Liyao Lyu

Department of Computational Mathematics, Science and Engineering
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Education

- **Michigan State University** — East Lansing, MI
  Ph.D., Department of Computational Mathematics, Science and Engineering; — *Sep 2020 - Present*
  Advisor: Huan Lei
- **UC Berkeley Extension** — Berkeley, CA
  Completed coursework in numerical solution of PDE and Mathematical Methods for Optimization; — *Jan 2019-May 2019*
- **Soochow University** — Suzhou, Jiang Su
  Bachelor of Science(BS): Mathematics — *Sep. 2016 - Jul. 2020*
  Advisor: Jingrun Chen

Publication List (Google Scholar)

1. Liyao Lyu, Huan Lei. **On the generalization ability of coarse-grained molecular dynamics models for non-equilibrium processes**, *arXiv: 2409.11519*, 2024.
2. Sengwei Liang, Liyao Lyu, Chunmei Wang, Haizhao Yang. **Reproducing activation function for deep learning**, *Communications in Mathematical Sciences*, 2024.
3. Liyao Lyu, Huan Lei. **Consensus-based construction of high-dimensional free energy surface**, *arXiv: 2311.05009*, 2023.
4. Liyao Lyu, Huan Lei. **Construction of coarse-grained molecular dynamics with many-body non-Markovian memory**, *Physical Review Letters*, 2023
5. Liyao Lyu, Zhen Zhang, Minxin Chen, Jingrun Chen. **MIM: A deep mixed residual method for solving high-order partial differential equations**, *Journal of Computational Physics*, 2022.
6. Jingrun Chen, Shi Jin, Liyao Lyu. **A Consensus-Based Global Optimization Method with Adaptive Momentum Estimation**, *Communications in Computational Physics*, 2022.
7. Liyao Lyu, Zheng Chen. **Local discontinuous Galerkin methods with novel basis for fractional diffusion equations with non-smooth solutions**, *Communications on Applied Mathematics and Computation*, 2022.
8. Jingrun Chen, Shi Jin, Liyao Lyu. **A Deep Learning Based Discontinuous Galerkin Method for Hyperbolic Equations with Discontinuous Solutions and Random Uncertainties**, *Journal of Computational Mathematics*, 2023.
9. Liyao Lyu, Keke Wu, Rui Du, Jingrun Chen. **Enforcing Exact Boundary and Initial Conditions in the Deep Mixed Residual Method**, *CSIAM Transactions on Applied Mathematics*, 2021.
10. Jingrun Chen, Rui Du, Panchi Li, Liyao Lyu. **Quasi-Monte Carlo sampling for machine-learning partial differential equations**, *Numerical Mathematics: Theory, Methods and Applications*, 2021
11. Liyao Lyu, Zhiwen Zhang, Jingrun Chen. **A Qmc-Deep Learning Method for Diffusivity Estimation in Random Domains**. *Numerical Mathematics: Theory, Methods and Applications*, 2020.

Visiting Position

- **University of Massachusetts Dartmouth** — MA, USA
  Host *Zheng Chen.* Local Discontinuous Galerkin Method for Fractional Diffusion Equation — *Aug 2019 - Nov 2019*
- **Hong Kong University of Science and Technology** — Hong Kong
  Host *Yang Xiang.* — *Jul 2019 - Aug 2019*

Professional Service

- Reviewer: SIAM Journal on Optimization

Teaching

Teaching assistant at Michgan State University

- CMSE 801 Numerical Linear Algebra, Fall 2024-2025
- CMSE 803 Numerical Methods for Differential Equations, Fall 2024-2025

Invited Talks

Machine Learning based Coarse-Grained Models for Molecular Systems

SIAM Conference on Computational Science and Engineering (CSE25) 2025.03
CompMath PI Meeting 2024 (Poster) 2024.07
Scale Bridging Meeting and Workshop(Poster), Los Alamos, NM, USA 2024.05
Student Computational Math Seminar, The Ohio State University 2024.03
SIAM New York-New Jersey-Pennsylvania Section (SIAM-NNP), NJ, USA 2023.10
The 2023 SIAM Great Lakes Meeting, East Lansing, USA 2023.10

A Deep Learning Based Discontinuous Galerkin Method for Hyperbolic Equations with Discontinuous Solutions and Random Uncertainties

IMA Workshop on the Mathematical Foundation and Applications of Deep Learning,Virtual 2021.09