ANUJ KARPATNE

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Dept. of CS, Virginia Tech
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APPOINTMENTS

Associate Professor 2023 – present
Department of Computer Science, Virginia Tech

Dean's Fellow 2025 – present
College of Engineering, Virginia Tech

Faculty Fellow 2025 – present
College of Engineering, Virginia Tech

Assistant Professor 2018 – 2023
Department of Computer Science, Virginia Tech

PostDoctoral Associate 2017 – 2018
Kumar Research Group, University of Minnesota (UMN)

EDUCATION

PhD, Computer Science 2011 – 2017
University of Minnesota (UMN), Twin Cities
Thesis: "Predictive Learning with Heterogeneity in Populations"
Advisor: Vipin Kumar

Integrated M.Tech, Mathematics and Computing 2006 – 2011
Indian Institute of Technology Delhi (IITD)

RESEARCH INTERESTS

Knowledge-guided Machine Learning (KGML); AI for Science; Physics-informed Machine Learning.

FUNDING

Total Amount Across **10** External Grants: **$49,230,351**. Amount Responsible as Lead PI or Site PI: **$4,479,690**. Personal Share: **$3,720,526**.

- USDA National Institute of Food and Agriculture **(NIFA)**: "Enabling Farmer Discovery and Managing Critical Tradeoffs with the Emergence of National Scale Carbon Markets"; **Site PI**; **$10,000,000** (site amount and personal share: $499,525); Duration: 01/01/2025 to 12/31/2029; Collaborative project with Ohio State University as the lead institution.
- NSF-DBI-2412389: "**PIPP Phase II**: Community Empowering Pandemic Prediction and Prevention from Atoms to Societies (COMPASS)"; **co-PI**; **$18,000,000** (personal share: $664,698); Duration: 08/15/2024 to 08/14/2031; Collaborative project with Virginia Tech as the lead institution.
- NSF-IIS-2239328: "**CAREER**: Unifying Scientific Knowledge with Machine Learning for Forward, Inverse, and Hybrid Modeling of Scientific Systems"; **PI**; **$595,738**; Duration: 07/01/2023 to 06/30/2028.
- NSF-CCF-2200045: "**PIPP Phase I**: Community Informed Computational Prevention of Pandemics"; **co-PI**; **$1,000,000** (personal share: $146,976); Duration: 05/01/2022 to 10/31/2023.

- NSF-DEB-2213550: "Collaborative Research: MRA: Advancing process understanding of lake water quality to macrosystem scales with knowledge-guided machine learning"; **Site PI**; **$1,093,239** (site amount: $567,340; personal share: $302,842); Duration: 09/01/2022 to 08/ 31/2026; Collaborative project from the **Macrosystems Biology (MSB)** program with University of Wisconsin as lead institution.
- Naval Engineering Education Consortium (**NEEC**): "Seafloor Characterization From Free Fall Penetrometers Using Machine Learning"; **co-PI**; **$390,766** (personal share: $138,839); Duration: 04/01/2022 to 03/31/2025.
- NSF-OAC-2118240: "**HDR Institute**: Imageomics: A New Frontier of Biological Information Powered by Knowledge-Guided Machine Learning"; **Site PI**; **$14,969,077** (site amount: $1,340,635; personal share: $578,000); Duration: 10/01/2021 to 09/30/2026; Collaborative project with Ohio State University as the lead institution. I am one of the 4 co-PIs across 11 institutions of this project.
- NSF-IIS-2107332: "**III: Medium**: Physics-guided Machine Learning for Predicting Cell Trajectories, Shapes, and Interactions in Complex Dynamic Environments"; **Lead PI**; **$1,000,000** (personal share: $317,456); Duration: 10/01/2021 to 09/30/2025.
- NSF-OAC-1940247: "Collaborative Research: Biology-guided neural networks for discovering phenotypic traits"; **Site PI**; **$1,982,810** (site amount and personal share: $422,000); Duration: 10/01/2019 to 09/30/2022; Collaborative project from the **HDR Ideas Labs** program with Battelle as the lead institution.
- NSF-IIS-2026710: "**EAGER**: Collaborative Research: III: Exploring Physics Guided Machine Learning for Accelerating Sensing and Physical Sciences"; **Site PI**; **$198,721** (site amount and personal share: $54,452); Duration: 05/01/2020 to 04/30/2022; Collaborative project with Ohio State University as the lead institution.

