# 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)