Yangshuai Wang

Curriculum Vitae

Peng Tsu Ann Assistant Professor (Visiting Fellow)
Department of Mathematics, National University of Singapore

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Updated 24 October 2026

Academic Appointments

2024–present	National University of Singapore Peng Tsu Ann Assistant Professor (Visiting Fellow) Mentor: Prof. Weizhu Bao
2021–2024	University of British Columbia Postdoctoral Research and Teaching Fellow Supervisor: Prof. Christoph Ortner

Education

2016–2021	Shanghai Jiao Tong University Ph.D. in Computational Mathematics; supervisor: Lei Zhang
2012–2016	Sichuan University B.S.

Research Interests

Numerical analysis and scientific computing for multiscale molecular and materials simulation; atomistic-to-continuum and QM/MM coupling; error estimation and adaptive algorithms; machine-learned interatomic potentials; uncertainty quantification; scientific machine learning for partial differential equations.

Teaching

2026 Autumn	MA4230 - Matrix Computation (NUS); Lecturer.
2025 Autumn	MA4270 - Data Modeling and Computation (NUS); Lecturer.
2025 Autumn	MA4230 - Matrix Computation (NUS); Lecturer.
2025 Spring	MA5240 - Finite Element Method (NUS); Lecturer.
2024 Autumn	MA4230 - Matrix Computation (NUS); Lecturer.
2023 Autumn	MATH 100 (UBC); Instructor.

Journal Articles

[J29] Yanbo Zhan, **Yangshuai Wang**, Bing Hu, Hao Wang. *Construction and a Priori Analysis of a Linear Elasticity Enhanced Multiscale Coupling Method for a Defective Atomistic Chain*. Journal of Scientific Computing (accepted), 2026. [Record] | [Earlier preprint: arXiv:2502.17164]

[J28] Xiaoqing Liu, **Yangshuai Wang**, Lei Shen. *Configuration Selection and Matrix-Aware Optimization for Data-Efficient Atomistic Foundation Models*. Journal of Materials Informatics (accepted), 2026. [Record]

[J27] Jiale Linghu, **Yangshuai Wang**. *TensorSketch-Compressed High-Order Atomic Cluster Expansion Potentials: Accuracy, Mechanics, and Vibrational Thermodynamics*. The Journal of Physical Chemistry A (accepted), 2026. [Record]

[J26] **Yangshuai Wang**. *Geometry-conditioned basin initialization for variational quantum eigensolvers in strongly correlated molecules*. Physical Review A, 114:042421, 2026. [Publisher]

[J25] Xinyi Wei, **Yangshuai Wang**, Kai Jiang, Lei Zhang. *Amplitude Expansion Phase Field Crystal (APFC) Modeling based Efficient Dislocation Simulations using Fourier Pseudospectral Method*. Journal of Scientific Computing, 108:57, 2026. [Publisher]

[J24] Xinyi Wei, Julian Braun, **Yangshuai Wang**, Lei Zhang. *Higher-Order Boundary Conditions for Atomistic Dislocation Simulations*. SIAM Journal on Scientific Computing, 48(5):A2934–A2958, 2026. [Publisher]

[J23] Yifan Yu, Cheuk Hin Ho, **Yangshuai Wang**. *A Conformal Prediction Framework for Uncertainty Quantification in Physics-Informed Neural Networks*. Journal of Computational Physics, 114979, 2026. [Publisher]

[J22] Cheuk Hin Ho, Christoph Ortner, **Yangshuai Wang**. *Flexible Uncertainty Calibration for Machine-Learned Interatomic Potentials*. npj Computational Materials, 2026. [Publisher]

[J21] Peng Liu, Lidong Fang, **Yangshuai Wang**, Lei Zhang, Qingcheng Yang. *Concurrent Atomistic-Continuum Coupling via Physics-Informed Neural Networks (PINNs-CAC) with Adaptive Energy Weighting and Direct Boundary Encoding*. Applied Mathematical Modelling, 116931, 2026. [Publisher]

[J20] Xiaoqing Liu, **Yangshuai Wang**, Teng Zhao. *Beyond Adam: Disentangling Optimizer Effects in the Fine-Tuning of Atomistic Foundation Models*. AI for Science, 2(1), 2026. [Publisher]

[J19] Hao Wang, **Yangshuai Wang**. *Adaptive quasicontinuum methods and simulations for crystal defects with a theory based unified a posteriori error estimate*. Computer Physics Communications, 322:110085, 2026. [Publisher]

