

Xuanzhao Gao

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EDUCATION

Hong Kong University of Science and Technology, Hong Kong SAR, China

2021 -- now

P.h.D. in Individual Interdisciplinary Program, major in Applied Mathematics

Advisor: [Prof. Zecheng Gan](#); Co-advisor: [Prof. Jin-Guo Liu](#) & [Prof. Yang Xiang](#).

The University of Science and Technology of China, China

2017 -- 2021

B.S. in Condensed Matter Physics & B.S. in Computer Science

RESEARCH INTERESTS

I am interested in computational mathematics and scientific computing in general, with a particular focus on developing efficient numerical algorithms for modeling and simulating complex systems, emphasizing high-performance implementation. Specifically, I am engaged in research on fast summation algorithms tailored for long-range interactions. I have also concentrated on tensor network-based algorithms for combinatorial optimization problems and their potential applications in simulating quantum many-body systems.

PUBLICATIONS

Peer-reviewed Publications

[1] Z. Gan, X. Gao, J. Liang, and Z. Xu, Random batch Ewald method for dielectrically confined Coulomb systems, Arxiv Preprint Arxiv:2405.06333 (2025), accepted by SIAM Journal on Scientific Computing

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

[3] Z. Gan, X. Gao, J. Liang, and Z. Xu, Fast algorithm for quasi-2D Coulomb systems, Journal of Computational Physics **524**, 113733 (2025)

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

[5] X. Gao and Z. Gan, Broken symmetries in quasi-2D charged systems via negative dielectric confinement, The Journal of Chemical Physics **161**, (2024)

[6] 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 Letters **20**, 4610 (2020)

Manuscripts Under Review

[7] X. Gao, Q. Zhou, Z. Gan, and J. Liang, Accurate error estimates and optimal parameter selection in Ewald summation for dielectrically confined Coulomb systems, Arxiv Preprint Arxiv:2503.18126 (2025)

[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.

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

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)