

ZIJIE LI

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EDUCATION

Ph.D. in Mechanical Engineering,

Topic: AI for Science, Advisor: [Amir Barati Farimani](#)

Carnegie Mellon University, GPA: 4.00/4.00

January, 2020 - January, 2025 (expected)

B.E. in Theoretical and Applied Mechanics,

Sun Yat-sen University, GPA: 3.91/4.00

August, 2015 - May, 2019

WORKING EXPERIENCE

Research intern on diffusion models,

1. Diffusion feature extraction for multi-modal tasks

Extract visual representations from pretrained state-of-the-art diffusion model (PixArt, SD3) and benchmark their performance on image understanding task like captioning.

2. Turning text-to-image diffusion model (SD3 medium) into a image-text joint diffusion model

Modify the MMDIT backbone of SD3 and finetune it with joint diffusion target.

3. Training a 1.1B joint-diffusion model from scratch

Curate high quality data by filtering publicly available image-text dataset and generate synthetic captions. Training a customized MMDIT from scratch to do text-to-image generation and image-to-text understanding.

Mentor: [Linjie Yang](#), [Peng Wang](#)

TikTok, Seed-Image-Generation

May, 2024 - November, 2024

RESEARCH INTEREST

Neural PDE solver, Numerical simulation of PDEs and dynamical systems, Physics and numerical methods inspired design of neural networks, Diffusion models, Generative AI

PEER-REVIEWED PUBLICATIONS

(For the up-to-date publication list please refer to the [Google scholar](#), * denotes equal contribution)

1. Scalable Transformer for PDE surrogate modelling [[Paper](#)], [[Code](#)]

Advances on Neural Information Processing Systems 2023

Zijie Li, Dule Shu, A. Barati Farimani

2. Transformer for Partial Differential Equations' Operator Learning [[Paper](#)], [[Code](#)]

Transactions on Machine Learning Research (2023)

Zijie Li, Kazem Meidani, A. Barati Farimani

3. Denoise Pre-training on Non-equilibrium Molecules for Accurate and Transferable Neural Potentials

[[Paper](#)], [[Code](#)]

Journal of Chemical Theory and Computation (2023)

Yuyang Wang, Changwen Xu, **Zijie Li**, A. Barati Farimani

4. A physics-informed diffusion model for high-fidelity flow field reconstruction [[Paper](#)], [[Code](#)]

Journal of Computational Physics (2023)

Dule Shu*, **Zijie Li***, A. Barati Farimani

5. Hyena neural operator for partial differential equations [[Paper](#)], [[Code](#)]

APL Machine Learning (2023)

Saurabh Patil, **Zijie Li**, A. Barati Farimani

6. Graph Neural Network Accelerated Molecular Dynamics [Paper], [Code]
Journal of Chemical Physics (2022)
Zijie Li, Kazem Meidani, Prakarsh Yadav, A. Barati Farimani
7. TPU-GAN: Learning temporal coherence from dynamic point cloud sequences [Paper], [Code]
International Conference on Learning Representations 2022
Zijie Li, Tianqin Li, A. Barati Farimani
8. Prototype memory and attention mechanisms for few shot image generation [Paper], [Code]
International Conference on Learning Representations 2022
Tianqin Li*, Zijie Li*, Andrew Luo, Harold Rockwell, A. Barati Farimani, Tai Sing Lee
9. Graph neural network-accelerated Lagrangian fluid simulation [Paper], [Code]
Computers & Graphics (2022)
Zijie Li, A. Barati Farimani

CONFERENCE PRESENTATION

1. **Latent Neural PDE Solver for time-dependent system**
37th Annual Conference on Neural Information Processing Systems, AI for Science workshop
New Orleans, LA December 2023
2. **Factorized kernel attention for scalable PDE learning**
76th Annual Meeting of the Division of Fluid Dynamics, Washington DC November, 2023
3. **Mesh-agnostic PDE Operator Learning with Attention**
American Physical Society (APS) March 2023, Las Vegas, NV March, 2023
4. **Accelerating Lagrangian fluid simulation with graph neural networks**
International Conference on Learning Representations 2021 SimDL workshop, Virtual May, 2021
5. **Graph Neural Network for Lagrangian Fluid Simulation**
73th Annual Meeting of the Division of Fluid Dynamics, Virtual November, 2020

INDUSTRIAL COLLABORATION

- Transformer-based neural operator** (with Nvidia) September, 2023 - (In progress)
Contributing attention-based kernel integral and Transformer utilities to the open-source library: [neuraloperator](#).
- Physics-informed diffusion model** (with Nvidia) October, 2023 - March, 2024
Contributing physics-informed diffusion to Nvidia's physics+machine learning library: [Modulus](#).
- Neural operator for reaction-diffusion simulation** (with KLA Tencor) February, 2022 - December, 2022
Created a differentiable simulation pipeline for simulating reaction-diffusion data and studied different kinds of neural operator surrogates with physics-informed loss.

BOOK CHAPTERS

Graph Neural Networks for Molecules
A chapter for book "Machine Learning in Molecular Sciences" published by Springer Nature
Yuyang Wang, Zijie Li, Amir Barati Farimani

TEACHING EXPERIENCE

Teaching Assistant September, 2023 - December, 2023
24889 (Online certificate course): *Deep learning for engineers*

Teaching Assistant January, 2023 - May, 2023
24788: *Introduction to Deep Learning* & 24789: *Intermediate to Deep Learning*

SERVICE

Reviewer:

Conference: NeurIPS, ICLR,

Journal: Nature Machine Intelligence, IEEE Transactions on Neural Networks and Learning Systems

SKILLS

Programming: Python, Fortran, C++

Package: PyTorch, Deep Graph Library, Pytorch Geometric, Numba, Phiflow, OpenMM, JAX, JAX-MD, FENICS

Language: Mandarin (native), English (proficient)

SELECTED COURSEWORKS

Deep reinforcement learning and control, Numerical methods, Computer vision, Introduction to machine learning, Introduction to deep learning, Learning-based image synthesis, Engineering computation (C++), Computational fluid dynamics, Finite element analysis, Molecular simulation for materials