Arka **Daw**

PhD Student

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Research Interests

Deep Learning and Artificial Intelligence; Physics-Informed Machine Learning (Integrating scientific/physical knowledge with deep learning frameworks); AI for Science; Uncertainty Quantification; Semi-supervised Learning, Climate and Sustainability, Network Pruning.

Education

Virginia Tech — *Blacksburg, USA*

Ph.D. in Computer Science — *Aug. 2018 - May 2023 (Expected)*

- Adviser: Dr. Anuj Karpatne

Jadavpur University — *Kolkata, India*

B.Eng. in Electronics and Telecommunication — *Aug. 2014 - May 2018*

Work Experience

Virginia Tech — *Blacksburg, USA*

Research Assistant, Adviser: Dr. Anuj Karpatne — *Aug. 2018 - Present*

- Introduced a novel perspective of failure modes in Physics-informed Neural Networks (PINNs) called *"Propagation Hypothesis"*. A novel "Evolutionary Sampling" strategy was also proposed to adaptively emphasize on high error regions while being computationally efficient. *(Under submission.)*
- Designed a Physics-informed Discriminator for GANs, where physics supervision guides the learning of both generator and discriminator, and additionally stabilizes the training of GANs. *(Published at KDD 2021.)*
- Designed a novel deep learning architecture for seq-to-seq models to enforce physics-driven inductive bias in the modeling of lake temperature profiles. It improved the predictive performance by 20% while providing interpretable uncertainty estimates. *(Published at SDM 2020.)*
- Developed a single-stage structured pruning algorithm DAM that can can enforce L_0 sparsity. It not only achieves state-of-the-art performance on structured pruning for image classification tasks, but also on dimensionality reduction, and graph representation learning tasks. *(Published at NeurIPS 2021.)*
- Co-lead an interdisciplinary team that *invented single cell force-sensing platform* with applications in drug screening. I designed the deep learning tools that performed image-to-image translation using pix2pix and precise node tracking by combining object detectors with traditional CV. (Preprint available)
- Developing an iterative algorithm that can reveal non-discriminative regions in weakly-supervised semantic segmentation through stochastic transformations of the input images such as random cropping, multiplying the image with a binary mask, etc.

I.B.M. T.J. Watson Research Center — *Yorktown Heights, USA*

Research Intern, Adviser: Dr. Levente Klien, Dr. Kyongmin Yeo — *May 2022 - Aug. 2022*

- Developed a multi-task learning framework for source identification and field reconstruction of Advection-Diffusion Process from sparse sensor measurements. Designed a novel diffusive-masked convolution layer that mimics the process of diffusion for systematic reconstruction of the field. *(Published at ML4PS workshop at NeurIPS 2022, IEEE Big Data ADoCS 2022, and Patent disclosure submitted.)*

Amazon Web Services Inc. — *Seattle, USA*

Applied Scientist Intern, Adviser: Dr. John Konstantinides — *May 2021 - Aug. 2021*

- Developed Accelerated Causal Exploration (ACE) package that can significantly shorten the effort and time to design a robust *end-to-end causal inference* experiment while being flexible enough to adapt 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.

University of Münster — *Münster, Germany*

Research Intern, Adviser: Dr. Xiaoyi Jiang — *May 2017 - Aug. 2017*

- Designed a U-Net based framework for segmenting arteries and veins in retinal images. It demonstrated significant improvement in performance over traditional graph-based methods for segmenting arteries and veins.

Indian Statistical Institute — *Kolkata, India*

Undergraduate Research Assistant, Adviser: Dr. Swagatam Das — *May 2015 - Aug. 2016*

- Performed a study on the robustness of alternate distance metrics to noise and outliers for k-NN.

Publications

Peer-reviewed Conference Proceedings

4. **Arka Daw**, Jie Bu, Sifan Wang, Paris Perdikaris, and Anuj Karpatne. *"Mitigating Propagation Failures in PINNs using Evolutionary Sampling."* (under submission)
3. Jie Bu*, **Arka Daw***, M. Maruf*, and Anuj Karpatne. *"Learning Compact Representations of Neural Networks using DiscriminAtive Masking (DAM)."* In Proceedings of the 35th Conference on Neural Information Processing Systems (NeurIPS '21).**(*equal contribution)**
2. **Arka Daw***, M. Maruf*, and Anuj Karpatne. *"PID-GAN: A GAN Framework based on a Physics-informed Discriminator for Uncertainty Quantification with Physics."* In Proceedings of the 27th ACM SIGKDD Conference on Knowledge Discovery & Data Mining (KDD '21).**(*equal contribution)**
1. **Arka Daw** , R. Quinn Thomas, Cayelan C. Carey, Jordan S. Read, Alison P. Appling, and Anuj Karpatne. *"Physics-Guided Architecture (PGA) of Neural Networks for Quantifying Uncertainty in Lake Temperature Modeling."* In Proceedings of the 2020 SIAM International Conference on Data Mining (SDM '20) (pp. 532-540).

