

Guan-Horng Liu

🌐 [ghliu.github.io](https://github.com/ghliu) • ✉ ghliu@meta.com • ✎ [guanhorng_liu](#)

RESEARCH INTERESTS

- **Generative AI:** post-training, reinforcement learning, large reasoning language models
- **AI for Science:** Boltzmann distribution, diffusion sampler, molecular generation
- **Physics/Control:** Schrödinger bridge, dynamic optimal transport, stochastic optimal control

RESEARCH EXPERIENCE

Fundamental AI Research (FAIR), Meta

Research Scientist

New York, NY
09/2024 – present

- Awards: NeurIPS 2025 Oral [acceptance rate: 0.3%]

Fundamental AI Research (FAIR), Meta

Research Scientist Intern

New York, NY
Summer 2023

- Mentor: Ricky T. Q. Chen

NVIDIA Research

Research Scientist Intern

Santa Clara, CA
Summer 2022

- Mentor: Weili Nie, Arash Vahdat, Anima Anandkumar

EDUCATION

Georgia Institute of Technology

Ph.D. in Machine Learning (GPA: 4.0/4.0)

Atlanta, GA
07/2024

- Advisor: Evangelos A. Theodorou
- Awards: ICLR 2025 Oral [1.8%], NeurIPS 2022 Oral [1.9%], NeurIPS 2021 Spotlight [3.0%], ICML 2021 Oral [3.0%], ICLR 2021 Spotlight [3.8%]

Carnegie Mellon University

M.S. in Robotics (GPA: 4.0/4.0)

Pittsburgh, PA
05/2017

- Advisor: George Kantor

Tokyo Institute of Technology

Research Exchange Program (GPA: 4.0/4.0)

Tokyo, Japan
06/2014

- Advisor: Edwardo F. Fukushima

National Taiwan University

B.S. in Mechanical Engineering (GPA: 3.99/4.0)

Taipei, Taiwan
06/2013

- Advisor: Pei-Chun Lin
- Awards: Graduated Cum Laude, Best Paper in IEEE/SICE ISS 2013 [0.8%]

Last update: 11/2025

PUBLICATIONS

(*Equal contribution *Core contributors †Equal advising ‡Alphabetical order)

Preprints

- [P1] Functional Adjoint Sampler: Scalable Sampling on Infinite Dimensional Spaces,
B. Park, J. Lee, **G.-H. Liu**,
2025.
- [P2] Enhancing Diffusion-Based Sampling with Molecular Collective Variables,
J. Nam*, B. Máté, A. P. Toshev, M. Kaniselman, R. Gómez-Bombarelli, Ricky T. Q. Chen, B.
Wood, **G.-H. Liu***, B. K. Miller*,
2025.

Conference Papers

- [C1] Adjoint Schrödinger Bridge Sampler **[Oral, 0.3%]**
G.-H. Liu*, J. Choi*, Y. Chen, B. K. Miller, Ricky T. Q. Chen*
Advances in Neural Information Processing Systems (NeurIPS), 2025
- [C2] Non-equilibrium Annealed Adjoint Sampler
J. Choi*, Y. Chen, M. Tao, **G.-H. Liu***
Advances in Neural Information Processing Systems (NeurIPS), 2025
- [C3] Momentum Multi-Marginal Schrödinger Bridge Matching
P. Theodoropoulos, A. D. Saravanos, E. Theodorou†, **G.-H. Liu**†
Advances in Neural Information Processing Systems (NeurIPS), 2025
- [C4] MDNS: Masked Diffusion Neural Sampler via Stochastic Optimal Control
Y. Zhu*, W. Guo*, J. Choi, **G.-H. Liu**, Y. Chen, M. Tao
Advances in Neural Information Processing Systems (NeurIPS), 2025
- [C5] Adjoint Sampling: Highly-Scalable Diffusion Samplers via Adjoint Matching
A. J. Havens*, B. K. Miller*, B. Yan*, C. Domingo-Enrich, A. Sriram, D. S. Levine, B. M. Wood,
B. Hu, B. Amos, B. Karrer, X. Fu*, **G.-H. Liu***, Ricky T. Q. Chen*
International Conference on Machine Learning (ICML), 2025
- [C6] Feedback Schrödinger Bridge Matching **[Oral, 1.8%]**
P. Theodoropoulos, N. Komianos, V. Pacelli, **G.-H. Liu**†, E. Theodorou†
International Conference on Learning Representations (ICLR), 2025
- [C7] Generalized Schrödinger Bridge Matching
G.-H. Liu, Y. Lipman, M. Nickel, B. Karrer, E. Theodorou, Ricky T. Q. Chen
International Conference on Learning Representations (ICLR), 2024
- [C8] A Robust Differential Neural ODE Optimizer
P. Theodoropoulos, **G.-H. Liu**, T. Chen, A. D. Saravanos, E. Theodorou
International Conference on Learning Representations (ICLR), 2024
- [C9] Mirror Diffusion Models for Constrained and Watermarked Generation
G.-H. Liu, T. Chen, E. Theodorou†, M. Tao†
Advances in Neural Information Processing Systems (NeurIPS), 2023
- [C10] Deep Momentum Multi-Marginal Schrödinger Bridge
T. Chen, **G.-H. Liu**, M. Tao, E. Theodorou
Advances in Neural Information Processing Systems (NeurIPS), 2023

