

Yue Zhao

Department of Computational Mathematics, Science, and Engineering,
Michigan State University,
428 S Shaw Ln, East Lansing, MI 48824,
Phone: 586-436-0720
Email: zhaoyu14@msu.edu

Positions

Postdoctoral Researcher, Department of Computational Mathematics, Science, and Engineering, Michigan State University, 2023-now

Mentor: Prof. Huan Lei

Education

Ph.D., Mathematics, Shanghai Jiao Tong University, 2019-2023

Advisor: Prof. Zhenli Xu, Shanghai Jiao Tong University

Co-advisor: Prof. Xiaoping Wang, Hong Kong University of Science and Technology

Visiting scholar, Hong Kong University of Science and Technology, 2022.2-2023.1

B.S. Mathematics, Shanghai Jiao Tong University, 2015-2019

Research Interests

Multiscale modeling for structure-preserving machine learning models;

Fast algorithms in molecular dynamics and the Monte Carlo method;

Numerical methods for partial differential equations;

Hydrodynamics and interfacial problems;

Data assimilation and Bayesian inverse problems.

Awards

Wenjun Wu Scholarship, Shanghai Jiao Tong University, 2021

Weichai Power Scholarship, Shanghai Jiao Tong University, 2021

Second Prize of Zhiyuan honored Ph.D Students Academic Forum, Shanghai Jiao Tong University, 2021

Second Prize of the 8th National College Student Mathematics Competition (Final), China, 2017

Excellent Students Scholarship in University, Shanghai Jiao Tong University, 2015-2019

Publications

Peer-Reviewed Journal Articles

1. **Yue Zhao** and Huan Lei, Fast spectral separation method for kinetic equation with anisotropic non-stationary collision operator retaining micro-model fidelity. *arXiv:2510.15093*, 2025.
2. **Yue Zhao**, Joshua W. Burby, Andrew J. Christlieb and Huan Lei, Data-driven construction of a generalized kinetic collision operator from molecular dynamics. *Phys. Rev. Lett.*, 135(18):185101, 2025.
3. Zhenli Xu, **Yue Zhao** and Qi Zhou, Variance-reduced random batch Langevin dynamics. *J. Chem. Phys.*, 161(24):244110, 2024.
4. Jiuyang Liang, Zhenli Xu and **Yue Zhao**, Energy stable scheme for random batch molecular dynamics. *J. Chem. Phys.*, 160(3):034101, 2024.
5. Jiuyang Liang, Zhenli Xu and **Yue Zhao**, Improved random batch Ewald method in molecular dynamics simulations. *J. Phys. Chem. A*, 126(22):3583-3593, 2022.
6. Jiuyang Liang, Pan Tan, **Yue Zhao**, Lei Li, Shi Jin, Liang Hong and Zhenli Xu, Superscalability of the random batch Ewald method. *J. Chem. Phys.*, 156(1):014114, 2022.
7. Jiuyang Liang, Zhenli Xu and **Yue Zhao**, Random-batch list algorithm for short-range molecular dynamics simulations *J. Chem. Phys.*, 155(4):044108, 2021.
8. Shi Jin, Lei Li, Zhenli Xu and **Yue Zhao**, A random batch Ewald method for particle systems with Coulomb interactions. *SIAM J. Sci. Comput.*, 43(4):B937-B960, 2021.
9. Lei Li, Zhenli Xu, and **Yue Zhao**, A random-batch Monte Carlo method for many-body systems with singular kernels. *SIAM J. Sci. Comput.*, 42(3):A1486-A1509, 2020.

Work in Preparing

10. **Yue Zhao**, Guosheng Fu and Huan Lei, From MD to kinetic models: data-driven generalized collision operators in 1D3V plasmas

Teaching experience

Michigan State University

STT 351H, Probability and Statistics for Engineering, Fall 2025

Shanghai Jiao Tong University

TA, Numerical Analysis and Programming, Spring 2021

TA, Numerical Analysis and Programming, Spring 2020

TA, Mathematical Analysis I, Fall 2019

NYU Shanghai

TA, Math for Economics I and II, Fall 2021

Conference and Workshop Presentations

NSF Computational Math Meeting 2025, "Data-driven construction of the kinetic collision operator from molecular dynamics"(Poster), The University of Utah, Salt Lake City, 05/2025

CHARMNET meeting, Virginia Tech, 12/2024

CHARMNET meeting, "Learning Collision Operator From Micro-Scale Descriptions"(Poster), 12/2023

Mathematics in Action (MiA2021): Modeling and Analysis in Molecular Biology and Electrophysiology, Duke Kunshan University (Poster), 06/2021

The Forum on Mathematics and Industrial Innovations, Shanghai Science Hall, 03/2020

Annual Meeting of Shanghai Society for Industrial and Applied Mathematics, Fudan University, 11/2019

The 15th Shanghai Symposium on Scientific and Engineering Computing Methods, Shanghai Maritime University, 11/2019

Seminar Talks

"Data-driven Learning and Fast Computation of the Kinetic Collision Operator from Molecular Dynamics", The Great Lakes section of SIAM (GLSIAM), Illinois Institute of Technology, Chicago, IL USA, 09/2025

"Random-batch Ewald method", 2024 Joint Mathematics Meetings, San Francisco, CA USA, 01/2024

"Random-batch Ewald method", the 5th CSIAM Student Forum (CSIAM 2021 Annual Meeting), Hefei, China, 10/2021

"Random-batch Ewald method", Zhiyuan honored Ph.D Students Academic Forum (Second Prize), Shanghai Jiao Tong University, 07/2021