ABIN SHAKYA

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EDUCATION

Louisiana State University, Baton Rouge *Advisor: Dr. Bijaya Karki*
PhD in Computer Science : 4.0/4.0 GPA *Aug 2021 - May 2026 (Expected)*

Tribhuvan University, Kathmandu, Nepal *Advisor: Dr. Subarna Shakya*
BE in Computer Engineering: 3.6 GPA (US Scale) *Nov 2013 - Nov 2017*

PROFESSIONAL AND RESEARCH EXPERIENCE

Research Assistant (Ph.D.) *Aug 2021 – Present*
Louisiana State University, Baton Rouge, LA *Supervisor: Dr. Bijaya B. Karki*

- Developed an AI agent capable of parsing and analyzing scientific PDFs to extract polymer-related data and automatically generate a structured database of polymer properties and force fields for knowledge discovery and retrieval.
- Designed and implemented a GNN-based regression model using coarse-grained (MARTINI) topology graphs to predict structure–property and structure–interaction relationships in polymer–drug systems.
- Developed Weakly Supervised Graph Neural Networks for scalable **3D phase segmentation** in molecular dynamics simulations; accepted for Oral Presentation at KDIR 2025.
- Built Graph Neural Network-accelerated Molecular Dynamics to explore atom distribution in Earth's core.
- Developed an **active learning** framework for molecular dynamics that enhanced model generalization and made it feasible to model combinatorially complex chemical spaces.
- Developed deep learning-based potential energy models for molecular dynamics, facilitating simulations of Earth's interior, and authored the paper Insights into core-mantle differentiation from bulk Earth melt simulations. DOI: 10.1038/s41598-024-69873-8
- Built a two-level binning method to detect compositional shifts and verify core-mantle segregation—starting with spatial binning and refining clusters using hierarchical grouping and graph connectivity.

Senior Software Engineer *Oct 2017 – Sep 2021*
Sparrow Private Limited, Lalitpur, Nepal

- Joined as one of the first 5 engineers and helped scale the platform and engineering organization to over 50 members, transforming Khalti from a growing startup into a nationwide fintech ecosystem.
- Designed Khalti's unified API middleware, integrating fragmented third-party services into a scalable, maintainable service layer that cut partner onboarding time from weeks to hours and streamlined long-term operations.
- Built a fully automated financial reconciliation system for the accounts team, replacing manual, error-prone workflows. What previously took weeks or months to surface discrepancies became a daily automated reconciliation pipeline, drastically improving accuracy and financial transparency.
- Improved a high-traffic flight search system by shifting vendor integrations to an asynchronous request model and introducing intelligent caching—cutting worst-case latency by 6× while maintaining consistent performance under load.
- Automated financial reporting via a Django backend with Celery-based task scheduling and RabbitMQ as the message broker, enabling daily tracking of cash inflows/outflows and early detection of unresolved transactions—reducing reconciliation from weeks to continuous daily resolution and minimizing month-end accounting issues.
- Maintained staging infrastructure, deployment pipelines, and release automation, enabling rapid reproduction of client issues in test environments and accelerating customer onboarding.

SKILLS

Programming Languages:	**Python**, **C++**, Java, C, R, SML, SAS, SQL, MATLAB
Frameworks/Libraries:	**PyTorch, TensorFlow**, PyG, Django, Flask, PySpark, Pandas, NumPy, Scikit-Learn
Graph Machine Learning:	GCN, GAT, GraphSAGE, PNA, MPNNs, Graph Transformers, Equivariant GNNs, Link Prediction, Node Classification, Spatio-Temporal GNNs, PyG, Graph Sampling
Generative AI:	Pretraining and Fine-Tuning of Foundation Models, Normalizing Flows, Probabilistic Diffusion Models, VAEs, GANs, Transformers (GPT, BERT, T5, ViT)
Tools/Technologies/DB:	HPC, SLURM, Nginx, Redis, Amazon S3, SageMaker, MongoDB, SparkSQL, Apache Kafka, Apache Hadoop, RabbitMQ , PostgreSQL, LaTeX
MD Simulation:	LAMMPS, GROMACS, VASP, DeepMD-kit, DP-GEN, VMD

PAPERS, AWARDS AND RECOGNITIONS

- Shakya, A.*, Karki, B.B. (2025). Weakly Supervised Graph Neural Networks for Scalable 3D Phase Segmentation in Molecular Dynamics Simulations. [Accepted at KDIR 2025]
- Shakya, A.*, Ghosh, D.B., Jackson, C., Morra, G., Karki, B.B. (2024). Insights into core-mantle differentiation from bulk Earth melt simulations. Scientific Reports. DOI: 10.1038/s41598-024-69873-8.
- Shakya, A.*, Pokharel, A., Bhattarai, A., Sitikhu, P., Shakya, S. (2018). Real-Time Stock Prediction Using Neural Network. 8th International Conference, Confluence 2018— IEEE. ISBN: 978-1-5386-1720-5.
- Enrolled in a fully Funded PhD Program : NASA Emerging Worlds Research Grant, Computer Science, LSU, 2021/22
- **National Top 26th Rank** (out of 15,000+) in Engineering Entrance Examination — Full Merit Scholarship.