ZONGYI LI

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RESEARCH INTEREST

My research interest lies at the intersection of machine learning and physical science (AI for science), with a primary focus on solving partial differential equations (PDE). I aim to develop foundation models to solve scientific problems faster and more accurately. Specifically, I am working on operator learning methods for solving partial differential equations arising in fluid mechanics, solid mechanics, earth science, ultrasound imaging, and finance.

EDUCATION

California Institute of Technology Fall 2019 - Spring 2025 (Expected)
Pasadena, CA
Ph.D. in computer science, advised by Anima Anandkumar.

Washington University in St. Louis Fall 2015 - Spring 2019
St. Louis, MO
BS, double major in math and computer science with a minor in Jazz.
Highest distinction in mathematics and Ross Middlemiss award in mathematics.

EXPERIENCE

Nvidia: Research Internships (three times) Summer 2022, 2023, 2024
Mentored by Sanjay Choudhry, Anima Anandkumar, and Sylvia Chanak.
Worked on developing and applying machine learning models for scientific applications.

AWARDS

Jane Street Fellowship - Finalist	2024
Nvidia Fellowship	2023 - 2024
Amazon AI4Science Fellowship	2022 - 2023
PIMCO Fellowship	2021 - 2022
Kortschak Scholars Fellowship	2019 - 2021

PUBLICATIONS

Selected publications on machine learning

- **"Fourier neural operator for parametric partial differential equations"**.
  Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. *International Conference on Learning Representations*, 2021.
- **"Neural operator: Learning maps between function spaces"**.
  Nikola Kovachki, Zongyi Li, Burigede Liu, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. *Journal of Machine Learning Research*, 2021.
- **"Fourier neural operator with learned deformations for pdes on general geometries"**.
  Zongyi Li, Daniel Zhengyu Huang, Burigede Liu, and Anima Anandkumar. *Journal of Machine Learning Research*, 2023.
- **"Physics-informed neural operator for learning partial differential equations"**.
  Zongyi Li, Hongkai Zheng, Nikola Kovachki, David Jin, Haoxuan Chen, Burigede Liu, Kamyar Azizzadenesheli, and Anima Anandkumar. *ACM/JMS Journal of Data Science*, 2024.

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

Selected publications on scientific applications

- **"Geometry-informed neural operator for large-scale 3d pdes"**. Zongyi Li, Nikola Kovachki, Chris Choy, Boyi Li, Jean Kossaifi, Shourya Otta, Mohammad Amin Nabian, Maximilian Stadler, Christian Hundt, Kamyar Azizzadenesheli, et al.. *Advances in Neural Information Processing Systems*, 2023.
- **"Fourcastnet: A global data-driven high-resolution weather model using adaptive fourier neural operators"**. Jaideep Pathak, Shashank Subramanian, Peter Harrington, Sanjeev Raja, Ashesh Chattopadhyay, Morteza Mardani, Thorsten Kurth, David Hall, Zongyi Li, Kamyar Azizzadenesheli, et al.. *PASC '23: Proceedings of the Platform for Advanced Scientific Computing Conference*, 2023.
- **"U-FNO—An enhanced Fourier neural operator-based deep-learning model for multiphase flow"**. Gege Wen, Zongyi Li, Kamyar Azizzadenesheli, Anima Anandkumar, and Sally M Benson. *Advances in Water Resources*, 2022.
- **"AI-aided geometric design of anti-infection catheters"**. Tingtao Zhou, Xuan Wan, Daniel Zhengyu Huang, Zongyi Li, Zhiwei Peng, Anima Anandkumar, John F Brady, Paul W Sternberg, and Chiara Daraio. *Science Advances*, 2024.
- **"A learning-based multiscale method and its application to inelastic impact problems"**. Burigede Liu, Nikola Kovachki, Zongyi Li, Kamyar Azizzadenesheli, Anima Anandkumar, Andrew Stuart, and Kaushik Bhattacharya. *Journal of the Mechanics and Physics of Solids*, 2021.

Full publications in chronological order

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

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

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

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

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

. [6] **"Incremental fourier neural operator"**. Jiawei Zhao, Robert Joseph George, Yifei Zhang, Zongyi Li, and Anima Anandkumar. *TMLR*, 2024.

