

# Guan-Horng Liu

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## 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

### Meta Superintelligence Labs

*Research Scientist*

Menlo Park, CA

09/2024 – present

- RL/Science in post-training LLMs.
- Reward-driven Diffusion sampler (NeurIPS 2025 Oral [accept rate: 0.3%]).

### Meta FAIR Labs

*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

- 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

### Tokyo Institute of Technology

*Research Exchange Program (GPA: 4.0/4.0)*

Tokyo, Japan

06/2014

### National Taiwan University

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

Taipei, Taiwan

06/2013

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

*Last update: 02/2026*

## PUBLICATIONS

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

### Preprints

- [P1] Discrete Adjoint Schrödinger Bridge Sampler  
W. Guo\*, Y. Zhu\*, X. Du\*, J. Nam\*, Y. Chen†, R. Gomez-Bombarelli†, **G.-H. Liu†**, M. Tao†, J. Choi\*  
2025
- [P2] Functional Adjoint Sampler: Scalable Sampling on Infinite Dimensional Spaces  
B. Park, J. Lee, **G.-H. Liu**  
2025

### Conference Papers

- [C1] Discrete Adjoint Matching  
O. So\*, B. Karrer\*, C. Fan, Ricky T. Q. Chen\*, **G.-H. Liu\***  
*International Conference on Learning Representations (ICLR)*, 2025
- [C2] 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\*  
*International Conference on Learning Representations (ICLR)*, 2025
- [C3] 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
- [C4] Non-equilibrium Annealed Adjoint Sampler  
J. Choi\*, Y. Chen, M. Tao, **G.-H. Liu\***  
*Advances in Neural Information Processing Systems (NeurIPS)*, 2025
- [C5] Momentum Multi-Marginal Schrödinger Bridge Matching  
P. Theodoropoulos, A. D. Saravanos, E. Theodorou†, **G.-H. Liu†**  
*Advances in Neural Information Processing Systems (NeurIPS)*, 2025
- [C6] 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
- [C7] 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
- [C8] 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
- [C9] 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
- [C10] 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

- [C11] Mirror Diffusion Models for Constrained and Watermarked Generation  
**G.-H. Liu**, T. Chen, E. Theodorou<sup>†</sup>, M. Tao<sup>†</sup>  
*Advances in Neural Information Processing Systems (NeurIPS)*, 2023
- [C12] Deep Momentum Multi-Marginal Schrödinger Bridge  
T. Chen, **G.-H. Liu**, M. Tao, E. Theodorou  
*Advances in Neural Information Processing Systems (NeurIPS)*, 2023
- [C13] I<sup>2</sup>SB: Image-to-Image Schrödinger Bridge  
**G.-H. Liu**, A. Vahdat, D.-A. Huang, E. Theodorou, W. Nie<sup>†</sup>, A. Anandkumar<sup>†</sup>  
*International Conference on Machine Learning (ICML)*, 2023
- [C14] Deep Generalized Schrödinger Bridge [Oral, 1.9%]  
**G.-H. Liu**, T. Chen\*, O. So\*, E. Theodorou  
*Advances in Neural Information Processing Systems (NeurIPS)*, 2022
- [C15] Likelihood Training of Schrödinger Bridge using Forward-Backward SDEs Theory  
T. Chen\*, **G.-H. Liu**\*, E. Theodorou  
*International Conference on Learning Representations (ICLR)*, 2022
- [C16] Second-Order Neural ODE Optimizer [Spotlight, 3.0%]  
**G.-H. Liu**, T. Chen, E. Theodorou  
*Advances in Neural Information Processing Systems (NeurIPS)*, 2021
- [C17] Dynamic Game Theoretic Neural Optimizer [Oral, 3.0%]  
**G.-H. Liu**, T. Chen, E. Theodorou  
*International Conference on Machine Learning (ICML)*, 2021
- [C18] Differential Dynamic Programming Neural Optimizer [Spotlight, 3.8%]  
**G.-H. Liu**, T. Chen, E. Theodorou  
*International Conference on Learning Representations (ICLR)*, 2021
- [C19] 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
- [C20] 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
- [C21] 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
- [C22] 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)*, 2026
- [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<sup>‡</sup>, **G.-H. Liu**<sup>‡</sup>, V. Mikuni<sup>‡</sup>, B. Nachman<sup>‡</sup>, W. Nie<sup>‡</sup>  
*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 (×4), Top 5% in National Taiwan University ..... 2009 – 2014

## PRESS COVERAGE

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

## INVITED TALKS

### **Sampling with Schrödinger Bridge: An Adjoint-Matching Perspective**

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 – 2026), NeurIPS (2023 – 2025), L4DC (2023 – 2024), IJCAI (2024), AISTATS (2025)

## MENTORSHIP

<b>Byoungwoo Park</b> , KAIST (Preprint×1) .....	06/2025 – 01/2026
<b>Oswin So</b> , MIT (ICLR×1) .....	05/2025 – 12/2025
<b>Jaemoo Choi</b> , Georgia Tech (NeurIPS×1) .....	01/2025 – 08/2025
<b>Panagiotis Theodoropoulos</b> , Georgia Tech (NeurIPS×1, ICLR×2) .....	09/2023 – 07/2025