TAILIN WU

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Assistant professor of AI, Department of Engineering ◇ Westlake University

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WORK

Assistant Professor of AI, Department of Engineering Westlake University, Hangzhou, China	7/2023 – present
Postdoctoral Scholar in Computer Science Stanford University, Palo Alto, CA, USA	1/2020 – 5/2023 Advisor: Jure Leskovec

EDUCATION

Ph.D. in Physics Massachusetts Institute of Technology, USA Research: Machine Learning + Physics Thesis: [Intelligence, physics and information – the tradeoff between accuracy and simplicity in machine learning](#)	9/2012 – 11/2019 Advisors: Isaac Chuang, Max Tegmark
B.S. in Physics Peking University, Beijing, China	9/2008 – 7/2012 GPA: 3.83/4.00, top 3% out of 194 students

RESEARCH INTERESTS

My research vision is to develop machine learning (ML) methods for accelerating scientific simulation and discovery, while opening new frontiers in machine learning research (**AI + Science**). This lies in the interdisciplinary field of machine learning, scientific computing, and physical sciences.

Towards this goal, my past research has pioneered and made important advances to learning structured and compressed representations for accelerating large-scale and multi-scale simulations in physical sciences, including fluid, plasma, and more generic PDEs and N-body systems. My research has enabled ML-based surrogate models to scale to dynamical systems with two orders of magnitude higher dimensions and 15x faster than prior ML models. The ML models I developed are being deployed for fluid simulation in industry and will also be used for modeling laser-plasma systems in Stanford National Accelerator Laboratory (SLAC). Besides ML for simulation, I have introduced ML methods for discovering symbolic theories (published in a top physics journal) and relational structures from observations, and have theoretically revealed the origin of phase transition phenomena for the compression vs. prediction tradeoff in representation learning.

My future research aims to realize my vision via three thrusts: first, develop an *integrated and general-purpose ML pipeline and ecosystem* for accelerating simulation across physical sciences (mechanical engineering, materials, physics, biology). Second, building on top, develop *ML-based methods for accelerated inverse design for physical sciences* (e.g., controlled nuclear fusion design, drug design). Third, develop *knowledge-grounded and generalizable representations* for scientific discovery.

SELECTED AWARDS AND RECOGNITIONS

The paper "[Toward an Artificial Intelligence Physicist for Unsupervised Learning](#)" is featured in [MIT Technology Review](#) and [MotherBoard](#).

The paper "Toward an Artificial Intelligence Physicist for Unsupervised Learning" is published at *Physical Review E* as part of a *PRE Spotlight on Machine Learning in Physics*.

The paper "Discovering Nonlinear Relations with Minimum Predictive Information Regularization" is awarded the Best Poster Award at ICML 2019 Time Series Workshop.

The paper "Graph Information Bottleneck" is featured in Synced AI Technology & Industry Review.
The paper "Pareto-optimal data compression for binary classification tasks" is published as cover issue in *Entropy.*

Chinese National Scholarship (Top 2% in Peking University), 2011

Dean's Award for Academic Excellence of Peking University (Top 2%), 2009

Bronze Medal in the 2nd National Undergraduate Mathematics Contest (Finals), 2011

First Prize in the 2nd National Undergraduate Mathematics Contest (Beijing section), 2010

PUBLICATIONS AND PREPRINTS

Machine Learning for Simulation, Design, Control, and Discovery:

[1] L. Wei*, P. Hu*, R. Feng*, H. Feng, Y. Du, T. Zhang, R. Wang, Y. Wang, Z.M. Ma, T. Wu†, DiffPhyCon: A Generative Approach to Control Complex Physical Systems, NeurIPS 2024, (pdf), (openreview).

[2] T. Wu*†, T. Maruyama*, L. Wei*, T. Zhang*, Y. Du*, G. Iaccarino, J. Leskovec, "Compositional Generative Inverse Design." ICLR 2024 Spotlight (top 15% of accepted papers), (pdf), (openreview).

[3] H, Wang*, J. Li*, A. Dwivedi, K. Hara, T. Wu†, "BENO: Boundary-embedded Neural Operators for Elliptic PDEs." ICLR 2024 (pdf), (openreview).

[4] T. Wu*, W. Neiswanger*, H. Zheng*, S. Ermon, J. Leskovec, "Uncertainty Quantification for Forward and Inverse Problems of PDEs via Latent Global Evolution." AAAI 2024 oral (top 10% of accepted papers), (pdf).

