

Tianju Xue (薛添駒)

Ph.D., Princeton University

The Hong Kong University of Science and Technology
Clear Water Bay, Hong Kong
✉ cetxue@ust.hk

Research Interest

Computational Mechanics (AI + CAE; Topology Optimization)
Additive Manufacturing (Multi-scale Multi-physics Simulation; Metamaterial Design)
Machine Learning (Automatic Differentiation; Bayesian Methods)

Professional Experience

- 09/2023–**Assistant Professor**, *The Hong Kong University of Science and Technology*.
Now Civil and Environmental Engineering
2022–2023 **Postdoctoral Scholar**, *Northwestern University*.
Mechanical Engineering, Advisor: Prof. *Jian Cao*

Education

- 2017–2022 **Ph.D.**, *Princeton University*.
Civil and Environmental Engineering, Advisor: Prof. *Sigrid Adriaenssens*
Computer Science, Advisor: Prof. *Ryan P. Adams*
2013–2017 **B.Sc.**, *Shanghai Jiao Tong University*.
Mechanical Engineering (UM-SJTU Joint Institute), GPA - 3.80/4.0 (ranking 1/53)
2016 **Exchange Student**, *The University of Hong Kong*.
Mechanical Engineering

Peer-reviewed Publications

- [43] X. Wang, W. Xu, **T. Xue***, Solving contact problems using Fiber Monte Carlo, *Computational Mechanics*, 2026.
[42] B. Xu, **T. Xue***, P. Wriggers, A first-order virtual element method for third-medium contact, *Computer Methods in Applied Mechanics and Engineering*, 2026.
[41] W. Xu, Z. Xie, H. Lin, X. Wang, G. Mou, **T. Xue***, Style-constrained inverse design of microstructures with tailored mechanical properties using unconditional diffusion models, *International Journal for Numerical Methods in Engineering*, 2026.
[40] G. Mou, D. Dong, J. Chen, S. Zhang, S. Liu, Y. Lu, N. Auffray*, **T. Xue***, A planar orthotropic mechanical metamaterial with isotropic deviatoric elasticity, *International Journal of Mechanical Sciences*, 2026.
[39] J. Cheng, L. Huang, Z. Xiao, K. Jiang, Z. Ma, Q. Chen*, C. Wang, **T. Xue**, N. Hu*, Revealing high-dimensional geometry–property relations in architected lattices via clustering-enabled explainable artificial intelligence, *Computers & Structures*, 2026.
[38] J. Fang, W. Ji*, **T. Xue**, Y. Wang, J. Zhao, Y. Jiang, C.E. Choi*, A novel coupled MPM-SDM framework for simulating non-spherical objects in flow-type landslide, *Computers and Geotechnics*, 2026.
[37] B. Xu, Z. Cao, **T. Xue***, P. Wriggers, Virtual Element Method based on divergence-free projection for contact mechanics, *Finite Elements in Analysis and Design*, 2026.

