in incompressible flow simulations, incurs high computational costs due to the iterative solution of large-scale linear systems. To address this challenge, we introduce HyDEA (Hybrid Deep LEarning line-search directions and iterative methods for Accelerated solutions), a novel framework that synergizes deep learning with classical iterative solvers. It leverages the complementary strengths of a deep operator network (DeepONet) – capable of capturing large-scale features of the solution – and the conjugate gradient (CG) or a preconditioned conjugate gradient (PCG) (with Incomplete Cholesky, Jacobi, or Multigrid preconditioner) method, which efficiently resolves fine-scale errors. Specifically, within the framework of line-search methods, the DeepONet predicts search directions to accelerate convergence in solving sparse, symmetric-positive-definite linear systems, while the CG/PCG method ensures robustness through iterative refinement. The framework seamlessly extends to flows over solid structures via the decoupled immersed boundary projection method, preserving the linear system's structure. Crucially, the DeepONet is trained on fabricated linear systems rather than flow-specific data, endowing it with inherent generalization across geometric complexities and Reynolds numbers without retraining. Benchmarks demonstrate HyDEA's superior efficiency and accuracy over the CG/PCG methods for flows with no obstacles, single/multiple stationary obstacles, and one moving obstacle – using fixed network weights. Remarkably, HyDEA also exhibits super-resolution capability: although the DeepONet is trained on a 128×128 grid for Reynolds number $Re = 1000$, the hybrid solver delivers accurate solutions on a 512×512 grid for $Re = 10,000$ via interpolation, despite discretizations mismatch. In contrast, a purely data-driven DeepONet fails for complex flows, underscoring the necessity of hybridizing deep learning with iterative methods. HyDEA's robustness, efficiency, and generalization across geometries, resolutions, and Reynolds numbers highlight its potential as a transformative solver for real-world fluid dynamics problems.

Keywords: hybrid method, deep operator network, iterative method, incompressible flow, Poisson equation

A Novel Mesh-Based Data-Driven approach for Optimization of Tidal Turbine Blades

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ABSTRACT

As the global demand for renewable energy rises, tidal energy has emerged as a reliable and predictable source. Yet, optimizing the design of horizontal axis tidal turbine (HATT) blades to maximize their efficiency presents a formidable challenge. This paper addresses this challenge by introducing TurbineNet, an innovative data-driven model designed to enhance the prediction of hydrodynamic performance for blade shape optimization. Specifically, TurbineNet leverages a sophisticated mesh-based representation of blade, incorporating advanced mesh convolution and fully connected neural network layers to extract and analyze spatial and structural features. This approach achieves a remarkable prediction accuracy with an error margin of less than 2%. Integrating TurbineNet with free form deformation (FFD) and differential evolution (DE) optimization algorithms, the study optimizes the NREL S814 blade model to maximize its power coefficient. The optimization results demonstrate a substantial improvement, with at least a 20% increase in power coefficient across various tip speed ratios. Furthermore, incorporating complex blade surface deformations through FFD offers an additional improvement of nearly 1% compared to traditional optimization methods that focus exclusively on variations in twist and chord length. These findings underscore the efficacy of utilizing neural networks for blade design recognition and optimization, significantly enhancing both performance prediction and the design space for HATT blades. The study represents a significant advance in the application of neural networks to tidal turbine optimization, paving the way for future research to address practical design considerations such as inflow fluctuations, structural strength, and refined experimental validation.

Keywords: Horizontal axis tidal turbine (HATT); Shape optimization; Mesh convolution; Free form deformation; Neural Network; Differential evolution.

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Simulation of bond failure between FRP bar and concrete based on a full mesoscale model

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Abstract

The interfacial bond performance between FRP bars and concrete is critical to the structural load-bearing capacity and durability. To investigate the nonlinear bond behavior of the FRP–concrete interface, a three-dimensional full mesoscale finite element model for the FRP bar pullout specimen was developed, incorporating the geometric configuration of FRP bars, the mesostructure of concrete, and their interactions. The geometries of the FRP bar are established by reverse modeling, and the mesoscale model of the concrete block is simulated by a random aggregate generation algorithm. A comparison with conventional mesoscale interface models was also conducted, and the effects of various parameters on interfacial bond performance, including bond failure modes, bond–slip curves, and ultimate bond strength, were systematically analyzed. It is verified that the proposed approach is capable of capturing the fluctuated trend of the bond-slip curve, which is observed in the experiment but is difficult to simulate by a traditional finite element model. Results show that the surface morphology of FRP bars and the aggregate distribution in concrete have a significant influence on the bond behavior. The proposed model successfully reproduces the entire bond failure process and provides an effective tool for failure analysis of FRP–concrete structures.

Keywords: FRP bars; concrete; numerical simulation; interfacial bond–slip; full mesoscale model

Axial Compression Capacity Prediction Model of FRP-Steel-Concrete Composite Columns Based on Stacking Ensemble Learning

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Abstract : This study addresses the limitations of traditional theoretical formulas in predicting the axial compressive bearing capacity of FRP-steel-concrete composite columns, particularly their insufficient accuracy and the limited generalization ability of single machine learning models. A high-precision prediction model based on stacking ensemble learning is proposed. By integrating 661 sets of experimental data from multiple literature sources, a high-quality dataset covering 15 types of cross-sections was constructed. In terms of model construction, GBDT, RF, and CatBoost were selected as base learners, with linear regression serving as the meta-learner. The results demonstrate that the Stacking ensemble model significantly outperforms all base learners across performance metrics on the test set, with the feature importance ranking exhibiting a high degree of consistency with the mechanical mechanism of "compressive and confinement-induced strengthening in concrete." Additionally, an engineering-oriented prediction platform based on PyQt5 was developed, enabling "programming-free" parameter input and bearing capacity prediction, thereby effectively facilitating the transition from theoretical models to engineering applications. This research provides a high-precision and highly interpretable solution for predicting the axial compressive bearing capacity of composite structural columns, offering significant theoretical value and practical engineering implications.

Keywords : Stacking Ensemble; FRP-Steel-Concrete Composite; Axial Compression Bearing Capacity Prediction; Machine Learning; Predictive Platform

Macroscale and mesoscale modelling of interfacial debonding between FRP and concrete

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Abstract

Interfacial debonding between fiber-reinforced polymers (FRP) and concrete is one of the most common failure modes in externally bonded FRP (EBFRP)-strengthened concrete structures, typically occurring within a thin layer of concrete near the interface. This study presents two numerical approaches, i.e., the finite element method (FEM) and the scaled boundary finite element method (SBFEM), to simulate the interfacial debonding process between FRP and concrete. Numerical models at two different scales, namely the macroscale model and mesoscale model, are established. In the macroscale model, highly refined meshes are used in the region near the interface to capture the accurate debonding behavior of EBFRP-strengthened concrete. Quadtree meshes are employed in SBFEM to achieve multi-level subdomains with a fast transition, rather than free meshes in FEM. An integral-type nonlocal damage model is used to eliminate mesh sensitivity. The effects of various factors, including concrete strength, FRP stiffness, and bonding length, on the interfacial bonding performance are discussed. In the mesoscale model, the mesostructure of the concrete substrate is generated by a random walking algorithm. The effects of concrete heterogeneity and adhesive properties on the interfacial bonding performance are investigated. It is found that the impact of concrete heterogeneity cannot be neglected.

Keywords: Finite element method, scaled boundary finite element method, nonlocal damage, interfacial debonding, mesh-independent, fiber-reinforced polymer

Analysis of the Effect of an Electric Field on the Vibrational Properties of Hexagonal Boron Nitride and Boron Nitride Nanotubes

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Abstract

Many two-dimensional materials exhibit piezoelectric effects, enabling the modulation of nanoresonators through electric fields. This study takes hexagonal boron nitride and boron nitride nanotubes as examples and investigates the effect of electric fields on its thermal vibrations using classical molecular dynamics methods and semi-empirical quantum mechanics methods. The results indicate that in classical molecular dynamics, the influence of the electric field on vibrations primarily stems from electric field forces, whereas in semi-empirical quantum mechanics methods, both electric field forces and non-electric field forces play a role. In light of these findings, we have developed a force field suitable for both hexagonal boron nitride and boron nitride nanotubes, which accurately describes the contributions of both electric field forces and non-electric field forces to vibrations. The feasibility of transferring the force field parameters from hexagonal boron nitride to boron nitride nanotubes was discussed. The force field was tested under various conditions, including different sizes, pre-strains, forces, and electric fields, and the results were consistently satisfactory. Regarding boron nitride nanotubes, we further extended the analysis to investigate the influence of varying diameters and external electric fields on their breathing modes. Finally, the new force field was applied to analyze structures with dimensions closer to experimental scales, such as multi-walled boron nitride nanotubes and hexagonal boron nitride sheets supported on silicon substrates. This research provides a new perspective for studying the influence of electric fields on two-dimensional piezoelectric materials.

Keywords: force field, piezoelectricity, electric field, natural frequency

Advanced hygrothermal flexural analysis of functionally graded plates using generalized differential quadrature and higher-order Haar wavelet methods

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Abstract

This work presents an advanced numerical framework for the flexural analysis of functionally graded (FG) and functionally graded coated (FGC) thin plates subjected to hygrothermal environments. The formulation incorporates the coupled influence of temperature variation and moisture concentration on material properties, which are assumed to vary continuously through the thickness direction. To ensure high accuracy and computational efficiency, the Generalized Differential Quadrature Method (GDQM) and the Higher-Order Haar Wavelet Method (HOHWM) are employed. The proposed approach is validated against benchmark elasticity solutions and existing differential quadrature formulations, demonstrating excellent agreement. Numerical results confirm that the present methodology effectively captures hygrothermal effects while offering superior convergence, stability, and accuracy compared with conventional DQ techniques. The developed framework highlights the potential of GDQM and HOHWM as reliable and efficient tools for the analysis and design of FG and FGC structural components in advanced aerospace, marine, and thermo-mechanical applications.

