# Haibo Li

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## Current Position

Research Fellow, School of Mathematics and Statistics, The University of Melbourne, Sept. 2023 – now (supervisor: Hailong Guo)

## Research Interest

My research interests center around utilizing mathematical modeling and computational techniques to address challenging problems in scientific computing and data science. The research areas mainly include:

- Inverse and ill-posed problems
- Numerical linear algebra
- Scientific machine learning

## Academic Experience

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|---|---|
| Aug. 2024 – Oct. 2024 | • Visiting Scholar, Department of Mathematics, Johns Hopkins Univeristy (host: Fei Lu) |
| Aug. 2021 – Sept. 2023 | • Researcher, Computing System Optimization Lab, Huawei Technologies (joint with Institute of Computing Technology, Chinese Academy of Sciences) |
| Sept. 2015 – Jun. 2021 | • Ph.D. in Computational Mathematics, Department of Mathematical Sciences, Tsinghua University, China |
| | • *Thesis: Joint Bidiagonalization Algorithms for the Computation of Partial GSVDs and Discrete Ill-posed Problems with General-form Regularization* (supervisor: Zhongxiao Jia) |
| Sept. 2011 – Jun. 2015 | • Bachelor in mathematics, Taishan College (talent training project), Shandong University, China |

## Papers

Publications:

18 • **Haibo Li**. *Characterizing GSVD by singular value expansion of linear operators and its computation*, SIAM Journal on Matrix Analysis and Applications 46 (1), 439-465, 2025.

17 • Rongrong Liu, Zhuoqiang Guo, Qiuchen Sha, Tong Zhao, **Haibo Li**, Wei Hu, Lijun Liu, Guangming Tan, Weile Jia. *Large Scale Finite-Temperature Real-time Time Dependent Density Functional Theory Calculation with Hybrid Functional on ARM and GPU Systems*, International Parallel and Distributed Processing Symposium (IPDPS 2025)

16 • **Haibo Li**, Guangming Tan, Tong Zhao. *Backward error analysis of the Lanczos bidiagonalization with reorthogonalization*, Journal of Computational and Applied Mathematics, 116414, 2025.

15 • **Haibo Li**. *A new interpretation of the weighted pseudoinverse and its applications*, SIAM Journal on Matrix Analysis and Applications (accepted), 2024.

14 • **Haibo Li**. *A preconditioned Krylov subspace method for linear inverse problems with general-form Tikhonov regularization*, SIAM Journal on Scientific Computing, 46 (4), A2607-A2633, 2024.

13 • **Haibo Li**. *The joint bidiagonalization of a matrix pair with inaccurate inner iterations*, SIAM Journal on Matrix Analysis and Applications, 45 (1), 232–259, 2024.

12 • **Haibo Li**. *Double precision is not necessary for LSQR for solving discrete linear ill-posed problems*, Journal of Scientific Computing, 98 (3), 55, 2024.

## Papers (continued)

11 • Yujin Yan, **Haibo Li**, Tong Zhao, Lin-Wang Wang, Lin Shi, Tao Liu, Guangming Tan, Weile Jia, Ninghui Sun. *10-million atoms simulation of first-principle package LS3DF on Sugon supercomputer*, Journal of Computer Science and Technology, 39 (1), 45-62, 2024.

10 • Zhongxiao Jia, **Haibo Li**. *The joint bidiagonalization method for large GSVD computations in finite precision*, SIAM Journal on Matrix Analysis and Applications, 44 (1), 382–407, 2023.

9 • Zhongxiao Jia, **Haibo Li**. *The joint bidiagonalization process with partial reorthogonalization*, Numerical Algorithms (88), 965–992, 2021.

Preprints:

8 • Hailong Guo, **Haibo Li**. *Derivative estimation with RKHS for learning dynamics from time-series data*, 2025, submitted.

7 • **Haibo Li**, Fei Lu. *Automatic kernel regression and regularization for learning convolution kernels*, 2025, manuscript.

6 • **Haibo Li**. *Krylov iterative methods for linear least squares problems with linear equality constraints*, 2025, submitted.

5 • **Haibo Li**, Xingxing Wu, Liping Liu, Long Wang, Lin-Wang Wang, Guangming Tan, Weile Jia, *ALKPU: an active learning method for the DeePMD model with Kalman filter*, 2024, submitted.

4 • **Haibo Li**, Jinchao Feng, Fei Lu. *Scalable iterative data-adaptive RKHS regularization*, 2024, submitted.

3 • **Haibo Li**. *Projected Newton method for large-scale Bayesian linear inverse problems*, 2024, submitted to SIAM Journal on Optimization (minor revision).

