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 - March, 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 simple 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 training (including visual instruction tuning), reach competitive performance on various vision-language benchmarks (VQAv2, POPE, MME, etc). [Preprint]
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 (Geneval score: 0.39) and image-to-text understanding (around 60 percent accuracy on VQAv2-val 32-shot).

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 - May, 2024
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, ICML
Journal: Nature Machine Intelligence, IEEE Transactions on Neural Networks and Learning Systems, Transaction on Machine Learning Research

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