Keywords: Functionally graded plates; Hygrothermal loading; Bending analysis; Generalized Differential Quadrature Method (GDQM); Higher-Order Haar Wavelet Method (HOHWM); Flexural behavior

Hybrid depth physics-informed neural network for solving partial differential equation

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Abstract

Physics-informed neural networks (PINNs) have emerged as a promising tool for solving complex partial differential equations, but conventional PINNs struggle with slow convergence, gradient vanishing, and poor handling of localized physical features. This paper proposes a hybrid depth physics-informed neural network (hd-PiNN) for solving partial differential equation. The proposed hd-PiNN introduces a hybrid-depth framework that integrates deep and shallow sub-networks in parallel. The deep sub-network captures global physical characteristics, ensuring a comprehensive understanding of the system, while the shallow neural network focuses on localized details and small-scale physical features, improving approximation accuracy in complex regions. In addition, a nested activation function is introduced in the shallow sub-network to further improve feature extraction, allowing it to efficiently capture complex features using shallower layers. This reduces dependence on deep networks and enhances the model's ability to reflect the system's underlying dynamics more effectively. By incorporating hybrid-depth structures, hd-PiNN balances depth and locality, enabling it to achieve more precise solutions, improve convergence rates, and enhance overall computational stability. Theoretical analysis demonstrates that hd-PiNN avoids suboptimal convergence with appropriate initialization. The proposed approach is validated across multiple PDEs, including heat transfer scenarios with complex boundaries, Allen-Cahn equation, and fluid dynamics. Results show that hd-PiNN exhibits the superior capabilities in approximating and capturing intricate system features. These findings underscore the computational efficiency and potential of hd-PiNN in tackling real-world and complex problems

Keywords: Physics-informed neural network, nested activation function, hybrid depth blocks, partially known physical laws.

Vibrational analysis of sp^3 carbon nanostructures via atomistic simulations and continuum mechanics models

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Abstract

In past years, nanoelectromechanical systems (NEMS) attract interest from broad fields. The excellent vibrational properties of low-dimensional nanomaterials are crucial, which allows the detection of minute frequency shift under external perturbations. Recently, low dimensional sp^3 carbon nanostructures have attracted increasing attention, due to their unique properties. 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. Based on continuum mechanics 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 diamond nanosheets are studied. It is found that the Mindlin plate model can effectively predict the natural frequencies of diamond nanosheets with different thicknesses under different boundary conditions.

This work provides a comprehensive understanding of the vibrational properties of diamane and diamond nanosheets, which should be beneficial to the design and fabrication of ultrasensitive nanoresonators.

Keywords: Diamane and diamond nanosheets, molecular dynamics simulations, Kirchhoff plate model, Mindlin plate model

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Numerical Simulation and Theoretical Prediction of Ultimate Tensile Capacity for Screw Piles

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Abstract

Screw piles have gained widespread application due to their superior installation efficiency and load-bearing capacity. The discrete element method (DEM) serves as a powerful tool for investigating screw pile installation processes and bearing mechanisms. However, current DEM applications face limitations in computational efficiency and boundary condition simulation, while the unique structural configuration of screw piles introduces complexities in ultimate uplift capacity prediction that require further refinement. This study employs the DEM to simulate both the installation and pullout behavior of screw piles. An elastic boundary method was developed that enhances computational efficiency without compromising accuracy. The findings demonstrate that ultimate uplift capacity exhibits an inverse relationship with pile shaft diameter, a positive correlation with helix diameter and quantity, and a nonlinear dependence on helix spacing ratio. Either conventional cylindrical shear or the individual bearing model suffers from significant limitations. This study enhanced methodology introduces a transitional behavior mechanism where: (i) both cylindrical shear and individual bearing models coexist and interact complementarily at small spacings through a weighting function, and (ii) pure individual bearing dominates at larger spacings. This advancement overcomes fundamental shortcomings of traditional approaches and achieves superior prediction accuracy, providing more reliable design tools for engineering practice.

Keywords: Screw pile, discrete element method, ultimate uplift capacity, cylindrical shear model, individual bearing model

GPU-accelerated MPM-LSDEM approach for particle-continuum interaction

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Abstract

Aiming at the challenges of numerical stability and computational efficiency in modeling of complex interactions between irregularly shaped particles and large-deformation continua, this study proposes a unified framework based on GPU-parallelized material point method-level set discrete element method (MPM-LSDEM). By deeply integrating LSDEM's geometric representation capability for irregular particles and MPM's advantage in large-deformation analysis of multiphase media (elastoplastic solids/non-Newtonian fluids), this framework establishes a coupled particle-continuum multiscale simulation system. Key innovations include: (1) Constructing multi-level dynamically linked cells based on a double-layer Verlet neighbor list to enhance contact detection efficiency for polydisperse particles; (2) Establishing an energy-conserving contact model with barrier function constraints to effectively suppress contact penetration and ensure numerical robustness of interfacial interactions; (3) Designing a dynamic GPU memory partitioning strategy to optimize MPM background grid management, improving computational efficiency by two orders of magnitude for large-scale multiphase coupling problems. Through systematic numerical validation, this framework has been successfully applied to multiple typical scenarios such as particle-structure collisions and soil-fluid coupling, demonstrating exceptional computational accuracy and accelerated performance, thereby providing an efficient solution for modeling complex multiphase coupled systems.

Keywords: Granular material, Level-set DEM, MPM, GPU parallel computing, Particle-continuum interaction

Self-consistent Clustering Analysis-Based Dual-scale Ablation Mechanism and Performance Prediction of Silica Fiber-Reinforced Phenolic Resin Composites (SiFPRCs)

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Abstract

Silica Fiber-Reinforced Phenolic Resin Composites (SiFRPC) are widely utilized in thermal protection systems and structural materials for hypersonic vehicles due to their superior insulation and ablation resistance. A profound understanding of the ablation mechanisms and numerical analysis of SiFRPC holds significant theoretical and engineering value. This study first employed high-precision in-situ CT technology to explore the micro-ablation characteristics of SiFRPCs under oxyacetylene ablation conditions, including the evolution of microstructures, porosity, and microcracks, revealing the ablation performance along the thickness direction, such as regional layer thickness and layer-wise porosity distribution. Within the framework of non-equilibrium thermodynamics, a cross-scale consistent variational model coupling heat conduction and pyrolysis characteristics of SiFRPCs was developed, implemented via a nonlinear finite element method for thermo-mechanical co-simulation across scales. To efficiently simulate the coupled thermo-mechanical ablation process, this study advanced a multiscale incremental solution technique based on homogenization theory and a self-consistent clustering algorithm. By reducing the high-fidelity RVE to a cluster-based RVE during the offline phase, a new clustering solution strategy integrating strain concentration tensors and thermal concentration tensors was formulated, assessing the thermo-mechanical interaction tensors between clusters. During the online phase, by solving the cluster-based discrete incremental LS equations, the ablation response and performance evolution of SiFRPCs were precisely simulated. The theoretical models and solution techniques developed in this study comprehensively consider various thermal dissipation mechanisms such as the thermal decomposition of phenolic resin, thermal blocking effect, phase change in silica fibers, carbon-silica reaction, and oxidation processes. Comparisons between model predictions and experimental results demonstrate that the model considering thermal dissipation effects accurately describes the ablation behavior. This research provides robust theoretical support and a design foundation for the development of high-performance materials for thermal protection systems.

Multi-scale collaborative optimization design method for multi-layer thermal protection structures

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Abstract

This study introduces an innovative concurrent optimization framework utilizing the Generalized Multiscale Finite Element Method (GMsFEM) to optimize the balance between thermal insulation and load-bearing capabilities in Integrated Thermal Protection Systems (ITPS). First, we detail the application of GMsFEM for efficient and accurate analysis of hierarchical ITPS, including the construction of numerical basis functions and the computation of equivalent structural matrices. Second, to balance design flexibility with computational efficiency, we develop a parameterized lattice characterization model that rapidly predicts the equivalent stiffness matrix, thermo-mechanical coupling matrix, heat conduction matrix, and heat capacity matrix. Third, a concurrent optimization model is established to simultaneously optimize lattice layout and configuration. To address limitations of standard optimization methods, which often overly restrict maximum backface temperature, we formulate the objective function as a combination of structural compliance and a penalty term for mechanical compliance. This approach prevents the design domain from being dominated by low load-bearing insulation materials. Consequently, the proposed method achieves an effective balance between thermal insulation and structural performance at a manageable computational cost. Finally, a representative numerical example demonstrates the efficacy of the proposed concurrent optimization approach, showing significant improvements in the thermal protection performance of ITPS through optimized lattice layout and configuration.

Plant-inspired Crashworthiness Design for Composite Materials

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Abstract

This study takes inspiration from the coconut in nature to study the crash-resistance design of the structure. In terms of theoretical research, Hashin and Tsai-Wu criteria were used to quantitatively analyze the mechanical behavior and energy absorption mechanism of coconut peel materials from different angles, and it was found that the macroscopic ordered arrangement of fibers was the key factor affecting energy absorption. In addition, the effect of fiber arrangement on the stress wave propagation and the stress wave propagation in the variable cross-section were revealed by establishing the coconut model and the fluid-structure coupling model of the ecological structure in free fall. Based on the discovery and interpretation, a biologically inspired mechanical model is proposed to guide the design and preparation of biomimetic energy-absorbing structures of composite materials. This model improves the energy absorption capacity per unit mass of the composite structure.

Keywords: Plant, Stress wave, Energy absorption, Composite Structure, Crashworthines

Programming nonlinear thermo-mechanical intelligence via topology optimization

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Abstract

Nonlinear material behaviors play a crucial role in many modern applications, and the ability to precisely program the nonlinear responses of materials and structures offers significant benefits. Here, we employ state-of-the-art topology optimization (TO) techniques to inverse design nonlinear force–displacement curves, three-dimensional deformation modes, and temperature-tunable nonlinear behaviors. This approach enables the creation of multimaterial structures with complex geometries that accurately realize prescribed target responses. The optimized designs are fabricated through innovative mold-and-casting methods as well as multimaterial 3D printing, with the resulting specimens successfully reproducing the intended complex behaviors. Together, the TO-based inverse design and fabrication strategy establishes a systematic route for customizing virtually any desired nonlinear behavior.

