Rajan Gyawali

Ph.D. candidate in Computer Science, University of Missouri, Columbia, MO
rgkg2@missouri.edu | rajangyawali.github.io | Google Scholar | github.com/rajangyawali | linkedin.com/in/rajangyawali

Research summary

Machine learning for noisy, label-scarce scientific data: multimodal deep learning and foundation-model adaptation, learning from scarce and unreliable supervision, benchmarks and evaluation, and self-improving LLM agents. Most work is in cryo-EM protein structure determination.

Education

2022 – May 2027 **Ph.D. in Computer Science**
University of Missouri, Columbia, MO
Advisor: Dr. Jianlin Cheng. Focus: deep learning, computational biology and bioinformatics. GPA 4.0. Expected May 2027.

2017 – 2019 **M.Sc. in Electronics and Communication Engineering**
Tribhuvan University, Kathmandu, Nepal
Specialization in information and communication, with distinction. Thesis: employee face recognition with region proposal networks and Faster R-CNN (96.0% accuracy on the ChokePoint dataset).

2012 – 2016 **B.E. in Electronics and Communication Engineering**
Himalaya College of Engineering, Tribhuvan University, Kathmandu, Nepal
With distinction. Final project: a brain-controlled wheelchair using a NeuroSky MindWave brain–computer interface.

Research experience

Jun – Aug 2026 **Applied Scientist II Intern**
Amazon, San Diego, CA
Built a training-free, self-evolving framework for URL-based scam and phishing detection, driven by adversarial self-play among four LLM agents: an attacker that synthesizes novel phishing pages and URL attack patterns, an oracle that certifies ground-truth labels, a detector, and a reflector that distills reusable detection strategies. Strategies learned from synthetic attacks transferred to real-world scam URLs and phishing pages, outperforming existing baselines on public and internal benchmarks without retraining while keeping false-positive rates low.

Aug 2022 – present **Graduate Research Assistant**
Bioinformatics and Machine Learning Lab, University of Missouri, Columbia, MO
MICA: multimodal atomic model building from cryo-EM maps and AlphaFold3 predictions; average TM-score of 0.93 on recently released high-resolution cryo-EM density maps. CryoSegNet: particle picking with the Segment Anything Model and an attention-gated U-Net, surpassing crYOLO and Topaz. CryoPPP and CryoVirusDB: expert-labeled benchmark datasets for particle picking. Contributions to CryoTransformer, CryoFSL, macromolecule identification in cryo-ET tomograms, and protein–ligand binding prediction with E(n)-equivariant graph neural networks. Distributed training with PyTorch DDP on multi-node, multi-GPU clusters (Slurm, LSF).

Publications **(* equal contribution)**

[1] Biplab Poudel, **Rajan Gyawali**, Ashwin Dhakal, Jianlin Cheng, D. Xu. CryoFSL: a few-shot learning framework for robust protein particle picking in cryo-EM micrographs. *Briefings in Bioinformatics*, 27(3), bbag285 (2026). doi:10.1093/bib/bbag285.

[2] **Rajan Gyawali**, Ashwin Dhakal, Liguo Wang, Jianlin Cheng. CryoVirusDB: An Annotated Dataset for AI-Based Virus Particle Identification in Cryo-EM Micrographs. *Viruses*, 18(2), 224 (2026). doi:10.3390/v18020224.

[3] Ashwin Dhakal*, **Rajan Gyawali***, J. Selvaraj*, Jianlin Cheng. AI tools for cryo-EM: Protein particle picking, density map enhancement, and atomic model building. *Progress in Molecular Biology and Translational Science*, 223, 71–113 (2026).

[4] **Rajan Gyawali**, Ashwin Dhakal, Jianlin Cheng. Multimodal deep learning integration of cryo-EM and AlphaFold3 for high-accuracy protein structure determination. *Communications Chemistry*, 8(1), 320 (2025). doi:10.1038/s42004-025-01718-5.

[5] Ashwin Dhakal*, **Rajan Gyawali***, Liguo Wang, Jianlin Cheng. Artificial intelligence in cryo-EM protein particle picking: recent advances and remaining challenges. *Briefings in Bioinformatics*, 26(1), bbaf011 (2025). doi:10.1093/bib/bbaf011.

[6] **Rajan Gyawali**, Ashwin Dhakal, Liguo Wang, Jianlin Cheng. CryoSegNet: accurate cryo-EM protein particle picking by integrating the foundational AI image segmentation model and attention-gated U-Net. *Briefings in Bioinformatics*, 25(4), bbae282 (2024). doi:10.1093/bib/bbae282.

