ZONGYI LI

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RESEARCH INTEREST

My research interests lie at the intersection of machine learning and physical sciences (AI for science). Specifically, I work on neural operators for learning solution operators in partial differential equations (PDEs) that arise in fluid mechanics and earth sciences. Neural operators model physical simulations with chaotic behaviors and complex geometries, and they have applications in weather forecasting, carbon storage, and aerodynamics simulation.

APPOINTMENTS

Assistant Professor, NYU Courant Fall 2026 (expected)
Mathematics and Data Science. Courant Institute of Mathematical Sciences
Center for Atmosphere Ocean Science (CAOS) and Center for Data Science (CDS)

Postdoctoral Associate, MIT 2025 - 2026
Computer Science and Artificial Intelligence Laboratory (CSAIL). Hosted by Kaiming He

EDUCATION

Ph.D., Caltech 2019 - 2025
Computing and Mathematical Science. Advised by Anima Anandkumar
Milton and Francis Clauser Doctoral Prize (best thesis award)

B.S., Washington University in St. Louis 2015 - 2019
Mathematics and Computer Science
Highest distinction in mathematics and Ross Middlemiss award in mathematics

WORK EXPERIENCE

Research Internships, Nvidia Summer 2022, 2023, 2024
Mentored by Sylvia Chanak, Anima Anandkumar, and Sanjay Choudhry respectively
Worked on developing machine learning models for scientific applications

AWARDS

MIT-Novo Nordisk AI Fellowship 2025
Milton and Francis Clauser Doctoral Prize 2025
(Awarded to a single Caltech Ph.D. graduate whose thesis exhibits the highest originality)
Caltech Graduate Teaching and Mentoring Award 2025
Jane Street Fellowship - Finalist 2024
Nvidia Fellowship 2023
Amazon AI4Science Fellowship 2022
PIMCO Fellowship 2021
Kortschak Scholars Fellowship 2019

PUBLICATIONS

[1] Kamyar Azizzadenesheli, Nikola Kovachki, **Li, Zongyi**, Miguel Liu-Schiaffini, Jean Kossaifi, and Anima Anandkumar. "Neural operators for accelerating scientific simulations and design". In: *Nature Reviews Physics* (2024), pp. 1–9.

[2] Vignesh Gopakumar, Stanislas Pamela, Lorenzo Zanisi, **Li, Zongyi**, Anima Anandkumar, and MAST Team. "Fourier neural operator for plasma modelling". In: *Nuclear Fusion* (2024).

[3] Samuel Lanthaler, **Li, Zongyi**, and Andrew M Stuart. "The nonlocal neural operator: Universal approximation". In: *Constructive Approximation* (2024).

[4] **Li, Zongyi**, Hongkai Zheng, Nikola Kovachki, David Jin, Haoxuan Chen, Burigede Liu, Kamyar Azizzadenesheli, and Anima Anandkumar. "Physics-informed neural operator for learning partial differential equations". In: *ACM/JMS Journal of Data Science* 1.3 (2024), pp. 1–27.

[5] Md Ashiqur Rahman, Robert Joseph George, Mogab Elleithy, Daniel Leibovici, **Li, Zongyi**, Boris Bonev, Colin White, Julius Berner, Raymond A Yeh, Jean Kossaifi, et al. "Pretraining codomain attention neural operators for solving multiphysics pdes". In: *Advances in Neural Information Processing Systems (Neurips)*. 2024.

[6] Jiawei Zhao, Robert Joseph George, Yifei Zhang, **Li, Zongyi**, and Anima Anandkumar. "Incremental fourier neural operator". In: *Transactions on Machine Learning Research (TMLP)* (2024).

[7] Tingtao Zhou, Xuan Wan, Daniel Zhengyu Huang, **Li, Zongyi**, Zhiwei Peng, Anima Anandkumar, John F Brady, Paul W Sternberg, and Chiara Daraio. "AI-aided geometric design of anti-infection catheters". In: *Science Advances* 10.1 (2024), eadj1741.

[8] **Li, Zongyi**, Daniel Zhengyu Huang, Burigede Liu, and Anima Anandkumar. "Fourier neural operator with learned deformations for pdes on general geometries". In: *Journal of Machine Learning Research* 24.388 (2023), pp. 1–26.