- [36] Y. Cheng, S. Sun, **T. Xue**, C. Ding, S. Mao*, ExDORGP: a high-efficiency data-driven method for uncertainty quantification for lithium-ion batteries, *Acta Mechanica Sinica*, 2026.
- [35] Y. Liu, W. Xu, Y. Xu, K. Sun, B. Ding, **T. Xue***, Y. Chen*, Frequency-domain Bayesian inference for identifying high-dimensional nonlinear mechanical properties of heterogeneous materials, *Journal of the Mechanics and Physics of Solids*, 2026.
- [34] B. Xu, **T. Xue***, P. Wriggers, Three-dimensional third medium contact model for hyperelastic contact and pneumatically actuated systems, *Journal of the Mechanics and Physics of Solids*, 2026.
- [33] E. Lale, J. Eliáš*, K. Yu, M. Troemner, M. Středulová, J. Khoury, **T. Xue**, I. Koutromanos, A. Fascetti, B. Ayhan, B. Chen, G. Di Luzio, Y. Lyu, M. Pathirage, G. Pijaudier-Cabot, L. Shen, A. Tasora, L. Yang, J. Zhong, G. Cusatis, Lattice discrete particle model (LDPM): comparison of various time integration solvers and implementations, *International Journal for Numerical and Analytical Methods in Geomechanics*, 2026.
- [32] W. Xu, K. Yang, Y. Zhang, W. Zhang, S. Sun, S. Mao, **T. Xue***, DiffLiB: High-fidelity differentiable modeling of lithium-ion batteries and efficient gradient-based parameter identification, *Structural and Multidisciplinary Optimization*, 2026.
- [31] Z. Xie, Z. Fu, J. Zhang, K. Zhang*, T. Zeng, Y. Wu*, S. Liao, X. Li, and **T. Xue***, Sim-to-real diffusion models for microstructure prediction in metal additive manufacturing, *Engineering with Computers*, 2026.
- [30] **T. Xue***, Implicit differentiation with second-order derivatives and benchmarks in finite-element-based differentiable physics, *Computer Physics Communications*, 2026.
- [29] W. Zhang, C. Liu, Y. Weng, **T. Xue***, J. Zhao, A differentiable material point method solver for the modeling, simulation and analysis of extrusion-flow process for 3D concrete printing, *Additive Manufacturing*, 2026.
- [28] F. Hu, R. Zhou, K. Ryou, R. Zha, S. Niezgoda, **T. Xue**, J. Cao*, An Efficient Graphical Processing Unit-Accelerated Calibration of Crystal Plasticity Model Parameters by Multi-Objective Optimization With Automatic Differentiation-Based Sensitivities, *Journal of Applied Mechanics*, 2026.
- [27] N. Liu, **T. Xue**, J. Qiu*, Multi-scale modeling of hydrogel-based concrete formed under the ambient environment and the extremely harsh environment of Mars, *Journal of the Mechanics and Physics of Solids*, 2025.
- [26] F. Hu, S. Niezgoda, **T. Xue***, J. Cao*, Efficient GPU-computing simulation platform JAX-CPFEM for differentiable crystal plasticity finite element method, *npj Computational Materials*, 2025.
- [25] D. Quispe, D. Kozjeka, M. Mozaffara, **T. Xue**, J. Cao*, AI-enabled manufacturing process discovery, *PNAS Nexus*, 2025.
- [24] J. Cao*, M. Bambach, M. Merklein, M. Mozaffar, **T. Xue**, Artificial intelligence in metal forming, *CIRP Annals*, 2024.
- [23] S. Liao, **T. Xue**, J. Cao*, Deep learning based reconstruction of transient 3D melt pool geometries in laser powder bed fusion from coaxial melt pool images, *Manufacturing Letters*, 2024.
- [22] X. Wu, **T. Xue***, S. Mao*, G-code Net: Learning-based rational design and optimization for additively manufactured structures, *MRS Communications*, 2024.
- [21] J. Choi, **T. Xue***, S. Liao, J. Cao*, Accelerating phase-field simulation of three-dimensional microstructure evolution in laser powder bed fusion with composable machine learning predictions, *Additive Manufacturing*, 2024.