[5] T. Wu*, T. Maruyama*, Q. Zhao*, G. Wetzstein, J. Leskovec, "Learning Controllable Adaptive Simulation for Multi-resolution Physics." ICLR 2023 Spotlight (pdf), (openreview), (slides).

[6] T. Wu, Max Tegmark, "Toward an Artificial Intelligence Physicist for Unsupervised Learning." *Physical Review E* 100 (3), 033311. Featured in PRE Spotlight on Machine Learning in Physics, (journal), (pdf), (code). Featured in MIT Technology Review and MotherBoard, (media), (media).

[7] T. Wu, T. Maruyama, J. Leskovec, "Learning to Accelerate Partial Differential Equations via Latent Global Evolution." In *36th Conference on Neural Information Processing Systems* (NeurIPS 2022a), (pdf), (poster), (code), (project page).

[8] T. Wu, M. Tjandrasuwita, Z. Wu, X. Yang, K. Liu, R. Sosič, J. Leskovec, "ZeroC: A Neuro-Symbolic Model for Zero-shot Concept Recognition and Acquisition at Inference Time." In *36th Conference on Neural Information Processing Systems* (NeurIPS 2022b), (pdf), (poster), (code), (project page).

[9] T. Wu, Q. Wang, Y. Zhang, R. Ying, K. Cao, R. Sosič, R. Jalali, H. Hamam, M. Maucec, J. Leskovec: Learning Large-scale Subsurface Simulations with a Hybrid Graph Network Simulator. In *Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining* pp. 4184-4194 (SIGKDD 2022), (pdf), (project page). Also presented as a 10min long talk at ICLR 2022 AI for Earth and Space Sciences workshop (poster).

[10] I. Lázaro, A. Anastasaki, H. Ardoña, M. Arguilla, ...Tailin Wu, ..et al. "35 challenges in materials science being tackled by PIs under 35 (ish) in 2024." Matter 7, no. 11 (2024): 3699-3706. (paper), (journal).

[11] X. Zhang, … T. Wu (31th/63 author), … S. Ji: Artificial Intelligence for Science in Quantum, Atomistic, and Continuum Systems, *in submission*, arXiv preprint arXiv:2307.08423 (2023).

[12] T. Wu, M. Sun, J. Chou, P. R. Samala, S. Cholsaipant, S. Kivelson, J. Yau, Z. Ying, E. P. Alves, J. Leskovec, F. Fiuza, "Learning Efficient Hybrid Particle-continuum Representations of Non-equilibrium N-body Systems." Under Review, (pdf). Also accepted in NeurIPS 2022 AI4Science workshop, (workshop pdf), (poster).

[13] J. Chou, T. Wu, S. Kivelson, J. Yau, R. Ying, E. P. Alves, J. Leskovec, F. Fiuza, "Accelerating predictive modeling of laser-driven ion acceleration with deep learning", APS Division of Plasma Physics Meeting Abstracts.

[14] S. M. Udrescu, A. Tan, J. Feng, O. Neto, <u>T. Wu</u>, M. Tegmark, "AI Feynman 2.0: Pareto-optimal Symbolic Regression Exploiting Graph Modularity." In *34th Neural Information Processing Systems* (NeurIPS 2020b). Oral presentation, (paper), (code).

[15] <u>T. Wu</u>, T. Breuel, M. Skuhersky, J. Kautz, "Discovering Nonlinear Relations with Minimum Predictive Information Regularization." ICML 2019 Time Series Workshop, Best Poster Award, (pdf), (workshop pdf), (poster), (code).

[16] D. Zeng*, <u>T. Wu</u>*, J. Leskovec, "ViRel: Unsupervised Visual Relations Discovery with Graph-level Analogy." In ICML 2022 Beyond Bayes: Paths Towards Universal Reasoning Systems Workshop, (pdf), (project page).

[17] M. Skuhersky, <u>T. Wu</u>, E. Yemini, A. Nejatbakhsh, E. Boyden, M. Tegmark, "Toward a More Accurate 3D Atlas of C. elegans Neurons", *BMC Bioinformatics* 23 (1), 1-18, (pdf).

Representation Learning:

[18] <u>T. Wu</u>*, H. Ren*, P. Li, J. Leskovec, "Graph Information Bottleneck." In *34th Neural Information Processing Systems* (NeurIPS 2020a). (paper), (project page), (code). Featured in Synced AI Technology & Industry Review, (media).

