Yuejia **Zhang** | Ph.D. Candidate in Computational Mathematics

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Research Profile

Ph.D. candidate focusing on high-performance scientific computing for numerical linear algebra in electronic structure calculations, in particular wavefunction-based methods for strongly-correlated quantum systems. Developer of the CDFCI software package, integrating coordinate-descent based methods for full configuration interaction (FCI) calculations of fermionic Hamiltonians. Extensive experience with large-scale eigensolvers, sparse linear solvers, and tensor-train-based methods. Proficient in C/C++, Python and MATLAB, with a strong background in HPC software engineering and algorithmic performance optimization.

Research Interests

- Electronic structure calculations for strongly correlated quantum systems: FCI methods using coordinate gradient descent to preserve sparsity, alongside tensor-based methods (e.g., DMRG) with low-rank approximation.
- Practical numerical linear algebra algorithms for linear systems and eigenvalue problems, with a focus on the use of tensor trains and quantized tensor trains in high-dimensional problems.
- Large-scale scientific software development and algorithmic performance optimization.

Education

Fudan University **Shanghai**
Ph.D. in Computational Mathematics *2021–2026 (expected)*
Supervisors: *Prof. Weiguo Gao, Prof. Yingzhou Li*
Thesis in Preparation: *High-Performance Multi-Coordinate Descent Framework for Full Configuration Interaction Eigenvalue Problems: Theory, Algorithms, and Software*

Fudan University **Shanghai**
B.Sc. in Data Science *2016–2021*
Relevant Coursework: Numerical Linear Algebra, Quantum Chemistry, Optimization, Machine Learning

Research Experience

Fudan University **Shanghai**
Ph.D. Student *2021–Present*
- Lead developer of multi-coordinate descent FCI method (mCDFCI), designed multi-coordinate-descent parallel eigensolvers achieving state-of-the-art performance
- Lead developer of the CDFCI software suite in C++, integrating coordinate-descent-based methods such as CDFCI, mCDFCI, XCDFCI (for excited states) and OptOrbFCI (for orbital compression)
- Maintained multi-node HPC cluster (Slurm, CUDA, NFS, networking)

EPFL **Lausanne, Switzerland**
Visiting Ph.D. Student, Supervisor: Prof. Laura Grigori *2023–2024*
- Developed block-aware DMRG algorithms in Julia
- Designed optimized tensor contraction pipelines for distributed-memory HPC

Publications

[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.

Manuscripts in Preparation

[1] Yuejia Zhang, Zhe Wang, Jianfeng Lu, Yingzhou Li. *CDFCI: High-Performance Parallel Software for Eigenvalue Problems in Many-Body Schrödinger Equation.* In preparation for ACM TOMS, 2026.

Selected Talks and Presentations

CDFCI: High-Performance Parallel Software for Eigenvalue Problems in Many-Body Schrödinger Equation

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)

Hybrid Subgraph Matching Framework

ICDE 2022 (May 2022)

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, VTune, profiling
- **Languages:** Chinese (Native), English (C1), French (C1)

Professional Service

Teaching Assistant: MATH20007.01, Numerical Algorithms with Case Studies I, *Fall 2025*

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

Teaching Assistant: DATA130002h, Numerical Algorithms with Case Studies I, *Fall 2023*

Student Organizer, Applied Math PhD Seminar, Fudan University, *Spring 2023*

Teaching Assistant: MATH130165h, Numerical Linear Algebra and Optimization, *Spring 2022*