Yukuan **Hu**

Ph.D. in Computational Mathematics

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Education

Academy of Mathematics and Systems Science (AMSS), Chinese Academy of Sciences (CAS) — *Beijing, China*
Ph.D. in Computational Mathematics — *2019.09 - 2024.06*
Supervisor: Prof. Xin Liu

School of Mathematical Sciences, Tongji University — *Shanghai, China*
B.Sc. in Mathematics and Applied Mathematics — *2015.09 - 2019.06*
Thesis advisor: Prof. Junfeng Yin

Academic Experience

CERMICS, École nationale des ponts et chaussées, Institut Polytechnique de Paris — *Champs-sur-Marne, France*
Postdoctoral Fellow — *2024.09 - Present*
Advisor: Prof. Eric Cancès

Department of Applied Mathematics, The Hong Kong Polytechnic University — *Hong Kong, China*
Research Associate — *2024.07 - 2024.08*
Host: Prof. Zaikun Zhang

Research Interests

- **Numerical optimization**
- **Computational quantum chemistry**
- **Computational materials science**

My interests focus on developing numerical optimization methods for scientific and engineering applications. Recently, I have been working on the topics in computational quantum chemistry and computational materials science, including electronic excited states calculations, electronic energy landscape analysis, strongly correlated electrons calculations, and structure relaxation with physical constraints.

Publications & Preprints

1. Critical point search and linear response theory for computing electronic excitation energies of molecular systems. Part I: General framework, application to Hartree-Fock and DFT
   arXiv preprint arXiv:2025.16420, 2025 (preprint)
   Laura Grazioli, **Yukuan Hu**, Eric Cancès

2. Sampling-based approaches for multi-block optimization problems over transport polytopes
   Mathematics of Computation, 2025, 94(353): 1281–1322 (doi, preprint)
   Yukuan Hu, Mengyu Li, Xin Liu, Cheng Meng

3. Complexity of tensor product functions in representing antisymmetry
   arXiv preprint arXiv:2501.05958, 2025 (preprint)
   Yuyang Wang, **Yukuan Hu**, Xin Liu

4. The exactness of the ℓ_1 penalty function for a class of mathematical programs with generalized complementarity constraints
   Fundamental Research, 2024, 4(6): 1459–1464 (doi, preprint)
   Yukuan Hu, Xin Liu

5. Projected gradient descent algorithm for *ab initio* crystal structure relaxation under a fixed unit cell volume
   Physical Review B, 2024, 109(22): 224109 (14 pages) (doi, preprint)
   Yukuan Hu, Junlei Yin, Xingyu Gao, Xin Liu, Haifeng Song

6. The convergence properties of infeasible inexact proximal alternating linearized minimization
Science China Mathematics, 2023, 66(10): 2385–2410 (doi, preprint)
Yukuan Hu, Xin Liu

7. A global optimization approach for multimarginal optimal transport problems with Coulomb cost
SIAM Journal on Scientific Computing, 2023, 45(3): A1214–A1238 (doi, preprint)
Yukuan Hu, Huajie Chen, Xin Liu

8. Force-based gradient descent method for *ab initio* atomic structure relaxation
Physical Review B, 2022, 106(10): 104101 (10 pages) (doi, preprint)
Yukuan Hu, Xingyu Gao, Yafan Zhao, Xin Liu, Haifeng Song

Patents & Copyrights

1. 晶体结构弛豫软件包 ProME-SuRe
Description: A suite for crystal structure relaxation; static-link library files are available upon request
CN Software Copyright, 2023, 2023SR1558824
Xingyu Gao, Xin Liu, **Yukuan Hu**, Haifeng Song, Xin Chen, Yuechao Wang, Lifang Wang

2. 固定晶格体积晶体结构弛豫的计算方法及装置
Description: Computational methods and apparatus for crystal structure relaxation with a fixed unit cell volume
CN Patent, 2023, ZL 202211210741.3
Xingyu Gao, Xin Liu, Haifeng Song, **Yukuan Hu**, Xin Chen, Yuechao Wang, Jun Fang, Lifang Wang, Le Zhang

3. 原子结构弛豫的非单调线搜索方法及装置
Description: Computational methods and apparatus for atomic structure relaxation
CN Patent, 2022, ZL 202111534901.5
Xingyu Gao, Xin Liu, Haifeng Song, **Yukuan Hu**, Jun Fang, Zhen Yang, Yafan Zhao, Lifang Wang, Haifeng Liu

Selected Projects

As a member

2024.09 – 2026.08 Extremely-scale Mathematically-based Computational Chemistry (**EMC2**) *EU Horizon 2020, ERC*

Selected Presentations

2025.08 The 15th International Conference on Numerical Optimization and Numerical Linear Algebra *Harbin, China*
2025.07 The 8th International Conference on Continuous Optimization (**ICCOPT 2025**) *Los Angeles, USA*
2025.06 The 22nd Conference on Advances in Continuous Optimization (**EUROPT 2025**) *Southampton, UK*
2024.07 The First Forum for Ph.D. Students in Computational Mathematics *Beijing, China*
2023.10 The 21st Annual Meeting of China Society for Industrial and Applied Mathematics (**CSIAM 2023**) *Kunming, China*
2023.08 The 10th International Congress on Industrial and Applied Mathematics (**ICIAM 2023**) *Tokyo, Japan*
2023.08 The 14th International Conference on Numerical Optimization and Numerical Linear Algebra *Taiyuan, China*
2023.06 Applied Math Ph.D. Seminar at Fudan University *Shanghai, China*

Selected Honors & Awards

2025.09 **CAS Excellent Ph.D. Dissertation** (**TOP 78 in CAS**, **TOP 2 in AMSS**) *CAS*
2024.11 **CAS President's Special Award** (10,000 CNY, **TOP 59 in CAS**, **TOP 2 in AMSS**) *CAS*
2023.11 Beijing Mathematical Society (BMS) Excellent Youth Paper (**the only Ph.D. candidate selected**) *BMS*
2023.11 Zhu Li Yuehua Outstanding Doctoral Student Award (5,000 CNY) *University of CAS*
2023.09 AMSS President's Special Award (32,000 CNY, **TOP 4 in AMSS**) *AMSS*
2023.04 Financial Support Program *ICIAM 2023*
2022.09 Loo-Keng Hua Scholarship (**100,000 CNY**) *AMSS*
2021.09 Loo-Keng Hua Scholarship (**100,000 CNY**) *AMSS*

Professional Activities

Conference organizations

2025.06 **Session Chair** for "*Advances in Manifold Optimization*", EUROPT 2025 *Southampton, UK*

Referee for journals

- IEEE Transactions on Signal Processing
- The Innovation
- Numerical Functional Analysis and Optimization
- npj Unconventional Computing

Skills

Languages	Chinese (mother tongue), English (professional fluency), French (beginner)
Programming	Python, Fortran, C, MATLAB, LaTeX, Shell
Parallel Computing	MPI, OpenMP