Nabin Giri

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 Google Scholar

Revised: August 2, 2025

EDUCATION

University of Missouri January 2021 – May 2025

Ph.D. in Computer Science, Minor in Statistics

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)

University of Central Missouri May 2018 – May 2020

2024

Warrensburg, MO

Bangalore, India

Berkeley, CA

Columbia, MO

Seattle, WA

San Diego, CA

Warrensburg, MO

Spring 2024

Masters of Science in Computer Science - Thesis Track

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

Thesis: Recommendation System Using Factorization Model and MapReduce Framework

Bangalore University

May 2011 – May 2014

Bachelors of Computer Application - First Class Honors

Semester Projects: Supermarket Management System & Online Admission System

EXPERIENCE

Lawrence Berkeley National Laboratory

June 2025 – Present

Machine Learning Postdoctoral Scholar

University of Missouri January 2021 – May 2025

Graduate Researcher at Bioinformatics and Machine Learning Lab

Amazon.com Inc. May 2024 – August 2024

Applied Scientist II Intern

BIOVIA - Dassault Systèmes May 2023 – August 2023

 $Scientific\ Software\ Development\ Intern$

University of Central Missouri May 2018 – May 2020

Graduate Student Worker (GSW) - James C Kirkpatrick Library

Max International March 2017 – April 2018

System Engineer, Head of Department Kathmandu, Nepal

Capgemini October 2014 – October 2016

Software Engineer Bangalore, India

Software Brighteen

TEACHING

Machine Learning for Biomedical Informatics

Course Level: CMP_SC 8180 (INFOINST 8880) 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 2^{nd} out of 15 participants in the competition	$Microsoft\ Partner\ Meet\ Nepal$

SERVICE

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 Biomedic Program Committee and Manuscript Reviewer	cine (BIBM) 2023 - 2025
Briefings in Bioinformatics Manuscript Reviewer	2022 - Present
IEEE/ACM Transactions on Computational Biology and Bioinfo	formatics
Manuscript Reviewer	2022 - Present
Undergraduate Research Forum Research Abstract Reviewer	University of Missouri (MU) 2022
Upsilon Pi Epsilon-Gamma Chapter Member	University of Missouri (MU) 2021 - Present
MU Nepalese Student Association Member	University of Missouri (MU) 2021 - Present
Nepalese UCM Association President	University of Central Missouri (UCM) 2018 - 2020
Association for Computing Machinery (ACM) Member	University of Central Missouri (UCM) 2018 - 2019
International Student Services International Students Ambassador	University of Central Missouri (UCM) 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 Dana-Farber Cancer Institute, Harvard Medical School	2025 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 Artificial Intelligence Department, Brookhaven National Laboratory	$egin{array}{c} oldsymbol{2025} \ Upton,\ NY \end{array}$
De novo Protein Structure Modeling for CryoEM using 3D Trans	
Intelligent Systems For Molecular Biology (ISMB). Presented by Dr. Jianlin Ch	teng Montreal, Canada
Deep Learning for Modeling Protein Atomic Structures from Constitution of Electrical Engineering and Computer Science	ryo-EM Maps 2024 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	n Cryo-EM Maps 2024

 $University\ of\ Missouri$

 $CryoEM\ Super\ Group,\ Department\ of\ Biochemistry$

Improving Relevance Prediction with Multimodal Models	$\boldsymbol{2024}$
Amazon Science	Seattle, WA
De Novo Protein Structure Modeling for Cryo-EM Maps Using 3D Transformer and HM $BIOVIA$	IM 2024 Virtual
Conformational Sampling with Alpha Fold and Diffusion-Based Protein-Ligand Modeling $\it BIOVIA$	$egin{array}{c} oldsymbol{2024} \ Virtual \end{array}$
Cryo2StructData: Large Labeled Cryo-EM Dataset for AI-Based Protein Structure Mod $BIOVIA$	leling 2023 Virtual
Modeling Protein-Ligand interaction from cryo-EM data, Templates and Deep Learning Organized by EMDataResource, presented the work developed for the 2021 Ligand Model Challenge	
Three Minute Thesis (3MT)	2020
Presented Master's Thesis Research University of C	entral 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