[J18] Xiaoqing Liu, Kehan Zeng, Zedong Luo, **Yangshuai Wang**, Teng Zhao, Zhenli Xu. *Fine-Tuning Universal Machine-Learned Interatomic Potentials: A Tutorial on Methods and Applications*. Journal of Applied Physics, 139:041101, 2026. [Publisher] | [arXiv:2506.21935]

[J17] Xi'an Li, Jinran Wu, Xiao Ning, **Yangshuai Wang**, Lei Zhang. *Bayesian Physics-Informed Neural Networks to Solve the PDEs with Noise or Incomplete Constraints*. The Innovation Informatics (Editorial), 2:100039, 2026. [Publisher]

[J16] **Yangshuai Wang**, Drake Clark, Sambit Das, Ziyan Zhu, Daniel Massatt, Vikram Gavini, Mitchell Luskin, Christoph Ortner. *An Atomic Cluster Expansion Potential for Twisted Multilayer Graphene*. Machine Learning: Science and Technology, 6:045040, 2025. [Publisher]

[J15] Ilyes Batatia et al. (including **Yangshuai Wang**). *A Foundation Model for Atomistic Materials Chemistry*. The Journal of Chemical Physics, 163:184110, 2025. [Publisher]

[J14] Julian Braun, Christoph Ortner, **Yangshuai Wang**, Lei Zhang. *Higher Order Far-Field Boundary Conditions for Crystalline Defects*. SIAM Journal on Numerical Analysis, 63(2), 2025. [Publisher]

[J13] Tina Torabi, Christoph Ortner, **Yangshuai Wang**. *Surrogate models for vibrational entropy based on a spatial decomposition*. Multiscale Modeling and Simulation, 23(1), 2025. [Publisher]

[J12] **Yangshuai Wang**. *A Posteriori Analysis and Adaptive Algorithms for Blended Type Atomistic-to-Continuum Coupling with Higher-Order Finite Elements*. Computer Physics Communications, 310:109533, 2025. [Publisher]

[J11] Kejie Fu, Mingjie Liao, **Yangshuai Wang**, Jianjun Chen, Lei Zhang. *MeshAC: A 3D Mesh Generation and Adaptation Package for Multiscale Coupling Methods*. Computer Physics Communications (Computer Programs in Physics), 310:109523, 2025. [Publisher]

[J10] **Yangshuai Wang**, James Kermode, Christoph Ortner, Lei Zhang. *A Posteriori Error Estimate and Adaptivity for QM/MM Models of Crystalline Defects*. Computer Methods in Applied Mechanics and Engineering, 428:117097, 2024. [Publisher]

[J9] **Yangshuai Wang**, Shashwat Patel, Christoph Ortner. *A Theoretical Case Study of the Generalisation of Machine-learned Potentials*. Computer Methods in Applied Mechanics and Engineering, 422:116831, 2024. [Publisher]

[J8] **Yangshuai Wang**, Hao Wang. *Efficient a Posteriori Error Control of a Consistent Atomistic/Continuum Coupling Method for Two Dimensional Crystalline Defects*. Journal of Scientific Computing, 97:51, 2023. [Publisher]

[J7] Derek Olson, Christoph Ortner, **Yangshuai Wang**, Lei Zhang. *Elastic Far-field Decay from Dislocations in Multilattices*. Multiscale Modeling and Simulation, 21(4), 2023. [Publisher]

[J6] Christoph Ortner, **Yangshuai Wang**. *A Framework for a Generalisation Analysis of Machine-learned Interatomic Potentials*. Multiscale Modeling and Simulation, 21:1053–1080, 2023. [Publisher]

[J5] Kejie Fu, Mingjie Liao, **Yangshuai Wang**, Jianjun Chen, Lei Zhang. *Adaptive multigrid strategy for geometry optimization of large-scale three dimensional molecular mechanics*. Journal of Computational Physics, 485:112113, 2023. [Publisher]

[J4] Huajie Chen, Christoph Ortner, **Yangshuai Wang**. *QM/MM Methods for Crystalline Defects. Part 3: Machine-learned MM Models*. Multiscale Modeling and Simulation, 20:1490–1518, 2022. [Publisher]

[J3] **Yangshuai Wang**, Huajie Chen, Mingjie Liao, Christoph Ortner, Hao Wang, Lei Zhang. *A Posteriori Error Estimates for Adaptive QM/MM Coupling Methods*. SIAM Journal on Scientific Computing, 43:A2785–A2808, 2021. [Publisher]

[J2] **Yangshuai Wang**, Lei Zhang, Hao Wang. *A Priori Analysis of a Higher Order Nonlinear Elasticity Model for an Atomistic Chain with Periodic Boundary Condition*. IMA Journal of Numerical Analysis, 41(2):1465–1495, 2021. [Publisher]

