Ankit Shrivastava

Computational and Machine Learning Scientist

Knoxville, TN, USA
www.ashriva.in
ashriva16

Applied Mathematician at Computational Science and Mathematics Division at Oak Ridge National Lab. I specialize in scientific machine learning, uncertainty quantification, computational modeling to address diverse research challenges in engineering.

Education

2017–21 **PhD in Computational Mechanics**, *Carnegie Mellon University*, Pittsburgh, USA
- Thesis: Elucidating the origin of heterogeneous stresses in granular and microstructured materials using data science methods.
- Advisors: Prof. Kaushik Dayal, Prof. Hae Young Noh

2019–21 **MS in Machine Learning**, *Carnegie Mellon University*, Pittsburgh, USA

2015–17 **MS in Computational Science**, *Indian Institute of Science*, Bangalore, India
- Thesis: Numerical study of magneto-hydrodynamics for turbulent flow using the projection-based variational multiscale finite element method.
- Advisor: Prof. Sashikumaar Ganesan

2009–13 **BS in Civil Engineering**, *Indian Institute of Technology*, Kharagpur, India
- Thesis: Numerical computation of flow in open channel cross sections.
- Advisor: Prof. Anirban Dhar

Professional Experience

Nov 24–Present **Postdoctoral Fellow**, *Oak Ridge National Laboratory*, Oak Ridge, TN, USA
- Developing an active learning microservice for efficient experimental design.
- Developing a Python-based solution for blackout avoidance in power grids through adaptive policy design.

2022– Oct 24 **Postdoctoral Fellow**, *Sandia National Laboratories*, Livermore, California, USA
- Design of multimodal machine learning, Bayesian optimization, manifold learning, and signal processing methods for materials and mechanics problems.

2014–15 **Structural Engineer**, *Thornton Tomasetti*, Mumbai, India

2013–14 **Senior Analyst**, *Eastbrook Landholdings*, Bhubaneswar, India

Honors and Awards

2024 NSF travel award, *The Industrialization of SciML by the Institute for Computational and Experimental Research in Mathematics*

2023 Conference travel award, *Mechanistic Machine Learning and Digital Engineering for Computational Science Engineering*

2023 Conference travel award, *US National Congress on Computational Mechanics*

2019 Fenves travel grant, Civil Engineering Department, CMU

2017 Dean's fellowship, Civil Engineering Department, CMU

2015 Ministry of Human Resource Development Scholarship, Govt. of India

2012 IBM Centennial research fellowship, IIT Kharagpur

Publications

Google Scholar
ORCiD: 0000-0003-4445-8817
ResearcherID: AFY-6130-2022

Peer-Reviewed Journal Articles

2025 **A. Shrivastava**, K. Dayal, and H. Y. Noh. "The Roles of Size, Packing, and Cohesion in the Emergence of Force Chains in Granular Packings". In: *Journal of Applied Mechanics* (2025).

2024 **A. Shrivastava**, M. Kalaswad, J. O. Custer, D. P. Adams, and H. N. Najm. "Bayesian optimization for stable properties amid processing fluctuations in sputter deposition". In: *Journal of Vacuum Science & Technology A* (2024).

2023 S. Desai, **A. Shrivastava**, M. D'Elia, H. N. Najm, and R. Dingreville. "Trade-offs in the latent representation of microstructure evolution". In: *Acta Materialia* (2023).

2022 **A. Shrivastava**, J. Liu, K. Dayal, and H. Y. Noh. "Predicting peak stresses in microstructured materials using convolutional encoder-decoder learning". In: *Mathematics and Mechanics of Solids* (2022).

Conference Proceedings

2022 R. Arora and **A. Shrivastava**. "Spatio-temporal super-resolution of dynamical systems using physics-informed deep-learning". In: *AAAI Workshop on AI to Accelerate Science and Engineering*. 2022.

2021 A. Muhammed, **A. Shrivastava**, and B. Biswas. "A parallel Galerkin's moment-based method for finding the resistance of HVDC grounding electrode". In: *22nd International Symposium on High Voltage Engineering (ISH 2021)*. 2021.

Technical Expertise

Machine learning: PyTorch, Tensorflow, R, BoTorch, Bayesian optimization, dimensionality reduction, CNN, PINNs, GenAI, Image and Signal processing

Computing: Python, C, C++, CUDA, OPEN-MP, MPI

Simulations: FEniCS, LAMMPS, Finite element, Molecular dynamics

Selected Projects (** ongoing)

- ** **Multimodal machine learning with small datasets:** Developing a novel multimodal machine learning approach to predict thin film properties and structural information from processing conditions. Used PCA, signal-processing, and autoencoders for joint latent representations of multimodal datasets.
- **Multi constrained Bayesian optimization:** Created a Python-based Bayesian optimization algorithm with a tailored optimization function to drive the development of semiconductor thin film design. The manuscript is currently under review for publication.
- **Physics-informed deep-learning for dynamical systems:** Collaborated and published a physics-informed deep learning-based super-resolution framework, enhancing the spatio-temporal resolution of time-dependent partial differential equation solutions. The publication appeared in the AAAI Workshop.