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

. [8] **"Fourier neural operator with learned deformations for pdes on general geometries"**.
Zongyi Li, Daniel Zhengyu Huang, Burigede Liu, and Anima Anandkumar. *Journal of Machine Learning Research*, 2023.

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

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

. [11] **"Forecasting subcritical cylinder wakes with Fourier Neural Operators"**.
Peter I Renn, Cong Wang, Sahin Lale, Zongyi Li, Anima Anandkumar, and Morteza Gharib. *arXiv preprint arXiv:2301.08290*, 2023.

. [12] **"Real-time high-resolution CO 2 geological storage prediction using nested Fourier neural operators"**.
Gege Wen, Zongyi Li, Qirui Long, Kamyar Azizzadenesheli, Anima Anandkumar, and Sally M Benson. *Energy & Environmental Science*, 2023.

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

. [14] **"An adversarial active sampling-based data augmentation framework for manufacturable chip design"**.
Mingjie Liu, Haoyu Yang, Zongyi Li, Kumara Sastry, Saumyadip Mukhopadhyay, Selim Dogru, Anima Anandkumar, David Z Pan, Brucek Khailany, and Haoxing Ren. *Neural Information Processing Systems ML for Systems Workshop*, 2022.

. [15] **"Fourier continuation for exact derivative computation in physics-informed neural operators"**.
Haydn Maust, Zongyi Li, Yixuan Wang, Daniel Leibovici, Oscar Bruno, Thomas Hou, and Anima Anandkumar. *arXiv preprint arXiv:2211.15960*, 2022.

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

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

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

. [19] **"Large scale mask optimization via convolutional fourier neural operator and litho-guided self training"**.
Haoyu Yang, Zongyi Li, Kumara Sastry, Saumyadip Mukhopadhyay, Anima Anandkumar, Brucek Khailany, Vivek Singh, and Haoxing Ren. *arXiv preprint arXiv:2207.04056*, 2022.

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

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

. [22] **"Neural operator: Learning maps between function spaces"**.
Nikola Kovachki, Zongyi Li, Burigede Liu, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. *Journal of Machine Learning Research*, 2021.

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

. [24] **"Markov neural operators for learning chaotic systems"**.
Zongyi Li, Miguel Liu-Schiaffini, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. *Advances in Neural Information Processing Systems, 2022*, 2021.

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

. [26] **"Neural operator: Graph kernel network for partial differential equations"**.
Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. *ICLR 2020 Workshop on Integration of Deep Neural Models and Differential Equations*, 2020.

. [27] **"Multipole graph neural operator for parametric partial differential equations"**.
Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Andrew Stuart, Kaushik Bhattacharya, and Anima Anandkumar. *Advances in Neural Information Processing Systems*, 2020.

. [28] **"Learning Abduction Using Partial Observability"**.
Brendan Juba, Zongyi Li, and Evan Miller. *Proceedings of the AAAI Conference on Artificial Intelligence*, 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.

- 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

Scale-consistency in operator learning

- American Physical Society (APS) Division of Plasma Physics Meeting — Oct 2024
- U Michigan 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
- UCSD, guest lecture in Machine Learning for Physical Science — April, 2022,

Physics-informed neural operator

- Carnegie Mellon University, 'NSF AI Planning Institute for Data Discovery in Physics — Sep 2021
- Carnegie Mellon University, 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 20, 2020.

SERVICES

Reviewer: Neurips, ICLR, ICML, AAAI, JMLR, JCP, CMAME, SIAM JUQ.

MENTORING

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

- Michael Chen (2024 -)
- Xinyi Li (2024 -)
- Reva Dhillon (2024 -)
- Vansh Tibrewal (2023 -)
- Catherine Deng (2023)
- Haydn Maust (2022)
- Kimia Hassibi (2022 $\rightarrow$ MIT PhD)
- David Jin (2021 $\rightarrow$ MIT PhD)
- Derek Qin (2021 $\rightarrow$ Databricks)
- Miguel Liu-Schiaffini (2021 -)