[9] **Li, Zongyi**, Nikola Kovachki, Chris Choy, Boyi Li, Jean Kossaifi, Shourya Otta, Mohammad Amin Nabian, Maximilian Stadler, Christian Hundt, Kamyar Azizzadenesheli, et al. "Geometry-informed neural operator for large-scale 3D PDEs". In: *Advances in Neural Information Processing Systems (Neurips)* 36 (2023).

[10] Jaideep Pathak, Shashank Subramanian, Peter Harrington, Sanjeev Raja, Ashesh Chattopadhyay, Morteza Mardani, Thorsten Kurth, David Hall, **Li, Zongyi**, Kamyar Azizzadenesheli, et al. "Fourcastnet: A global data-driven high-resolution weather model using adaptive fourier neural operators". In: *PASC '23: Proceedings of the Platform for Advanced Scientific Computing Conference*. 2023.

[11] Gege Wen, **Li, Zongyi**, Qirui Long, Kamyar Azizzadenesheli, Anima Anandkumar, and Sally M Benson. "Real-time high-resolution CO 2 geological storage prediction using nested Fourier neural operators". In: *Energy & Environmental Science* 16.4 (2023), pp. 1732–1741.

[12] Colin White, Julius Berner, Jean Kossaifi, Mogab Elleithy, David Pitt, Daniel Leibovici, **Li, Zongyi**, Kamyar Azizzadenesheli, and Anima Anandkumar. "Physics-informed neural operators with exact differentiation on arbitrary geometries". In: *The Symbiosis of Deep Learning and Differential Equations III*. 2023.

[13] **Li, Zongyi**, Miguel Liu-Schiaffini, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. "Markov neural operators for learning chaotic systems". In: *Advances in Neural Information Processing Systems (Neurips)*. 2022.

[14] Yuanyuan Shi, **Li, Zongyi**, Huan Yu, Drew Steeves, Anima Anandkumar, and Miroslav Krstic. "Machine learning accelerated pde backstepping observers". In: *2022 IEEE 61st Conference on Decision and Control (CDC)*. IEEE. 2022, pp. 5423–5428.

[15] Anda Trifan, Defne Gorgun, **Li, Zongyi**, Alexander Brace, Maxim Zvyagin, Heng Ma, Austin R Clyde, David A Clark, Michael Salim, David Hardy, et al. "Intelligent Resolution: Integrating Cryo-EM with AI-driven Multi-resolution Simulations to Observe the SARS-CoV-2 Replication-Transcription Machinery in Action". In: *The International Journal of High Performance Computing Applications* (2022).

[16] Gege Wen, **Li, Zongyi**, Kamyar Azizzadenesheli, Anima Anandkumar, and Sally M Benson. "U-FNO—An enhanced Fourier neural operator-based deep-learning model for multiphase flow". In: *Advances in Water Resources* 163 (2022), p. 104180.

[17] Haoyu Yang, **Li, Zongyi**, Kumara Sastry, Saumyadip Mukhopadhyay, Mark Kilgard, Anima Anandkumar, Brucek Khailany, Vivek Singh, and Haoxing Ren. "Generic lithography modeling with dual-band optics-inspired neural networks". In: *Proceedings of the 59th ACM/IEEE Design Automation Conference*. 2022, pp. 973–978.

[18] John Guibas, Morteza Mardani, **Li, Zongyi**, Andrew Tao, Anima Anandkumar, and Bryan Catanzaro. "Adaptive Fourier Neural Operators: Efficient Token Mixers for Transformers". In: *International Conference on Learning Representations, 2022*. 2021.

[19] Nikola Kovachki, **Li, Zongyi**, Burigede Liu, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. "Neural operator: Learning maps between function spaces". In: *Journal of Machine Learning Research* (2021), pp. 89–1.

[20] **Li, Zongyi**, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. "Fourier neural operator for parametric partial differential equations". In: *International Conference on Learning Representations*. 2021.

[21] Burigede Liu, Nikola Kovachki, **Li, Zongyi**, Kamyar Azizzadenesheli, Anima Anandkumar, Andrew Stuart, and Kaushik Bhattacharya. "A learning-based multiscale method and its application to inelastic impact problems". In: *Journal of the Mechanics and Physics of Solids* (2021).