TEACHING

Instructor for "CS 5806: Machine Learning II", Virginia Tech, Spring 2025.

Instructor for "CS 3654: Introduction to Data Analytics and Visualization", Virginia Tech, Fall 2024.

Instructor for "CS 5805: Machine Learning I", Virginia Tech, Spring 2024.

Instructor for "CS 6814: Science-guided Machine Learning", Virginia Tech, Fall 2023.

Instructor for "CS 4664: Data-Centric Computing Capstone", Virginia Tech, Fall 2022.

Instructor for "CS (STAT) 5525: Data Analytics I", Virginia Tech, Spring 2022.

Instructor for "CS (STAT) 5525: Data Analytics I", Virginia Tech, Fall 2021.

Instructor for "CS (STAT) 5525: Data Analytics I", Virginia Tech, Spring 2021.

Instructor for a session on "Science Guided Machine Learning" at the Geilo Winter School, Norway (conducted virtually), 2021.

Instructor for "CS 6804: Science-guided Machine Learning", Virginia Tech, Fall 2020.

Instructor for "CS 4824 / ECE 4424: Machine Learning", Virginia Tech, Spring 2020.

Instructor for "CS(STAT) 5525: Data Analytics I", Virginia Tech, Fall 2019.

Instructor for "CS(STAT) 5525: Data Analytics I", Virginia Tech, Spring 2019.

Instructor for "CS 6804: Machine Learning Meets Physics", Virginia Tech, Fall 2018.

Instructor for Summer School on "Intelligent Systems for Geosciences (IS-GEO)", UT Austin, 2017.

HONORS AND AWARDS

Received the **Faculty Fellow** award for Excellence in Research from College of Engineering (COE) at Virginia Tech in 2025.

Recognized by a **NAIRR Pilot Award** invited to speak at the **White House** in 2024.

Received the **NSF CAREER Award** in 2023.

Received the **Outstanding New Assistant Professor Award** by the College of Engineering at Virginia Tech in 2022.

Received the **Rising Star Faculty Award** by the Department of Computer Science at Virginia Tech in 2021.

Named the **Inaugural Research Fellow** by the Intelligent Systems for Geosciences (IS-GEO), sponsored by Petrobras, for 2019.

Recipient of the **Doctoral Dissertation Fellowship** by the University of Minnesota for 2015.

Recipient of University of Minnesota Informatics Institute **(UMII) Graduate Fellowship** for 2015.

Recipient of **Student Travel Awards** at SIAM International Conference on Data Mining (SDM) 2014 and 2015, IEEE International Conference on Data Mining (ICDM) 2015, Conference on Intelligent Data Understanding (CIDU) 2012, and Climate Informatics Workshop 2013, 2014, and 2016.

Recipient of two consecutive **Director's Merit Awards** at IIT Delhi.

MEDIA COVERAGE

Marissa Pederson, "CS&E Alum Anuj Karpatne Featured at White House Event for AI Research," *UMN CSE Department News*, June 2024 Web Link.

Jeffrey Mervis, "New U.S. AI network aims to make supercomputers available to more researchers," *Science News*, May 2024 Web Link.

Mike Allen, "VA Tech Researchers on Quest for Clean Water," *The Roanoke Star*, July 2024 Web Link.

Barbara Micale, "Sanghani Center and CAIA cultivate transdisciplinary research in agriculture, AI, and data analytics," *VT News*, April 2024 Web Link.

Tonia Moxley, "Making a CAREER on bridging scientific knowledge and AI," *VT News*, August 2023 Web Link.

