

# 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

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  $\ell_1$  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

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### 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 Presentations

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

## Selected Honors & Awards

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

## Skills

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<b>Languages</b>	Chinese (mother tongue), English (professional fluency)
<b>Programming</b>	Fortran, C, MATLAB, Shell, Python, $\text{\LaTeX}$
<b>Parallel Computing</b>	MPI, OpenMP

## Professional Activities

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### Referee for Journals

- IEEE Transactions on Signal Processing