Rajan Gyawali

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Education

University of Missouri | Columbia, MO — Aug 2022 – Dec 2026 (Expected)

PhD in Computer Science | Emphasis: Deep Learning, Computational Biology and Bioinformatics

Advisor: Dr. Jianlin Cheng

Tribhuvan University | Kathmandu, Nepal — 2017 – 2019

Masters of Science in Information and Communication Engineering

Research Experience

Graduate Researcher — August 2022 – Present

Bioinformatics and Machine Learning Lab, University of Missouri — *Columbia, MO*

- Developed MICA, a multimodal deep learning method integrating cryo-EM density maps and AlphaFold3 structures for automated 3D atomic modeling of protein complexes using encoder-decoder architecture with feature pyramid networks, outperforming state-of-the-art methods
- Designed CryoSegNet, a deep learning method integrating Segment Anything Model (SAM) with attention-gated U-Net for automated protein particle detection from cryo-EM micrographs, achieving 7-14% improvement in 3D reconstruction resolution (3.32Å) over state-of-the-art methods
- Curated CryoPPP, a 2.6TB benchmark dataset (9,893 micrographs, 300K+ labels, 34 proteins) for training AI models in cryo-EM protein particle picking, now widely adopted as a standard dataset with 45+ citations
- Developed CryoVirusDB, an annotated dataset for AI-based virus particle identification in cryo-EM micrographs, enabling automated detection and classification of icosahedral virus structures
- Contributed to protein-ligand binding structure prediction using E(n)-equivariant graph neural networks
- Contributed to CryoTransformer, a detection transformer-based method achieving 0.747 F1-score for automated protein particle detection in cryo-EM micrographs
- Contributed to CryoFSL, a few-shot learning framework reducing labeling requirements by 95% for robust protein particle picking in cryo-EM micrographs
- Contributed to adapting Segment Anything Model (SAM) through prompt-based learning for enhanced protein identification in cryo-EM micrographs
- Trained and optimized deep learning models including Graph Neural Networks (GNNs), E(n)-equivariant networks, diffusion models using distributed data parallel training across multi-node multi-GPU HPC clusters (Slurm, LSF)
- Developed process-based parallelism scripts for large-scale data preprocessing across multiple HPC cluster nodes

Professional Experience

Telecommunications Engineer — May 2018 – June 2022

Nepal Telecom — *Kathmandu, Nepal*

- Developed Wireless KPI Analytics Tool, a full-stack Django web application with RESTful APIs for automated analysis and visualization of key performance indicators across 5000+ network elements, eliminating manual processing and reducing analysis time from days to minutes
- Designed and implemented automated data pipelines using Python and SQL for processing large-scale network performance data (10+ GB daily), including data extraction, transformation, statistical analysis, and visualization

- Configured and maintained Linux servers for application deployment, including hands-on experience with PostgreSQL/MySQL database installation, configuration, performance tuning, and backup automation
- Built predictive models for network anomaly detection and performance forecasting using time-series analysis and LSTM models, improving network reliability by 15%
- Automated daily redundant tasks including report generation, network status monitoring, and alert systems using Python scripting and task scheduling, reducing manual workload by 80% and improving response time
- Developed interactive dashboards and visualization tools using Matplotlib, Plotly, and Pandas for real-time network monitoring and performance reporting to management and technical teams
- Conducted data-driven analysis of network traffic patterns and user behavior to optimize resource allocation and capacity planning for telecommunications infrastructure
- Prepared technical documentation, performance reports, and data-driven recommendations for network optimization projects and infrastructure upgrades

Technical Skills

Deep Learning Architectures: CNNs, Vision Transformers, U-Net, ResNet, attention mechanisms, encoder-decoder architectures, Graph Neural Networks (GNNs), E(n)-equivariant networks, generative models, diffusion models, detection transformers, few-shot learning, transfer learning, prompt-based learning

Frameworks & Libraries: PyTorch, PyTorch Lightning, PyTorch Geometric, Deep Graph Library (DGL), TensorFlow, scikit-learn, NumPy, Pandas, SciPy, Matplotlib, Plotly