Barbara Micale, "Scientists partner on multi-university grant to establish a field of 'imageomics'," *VT News*, March 2022 Web Link.

Barbara Micale, "Researchers receive grant to predict the mechanics of living cells," *VT News*, October 2021 Web Link.

ADVISING AND MENTORING ROLES

Current Ph.D Students (8 in total):

- *Medha Sawhney*, Dept. of Computer Science, Virginia Tech (Fall 2021 – present).
- *Kazi Sajeed Mehrab*, Dept. of Computer Science, Virginia Tech (Fall 2022 – present).
- *Abhilash Neog*, Dept. of Computer Science, Virginia Tech (Fall 2022 – present).
- *Mridul Khurana*, Dept. of Computer Science, Virginia Tech (Fall 2022 – present).
- *Sepideh Fatemi Khorasgani*, Dept. of Computer Science, Virginia Tech (Spring 2024 – present).
- *Blessy Antony*, Dept. of Computer Science (co-advised with Prof. T.M. Murali), Virginia Tech (Fall 2023 – present).

- *Amartya Dutta*, Dept. of Computer Science (co-advised with Prof. T.M. Murali, Virginia Tech (Fall 2025 – present).
- *Snehal More*, Dept. of Forest Resources and Environmental Conservation (co-advised with Prof. Randolph Wynne), Virginia Tech (Fall 2019 – present).

Graduated Ph.D. students (5 in total):

- *Md Abdullah Al Maruf*, Ph.D. in Computer Science, Virginia Tech, Graduated in Fall 2024, First Employment: Amazon Research.
- *Arka Daw*, Ph.D. in Computer Science, Virginia Tech, Graduated in Fall 2023, First Employment: Distinguished Staff Fellow (DSF) at Oak Ridge National Laboratory.
- *Mohannad Elhamod*, Ph.D. in Computer Science, Virginia Tech, Graduated in Spring 2023, First Employment: Clinical Assistant Professor in the Questrom School of Business at Boston University.
- *Jie Bu*, Ph.D. in Computer Science, Virginia Tech, Graduated in Spring 2023, First Employment: Apple Research.
- *Nikhil Muralidhar*, Ph.D. in Computer Science (co-advised with Prof. Naren Ramakrishnan), Virginia Tech, Graduated in Summer 2022, First Employment: Tenure-track Assistant Professor in Computer Science at Stevens Institute of Technology.

Graduated M.S. students (11 in total):

- *Aanish Pradhan*, M.S. in Computer Science, Virginia Tech, Graduated in Spring 2025.
- *Harish Babu Manogaran*, M.S. in Electrical and Computer Engineering (co-advised with Dr. Lynn Abbott), Virginia Tech, Graduated in Fall 2024, First Employment: Stealth Startup in California on Augmented Reality + AI.
- *Suredrabikram Thapa*, M.S. in Computer Science (co-advised with Dr. Abhijit Sarkar), Virginia Tech, Graduated in Summer 2023, First Employment: Research Faculty at Virginia Tech Transportation Institute (VTTI).
- *Naveen Gupta*, M.S. in Computer Science, Virginia Tech, Graduated in Spring 2023, First Employment: Hughes Network.
- *Hirva Bhagat*, M.S. in Computer Science (co-advised with Prof. Lynn Abbott), Virginia Tech, Graduated in Spring 2023, First Employment: Goldman Sachs.
- *Prathamesh Kalyan Mandke*, M.Eng. in Electrical and Computer Engineering (co-advised with Prof. Lynn Abbott), Virginia Tech, Graduated in Spring 2021, First Employment: Qualcomm.
- *Reza Sepasdar*, M.S. in Computer Science (co-advised with Prof. Maryam Shakiba), Virginia Tech, Graduated in Spring 2021, First Employment: IMS Engineers.
- *Ioannis Papakis*, M.S. in Computer Science (co-advised with Dr. Abhijit Sarkar), Virginia Tech, Graduated in Spring 2021, First Employment: Bertrandt.
- *Arya Shahadi*, M.S. in Computer Science (co-advised with Prof. Bahareh Nojabaei), Virginia Tech, Graduated in Spring 2021, First Employment: Lowe's.
- *Sandhya Bhaskar*, M.S. in Electrical and Computer Engineering (co-advised with Prof. Kevin Kochersberger), Virginia Tech, Graduated in Spring 2020, First Employment: Ford Research.
- *Zheng Li*, M.S. in Computer Science, Virginia Tech, Graduated in Spring 2020, First Employment: Vanguard.

