Nabin Giri

Berkeley, CA

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Revised :   August 2, 2025

EDUCATION

University of Missouri
Ph.D. in Computer Science, Minor in Statistics
January 2021 – May 2025
Columbia, MO

Emphasis: *Deep Learning and Structural Biology*

Dissertation: *Deep Learning for Modeling Protein Atomic Structures from cryo-EM Density Maps*

Summer Schools: *Oxford Machine Learning & London Geometry and Machine Learning*   *2022, 2023*

Seminar: *Preparing Future Faculty Seminar (Spanned one academic semesters)*   *2024*

University of Central Missouri
Masters of Science in Computer Science - Thesis Track
May 2018 – May 2020
Warrensburg, MO

Workshop: *Graduate Research Workshop Series (Spanned one academic semester)*

Thesis: *Recommendation System Using Factorization Model and MapReduce Framework*

Bangalore University
Bachelors of Computer Application - First Class Honors
May 2011 – May 2014
Bangalore, India

Semester Projects: *Supermarket Management System & Online Admission System*

EXPERIENCE

Lawrence Berkeley National Laboratory
Machine Learning Postdoctoral Scholar
June 2025 – Present
Berkeley, CA

University of Missouri
Graduate Researcher at Bioinformatics and Machine Learning Lab
January 2021 – May 2025
Columbia, MO

Amazon.com Inc.
Applied Scientist II Intern
May 2024 – August 2024
Seattle, WA

BIOVIA - Dassault Systèmes
Scientific Software Development Intern
May 2023 – August 2023
San Diego, CA

University of Central Missouri
Graduate Student Worker (GSW) - James C Kirkpatrick Library
May 2018 – May 2020
Warrensburg, MO

Max International
System Engineer, Head of Department
March 2017 – April 2018
Kathmandu, Nepal

Capgemini
Software Engineer
October 2014 – October 2016
Bangalore, India

TEACHING

Machine Learning for Biomedical Informatics
Course Level: CMP_SC 8180 (INFOINST 8880)
Spring 2024
University of Missouri

PUBLICATIONS (First-author papers numbered in red.)

- [13] **A labeled dataset for AI-based cryo-EM map enhancement.** **Nabin Giri**, Xiao Chen, Liguo Wang, and Jianlin Cheng. *Computational and Structural Biotechnology Journal. 2025.*

- [12] **Atomic Protein Structure Modeling from Cryo-EM Using Multi-Modal Deep Learning and AlphaFold3.** **Nabin Giri** and Jianlin Cheng. bioRxiv *2025.*

- [11] **Protein-Ligand Structure and Affinity Prediction in CASP16 Using a Geometric Deep Learning Ensemble and Flow Matching.** Alex Morehead, Jian Liu, Pawan Neupane, **Nabin Giri** and Jianlin Cheng. *Proteins: Structure, Function, and Bioinformatics, 2025.*

- [10] **De novo atomic protein structure modeling for cryoEM density maps using 3D transformer and HMM.** **Nabin Giri** and Jianlin Cheng. *Nature Communication, 2024.*

- [9] **Cryo2StructData: A Large Labeled Cryo-EM Density Map Dataset for AI-based Modeling of Protein Structures.** **Nabin Giri**, Liguo Wang, and Jianlin Cheng. *Nature Scientific Data, 2024. Dataset available in* **Harvard Dataverse.**

- [8] **Outcomes of the EMDataResource cryo-EM Ligand Modeling Challenge.** Catherine L. Lawson, Andriy Kryshtafovych, Grigore D. Pintilie, Stephen K. Burley,. . ., **Nabin Giri**,. . ., Helen M. Berman, and Wah Chiu. *Nature Methods, 2024.*

- [7] **Deep Learning for Protein-Ligand Docking: Are We There Yet?** Alex Morehead, **Nabin Giri**, Jian Liu and Jianlin Cheng. *ICML AI4Science, 2024.*

- [6] **Impact of AlphaFold on Structure Prediction of Protein Complexes: The CASP15-CAPRI Experiment** Marc F. Lensink, Guillaume Brysbaert, Nessim Raouraoua,. . ., **Nabin Giri**,. . ., Sameer Velankar and Shoshana J. Wodak. *PROTEINS: Structure, Function, and Bioinformatics, 2023.*

- [5] **Combining pairwise structural similarity and deep learning interface contact prediction to estimate protein complex model accuracy in CASP15** Raj S. Roy, Jian Liu, **Nabin Giri**, Zhiye Guo and Jianlin Cheng. *PROTEINS: Structure, Function, and Bioinformatics, 2023. [Ranked First in CASP15]*

- [4] **Deep learning for reconstructing protein structures from cryo-EM density maps: recent advances and future directions** **Nabin Giri**, Raj S. Roy, and Jianlin Cheng. *Current Opinion in Structural Biology, 2023.*

- [3] **Improving Protein-Ligand Interaction Modeling with cryo-EM Data, Templates, and Deep Learning in 2021 Ligand Model Challenge** **Nabin Giri** and Jianlin Cheng. *Biomolecules, 2023.*