Computational Biology & Structural Biology: Cryo-EM structure determination, protein structure prediction, protein-ligand binding, virus particle identification, PyRosetta, UCSF ChimeraX, PyMOL, RDKit, Open Babel, Clustal Omega, RELION, CryoSPARC, Biopython, AlphaFold

Distributed Computing & HPC: Multi-node multi-GPU training (DDP), HPC cluster management (Slurm, LSF), parallel data processing, distributed model training

Programming Languages: Python (expert), C++, Bash, R, SQL

Data Analysis & Visualization: Statistical analysis, time-series analysis, predictive modeling, data pipelines, dashboard development, data visualization

Development Tools: Git/GitHub, Linux, Docker, Django, Visual Studio, Jupyter, Weights & Biases (W&B), TensorBoard

Publication

[1] **Gyawali, R.**, Dhakal, A., Wang, L., & Cheng, J. (2026). CryoVirusDB: An Annotated Dataset for AI-Based Virus Particle Identification in Cryo-EM Micrographs. *Viruses, 18(2), 224.*

[2] **Gyawali, R.**, Dhakal, A., & Cheng, J. (2025). Multimodal deep learning integration of cryo-EM and AlphaFold3 for high-accuracy protein structure determination. *Communications Chemistry, 8(1), 320.*

[3] Dhakal, A.*, **Gyawali, R.***, Wang, L., & Cheng, J. (2025). Artificial intelligence in cryo-EM protein particle picking: recent advances and remaining challenges. *Briefings in Bioinformatics, 26(1).*

[4] Poudel, B., **Gyawali, R.**, Dhakal, A., Cheng, J., & Xu, D. (2025). CryoFSL: An Annotation-Efficient, Few-Shot Learning Framework for Robust Protein Particle Picking in Cryo-EM Micrographs. *bioRxiv.*

[5] **Gyawali, R.**, Dhakal, A., Wang, L., & Cheng, J. (2024). 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.*

[6] Dhakal, A., **Gyawali, R.**, Wang, L., & Cheng, J. (2024). CryoTransformer: a transformer model for picking protein particles from Cryo-EM micrographs. *Bioinformatics, 40(3), btae109.*

[7] He, F., Yang, Z., Gao, M., Poudel, B., Dhas, N.S.E.S., **Gyawali, R.**, Dhakal, A., et al. (2024). 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).*

[8] Dhakal, A.*, **Gyawali, R.***, Wang, L., & Cheng, J. (2023). A large expert-curated cryo-EM image dataset for machine learning protein particle picking. *Scientific Data, 10(1), 392.*

[9] Dhakal, A.*, **Gyawali, R.***, & Cheng, J. (2023). Predicting protein-ligand binding structure using E(n) Equivariant graph neural networks. *bioRxiv, 2023.08.06.552202.*

[10] **Gyawali, R.**, & Pant, D.R. (2019). An Approach for the Employee Face Recognition by RPN and Faster R-CNN Techniques. *Proceedings of IOE Graduate Conference, 2019-Summer, 6, 231.*

*****Equal contribution*

Talks & Presentations

CryoSegNet: AI-based method for proteins particle picking from cryo-EM density micrographs 2024
Cryo-EM Super Group *University of Missouri*

A large expert-curated cryo-EM image dataset for machine learning protein particle picking 2024
RECOMB Conference (poster presentation) *Cambridge, MA*

Honors and Awards

Dean's Fellowship, University of Missouri 2022

Graduate Scholarship, Tribhuvan University 2017

Undergraduate Scholarship, Tribhuvan University 2012

Professional Service and Other Involvements

Manuscript Reviewer:

NeurIPS, Briefings in Bioinformatics, BMC Bioinformatics, Communications Chemistry

President, University of Missouri Nepalese Students Association May 2025 – April 2026

Treasurer, University of Missouri Nepalese Students Association May 2024 – April 2025

Member, Academic Affairs Committee, University of Missouri August 2023 – May 2024