PROFESSIONAL SERVICE

Associate Editor for the ACM Transactions on Knowledge Discovery from Data (TKDD) journal: 2024 — present.

Co-Editor-in-Chief (EiC) of the ACM Special Interest Group in Artificial Intelligence (SIGAI) quarterly newsletter, "AI Matters": 2019 — present.

Senior Program Committee Member for AAAI 2025, AAAI 2024, KDD 2023, SDM 2025, SDM 2024, SDM 2023, SDM 2022.

Poster Co-chair for KDD 2022, IEEE Big Data 2020.

Workshop Co-chair for SDM 2024, KDD 2019.

Co-organizer for the following workshops, symposiums, and tutorials:

- "Workshop on GenAI4Science: Integrating Scientific Knowledge into Generative AI' at the University of Minnesota, 2025.
- "GenAI Day" in the College of Science & Engineering at the University of Minnesota, sponsored by the Data Science Initiative, 2025.
- "Second Bridge Program on Knowledge-guided Machine Learning" at AAAI 2025.
- "Second Workshop on Imageomics" at AAAI 2025.
- "Knowledge-guided Machine Learning Workshop (KGML2024)" at University of Minnesota, 2024.
- "Summer Tutorial on Knowledge-guided Machine Learning (KGML)" at Oak Ridge National Laboratory (ORNL), July 2024.
- "Bridge Program on Knowledge-guided Machine Learning" at AAAI 2024.
- "First Workshop on Imageomics" at AAAI 2024.
- "First European Knowledge-Guided Machine Learning Workshop" at ECML-PKDD 2023.
- "Workshop on Synergy of Machine Learning and Physical Sciences" at ICML 2023.
- "Third Symposium on Knowledge-guided Machine Learning" held as part of the AAAI Fall Symposium Series 2022.
- "International Sustainable AI Workshop (ISAW)" held in conjunction with IEEE International Conference on Data Mining (ICDM) 2022.
- "Second Symposium on Science-guided AI" held as part of the AAAI Fall Symposium Series 2021.
- Symposium on "Combining Artificial Intelligence and Machine Learning with Physics Sciences" held as part of the AAAI Spring Symposium Series 2021.
- Session on "Knowledge Guided Machine Learning in Biology" in the Great Lakes Bioinformatics (GLBIO) Conference 2021.
- Tutorial on "Physics-Guided AI for Large-Scale Spatiotemporal Data" at KDD 2021.
- Symposium on "Physics-guided AI for Accelerating Scientific Discovery" held as part of the AAAI Fall Symposium Series 2020.
- Session on "How AI and Knowledge Centers are Changing Societal Views of Critical Earth Resources" at *American Association for the Advancement of Science (AAAS) Annual Meeting*, 2019.
- Workshop on "Fragile Earth: Theory Guided Data Science to Enhance Scientific Discovery (FEED)" at *KDD*, 2018.

Convener for session on "Intelligent Systems for Geosciences: Accelerating Discovery and Building Community" at *AGU Fall Meeting*, 2017.

Program Committee Member for the following workshops and conferences:

- *NAIRR* Pilot Annual Meeting 2025, *AAAI* 2023, 2022, 2021, 2020 (AI for Social Impact Track), 2019; *KDD* 2022, 2021, 2020, 2019, 2018; *SDM* 2021, 2020, 2019; *AISTATS* 2024, 2023; *PAKDD* 2024; *SDM Workshop on Mining Big Data in Climate and Environment* 2017; *IEEE Big Data* 2020; *IJCAI* 2020, 2013; ICDM 2024.