[19] <u>T. Wu</u>, I. Fischer, "Phase Transitions for the Information Bottleneck in Representation Learning." In *International Conference on Learning Representations* (ICLR 2020), (pdf).

[20] <u>T. Wu</u>, I. Fischer, I. L. Chuang, M. Tegmark, "Learnability for the Information Bottleneck." In *Uncertainty in Artificial Intelligence* (UAI 2019) (pp. 1050-1060). PMLR, (pdf), (poster). An extended version published in Entropy 21(10), 924, special issue "Information-Theoretic Approaches to Computational Intelligence".

[21] M. Tegmark, <u>T. Wu</u>, "Pareto-optimal data compression for binary classification tasks." *Entropy* 22.1 (2019): 7. Featured as cover issue, (pdf).

[22] C. Northcutt*, <u>T. Wu</u>*, I. L. Chuang, "Learning with Confident Examples: Rank Pruning for Robust Classification with Noisy Labels". In *Uncertainty in Artificial Intelligence*, Sydney, Australia (UAI 2017), (pdf), (code).

[23] <u>T. Wu</u>, J. Peurifoy, I. L. Chuang, M. Tegmark, "Meta-learning Autoencoders for Few-shot Prediction". arXiv preprint arXiv:1807.09912, (pdf).

Prior physics-centered publications:

[P1] D. Gangloff*, M. Shi*, <u>T. Wu</u>*, A. Bylinskii, B. Braverman, M. Gutierrez, R. Nichols, J. Li, K. Aichholz, M. Cetina, L. Karpa, B. Jelenković, I. L. Chuang, V. Vuletić, "Preventing and Reversing Vacuum-Induced Optical Losses in High-Finesse Tantalum (V) Oxide Mirror Coatings." *Optics Express* 23(14).

[P2] H. Zhang, M. Gutierrez, G. H. Low, R. Rines, J. Stuart, <u>T. Wu</u>, I. L. Chuang, "Iterative Precision Measurement of Branching Ratios Applied to 5P states in 88Sr+." *New Journal of Physics*, 18(12):123021, 2016.

[P3] G. Si, <u>T. Wu</u>, Q. Ouyang, Y. Tu, "Pathway-based mean-field model for Escherichia coli chemotaxis." *Physical Review Letters*, 109, 048101 (2012).

[P4] X. Zhu, G. Si, N. Deng, Q. Ouyang, <u>T. Wu</u>, Z. He, L. Jiang, C. Luo, Y. Tu, "Frequency-Dependent Escherichia coli Chemotaxis Behavior." *Physical Review Letters*, 108, 128101 (2012).

INVITED TALKS AND PRESENTATIONS

- *Design and control of physical systems based on diffusion generation models*
  2024 Chinese Physical Society Fall Meeting, Oct 2024

- *Learning adaptive and compositional models for multi-resolution simulation and inverse design*
  IMS-NTU joint workshop on Applied Geometry for Data Sciences Part I, Oct 2024

- *Compositional inverse design and control with diffusion generative models*
  Shanghai Institute for Mathematics and Interdisciplinary Sciences, June 2024

- *Uncertainty Quantification for Forward and Inverse Problems of PDEs via Latent Global Evolution*
  SIAM Conference on Uncertainty Quantification (UQ24), March 2024

- *Compositional generative inverse design*
  AI4Science Talks, February 2024

- *Machine learning for accelerating scientific simulation, design and control*
  Annual Meeting of Peking University Center for Quantitative Biology, January 2024

- *GNN for scientific simulations: towards adaptive multi-resolution simulators and a foundation neural operator*
  LoG Shanghai Meetup, November 2023

- *Machine learning of structured representations for accelerating scientific discovery and simulation*
  CPS Fall Meeting, August 2023

- *Graph Neural Networks for Accelerating Large-scale Simulations*
  AI for Science Summit 2023, August 2023

- *Phase transitions in the universal tradeoff between accuracy and simplicity in machine learning*
  HK Satellite of StatPhys28, August 2023

- *Machine learning of structured representations for accelerating scientific discovery and simulation*
  Tsinghua University, June 2023

- *Graph Neural Networks for Accelerating Large-scale Simulations*
  The First Workshop on AI-enabled Scientific Computing, June, 2023

- *AI + Science: motivations, advances, and open questions*
  Swarma, March, 2023 (slides)