- [20] X. Sun, G. Roeder, **T. Xue**, R. P. Adams, S. Rusinkiewicz, More Stiffness with Less Fiber: End-to-End Fiber Path Optimization for 3D-Printed Composites, *Proceedings of the 8th ACM Symposium on Computational Fabrication*, 2023.
- [19] J. Shao, A. Samaei, **T. Xue**, X. Xie, S. Guo, J. Cao, E. MacDonald, Z. Gan*, Additive friction stir deposition of metallic materials: process, structure and properties, *Materials & Design*, 2023.
- [18] **T. Xue**, S. Liao, Z. Gan, C. Park, X. Xie, W. K. Liu, J. Cao*, JAX-FEM: A differentiable GPU-accelerated 3D finite element solver for automatic inverse design and mechanistic data science, *Computer Physics Communications*, 2023.
- [17] C. Park, Y. Lu, S. Saha, **T. Xue**, J. Guo, S. Mojumder, D. W. Apley, G. J. Wagner, W. K. Liu*, Convolution Hierarchical Deep-learning Neural Network (C-HiDeNN) with Graphics Processing Unit (GPU) Acceleration, *Computational Mechanics*, 2023.
- [16] S. Liao, J. Jeong, R. Zha, **T. Xue**, J. Cao*, Simulation-guided feedforward-feedback control of melt pool temperature in directed energy deposition, *CIRP Annals*, 2023.
- [15] S. Liao, **T. Xue**, J. Jeong, S. Webster, K. Ehmann, J. Cao*, Hybrid full-field thermal characterization of additive manufacturing processes using physics-informed neural networks with data, *Computational Mechanics*, 2023.
- [14] M. Mozaffar, S. Liao, J. Jeong, **T. Xue**, J. Cao*, Differentiable simulation for material thermal response design in additive manufacturing processes, *Additive Manufacturing*, 2023.
- [13] **T. Xue**, S. Adriaenssens, S. Mao*, Learning the nonlinear dynamics of soft mechanical metamaterials with graph networks, *International Journal of Mechanical Sciences*, 2023.
- [12] **T. Xue**, Z. Gan, S. Liao, J. Cao*, Physics-embedded graph network for accelerating phase-field simulation of microstructure evolution in additive manufacturing, *npj Computational Materials*, 2022.
- [11] **T. Xue**, S. Mao*, Mapped shape optimization method for rational design of cellular mechanical metamaterials under large deformation, *International Journal for Numerical Methods in Engineering*, 2022.
- [10] X. Sun, **T. Xue**, S. M. Rusinkiewicz, R. P. Adams, Amortized Synthesis of Constrained Configurations Using a Differentiable Surrogate, *NeurIPS*, 2021.
- [9] **T. Xue**, S. Adriaenssens, S. Mao*, Mapped phase field method for brittle fracture, *Computer Methods in Applied Mechanics and Engineering*, 2021.
- [8] **T. Xue**, W. C. Sun, S. Adriaenssens, Y. Wei, C. Liu*, A new finite element level set reinitialization method based on the shifted boundary method, *Journal of Computational Physics*, 2021.
- [7] A. Beatson, J. T. Ash, G. Roeder, **T. Xue**, R. P. Adams, Learning Composable Energy Surrogates for PDE Order Reduction, *NeurIPS*, 2020.
- [6] **T. Xue***, T. J. Wallin, Y. Menguc, S. Adriaenssens, M. Chiaramonte*, Machine learning generative models for automatic design of multi-material 3D printed composite solids, *Extreme Mechanics Letters*, 2020.
- [5] **T. Xue**, A. Beatson, S. Adriaenssens, R. P. Adams, Amortized Finite Element Analysis for Fast PDE-Constrained Optimization, *ICML*, 2020.
- [4] **T. Xue***, A. Beatson, M. Chiaramonte*, G. Roeder, J. T. Ash, Y. Menguc, S. Adriaenssens, R. P. Adams, S. Mao*, A data-driven computational scheme for the nonlinear mechanical properties of cellular mechanical metamaterials under large deformation, *Soft Matter*, 2020.
- [3] Y. Wan, **T. Xue**, Y. Shen*, The successive node snapping scheme for an evolving branched curve in 2D and 3D, *Computer-Aided Design*, 2019.

- [2] Y. Wan, **T. Xue**, Y. Shen*, The successive node snapping scheme: A method to obtain conforming meshes for an evolving curve in 2D and 3D, *Finite Elements in Analysis and Design*, 2019.
- [1] M. Ma, **T. Xue**, S. Chen, Y. Guo*, Y. Chen, H. Liu, Features of structural relaxation in diblock copolymers, *Polymer Testing*, 2017.