Information Geometry Perspective on Constitutive Models and Its Inspired Dual-Space Model Optimization

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Abstract

Advanced medical solutions rely on dependable biomechanical modeling. An enduring challenge in the constitutive modeling of soft tissue is delicately balancing model complexity, goodness-of-fit, and parameter identifiability, all of which impact the reliability of material behavior predictions under mechanical loading. It is established that biomechanical constitutive models, whether physically motivated or neural network derived, are typically sloppy from the information theory perspective. By analyzing the sensitivity matrix associated with posterior distributions of the constitutive parameters, a consistent pattern revealing the regularity in parameter combinations across experimental protocols characterizing tissue mechanical behavior and prior beliefs with varying levels of informativeness is discovered. The discovered pattern inspires to construct a sloppiness-based parameter hyperspace and proposes a model reduction program that performs model optimization by exploring four sub-hyperspaces. The proposed program offers a guide for effectively simplifying models while tightly ensuring parameter identifiability and prediction accuracy. Clear improvements are showcased to the brain tissue constitutive models discovered by neural networks and a physically motivated constitutive model of the human patellar tendon.

Keywords: Constitutive, Model, Data, Machine Learning

Optimization design method of smart hydrogel double-layer structures and programmable metamaterials

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Abstract

Smart hydrogels, owing to their excellent biocompatibility and stimulus responsiveness, hold great potential in biomedicine, flexible electronics, and related areas. Nevertheless, the actuation of hydrogel-based composite structures involves nonlinear effects such as swelling deformation and contact, which makes conventional simulation-based design approaches computationally demanding and limits their ability to explore the design space. To overcome these challenges and support the application-oriented design of hydrogel devices, this study develops optimization methods for smart hydrogel double-layer structures and programmable metamaterials. For double-layer structures, the explicit optimization method under finite deformation is proposed, in which the structural outline and material distribution are described by moving morphable voids and components, and the degree of freedom removal technology is developed to ensure numerical convergence during intermediate design stages. The optimization formulation targeting nodal displacements after deformation is constructed to realize actuators with specific functions. For programmable metamaterials, the machine learning-driven optimization framework is proposed, where the back-propagation neural network is trained to map the geometric features of metamaterials to their mechanical responses, and combined with the multi-population genetic algorithm to efficiently achieve inverse design. Numerical and experimental results demonstrate that the proposed methods can achieve the optimization design of the hydrogel bionic double-layer structures with the specific actuation effects, as well as the efficient design of the hydrogel-based metamaterials with the specific negative hydration expansion effects and the hydrogel-based network metamaterials with the tissue-like mechanical responses.

Keywords: Hydrogel, optimization design, double-layer structure, metamaterial, finite deformation

An efficient approach to shape optimization of structures with viscous dampers for strain energy minimization

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Abstract

Vibration in machines, structures, and vehicles can cause safety and performance issues. Structural shape optimization provides an effective way to suppress vibration, especially under multiple frequency excitations. While modal analysis is efficient for response and sensitivity computations, the presence of dampers prevents decoupling of the equations of motion, limiting its applicability. This study proposes an efficient shape optimization approach for structures with viscous dampers. Using the material derivative and adjoint variable methods, we derive analytical shape gradients for integral objectives such as the total strain energy. The computational cost involves one modal analysis and the solution of a complex system of equations related to damper degrees of freedom. To ensure boundary smoothness during optimization, the H^1 gradient method is employed. A numerical example with HyperWorks and a self-developed program demonstrates the effectiveness of the proposed method, reducing strain energy to about 29% of the original value in a numerical example.

Keywords: Modal analysis, shape optimization, viscous damper, H^1 gradient method, damper arrangement

Robust Topology Optimization of FRP Composite Structures under Uncertain Dynamic Excitations

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Abstract

The growing demand for lightweight and multifunctional components in advanced industrial applications has accelerated the use of fiber-reinforced plastic (FRP) composites. However, their dynamic performance is highly sensitive to uncertainties in external excitations, often leading to excessive deformation and significant performance degradation. This paper introduces a robust topology optimization framework for FRP composite structures subjected to stochastic dynamic loading. The framework integrates a discrete material and thickness optimization (DMTO) strategy, enabling concurrent optimization of both equivalent thickness and fiber orientation parameters. An extended polynomial interpolation model and a rational approximation of material property (RAMP) scheme are adopted to parameterize the respective design fields. Excitation uncertainties are modelled via Monte Carlo sampling, while a new frequency-response based approach is developed to estimate the statistical characteristics efficiently, namely the mean and standard deviation of dynamic compliance. To enable efficient gradient-based optimization, a decoupled sensitivity analysis is derived, allowing the analytical computation of derivatives for both types of design variables. The proposed framework is validated through several numerical examples, including 2D composite panels and a 3D laminated plate. The results demonstrate that, compared to conventional deterministic designs, the robust design strategy significantly reduces the expected dynamic response while enhancing reliability under uncertain excitation.

Keywords: Robust topology optimization; FRP composites; DMTO; dynamic compliance; load uncertainty

**Concurrent Topology–Path Optimization and Vacuum-Assisted Reprocessing for
Continuous-Fiber 3D-Printed CFRP**

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Additive manufacturing (AM) enables the fabrication of carbon-fiber-reinforced polymer (CFRP) structures with complex, topology-optimized geometries, yet printed parts often suffer from low fiber volume fraction and elevated porosity that undermine mechanical performance. This work proposes an integrated, experimentally validated framework that couples optimization-driven design with vacuum-assisted thermal post-processing to address these limitations without increasing material cost. First, we develop a level-set-based concurrent optimization that simultaneously determines structural topology and AM-feasible, load-path-aligned filament trajectories under constraints on bead width, curvature, spacing, and deposition continuity. Continuous-fiber 3D-printed specimens produced with matched mass and process settings benchmark the optimized designs against empirically designed counterparts. Second, we introduce a one-atmosphere vacuum-assisted heating protocol that promotes interfacial consolidation, reduces void content, and improves bonding. Third, high-resolution micro-computed tomography (μ CT) reconstructs as-printed geometries for fidelity-aware finite-element simulations and quantitative defect analysis. Simulation predictions agree with experiments, confirming model reliability. Relative to baselines, the proposed optimization increases stiffness-to-mass ratio by 47.0–52.1%, while post-processing further reduces out-of-plane deformation by 10.8–26.8%. The resulting design–manufacture–scan–simulate loop translates topological efficiency into realized structural gains and provides a practical route to robust, high-performance CFRP components. Beyond the demonstrated cases, the workflow generalizes to common continuous-fiber AM platforms and accommodates process-specific constraints and property targets, offering a scalable, quality-aware pathway to cost-neutral performance improvement at component and system level.

High-Fidelity Process Modeling of Alumina Melt Pool Dynamics in Laser Powder Bed Fusion

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Abstract

Recent progress in high-fidelity process simulations has greatly improved the comprehension of melt pool dynamics in laser powder bed fusion (LPBF) of metallic materials. However, modeling alumina systems remains particularly challenging due to their distinct thermophysical properties and complex behavior under high-energy laser irradiation, making it difficult to develop accurate simulations that align with sparse experimental data. In this study, we combine operando synchrotron X-ray tomographic microscopy with computational fluid dynamics-discrete element method (CFD-DEM) simulations ^[1-2] to examine the melt pool behavior of alumina during LPBF. Real-time observations uncover a melt pool morphology that is notably shallow and broad, differing significantly from the deeper, narrower melt pools typically observed in metals. This phenomenon is attributed to alumina's low thermal conductivity, high absorptivity of laser energy, and inverse surface tension gradients, as validated by high-fidelity simulations. Critical mechanisms governing this behavior include restricted thermal diffusion, intensified surface-directed fluid flow, and vortex formation induced by heat transfer with the surrounding gas atmosphere. The effects of laser power and scanning speed on melt pool dimensions are systematically evaluated, resulting in the first computational process map and optimized parameter ranges for stable PBF-LB processing of alumina. These insights offer valuable guidance for refining additive manufacturing techniques for alumina and advancing their industrial adoption.

Keywords: Additive manufacturing, laser powder bed fusion, high-fidelity simulations, multi-material mixing

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Data-driven Thermo-mechanical Interfaces: Thermal Mismatch Induced Interface Debonding

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Abstract

In this work, a model-free data-driven framework is proposed to simulate interface debonding induced by the thermal mismatch. The material phase space is expanded and a new thermo-mechanical distance norm is formulated, incorporating three canonical conjugate pairs: traction–separation, temperature–internal energy, and temperature gradient–heat flux. The thermo-mechanical coupling interactions of interface are naturally encoded by the given material database and the complex constitutive relations are not necessary herein. The proposed data-driven is enriched by an internal variable-based parameterization to construct a time-evolving database for enforcing monotonic increase of interface damage evolution. Several numerical examples are provided to evaluate the accuracy and efficiency of the proposed approach. First, the thermo-mechanical data-driven model is benchmarked against classical finite element results, with convergence behavior analyzed in detail. Second, parametric studies are conducted on key interfacial properties, including superficial heat capacity and interfacial thermal conductivity, demonstrating the capability of the developed data-driven method to capture essential features of heat transfer across interfaces. Finally, the proposed framework is applied to simulate interface debonding driven by thermal mismatch in different cases, successfully capturing the coupled evolution of heat conduction and interfacial degradation. The results confirm that the data-driven formulation provides a novel numerical tool to describe the interplay between thermal fields and damage processes at material of interfaces.

Keywords: Data-driven computational mechanics, Multi-physics coupling, Thermal mismatch, Thermo-mechanical interfaces, History-dependent interface damage, Model-free

Acceleration of stiffness matrix numerical integration using a finite element inspired neural network

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Abstract. We observed that the vectorization rate of the stiffness matrix numerical integration is low in structure simulations. To overcome this issue, we propose a finite element inspired neural network architecture called FEINN that completely parallelize the numerical integration. FEINN replaces the quadrature loops with a data parallel calculation fed by an elemental quadrature point features matrix. Moreover, FEINN achieves performance trade-off by combining accurate FEM vectorization with fast neural network predictions. When applied to a large-scale model, FEINN achieved about threefold acceleration in the stiffness matrix calculation while maintaining accuracy in the final displacement results up to three decimal places.

Keywords: Structural analysis, Finite element method, Stiffness matrix, Gaussian quadrature, High performance computing, Deep learning

Several novel Physics-informed neural networks for solving varied PDEs

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Abstract

In recent years, deep learning has become ubiquitous and has attracted widespread attention in empowering various fields, especially the combination of artificial intelligence and traditional science. Physics-informed machine learning deeply integrates data with physical equations and solves partial differential equations using artificial intelligence algorithms. Compared with traditional numerical methods, Physics-informed machine learning shows significant advantages in engineering inverse analysis, high-dimensional nonlinear problems and so on. This talk introduces the recent advances in physics-informed machine learning from the authors' group, which includes several novel Physics-informed neural networks: 1) Physics-informed kernel function neural networks, 2) Curriculum-transfer learning-based physics-informed networks, and 3) Physics-informed Kolmogorov-Arnold networks.