[J1] Huajie Chen, Mingjie Liao, Hao Wang, **Yangshuai Wang**, Lei Zhang. *Adaptive QM/MM Coupling for Crystalline Defects*. Computer Methods in Applied Mechanics and Engineering, 354:351–368, 2019. [Publisher]

Conference Papers

[C4] Qinyi Zhang, Duanyu Feng, Hao Wang, **Yangshuai Wang**. *IADR: Interface-Augmented Neural Operator for Phase-Field Mean-Curvature Flow*. NeurIPS 2026 (accepted), 2026. [OpenReview]

[C3] Zhaohui Fu, Duanyu Feng, **Yangshuai Wang**. *LDD-RFM: Learnable Domain Decomposition for Random Feature Models via Variable Projection*. NeurIPS 2026 (accepted), 2026. [OpenReview]

[C2] Qinyi Zhang, Duanyu Feng, Ronghui Han, **Yangshuai Wang**, Hao Wang. *MicroEvoEval: A Systematic Evaluation Framework for Image-Based Microstructure Evolution Prediction*. Proceedings of the AAAI Conference on Artificial Intelligence, 40(2):1543–1551, 2026. [arXiv:2511.08955]

[C1] Shivangi Kamat, **Yangshuai Wang**. *Before Lean Checks: Candidate Exposure in Proof-Action Ranking*. ICML 2026, AI4Math Workshop, 2026. [Conference]

Books

[B1] Mitchell Luskin, Christoph Ortner, **Yangshuai Wang**. *Mathematical Modeling of Materials at the Atomic Scale*. Texts in Applied Mathematics, Springer Nature (under contract). [Record]

Preprints and Submitted Manuscripts

[P22] Chenyu Wang, **Yangshuai Wang**, Lei Zhang. *From Energy-Force Weighting to Primal-Dual Optimization of Machine-Learned Interatomic Potentials*. Preprint; under review, 2026. [arXiv:2610.00876]

[P21] Xingguo Wu, **Yangshuai Wang**, Zhenli Xu. *Moment-Informed Force Rescaling for Random-Batch Langevin Dynamics*. Preprint; under review, 2026. [arXiv:2609.18389]

[P20] Jiawen Yu, Chaohong Guan, Xiaoqing Liu, **Yangshuai Wang**, Hong Zhu, Xiaoqin Zeng. *Evaluating Universal Interatomic Potentials for Metallic Systems: From Elastic Response to Defect Energetics and Ideal Strength*. Preprint; under review, 2026. [Record]

[P19] Zhaohui Fu, **Yangshuai Wang**. *Optimal Sobolev Approximation by Deterministic and Random Shallow Sigmoidal Networks*. Preprint; under review, 2026. [arXiv:2608.19797]

[P18] Jiaye Chen, **Yangshuai Wang**, Weizhu Bao, Xiaogang Liu. *Autonomous Knowledge Distillation for an AI-Ready Knowledge Layer*. Preprint; under review, 2026. [Record]

[P17] Jiale Linghu, Hao Dong, **Yangshuai Wang**. *A Structure-Adaptive Random Feature Method for High-Dimensional Elliptic PDEs*. Preprint; under review, 2026. [arXiv:2607.19786]

[P16] Jiale Linghu, **Yangshuai Wang**. *Residual-Christoffel Sampling for Random Feature Collocation of Linear PDEs*. Preprint; under review, 2026. [arXiv:2607.13382]

[P15] Jiale Linghu, Hao Dong, **Yangshuai Wang**. *Trainable Photonic Measurement for Physics-Informed PDE Learning*. Preprint; under review, 2026. [arXiv:2606.18713]

[P14] Xi'an Li, Jiale Linghu, **Yangshuai Wang**. *Random-Feature Kalman Filtering for Linear PDE Data Assimilation*. Preprint; under review, 2026. [arXiv:2606.16086]

[P13] Jiale Linghu, **Yangshuai Wang**. *Liquid Random Feature Methods for Time-Dependent Partial Differential Equations*. Preprint; under review, 2026. [arXiv:2606.15571]

[P12] Tina Torabi, Jiale Linghu, **Yangshuai Wang**. *Local Surrogates for Harmonic Vibrational Entropy in Multilattices*. Preprint; under review, 2026. [arXiv:2605.26588]

[P11] Yifan Yu, **Yangshuai Wang**. *Geometry-Preserving Nudged Elastic Band and Dimer Methods under Anisotropic Force Uncertainty*. Preprint; under review, 2026. [arXiv:2605.24401]

[P10] Haoran Zhou, Zhaohui Fu, **Yangshuai Wang**, Xinlong Feng. *A Discrete-Time Random Feature Method for Nonlinear Evolution Equations with Implicit-Explicit Runge–Kutta Time Stepping*. Preprint; under review, 2026. [arXiv:2604.25502]

