

Yuejia Zhang | Computational Mathematics

Fudan University, Shanghai, China

✉ yuejiazhang21@m.fudan.edu.cn • 🌐 yuejiazhang.com • 🌐 ninotreve

Research Profile

Computational mathematician specializing in electronic-structure and quantum many-body calculations, with a particular focus on correlated many-electron eigenvalue problems. My research combines wave-function-based methods, numerical linear algebra, sparse computation, and parallel scientific computing. Lead developer of the CDFCI C++ software package, with experience turning numerical methods into tested, documented, and scalable research software.

Research Interests

- Numerical methods for electronic-structure and quantum many-body calculations, including configuration interaction and tensor-network methods.
- Correlated many-electron eigenvalue problems, including ground- and excited-state calculations and large-scale wave-function representations.
- High-performance scientific computing for large-scale electronic-structure and many-body calculations.

Education

Fudan University

Shanghai

Ph.D. Candidate in Computational Mathematics (degree expected Dec. 2026)

2021–2026

Supervisors: Prof. Weiguo Gao, Prof. Yingzhou Li

Thesis: Multi-Coordinate Descent Framework for Full Configuration Interaction Eigenvalue Problems: Theory, Algorithms, and Software (defended June 3, 2026)

Fudan University

Shanghai

B.Sc. in Data Science

2016–2021

Research Experience

Fudan University

Shanghai

Ph.D. Student

2021–2026

- Developed and analyzed the multi-coordinate descent FCI (mCDFCI) method for large-scale calculations of correlated many-electron states using sparse wave-function representations.
- Lead developer and maintainer of CDFCI, a C++17/OpenMP package for ground- and excited-state calculations of fermionic Hamiltonians, with a Python/PySCF interface.
- Performed large-scale FCI calculations with up to 2.07 billion variational determinants, supported by parallel implementations scaling to 128 CPU cores.

EPFL

Lausanne, Switzerland

Visiting Ph.D. Student, Supervisor: Prof. Laura Grigori

2023–2024

- Worked on parallel density-matrix renormalization group (DMRG) algorithms in Julia, exploiting block structure in matrix product states (MPS).
- Designed and optimized tensor-contraction pipelines for distributed-memory HPC.

Publications and Preprints

- [1]: **Yuejia Zhang**, Weiguo Gao, Yingzhou Li. *Parallel Multi-Coordinate Descent Methods for Full Configuration Interaction*. Journal of Chemical Theory and Computation 21(5), 2325–2337 (2025).
- [2]: **Yuejia Zhang**, Weiguo Zheng, Zhijie Zhang, Peng Peng, Xuecang Zhang. *Hybrid Subgraph Matching Framework Powered by Sketch Tree for Distributed Systems*. ICDE 2022.
- [3]: **Yuejia Zhang**, Zhe Wang, Jianfeng Lu, Yingzhou Li. *CDFCI: High-Performance Parallel Software for Quantum Many-Body Eigenvalue Problems*. arXiv:2605.04483, 2026. Under revision for ACM Transactions on Mathematical Software.

Selected Talks and Presentations

CDFCI: High-Performance Parallel Software for Quantum Many-Body Eigenvalue Problems

GAMM 2026 S26, Magdeburg, Germany (March 2026)

SIAM PP26, Berlin, Germany (March 2026)

Parallel Multi-Coordinate Descent for Full Configuration Interaction

SIAM LA24, Paris, France (May 2024)

GAMM 2024 S26, Magdeburg, Germany (March 2024)

ICIAM 2023, Tokyo, Japan (Aug 2023)

Honors and Awards

SIAM PP26 Student Travel Award (2026)

Goku Tech Scholarship, Fudan University (2025)

SIAM LA24 Student Travel Award (2024)

Second Prize — Linear Solver Optimization Competition (2024)

Third Prize — Low-Rank SVD Track, Greater Bay Area Cup (2022)

Tower Watson Scholarship, Fudan University (2022)

Outstanding Teaching Assistant, Fudan University (2022)

First Prize — Eigenvalue Solver Optimization, Pioneer Cup (2021)

Technical Skills

- **Programming:** C++, Python, MATLAB, R, Julia
- **HPC:** MPI, OpenMP, CUDA, Slurm, Intel VTune
- **Languages:** Chinese (Native), English (Fluent), French (Fluent)

Teaching and Academic Service

Teaching Assistant, Numerical Algorithms with Case Studies I, Fudan University *Fall 2025*

Teaching Assistant, Numerical Algorithms with Case Studies I, Fudan University *Fall 2023*

Teaching Assistant, Numerical Linear Algebra and Optimization, Fudan University *Spring 2022*

Student Organizer, Fudan Summer School on Scientific Computing, Fudan University *Summer 2025*

Student Organizer, Applied Math Ph.D. Seminar, Fudan University *Spring 2023*