Keywords: Physics-informed neural networks, Kolmogorov-Arnold networks, Physics-informed kernel functions

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A profile structure model based on model driven and data-driven coupling approach

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Abstract

Recent advancements in artificial intelligence and big data analytics have propelled computational mechanics into an era of intelligent computation, marked by synergistic integration of quantum-enhanced processing and data-driven methodologies. This evolution has catalyzed a paradigm shift from conventional numerical approaches to innovative multi-framework solutions. Particularly in composite material analysis, modern homogenization techniques employing a two-phase strategy involving offline microscopic analysis and online macroscopic computation demonstrate superior computational efficiency through intelligent resource allocation. This study presents a novel hybrid computational framework that synergistically combines multi-scale homogenization principles with adaptive single-scale finite element modelling. The proposed methodology enhances traditional data-driven homogenization through three key innovations: 1) Implementation of Carrera's Unified Formulation (CUF) for a dimensional reduction in complex structural modelling, 2) Development of a coupled data-model fusion architecture balancing physical principles with machine learning insights, and 3) Creation of an optimized computation workflow maintaining micron-scale accuracy while achieving microscale efficiency. The CUF-enhanced hybrid model was rigorously tested through deflection analysis of composite structures under cantilever and simply supported constraints. Validation against conventional FEM simulations and analytical benchmarks confirms the method's accuracy, with comparative studies revealing <5% deviation in displacement predictions while achieving 40-60% reduction in computational resource requirements. This integrated approach demonstrates particular efficacy in layered composite analysis, successfully addressing the accuracy-efficiency trade-off inherent in multi-scale modelling through intelligent dimensionality management and physics-informed machine learning strategies.

Keywords: Data-driven computational homogenization; Hierarchical data search; Carrera unified formula; Data-driven and model-driven coupling; Finite element method;

A Large Language Model-inspired Data-driven Mechanics Framework for Viscoelastic Soft Structures

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Abstract

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

Rapid Prediction of Textile Forming Deformation via a Graph-Based Learning Approach

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Abstract

Forming-induced defects are a critical issue in composites applications, leading to significant material waste and requiring costly experimental trials for their mitigation. While Finite Element (FE) simulations can accurately predict these defects, their prohibitive computational cost hinders rapid design optimization. Machine learning (ML) surrogate models offer a compelling alternative, promising the speed and accuracy of high-fidelity FE simulations [1]. However, their practical application is hindered because most existing models employ an end-to-end, 'black-box' learning approach that ignores the governing physical processes. This disregard for physics renders them data-hungry and case-specific, severely limiting their ability to generalize to new tool geometries without exhaustive retraining.

This study proposes a novel Graph Neural Network (GNN) simulator to overcome these limitations. The approach converts FE meshes into graph representations and models interactions between textile layers and tools as graph edges. Different from previous end-to-end methods, the proposed GNN-simulator learns the entire deformation process through a roll-out mechanism, enabling remarkable geometric generalization across diverse geometries. Numerical results demonstrate that our model, trained on a small dataset of simple geometries, accurately predicts complex deformation behavior on unseen, combined geometries, achieving two orders of acceleration in computation time relative to FE simulations. Moreover, GNNs naturally accommodate variable numbers of nodes, allowing scalability to different geometry sizes without re-training. The proposed GNN-simulator establishes a foundation for efficient, digitally-driven manufacturing of textile composites.

Keywords: Textile composite forming; Manufacturing process simulation; Machine learning; Graph Neural Networks

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A Large Language Model-inspired Data-driven Mechanics Framework for Viscoelastic Soft Structures

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Abstract

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

Improved artificial neural network algorithms and its engineering applications

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Abstract

In machine learning, the most commonly used and effective algorithm is the artificial neural network (ANN) algorithm, which has the advantages of fast computing speed, strong self-learning ability, good robustness etc.. Among the ANNs, back-propagating neural network (BPNN) is one of the most commonly used neural network, which is composed of multi-layer neurons connected to each other to form a network structure. However, due to the lack of theoretical support for the selection of initial parameters and activation function, it often leads to slow convergence and local optimization, and drags the convergence and generalization ability. At the same time, in the mechanical problems, it is difficult to solve some complex problems with complicated models. With the help of artificial neural network algorithms, the numerical computation efficiency can be effectively improved and a new solution can be provided for some complex mechanical problems. On the one hand, based on the loss function analysis of mechanics and the basic theory of fracture mechanics, this work proposes two different improvement schemes of BP algorithm. The selection of weights and thresholds and activation function are optimized respectively. Numerical analysis shows that the improved algorithm can improve the accuracy, convergence and efficiency of numerical results. On the other hand, a deep extended causal convolution network is constructed based on the WaveNet model to repair the missing experimental data of shale fracturing. The proposed new algorithms have higher accuracy, efficiency and convergence for solving the three-dimensional surface reconstruction problem and crack propagation problem. Moreover, the missing shale fracturing experimental data can also be repaired on the selected deep learning algorithms. The proposed method can be applied to fretting fatigue and non-destructive testing.

Keywords: improved back propagation algorithm; optimal weights and thresholds; crack problems; multilevel LSTM; fretting fatigue; non-destructive testing

FEM-PIKFNN for structural vibration induced underwater acoustic propagation

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Abstract

With the development of the field of ocean engineering, the impact of human activities on the ocean environment is increasing. Among them, marine structures such as ships and submarines inevitably generate various noises in the ocean environment during navigation and operations. Noise control of underwater structures and prediction of the acoustic field in the ocean environment is an active research field. This paper proposes a hybrid solver based on the finite element method and kernel method to analyze vibration and acoustic propagation of the underwater structure in the ocean environment. In the proposed hybrid solver, the finite element method (FEM) is employed to obtain the acoustic-vibration coupling response of the underwater structure, the normal wave model is used to obtain the underwater acoustic Green's function for far-field acoustic propagation. Based on near-field acoustic information and Green's function, the physics-informed kernel function neural network (PIKFNN) is used to predict the far-field acoustic propagation response in the ocean environment.

Keywords: Shallow physics-informed neural network, Physics-informed kernel function, Ocean acoustic propagation, Structural vibration

Novel Actuator Lines Method Accounting for Structural Geometries

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Abstract

Since Sørensen and Shen proposed the Actuator Line Model (ALM), their team and other scholars have developed and refined many other models based on ALM. However, there remains a significant discrepancy between the wind turbine wake results calculated based on ALM and the wind turbine wake results obtained from high-fidelity CFD simulations. This deficiency stems from multiple causes, but a key factor is the intrinsic limitation of the ALM which fails to account for the specific structural geometries of wind turbine components. This paper will reconstruct the lift and drag coefficient database for distinct wind turbine components, and further incorporate the original structural features of these components through discrete positioning of actuator points. This work leverages the open-source turbinesFoam solver to achieve comparable accuracy to high-fidelity CFD simulations while requiring significantly less computational resources.

Keywords: Actuator Line Model (ALM), wind turbine wake results, CFD

Unified theory and method for computational stochastic mechanics

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Abstract

Stochastic mechanics covers the topics of the stochastic structural analysis, random vibration, reliability assessment, reliability-based design optimization, and stochastic optimal control. Traditionally, stochastic response analysis of structures, reliability assessment, and reliability-based design optimization were solved using distinct methods. Furthermore, there was a lack of unified, efficient, and straightforward methods for addressing stochastic linear and nonlinear problems in static and dynamic structures. This study establishes a unified fundamental equation, namely the probability density integral equation, to characterize the propagation and evolution of uncertainties in space and time domains for general stochastic systems, based on the principle of probability conservation. Building upon this equation, statistical moment formulas for stochastic responses, as well as formulas for reliability and its sensitivity, are derived. The direct probability integral method is developed to address stochastic response analysis, reliability assessment, reliability-based design optimization, and optimal control for static/dynamic systems. As a unified and efficient method for stochastic mechanics, the direct probability integral method resolves challenges in the stochastic static and dynamic analysis of large-scale linear and nonlinear structures with up to 1000 random variables, as well as system reliability and dynamic reliability-based design optimization. Additionally, it is applicable to Gaussian/non-Gaussian, stationary/non-stationary stochastic excitations, and Markov/non-Markov systems, providing computational tools for the reliability and safety assessment, risk management, and digital and intelligent optimal design of large-scale structures.

Keywords: Stochastic mechanics; stochastic responses of structures; static and dynamic reliabilities; probability density integral equation; direct probability integral method

DPIM-based neural network model for stochastic acoustic-vibration response of underwater structure

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Abstract

Investigating the acoustic-vibration behavior of underwater structures in the random ocean environment poses significant challenges due to experimental costs and computational complexity. To address these issues, the singular boundary method and finite element method are first introduced to establish the numerical computational model for the acoustic-vibration response of underwater structures. However, analyzing the probability characteristics of the acoustic-vibration response of underwater structures in the random ocean environment is challenging. Therefore, this paper extends a novel stochastic analysis method, which is the direct probability integral method (DPIM), to address this issue. Recognizing both the difficulty of obtaining sufficient data for stochastic analysis and the high computational cost of the singular boundary method-finite element method model, a back-propagation neural network improved by particle swarm optimization (BPNN-PSO) model for predicting the acoustic-vibration response is established. Based on this, a novel DPIM-based neural network model (DPIM-NN) is further proposed. In the numerical example, the calculated results of DPIM-NN are compared with those of Monte Carlo simulation, which demonstrates the high accuracy of DPIM-NN. The results reveal the effects of various random parameters on the acoustic-vibration response of underwater structures.