[P9] Yihan Huang, **Yangshuai Wang**. *Analysis of Hessian Scaling for Local and Global Costs in Variational Quantum Algorithm*. Preprint; under review, 2026. [arXiv:2602.00783]

[P8] Yanbo Zhan, **Yangshuai Wang**, Xingyu Gao, Hao Wang. *Flexible Boundary Sequential Coupling for Atomistic Simulation of Crystal Defects*. Preprint, 2026. [Record]

[P7] Li Ding, Duanyu Feng, Chen Huang, **Yangshuai Wang**, Wenqiang Lei. *2D-ProteinRAG: Mitigating Intent-Context Misalignment in Homology-Based Protein Question Answering*. Preprint; under review, 2026. [Record]

[P6] Qingyu Meng, **Yangshuai Wang**. *Trainability-Oriented Hybrid Quantum Regression via Geometric Preconditioning and Curriculum Optimization*. Preprint; under review, 2026. [arXiv:2601.11942]

[P5] **Yangshuai Wang**, Yongfa Guo, Zedong Luo, Xiaoqing Liu, Cheng Chen, Qi Zhou, Teng Zhao, Zhenli Xu. *NanoTitan: An AI-Driven Memory-Efficient Platform for High-Performance Molecular Dynamics Simulation*. Preprint, 2025. [Record]

[P4] Xiaoqing Liu, Xinyu Yu, **Yangshuai Wang**, Zhe-Tao Sun, Zedong Luo, Kehan Zeng, Teng Zhao, Shou-Hang Bo, Zhenli Xu. *An AI-Ready Fine-Tuning Framework for Accurate Machine-Learning Interatomic Potentials in Solid –Solid Battery Interfaces*. Preprint; under review, 2026. [arXiv:2601.17847]

[P3] Xiaoqing Liu, Kehan Zeng, **Yangshuai Wang**, Teng Zhao. *A Study on the Fine-Tuning Performance of Universal Machine-Learned Interatomic Potentials (U-MLIPs)*. Preprint, 2025. [arXiv:2506.07401]

[P2] Junfeng Lu, Hao Wang, **Yangshuai Wang**. *Formulation and Analysis of Blended Atomistic to Higher-Order Continuum Coupling Methods for Crystalline Defects*. Preprint, 2025. [arXiv:2502.18854]

[P1] **Yangshuai Wang**, Gabor Csanyi, Christoph Ortner. *Many-Body Coarse-Grained Molecular Dynamics with the Atomic Cluster Expansion*. Preprint, 2025. [arXiv:2502.04661]

Doctoral Thesis

[T1] **Yangshuai Wang**. *Some Progress on Multi-scale Methods in Materials Modeling*. Shanghai Jiao Tong University, 2021. [Record]

Awards and Honors

2026	NeurIPS Top Reviewer
2021	Development Postdoctoral Scholarship for Outstanding Doctoral Graduates, Shanghai Jiao Tong University
2020	National Scholarship for Doctoral Students
2019	Qiushi Postgraduates Scholarship
2015–2021	Tanglixin Scholarship

Selected Talks and Conferences

April 2026	Invited talk, First China AI+New Materials Conference, Guangzhou
May 2025	Workshop on Mathematical Theory, Methods, and Applications in Materials Simulations, Tianyuan Mathematical Center in Science and Technology, Kunming
April 2025	Computational Multiscale Methods, Oberwolfach
October 2024	Invited talk, International Workshop on Data-driven Computational and Theoretical Materials Design, Shanghai
July 2024	Machine Learning in Multiscale and Reduced Order Methods for the Simulation of Physical Systems, SciCADE 2024, National University of Singapore
April 2024	Machine Learning Force Fields and Data-Driven Materials Informatics, Institute for Mathematical and Statistical Innovation, University of Chicago
April 2024	Application of Machine-Learned Interatomic Potentials in Atomic-Scale Simulations and Beyond, Data Science Seminar, University of Minnesota
February 2024	Enhancing Machine-Learned Interatomic Potentials in Materials Science: Progressing from Accuracy to Robustness, Hot Topics in AI for Sciences, Shanghai Jiao Tong University
May 2022	Error Propagation of Machine-Learned Interatomic Potentials, Machine-Learned Interatomic Potentials Mini-workshop, IPAM, UCLA

Scientific Software and Skills

Co-author of MeshAC, a three-dimensional mesh generation and adaptation package for multiscale coupling methods.

Programming: Julia, MATLAB, Python and LaTeX. Languages: Chinese and English.