Reviewer for the following conferences and journal proceedings:

- *ICLR 2025, ICCV 2025, CVPR 2025, NeurIPS 2019, ICML 2019, Medical Physics 2020, Remote Sensing of Environment 2019, Wiley Ecosphere 2018, IEEE Transactions on Knowledge and Data Engineering (TKDE) 2018, Elsevier: Information Sciences 2012.*

TALKS

[T45] "Foundations and Frontiers of Generative AI for Science," Opening Session in **Workshop on Generative AI for Science & Engineering** at the University of Minnesota, Minneapolis, August 13, 2025.

[T44] "Navigating Research Landscape in Knowledge-guided Machine Learning: Problems, Methods, and Emerging Opportunities," Keynote Talk at the **KGML Workshop at University of Michigan** sponsored by Schmidt Sciences AI in Science program, Ann Arbor, August 8, 2025.

[T43] "Knowledge-guided Machine Learning: Advancing AI for Science and the Science of AI by Incorporating Scientific Knowledge in AI," Invited Talk at the **AI for Science Day** at KDD conference, Toronto, August 6, 2025.

[T42] "Knowledge-guided Machine Learning for Discovering Biological Traits in the Emerging Field of Imageomics," **Keynote Talk** at the **AI for Biodiversity Symposium** at the **University of Florida**, Gainesville, April 10, 2025.

[T41] "Knowledge-guided Machine Learning: Current Trends and Opportunities for Incorporating Scientific Knowledge in Machine Learning," Invited Talk in the **Frontiers of Machine Learning and AI Seminar Series** at the **University of Southern California**, Los Angeles, March 12, 2025.

[T40] "Knowledge-guided Machine Learning: Current Trends and Opportunities for Incorporating Scientific Knowledge in Machine Learning," Invited Talk in the Seminar Series at the **Center for Limnology in University of Wisconsin**, Madison, February 12, 2025.

[T39] "Knowledge-guided Machine Learning: Current Trends and Opportunities for Incorporating Scientific Knowledge in Machine Learning," Invited Seminar Talk in the **Kotak IISc AI-ML Talk Series** at the **Indian Institute of Science (IISc)**, Bengaluru, India, January 7, 2025.

[T38] "Knowledge-guided Machine Learning: Current Trends and Future Prospects in Combining Scientific Knowledge with Machine Learning," Invited Seminar Talk at the **University of Michigan**, Ann Arbor, October 10, 2024.

[T37] "Knowledge-guided Machine Learning: Current Trends and Future Prospects for Applications in Environmental Sustainability," **Keynote Talk** at the **Fragile Earth: Generative and Foundational Models for Sustainable Development Workshop** held as part of the KDD conference, Barcelona, August 26, 2024.

[T36] "Toward Foundation Models in Science Powered by KGML," Invited Talk at **the 2nd NSF**

Workshop on AI-Enabled Scientific Revolution, Minneapolis, August 6, 2024.

[T35] "Knowledge-guided Machine Learning: Current Trends and Future Prospects in Combining Scientific Knowledge with Machine Learning," Invited Talk at the **COEAI-SPARC Workshop on Hybrid Physics-AI Models for Climate, Weather and Water at IIT Kharagpur**, (virtual talk), June 20, 2024.

[T34] "Knowledge-guided Machine Learning (KGML) for Discovering Biological Traits from Images," Invited Talk at the **iDigBio Advances in Digital Media Workshop at the Yale Peabody Museum**, (virtual talk), June 11, 2024.

[T33] "LakeGPT: A Foundation Model for Aquatic Sciences," Invited Talk at the **AI Expo for National Competitiveness**, May 7, 2024.