Keywords: underwater structure; random ocean environment; stochastic analysis; improved neural network model; direct probability integral method

Structural Design and Intelligent Optimization of a Combined Seismic Metamaterial

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Abstract

Seismic metamaterials, as artificially engineered periodic structures, effectively attenuate destructive Rayleigh surface waves that pose a threat to structural safety. However, how to design seismic metamaterials with a wide band gap in the low-frequency band remains a major engineering challenge. This paper proposes a combined seismic metamaterial composed of concrete columns and multiple-layer composite material structures, which exhibits superior bandgap characteristics compared to traditional combined seismic metamaterials. Furthermore, in order to simultaneously improve the low-frequency wide bandgap performance of the proposed seismic metamaterials, a multiple-objective optimization framework was established, combining the Q-learning algorithm with Kriging surrogate model to optimize the width and lower bound frequency of the bandgap. Following structural optimization, the bandgap exhibits a 67.76% width expansion accompanied by a 23.79% reduction in the lower limit. Transmission spectrum calculations and displacement analyses across various excitation frequencies confirm the isolation characteristics of the optimized metamaterial. In addition, analysis using the Jiuzhaigou seismic record demonstrates that the optimized combined seismic metamaterial effectively attenuates seismic wave energy.

Keywords: Combined seismic metamaterials, Rayleigh wave attenuation, Bandgap, Multiple-objective optimization

Rare event probability and global reliability sensitivity analysis for engineering structures based on direct probability integral method

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Abstract

Efficient and accurate evaluations of the rare event probability and global reliability sensitivity are crucial yet challenging tasks for the safety design of static and dynamic structures with uncertainties. This study establishes a novel level-wise representative points increment strategy for direct probability integral method (DPIM), which calculates accurately rare event probabilities (less than 10^{-3}). Additionally, the single-loop algorithm based on DPIM for global reliability sensitivity analysis is proposed. Firstly, it is clarified that the error in reliability assessment using DPIM is caused by the imprecise simulation of important subdomains. The idea of increasing the number of important points is advanced to improve the precision of reliability assessment. Subsequently, inspired by subset simulation, the level-wise representative points increment strategy is proposed. This strategy effectively and adaptively adds representative points within important subdomains by selecting new points from the low-level points. Embedding the points increment strategy into DPIM forms a unified and efficient method for rare event estimations of static and dynamic structures. Secondly, the DPIM is extended to efficiently calculate global reliability sensitivity with a single evaluation of reliability. Finally, the accuracy and efficiency of the proposed method are demonstrated in three typical examples by comparing with Monte Carlo simulation (MCS), Quasi-MCS and importance sampling. The results indicate that the proposed strategy significantly improves the accuracy of reliability and global sensitivity assessment employing DPIM, and fulfils a versatile and precise analysis of rare event probabilities and reliability sensitivity in both static and dynamic systems.

Keywords: Rare event probability; direct probability integral method; level-wise representative points increment strategy; global reliability sensitivity

High-dimensional Reliability Analysis using Combined Dimensionality Reduction and Adaptive Sparse Polynomial Chaos Expansion

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Keywords: RELIABILITY ANALYSIS, POLYNOMIAL CHAOS EXPANSION, DIMENSIONALITY REDUCTION, PRINCIPAL COMPONENT ANALYSIS, SURROGATE MODEL

Abstract

Polynomial chaos expansion (PCE) is increasingly used for structural reliability analysis in various engineering fields. However, due to the curse of dimensionality, full PCE computation is often unaffordable for high-dimensional problems. In this paper, a combined dimensionality reduction based adaptive polynomial chaos expansion (CDR-PCE) is proposed for high-dimensional reliability analysis. Taking advantage of different kernel functions and low-fidelity model gradients to construct transformation matrix, a combined dimensionality reduction (CDR) method is first introduced to map high-dimensional input data to a low-dimensional space for effective dimension reduction. Then, an adaptive PCE model is constructed by employing the sparrow search algorithm to optimize the polynomial order and regularization parameter in the solving process of recently developed Bregman-iterative greedy coordinate descent. A novel CDR-PCE framework is finally conceived by incorporating the CDR method into the adaptive PCE model for enhancing both efficiency and accuracy. The performance of the proposed CDR-PCE is evaluated on two numerical examples of varying dimensionality and complexity through comparison with several state-of-the-art methods. Results show that the proposed method is superior to the benchmark algorithms in terms of accuracy, efficiency and robustness for high-dimensional reliability analysis.

Research on Adaptive Loss Physics-Informed Neural Network Algorithm Based on KAN Network for Heat Conduction Equation

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Abstract

Physics-Informed Neural Networks have shown potential in solving partial differential equations with fewer data requirements, but their performance and convergence are easily affected by loss weight selection. In the context of solving heat conduction equations, this paper innovatively applies KAN neural networks to PINN, referred to as PI-KAN and proposes an adaptive loss function weight adjustment method. This method dynamically adjusts the relative importance of individual loss terms at the start of each training iteration, avoiding dominance by a single loss component and achieving balanced optimization. Numerical experiments on 1D transient heat conduction equations verify the effectiveness of the proposed method. Compared with traditional PINNs based on fully connected neural networks, PI-KAN reduces the solution error, and the solution in the spatial domain has a significantly higher degree of agreement with the exact solution, with the L2 error reaching the order of 10^{-3} . Meanwhile, it improves the stability of the model. This study provides a new efficient approach for solving heat conduction equations, and has potential application value in related fields involving PDE solution.

Keywords: KAN neural network, Heat conduction equation, Physics-Informed Neural Network, Adaptive loss function, PDE solution

Mechanical Property Evaluation of Nuclear Fuel Assembly Spacer Grids under Extreme Service Conditions

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Abstract

As a structural support and restraint component for nuclear fuel rods, the spacer grid of a fuel assembly plays a crucial role in maintaining the overall mechanical stability of the assembly, and its mechanical properties are directly related to the safe operation of nuclear reactors. However, under extreme service conditions such as high temperature, intense irradiation, and impact loads, the spacer grid exhibits complex nonlinear responses, including material degradation and stiffness reduction, which weaken its load-bearing capacity, reduce service reliability, and impair the accuracy of performance predictions. To address this issue, this study systematically investigates the degradation mechanisms of spacer grid mechanical properties under extreme conditions. Through automated modeling and experimental validation, the study reveals the mechanisms of stiffness degradation and buckling mode evolution induced by factors such as material hardening and clamping force relaxation. A simplified beam-element model based on automated topology reconstruction is developed, with nonlinear connector elements introduced to represent the nonlinear contact constraints between the grid and fuel rods. The model's effectiveness is verified through static compression experiments. Furthermore, a constitutive model for zirconium alloy under high-temperature irradiation is established to quantitatively analyze degradation mechanisms such as material hardening, clamping force relaxation, irradiation-induced swelling of grid cells, and oxide film growth under fast neutron fluence. In addition, an explicit dynamic algorithm is employed to simulate the buckling response of the spacer grid under both single and repeated impact loads, assessing its adaptability to dynamic shock environments. By comprehensively considering irradiation-induced degradation factors, this study elucidates the dynamic mechanical behavior of spacer grids under extreme operating conditions. The results show that under such conditions, grid stiffness decreases by approximately 26%, dynamic buckling strength is reduced by about 19%, and the buckling mode shifts from transverse shear slip at the bottom to localized vertical strip buckling around the upper guide tube.

Keywords: Spacer grid, Automated modeling, High-temperature irradiation, Impact load, Dynamic buckling

Generalization Analysis of Direct Weights Inversion Method for Small datasets

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Abstract

This study presents a theoretical and numerical investigation of the generalization performance of the direct weights inversion method, a technique computationally efficient as established in previous studies, for solving inverse problems with limited data. The method directly maps the weights of a well-trained forward network to construct an inverse network explicitly. Going beyond efficiency, our rigorous analysis and experiments demonstrate that the approach retains strong generalization capability even with small datasets, owing to its unique inversion mechanism. Case studies across various domains confirm consistent and high accuracy in data-scarce settings. The work contributes an efficient solution for small-sample inverse problems, showing significant potential for practical applications where data acquisition is difficult."

Keywords: Computational inverse problem, surrogate model, direct weights inversion method, small-sample learning, generalization

Numerical Method for Irradiation Deformation of Rod-Bundle Fuel Assemblies Based on Beam Model

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Abstract

Due to the complex geometric structure and harsh service environment, studying the irradiation deformation of rod-bundle fuel assemblies in the core is challenging. Limited by current computational capabilities, it is difficult to simulate the overall irradiation deformation of fuel assemblies accurately using three-dimensional models. Therefore, an equivalent beam-model-based method has become a more effective approach for analyzing in-reactor deformation of assemblies. This study proposed a beam-model-based method for analyzing the irradiation deformation of rod-bundle fuel assemblies. Key components such as fuel rods, guide tubes, and grids were equivalently represented as beam elements based on mechanical equivalence principles. By considering the material properties of each component and their mechanical contact relationships, the effects of irradiation/creep and structural interactions were incorporated into the beam model, and the beam model suitable for the whole fuel assemblies was established. The model was verified using small-scale three-dimensional finite element models and validated with the actual data of irradiation measured by poolside inspection. The three-dimensional finite element validation showed that the computational error was controlled within 20%, while the poolside inspection data validation indicated that the maximum deviation was less than 2 mm, both within acceptable ranges. Using the established analysis method, a sensitivity analysis was conducted on the effects of hydraulic load, neutron fluence, temperature field, and compressive load on the irradiation deformation of fuel assemblies. The results demonstrated that hydraulic load and neutron fluence were key factors influencing assembly deformation under in-reactor conditions. As hydraulic load and neutron fluence increase, the lateral deformation behavior of fuel assemblies becomes more pronounced. The research outcomes provide an efficient analytical tool for predicting irradiation deformation of fuel assemblies and offer valuable insights for fuel assembly design and safety assessment.

Keywords: Rod-bundle fuel assembly; Irradiation deformation; Beam model; Mechanical constitutive law

Coupled Autoencoder for Joint Dimensionality Reduction and Inversion

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Abstract

The accurate acquisition of key parameters is a prerequisite for ensuring the high-performance optimized design of mechanical equipment. For parameters that are challenging to measure directly, they are often inferred based on simple and easy-to-measure high-dimensional response data. However, high-dimensional response data usually contain a large amount of redundant information, and dimensionality reduction is required to extract effective features. The traditional decoupled pipeline approach—first performing dimensionality reduction and then inverse calculation—suffers from insufficient adaptability between the reduced features and the inverse modeling task, compromising both accuracy and computational stability. To address this issue, the Coupled Autoencoder Inverse Method is proposed. First, an optimization strategy for dimensionality reduction using autoencoders is developed, where the bottleneck layer's dimension is determined by the cumulative variance contribution rate from principal component analysis, thereby retaining key information while minimizing dimensionality. Second, a neural network model is constructed that couples the autoencoder with the inverse problem solver. A composite loss function is defined to integrate the reconstruction loss of the autoencoder and the inverse calculation loss. A dynamic adaptive weighting strategy for the loss components is introduced based on Bayesian optimization to balance generalization ability and inverse prediction accuracy. Finally, a complete training framework for the Coupled Autoencoder Inverse Method is established and validated using a composite laminated plate as a case study. The results demonstrate that the proposed Coupled Autoencoder Inverse Method not only achieves high accuracy in parameter inversion but also exhibits excellent generalization and stability under small-sample conditions.

