

Yuejia Zhang | Computational Mathematics

Fudan University, Shanghai, China

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

Research Profile

Computational mathematician developing structure-exploiting algorithms and high-performance software for large-scale quantum many-body eigenvalue problems. My research combines numerical linear algebra, sparse and matrix-free computation, and scientific computing, with applications to configuration interaction and electronic-structure calculations. Lead developer of the CDFCI software package.

Research Interests

- Numerical methods for quantum many-body problems, including sparse many-body eigensolvers, excited-state computations, tensor-network methods, and electronic-structure calculations.
- Structure-exploiting numerical algorithms for large-scale eigenvalue problems, with emphasis on sparsity, symmetry, matrix-free computation, and high-performance computing.
- Numerical methods for electronic structure and quantum dynamics, including real-space discretizations, non-linear eigenvalue problems, and nonequilibrium many-body systems.

Education

Fudan University

Ph.D. in Computational Mathematics

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)

Shanghai

2021–2026

Fudan University

B.Sc. in Data Science

Shanghai

2016–2021

Research Experience

Fudan University

Ph.D. Student

Shanghai

2021–2026

- Developed the multi-coordinate descent FCI (mCDFCI) method, a parallel eigensolver for large-scale fermionic Hamiltonians that exploits sparsity in the many-body wavefunction.
- Lead developer and maintainer of CDFCI, a C++17/OpenMP software suite for sparse ground- and excited-state FCI calculations.

EPFL

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

Lausanne, Switzerland

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, Xuechang 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*