# Senwei Liang

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Google scholar | Github

## Research interests

My research interest spans several topics:

**Scientific machine learning:** modeling dynamical systems; solving high-dimensional PDE, Symbolic regression; Neural network approximation; Activation function.

**AI for science:** Transitional path sampling in chemical reaction; rare events; reinforcement learning-based optimization.

**Deep learning algorithm:** Regularization methods; Classification models; Foundation models; Explainable models; Graph neural networks; Network slimming; Diffusion models.

## Education

**Purdue University** — West Lafayette, IN
Doctor of Philosophy. Advisor: Prof. Haizhao Yang — Dec 2019 – 2022
Thesis: *Learning and Solving Differential Equations With Deep Learning*

**National University of Singapore** — Singapore
Master of Science. Advisor: Prof. Haizhao Yang — Aug 2017 – 2019
Thesis: *Regularization on Machine Learning*

**Sun Yat-Sen University** — Guangzhou, China
Bachelor of Science. Advisor: Prof. Lihua Yang — Aug 2013 – 2017

## Experience

**Lawrence Berkeley National Laboratory** — Berkeley, CA
Postdoc. Advisors: Prof. Chao Yang and Lin Lin — Aug 2022 – Present

**Computational Medical Imaging Laboratory** — Guangzhou, China
Research assistant. Advisor: Prof. Yao Lu — Jun 2016 – 2017

## Journal publications

[10] Optimizing Shot Assignment in Variational Quantum Eigensolver Measurement — 2024
L Zhu, ***S Liang***†, C Yang and X Li († joint first author)
Journal of Chemical Theory and Computation, 20, 6, 2390-2403 [PDF] [Code]

[9] Solving PDEs on Unknown Manifolds with Machine Learning — 2024
***S Liang***, SW Jiang, J Harlim and H Yang
Applied and Computational Harmonic Analysis, Volume 71, 101652 [PDF] [Code]

[8] Reproducing Activation Function for Deep Learning — 2024
***S Liang***, L Lyu, C Wang and H Yang
Communications in Mathematical Sciences, 22 (2), 285 – 314 [PDF] [Code]

[7] Learning Nonlinear Integral Operators via Recurrent Neural Networks and Its Application — 2024
H Bassi, Y Zhu, ***S Liang***, J Yin, CC Reeves, V Vlček and C Yang
Machine Learning with Applications 15, 100524 [PDF]

[6] Probing Reaction Channels via Reinforcement Learning — 2023
***S Liang***, AN Singh, Y Zhu, DT Limmer and C Yang
Machine Learning: Science and Technology 4 (4) [PDF] [Code]

[5] On Fast Simulation of Dynamical System with Neural Vector Enhanced Numerical Solver — 2023
Z Huang, ***S Liang***†, H Yang, L Lin († Joint first author)

Scientific reports 13 (1), 15254 [PDF][Code]

[4] Stationary Density Estimation of Ito Diffusions Using Deep Learning 2023
Y Gu, J Harlim, H Yang and ***S Liang**** (* Corresponding author)
SIAM Journal on Numerical Analysis 61 (1), 45-82 [PDF]

[3] Quantifying Spatial Homogeneity of Urban Road Networks via Graph Neural Networks 2022
J Xue, N Jiang, ***S Liang***, Q Pang, T Yabe, SV Ukkusuri and J Ma
Nature Machine Intelligence 4 (selected as cover paper)[PDF] [Code]

[2] Machine Learning for Prediction with Missing Dynamics 2021
J Harlim, SW Jiang, ***S Liang*** and H. Yang (Alphabetical order)
Journal of Computational Physics 428, 109922 [PDF] [Code]

[1] Drop-Activation: Implicit Parameter Reduction and Harmonic Regularization 2021
***S Liang***, Y Khoo and H Yang
Communications on Applied Mathematics and Computation 3, 293-311 [PDF] [Code]

## Conference proceedings

[5] Lottery Ticket Hypothesis for Attention Mechanism in Residual Convolutional Neural Network 2024
Z Huang, ***S Liang***†, M Liang, W He, H Yang and L Lin († joint first author)
IEEE International Conference on Multimedia & Expo [PDF] [Code]

[4] Stiffness-aware Neural Network for Learning Hamiltonian Systems 2022
***S Liang***, Z Huang and H Zhang
International Conference on Learning Representations [PDF]

[3] Blending Pruning Criteria for Convolutional Neural Networks 2021
W He, Z Huang, M Liang, ***S Liang*** and H Yang
International Conference on Artificial Neural Networks [PDF]

[2] DIANet: Dense-and-Implicit Attention Network 2020
Z Huang, ***S Liang***†, M Liang and H Yang († joint first author)
Proceedings of the AAAI Conference on Artificial Intelligence [PDF] [Code]

[1] Instance Enhancement Batch Normalization: An Adaptive Regulator for Batch Noise 2020
***S Liang***, Z Huang, M Liang and H Yang
Proceedings of the AAAI Conference on Artificial Intelligence [PDF] [Code]