Keywords: Parameter inversion, Dimensionality reduction, Neural network; Autoencoder; Composite material structure.

Optimized Bubble Suppression in Piezoelectric Jet Dispensing for Microelectronic Packaging

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Abstract

Piezoelectric dispensing is a widely adopted technique in the packaging of microelectronic integrated circuits. However, the formation of adhesive bubbles is an inevitable phenomenon that results in a reduced volume of dispensed glue relative to the design specifications. This discrepancy can lead to compromised bonding strength, disconnections in the adhesive line, and, in extreme cases, bubble rupture due to thermal expansion, thereby severely undermining encapsulation quality. This study investigates the underlying mechanisms of bubble formation and identifies the key parameters that influence this process. A novel strategy for bubble suppression is proposed, which involves the precise control of the firing pin movement within the piezoelectric nozzle. The study begins by analyzing the bubble generation mechanism, developing an electromechanical coupled dynamics model alongside a fluid dynamics model to simulate and evaluate the impact of the firing pin's upward motion on dispensing performance. Spray experiments were then conducted to validate the theoretical models. The results demonstrate that the air suction caused by the upward motion of the firing pin is the primary cause of bubble formation. The key factors affecting air back-suction and bubble generation are systematically analyzed and experimentally verified. Furthermore, the study employs folding lines and Bessel curves to optimize the driving waveform during the firing pin's uplifting phase to mitigate bubble formation. The findings indicate that the formation of bubbles is closely related to the upward motion of the firing pin within the injection valve. Effective suppression of bubble formation can be achieved by increasing the firing pin's stroke, reducing the uplifting speed, elongating the nozzle length, and minimizing the nozzle diameter. In addition, the optimized driving waveform significantly reduces the occurrence of adhesive bubbles compared to conventional waveforms.

Keywords: Jet dispensing; Hydrodynamic simulation analysis; Adhesive bubbles; Drive waveform optimization; suppression

A high-order accurate wavelet method for two-dimensional turbulence

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Abstract

Find a high accurate numerical solution of turbulent flows is still a challenge, especially for the problems with curved boundary. Although many finite difference methods can achieve a high-order accuracy, they have been consistently encountered serious difficulties in dealing with irregular domains. The finite volume method, which can effectively handle complicated boundaries and hence is most widely used in engineering, usually exhibits a limitation of second-order accuracy, because the computational complexity of the high-order schemes is too cumbersome. In this study, the wavelet multiresolution interpolation Galerkin method is extended to solve the two-dimensional Navier-Stokes equation. In such a method, the nonlinear term is treated as an independent function and then approximated directly by its wavelet expansion, similar to the treatment of the unknown function. Therefore, the approximations to the nonlinear term and unknown functions are their projection in the same subspace of L^2 space, resulting in a good accuracy, convergence, and stability of the proposed method. By simulating the two-dimensional homogeneous isotropic turbulence flows, the numerical results show that the present method can achieve forth-order accuracy. And compared with the several compact finite difference schemes, this wavelet method possesses a better accuracy while costing comparable computational time. More importantly, the proposed wavelet method can be extended to solve problems with curved boundary.

Keywords: Wavelet multiresolution interpolation, Meshfree method, high-order accuracy, turbulence

Wavelet solution for moving point heat source problems

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Abstract

The analysis of temperature fields induced by a moving point heat source is a fundamental topic in numerous scientific and engineering problems, such as laser sintering for 3D printing and welding. The temperature field exhibits extremely steep gradients in the vicinity of the point heat source, and these gradients move progressively with the motion of the source. Consequently, solving such problems requires the use of dynamically adaptive node distributions with local high refinement, which poses significant difficulties for mesh-quality-dependent methods like the Finite Element Method (FEM). Although existing meshless methods avoid the challenge of mesh generation, they themselves face issues such as difficulties in imposing essential boundary conditions and susceptibility to numerical oscillations near regions with large local gradients. In this study, the Wavelet Multiresolution Interpolation Galerkin Method is extended to solve moving point heat source problems. In this method, no mesh, including background mesh, is required. Essential boundary conditions can be directly imposed much like in the traditional FEM. Furthermore, benefiting from the properties of wavelet multiresolution analysis, the method can robustly capture local large gradients without generating significant numerical oscillations. Simultaneously, the method always represents the approximate solution at any given time based on a corresponding locally refined node distribution specific to that time instant. This eliminates the need for repeated interpolation and projection between different node distributions, effectively saving computational cost while ensuring approximation accuracy. Numerical tests demonstrate that the proposed wavelet multiresolution method possesses a better accuracy, efficiency, and stability than many existing numerical methods.

Keywords: Point heat source; Heat conduction; Local large gradient; Multiresolution analysis; Dynamic node distribution

Study on seismic resilience assessment method of a multi-story underground structure for ICCM

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Abstract

Unlike traditional seismic design methods, the seismic design method based on resilience focuses on both personnel safety and post-earthquake recovery. With the proposal of the "resilient urban and rural" plan, seismic resilience has also become one of the research hotspots in the current seismic design of underground structures. However, there is still a lack of research on seismic resilience assessment of underground structures. This article starts with seismic resilience, sorts out the methods for seismic resilience assessment, and uses the method provided in China's current "Standard for seismic resilience assessment of buildings" to evaluate the seismic resilience of an underground structure. Based on the resulting repair costs, repair time, and casualty indicators, the seismic resilience rating of the underground structure is evaluated, and the applicability and limitations of the method provided in the "Standard for seismic resilience assessment of buildings" are analyzed. The results show that the method provided in the "Standard for Evaluation of Seismic Resilience of Buildings" is applicable to this underground structure and can provide a reference for the seismic resilience assessment of other underground structures.

Keywords: underground structures, seismic resilience, Monte Carlo, resilience assessment

Acetone adsorption behavior on two-dimensional ZnO regulated by doping engineering: A DFT study

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Abstract

Breath analysis is a promising, non-invasive method for diagnosing various diseases including diabetes. Acetone is demonstrated as an effective biomarker for diabetes monitoring and estimation. The acetone sensing potential of 12 different elemental doped 2d ZnO nanosheets are systematically explored by DFT study. The calculation results show that Fe- and Ni doped 2d ZnO may act as ideal sensing materials for acetone.

Keywords: Acetone, 2D -ZnO, elemental doping, density functional theory, sensing

From Molecule to Membrane: Integrating Molecular Dynamics and In Vitro Experiments for Tyrosinase Inhibition Mechanism Discovery

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Abstract

Tyrosinase (TYR) is a key enzyme in melanin production and a crucial target for skin-whitening agents. Due to challenges in isolating pure human TYR, we constructed a homology model and evaluated the inhibitory effects of Ar-turmerone (A1) and its derivatives (A8 and B18) through in vitro assays and molecular dynamics (MD) simulations. Ar-turmerone reduced TYR activity by 19.2 % at 2.0×10^{-4} M, while bromine- and indole-modified turmerone (B18) exhibited the highest binding energy (-85.27 ± 15.73 kJ/mol). A DPPC lipid bilayer model revealed that indole modification enhances skin permeability by reducing the energy barrier by 11 kJ/mol. Methyl substitution increased binding free energy by 14.7 %. Our findings demonstrate that Ar-turmerone inhibits tyrosinase to prevent melanin synthesis and that rational side-chain modifications enhance both activity and permeability. This study provides mechanistic insights into Ar-turmerone's potential as a skin-whitening agent, guiding future food-derived drug development.

Keywords: Molecular dynamics simulations, skin whitening, Aromatic turmerone, drug delivery

The optimized Runge-Kutta-Chebyshev method for semi-discretizations of hyperbolic conservation equations

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Abstract

Explicit time-marching method with the stability interval as large as possible is desirable for solving the semi-discretizations of hyperbolic conservation equations. The Runge-Kutta-Chebyshev (RKC) methods for the ordinary differential equation take advantage of the properties of the Chebyshev polynomials and hence their stability intervals are extended much larger than the traditional ones. Based on the requirements of low-dissipation and low-dispersion for solving the hyperbolic equations, a family of optimized Runge-Kutta-Chebyshev method is constructed by minimizing the error function. Several numerical experiments show that, for simulating the complex flow fields, the new method has improved performances, such as the capability of maintaining vortex shape, the robustness.

Keywords: Runge-Kutta-Chebyshev method, time-marching method, hyperbolic conservation equations, complex flow field

Surface Strengthening of Laser Additive Manufactured AlSi10Mg Alloy: A Multiscale Numerical Simulation Study Based on SPH-FEM Coupling

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Abstract

AlSi10Mg alloy is widely used in aerospace load-bearing components and automotive lightweight applications due to its excellent comprehensive properties. With the advancement of additive manufacturing (AM), the capability to fabricate complex-shaped components from this alloy has been significantly improved. However, the irregular surfaces of these components pose challenges for conventional strengthening techniques to achieve uniform and efficient surface treatment, resulting in critical issues in surface strengthening and precision machining of laser additive manufactured AlSi10Mg parts. To address this problem, this study proposes a multiscale numerical simulation method coupling Smoothed Particle Hydrodynamics (SPH) and the Finite Element Method (FEM) for multi-physics modeling of the abrasive water jet (AWJ) strengthening process. The SPH method is employed to simulate the dynamic impact behavior of the abrasive-fluid multiphase flow, while the FEM is used to characterize the elastoplastic deformation and damage evolution of the substrate. A finite element model of AWJ impacting AlSi10Mg alloy was established on the Abaqus software platform. Systematic simulations were conducted under various process parameters, including jet pressures ranging from 10 to 40 MPa and standoff distances from 10 to 20 mm, to analyze the distribution characteristics of stress and strain fields. The simulation results indicate that jet pressure significantly influences the surface stress state after strengthening; increasing pressure leads to a notable rise in residual compressive stress. In contrast, increasing the standoff distance causes attenuation of the jet impact energy, correspondingly reducing the residual compressive stress. Further analysis of the strain and stress fields reveals a significant positive correlation between jet pressure and the mechanical response: as the pressure increases from 10 MPa to 40 MPa, the peak plastic strain, its distribution range, the absolute value of residual stress, and the extent of high-stress regions all expand markedly, indicating more intense material deformation and stress response. Based on these findings, the parameter combination of 40 MPa jet pressure and 15 mm standoff distance yields the optimal strengthening effect, under which the most significant plastic strain and stress responses are observed.

