

Ansh Sharma

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EXPERIENCE

Genesis Therapeutics

San Francisco, CA

Senior Machine Learning Research Engineer

Aug. 2024 – Present

- Core contributor to **PEARL**, a **generative diffusion model** for structure-based drug discovery; achieved SOTA performance surpassing **AlphaFold3** and open-source baselines on protein-ligand cofolding benchmarks.
- Designed **equivariant architectural components** and explored **scaling laws** to improve performance, leveraging geometric inductive biases for high-fidelity structural predictions.
- Developed end-to-end **training and evaluation infrastructure** for ML-based binding affinity prediction, facilitating high-velocity research on hit-identification and lead-optimization tasks.
- Scoped, designed, and mentored a research internship project on **parameter efficient fine-tuning (LoRA/TLoRA)**, resulting in production-ready adaptations for program-specific model deployments.

AbbVie

Chicago, IL

Machine Learning Research Intern - Pharma R&D

Jan. 2022 – May 2024

- Designed an end-to-end **GNN-based pipeline** to automate 3D molecular structure prediction from **NMR spectra**, replacing manual scientist-led alignment with an automated deep learning workflow.
- Developed ML-based biomarkers for patient stratification using **multi-modal genomic and radiomic data** for ABBV-CLS-628, which has successfully progressed to a **Phase II clinical trial**.
- Implemented **self-supervised contrastive learning** frameworks for representation learning on high-content **cell-painting datasets** to support downstream chemical tasks.
- Built **scalable distributed training pipelines** on AWS to process and featurize terabyte-scale molecular perturbation and imaging datasets.

Amazon

New York City, NY

SDE Intern - Amazon Translate (Applied Science Team)

May 2023 – Aug. 2023

- Evaluated and fine-tuned **Large Language Models (LLMs)** as automated judges for translation quality, improving correlation with human judgment over traditional heuristic metrics.
- Fine-tuned models for cross-lingual unit conversion and normalization, improving the interpretability and accuracy of translated technical specifications.
- Deployed LLM-based scoring workflows into production inference pipelines for model evaluation and monitoring.

Argonne National Laboratory

Chicago, IL

Visiting Student Researcher

Oct. 2022 – May 2023

- Optimized AlphaFold2 inference on the NCSA Delta supercomputer, achieving a **73% runtime reduction** through multi-GPU scheduling, mixed-precision (FP16), and CPU parallelization.
- Created containerized distributed computing endpoints (Singularity) to enable large-scale protein structure prediction for biomedical researchers at Argonne and partner institutions.

SELECTED PUBLICATIONS

PEARL: A Generative Model for Structure-based Drug Discovery, ArXiv (2025)

EarthGen: Generating the World from Top-Down Views, ArXiv (2024)

YoutubePD: A Multimodal Benchmark for Parkinson's Disease Analysis, NeurIPS (2023)

EDUCATION

University of Illinois at Urbana-Champaign

Champaign, IL

B.S. in Computer Science, Chancellor's Scholar (GPA: 4.0/4.0)

May 2024

Selected Awards: Bronze Tablet (2024), John R. Pasta Outstanding Undergraduate Award (2023), Regeneron ISEF Finalist (2021), USAPhO Top 50 (2021), Putnam Top 500 (2020), USAJMO Qualifier (2019)

TECHNICAL SKILLS

Languages & Tools: Python, C++, CUDA, SQL, Linux, Git, Docker, AWS, GCP, PySpark, Slurm

ML & Scientific Computing: PyTorch, JAX, NumPy, Pandas, SciPy, OpenCV, RDKit, BioPython

Research Areas: Geometric DL, Diffusion Models, Protein Structure Prediction, Molecular Docking, Scaling Laws