# Yangshuai Wang

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## Career

- **National University of Singapore** Singapore
  *Peng Tsu Ann Assistant Professor (Visiting Fellow)* *July 2024 – Now*
- **University of British Columbia** Vancouver, Canada
  *Postdoctoral Research and Teaching Fellow* *Dec. 2021 – July 2024*

## Education

- **Shanghai Jiao Tong University** Shanghai, China
  *Ph.D. in Mathematics; GPA: 3.95/4.0* *Sept. 2016 – Dec. 2021*
- **Sichuan University** Sichuan, China
  *B.S. in Computational Mathematics; GPA: 92.5/100* *Sept. 2012 – June 2016*

## Research Interests

My research interests encompass numerical analysis and scientific computing applied to molecular modeling and simulations in materials science, with a focus on:

- **Mathematical theory of machine-learned interatomic potentials**: generalisation error analysis; uncertainty quantification and active learning; inverse problems;
- **Modeling and simulations of machine-learned interatomic potentials**: crystalline defects (dislocations, grain-boundaries and random alloys); 2D materials; vibrational entropy; coarse-grained molecular dynamics; accelerated molecular dynamics;
- **Analysis and applications of multi-scale coupling methods**: *a priori* analysis, *a posteriori* error control and adaptive algorithm design for atomistic-to-continuum (A/C) and quantum mechanics/molecular mechanics (QM/MM) coupling methods;
- **Mathematical modeling of materials at atomic scale**: boundary conditions of defect simulations; regularity estimate of defect equilibrium; multi-lattices modeling; Cauchy-Born rule;
- **Scientific machine learning**: data-driven and machine learning techniques to solve partial differential equations (PDEs) and related scientific and mathematical problems.

## Publications

- (**Book**) Mitchell Luskin, Christoph Ortner and **Yangshuai Wang**, *Mathematical Modeling of Materials at the Atomic Scale*, Book Series Texts in Applied Mathematics, **Springer Nature**, under the contract.
- (Corresponding author) Julian Braun, Christoph Ortner, **Yangshuai Wang** and Lei Zhang, *Higher Order Far-Field Boundary Conditions for Crystalline Defects*, accepted by **SIAM J Numer. Anal.**, 2024.
- (Corresponding author) Tina Torabi, Christoph Ortner and **Yangshuai Wang**, *Surrogate models for vibrational entropy based on a spatial decomposition*, accepted by **Multiscale Model. Simul.**, 2024.

- **Yangshuai Wang**, James Kermode, Christoph Ortner and Lei Zhang, *A Posteriori Error Estimate and Adaptivity for QM/MM Models of Crystalline Defects*, **Comput. Methods Appl. Mech. Engrg.**, 428:117097, 2024.
- **Yangshuai Wang**, Shashwat Patel and Christoph Ortner, *A Theoretical Case Study of the Generalisation of Machine-learned Potentials*, **Comput. Methods Appl. Mech. Engrg.**, 422:116831, 2024.
- **Yangshuai Wang** and Hao Wang, *Efficient a Posteriori Error Control of a Consistent Atomistic/Continuum Coupling Method for Two Dimensional Crystalline Defects*, **J. Sci. Comput.**, 97:51, 2023.
- (Corresponding author) Derek Olson, Christoph Ortner, **Yangshuai Wang** and Lei Zhang, *Elastic Far-field Decay from Dislocations in Multilattices*, **Multiscale Model. Simul.**, 21(4), 2023.
- (Corresponding author) Christoph Ortner and **Yangshuai Wang**, *A Framework for a Generalisation Analysis of Machine-learned Interatomic Potentials*, **Multiscale Model. Simul.**, 21:1053-1080, 2023.
- (Corresponding author) Kejie Fu, Mingjie Liao, **Yangshuai Wang**, Jianjun Chen and Lei Zhang, *Adaptive Multigrid Strategy for Large-scale Molecular Mechanics Optimization*, **J. Comp. Phys.**, 485:112113, 2023.
- (Corresponding author) Huajie Chen, Christoph Ortner and **Yangshuai Wang**, *QM/MM Methods for Crystalline Defects. Part 3: Machine-learned MM Models*, **Multiscale Model. Simul.**, 20:1490-1518, 2022.
- **Yangshuai Wang**, Huajie Chen, Mingjie Liao, Christoph Ortner, Hao Wang and Lei Zhang, *A Posteriori Error Estimates for Adaptive QM/MM Coupling Methods*, **SIAM J Sci. Comp.**, 43:A2785-A2808, 2021.
- **Yangshuai Wang**, Hao Wang and Lei Zhang, *A Priori Analysis of a Higher Order Nonlinear Elasticity Model for an Atomistic Chain with Periodic Boundary Condition*, **IMA J. Numer. Anal.**, 41:1465-1495, 2020.
- (Alphabetic order) Huajie Chen, Mingjie Liao, Hao Wang, **Yangshuai Wang** and Lei Zhang, *Adaptive QM/MM Coupling for Crystalline Defects*, **Comput. Methods Appl. Mech. Engrg.**, 354:351-368, 2019.