Keywords: AlSi10Mg alloy, surface strengthening, SPH-FEM coupling, residual stress

SPH Simulation of Dual Roller Cutters Penetrating into Coal Seam with Hard Nodules

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Abstract

This study establishes a numerical model of coal seams containing hard nodules based on the Smoothed Particle Hydrodynamics (SPH) method, and develops an SPH simulation framework for the rock-breaking process using dual roller cutters. A self-developed Fortran program was implemented to integrate the following key computational modules: An elastoplastic constitutive model for coal-rock composites, A dynamic fracture failure criterion, A cutter-coal/rock contact algorithm. Specifically, the coal matrix is governed by a modified Drucker-Prager model, while the hard nodules are characterized by a hybrid failure model to capture their dynamic damage evolution during low-velocity penetration. A comparative analysis was conducted between the proposed hybrid model and the conventional Johnson-Holmquist (JH-II) model under varying penetration velocities, highlighting their distinct responses to strain rate effects and fragmentation patterns.

The simulation systematically investigates the evolution mechanisms of dynamic fracture patterns in coal seams under the following operational parameters: Cutter spacing: 20–100 mm, Tip width: 40–80 mm, Penetration velocity: 0.5–2 m/s, Cutter-nodule alignment: Centered configuration, Offset configuration. The study reveals that nodules significantly alter crack propagation paths, causing the main crack to exhibit core-circumventing bifurcation characteristics. Their size and spatial distribution directly govern the morphology of the fracture zone; The cutter width critically governs stress distribution: When the cutter width increases from 40 mm to 60 mm, the peak normal force rises significantly. At the critical width of 80 mm, the tool induces "edge-localized fragmentation", with the crack density around nodules notably higher compared to narrower cutters. When cutter spacing falls below the critical threshold, a synergistic fragmentation effect emerges, reducing the peak penetration force. Conversely, direct alignment of cutters with nodules induces localized stress concentration, amplifying normal force fluctuation magnitudes compared to offset conditions. The research findings reveal the multi-scale mechanical mechanisms governing fragmentation in coal seams containing nodules, establishing a theoretical foundation for optimizing disc cutter parameters.

Keywords: Smoothed Particle Hydrodynamics (SPH), Hybrid failure model; Johnson-Holmquist (JH-II) damage model, Cutter penetration, Coal seams with hard nodules, Dynamic crack propagation, Rock fragmentation simulation.

Application of the lattice Boltzmann flux solver in large-scale hydrodynamic numerical problems

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Abstract

In engineering, the fluid-structure interaction and the enormous computational cost involved in large-scale hydrodynamic problems present significant challenges for numerical simulations. To address these issues, this work proposes a numerical method based on the lattice Boltzmann flux solver (LBFS). The method employs the immersed boundary method to capture the contact lines between the solids and multiphase flows, and leverages a multi-GPU platform to achieve efficient data transfer and parallel computation across devices. The verification results demonstrate that the parallel efficiency of multi-GPU compared to single-GPU reaches 85%, achieving extremely high computational efficiency while maintaining consistent computational accuracy. Two numerical cases of water entry successfully verify the accuracy in simulating the trans-media problems. Finally, the method is applied to simulate an engineering problem of aircraft landing, analyzing the structural motion response and hydrodynamic loads. This case uses a full-scale model and hundreds of millions of flow field grids, yet can be completed in a short time on a single workstation. In summary, the method exhibits robustness and ultra-efficient computational performance, with the potential to solve large-scale engineering problems.

Key words: lattice Boltzmann flux solver, immersed boundary method, multi-GPU, aircraft landing

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Effect of Particle Shape on Cohesion and Friction Angle in Clay studied by DEM Biaxial Shear Simulations

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Abstract

Cohesion and friction angle are key strength parameters of soils, yet their micromechanical origin remains unclear. In particular, the influence of clay particle shape on these parameters is still insufficiently understood. Here we systematically examine the effect of particle elongation using 2-D DEM biaxial shear simulations, considering both normally consolidated (NC) and over-consolidated (OC) samples. Biaxial specimens are generated via isotropic compression and uniaxial (one-dimensional) compression, and the interparticle mechanics combine a DLVO non-contact interaction with a linear contact law. We compare circular particles with elongated particles formed by clumping two equal circles. OC specimens are prepared with the same non-dimensional pre-consolidation stress of $p/k_n=0.064$ where k_n is the normal contact stiffness. It was observed that not only OC but also NC specimens exhibit bulk cohesion, because the adopted DLVO interaction does not have an energy barrier and accordingly allows self-agglomeration without external compression. The cohesion in OC specimens is slightly larger than that of NC specimens because the former is denser than the latter. As a result, the failure envelope of the OC specimens is larger than that of the NC specimens, which is in accordance with the actual clay behaviour.

Keywords: Cohesion, Friction angle, Clay particle shape, DLVO theory, Bi-axial shear test.

Impact of Physical Constraints on Spatio-Temporal Neural Networks for Predicting Cylinder Water Entry Flow Fields

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Abstract

To address the physical inconsistency and long-term instability of data-driven models in cylinder water entry multiphase flow prediction, this study proposes a Physics-Informed Spatio-Temporal Graph Neural Network (PI-STGNN). The model integrates the mass conservation law and the Volume of Fluid (VOF) transport equation as soft constraints into a framework combining a Graph Neural Network (GNN) and a Long Short-Term Memory (LSTM) network. Through systematic comparative experiments, we demonstrate that a mixed-constraint model, combining both physical laws, achieves the best overall performance. While maintaining data fidelity that is nearly on par with a purely data-driven baseline, the mixed-constraint model demonstrates superior long-term stability in autoregressive predictions and significantly better adherence to physical principles. The model's strong generalization capability is also verified for cases with different physical parameters. Our findings confirm that integrating multi-physics prior knowledge into spatio-temporal neural networks is a promising approach for developing reliable and efficient surrogate models for water entry flow field prediction.

Keywords: Physics-Informed Neural Network, Multiphase Flow, Water Entry, Surrogate Model.

A multiscale continuum model for the mechanics of cross-linked elastomer composites reinforced with nanofibers

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Abstract

Molecular dynamics (MD)-guided parameterization of constitutive equations serves as a vital bridge between microscale structures and macroscale mechanical behavior in elastomer composites. Conventional continuum models often depend on empirically fitted parameters, which may fail to capture key physical phenomena such as molecular chain orientation, filler-matrix interactions, and temperature-dependent effects. By harnessing MD simulations, these parameters can be systematically derived from all-atom or coarse-grained models, enabling constitutive equations that are not only predictive but also adaptable to variations in material composition and service conditions.

A multiscale continuum model is presented for the mechanics of cross-linked elastomer composites reinforced with randomly oriented nanofibers. The hyperelastic response of the cross-linked elastomer is characterized by using the Arruda-Boyce model and the kinematics of the filled nanofibers are described via the first and second gradient of continuum deformations. The shear lag theory and Krenchel orientation parameters are incorporated into the continuum models to characterize the size and orientation effects of the nanofibers. Particularly, a non-uniform interface stiffness function is proposed to refine the constitutive equation for nanofiber-filled cross-linked elastomer composites, accounting for interface debonding damage. Subsequently, all-atom and coarse-grained MD simulations are performed to obtain the microstructural parameters of the proposed nanofiber-reinforced cross-linked elastomer continuum models, such as the macro-micro transition factor, the physical parameters of cross-linked elastomer networks, and the interfacial shear stress between nanofibers and the elastomer. The comparison with experimental data shows that the predicted values of the constitutive equation for nanofiber-filled cross-linked elastomer considering interface debonding damage are in good agreement with the experimental results, demonstrating the reliability of the developed constitutive equation and multiscale method.

The present constitutive equation of cross-linked elastomer composites reinforced with randomly oriented nanofibers can be further extended to study the influence of surface properties of nanofibers, such as defects and surface modification, which can achieve a directional optimization of interfacial properties of elastomer composites and provide theoretical basis for the design of high-performance elastomers.

Keywords: Multiscale modeling, elastomer network theory; molecular dynamics simulations

An efficient approach to shape optimization of structures with viscous dampers for strain energy minimization

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Abstract

Vibration in machines, structures, and vehicles can cause safety and performance issues. Structural shape optimization provides an effective way to suppress vibration, especially under multiple frequency excitations. While modal analysis is efficient for response and sensitivity computations, the presence of dampers prevents decoupling of the equations of motion, limiting its applicability. This study proposes an efficient shape optimization approach for structures with viscous dampers. Using the material derivative and adjoint variable methods, we derive analytical shape gradients for integral objectives such as the total strain energy. The computational cost involves one modal analysis and the solution of a complex system of equations related to damper degrees of freedom. To ensure boundary smoothness during optimization, the H^1 gradient method is employed. A numerical example with HyperWorks and a self-developed program demonstrates the effectiveness of the proposed method. In this example, both shape optimization and damper arrangement optimization were conducted simultaneously, which reduced the strain energy to approximately 90% of its original value.

Keywords: Modal analysis, shape optimization, viscous damper, H^1 gradient method, damper arrangement

Layout design of complex multi-connected fluid channel system with multi-material topology optimization method

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Abstract

Piping systems are critical functional structures in aerospace vehicles, where multiple independent channels transport diverse liquid working fluids to designated locations for specific tasks. These systems exhibit a "multi-inlet-multi-outlet, directed-connection" topological characteristic and require "path-independent, medium-isolated" functional performance. To address these design challenges and achieve drag-reduction-optimized layout design, this study proposes a layout optimization method for complex multi-connected fluid channel systems based on a multi-material interpolation model. The method employs multiple design variable fields to define solid materials and distinct fluid phases, establishes a spatially continuous mapping between maximum inverted permeability and fluid volume fractions for individual channels, and assigns independent laminar flow physics, boundary conditions, and fluid governing equations to inlets/outlets with predefined connectivity relationships. Sensitivity analysis is performed via the discrete adjoint method to solve the optimization problem. Numerical validation through simple and complex cases demonstrates the feasibility and effectiveness of the framework. Comparative analysis of results provides empirical guidelines for model parameter settings, laying a foundation for future mathematical and simulation-based research.