- [C11] I²SB: Image-to-Image Schrödinger Bridge
G.-H. Liu, A. Vahdat, D.-A. Huang, E. Theodorou, W. Nie[†], A. Anandkumar[†]
International Conference on Machine Learning (ICML), 2023
- [C12] Deep Generalized Schrödinger Bridge **[Oral, 1.9%]**
G.-H. Liu, T. Chen*, O. So*, E. Theodorou
Advances in Neural Information Processing Systems (NeurIPS), 2022
- [C13] Likelihood Training of Schrödinger Bridge using Forward-Backward SDEs Theory
T. Chen*, **G.-H. Liu***, E. Theodorou
International Conference on Learning Representations (ICLR), 2022
- [C14] Second-Order Neural ODE Optimizer **[Spotlight, 3.0%]**
G.-H. Liu, T. Chen, E. Theodorou
Advances in Neural Information Processing Systems (NeurIPS), 2021
- [C15] Dynamic Game Theoretic Neural Optimizer **[Long talk, 3.0%]**
G.-H. Liu, T. Chen, E. Theodorou
International Conference on Machine Learning (ICML), 2021
- [C16] Differential Dynamic Programming Neural Optimizer **[Spotlight, 3.8%]**
G.-H. Liu, T. Chen, E. Theodorou
International Conference on Learning Representations (ICLR), 2021
- [C17] Variational Inference MPC using Tsallis Divergence
Z. Wang*, O. So*, J. Gibson, B. Vlahov, M. S. Gandhi, **G.-H. Liu**, E. Theodorou
Robotics: Science and Systems (RSS), 2021
- [C18] Learning End-to-end Multimodal Sensor Policies for Autonomous Navigation
G.-H. Liu, A. Siravuru, S. Prabhakar, M. Veloso, G. Kantor
Conference on Robot Learning (CoRL), 2017
- [C19] Autonomous Control of the WAM-V Catamaran Type USV: Propulsion System Design
G.-H. Liu, A. Y. Yasutomi, A. Holgado, E. F. Fukushima
Annual Conference of the Robotics Society of Japan, 2014
- [C20] Design of a Kangaroo Robot with Dynamic Jogging Locomotion **[Best Paper Award, 0.8%]**
G.-H. Liu, H.-Y. Lin, H.-Y. Lin, S.-T. Chen, P.-C. Lin
IEEE/SICE International Symposium on System Integration (ISS), 2013

Journal Papers

- [J1] Optimal Control Theoretic Neural Optimizer: From Backpropagation to Dynamic Programming
G.-H. Liu, T. Chen, E. Theodorou
Transactions on Pattern Analysis and Machine Intelligence (TPAMI), 2025
- [J2] Optimal Transport for Generating Transition States in Chemical Reactions
C. Duan*, **G.-H. Liu***, Y. Du*, T. Chen, Q. Zhao, H. Jia, C. P. Gomes, E. Theodorou, H. J. Kulik
Nature Machine Intelligence, 2025
- [J3] Improving Generative Model-based Unfolding with Schrödinger Bridges
S. Diefenbacher[‡], **G.-H. Liu[‡]**, V. Mikuni[‡], B. Nachman[‡], W. Nie[‡]
Physical Review D, 2024
- [J4] A Bio-Inspired Hopping Kangaroo Robot with an Active Tail
G.-H. Liu, H.-Y. Lin, H.-Y. Lin, S.-T. Chen, P.-C. Lin
Journal of Bionic Engineering, 2014