Grants

- 2026-2027 **HKUST**, *Bridge Gap Fund*, PI, HKD 362,300.
AI Agents for Additive Manufacturing Simulation and Topology Optimization Based on JAX-FEM Express
- 2026-2029 **NSFC/RGC**, *Joint Research Scheme*, PI, HKD 1,142,400.
Resolving the toughening mechanisms of fracture-resistant mechanical metamaterials and their inverse design using deep generative models
- 2025-2027 **NSFC**, *Young Scientist Fund*, PI, RMB 300,000.
Inverse optimization of process parameters for metal additive manufacturing based on differentiable programming techniques
- 2025-2027 **RGC**, *Early Career Scheme*, PI, HKD 497,603.
Structural topology optimization with aesthetic value based on conditional diffusion models
- 2025-2026 **ITF**, *Seed Project*, PI, HKD 1,588,280.
DeepFEM: A GPU-Accelerated Finite Element Modeling and Simulation Toolkit for Products of AI for Science
- 2025-2026 **RGC**, *Young Collaborative Research Fund*, Co-PI, HKD 1,591,333 (share: 320,000).
Living Building Material-Based Extra-Terrestrial Construction Technology for Resource-Starved and Extremely Harsh Environments
- 2025-2028 **RGC**, *Collaborative Research Fund*, Co-PI, HKD 4,078,834 (share: 800,000).
Disaster reconstruction of landslides for rapid rescue of buried objects using differentiable physics-guided machine learning
- 2024-2028 **Beijing DP Technology Co., Ltd**, *Industrial Donation*, PI, RMB 500,000.
Development of a macroscopic computational platform based on automatic differentiation techniques

Teaching

- 2024-Now **Course Instructor**, The Hong Kong University of Science and Technology.
CIVL5830 Advanced Mechanics of Materials
CIVL5390 Finite Element Methods
CIVL4370 Computer Methods of Structural Analysis
CIVL2110 Statics
- 2017-2021 **Graduate Teaching Assistant**, Princeton University.
SML201 Introduction to Data Science
COS424 Fundamentals of Machine Learning
CEE205 Mechanics of Solids
- 2013-2017 **Undergraduate Teaching Assistant**, Shanghai Jiao Tong University.
VM382 Mechanical Behaviour of Materials
VP140 Physics

Internships

- 2020 **Quantitative Researcher**, Sixie Capital, Shanghai.
Statistical analysis of market data: Seeking investment alpha
- 2019 **Research Intern**, Facebook Inc., Redmond.
AR/VR at Facebook Reality Labs: Deep learning for 3D-printed material design
- 2017 **Product Design Engineer**, Apple Inc., Shanghai.
Apple accessories team: Keyboard design and manufacturing

Reviewing

PNAS; Nature Materials; npj Computational Materials; npj Advanced Manufacturing; npj Artificial Intelligence; Computational Mechanics; Extreme Mechanics Letters; Journal of Computing and Information Science in Engineering; Journal of Manufacturing Science and Engineering; International Journal of Plasticity; Physics of Fluids; Advanced Engineering Materials; Engineering Structures; Computational Materials Science; NeurIPS; Thin-Walled Structures; Finite Elements in Analysis and Design; Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences; International Journal of Mechanical Sciences; Materials & Design; Additive Manufacturing; Journal of Manufacturing Processes; Structures; International Journal of Solids and Structures; Composites Part B: Engineering.

Editorial Service

Editorial Board Member, *Journal of Mechanoinformatics (JMechI)*, OAE Publishing, 2026–present.

Selected Honors

- 2026 **Silver Medal in AI4S Agent Hackathon** (by Beijing DP Technology Co., Ltd)
- 2025 **Winner of NIST AM Bench 2025** (1st place in baseplate deflection prediction & 2nd place in residual elastic strains prediction)
- 2022 **Gordon Y.S. Wu Fellowships** (A highly prestigious award at Princeton University)
- 2021 **Student Competition Winner** (by U.S. Association for Computational Mechanics)
- 2016 **Merit Student Model (三好学生标兵)** (Top honor at Shanghai Jiao Tong University, 10 awardees each year (undergraduate and graduate students combined))
- 2016 **Shanghai Scholarship (上海市奖学金)** (Top scholarship for students in Shanghai)
- 2015 **National Scholarship (国家奖学金)** (Top scholarship for students in China)

Memberships

Member of the U.S. Association for Computational Mechanics (USACM)
Member of the Hong Kong Society of Theoretical and Applied Mechanics (HKSTAM)
Member of American Society of Civil Engineers (ASCE)
Director of the ASCE Greater China Section (ASCE-GC)

Software

JAX-AM An open-source Python library for numerical simulations in additive manufacturing with GPU acceleration and automatic sensitivity analysis.

JAX-FEM A GPU-accelerated differentiable finite element package based on JAX.