[7] Ashwin Dhakal, **Rajan Gyawali**, Liguo Wang, Jianlin Cheng. CryoTransformer: a transformer model for picking protein particles from cryo-EM micrographs. *Bioinformatics*, 40(3), btae109 (2024). doi:10.1093/bioinformatics/btae109.

[8] F. He, Z. Yang, M. Gao, B. Poudel, N. S. E. S. Dhas, **R. Gyawali**, A. Dhakal, et al. Adapting Segment Anything Model (SAM) through prompt-based learning for enhanced protein identification in cryo-EM micrographs. *IEEE International Conference on Medical Artificial Intelligence (MedAI)*, 9–20 (2024).

[9] Ashwin Dhakal*, **Rajan Gyawali***, Liguo Wang, Jianlin Cheng. A large expert-curated cryo-EM image dataset for machine learning protein particle picking. *Scientific Data*, 10(1), 392 (2023). doi:10.1038/s41597-023-02280-2.

[10] Ashwin Dhakal*, **Rajan Gyawali***, Jianlin Cheng. Predicting protein–ligand binding structure using E(n) equivariant graph neural networks. *bioRxiv*, 2023.08.06.552202 (2023). doi:10.1101/2023.08.06.552202.

[11] **Rajan Gyawali**, Dibakar Raj Pant. An Approach for the Employee Face Recognition by RPN and Faster R-CNN Techniques. *Proceedings of IOE Graduate Conference*, 2019-Summer, 6, 231–237 (2019).

Software and datasets

MICA	Automated atomic model building from cryo-EM maps and AlphaFold3 predictions. github.com/jianlin-cheng/MICA
CryoSegNet	Protein particle picking with SAM and an attention-gated U-Net. github.com/jianlin-cheng/CryoSegNet
CryoTransformer	Particle picking with a ResNet and transformer detector. github.com/jianlin-cheng/CryoTransformer
CryoPPP	Benchmark of 9,893 labeled micrographs from 34 EMPIAR protein datasets. github.com/BioinfoMachineLearning/cryoppp
CryoVirusDB	Labeled virus particles in 9,941 cryo-EM micrographs. github.com/BioinfoMachineLearning/CryoVirusDB

Teaching and mentoring

2026 – present **Undergraduate research mentor**
Bioinformatics and Machine Learning Lab, University of Missouri
Mentors undergraduate researchers in deep learning–based image segmentation.

2016 – 2022 **Instructor of record (Assistant Lecturer, Lecturer, Adjunct Lecturer)**
Himalaya College of Engineering, Tribhuvan University, Kathmandu, Nepal
Instructor of record for eight undergraduate engineering courses, with 36–48 students each. Designed Python training and supervised final-year projects.

Other experience

May 2018 – Jun 2022 **Telecommunications Engineer**
Nepal Telecom, Kathmandu, Nepal
Built the Wireless KPI Analytics Tool, a Django application with REST APIs that automated analysis across 5,000+ network elements and cut analysis time from days to minutes. Designed Python and SQL pipelines for 10+ GB of daily network data, and LSTM models for anomaly detection and forecasting that improved network reliability by 15%.

Honors and awards

2026 Outstanding Doctoral Student Award, EECS Department, University of Missouri

2024 EECS Excellence Travel Grant, University of Missouri

2022 Dean's Fellowship, University of Missouri

2018 First rank, engineer recruitment examination, Public Service Commission, Nepal

2017 Graduate Scholarship, Tribhuvan University

2012 Undergraduate Scholarship, Tribhuvan University

Golden Jubilee Scholarship for undergraduate study, Embassy of India, Kathmandu

Talks

2024 CryoSegNet: AI-based method for protein particle picking from cryo-EM micrographs. Invited talk, Cryo-EM Super Group, University of Missouri.

2024 A large expert-curated cryo-EM image dataset for machine learning protein particle picking. Poster, RECOMB 2024, Cambridge, MA.

Service and leadership

Reviewer NeurIPS; Bioinformatics, Briefings in Bioinformatics, BMC Bioinformatics, Biochemical and Biophysical Research Communications, Communications Chemistry, IUCrJ, Patterns, Scientific Data, Scientific Reports.

2024 – 2026 President (2025 – 2026) and Treasurer (2024 – 2025), Nepalese Students Association, University of Missouri.

2023 – 2024 Member, Academic Affairs Committee, University of Missouri.