- **CUDA based evolutionary optimization:** Developed a parallelized code utilizing CUDA for NVIDIA GPUs, optimizing the traveling salesman problem through a hybrid ant colony optimization - river flow dynamics. The parallelization improved computation speedup by 25x for task parallelism and a remarkable 120x enhancement when employing data parallelism.
- **Active learning in graph-based semi-supervised learning:** Implemented active learning to choose optimized labels for semi-supervised learning. Active learning utilized a clique overlap centrality to improve the diversity of labels.
- **Convolutional encoder decoder deep learning:** Developed a Python-based image-based cluster detection and convolutional deep learning algorithm to identify and characterize high-stress clusters in material images. Implemented saliency mapping algorithms to interpret the model's behavior, unveiling critical insights in a publication.
- **Multi-scale finite element in multi-physics problem:** Implemented a projection-based variational multiscale parallelized FEM solver in C++ with MPI for a modified Navier-Stokes equation coupled with a heat equation. This project focused on studying heat transfer through liquid metal under high turbulence, addressing convergence issues encountered by standard finite element and finite volume schemes.
- **MPI based parallelized linear algebra solver:** Implemented an MPI-based numerical solver in C++ for a computational electromagnetics problem, achieving a significant 5.86x speedup. Published the work at the 2021 International Conference on High Voltage Engineering proceedings.

Editorial Work

Journals Reviewed

- *Scientific Reports* 2
- *Mathematics and Mechanics of Solids* 3
- *International Journal for Uncertainty Quantification* 2
- *Journal of the Mechanics and Physics of Solids* 2
- *Journal of Vacuum Science & Technology A: Vacuum, Surfaces, and Films* 2
- *Journal of Applied Mechanics* 1

Teaching and Mentoring

Teaching Assistantships

2018-20 Structural Dynamics and Vibrations, **Carnegie Mellon University**

Guest Lectures

2024 "Machine learning algorithms for Inverse design." In: *Deparment of Mechanical Engineering, Indian Institute of Technology, Bombay*. 2024.

Professional Activities

Session Chair

2024 "Data Sciences and Related Methods". In: *Mathematics of Materials 2024, Society for Industrial and Applied Mathematics*. 2024.

Minisymposia Co-organised

2024 "Machine learning algorithms for accelerating material characterization, discovery, design, and manufacturing processes". In: *World Congress of Computational Mechanics*. 2024.

2024 "Accelerating analysis and design of complex materials via novel numerical methods and machine learning techniques". In: *Mathematics of Materials 2024, Society for Industrial and Applied Mathematics*. 2024.

2024 "Machine learning's role in uncovering insights from heterogeneous materials data". In: *Mathematics of Materials 2024, Society for Industrial and Applied Mathematics*. 2024.

2023 "Integrating machine learning and numerical methods to accelerate engineering design". In: *Mechanistic Machine Learning and Digital Engineering for Computational Science, Engineering and Technology*. 2023.

Professional Speaking Engagements

Invited Talks

2024 "Enabling Material Discovery: Harnessing Multimodal Machine Learning Algorithms for Inverse Design." In: *Mathematics in Computation (MiC) seminar, Oak Ridge National Laboratory*. 2024.

2024 "Mulitmodal machine learning with small datasets for process strcture property modeling". In: *International Workshops on Advances in Computational Mechanics, Kitakyushu, Japan*. 2024.

2022 "Predicting stress hotspots in polycrystalline materials from microstructural features using deep learning". In: *MIrACLE seminar, Air Force Research Laboratory, Ohio, USA*. 2022.

2021 "Predicting stress hotspots in polycrystalline materials from microstructural features using deep learning". In: *Crunch seminar, Department of Applied Mathematics, Brown University*. 2021.

2021 "Predicting stress hotspots in polycrystalline materials from microstructural features using deep learning". In: *Physics and Chemistry of Materials Group Seminar, Los Alamos National Laboratory, NM, USA*. 2021.

Contributed Presentations

2023 "Analyzing latent dimensional representations of microstructure evolution". In: *The Minerals, Metals, and Materials Society*. 2023.

2023 "Bayesian optimization-assisted sputter deposition of Molybdenum thin films". In: *International Conference on Metallurgical Coatings and Thin Films*. 2023.

2023 "Modeling process structure property relationships in Mo thin films from multi-modal data using machine learning". In: *U.S. National Congress on Computational Mechanics*. 2023.

2023 "Predicting microstructure from physical vapor deposition process conditions using machine learning." In: *Mechanistic Machine Learning, and Digital Engineering for Computational Science, Engineering and Technology*. 2023.

2023 "Spatio-temporal super-resolution of dynamical systems using physics-informed deep-learning". In: *Mechanistic Machine Learning, and Digital Engineering for Computational Science, Engineering and Technology*. 2023.

2023 "Spatio-temporal super-resolution of dynamical systems using physics-informed deep-learning". In: *Machine Learning/Deep Learning Workshop, Sandia National Laboratory*. 2023.

2021 "Predicting microstructure from physical vapor deposition process conditions using machine learning." In: *Mechanistic Machine Learning and Digital Engineering for Computational Science, Engineering and Technology*. 2021.

2020 "Predicting Stress Hotspots Inside Microstructures Using Deep Learning". In: *Materials Science & Technology conference*. 2020.

Poster

2020 "Identifying microstructural features that drive stress hot-spots using a data mining approach". In: *NextManufacturing Center Virtual Membership Meeting & Research Expo*. 2020.

2019 "Identifying microstructural features that drive stress hotspots using a data mining approach". In: *Engineering Mechanics Institute Conference*. 2019.

Referees

- **Dr. Juan M Restrepo**
  Section Head, Mathematics In Computation, Oak Ridge National Laboratory
  Oak Ridge, CA, US
  Email: restrepojm@ornl.gov
- **Dr. Habib N Najm**
  Senior Scientist, Sandia National Laboratories
  Livermore, CA, US
  Email: hnnajm@sandia.gov
- **Prof. Kaushik Dayal**
  Professor, Civil & Environmental Engineering, Carnegie Mellon University
  Pittsburgh, PA, US
  Email: Kaushik.Dayal@cmu.edu
- **Prof. Hae Young Noh**
  Associate Professor, Civil & Environmental Engineering, Stanford University
  Stanford, CA, US
  Email: noh@stanford.edu