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Ashim Paudel

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EDUCATION

MS in Computer Science | Louisiana State University | Expected Dec 2026

GPA: 4.0 | Relevant Courses: Machine Learning, Deep Learning, Applied LLM Development, Computational Chemistry

BS in Computer Science | Mississippi State University | May 2022

GPA: 3.41 | Relevant Courses: DBMS, Programming Languages, AI Robotics, Algorithms, Microprocessors

TECHNICAL SKILLS

Programming Languages:	Python, C, C++, Java, MATLAB, Bash
Frameworks/Libraries:	PyTorch, TensorFlow, Scikit-Learn, Transformers, OpenCV, NumPy, Pandas
Graph Machine Learning:	GCN, GAT, Link Prediction, Node Classification
Scientific Computing:	NAMD, GROMACS, VMD, HPC, SLURM
DB/Tools/Technologies:	MySQL, SparkSQL, Apache Kafka, Apache Hadoop, Vector DB, Git, Docker

EXPERIENCE

Graduate Research Assistant

Jan 2025 – Present

Louisiana State University, Baton Rouge, LA

- Developed and implemented a graph neural network (GNN) regression model leveraging coarse-grained (MARTINI) topology graphs to predict structure–property relationships in polymer–drug systems.
- Developed an automated AI pipeline for extracting structured polymer-related data from scientific documents and implemented a Python-based RAG chatbot using Chroma vector stores to deliver accurate Q&A over the engineered dataset.
- Implemented agentic AI systems to automate molecular simulation tasks, from structure parsing and configuration generation to automated analysis of simulation results.
- Conducted molecular dynamics simulations of polymer–drug systems, generating topologies, preparing solvated models, and performing structural analyses (e.g. Rg, SASA).

Software Engineer

Jul 2022 – Jan 2024

Orbbec, Troy, MI

- Developed a real-time image processing pipeline in C++ for converting RGB-D images into stereoscopic view. Integrated Orbbec's proprietary algorithm, leveraging OpenCV and Boost for efficient multi-threaded data handling, and used StereoKit for XR rendering across VR platforms.
- Developed 'The Eye for AIs,' an advanced image processing application that isolates objects, computes volumes, and performs detailed analysis using color and depth images from a depth camera. Leveraged vision language models (VLMs) and large language models (LLMs) to segment and interpret regions of interest from images.
- Led integration of a tailored LLM API into a customer chatbot application. Improved technical response accuracy by 18% by fine-tuning the LLM model using the company software development kit, product specifications, and API documentation.
- Led the design of an iOS prototype to capture and transmit synchronized RGB camera and LiDAR depth sensor data over the network to perform real-time stereoscopic 3D reconstruction. Conducted in-depth research on Apple's LiDAR sensor and depth APIs.
- Collaborated with Nvidia to evaluate the compatibility of their body and hand-tracking technologies with the Orin and Jetson Nano platforms. Conducted thorough testing of Orbbec SDKs, documenting test cases, outcomes, and errors.

Undergraduate Research Assistant

Aug 2021 – May 2022

Mississippi State University, Starkville, MS

- Developed and validated a multi-UE LTE testbed using SDR (USRP B205mini) and srsRAN, demonstrating dual UE attachment to a single base station near 3.5 GHz and resolving inter-UE communication issues through RF parameter optimization.
- Conducted LTE experiments on Ubuntu, evaluated SDR device compatibility, and mentored undergraduate researchers in configuring and testing srsLTE/srsRAN systems.

PUBLICATIONS

- Paudel, A., Shakya, A., et al. "A structured dataset of polymers in molecular dynamics simulations extracted by LLM-assisted text mining." ChemRxiv (2026). <https://doi.org/10.26434/chemrxiv.15000400/v1>. Submitted to Nature Scientific Data.