[T32] "LakeGPT: A Foundation Model for Aquatic Sciences," Invited Talk at a **White House Event Sponsored by OSTP**, May 6, 2024.

[T31] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **Department of Statistics Seminar Series at Virginia Tech**, February 14, 2024.

[T30] "Knowledge-guided Machine Learning: Overview and Applications of Combining Scientific Knowledge with Machine Learning," Invited Talk in the **ORNL Core Universities AI Workshop**, November 1, 2023.

[T29] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **Earth Science Information Partners (ESIP) Machine Learning Cluster Meeting**, (virtual talk), October 20, 2023.

[T28] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **NSF-funded Machine Learning Potentials - StAtus and FuturE (MLP-SAFE) Workshop**, (virtual talk), July 19, 2023.

[T27] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the Seminar Series in the **Department of Mathematics Seminar Series at the University of California Santa Barbara**, (virtual talk), February 17, 2023.

[T26] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Guest Lecture in **Graduate Course on Exploratory Methods in Planetary Science at Louisiana State University**, (virtual talk), February 16, 2023.

[T25] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," **Keynote Talk** at the **17th Workshop on Spatial and Spatiotemporal Data Mining (SSTDM) at International Conference on Data Mining (ICDM) 2022**, Orlando, FL (virtual talk), November 28, 2022.

[T24] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **ORNL Core Universities AI Workshop**, October 28, 2022.

[T23] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **Dynamic Data Driven Applications**

Systems (DDDAS) Conference at MIT (virtual talk), October 6, 2022.

[T22] "Knowledge-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," **Graduate Seminar Series in the Department of Computer Science at Virginia Tech**, September 9, 2022.

[T21] "Science-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **AI-guided Materials Thrust Workshop organized by the College of Engineering at Virginia Tech**, April 8, 2022.

[T20] "Science-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **ML/AI Speaker Series of the Dept. of Civil and Environmental Engineering at Virginia Tech**, Feb 25, 2022.

[T19] "Biology-guided Neural Networks: Integrating Biological Knowledge with Neural Networks for Discovering Phenotypic Traits from Fish Images," Invited Talk in the **Session on Aquatic Sciences of the NSF-funded Second Workshop on Knowledge Guided Machine Learning**, August 10, 2021.

[T18] "Science-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **Seminar Series of the Dept. of Earth System Science at Stanford University**, April 21, 2021.

[T17] "Science-guided Machine Learning: Advances in An Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **"Small Data Approaches in Earthquake Engineering" Session at the Earthquake Engineering Research Institute (EERI) Annual Meeting**, March 25, 2021.

[T16] "Science-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk as a **Featured Speaker in the University of Idaho Institute for Modeling Collaboration and Innovation Seminar Series**, March 11, 2021.

[T15] "Science-guided Machine Learning: Advances in An Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk at the **Engineering Mechanics Seminar Series in the Dept. of Biomedical Engineering and Mechanics (BEAM) at Virginia Tech**, January 27, 2021.

[T14] "Science-guided Machine Learning: Advances in An Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk at the **Indian Symposium on Machine Learning (IndoML)**, December 18, 2020.

[T13] "Science-guided Machine Learning: Advances in An Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk in the **Plenary Session of the NSF-funded Workshop on Knowledge Guided Machine Learning: A Framework for Accelerating Scientific Discovery**, August 18, 2020.

[T12] "Physics-guided Machine Learning: Advances in an Emerging Paradigm Combining Scientific Knowledge with Machine Learning," Invited Talk at the **Macromolecules Innovation Institute (MII) Workshop on "Learning About Machine Learning"**, November 4, 2019.

[T11] "Theory-guided Data Science: Foundations of an Emerging Paradigm Combining Physics and Machine Learning," **Keynote Talk** at **DARPA Physics of AI (PAI) Review Meeting**, Ann Arbor, MI, October 2, 2019.

[T10] "Theory-guided Data Science: How Can Machine Learning and Physical Knowledge Come Together to Accelerate Scientific Discovery," Invited Talk at **Oak Ridge National Lab (ORNL) AI Workshop**, Oak Ridge, TN, September 20, 2019.

