

# ZIJIE LI

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## EDUCATION

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### Ph.D. in Mechanical Engineering,

Carnegie Mellon University, GPA: 4.00/4.00

January, 2020 - December, 2024 (expected)

### B.E. in Theoretical and Applied Mechanics,

Sun Yat-sen University, GPA: 3.91/4.00

August, 2015 - May, 2019

## RESEARCH INTEREST

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Neural PDE solver, Numerical simulation of PDEs, Physics and numerical methods inspired design of neural networks

## PUBLICATIONS

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

1. Scalable Transformer for PDE surrogate modelling [[Paper](#)]  
*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. Graph Neural Network Accelerated Molecular Dynamics [[Paper](#)], [[Code](#)]  
*Journal of Chemical Physics (2022)*  
**Zijie Li**, Kazem Meidani, Prakarsh Yadav, A. Barati Farimani
6. 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
7. 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
8. Graph neural network-accelerated Lagrangian fluid simulation [[Paper](#)], [[Code](#)]  
*Computers & Graphics (2022)*  
**Zijie Li**, A. Barati Farimani

## CONFERENCE PRESENTATION

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1. **Factorized kernel attention for scalable PDE learning**  
76th Annual Meeting of the Division of Fluid Dynamics, Washington DC  
November, 2023

2. **Mesh-agnostic PDE Operator Learning with Attention**  
American Physical Society (APS) March 2023, Las Vegas, NV March, 2023
3. **Accelerating Lagrangian fluid simulation with graph neural networks**  
International Conference on Learning Representations 2021 SimDL workshop, Virtual May, 2021
4. **Graph Neural Network for Lagrangian Fluid Simulation**  
73th Annual Meeting of the Division of Fluid Dynamics, Virtual November, 2020

#### BOOK CHAPTERS

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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

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Teaching Assistant	September, 2023 - December, 2023
24889 ( <i>Online certificate course</i> ): Deep learning for engineers	
Teaching Assistant	January, 2023 - May, 2023
24788: <i>Introduction to Deep Learning</i> & 24789: <i>Intermediate to Deep Learning</i>	

#### SERVICE

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**Reviewer:** NeurIPS, Nature Machine Intelligence, IEEE Transactions on Neural Networks and Learning Systems

#### SKILLS

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**Programming:** Python, Fortran, C++  
**Package:** PyTorch, Deep Graph Library, Pytorch Geometric, Numba, Phiflow, OpenMM, JAX  
**Language:** Mandarin (native), English (proficient)

#### SELECTED COURSEWORKS

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