- *Learning Controllable Adaptive Simulation for Multi-resolution Physics*
  Stanford Data for Sustainability Conference 2023, April, 2023 (slides)

- *Steps toward an AI scientist: neuro-symbolic models for concept generalization and theory learning*
  AAAI 2023 Symposium of Computational Approaches to Scientific Discovery, March, 2023 (slides)

- *Graph Neural Networks for Accelerating Large-scale Simulations*
  IBiM, March, 2023 (slides)

- *Learning Controllable Adaptive Simulation for Multi-resolution Physics*
  TechBeat, March, 2023 (slides), (video)

- *Graph Neural Networks for Large-scale Simulations*
  Stanford HAI Climate-Centred Student Affinity Group, February, 2023 (slides)

- *ZeroC: A Neuro-Symbolic Model for Zero-shot Concept Recognition and Acquisition at Inference Time*
  AI Time, February, 2023 (slides)

- *Learning to Accelerate Large-scale Physical Simulations in Fluid and Plasma Physics*
  Data-driven Physical Simulations (DDPS) seminar at Lawrence Livermore National Laboratory, June, 2022 (video)
  SIAM 2022 Conference on Mathematics of Data Science, September, 2022

- *Learning to accelerate simulation and inverse optimization of PDEs via latent global evolution*
  Stanford Computer Science ML lunch, June, 2022, (slides)

- *Steps toward an AI scientist: neuro-symbolic models for zero-shot learning of concepts and theories*
  BIGAI Cognitive Group seminar, December, 2022

- *AI Physicist and Machine Learning for Simulations*
  Guest lecture at Caltech CS159: Advanced Topics in Machine Learning, April, 2022 (slides)

- *Machine learning of physics theories*
  Alan Turing Institute, Machine Learning and Dynamical Systems Seminar, December, 2021

- *Graph Information Bottleneck*
  Beijing Academy of Artificial Intelligence (BAAI), October, 2021

- *Machine learning of physics theories and its universal tradeoff between accuracy and simplicity*
  [Workshop on Artificial Scientific Discovery 2021](#), June, 2021, ([video](#)), ([slides](#))
- *Machine Learning of Physics Theories*
  Summer school at Max Planck Institute for the Science of Light, April, 2021
- *Phase transitions on the tradeoff between prediction and compression in machine learning*
  Stanford Computer Science ML lunch, June, 2022
- *Learning to accelerate the simulation of PDEs*
  [CLARIPHY Topical Meetings](#), *March, 2021*
- *Machine Learning of Physics Theories*
  [Seminar Series of SJTU Institute of Science](#), February, 2021
- *Phase transitions on the universal tradeoff between prediction and compression in machine learning*
  [Math Machine Learning seminar MPI MIS + UCLA](#), February, 2021
- *Machine learning of physics theories and its universal tradeoff between accuracy and simplicity*
  Los Alamos National Laboratory, October, 2020
- *Phase transitions for the information bottleneck*
  Secure Learning Lab at Department of Computer Science, UIUC, February, 2020
- *Toward an AI Physicist for Unsupervised Learning*
  Poster presentation at the inauguration of MIT Stephen Schwarzman College of Computing, February, 2019

Workshop Organizing:

[NeurIPS 2024 Safe Generative AI Workshop](#)
- Co-organizer and program chair

[ICLR 2021 Deep Learning for Simulation Workshop (simDL)](#)
- Lead organizer and program chair

REVIEWERS FOR JOURNALS AND CONFERNCES

Journals:
- Proceedings of the National Academy of Sciences (PNAS)
- Nature Machine Intelligence
- Nature Communications
- Nature Scientific Reports
- Science Advances
- Neural Computation
- Patterns (by Cell Press)
- iScience (by Cell Press)
- IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)
- IEEE Transactions on Audio, Speech and Language Processing (T-ASL)
- IEEE Transactions on Network Science and Engineering
- IEEE Signal Processing Letters
- IEEE International Symposium on Information Theory (ISIT)
- Journal of Petroleum Science and Engineering
- Patterns
- Physica D

Conferences:
- NeurIPS 2024, NeurIPS 2022, NeurIPS 2021, NeurIPS 2020

- ICML 2024, ICML 2023, ICML 2022, ICML 2021, ICML 2020
- ICLR 2024, ICLR 2023, ICLR 2022
- SIGKDD 2023, SIGKDD 2022
- AAAI 2024
- SIAM 2024 International Conference on Data Mining (SDM'24)
- TMLR
- Learning on Graph Conference 2022, 2024

EXPERIENCES

Stanford Network Analysis Project (SNAP) lab
1/2020 – Present
Postdoctoral scholar (advisor: Jure Leskovec)
Stanford, Palo Alto, CA
- Developed machine learning methods to accelerate large-scale simulations, and developed method to improve representation learning on graphs. Led collaborations with Stanford National Accelerator Laboratory for multi-scale laser-plasma simulations, and with Aramco for large-scale subsurface fluid simulations.

