

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

Fudan University, Shanghai, China

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## Research Profile

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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

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- 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

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### Fudan University

*Ph.D. in Computational Mathematics*

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*

Shanghai

2021–2026 (expected)

### Fudan University

*B.Sc. in Data Science*

Relevant Coursework: Numerical Linear Algebra, Quantum Chemistry, Optimization, Machine Learning

Shanghai

2016–2021

## Research Experience

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### Fudan University

*Ph.D. Student*

- 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)

Shanghai

2021–Present

### EPFL

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

- Exploiting block structure in the Matrix Product State (MPS) for parallel Density Matrix Renormalization Group (DMRG) algorithm in Julia
- Designed optimized tensor contraction pipelines for distributed-memory HPC

Lausanne, Switzerland

2023–2024

## Publications

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- [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.

## Preprints

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- [1] Yuejia Zhang, Zhe Wang, Jianfeng Lu, Yingzhou Li. *CDFCI: High-Performance Parallel Software for Eigenvalue Problems in Many-Body Schrödinger Equation*. arXiv:2605.04483, 2026.

## Selected Talks and Presentations

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- 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

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- 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

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- **Programming:** C++, Python, MATLAB, R, Julia
- **HPC:** MPI, OpenMP, CUDA, Slurm, VTune, profiling
- **Languages:** Chinese (Native), English (C1 level), French (C1 level)

## Professional Service

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- 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*