[T9] "Physics-guided Data Science: Challenges and Opportunities in Combining Machine Learning with Physical Knowledge in Geosciences," Invited Talk at the **Virginia Tech Office of GIS and Remote Sensing (OGIS) Research Symposium**, April 26, 2019.

[T8] Lightning Talk Representing the NSF Expeditions project: "Understanding Climate Change: A Data-driven Approach" at the **NSF Expeditions in Computing PI Meeting: 10 Years of Transforming Science and Society**, Washington D.C., December 10, 2018.

[T7] "Theory-guided Data Science: A New Paradigm for Scientific Discovery from Data," Invited Talk at **UCLA IPAM Workshop on HPC for Computationally and Data-Intensive Problems**, November 9, 2018.

[T6] "Theory-guided Data Science: A New Paradigm for Scientific Discovery from Data," Invited Talk at **IS-GEO Seminar for Energy Industry (with support from Petrobras) at Texas Advanced Computing Center (TACC)**, September 20, 2018.

[T5] "Theory-guided Data Science: A New Paradigm for Scientific Discovery Combining Physics with Machine Learning," Invited CISL Seminar Talk at **National Center for Atmospheric Research (NCAR)**, May 3, 2018.

[T4] "Theory-guided Data Science: A New Paradigm for Scientific Discovery from Data," Invited Talk at **Oak Ridge National Laboratory (ORNL)**, March 6, 2018.

[T3] "How Can Physics Inform Deep Learning Methods in Earth System Science?: Recent Progress and Future Prospects," **Keynote Talk** at **ICDM Workshop on Data Mining in Earth System Science**, November 18, 2017.

[T2] "Theory-guided Data Science: A New Paradigm for Scientific Discovery in the Era of Big Data," Invited Talk at **American Institute of Chemical Engineers (AIChE) Annual Meeting**, October 30, 2017.

[T1] "Global Monitoring of Inland Surface Water Dynamics Using Remote Sensing Data," Invited Talk at **96th American Meteorological Society Annual Meeting**, January 11–14, 2016.

PANEL DISCUSSIONS

[PD8] "Data-Centric Machine Learning in Climate Applications," Panel Discussion at the **ICLR Tackling Climate Change with Machine Learning Workshop**, Singapore, April 28, 2025.

[PD7] "Interpretability and Inductive Bias in ML for Physical Sciences," Panel Discussion at the **NeurIPS Machine Learning for Physical Sciences Workshop**, New Orleans, LA, December 15, 2023.

[PD6] "Leveraging AI to Extend Specimen Networks," Panel Discussion at the **Fifth Annual Digital Data Conference Organized by iDigBio**, Virtual, June 9, 2021.

[PD5] " AI Research Challenges in Accelerating Material Science and Engineering," Panel Discussion at the **NSF-funded Workshop on Accelerating Materials Discovery, Design, and Synthesis: A Grand Challenge for Artificial Intelligence**, Virtual, April 9, 2021.

[PD4] "Data Mining Challenges and Opportunities for Earth Science," Panel Discussion at the **ACM SIGKDD 2019 Earth Day Session**, Anchorage, AK, August 5, 2019.

[PD3] "Augmenting Advances in the Next Century: Why AI and Knowledge-Centered Research in Geosciences Is Important Now and How It Will Change the Next Century I," Panel Discussion Session at the **American Geophysical Union (AGU) Annual Meeting**, Washington D.C., December 10, 2018.

[PD2] "Theory-guided Data Science: A New Paradigm for Scientific Discovery," Panel Discussion at the **International Conference on Scientific and Statistical Database Management (SSDBM)**, June 29, 2017.

[PD1] "Understanding and Narrowing Gaps Between Data Science and Mechanistic Theories in Physical Sciences," Panel Discussion at the **SDM Workshop on Mining Big Data in Climate and Environment**, April 29, 2017.