Book Chapters

2. **Arka Daw** , R. Quinn Thomas, Cayelan C. Carey, Jordan S. Read, Alison P. Appling, and Anuj Karpatne,*"Incorporating monotonic constraints in the architecture of neural networks for quantifying uncertainty in lake temperature modeling,"* In *"Knowledge-guided Machine Learning Accelerating Discovery using Scientific Knowledge and Data,"* A. Karpatne, R. Kanan and V. Kumar (Eds.), CRC Press, 2022.

1. **Arka Daw**, Anuj Karpatne, William Watkins, Jordan Read, Vipin Kumar, *"Physics-guided Neural Networks (PGNN): An Application in Lake Temperature Modeling,"* In *"Knowledge-guided Machine Learning Accelerating Discovery using Scientific Knowledge and Data,"* A. Karpatne, R. Kanan and V. Kumar (Eds.), CRC Press, 2022.

Peer-reviewed Workshop Proceedings

7. **Arka Daw**, Kyongmin Yeo, Anuj Karpatne and Levente Klein. *"Source Identification and Field Reconstruction of Advection-Diffusion Process from Sparse Sensor Measurements."* In Machine Learning and the Physical Sciences (ML4PS) Workshop at NeurIPS 2022.

6. **Arka Daw**, Kyongmin Yeo, Anuj Karpatne and Levente Klein. *"Multi-task Learning for Source Attribution and Field Reconstruction for Methane Monitoring."* In Digital Twins for Accelerated Discovery of Climate and Sustainability workshop (ADoCS) at IEEE Big Data 2022.

5. **Arka Daw**, Jie Bu, Sifan Wang, Paris Perdikaris and Anuj Karpatne. *"Rethinking the Importance of Sampling in Physics-informed Neural Networks."* In 3rd symposium on Knowledge-Guided AI (KGML) at Association for the Advancement of Artificial Intelligence (AAAI) 2022.

4. **Arka Daw***, M. Maruf*, and Anuj Karpatne. *"PID-GAN: A GAN Framework based on a Physics-informed Discriminator for Uncertainty Quantification with Physics."* In 2nd symposium on Science-Guided AI (SGAI) at Association for the Advancement of Artificial Intelligence (AAAI) 2021. **(*equal contribution)**

3. **Arka Daw**, M. Maruf, and Anuj Karpatne., *"Physics-Informed Discriminator (PID) for Conditional Generative Adversarial Nets"*. In Machine Learning and the Physical Sciences (ML4PS) Workshop at NeurIPS 2020.

2. **Arka Daw** , R. Quinn Thomas, Cayelan C. Carey, Jordan S. Read, Alison P. Appling, and Anuj Karpatne. *"Physics-Aware Architecture for Neural Networks for Uncertainty Quantification in Lake Temperature Modelling"*. In 3rd Physics Informed Machine Learning (PIML) Workshop 2020 at Los Alamos National Laboratory (LANL).

1. **Arka Daw**, and Anuj Karpatne. *"Physics-aware Architecture of Neural Networks for Uncertainty Quantification: Application in Lake Temperature Modeling."* In Fragile Earth (FEED) Workshop in 2019 Knowledge Discovery and Data Mining (KDD) Conference.

Preprint

1. Abinash Padhi*, **Arka Daw***, Medha Sawhney, Maahi M. Talukder, Atharva Agashe, Sohan Kale, Anuj Karpatne and Amrinder Nain. *"Deep Learning Enabled Label-free Cell Force Computation in Deformable Fibrous Environments"*. **(*equal contribution)**

Invited Talks

September 2022	**"Uncertainty quantification with Physics-informed Machine Learning"**, Allan Turing Institute, London, UK.
December 2021	**"Advanced Topics in Deep Learning"**, guest lecture for CS 5525 (Data Analytics), Virginia Tech.
July 2020	**"Deep Learning for Mechanobiologists: A Case Study on using Generative Models for Estimating Single Cell Forces"**, Department of Mechanical Engineering, Virginia Tech.

Honors & Awards

2020	SIAM Data Mining (SDM) Doctoral Forum Travel Award	*Blacksburg, USA*
2019	Knowledge Discovery and Data Mining (KDD) Conference Travel Grant	*Blacksburg, USA*
2017	DAAD-WISE (German Academic Exchange Services) Fellowship	*Münster, Germany*
2014	'INSPIRE' Scholarship, MHRD Department, Govt. of India.	*Delhi, India.*

Technical Skills

Languages	Python, MATLAB, Java, C., SQL
Deep Learning Frameworks	PyTorch, JAX, Tensorflow, Keras.
Relevant coursework	Deep Learning, Graph Machine Learning, Data Analytics - I/II, Advanced Machine Learning, Theory of Algorithms.

Service

Reviewer	IEEE-TNNLS (2020,2021), SGAI-AAAI (2021,2022), ML4PS-NeurIPS (2021, 2022), AI4Science-NeurIPS (2022).
External Reviewer	SIGKDD 2021, 2022
PC Member	SGAI-AAAI 2021, 2022
Session Chair	SDM 2021 (Spatiotemporal Data -II).
Student Volunteer	SIGKDD 2019