Yadi Cao

Postdoctoral researcher, CSE, UCSD; Email: yadicao95@gmail.com; Website: https://eydcao.github.io/.

Research Focus

AI4Science, AI for fusion, numerical methods, computational fluid dynamics, and computational mechanics

Bio

Yadi Cao develops novel **AI methods to scale up engineering research by reducing experimental costs and labor of experts**. Using techniques like surrogate modeling, active sampling, and agentic workflows, his research has made a significant impact in fusion energy and computational fluid dynamics: **TGLF-SiNN**, which delivers a **180x computational speedup** for fusion simulations and is **integrated into General Atomics' tokamak pipeline**, and **BSMS-GNN**, which enables learning realistic **turbomachinery simulations on million-node meshes**.
Yadi is a postdoctoral researcher at UCSD with Professor Rose Yu. He completed his Ph.D. at UCLA, co-advised by Professors Chenfanfu Jiang and Demetri Terzopoulos. He is seeking a tenure-track faculty position and is open to collaboration and mentoring opportunities.

Education

University of California, Los Angeles (UCLA) — Los Angeles, CA
Ph.D. in Computer Science — *2021–2024*
- Thesis: Advancing physics-based simulations: Integrating conventional and machine learning approaches for enhanced computational efficiency
- Advisors: Chenfanfu Jiang (Applied Math) and Demetri Terzopoulos (Computer Science)

University of British Columbia (UBC) — Kelowna, BC, Canada
MASc in Mechanical Engineering — *2016–2018*
- Thesis: Analytical and numerical study of plug flow inside round/concentric microchannels
- Advisor: Sunny Ri Li (Mechanical Engineering)

University of Science and Technology of China (USTC) — Hefei, Anhui, China
BEng — *2012–2016*

Publications [Google Scholar] [Total Citations: 375, h-index: 10]

Journal Articles

- **Cao, Y***, Liu, Y* (equal contribution), Yang, L, Yu, R, Schaeffer, H, Osher, S. VICON: Vision In-Context Operator Networks for Multi-Physics Fluid Dynamics Prediction. TMLR (Transactions on Machine Learning Research), 2026.
- Wang, P, **Cao, Y**, Russell, C, Shen, Y, Luo, J, Zhang, M, Heng, S, Luo, X. Delta: Dual Consistency Delving with Topological Uncertainty for Active Graph Domain Adaptation. TMLR, 2025.
- **Cao, Y**, Zhao, Y, Li, M, Yang, Y, Choo, J, Terzopoulos, D, Jiang, C. Unstructured Moving Least Squares Material Point Methods: A Stable Kernel Approach with Continuous Gradient Reconstruction on General Unstructured Tessellations. Computational Mechanics (IF: 4.1), 2024.
- **Cao, Y**, Chen, Y, Li, M, Yang, Y, Zhang, X, Aanjaneya, M, Jiang, C. An Efficient B-Spline Lagrangian/Eulerian Method for Compressible Flow, Shock Waves, and Fracturing Solids. ACM TOG (SIGGRAPH, IF: 7.8), 2022.
- **Cao, Y**, Gao, X, Li, R. A Liquid Plug Moving in an Annular Pipe: Heat Transfer Analysis. International Journal of Heat and Mass Transfer (IF: 6.4), 2019.
- **Cao, Y**, Li, R. A Liquid Plug Moving in an Annular Pipe: Flow Analysis. Physics of Fluids (IF: 4.3), 2018. **Editor's Pick**.
- Fang, Y, Li, M, **Cao, Y**, Li, X, Wolper, J, Yang, Y, Jiang, C. Augmented Incremental Potential Contact for Sticky Interactions. IEEE TVCG (IF: 6.5), 2023.