PUBLICATIONS

Note: Authors that are my direct advisees are underlined.

BOOKS

[B2] **A. Karpatne**, R. Kannan, and V. Kumar (Eds.), "Knowledge-guided Machine Learning: Accelerating Discovery using Scientific Knowledge and Data," *Data Mining and Knowledge Discovery Series of Chapman and Hall/CRC Press*, ISBN-9780367693411, 2022.

[B1] P. Tan, M. Steinbach, **A. Karpatne**, and V. Kumar "Introduction to Data Mining (2^{nd} Ed.)," *Pearson Addison–Wesley*, ISBN-13: 978-0133128901, 2018.

JOURNAL ARTICLES

[J31] **A. Karpatne**, A. Deshwal, X. Jia, W. Ding, M. Steinbach, A. Zhang, and V. Kumar, "AI-enabled scientific revolution in the age of generative AI: second NSF workshop report," *npj Artificial Intelligence*, 1, 18, 2025.

[J30] S. Lynch, J. LaMountain, B. Fan, J. Bu, A. Raju, D. Wasserman, **A. Karpatne**, and V. Podolskiy, "Physics-Guided Hierarchical Neural Networks for Maxwell's Equations in Plasmonic Metamaterials," *ACS Photonics*, 12(8), 4279-4288, 2025 (Impact Factor: 6.7).

[J29] B. McAfee, A. Pradhan, A. Neog, S. Fatemi, R. Hensley, M. Lofton, **A. Karpatne**, C. Carey, and P. Hanson, "LakeBeD-US: a benchmark dataset for lake water quality time series and vertical profiles," *Earth System Science Data*, 17, 3141-3165, 2025 (Impact Factor: 11.2).

[J28] M.A. Balk, J. Bradley, M. Maruf, B. Altintaş, Y. Bakiş, H.L. Bart Jr, D. Breen, C.R. Florian, J. Greenberg, **A. Karpatne**, K. Karnani, P. Mabee, J. Pepper, D. Jebbia, T. Tabarin, X. Wang, and H. Lapp, "A FAIR and modular image-based workflow for knowledge discovery in the emerging field of imageomics," *Methods in Ecology and Evolution*, 15, 1129–1145, 2024 (Impact Factor: 7.78).

[J27] M. Sawhney, B. Karmarkar, E.J. Leaman, A. Daw, **A. Karpatne**, and B. Behkam, "Motion Enhanced Multi-Level Tracker (MEMTrack): A Deep Learning-Based Approach to Microrobot Tracking in Dense and Low-Contrast Environments," *Advanced Intelligent Systems*, 6: 2300590, 2024 (Impact Factor: 6.8).

[J26] L. Bass, L.H. Elder, D.E. Folescu, N. Forouzesh, I.S. Tolokh, **A. Karpatne**, and A.V. Onufriev, "Improving the Accuracy of Physics-Based Hydration-Free Energy Predictions by Machine Learning the Remaining Error Relative to the Experiment," *Journal of Chemical Theory and Computation*, 20 (1), 396-410, 2024 (Impact Factor: 5.7).

[J25] R. Ladwig, A. Daw, E.A. Albright, C. Buelo, **A. Karpatne**, M.F. Meyer, A. Neog, P.C.

Hanson, and H.A. Dugan, "Modular Compositional Learning Improves 1D Hydrodynamic Lake Model Performance by Merging Process-based Modeling with Deep Learning," *Journal of Advances in Modeling Earth Systems (JAMES)*, 16, e2023MS003953, 2024 (Impact Factor: 6.8).

[J24] J. Zhang, P. Srivatsa, F. H. Ahmadzai, Y. Liu, X. Song, **A. Karpatne**, Z. Kong, and B. N. Johnson, "Improving Biosensor Accuracy and Speed Using Dynamic Signal Change and Theory-guided Deep Learning," *Biosensors and Bioelectronics*, 246, 115829, 2024 (Impact Factor: 12.6).

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