2 • **Haibo Li**. *Generalizing the SVD of a matrix under non-standard inner product and its applications to linear ill-posed problems*, 2023, submitted to Applied Mathematics and Computation (major revision).

1 • **Haibo Li**. *Subspace projection regularization for large-scale Bayesian linear inverse problems*, 2023, submitted.

## Presentations

• Invited talk: *Scalable iterative data-adaptive RKHS regularization*, The Eighth Young Scholar Symposium, East Asia Section of Inverse Problems International Association, Nov. 17, 2024.

• Invited talk: *Projected Newton method for large-scale Bayesian linear inverse problems*, School of Sciences, Great Bay University, Nov. 6, 2024.

• Invited talk: *Projected Newton method for large-scale Bayesian linear inverse problems*, School of Mathematics, Hunan University, Nov. 5, 2024.

• Talk: *Scalable iterative data-adaptive RKHS regularization*, Applied Math Seminar at Lehigh University, Oct. 24, 2024.

• Talk: *A preconditioned Krylov subspace method for regularizing linear inverse problems*, Data Science Seminar at Johns Hopkins University, Oct. 02, 2024.

• Talk: *Subspace projection regularization for high-dimensional Bayesian inverse problems*, MATRIX research program: Multivariate Dependence Modeling: Theory and Applications, Jul. 30, 2024.

• Talk: *Scalable iterative data-adaptive RKHS regularization*, International Conference on Scientific Computation and Differential Equations (SciCADE 2024), Jul. 16, 2024.

• Talk: *Subspace Projection Regularization: preconditioned Golub-Kahan bidiagonalization methods for regularizing linear inverse problems*, The 67th Annual Meeting of the Australian Mathematical Society (AustMS 2023), Dec. 2023.

• Talk: *A mixed precision variant of LSQR for solving discrete linear ill-posed problems*, Research Center for Mathematics and Interdisciplinary Sciences, Shandong University, Mar. 2023.

• Talk: *A Kalman filter based optimizer for training the neural network force field with first-principles accuracy*, Forum for High Performance Computing and Industrial Material Simulations, CCF HPC China, Dec. 2022.

- Talk: *The joint bidiagonalization process with reorthogonalization*, Forum for Doctoral Students, Tsinghua University, May 2020.
- Talk: *Introduction to iterative algorithms for solving large scale ill-posed problems*, Forum in Mathematics and Interdisciplinary Sciences, Research Center for Mathematics and Interdisciplinary Sciences, Shandong University, Nov. 2019.
- Technical report: *Preconditioned MINRES algorithm: basic theory and implementation*, CAEP Software Center for High Performance Numerical Simulation, Sep. 2019

## Academic service

Reviewer of journals:

- Reviewer for Mathematical Reviews (No. 161348)
- SIAM Journal on Matrix Analysis and Applications
- BIT Numerical Mathematics
- Numerical Algorithms

Reviewer of conferences:

- The International Conference for High Performance Computing, Networking, Storage, and Analysis (SC22), 2022
- The 13th International Conference on Electronics, Communications and Networks (CECNet 2023), 2023

Reviewer of grants:

- International reviewer for Czech Science Foundation (Czech Republic).

## Teaching Experience

- Stochastic Mathematical Methods (for undergraduates), teaching assistant, Tsinghua University. 2015.9-2016.1
- Stochastic Mathematical Methods (for undergraduates), teaching assistant, Tsinghua University. 2016.2-2016.6
- Linear Algebra (for undergraduates), teaching assistant, Tsinghua University. 2016.9-2017.1
- Calculus (for undergraduates), teaching assistant, Tsinghua University. 2017.2-2017.6
- Advanced Numerical Analysis (for postgraduates), teaching assistant, Tsinghua University. 2017.9-2018.1
- Calculus (for undergraduates), teaching assistant, Tsinghua University. 2018.2-2018.6
- Numerical Analysis (for postgraduates), teaching assistant, Tsinghua University. 2018.9-2019.1

## Supervision of students

Master students
- Jiayue Ma, The University of Melbourne, 2024 – now (Co-supervised with Dr. Hailong Guo)
- Bohan Sun, The University of Melbourne, 2025 – now (Co-supervised with Dr. Wei Huang)

## Skills

Programming
- Advanced: MATLAB, Python
  Basic: C/C++, Linux, JAX

Language
- English, Chinese

## Awards

- Small Grant Proposal for *Research Project: Data-driven methods for learning dynamics from observations*, funded by School of Mathematics and Statistics, University of Melbourne, 2024

## Awards (continued)

- Professor Maurice H. Belz Fund, funded by School of Mathematics and Statistics, University of Melbourne, 2024