

# Arka Daw

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Distinguished Staff Fellow at Oak Ridge National Lab (ORNL)

## RESEARCH INTERESTS

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My research spans several key areas in deep learning from integrating scientific knowledge into AI models for tackling complex scientific problems to ensuring their safety and trustworthiness. Lately, my efforts have primarily focused on the development and evaluation of large-scale multi-modal foundational models.

## EDUCATION

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- **Virginia Tech** Aug. 2018 - Dec. 2023  
*Ph.D. in Computer Science*  
◦ Advisor: [Anuj Karpatne](#)  
◦ Thesis: *Physics-informed Machine Learning with Uncertainty Quantification.*  
Blacksburg, USA
- **Jadavpur University** Aug. 2014 - May 2018  
*B.Eng. in Electronics Engineering*  
Kolkata, India

## SELECTED PUBLICATIONS

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Visit my Google Scholar [pz2Nm8AAAAAJ](https://scholar.google.com/citations?user=pz2Nm8AAAAAJ) for a complete list

- VLM4Bio: A Benchmark Dataset to Evaluate Pretrained Vision-Language Models for Trait Discovery [NeurIPS, 2024](#)  
from Biological Images.  
M. Maruf, **A. Daw**, K.S. Mehrab, H. Manogaran, A. Neog, M. Sawhney, M. Khurana, ..., A. Karpatne
- Hierarchical Conditioning of Diffusion Models Using Tree-of-Life for Studying Species Evolution. [ECCV, 2024](#)  
M. Khurana, **A. Daw**, M. Maruf, J. Uyeda, W. Dahdul, C. Charpentier, ..., A. Karpatne
- Modular Compositional Learning Improves 1D Hydrodynamic Lake Model Performance by Merging Process-Based Modeling With Deep Learning. [JAMES, 2024](#)  
R. Ladwig, **A. Daw**, E. Albright, C. Buelo, A. Karpatne, M. Meyer, A. Neog, P. Hanson, H. Dugan
- Motion Enhanced Multi-Level Tracker (MEMTrack): A Deep Learning-Based Approach to Microrobot Tracking in Dense and Low-Contrast Environments. [AIS, 2024](#)  
M. Sawhney, B. Karmarkar, E. Leaman, **A. Daw**, A. Karpatne, B. Behkam
- Mitigating propagation failures in physics-informed neural networks using R3 sampling. [ICML, 2023](#)  
**A. Daw**, J. Bu, S. Wang, P. Perdikaris, A. Karpatne
- Multi-task learning for source attribution and field reconstruction for methane monitoring. [IEEE BigData, 2022](#)  
**A. Daw**, K. Yeo, A. Karpatne, L. Klein
- Physics-guided neural networks (PGNN): An application in lake temperature modeling. [KGML, 2022](#)  
**A. Daw**, A. Karpatne, W. Watkins, J. Read, V. Kumar
- Learning compact representations of neural networks using discriminative masking (DAM). [NeurIPS, 2021](#)  
J. Bu\*, **A. Daw\***, M. Maruf\*, A. Karpatne (\*equal contribution)
- PID-GAN: GAN framework based on Physics-informed Discriminator for Uncertainty Quantification. [KDD, 2021](#)  
**A. Daw**, M. Maruf, A. Karpatne
- Physics-guided architecture (PGA) of neural networks for quantifying uncertainty in lake temperature modeling. [SDM 2021](#)  
**A. Daw**, R. Thomas, C. Carey, J. Read, A. Appling, A. Karpatne

### Selected Preprints:

- AI-generated Image Detection: Passive or Watermark? [2024](#)  
M. Guo, Y. Hu, Z. Jiang, Z. Li, A. Sadovnik, **A. Daw**, N. Gong
- Unified Framework for Forward and Inverse Problems in Subsurface Imaging using Latent Space Translations. [2024](#)  
N. Gupta\*, M. Sawhney\*, **A. Daw\***, Y. Lin, A. Karpatne (\*equal contribution)
- What Do You See in Common? Learning Hierarchical Prototypes over Tree-of-Life to Discover Evolutionary Traits. [2024](#)  
H. Manogaran, M. Maruf, **A. Daw**, K.S. Mehrab, C. Charpentier, ..., A. Karpatne
- Fish-Vista: A Multi-Purpose Dataset for Understanding & Identification of Traits from Images [2024](#)  
K.S. Mehrab\*, M. Maruf\*, **A. Daw\***, H. Manogaran, A. Neog, M. Khurana, ..., A. Karpatne
- Beyond Discriminative Regions: Saliency Maps as Alternatives to CAMs for Weakly Supervised Semantic Segmentation [2023](#)  
M. Maruf, **A. Daw**, A. Dutta, J. Bu, A. Karpatne

