

# Xuanzhao Gao

Center for Computational Mathematics, Flatiron Institute, New York, NY, USA

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## RESEARCH INTERESTS

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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

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**Hong Kong University of Science and Technology, Hong Kong SAR, China** 2021 -- 2025  
*P.h.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

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### Flatiron Research Fellow

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

## PUBLICATIONS

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### 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

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**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

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**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

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**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

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

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