

# Yukuan HU

PH.D. IN COMPUTATIONAL MATHEMATICS

Yip Kit Chuen Bldg., The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, China

✉ (+86) 18810512770 | ✉ ykhu@lsec.cc.ac.cn | 🌐 <https://huyukuan.github.io> | ⚡ GitHub | ⚡ Google Scholar



## 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. **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
2. **Sampling-based approaches for multi-block optimization problems over transport polytopes**  
*Mathematics of Computation*, 2024+, accepted ([preprint](#))  
**Yukuan HU**, Mengyu LI, Xin LIU, Cheng MENG
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

---

### 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

---

10/2023	The 21st Annual Meeting of China Society for Industrial and Applied Mathematics (CSIAM 2023)	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 (ICNONLA 2023)	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 RMB)	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	University of CAS
09/2023	AMSS President's Special Award (32,000 RMB)	AMSS
04/2023	Financial Support Program	ICIAM 2023
09/2022	Loo-Keng Hua Scholarship (100,000 RMB)	AMSS
09/2021	Loo-Keng Hua Scholarship (100,000 RMB)	AMSS

## Skills

---

<b>Languages</b>	Chinese (mother tongue), English (professional fluency)
<b>Programming</b>	Fortran, C, MATLAB, Shell, Python, L <sup>A</sup> T <sub>E</sub> X
<b>Parallel Computing</b>	MPI, OpenMP

## Professional Activities

---

### Referee for Journals

- IEEE Transactions on Signal Processing