Conference Proceedings

- Lyu, B*, **Cao, Y*** (equal contribution), Watson-Parris, D, Bergen, L, Berg-Kirkpatrick, T, Yu, R. Adapting While Learning: Grounding LLMs for Scientific Problems with Intelligent Tool Usage Adaptation. ICML 2025.
- Sun, F, Huang, Z, **Cao, Y**, Luo, X, Wang, W, Sun, Y. DoMiNO: Down-scaling Molecular Dynamics with Neural Graph Ordinary Differential Equations. ICLR 2025 Workshop on Machine Learning Multiscale Processes, 2025.
- **Cao, Y**, Chai, M, Li, M, Jiang, C. Efficient Learning of Mesh-Based Physical Simulation with Bi-Stride Multi-Scale Graph Neural Network. ICML 2023.
- Li, X, **Cao, Y**, Li, M, Yang, Y, Schroeder, C, Jiang, C. PlasticityNet: Learning to Simulate Metal, Sand, and Snow for Optimization Time Integration. **Spotlight**, NeurIPS 2022.
- Maheshwari, S, Mohanty, A, **Cao, Y**, Razu, S, McCulloch, A, Yu, R. BIGE: Biomechanics-informed GenAI for Exercise Science. L4DC 2025.
- Huang, Z, Zhao, W, Gao, J, Hu, Z, Luo, X, **Cao, Y**, Chen, Y, Sun, Y, Wang, W. Physics-Informed Regularization for Domain-Agnostic Dynamical System Modeling. NeurIPS 2024. **Best Paper Award**, NeurIPS DLDE workshop 2023.

Under Review Journal Articles

- **Cao, Y***, Zhang, F*, Liu, W* (equal contribution), Neiser, T, Meneghini, O, Smith, S, Nazikian, R, Sammuli, B, Yu, R. TGLF-SINN: Deep Learning Surrogate Model for Accelerating Turbulent Transport Modeling in Fusion. ArXiv: 2509.07024. NeurIPS ML4PS workshop. In submission to Nuclear Fusion (IF: 4.0).
- Yue, L, Somasekharan, N, Zhang, T, **Cao, Y**, Pan, S. Foam-Agent 2.0: An End-to-End Composable Multi-Agent Framework for Automating CFD Simulation in OpenFOAM. ArXiv: 2509.18178. NeurIPS ML4PS workshop. In submission to Nature Machine Intelligence (IF: 23.9).
- Ding, Y, Wu, K, **Cao, Y**, Magdon-Ismail, M, Gao, J. Computing Equilibria in Complex Systems with Billions of Interactions. In submission to PNAS NEXUS (IF: 3.8).

Preprints

- Wang, H, **Cao, Y**, Huang, Z, Liu, Y, Hu, P, Luo, X, Song, Z, Zhao, W, Liu, J, Sun, J, Zhang, S. Recent Advances on Machine Learning for Computational Fluid Dynamics: A Survey. ArXiv: 2408.12171.
- Somasekharan, N, Yue, L, **Cao, Y**, Li, W, Emami, P, Bhargav, P S, Acharya, A, Xie, X, Pan, S. CFD-LLMBench: A Benchmark Suite for Evaluating Large Language Models in Computational Fluid Dynamics. ArXiv: 2509.20374.
- Yang, J, Bhat, M, Hu, B, **Cao, Y**, Dehmamy, N, Walters, R, Yu, R. Discovering Symbolic Differential Equations with Symmetry Invariants. ArXiv: 2505.12083.
- Zhang, Y, **Cao, Y**, Sun, S, Yu, R. CAED-Agent: An Agentic Framework to Automate Simulation-Based Experimental Design.

Academic and Technical Talks

Building the Cost-Aware Scientific Agent
CSE-259 AI Seminar, UCSD (Host: Prithviraj Ammanabrolu) — *Oct, 2025*

Efficient Learning of Multi-Physics Simulation by Vision In-Context Operator Learning
SIAM UQ26 Mini-Symposium on In-context learning for PDEs and inverse problems (Host: Fei Lu) — *Mar, 2026*
Yale Lu Group Reading Group (Host: Lu Lu) — *Aug, 2025*
Algorithms for Multiphysics Models in the Post-Moore's Law Era, LANL (Host: Brian O'Shea) — *Jun, 2025*

Physics-Guided AI and Its Applications to Fusion
Lyncean Group of San Diego (Host: Bill Hagan) — *Jan, 2026*
Lawrence Livermore National Laboratory (Host: Ben Zhu) — *Dec, 2025*
CAST (Chinese Association for Science & Technology) (Host: Yongfeng Wu) — *Aug, 2025*
UCSD MAE+CER Winter 2025 Energy Seminar, UCSD (Host: George Tynan) — *Feb, 2025*
National Artificial Intelligence Research Resource Virtual Session Panelists (Host: Nitin Sukhija) — *Oct, 2024*

