

# CHAORAN CHENG

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## EDUCATION

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**Ph.D. Candidate in Computer Science, University of Illinois Urbana-Champaign** IL, US  
Computer Science, The Grainger College of Engineering Aug. 2021 – present

**B.S. in Computer Science, Peking University** Beijing, China  
School of Electronics Engineering and Computer Science Sept. 2018 – July 2021  
- *Turing Class*, with degree *summa cum laude*

**Peking University** (transferred to new college) Beijing, China  
College of Chemistry and Molecular Engineering Sept. 2017 – Aug. 2018

## RESEARCH EXPERIENCE

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**University of Illinois Urbana-Champaign** IL, US  
Ph.D. candidate of Professor [Ge Liu](#) Aug. 2021 – present

- Geometric Deep Learning for Biomolecules. Combining amino acid sequence information, three-dimensional coordinate information, and phylogenetic information to build a large-scale model on protein structure prediction.
- Generative Modeling in Biological Domains. Extending generative models to both the continuous and discrete modalities for biological applications including protein structure-sequence co-design.

**Peking University**, Institute of Network Computing and Information Systems Beijing, China  
Research Assistant to Professor [Ming Zhang](#) May 2020 – June 2021

## TEACHING & OTHER RESEARCH ACTIVITY

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**Teaching Assistant**, for UIUC CS 444, *Deep Learning for Computer Vision*, Fall 2023  
**Workflow Chair**, for NeurIPS GLFrontiers Workshop 2023

## WORK EXPERIENCE

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**Amazon AWS AI** San José, CA, USA  
Applied Scientist Intern under Dr. [Bernie Wang](#) May 2024 – Aug. 2024

**Microsoft Research AI4Science** Beijing, China  
Research Intern under Dr. [Tong Wang](#) May 2023 – Jan. 2024  
Developed the [AI2BMD](#) framework for protein molecular dynamics simulation with *ab initio* accuracy.

## SELECTED PUBLICATION

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Gradient-Free Generation for Hard-Constrained Systems  
**Chaoran Cheng**, Boran Han, Danielle C. Maddix, Abdul Fatir Ansari, Andrew Stuart, Michael W. Mahoney, Bernie Wang, *ICLR 2025*

Training Free Guided Flow-Matching with Optimal Control  
Luran Wang, **Chaoran Cheng**, Yizhen Liao, Yanru Qu, Ge Liu, *ICLR 2025*

Online Reward-Weighted Fine-Tuning of Flow Matching with Wasserstein Regularization  
Jiajun Fan, Shuaike Shen, **Chaoran Cheng**, Yuxin Chen, Chumeng Liang, Ge Liu, *ICLR 2025*

Ab initio characterization of protein molecular dynamics with AI2BMD  
Tong Wang, Xinheng He, Mingyu Li, Yatao Li, Yusong Wang, Ran Bi, **Chaoran Cheng**, Xiangzhen Shen, Jiawei Meng, He Zhang, Bin Shao, Haiguang Liu, Zun Wang, Shaoning Li, Tie-Yan Liu, *Nature*

Categorical Flow Matching on Statistical Manifolds  
**Chaoran Cheng**, Jiahao Li, Jian Peng, Ge Liu, *NeurIPS 2024*

Neural P<sup>3</sup>M: A Long-Range Interaction Modeling Enhancer for Geometric GNNs

Yusong Wang, **Chaoran Cheng**, Shaoning Li, Yuxuan Ren, Bin Shao, Ge Liu, Pheng-Ann Heng, Nanning Zheng, *NeurIPS 2024*

Gradient-Free Generation for Hard-Constrained Systems

**Chaoran Cheng**, Boran Han, Danielle C. Maddix, Abdul Fatir Ansari, Andrew Stuart, Michael W. Mahoney, Bernie Wang, *under peer review, 2024*

Training Free Guided Flow-Matching with Optimal Control

Luran Wang, **Chaoran Cheng**, Yizhen Liao, Yanru Qu, Ge Liu, *under peer review, 2024*

Full-Atom Peptide Design based on Multi-modal Flow Matching

Jiahao Li, **Chaoran Cheng**, Zuofan Wu, Ruihan Guo, Shitong Luo, Zhizhou Ren, Jian Peng, Jianzhu Ma, *ICML 2024*

Equivariant Neural Operator Learning with Graphon Convolution

**Chaoran Cheng**, Jian Peng, *NeurIPS 2023 (Spotlight)*

Equivariant Point Set Analysis via Learning Orientations for Message Passing

Shitong Luo, Jiahao Li, Jiaqi Guan, Yufeng Su, **Chaoran Cheng**, Jian Peng, Jianzhu Ma, *CVPR 2022*

#### ADDITIONAL INFORMATION

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**Languages:** Mandarin (native), German (novice)

**Computer Skills:** Python and PyTorch (skillful); C and C++ (skillful); JavaScript, CSS, and HTML (familiar)

**Interests:** Art and music, passed Tenth Grade (the highest grade of an amateur) of the piano