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   *09/2019 - 06/2024*
Supervisor: Prof. Xin Liu

School of Mathematical Sciences, Tongji University   *Shanghai, China*
B.Sc. in Mathematics and Applied Mathematics   *09/2015 - 06/2019*
Thesis advisor: Prof. Junfeng Yin

Academic Experience _____

CERMICS, École nationale des ponts et chaussées   *Champs-sur-Marne, France*
Postdoctoral Fellow   *09/2024 - Present*
Host: Prof. Eric Cancès

Department of Applied Mathematics, The Hong Kong Polytechnic University   *Hong Kong, China*
Research Associate   *07/2024 - 08/2024*
Host: Prof. Zaikun Zhang

Research Interests _____

- **Numerical optimization**
- **Computational materials science**
- **Machine learning**

My interests focus on developing numerical optimization methods for scientific and engineering applications. Recently, I have been working on the topics in computational materials science, including strongly correlated electrons systems and structure relaxation with physical constraints, as well as machine learning-based approaches. Motivated by the ubiquitous large-scale applications, I also pay attention to the development and analysis of first-order optimization methods.

Publications & Preprints _____

1. Sampling-based approaches for multi-block optimization problems over transport polytopes
   Mathematics of Computation, 2024, published online (doi, preprint)
   Yukuan Hu, Mengyu Li, Xin Liu, Cheng Meng

2. 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

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

4. 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

5. The exactness of the ℓ_1 penalty function for a class of mathematical programs with generalized complementarity constraints
   Fundamental Research, 2023, published online (doi, preprint)
   Yukuan Hu, Xin Liu

6. 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 201111534901.5
   Xingyu Gao, Xin Liu, Haifeng Song, **Yukuan Hu**, Jun Fang, Zhen Yang, Yafan Zhao, Lifang Wang, Haifeng Liu

Selected Presentations

07/2024	The First Forum for Ph.D. Students in Computational Mathematics	*Beijing, China*
10/2023	The 21st Annual Meeting of China Society for Industrial and Applied Mathematics	*Kunming, China*
08/2023	The 10th International Congress on Industrial and Applied Mathematics (ICIAM 2023)	*Tokyo, Japan*
08/2023	The 14th International Conference on Numerical Optimization and Numerical Linear Algebra	*Taiyuan, China*
06/2023	Applied Math Ph.D. Seminar at Fudan University	*Shanghai, China*

Selected Honors & Awards

11/2024	CAS President's Special Award (10,000 CNY)	*CAS*
11/2023	Beijing Mathematical Society (BMS) Excellent Youth Paper (the only Ph.D. candidate selected)	*BMS*
11/2023	Zhu Li Yuehua Outstanding Doctoral Student Award (5,000 CNY)	*University of CAS*
09/2023	AMSS President's Special Award (32,000 CNY)	*AMSS*
04/2023	Financial Support Program	*ICIAM 2023*
09/2022	Loo-Keng Hua Scholarship (100,000 CNY)	*AMSS*
09/2021	Loo-Keng Hua Scholarship (100,000 CNY)	*AMSS*

Skills

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

Professional Activities

Referee for Journals

- IEEE Transactions on Signal Processing