## RESEARCH EXPERIENCE

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- **Oak Ridge National Lab (ORNL)** Jan 2024 - Present  
Oak Ridge, TN  
*Distinguished Staff Fellow*
  - Developing a Hessian-based topological characterization of the adversarial loss landscape to **understand adversarial vulnerabilities**.
  - Developed an **adversarial attack on CLIP** called “Hiding-in-plain Sight (HiPS)” attack that can selectively conceal target object(s), as if it was absent from the scene. (*Published at NeurIPS 2024.*)
  - Developing and evaluating **two different multi-modal foundational models**, one for lake modeling (LakeGPT) and another for geospatial applications (EarthMFM).
  - Collaborated on accelerating trait discovery using **conditional diffusion models** with phylogenetic knowledge in the form of hierarchical embeddings. (*Published at ECCV 2024.*)
  - Enhanced performance of **vision language models (VLMs)** for discovering biological traits through **prompting, in-context learning, and instruction tuning** that leverages the scientific knowledge. (*Published at NeurIPS 2024.*)
- **IBM Research** May 2022 - Aug. 2022  
Yorktown Heights, NY  
*Research Intern*
  - Developed a **multi-task learning framework** for source identification and field reconstruction of Advection-Diffusion Process from **sparse sensor measurements** using novel diffusive-masked convolution layer. (*Published at NeurIPS 2022, IEEE Big Data 2022, and Patent disclosure submitted.*)
- **Amazon AWS (Lambda Team)** May 2021 - Aug. 2021  
Seattle, WA  
*Applied Scientist Intern*
  - Developed **Accelerated Causal Exploration (ACE)** package that significantly shortens the time to design a robust *end-to-end causal inference* experiment while being easily adaptable to a wide range of use-cases.
  - Lead the causal analysis and investigation of a **critical performance issue with AWS Lambda’s distributed worker fleet**, and suggested corrective measures.
- **Virginia Tech** Dec. 2018 - Dec. 2023  
Blacksburg, VA  
*Graduate Research Assistant*
  - Introduced a **new failure modes in Physics-informed Neural Networks (PINNs)** called “*Propagation Hypothesis*” and a new “R3 sampling” strategy to adaptively emphasize on high error regions. (*Published at ICML 2023.*)
  - Designed **two different uncertainty quantification methods** for physics-informed machine learning: PID-GAN and PGA-LSTM (*Published at KDD 2021 and SDM 2020.*)

## INVITED TALKS

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- “Knowledge Guided Machine Learning for Partial Differential Equations”, at ORNL Summer Tutorial, July 2024.
- “Exploring the frontiers of Physics-informed Machine Learning for Complex Scientific Problems”, at ORNL Discrete Algorithms Group, March 2023.
- “Uncertainty quantification with Physics-informed Machine Learning”, Allan Turing Institute, London, UK, September 2022.
- “Advanced Topics in Deep Learning”, Guest Lecture for CS 5525 (Data Analytics), Virginia Tech, Dec. 2021.
- “Deep Learning for Mechanobiologists: A Case Study on using Generative Models for Estimating Single Cell Forces”, Department of Mechanical Engineering, Virginia Tech, July 2020.

## AWARDS AND HONORS

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- Distinguished Staff Fellowship (Alvin M. Weinberg Fellow), ORNL. 2024
- NeurIPS Top 1% Reviewer 2023
- Kafura Graduate Fellowship, Virginia Tech 2023
- SDM Doctoral Forum & KDD Travel Grants 2019, 2020
- DAAD-WISE (German Academic Exchange Services) Fellowship 2017
- INSPIRE Scholarship, MHRD Department, Govt. of India. 2014

## ACADEMIC SERVICE

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- **Reviewer:** NeurIPS, ICLR, ICML, AAAI, IJCAI, KDD, SDM. 2021-Present
- **PC Member:** KGML at ECML-PKDD, SGAI-AAAI 2021-2023
- **Organizing Committee:** KGML Summer Tutorial at ORNL 2024, KGML-Workshop & KGML-Brige Program at AAAI 2023-24 2023, 2024
- **Session Chair:** SDM Spatiotemporal Data-II 2021

## TECHNICAL SKILLS

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\* Python, PyTorch, Tensorflow, JAX, Keras, MATLAB, SQL, SageMaker, S2, EC2, DeepSpeed.