Workshop Papers & Technical Reports

- [W1] Large-Scale Optimization for DNN Architecture: A Dynamical System Theory
G.-H. Liu
Georgia Tech Machine Learning Ph.D. Thesis, 2024
- [W2] Augmented Bridge Matching
V. D. Bortoli, **G.-H. Liu**, T. Chen, E. Theodorou, W. Nie
Preprint, 2023
- [W3] Improved Sampling via Learned Diffusions
L. Richter*, J. Berner*, **G.-H. Liu**
ICML Workshop on New Frontiers in Learning, Control, Dynamical Systems, 2023
- [W4] Spatio-Temporal Differential Dynamic Programming for Control of Fields
E. N. Evans, O. So, A. P. Kendall, **G.-H. Liu**, E. Theodorou
Preprint, 2021
- [W5] Deep Learning Theory Review: An Optimal Control and Dynamical Systems Perspective
G.-H. Liu, E. Theodorou
Preprint, 2019
- [W6] High Dimensional Planning and Learning for Off-Road Driving
G.-H. Liu
CMU Robotics Institute Master Thesis, 2017

PATENTS

Conditional Diffusion Model for Data-to-Data Translation

U.S. Patent Application No. 18/431,527 08/2024

HONORS & AWARDS

Fellowships & Scholarships

AE Graduate Research Fellowship, Georgia Tech 2022 – 2023
Study Abroad Scholarship, Ministry of Education, Taiwan 2019 – 2021
Student Exchange Scholarship, JASSO, Japan 2013

Awards & Prizes

Best Paper Award, IEEE/SICE ISS 2013
Third Prize, Chuian-Yan Thesis Paper Competition, Taiwan 2013
Presidential Awards ($\times 4$), Top 5% in National Taiwan University 2009 – 2014

PRESS COVERAGE

Meta AI Blog: A breakthrough in highly scalable, reward-driven generative modeling 05/2025
Chemistry World: AI predicts transition states with exceptional precision 05/2025
MIT News: New model predicts a chemical reaction’s point of no return 04/2025
Nature Machine Intelligence: Cover photo on Volume 7 Issue 4 04/2025

INVITED TALKS

Sampling with Schrödinger Bridge: An Adjoint-Matching Perspective

NeurIPS (Oral talk, 0.3%)	12/2025
Princeton University, Princeton Center of Theoretical Science	11/2025
International Seminar on Monte Carlo Methods	11/2025
Flatiron Institute, Center for Computational Mathematics	08/2025
Microsoft Research, Generative Modeling & Sampling Seminar	07/2025

Learning Scalable Diffusion Models using Optimality and Constraint Structures

Learning on Graphs NYC Meetup	11/2024
CS5785 Applied Machine Learning, Cornell Tech (Host: Brandon Amos)	09/2024
AMLab, University of Amsterdam	05/2024
Sony AI	04/2024
National Taiwan University (Host: Shao-Hua Sun)	04/2024
Appier Group Inc.	01/2024
School of Industrial and Systems Engineering, Georgia Tech (Host: Yao Xie)	12/2023
FAIR, Meta AI	11/2023
Nvidia Research	10/2023

Mirror Diffusion Models

Learning on Graphs and Geometry Reading Group	10/2023
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(Generalized) Schrödinger Bridge

AE8803 Optimal Transport Theory & Applications, Georgia Tech (Host: Yongxin Chen) ...	04/2025
Learning on Graphs and Geometry Reading Group	02/2023
NeurIPS Workshop on Score-Based Methods	12/2022
Rough Path Interest Group, Alan Turing Institute	11/2022
IBM Research Seminar	11/2022
School of Mathematics, Georgia Tech (Host: Molei Tao)	11/2021

Optimal Control Theoretic Neural Optimizer

AE4803 Robotic Systems and Autonomy, Georgia Tech (guest lecture)	10/2022
Rough Path Interest Group, Alan Turing Institute	12/2021
Machine Learning PhD Seminar, Georgia Tech (contributed talk)	10/2021
NeurIPS Workshop on Optimization for Machine Learning (spotlight talk)	12/2020

ACADEMIC SERVICES

Co-organizer:	NeurIPS 2025 Workshop on Frontiers in Probabilistic Inference: Sampling Meets Learning ICML 2024 Workshop on Structured Probabilistic Inference & Generative Modeling ICML 2023 Workshop on New Frontiers in Learning, Control, and Dynamical Systems
Area Chair:	NeurIPS 2023 Workshop on AI for Scientific Discovery: From Theory to Practice
Reviewer:	ICLR (2024 – 2025), ICML (2023 – 2025), NeurIPS (2023 – 2025), L4DC (2023 – 2024), IJCAI (2024), AISTATS (2025)

MENTORSHIP

Oswin So , Massachusetts Institute of Technology	05/2025 – present
Byoungwoo Park , Korea Advanced Institute of Science & Technology	06/2025 – present
Jaemoo Choi , Georgia Tech (NeurIPS×1)	01/2025 – present
Panagiotis Theodoropoulos , Georgia Tech (NeurIPS×1, ICLR×2)	09/2023 – 07/2025