Xuanzhao Gao

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RESEARCH INTERESTS

I am interested in applied and computational mathematics in general, working on the following topics:
- Boundary integral equations for complex geometries.
- Fast summation algorithms for long-range interactions.
- Tensor network-based algorithms for combinatorial optimization problems.

EDUCATION

Hong Kong University of Science and Technology, Hong Kong SAR, China *2021 -- 2025*
Ph.D. in Individual Interdisciplinary Program, major in Applied Mathematics. Thesis advisors: Zecheng Gan, Jinguo Liu, and Yang Xiang

The University of Science and Technology of China, China *2017 -- 2021*
B.S. in Condensed Matter Physics & B.S. in Computer Science. Undergraduate thesis advisor: Xianhui Chen

POSITIONS

Flatiron Research Fellow
Center for Computational Mathematics, Flatiron Institute, Simons Foundation, New York, NY, USA 2025 -- now

PUBLICATIONS

Peer-reviewed Publications

[1] X. Gao, Q. Zhou, 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**, 5890 (2025)

[2] Z. Gan, X. Gao, J. Liang, and Z. Xu, Random batch Ewald method for dielectrically confined Coulomb systems, SIAM J. Sci. Comput. **47**, B846 (2025)

[3] X. Gao, X. Li, and J. Liu, Programming guide for solving constraint satisfaction problems with tensor networks, Chinese Physics B **34**, 50201 (2025)

[4] Z. Gan, X. Gao, J. Liang, and Z. Xu, Fast algorithm for quasi-2D Coulomb systems, J. Comput. Phys. **524**, 113733 (2025)

[5] M. Roa-Villescas, X. Gao, S. Stuijk, H. Corporaal, and J.-G. Liu, Probabilistic inference in the era of tensor networks and differential programming, Phys. Rev. Res. **6**, 33261 (2024)

[6] X. Gao and Z. Gan, Broken symmetries in quasi-2D charged systems via negative dielectric confinement, J. Chem. Phys. **161**, (2024)

[7] Z. Nie, X. Gao, Y. Ren, S. Xia, Y. Wang, Y. Shi, J. Zhao, and Y. Wang, Harnessing hot phonon bottleneck in metal halide perovskite nanocrystals via interfacial electron-phonon coupling, Nano Lett. **20**, 4610 (2020)

Manuscripts Under Review

[8] 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 Preprint Arxiv:2412.04595 (2024)

[9] X. Gao, Y.-J. Wang, P. Zhang, and J.-G. Liu, Automated discovery of branching rules with optimal complexity for the maximum independent set problem, Arxiv Preprint Arxiv:2412.07685 (2024)

In Draft (preprint available upon request)

[10] X. Gao, Z. Gan, and Y. Li, Efficient particle-based simulations of Coulomb systems under dielectric nanoconfinement, (2025)

SOFTWARE PACKAGES

ExTinyMD.jl: A framework for molecular dynamics simulations.

EwaldSummations.jl: A comprehensive implementation of the Ewald summation method for electrostatic interactions in both triply and doubly periodic systems with and without dielectric mismatches.

ChebParticleMesh.jl: A suite of highly efficient tools for the widely used Particle-Mesh methods applicable to systems with arbitrary dimensions and periodicity.

TropicalNumbers.jl: A refined implementation of the tropical semiring.

CuTropicalGEMM.jl: A GPU-accelerated implementation of the tropical matrix multiplication.

TreeWidthSolver.jl: A collection of tools for calculating the exact tree width and tree decomposition of a given graph.

OptimalBranching.jl: A framework for automated discovery of optimal branching rules for the branch-and-bound algorithm.

OPEN SOURCE PROJECTS

Google Summer of Code 2024, The Julia Language
Contributed to the project "Tensor network contraction order optimization and visualization" released by the Julia Language community in GSoC 2024.

Open Source Promotion Plan 2023, JuliaCN
Contributed to the project "TropicalGEMM on GPU" released by the JuliaCN community in OSPP 2023.

PRESENTATIONS AND POSTERS

The 14th CSCM Annual Conference, Invited Talk *August 17-21, 2025*
A Fast Spectral Sum-of-Gaussians Method for Electrostatic Summation in Quasi-2D Systems

JuliaCN Meetup 2024, Invited Talk *Nov 2-3, 2024*
TreeWidthSolver.jl: From Treewidth to Tensor Network Contraction Order

SciCADE 2024, Contributed Talk *July 15-19, 2024*
Fast Algorithm for Quasi-2D Coulomb Systems

JuliaCN Meetup 2023, Contributed Talk *Dec 9, 2023*
How to Implement Generic Matrix-Mul with Generic Element Types on GPU?

ICIAM 2023, Poster *August 20-25, 2023*
Random Batch Quasi-Ewald Method for the Simulations of Charged Particles under Dielectric Confinement

SKILLS

Programming Languages: Julia (proficient), Python, C/C++, CUDA

Languages: Mandarin Chinese (native), English (proficient)