Qi Zhou

qizhou1729.github.io
https://github.com/qizhou1729
zhouqi1729@sjtu.edu.cn

Educational Background

Shanghai Jiao Tong University Sept. 2018 – June 2022

Bachelor — Major: Mathematics and Applied Mathematics (Wen-Tsun Wu's class)
Minor: Computer Science and Technology

Shanghai Jiao Tong University Sept. 2022 – Now

Ph.D. Candidate (Combined Master and Doctoral) — Computational Mathematics (Advisor: Zhenli Xu)

CCM, Flatiron Institute, Simons Foundation May 2025 – Aug. 2025

Intern Research Associate (Mentor: Shidong Jiang)

Academic Grade

- GPA: 4.00/4.00
- Rank **1** over **79** students.
- Graduate courses (Courses in bold received a full mark):
  - *General Fundamental Courses:* English for Academic Purposes (A), Scientific Writing, Integrity and Ethics (A), Specialized English (A+).
  - *Core Courses:* **Analysis (A+)**, **Scientific Computing (A+)**, **Partial Differential Equations (A+)**, Measure Theory and Probability (A+).
  - *Elective Courses:* **Algebraic Combinatorics (A+)**, Integrability and Bifurcation Theory of Dynamical Systems (A+), **Advanced Computation Methods (A+)**, Applied Mathematical Methods (A+), Variational Methods and Degree Theory (A+).
  - *Frontier Courses:* Additive Combinatorics in Number Theory (A+), High-Performance Computation for Differential Equations (A+).

Research Interest and Publications

I am currently interested in fast algorithms of molecular dynamics (MD) simulation, especially scalable algorithms for general interaction kernels. Also, I consider the design of specialized MD hardwares and supercomputers and the application of new algorithms, expected to approach the SOTA. I am also interested in other fast algorithms such as convolution equations and non-local interactions. Publications are listed as follows:

1. (Alphabetic order) J. Liang, Z. Xu and **Q. Zhou**, Random batch sum-of-Gaussians method for molecular dynamics simulations of particle systems, *SIAM J. Sci. Comput.*, 45 (2023), B591-B617.
2. (Alphabetic order) J. Liang, Z. Xu and **Q. Zhou**, Error estimate of the u-series method in molecular dynamics simulations, *Appl. Comput. Harmon. Anal.* 77 (2025) 101.
3. W. Gao, T. Zhao, Y. Guo, J. Liang, H. Liu, M. Luo, Z. Luo, W. Qin, Y. Wang, **Q. Zhou**, S. Jin and Z. Xu, RBMD: A molecular dynamics package enabling to simulate 10 million all-atom particles in a single graphics processing unit, *Comm. Comp. Phys.*, in press. arxiv:2407.09315.
4. (Alphabetic order) Z. Xu, Y. Zhao and **Q. Zhou**, Variance-reduced random batch Langevin dynamics, *J. Chem. Phys.*, 161(2024), 244110.
5. (Alphabetic order) X. Gao, S. Jiang, J. Liang, Z. Xu and **Q. Zhou**, A fast spectral sum-of-Gaussians method for electrostatic summation in quasi-2D systems, arXiv:2412.04595.
6. (Alphabetic order) Y. Lin, Z. Xu, Y. Zhang and **Q. Zhou**, Weighted balanced truncation method for approximating kernel functions by exponentials, *Phys. Rev. E*, 112 (2025), 015302.
7. X. Gao[1], **Q. Zhou**[1], Z. Gan* and J. Liang*, Accurate error estimates and optimal parameter selection in Ewald summation for dielectrically confined Coulomb systems, *J. Chem. Theory Comput.*, 21 (12) (2025), 5890-5904. **Special issue "Developments of Theoretical and Computational Chemistry Methods in Asia"**.

8. Y. Tu, H. Tian, L. Shi and **Q. Zhou**, SchulzNN: A neural network-based matrix inversion solver inspired by Schulz iteration, submitted.
9. **Q. Zhou**, T. Wu, J. Liu, Q. Sun, H. Xie and Z. Xu, Sum-of-Gaussians tensor neural networks for high-dimensional Schrödinger equation, arXiv:2508.10454.
10. W. Gao, **Q. Zhou***, Q. Zhang and Z. Xu*, Symmetry-preserving random batch Ewald method for constant-potential simulation of electrochemical systems, arXiv:2509.24742.

PATENT

1. Co-inventor, "A Random batch sum-of-Gaussians method for molecular dynamics simulations of particle systems", Patent number: ZL 2022 1 0449795.9.
2. Co-inventor, "A molecular dynamics simulation system", Publication number: CN120183519A

AWARD AND SCHOLARSHIPS

Zhiyuan honorary scholarship	Apr. 2019
Honorable mentioned in 2019 MCM/ICM	Apr. 2019
The third prize (provincial level) in 2019 CUMCM	Oct. 2019
The first prize (national level) of the 11-th Chinese mathematics competition, qualified for final	Nov. 2019
Finalist in 2020 MCM/ICM	Apr. 2020
Distinguished prize in 2nd Alibaba international mathematics competition	July 2020
Chia-Chiao Lin bronze medal in 11-th Yau's mathematics competition	Oct. 2020
Distinguished prize in 11-th Yau's mathematics competition (Analysis)	Nov. 2020
The second prize (provincial level) in 2020 CUMCM	Nov. 2020
The first prize (national level) of the 12-th Chinese mathematics competition	Dec. 2020
The second prize of the 11-th final Chinese mathematics competitions	Apr. 2021
Outstanding winner, COMAP scholarship and SIAM award in 2021 MCM/ICM	Apr. 2021
Chia-Chiao Lin silver medal in 12-th Yau's mathematics competition	May 2021
Baosteel outstanding student scholarship	Sept. 2021
The 5-th Sensetime scholarship	Nov. 2021
The third prize (collegiate level) of 3rd SJTU life science innovation competition	Dec. 2021
The second scholarship of outstanding undergraduate in SJTU	Dec. 2021
Distinguished prize in 13-th Yau's mathematics competition (Analysis)	Aug. 2022
Distinguished prize in 13-th Yau's mathematics competition (Applied Math)	Aug. 2022
First-class graduate scholarship	Dec. 2022
National scholarship for graduate (M.S.)	Sept. 2023
SJTU merit student	Oct. 2023
First-class graduate scholarship	Dec. 2023
Bonditech spark scholarship	May 2024
Excellent oral presentation in the 8-th CSIAM Student Forum	Oct. 2024
Huatai securities technology scholarship	Nov. 2024
Best oral presentation in the 6-th greater bay area symposium on soft and living matter	Jan. 2025
National scholarship for graduate (Ph.D.)	Sept. 2025