Department of Physics, MIT
9/2012 – 11/2019
Ph.D. Candidate (advisors: Isaac Chuang, Max Tegmark)
MIT, Cambridge, MA
- Thesis research on Machine learning + Physics: (1) ML $\Rightarrow$ Physics: developed machine learning techniques for discovering governing laws and relational structures of a system; (2) Physics $\Rightarrow$ ML: theoretically studied the compression vs. prediction tradeoff in representation learning.

Google AI
6/2019 – 8/2019
Research Intern (advisor: Ian Fischer)
Google, Mountain View, CA
- Theoretically studied the prediction-compression tradeoff and phase transitions of Information Bottleneck (IB) for representation learning, and showed how it can help reveal the structure of the learning problem (published in ICLR 2020).

NVIDIA Research
6/2018 – 8/2018
Research Intern (advisors: Thomas Breuel, Jan Kautzin)
NVIDIA, Santa Clara, CA
- Introduced a method to learn causal relations from observational time series, demonstrated its scalability for nonlinear, complex time series (ICML 2019 Time Series Workshop, Best Poster Award).

Department of Physics, MIT and MIT-Harvard Center for Ultracold Atoms
9/2012 – 1/2016
Research assistant on quantum computing (advisor: Isaac Chuang)
MIT, Cambridge, MA
- Participated in building the setup that strongly couples photons and atomic ions for enabling networks of quantum computing nodes. Introduced a method for solving the long-standing problem of vacuum-induced optical losses in high-finesse cavities.

TEACHING

- **Teacher,** *Frontiers in Computer Science and Technology* (for PhD students at Westlake University), 2024 Spring.
  Course website: ai4s.lab.westlake.edu.cn/course
- **Guest Lecturer**, *AI Physicist and Machine Learning for Simulations*, for Caltech CS159: Advanced Topics in Machine Learning, April, 2022.
- **Teaching Assistant,** MIT 8.01: *Classical Mechanics*, responsible developing part of the online interactive sessions for providing additional materials and automatic grading, and in-person tutoring, September to December, 2016.
- **Teaching Assistant,** MIT 8.02: *Electricity and Magnetism*, responsible developing part of the online interactive sessions for providing additional materials and automatic grading, and in-person tutoring, February to May, 2017.

SKILLS

- **Proficient in Python & PyTorch: written over 300,000 lines of high-quality code in my projects. Selected open-sourced projects:**
  - CinDM (ICLR 2024 spotlight): https://github.com/AI4Science-WestlakeU/cindm
  - LAMP (ICLR 2023 spotlight): https://github.com/snap-stanford/lamp
  - LE-PDE (NeurIPS 2022): https://github.com/snap-stanford/le_pde
  - ZeroC (NeurIPS 2022): https://github.com/snap-stanford/zeroc
  - GIB (NeurIPS 2020): https://github.com/snap-stanford/GIB
  - AI Physicist (Physical Review E): https://github.com/tailintalent/AI_physicist
  - Causal Learning (ICML 2019 workshop): https://github.com/tailintalent/causal
  - Pytorch_net Library: https://github.com/tailintalent/pytorch_net
- **Proficient in developing:**
  - Graph neural networks, energy-based models, and building training pipelines (for supervised and reinforcement learning).
  - Have experience in multi-GPU training and inference for Graph Neural Networks (over millions of nodes per time step)

SERVICE

- **Mentor,** Stanford CS undergraduate mentoring program for students from underrepresented backgrounds, 2021.
- **Mentor,** Stanford summer undergraduate research program.
- **Program committee**, ICLR 2021 Deep Learning for Simulation Workshop (simDL), 2021.
- **Co-president**, MIT Chinese Student and Scholar Association, 2015-2016.
- **Executive board member**, MIT Chinese Student and Scholar Association, 2014-2016.