- [2] **DRLComplex: Reconstruction of protein quaternary structures using deep reinforcement learning** Elham Soltanikazemi, Raj S. Roy, Farhan Quadir, **Nabin Giri**, Alex Morehead, and Jianlin Cheng. *The International Conference on Intelligent Biology and Medicine (ICIBM), 2022.*

- [1] **High-Performance Deep Learning Toolbox for Genome-Scale Prediction of Protein Structure and Function** Mu Gao, Peik Lund-Andersen, .., **Nabin Giri**,. . ., Jianlin Cheng and Ada Sedova. *IEEE/ACM Workshop on Machine Learning in High Performance Computing Environments (MLHPC), 2021.*

AWARDS

Outstanding PhD Student Award	**2025**
College of Engineering	*University of Missouri*
Graduate Research Award	**2020**
Graduate Education and Research	*University of Central Missouri*
Graduate Housing Scholarship	**2020**
Webb Housing	*University of Central Missouri*
Conference Scholarship - Gold Pass	**2019**
Strata Data Conference	*O'Reilly Media, Inc*
Microsoft Partner Meet	**2018**
Ranked 2nd out of 15 participants in the competition	*Microsoft Partner Meet Nepal*

SERVICE

The Protein Journal
Manuscript Reviewer   *2025 - Present*

GigaScience
Manuscript Reviewer   *2025 - Present*

International Journal of Biological Macromolecules
Manuscript Reviewer   *2024 - Present*

Neural Information Processing Systems (NeurIPS)
Manuscript Reviewer   *2023 - Present*

IEEE International Conference on Bioinformatics and Biomedicine (BIBM)
Program Committee and Manuscript Reviewer   *2023 - 2025*

Briefings in Bioinformatics
Manuscript Reviewer   *2022 - Present*

IEEE/ACM Transactions on Computational Biology and Bioinformatics
Manuscript Reviewer   *2022 - Present*

Undergraduate Research Forum   **University of Missouri (MU)**
Research Abstract Reviewer   *2022*

Upsilon Pi Epsilon-Gamma Chapter   **University of Missouri (MU)**
Member   *2021 - Present*

MU Nepalese Student Association   **University of Missouri (MU)**
Member   *2021 - Present*

Nepalese UCM Association   **University of Central Missouri (UCM)**
President   *2018 - 2020*

Association for Computing Machinery (ACM) **University of Central Missouri (UCM)**
Member   *2018 - 2019*

International Student Services   **University of Central Missouri (UCM)**
International Students Ambassador   *2018 - 2019*

INVITED TALKS AND PRESENTATIONS

Modeling Atomic Structures from Cryo-EM Maps   **2025**
Phenix Group, Lawrence Berkeley National Laboratory   *Virtual*

Modeling Atomic Structures from Cryo-EM Maps   **2025**
Dana–Farber Cancer Institute, Harvard Medical School   *Virtual*

Modeling Atomic Structures from Cryo-EM Maps   **2025**
Computational Biosciences Group, Lawrence Berkeley National Laboratory   *Berkeley, CA*

Modeling Atomic Structures from Cryo-EM Maps   **2025**
Artificial Intelligence Department, Brookhaven National Laboratory   *Upton, NY*

De novo Protein Structure Modeling for CryoEM using 3D Transformer & HMM   **2024**
Intelligent Systems For Molecular Biology (ISMB). Presented by Dr. Jianlin Cheng   *Montreal, Canada*

Deep Learning for Modeling Protein Atomic Structures from Cryo-EM Maps   **2024**
Department of Electrical Engineering and Computer Science   *University of Missouri*

Mizzou Tigers Summer Internship Experiences   **2024**
Electrical Engineering and Computer Science Graduate Student Association   *University of Missouri*

Cryo2Struct: AI-Based Modeling of 3D Atomic Structures from Cryo-EM Maps   **2024**
CryoEM Super Group, Department of Biochemistry   *University of Missouri*

Improving Relevance Prediction with Multimodal Models 2024
Amazon Science *Seattle, WA*

De Novo Protein Structure Modeling for Cryo-EM Maps Using 3D Transformer and HMM 2024
BIOVIA *Virtual*

Conformational Sampling with AlphaFold and Diffusion-Based Protein-Ligand Modeling 2024
BIOVIA *Virtual*

Cryo2StructData: Large Labeled Cryo-EM Dataset for AI-Based Protein Structure Modeling 2023
BIOVIA *Virtual*

Modeling Protein-Ligand interaction from cryo-EM data, Templates and Deep Learning 2021
Organized by EMDataResource, presented the work developed for the 2021 Ligand Model Challenge *Virtual*

Three Minute Thesis (3MT) 2020
Presented Master's Thesis Research *University of Central Missouri*

PRESS

Paving the way for new treatments
University of Missouri, College of Engineering. September, 2024

De novo atomic protein structure modeling for cryoEM density maps - Behind the Paper
Nature Portfolio Communities. July, 2024

Journey into Nabin Giri's BIOVIA Internship: Conformational Sampling with AlphaFold
BIOVIA. September, 2023

Mizzou team ranks first in category at CASP15 protein prediction competition **University of Missouri, College of Engineering. January, 2023**