Keywords: Topology optimization, Multi-Material Interpolation Model, Laminar Flow and Multi-Physics Coupling , Optimal Design of Piping Systems

Feature-driven topology optimization of complex fluid channel network with predefined inlet-outlet pairings

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Abstract

This paper proposes a feature-driven methodology for optimizing multi-connected pipeline layouts, addressing two critical limitations of conventional flow resistance minimization approaches: precise directional matching of multiple inlet-outlet pairs in complex systems, and guaranteed avoidance of 3D spatial interference with controlled minimum separation distances. The method utilizes worm-inspired features—parametric 3D spatial entities defined via B-spline-based variable cross-sections swept along central spines—which offer exceptional deformability and controllability for pipeline routing. Key methodological implementations include: (1) enforcing inlet-outlet connectivity through fixed terminal control points, (2) implementing minimum distance constraints via implicit level-set functions to ensure separation distance compliance, and (3) achieving flow resistance minimization as the primary optimization objective. The effectiveness and generality of the method are validated through two numerical examples.

Keywords: Topology optimization, Feature-driven method, Fluid channel, Distance control

Transformed Tensor Decomposition Method for Topology Optimization

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Abstract

In this paper, we propose a transformed tensor decomposition method for topology optimization. A transform is performed to the density variable to manipulate its range. The transformed variable is then decomposed as the sum of a number of modes, each in a variable separated form. In this way, the number of design variables in discrete form and the optimization time used in each iteration are considerably reduced. Numerical tests are performed to illustrate the nice features of the proposed method with evidence for solving the problems of checkerboard and mesh-dependency.

Keywords: Tensor decomposition, Topology optimization, Reduced-order modeling

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Mechanical response of protein-embedded vesicles under osmotic pressure: A Monte Carlo simulation

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Abstract

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.

A Robust E-CUSP Method for Compressible Fluid-Solid Multiphase Diffuse Interface Model

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Abstract

Compressible fluid-solid multiphase problems are widespread in nature and engineering. Their numerical simulation is challenging due to the simultaneous presence of interfaces and structures like shocks and expansion waves in both fluids and solids. This paper develops an energy-convective upwind and split pressure (E-CUSP) scheme for solving compressible fluid-solid diffuse interface models. The scheme's robustness is enhanced by adaptively adding numerical dissipation in the subsonic region, effectively suppressing non-physical oscillations near solid shocks. Simultaneously, an interface switch function is designed to avoid introducing excessive numerical dissipation near interfaces, ensuring high interface resolution. Numerical results demonstrate that the developed E-CUSP scheme can sharply capture shocks and expansion waves in both solids and fluids while maintaining clear material interfaces. Compared to the HLLD Riemann solver, the new scheme better suppresses non-physical oscillations near solid shocks and avoids the issue of increased oscillations with grid refinement observed in HLLD. Since the E-CUSP scheme avoids complex calculations of post-wave physical quantities, the computational cost is reduced, leading to improved computational efficiency.

Keywords: Multiphase diffuse interface model; Compressible fluid-solid interaction; Riemann solver; E-CUSP scheme.

Machine-learning enabled atomic insights into the phase diagram of Lead zirconate titanate

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Abstract

Lead zirconate titanate ($\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$, PZT) is a cornerstone material in sensors, actuators, and energy harvesting due to its superior piezoelectric properties. The origin of its exceptional performance at the morphotropic phase boundary (MPB) is intimately linked to the complex interplay of polar phases, yet a precise atomic-scale understanding remains challenging.

In this work, we develop a high-dimensional neuroevolution potential (NEP) for PZT using an active learning framework trained on first-principles data. The potential achieves density functional theory (DFT) accuracy in energies and atomic forces, and successfully reproduces the experimental temperature-composition phase diagram, including the MPB region (x : 0.44-0.54). Crucially, large-scale molecular dynamics simulations reveal that the MPB exhibits a rich diversity of local polarization orientations, facilitating easy rotation of the polarization vector. This intrinsic structural heterogeneity is identified as a key factor underpinning the enhanced piezoelectric response.

The developed NEP model provides a robust and efficient platform for atomic-scale investigations of domain dynamics and defect effects in PZT, offering fundamental insights for the design of advanced ferroelectric materials.

Keywords: Lead zirconate titanate, machine learning potential, phase diagram, molecular dynamics

Density of States Engineering: A Physics-Inspired Framework for Efficient Topology Optimization of Phononic Bandgaps

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Abstract

Phononic crystals are widely used in acoustic devices, vibration reduction and other fields, and topology optimization is an effective methodology for their structural design. Most existing studies design phononic crystals via topology optimization based on the extrema of dispersion curves, but the objective function constructed thereby has unclear physical meaning and requires additional constraints for prescribed band gap optimization. To address this, this work proposes a novel objective function based on the density of states concept migrated from solid-state physics, which is closely associated with the physical essence of band gaps (zero density of states corresponds to band gap ranges). Derived and simplified using density of states in specific frequency ranges, the objective function incorporates a Gaussian function to achieve continuity and differentiability. Numerical examples verified via the TS-MMC topology optimization method show that the objective function can accurately reflect the width and position of band gaps for low-contrast materials, and its design results for high-contrast materials are highly consistent with existing studies. This framework is expected to simplify the optimization process, enable the design of various band gaps by limiting the integral range of the objective function, and achieves performance comparable to the current state-of-the-art (SOTA).

Keywords: Phononic crystal, Topology optimization, Density of states, Band gap engineering, TS-MMC method

Nonlinear Flutter Analysis of Orthotropic Laminated Thin Rectangular Plates

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Abstract

This paper focuses on the nonlinear flutter behaviors of laminated orthotropic thin rectangular plates under the influence of aerodynamic loading. The aerodynamic load is determined by the first-order piston theory. Applying Reddy's shear deformation plate theory, Hamilton's principle, and the Galerkin method, a set of ordinary differential equations (ODEs) can be derived. Besides solving the set of linear ODEs as an eigenvalue problem, the other more general nonlinear ODEs is solved numerically via the pseudo-arclength continuation algorithm. Both linear and nonlinear flutter analyses are carried out in this study. Results show that the nonlinear flutter boundary is lower than the linear flutter boundary.

Keywords: flutter, geometric nonlinearities, limit cycle oscillation, orthotropic laminated plate, Reddy's shear deformation plate theory

Symplectic Contact Analysis of Inhomogeneous Media

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Abstract

High-throughput characterization techniques for multi-field coupling based on functionally graded materials have significantly advanced materials science. However, accurately and efficiently quantifying multiple fundamental property parameters at all sample points across a gradient remains a major challenge. This poster aims to establish a theoretical foundation for further development of high-throughput material characterization from the perspective of contact mechanics in inhomogeneous media. Previous studies in contact mechanics have predominantly focused on half-plane/half-space with vertical material gradients, while theoretical frameworks for horizontally graded materials remain underdeveloped. Moreover, theories based on half-plane/half-space assumptions often fail to reflect physical reality due to boundary effects.

To address these issues, this poster introduces a symplectic framework into contact mechanics, establishing a symplectic system for finite-sized inhomogeneous media. A series of explicit analytical solutions for contact problems are derived and extended to multi-field coupling scenarios. For horizontally graded materials, it is proposed and demonstrated that the quasi-Hamiltonian operator and its dual operator conform the dual Hamiltonian transformation, and their eigenvectors satisfy the dual adjoint symplectic orthogonality. Given that contact problems involve boundary nonlinearity, a strategy for determining contact regions in inhomogeneous media is developed based on the symplectic approach. All theoretical results are validated through finite element simulations, confirming their accuracy and effectiveness. Furthermore, leveraging neural operator learning, an inverse problem solution is also presented within the established symplectic contact mechanics framework. **Keywords:** flutter, geometric nonlinearities, limit cycle oscillation, orthotropic laminated plate, Reddy's shear deformation plate theory

Keywords: Symplectic framework; contact analysis; quasi-Hamiltonian operator; dual Hamiltonian transformation

SPH method with self-contact treatment for simulation of transient deformation of soft structures

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Abstract

Simulation of deformation of soft structures are generally required for the design of structural components (for example, actuators) of soft robots. During the simulation, large deformation and self-contact phenomena are usually encountered. To effectively simulation these phenomena, an SPH method with self-contact treatment is developed. In the method, a mesh-based nearest neighboring particle search (MNNPS) algorithm is proposed to overcome the non-physical interaction between particles near self-contact regions, and a penalty-based contact algorithm is used to treat contact interactions. The hourglass control technique combined with the particle shifting technique is employed to enhance the numerical stability of SPH method for large deformation simulation. The present SPH method is used to calculate several numerical examples, including oscillation of an elastic plate, expansion of a single-chamber soft structure and bending of a multi-chamber soft pneumatic actuator. It is found that the present method can produce good accuracy and has strong capability in simulating large deformation of soft structures. It can effectively capture the self-contact behavior of soft actuator and predict its deformation well.

Keywords: Self-contact, soft structure, SPH method, simulation

Topology Optimization with Node Density Adaptation and Geometric Multigrid Solving

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Abstract

This study proposes an adaptive nodal density Solid Isotropic Material with Penalization (SIMP) method for topology optimization to improve computational efficiency by overcoming the high cost of fixed meshes. By decoupling the density mesh from the analysis mesh, our method eliminates the need for generating complex unstructured analysis meshes and effectively mitigates discontinuities in the density field. Providing a practical framework for large-scale structural optimization, the proposed approach achieves a greater than 50% reduction in computational complexity and computational scale of that required by a uniformly refined mesh. Optimization results for truss and cantilever beam structures under various working conditions demonstrate that this method enhances computational accuracy with fewer fine-scale features, yielding clearer structures with less computational effort. These results highlight the method's robustness and practical manufacturability.

Keywords: Adaptive refinement; Nodal density; SIMP; Quadtree; Shepard interpolation



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