Advancing Physics-based Simulation with Unstructured Discretization and Machine Learning
UCLA Level Set Lab Reading Group (Host: Stanley Osher) — *Feb, 2024*
UCSD Rose STL Lab Reading Group (Host: Rose Yu) — *Jan, 2024*
Yale Lu Group Reading Group (Host: Lu Lu) — *Jan, 2024*
Caltech Anima AI + Science Lab Reading Group (Host: Anima Anandkumar) — *Jan, 2024*

Industry Experience

Google Student Researcher 2023–2024
Google *Los Angeles, CA*
Research Intern 2022
Snap *Los Angeles, CA*
SDE Intern 2021
Taichi Graphics *Beijing, China*
CAE/FEM Software Research Developer 2019–2020
shonCloud Tech/shonDynamics *Suzhou, Jiangsu, China*

Teaching

Teaching Fellow at University of California, Los Angeles
Operating Systems Principles (CS 111) (Instructors: Paul Eggert, Peter Reiher) *6 Quarters, 2022–2024*
Introduction to Algorithms and Complexity (CS 180) (Instructor: Matthew Ferland) *Summer 2023*
Teaching Assistant at University of British Columbia
Heat Transfer Applications (ENGR385) (Instructor: Ri Li) *Spring 2018*
Measurement Principles in Thermal Fluids (ENGR479) (Instructor: Ri Li) *Winter 2018*
Matter and Energy (APSC182) (Instructors: Shelir Ebrahimi, John Brereton) *2 Semesters, 2016–2017*

Mentoring

Current Mentees

- **Undergraduate Students:**
  - Lucas Hlaing (UCSD)
  - Zach Lawrence (UCSD)

Alumni

- **Undergraduate Students:**
  - Chloe Huang (University of Michigan; next stop: PhD student at Rose Lab)
  - Wesley Liu (UCSD; next stop: Master's student at USC)
  - Yang Zhang (Peking University)
  - Leo Lai (CUHK-Shenzhen)
  - Bohan Lyu (Tsinghua University; next stop: visiting student at Princeton University)
  - Darin Djapri (UCSD; next stop: continuing study at UCSD)
  - Yuwei Ren (UCSD; next stop: continuing study at UCSD)
- **Master's Students:**
  - Futian Zhang (UCSD; next stop: Software Engineer at ServiceNow)
  - Shubh Maheshwari (UCSD)
  - Howard Tsai (UCSD)

Programs

Gear Up2Research (GEAR) 2025
UCSD *San Diego, CA*

Early Research Scholars Program (ERSP) 2024–2025
UCSD *San Diego, CA*

Summer Training Academy for Research Success (STARS) 2024–2025
UCSD *San Diego, CA*

Awards and Honors

UCLA Non-residential Tuition Grant 2022–2024
UCLA Graduate Fellowship 2021
UBC Graduate Fellowship 2017–2018
NSERC Funding for Exchange Research 2017
USTC Alumni Fellowship of B.C. Canada 2017
Bronze Prize, Zhongwei-cup Energy & Environment Protection Contest 2015
Silver Prize, National Outstanding Undergraduate Scholarship 2013–2014

Research Community Service

Area Chair

- NeurIPS, AI for Science Workshop (2025)

Program Committee

- AAAI (2025, 2026)
- IJCAI (2024)

Reviewer (excluding committee services listed above)

- CVPR (2026)
- ICLR (2024-2026)
- ICML (2024-2025)
- NeurIPS (2023, 2025)
- JMLR (Journal of Machine Learning Research) (2025)
- TMLR (Transactions on Machine Learning Research) (2025)
- ACM SIGGRAPH (2024-2025)
- IEEE Transactions on Visualization and Computer Graphics (2025)
- ICLR Workshop: Tackling Climate Change with Machine Learning (2025)
- Pacific Graphics (2022, 2024)
- Physics of Fluids (2018-2024)