# Yue Zhao

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## Employment

- **Michigan State University**     08/2023 - now
  Postdoctoral Researcher
  - *Mentor*: Prof. Huan Lei

## Education

- **Shanghai Jiao Tong University**     09/2019 – 06/2023
  Ph.D. in Mathematics
  - *Advisor*: Prof. Zhenli Xu
  - *Co-advisor*: Prof. Xiaoping Wang
- **Hong Kong University of Science and Technology**     02/2022 - 01/2023
  Visiting scholar
- **Shanghai Jiao Tong University**     09/2015 - 06/2019
  B.S. in Mathematics

## 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.

## Publications (Google Scholar)

[*] Corresponding author; [†] Co-first author; other authors listed a-z.

*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 Preparation*

10. **Yue Zhao**[†], Guosheng Fu and Huan Lei, From molecular dynamics to kinetic models: data-driven generalized collision operators in 1D3V plasmas, preprint, 2025.

# Awards

- **Wenjun Wu Scholarship** 2021
  Shanghai Jiao Tong University
- **Weichai Power Scholarship** 2021
  Shanghai Jiao Tong University
- **Second Prize of Zhiyuan honored Ph.D Students Academic Forum** 2021
  Shanghai Jiao Tong University
- **First Prize in the 8th National College Student Mathematics Competition** 2017
  **Second Prize in the Final Round**
  Chinese Mathematical Society
- **Excellent Students Scholarship in University** 2015-2019
  Shanghai Jiao Tong University

# Academic Service

*Journal Reviewer:*

- Advances in Applied Mathematics and Mechanics
- IEEE Transactions on Parallel and Distributed Systems
- IEEE Transactions on Industrial Electronics

*Conference Reviewer:*

- ICLR 2025 Workshop on Machine Learning for Molecules and Materials

# Seminar Talks

- **The Great Lakes section of SIAM (GLSIAM)** 09/2025
  "Data-driven Learning and Fast Computation of the Kinetic Collision Operator from Molecular Dynamics"
  Illinois Institute of Technology, Chicago, IL, USA.
- 2024 **Joint Mathematics Meetings** 01/2024
  "Random-batch Ewald method"
  San Francisco, CA, USA.
- **CSIAM** 2021 **Annual Meeting (Student Forum)** 10/2021
  "Random-batch Ewald method"
  Hefei, China.
- **Zhiyuan honored Ph.D Students Academic Forum (Second Prize)** 07/2021
  "Random-batch Ewald method"

Shanghai Jiao Tong University, Shanghai, China.

## Conference and Workshop Presentations

- **NSF Computational Math Meeting** 05/2025
  "Data-driven construction of the kinetic collision operator from molecular dynamics" (Poster)
  The University of Utah, Salt Lake City, UT, USA.
- **CHARMNET meeting** 12/2024
  Virginia Tech, Blacksburg, VA, USA.
- **CHARMNET meeting** 12/2023
  "Learning Collision Operator From Micro-Scale Descriptions" (Poster)
  Michigan State University, East Lansing, MI, USA.
- **Mathematics in Action (MiA**2021**)** 06/2021
  "Random-batch Ewald method" (Poster)
  Duke Kunshan University, Kunshan, Jiangsu, China.
- **The Forum on Mathematics and Industrial Innovations** 03/2020
  Shanghai Science Hall, Shanghai, China.
- **Annual Meeting of Shanghai Society for Industrial and Applied Mathematics** 11/2019
  Fudan University, Shanghai, China.
- 15**th Shanghai Symposium on Scientific and Engineering Computing Methods** 11/2019
  Shanghai Maritime University, Shanghai, China.

## Teaching experience

*Michigan State University*

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

*Shanghai Jiao Tong University*

- **Teaching Assistant**, Numerical Analysis and Programming Spring 2021
- **Teaching Assistant**, Numerical Analysis and Programming Spring 2020
- **Teaching Assistant**, Mathematical Analysis I Fall 2019

*NYU Shanghai*

- **Teaching Assistant**, Math for Economics I and II Fall 2021