Dibyajyoti Chakraborty

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Research Statement

My research focuses on building efficient deep learning systems for real-world impact. I am passionate about developing machine learning solutions that translate from theoretical advances to practical tools, empowering individuals and organizations to make better-informed and impactful decisions.

Education

Pennsylvania State University, State College, PA, United States *Aug 2023 – present*
Ph.D. in Information Sciences and Technology (Data Science AI Track)

Indian Institute of Technology Bombay, Mumbai, India *Aug 2021 – Jul 2023*
M.Tech. in Mechanical Engineering

National Institute of Technology, Jamshedpur, India *Jul 2015 – May 2019*
B.Tech. in Mechanical Engineering

Research Experience

NVIDIA *Santa Clara, CA, USA*
Physics ML Research Intern *May 2025 – Aug 2025*

State-of-the-art AI Weather Forecasting

- Developed the Mixture of Weather Experts (MoWE) framework, integrating existing AI forecasting architectures with a Vision Transformer-based gating network that learns spatiotemporal adaptive weights conditioned on forecast lead time.
- Achieved up to 10% lower RMSE than the best individual expert (Aurora) at a 48-hour horizon, and extended MoWE to a probabilistic version using a hidden Markov Model trained with CRPS, providing a computationally efficient alternative to current probabilistic forecasting models.
- Released MoWE implementation through NVIDIA Earth2Studio and PhysicsNeMo libraries, enabling community adoption and reproducibility.

Los Alamos National Lab *Los Alamos, NM, USA*
Graduate Research Intern *May 2024 – Aug 2024*

AI surrogate for Chaotic Systems

- Designed lightweight time-series forecasting models for high-dimensional chaotic systems using Koopman operator theory.
- Developed a spectral loss-based vision transformer to mitigate spectral bias, improving spectral fidelity and stability.
- Applied implicit neural fields for 1500× compression of high-dimensional climate data, achieving memory-efficient representation, which is used by forecasting models.

The Pennsylvania State University *State College, PA, USA*
Graduate Research Assistant *Aug 2023 – present*

Deep Learning for Dynamical Systems

- Designed the Multi-step Penalty (MP) Optimization algorithm to enable long-term stable predictions of chaotic systems.
- Applied MP to Neural ODEs, Fourier Neural Operators, and UNets for climate and ocean modeling, achieving stable autoregressive rollouts.
- Proposed a Binned Spectral Power (BSP) Loss to preserve invariant metrics in turbulence surrogate modeling.

Generative AI for Atmospheric Super-resolution

- Trained Elucidated Diffusion Models (EDM) on 64 A100 GPUs and utilized posterior sampling for test-time atmospheric super-resolution and data assimilation.
- Developed a score-based Bayesian fusion framework that integrates ERA5 reanalysis, IGRA radiosondes, and emulator output, improving spatio-temporal fidelity with uncertainty quantification.

Hybrid Methods for Turbulence Simulations

- Developed differentiable-PDE solvers coupled with deep learning closure modeling for turbulence simulations.
- Demonstrated that hybrid solver-in-the-loop strategies outperform traditional offline training as well as physics based closure modeling, producing generalizable models across varying Reynolds numbers and flow parameters.

Indian Institute of Technology, Bombay *Mumbai, India*
Masters Thesis *Dec 2021 – May 2023*

Anti-derivatives using neural networks

- Developed an algorithm (DNNI - Deep Neural Network Integration) for computing the anti-derivatives of functions using **neural networks**
- Created and **open sourced** a python package that can be used to implement the DNNI algorithm.

Quantum Linear Algebra

- Researched various **quantum algorithms** and executed them on IBM's quantum computers.
- Implemented the quantum algorithm (HHL) for solving a system of linear equations on simulators and IBM's quantum computer.

Professional Experience

Engineers India Limited *Delhi, India*
Engineer *Nov 2019 – July 2021*

Dhobi-Durgapur Pipeline Project

- Managed 50+ personnel in the construction of an 86 km natural gas pipeline, overseeing project milestones and ensuring pipeline quality using advanced Non-Destructive Testing(NDT) methods and high-pressure hydro-testing.

Publications

Chakraborty, D., Maulik, R., Harrington, P., Foster, D., Nabian, M. A., & Choudhry, S. (2025). MoWE: A Mixture of Weather Experts. preprint

Chakraborty, D., Guan, H., Stock, J., Arcomano, T., Cervone, G., & Maulik, R. (2025). Multimodal Atmospheric Super-Resolution With Deep Generative Models. preprint

Chakraborty, D., Mohan, A. T., & Maulik, R. (2025). Binned Spectral Power Loss for Improved Prediction of Chaotic Systems. preprint (in review)

Shankar, V., **Chakraborty, D.**, Viswanathan, V., & Maulik, R. (2025). Differentiable turbulence: Closure as a partial differential equation constrained optimization. Physical Review Fluids, 10(2), 024605.

Chakraborty, D., Chung, S. W., Arcomano, T., & Maulik, R. (2024). Divide and conquer: Learning chaotic dynamical systems with multistep penalty neural ordinary differential equations. Computer Methods in Applied Mechanics and Engineering, 117442.

Chakraborty, D., Barwey, S., Zhang, H., & Maulik R. (2024). A note on the error analysis of data-driven closure models for large eddy simulations of turbulence. preprint (in review)

Chakraborty D., Gopalakrishnan S.(2023). Computing Anti-Derivatives using Deep Neural Networks. preprint (in review)

Achievements

- Institute Silver Medal, Indian Institute of Technology Bombay (Rank 1/75 in Masters).
- Ashok Chaturvedi Memorial Prize for outstanding master's student at Indian Institute of Technology Bombay.
- Best Paper & Best Poster Awards, Conference on Applied AI and Scientific Machine Learning (CASML) 2024.
- Finalist, Best Paper, World Congresses on Computational Mechanics (WCCM) 2024; Best Poster, USACM UQ-MLIP 2024.
- Travel awards: SIAM-DS 2025, UQ-MLIP 2024, APS DFD 2023, SIAM NNP 2024.
- Invited talks - Seminar Series, CRUNCH group, Brown University; DTL SciML Workshop, Texas A&M Institute of DS.

Skills

Languages: Python, C++, Julia, MATLAB **Packages:** PyTorch, Jax, TensorFlow, Keras, Dask, Xarray, Scikit-learn

Algorithms: Diffusion Models, Vision Transformers, GNN, CNN, Neural Operators, VAE, GAN, RNN, LSTM, NLP, LLMs

Others: Github, OpenFOAM, Ansys.