## Preprints

- Xinyi Wei, **Yangshuai Wang**, Kai Jiang and Lei Zhang, *Amplitude Expansion Phase Field Crystal (APFC) Modeling based Efficient Dislocation Simulations using Fourier Pseudospectral Method*, arXiv preprint, arXiv:2410.22720, 2024.
- **Yangshuai Wang**, *A Posteriori Analysis and Adaptive Algorithms for Blended Type Atomistic-to-Continuum Coupling with Higher-Order Finite Elements*, arXiv preprint, arXiv:2308.16467, 2023.
- (Corresponding author) Hao Wang and **Yangshuai Wang**, *Adaptive Multiscale Coupling Methods of Molecular Mechanics Based on a Unified Framework of a Posteriori Error Estimates*, arXiv preprint, arXiv:2309.13255, 2023.
- Ilyes Batatia, Philipp Benner, Yuan Chiang, Alin M. Elena, Dávid P. Kovács, and Janosh Riebesell et al. (62 authors not shown), *A Foundation Model for Atomistic Materials Chemistry*, **Nature (under review)**, arXiv preprint, arXiv:2401.00096, 2024.

- (Corresponding author) Kejie Fu, Mingjie Liao, **Yangshuai Wang**, Jianjun Chen and Lei Zhang, *MeshAC: A 3D Mesh Generation and Adaptation Package for Multiscale Coupling Methods*, arXiv preprint, arXiv:2402.09446, 2024.

## Selected Awards and Honors

- 2021 **Development Postdoctoral Scholarship for Outstanding Doctoral Graduates from Shanghai Jiao Tong University**
- 2020 **National Scholarship for Doctoral Students**
- 2019 **Qiushi Postgraduates Scholarship**
- 2015 - 2021 **Tanglixin Scholarship**

## Research Funding

- 2023-2026 Analysis and applications of multiscale coupling methods for crystalline defects, **National Natural Science Foundation of China No. 12271360**, co-PI.

## Teaching Experience

- Aug. 2024 - Nov. 2024 Instructor, MA4230 Matrix Computation, NUS.
- Sept. 2023 - Dec. 2023 Instructor, MATH 100 Calculus, UBC.
- Feb. 2019 - June 2019 Teaching Assistant, Numerical Methods for Differential Equations, SJTU.
- Feb. 2018 - June 2018 Teaching Assistant, Applied Mathematics Methods, SJTU.
- Feb. 2017 - June 2017 Teaching Assistant, Scientific Computing, SJTU.

## Skills

- **Languages**: Chinese, English
- **Programming**: Julia, Matlab, Python, LaTeX

## Selected Conferences and Talks

- July 2024 Machine Learning in Multiscale and Reduced Order Methods for the Simulation of Physical Systems, International Conference on Scientific Computation and Differential Equations (SciCADE 2024), National University of Singapore.
- June 2024 Advancing Molecular Simulations with Machine-Learned Interatomic Potentials, Beijing Normal University.
- May 2024 Using Uncertainty Quantification to Improve Learning in Atomistic Modeling, SIAM Conference on Mathematical Aspects of Materials Science, Pittsburgh.

- Apr. 2024 Machine Learning Force Fields, Data-Driven Materials Informatics, Institute for Mathematical and Statistical Innovation, University of Chicago.
- Apr. 2024 Application of machine-learned interatomic potentials in atomic-scale simulations and beyond, Data Science Seminars, University of Minnesota.
- Feb. 2024 Enhancing Machine-Learned Interatomic Potentials in Materials Science: Progressing from Accuracy to Robustness, Hot Topics in AI for Sciences, Shanghai Jiao Tong University.
- Jan. 2024 Application of machine-learned interatomic potentials in atomic-scale simulations and beyond, Model Reduction and Simulation at Atomic Scale, University of Warwick.
- Aug. 2023 Analysis, Methods and Applications in Complex Materials, mini-symposium in ICIAM 2023, co-organizer, Waseda University.
- Mar. 2023 "Atomic Cluster Expansion with and without Atoms", Beijing Normal University, online.
- Oct. 2022 Atomic Cluster Expansion (ACE) Seminar, University of Cambridge, online, "A Framework for a Generalisation Analysis of Machine-learned Interatomic Potentials (MLIPs)".
- Aug. 2022 Computational Methods in Applied Mathematics (CMAM 2022) in TU Wien, online, "A Framework for a Generalisation Analysis of Machine-learned Interatomic Potentials (MLIPs)".
- May 2022 Machine-learned Interatomic Potentials Mini-workshop, IPAM UCLA, "Error Propagation of Machine-learned Interatomic Potentials (MLIPs)".
- Nov. 2021 Workshop on Computational Materials Science, Sichuan University, online, "A Posteriori Error Estimates for Adaptive QM/MM Coupling Methods".
- Apr. 2021 International Workshop on Mathematical Theory, Methods and Application in Materials Simulation, Shanghai Jiao Tong University, "The Applications of Data-driven Interatomic Potentials to QM/MM Coupling Methods".
- June 2020 Workshop on Materials Modeling, University of Warwick-Shanghai Jiao Tong University-University of British Columbia, online, "Adaptive QM/MM Coupling Methods".
- July 2019 Top-notch Doctoral Seminar in Computational and Applied Mathematics, Peking University, "Some Recent Progress on Multiscale Coupling Methods".

## References


- Weizhu Bao, Professor, Department of Mathematics, NUS, matbaowz@nus.edu.sg
- Mitchell Luskin, Professor, Department of Mathematics, UMN, luskin@umn.edu
- Gabor Csanyi, Professor, Department of Engineering, Cambridge, gc121@cam.ac.uk
- Christoph Ortner, Professor, Department of Mathematics, UBC, ortner@math.ubc.ca
- Ping Lin, Professor, Mathematics, School of Science and Engineering, Dundee, P.Lin@dundee.ac.uk
- James Kermode, Professor, School of Engineering, Warwick, J.R.Kermode@warwick.ac.uk
- Lei Zhang, Professor, INS and Mathematics, SJTU, lzhang2012@sjtu.edu.cn
- Huajie Chen, Professor, School of Mathematics, Beijing Normal, chen.huajie@bnu.edu.cn