

# TAILIN WU

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Department of Computer Science ◇ Stanford University

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## EDUCATION

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### Postdoctoral Scholar in Computer Science

1/2020 – Present

Stanford University, Palo Alto, CA

Advisor: Jure Leskovec

### Ph.D. in Physics

9/2012 – 11/2019

Massachusetts Institute of Technology, Cambridge, MA

Advisors: Isaac Chuang, Max Tegmark

### Research: Machine Learning + Physics

Thesis: [Intelligence, physics and information – the tradeoff between accuracy and simplicity in machine learning](#)

### B.S. in Physics

9/2008 – 7/2012

Peking University, Beijing, China

GPA: 3.83/4.00, top 3% out of 194 students

## RESEARCH INTERESTS

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My research vision is to develop machine learning (ML) methods for accelerating large-scale scientific simulation and discovery, while opening new frontiers in machine learning research (**ML + 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., mechanical design, molecular design). Third, develop *knowledge-grounded and generalizable representations* for scientific discovery.

## SELECTED AWARDS AND RECOGNITIONS

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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*.

Best Poster Award for the paper “[Discovering Nonlinear Relations with Minimum Predictive Information Regularization](#)” at [ICML 2019 Time Series Workshop](#).

Cover issue for the paper “[Pareto-optimal data compression for binary classification tasks](#)” in *Entropy*.

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

Chinese National Undergraduate Endowment for Innovational Research, 2010

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

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### Machine Learning for Simulation and Discovery:

[1] [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](#)).

[2] [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](#)).

[3] [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](#)).

[4] [T. Wu](#)<sup>\*</sup>, T. Maruyama<sup>\*</sup>, Q. Zhao<sup>\*</sup>, G. Wetzstein, J. Leskovec, “Learning Controllable Adaptive Simulation for Multi-resolution Physics.” ICLR 2023, **spotlight** ([pdf](#)). Also accepted in NeurIPS 2022 AI4Science workshop, ([workshop pdf](#)), ([poster](#)).

[5] [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 in KDD 2023, ([pdf](#)). Also accepted in NeurIPS 2022 AI4Science workshop, ([workshop pdf](#)), ([poster](#)).

[6] 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](#).

[7] [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](#)).

[8] S. M. Udrescu, A. Tan, J. Feng, O. Neto, [T. Wu](#), 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](#)).

[9] [T. Wu](#), 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](#)).

[10] D. Zeng<sup>\*</sup>, [T. Wu](#)<sup>\*</sup>, 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](#)).

[11] M. Skuhersky, T. Wu, 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:

[12] T. Wu<sup>\*</sup>, H. Ren<sup>\*</sup>, P. Li, J. Leskovec, "Graph Information Bottleneck." In *34th Neural Information Processing Systems* (NeurIPS 2020a). ([paper](#)), ([project page](#)), ([code](#)).

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

[14] T. Wu, 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".

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

[16] C. Northcutt<sup>\*</sup>, T. Wu<sup>\*</sup>, 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](#)).

[17] T. Wu, 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<sup>\*</sup>, M. Shi<sup>\*</sup>, T. Wu<sup>\*</sup>, 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, T. Wu, 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, T. Wu, 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, T. Wu, Z. He, L. Jiang, C. Luo, Y. Tu, "Frequency-Dependent *Escherichia coli* Chemotaxis Behavior." *Physical Review Letters*, 108, 128101 (2012).

## INVITED TALKS AND PRESENTATIONS

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- *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 Large-scale Subsurface Simulations with a Hybrid Graph Network Simulator*  
Stanford HAI Climate-Centered AI Affinity Group, January, 2023.
- *Learning to accelerate simulation and inverse optimization of PDEs via latent global evolution*  
Stanford Computer Science ML lunch, June, 2022, ([slides](#))
- *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:**

[ICLR 2021 Deep Learning for Simulation Workshop \(simDL\)](#)

- Lead organizer and program chair

## **REVIEWERS FOR JOURNALS AND CONFERNCES**

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### **Journals:**

- Proceedings of the National Academy of Sciences (PNAS)
- Nature Machine Intelligence
- Nature Communications
- Science Advances
- Scientific Reports
- Neural Computation
- IEEE Signal Processing Letters
- IEEE International Symposium on Information Theory (ISIT)
- IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)
- IEEE Transactions on Network Science and Engineering
- Journal of Petroleum Science and Engineering
- Physica D
- MDPI Journals (Entropy, Algorithm)

### **Conferences:**

- NeurIPS 2022, NeurIPS 2021, NeurIPS 2020
- ICML 2022, ICML 2021, ICML 2020
- ICLR 2023, ICLR 2022

- SIGKDD 2022
- TMLR
- Learning on Graph Conference 2022

## EXPERIENCES

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**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).

## TEACHING

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- **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.

## SERVICE

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- **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.

## SKILLS

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- **Proficient in Python & PyTorch: written over 300,000 lines of high-quality code in my projects. Sample open-sourced projects:**
  - LE-PDE (NeurIPS 2022): [https://github.com/snap-stanford/le\\_pde](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](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](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)