[22] **Li, Zongyi**, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Andrew Stuart, Kaushik Bhattacharya, and Anima Anandkumar. "Multipole graph neural operator for parametric partial differential equations". In: *Advances in Neural Information Processing Systems (Neurips)* 33 (2020), pp. 6755–6766.

[23] Brendan Juba, **Li, Zongyi**, and Evan Miller. "Learning Abduction Using Partial Observability". In: *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 32. 1. 2018.

SOFTWARE

- Neural Operator Library (founder, 2k stars) `https://github.com/neuraloperator`
- Modulus Library `https://github.com/NVIDIA/modulus`
- Clima Library `https://github.com/CliMA/TurbulenceConvection.jl`
- Tensorly Library `https://github.com/tensorly/tensorly`

MEDIA COVERAGE

- MIT Tech Review: AI has cracked a key mathematical puzzle for understanding our world.
- Quanta Magazine: Latest Neural Nets Solve World's Hardest Equations Faster Than Ever Before.
- Quanta Magazine: The Year in Math and Computer Science.
- Towards Data Science: AI has unlocked a key scientific hurdle in predicting our world.
- Medium: Artificial Intelligence Can Now Solve Partial Differential Equations.

INVITED TALKS

Neural operator for scientific computing

- UCLA, hosted by Yizhou Sun and Wei Wang — Nov 2024
- UChicago, hosted by Pedram Hassanzadeh — Oct 2024

Scale-consistency in operator learning

- Rising Stars in Data Science workshop at UCSD — Nov 2024
- American Physical Society (APS) Division of Plasma Physics Meeting — Oct 2024
- UMichigan SciFM Summer School — July 2024

Automative and aerodynamics design using machine learning

- NVIDIA GTC (Graduate Fellowship recipient talk) — March 2024
- Caltech AI Bootcamp — March 2024

- Jizhi Swarma seminar May 2023

Deformed spectral methods for general geometries
- PIMCO investment talk July 2022
- CVPR Tutorial on neural fields June 2022

Neural operator for scientific computing
- UCSD, guest lecture in Machine Learning for Physical Science (Yuanyuan Shi) April 2022
- Caltech, guest lecture in Representation Learning for Science (Yisong Yue) April 2022

Physics-informed neural operator
- CMU, NSF AI Planning Institute for Data Discovery in Physics Sep 2021
- CMU, ML in Fluid Dynamics series DARPA-E and CMU SciML webinar June 2021

Fourier neural operator
- Caltech, CMX Student/Postdoc seminars Feb 2021
- University of Toronto, "AI in robotics reading group" Oct 2020

SERVICES

Reviewer:
- Machine Learning: Neurips, ICLR, ICML, AAAI, TPAMI, JMLR
- Computational Physics: COMMSPHYS, JCP, CMAME, APS-PRR, APS-PRF
- Applied Math: SIAM-JUQ, SIAM-SISC
- Geo-Physics: JGR-ML

Coordinator: AI4Science weekly group meetings at Caltech 2020-2024

TEACHING

Teaching Assistant at California Institute of Technology
- CS 165: Foundations of Machine Learning and Statistical Inference
  Winter 2021 (Head TA), Winter 2022, Winter 2023 (Head TA), Winter 2024

Teaching Assistant at Washington University in St. Louis
- CSE 513: Theory of Artificial Intelligence and Machine Learning
  Spring 2018
- CSE 347: Analysis of Algorithms
  Spring 2019 (Head TA), Fall 2017
- CSE 247: Basics of Algorithms
  Spring 2017

MENTORING

I regularly mentor and collaborate with undergraduate students through Caltech's Summer Undergraduate Research Fellowships (SURF) program.

- David Jin (2021 → MIT PhD)
- Derek Qin (2021 → Databricks)
- Miguel Liu-Schiaffini (2021-2023 → Stanford PhD)
- Kimia Hassibi (2022 → MIT PhD)
- Haydn Maust (2022)

- Zelin Zhao (2023 → Gatech PhD)
- Catherine Deng (2023-2024 → Stanford PhD)
- Vansh Tibrewal (2023-2024)
- Xinyi Li (2024 → Caltech PhD)
- Reva Dhillon (2024)
- Michael Chen (2025)