Nikhil Dhiman

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SUMMARY

Researcher in machine learning developing knowledge-guided, interpretable, and generalizable AI through generative modeling, data selection, and causal optimization for scientific and societal discovery.

EDUCATION

Master's in Computer Science — GPA: 4/4
California State University, Los Angeles, California, USA — *Aug 2024 – May 2026*
Thesis: Physics-Guided Active Learning for New Ligand Discovery
Advisor: Dr. Negin Forouzesh

Bachelor of Technology in Computer Science — GPA: 3.7/4
Dr. A.P.J. Abdul Kalam Technical University, India — *Aug 2016 – May 2020*
Thesis: Predictive big data analysis in healthcare

RESEARCH EXPERIENCE

Graduate Research Assistant — Aug 2024 – Present
Computational Molecular Biology Lab, California State University – Los Angeles — *Los Angeles, CA*

- Conducting **NSF and NIH-funded research** in computational biology and structure-based drug discovery using generative modeling guided by protein pocket geometry and molecular interactions.
- Developed a **physics-guided active learning framework** integrating molecular docking, solvation modeling, and generative design, improving binding affinity by 4.3%, reducing solvation energy by 29%, and increasing synthetic accessibility by 5.5%.
- Cross-disciplinary collaboration on ML-driven modeling for generalizable and interpretable drug discovery.

Software Engineer – Research & Development — Jan 2020 – Jul 2024
Appventurez Mobitech Private Limited — *Noida, India*

- Developed and benchmarked optimization models to improve computational efficiency in large-scale machine learning pipelines, reducing runtime by 15% while maintaining accuracy across datasets.
- Designed and implemented scalable learning architectures with distributed training and performance profiling, enhancing model stability, convergence speed, and generalization.
- Adapted and deployed research-grade ML frameworks in production environments, validating reliability and performance through extensive empirical evaluation.

Undergraduate Researcher — Jan 2018 – Jul 2020
Internet of Things Lab, ABES Institute of Technology — *Noida, India*

- Developed an IoT-based child welfare monitoring system integrating embedded sensors and cloud platforms for real-time tracking and long-term welfare assessment.
- Presented the project at the Smart India Hackathon (SIH 2019), recognized for its societal impact and innovative application of IoT for minimizing child labor.

PUBLICATIONS

- **Dhiman, N.**, Sagar, D., & Forouzesh, N. (2026). *Physics-Guided Active Learning for New Ligand Discovery. Biophysical Journal. [Under Review]*

- **Dhiman, N.**, Sagar, D., & Forouzesh, N. (2025). *Physics-Guided Active Learning for New Ligand Discovery.* In *Proceedings of the 6th ACM International Conference on Bioinformatics, Computational Biology and Health Informatics (BCB Companion '25)*, pp. 1–7. ACM. *[Accepted, Conference Proceeding]*

- **Dhiman, N.**, Baldesco, U., Sagar, D., & Forouzesh, N. (2025). *[Physics-Guided Deep Generative Model for New Ligand Discovery](#). Biophysical Journal, 124*(3).

- **Dhiman, N.**, Sharma, N., & Vashisth, V. (2023). *[DeepSecure: A Real-Time Deep Learning-Based System for Enhancing Cybersecurity in Social Media through DeepFake Detection using LSTM and ResNext CNN](#). International Research Journal of Engineering and Technology (IRJET).*

- Tiwari, U. K., **Dhiman, N.**, & Tandon, N. (2020). *[Predictive Big Data Analysis in Healthcare](#). AEGAEUM Journal.*

Teaching Experience

Teaching Assistant – CS4961/CS4962 Senior Design   *Fall 2025 & Spring 2026*
California State University – Los Angeles
- Supervised and mentored a team of 12 senior undergraduate students from diverse backgrounds developing the *AMBER* RAG-Based Generative AI Support System, integrating retrieval-augmented generation with large language models for scientific research support.
- Led weekly design reviews and mentored students in building scalable AI systems from research concepts.

Instructor – Intro to Machine Learning   *Summer 2025*
COMB Lab, California State University – Los Angeles
- Mentored two undergraduate researchers through the **NSF-PREC Program**, focusing on deep learning applications in computational biology.
- Guided students in applying machine learning to research at the intersection of AI and life science.

Presenter

- *ACM-BCB (CSBW)* (2025) – Paper Presentation
- *Biophysical Society Annual Meeting* (2025) – Poster Presentation

Awards & Honors

- Best Paper & Presentation Award (1st Place), "Physics-Guided Active Learning for New Ligand Discovery," ACM-BCB (CSBW) 2025 Conference, Philadelphia, USA
- Non-resident Tuition Fee Waiver Award- AY 2025-26, California State University, Los Angeles, USA
- Ranked Top 5 in Computer Science, ABES Institute of Technology, Ghaziabad, India
- Best R&D Project Award 2021, Appventurez Mobitech Private Limited, Noida, India

Technical Skills

Programming Languages: Python, Java, C++, Bash, SQL
Machine Learning & Deep Learning: Generative Models (CVAE, GANs, Diffusion Models), Self-Supervised Learning, Transfer Learning, Active Learning, Dimensionality Reduction (PCA, UMAP), PyTorch, TensorFlow
Scientific Computing: NumPy, SciPy, Pandas, Matplotlib, RDKit, PyMOL
Large Language Models & AI Agents: Retrieval-Augmented Generation (RAG), Multi-Agent Collaboration, Context-Aware Agents, Alignment & Post-Training (RLHF, DPO), Model Efficiency (Quantization, Distillation, Pruning), On-Device Inference (llama.cpp, MLC LLM)
Computational Modeling & Simulation: Physics-Guided Learning, Molecular Docking (GNINA, DiffDock), Molecular Dynamics (Amber, OpenMM), Structure-Based Drug Discovery
Cloud Computing & HPC: Distributed & Parallel Computing, GPU, AWS, Azure, GCP, Docker, HPC Servers
Tools: Data Management, Git, Experiment Tracking, Scientific Visualization, Documentation (LaTeX, Overleaf)

Reviewer

- *NeurIPS (ML4PS)* (2025) – Contributed to peer review under supervision of PI, Dr. N. Forouzesh
- *ACM-BCB (CSBW)* (2025) – Contributed to peer review under supervision of PI, Dr. N. Forouzesh
- *Journal of Engineering Research and Reports* (Mar 2025) – Peer Reviewer
- *Asian Journal of Research in Computer Science* (Dec 2024) – Peer Reviewer

Membership of Professional Societies

- Association for Computing Machinery (ACM)
- Biophysical Society
- Mathematics Engineering Science Achievement (MESA)