Yang KUANG

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Work Experience

Associate Professor 2021.09–present
School of Mathematics and Statistics, Guangdong University of Technology

Research Fellow 2019.08–2021.08
Department of Mathematics, National University of Singapore; Host: Prof. Zhenning Cai.

Education

PhD in Computational Mathematics, University of Macau 2016.08–2019.07
Advisor: Prof. Guanghui Hu

MSc in Computational Mathematics, University of Macau 2013.09–2016.06
Advisor: Prof. Guanghui Hu

BSc in Information and Computational Science, Wuhan University 2009.09–2013.06

Research Interests

Efficient numerical methods for electronic structure and related quantum models, with a focus on multiple approximation spaces, adaptive finite elements, and eigenvalue algorithms. I also study the validity and regularization of complex Langevin methods.

Submitted

1. Pengfei Hao, Renfeng Peng, Yang Kuang, and Bin Gao, *High-dimensional extreme eigenvalue problems: low-rank tensor parametrization and optimization*, arXiv preprint arXiv:2609.30138, 2026. (link)

Refereed Journal Articles

1. Mingzhe Li, Yang Kuang*, and Zhicheng Hu, *A multi-mesh adaptive finite element method for solving the Gross-Pitaevskii equation*, Advances in Applied Mathematics and Mechanics, accepted. (link)
2. Yang Kuang and Guanghui Hu, *A novel splitting strategy to accelerate solving generalized eigenvalue problem from Kohn–Sham density functional theory*, Computer Physics Communications, 322, 110056, 2026. (link)
3. Tao Wang, Yang Kuang*, Ran Zhang, and Guanghui Hu, *A hierarchical splines-based h-adaptive isogeometric solver for all-electron Kohn–Sham equation*, Journal of Computational Physics, 534, 114003, 2025. (link)
4. Zheming Luo and Yang Kuang*, *A high-order accurate moving mesh finite element method for the radial Kohn–Sham equation*, Molecular Physics, 2025. (link)
5. Yang Kuang, Yedan Shen, and Guanghui Hu, *Towards chemical accuracy using a multi-mesh adaptive finite element method in all-electron density functional theory*, Journal of Computational Physics, 518, 113312, 2024. (link)
6. Zhenning Cai, Jingwei Hu, Yang Kuang, and Bo Lin, *An entropic method for discrete systems with Gibbs entropy*, SIAM Journal on Numerical Analysis, 60(4), 2345–2371, 2022. (link)
7. Bin Gao, Guanghui Hu, Yang Kuang*, and Xin Liu, *An orthogonalization-free parallelizable framework for all-electron calculations in density functional theory*, SIAM Journal on Scientific Computing, 44(3), B723–B745, 2022. (link)

8. Zhenning Cai, Yang Kuang*, and Hong Kiat Tan, *Regularization of the complex Langevin method*, Physical Review D, 105, 014508, 2022. (link)
9. Zhenning Cai, Xiaoyu Dong, and Yang Kuang, *On the validity of complex Langevin method for path integral computations*, SIAM Journal on Scientific Computing, 43(1), A685–A719, 2021. (link)
10. Yang Kuang, Yedan Shen, and Guanghui Hu, *An adaptive finite element method for Kohn–Sham and time-dependent Kohn–Sham equations*, Journal on Numerical Methods and Computer Applications, 42(1), 33–55, 2021 (in Chinese). (link)
11. Yang Kuang and Guanghui Hu, *On stabilizing and accelerating SCF using ITP in solving Kohn–Sham equation*, Communications in Computational Physics, 28(3), 999–1018, 2020. (link)
12. Yedan Shen, Yang Kuang, and Guanghui Hu, *An asymptotic-based adaptive finite element method for Kohn–Sham equation*, Journal of Scientific Computing, 79(1), 464–492, 2019. (link)
13. Yang Kuang and Guanghui Hu, *An adaptive FEM with ITP approach for steady Schrödinger equation*, International Journal of Computer Mathematics, 95(1), 187–201, 2018. (link)

Research Funding

- NSFC General Program, No. 12671469, 2027.01–2030.12.
- NSFC Tianyuan Fund, No. 12326362, 2024.01–2024.12 (with Prof. Tao Tang).
- NSFC Young Scientists Fund-Type C, No. 12201130, 2023.01–2025.12.
- Natural Science Foundation of Guangdong Province, No. 2026A1515011703, 2026.01–2028.12.
- Guangzhou Municipal Science and Technology Bureau, No. 2023A04J1321, 2023.04–2025.03.

Visiting Experience

- 2024.03.01–2024.12.31: Institute for Advanced Study, Beijing Normal-Hong Kong Baptist University (BNBU); Host: Prof. Tao Tang.
- 2023.07.07–2023.08.13: Academy of Mathematics and Systems Science, Chinese Academy of Sciences; Host: Dr. Bin Gao.
- 2019.03.20–2019.04.10: Department of Mathematics, National University of Singapore; Host: Prof. Zhenning Cai.

Talks

1. "Some numerical methods for all-electron density functional theory," Workshop on Mathematical Theory, Methods and Applications in Materials Simulation, Tianyuan Mathematical Center, Kunming, May 2025.
2. "Multi-mesh adaptive finite elements for the Kohn–Sham equation," Workshop on Numerical Methods and Applications for Fluid Mechanics, Nanjing University of Aeronautics and Astronautics, Nanjing, December 2023.
3. "Multi-mesh adaptive finite element methods for eigenvalue problems," CSIAM 2023, Kunming, October 14, 2023.
4. "A multi-mesh adaptive finite element method for Kohn–Sham equation," ICIAM 2023, Tokyo, August 22, 2023.
5. "A multi-mesh adaptive finite element method for Kohn–Sham equation," TM21, CSIAM 2022, November 19, 2022.
6. "An orthogonalization-free parallelizable framework for all-electron calculations," BNU-UIC Research Center for Mathematics seminar, April 1, 2021.
7. "Numerical investigations of complex Langevin dynamics," 9th Symposium on Applied and Computational Mathematics, SIAM Student Chapter at NUS, June 17, 2020.

8. "An orthonormalization-free parallelizable algorithm for electronic structure calculation," Workshop on Electronic Structure Calculations, Fudan University, November 10, 2019.
9. "An efficient and adaptive finite element method for Kohn–Sham equation," Joint Annual Conference of Physical Societies in the Guangdong-Hong Kong-Macao Greater Bay Area, University of Macau, July 28, 2018.
10. "An efficient and adaptive finite element method for Kohn–Sham equation," 13th SIAM East Asian Section Conference, University of Tokyo, June 24, 2018.

Teaching Experience

School of Mathematics and Statistics, Guangdong University of Technology 2021.09–present

- Spring: Numerical Analysis; Mathematical Modeling; Algorithm Design and Analysis.
- Autumn: Wavelet Analysis; Linear Algebra.

Department of Mathematics, University of Macau 2013.09–2019.07

- MATB 221, Mathematical Analysis II (tutorials; Spring 2014, 2017, 2018).
- MATB 212, Mathematical Analysis I (tutorials; Autumn 2013, 2016, 2017).
- EDUC 491, Seminar (tutorials; Autumn 2013).

Skills

- Programming: C/C++, Python, MATLAB, Mathematica, LaTeX.
- High-performance computing: Linux, shell scripting.
- Parallel computing: OpenMP, Open MPI.