## Manuscripts

[10] Solving High-Dim. Partial Integral Differential Equations with Finite Expression Method 2024
G Hardwick, ***S Liang*** and H Yang
In preparation [PDF]

[9] Learning Biological Systems with Finite Expression Method 2024
J Du, ***S Liang*** and C Wang
In preparation [PDF]

[8] Learning Hamiltonian with Finite Expression Method 2024
J Lai, ***S Liang*** and C Wang
In preparation [PDF]

[7] QuGStep: Refining Step Size Selection for Gradient-Based Quantum Optimization 2024
***S Liang***, L Zhu, X Li and C Yang
In preparation [PDF]

[6] Piecewise Local PCA for Nonlinear Embedding and Collective Variables 2024
***S Liang*** and C Yang
In preparation [PDF]

[5] Effective Many-body Interactions in Reduced-Dimensionality Spaces through Neural Nets 2024
***S Liang***, K Kowalski, C Yang and NP Bauman

arXiv:2407.05536 [PDF]

[4] Artificial-Intelligence-Driven Shot Reduction in Quantum Measurement 2024
***S Liang***, L Zhu, C Yang and X Li
arXiv:2405.02493 [PDF] [Code]

[3] Finite Expression Method for Solving High-Dimensional Partial Differential Equations 2022
***S Liang*** and H Yang
arXiv:2206.10121 [PDF] [Code]

[2] Layer-wise Shared Attention Network on Dynamical System Perspective 2022
Z Huang, ***S Liang***, M Liang, W He and L Lin
arXiv:2210.16101 [PDF]

[1] Altersgd: Finding Flat Minima for Continual Learning by Alternative Training 2021
Z Huang, M Liang, ***S Liang*** and W He
arXiv:2107.05804 [PDF]

## Awards

- Travel Award, SIAM Northern and Central California Sectional Meeting 2024
- Travel Award, International Congress on Industrial and Applied Mathematics 2023
- Outstanding Reviewer, Computer Vision and Pattern Recognition Conference 2022
- Grad Student Travel Grant, American Mathematical Society 2022
- Ross-Lynn Fellowship, Purdue University 2021 – 2022
- Top Graduate Tutors, Department of Mathematics, National University of Singapore 2020
- Thirty-fourth AAAI Conference Scholarship 2020
- Samsung Scholarship, Samsung 2015 – 2016
- Outstanding Student Scholarship, Sun Yat-sen University 2013 – 2017
- National Scholarship, Ministry of Education of China 2013 – 2014

## Invited Presentation in Conference and Workshop

- Studying rare chemical reactions via deep learning, Postdoc Symposium, Berkeley lab 2024
- Identifying reaction channels via reinforcement learning, ICIAM, Waseda University 2023
- Identifying reaction channels via reinforcement learning, Postdoc Symposium, Berkeley lab 2023
- Solving PDEs on unknown manifolds with machine learning, AMS Sectional meeting, Purdue University 2022
- Solving PDEs on unknown manifolds with machine learning, Joint Mathematics Meetings, Seattle WA 2022
- Solving PDEs on unknown manifolds with machine learning, 4th Annual Meeting of the SIAM Texas-Louisiana Section, South Padre Island, Texas 2021
- Regularization Methods of Deep Learning for Image Classification, Workshop on "High-Dimensional Learning and Computation in Physics", National University of Singapore 2019
- Solving PDEs on Unknown Manifolds with Machine Learning, SIAM Southeastern Atlantic Section Conference, Auburn University 2021
- Solving PDEs on Unknown Manifolds with Machine Learning, IMA Workshop on the Mathematical Foundation and Applications of Deep Learning, Purdue University 2021

## Technologies

**Languages:** Python, Matlab

**Software:** Matlab, Meshlab

## Developed Software Package

**Deep Attention Neural Networks:** A collection of popular self-attention neural networks for image classification, boasting over 160 stars on GitHub. [Link]

**Finite Expression Method:** The implementation of the finite expression method for a variety of problems, including solving high-dimensional PDEs, eigenvalue problems, and more. [Link]

## Academic Service

**Conference reviewer:**

- NeurIPS Workshop FM4Science (Foundation Models for Science) 2024
- European Conference on Computer Vision (ECCV) 2022
- Conference on Computer Vision and Pattern Recognition (CVPR) 2022, 2021
- AAAI Conference on Artificial Intelligence 2021
- International Conference on Artificial Neural Networks (ICANN) 2021, 2022

**Journal reviewer:**

- Journal of Scientific Computing (JOMP)
- Journal of Vibration and Control

**Organizer:**

- Symposium at SIAM Conference on Computational Science and Engineering 2025
- Symposium at AMS Sectional meeting, Purdue University 2022
- Symposium at 4th Annual Meeting of the SIAM Texas-Louisiana Section 2021