

RYAN LIU

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EDUCATION

California Institute of Technology

September, 2025 - Present

Ph.D. in Physics. Advisor: Hsin-Yuan Huang.

University of California, Berkeley

August 2021 - May 2025

B.A., Physics and Computer Science, *Higest Distinction in General Scholarship*

GPA: 4.00/4.00

HONORS AND AWARDS

National Science Foundation Graduate Research Fellowship (NSF GRFP).

2025

Field of study: Physics and Astronomy; Artificial Intelligence

Highest Distinction in General Scholarship.

2025

College of Letters and Science and College of Computing, Data Science, and Society.

Gold Medal, European Physics Olympiad

2020

Ranked 15th internationally and 1st among the Taiwan National Team.

PUBLICATION

Ryan Liu, Eric Qu, Toby Kreiman, Sam Blau, Aditi S. Krishnapriyan. (2025). “From Evaluation to Design: Using Potential Energy Surface Smoothness Metrics to Guide Machine Learning Interatomic Potential Architectures” *Accepted to ICML 2026*.

Ryan Liu, Abhijith Gandrakota, Jennifer Ngadiuba, Maria Spiropulu, Jean-Roch Vlimant. (2023). “Fast Particle-based Anomaly Detection Algorithm with Variational Autoencoder” *Accepted to NeurIPS Machine Learning and the Physical Sciences Workshop 2023*.

Ryan Liu, Abhijith Gandrakota, Jennifer Ngadiuba, Maria Spiropulu, Jean-Roch Vlimant. (2023). “Efficient and Robust Jet Tagging at the LHC with Knowledge Distillation” *Accepted to NeurIPS Machine Learning and the Physical Sciences Workshop 2023*.

Ryan Liu, Paolo Calafiura, Steven Farrell, Xiangyang Ju, Daniel Thomas Murnane, Tuan Minh Pham (2023). “Hierarchical Graph Neural Networks for Particle Track Reconstruction” *Accepted to 21st International Workshop on Advanced Computing and Analysis Techniques in Physics Research*.

RESEARCH PROJECT

Wasserstein Data Synthesis Pipeline for Solver-Free Operator Learning

Caltech

September 2025 - Present

Proposed WaSP, a novel solver-free training framework for operator learning with applications in PDE. Showed negative theorems for existing solver-free training frameworks, including regularity-variance tradeoff for physics-informed learning and structural distribution shift for manufactured data.

Proved a step-wise error propagation bound for WaSP to motivate it theoretically.

Achieved uniformly improved accuracy over baselines and ablations on various PDE benchmarks.

From Evaluation to Design: Using Potential Energy Surface Smoothness Metrics to Guide MLIP Architectures

BAIR

May 2024 - July 2026

Proposed Bond Smoothness Characterization Test to evaluate potential energy surface smoothness.

Designed Minimally biased Differentiable Scalable Attention Interatomic Potential, “MinDScAIP”.

Proposed Diff-kNN algorithm and smoothness-oriented designs to improve physical soundness of MLIPs.

Achieved new state-of-the-art on SPICE MACE-OFF (molecules) and Matbench Discovery (materials).

Fast Anomaly Detection with Variational Autoencoder for CMS L1T

Caltech SURF, Fermilab

June 2023 - August 2023

Designed a decoding framework for particle-based autoencoders based on conditional VAE.

Proposed a training technique to facilitate encoder-only inference of anomaly detection with VAE.

Demonstrated a 2x improvement in signal efficiency compared with n-subjettiness.

Transfer Inductive Biases with Knowledge Distillation

Caltech SURF, Fermilab

June 2023 - August 2023

Showed knowledge distillation can improve the accuracy of a light-weight jet tagger.

Demonstrated knowledge distillation can improve robustness through inducing bias.

Hierarchical Graph Neural Networks for Particle Track Reconstruction

LBNL

April 2022 - October 2022

Designed and implemented a Hierarchical GNN for charged particle tracking.

Outperformed the graph segmentation algorithm in Exa.TrkX pipeline on the TrackML dataset.

Demonstrated superior robustness against graph construction inefficiency.

High Performance Graph Segmentation for ATLAS GNN Track Reconstruction

LBNL

May 2024 - October 2024

Analyzed failure modes of connected components as the graph segmentation algorithm.

Designed CC+JR algorithm that achieved three-fold faster inference and 0.9% efficiency improvement.

Simulation for Level-1 Trigger Foundation Model (COLLIDE-2V)

Fermilab

February 2024 - May 2024

R&D for generating a large event-level dataset supporting dual-view with fast simulation tools.

GRADUATE COURSEWORK

Caltech

Quantum Learning Theory, Foundation of Machine Learning

UC Berkeley

Deep Reinforcement Learning, Quantum Theory of Measurement, Theoretical Statistics

National Taiwan University (*through Precollege Program*)

Machine Learning, Quantum Information and Computation, General Relativity, Computational Physics