PRANOY RAY

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OVERVIEW

Computational Materials & Data Scientist specializing in Materials Informatics using Bayesian statistics for multiscale modeling. Expertise includes developing efficient feature engineering methods for robust materials process-structure-property relationships, and integrating physics-based constraints with data-driven AI/ML models on HPC systems. Innovative R&D professional with a track record of driving technical deliverables and leading diverse teams in fast-paced research environments. Presently a final year PhD candidate, expecting to graduate in May 2026 (Spring).

EDUCATION

- Ph.D: Mechanical Engineering, Georgia Institute of Technology - Atlanta, USA (2026)
  - *Advisor*: Dr. Surya R. Kalidindi
  - *Thesis Title*: "Computationally efficient voxelized approaches for structure-property relationships in molecular systems"
- MS: Computational Science and Engineering, Georgia Institute of Technology - Atlanta, USA (2024)
- B.Tech: Metallurgical & Materials Engineering, National Institute of Technology - Durgapur, India (2020)

PROFESSIONAL CERTIFICATIONS

- Management of Technology (MOT), Scheller College of Business, GeorgiaTech - Atlanta, USA (2025)
- Computational Materials Science & Engineering (CMSE), School of MSE, GeorgiaTech - Atlanta, USA (2023)

TECHNICAL SKILLS

- **Machine Learning/AI:** Neural Networks, Gaussian Process Regression, Normalizing Flows, Autoencoder, Convolutions
- **Programming & Data Science:** Python (with key libraries like PyTorch, GPyTorch, BOTorch, Pyvista, SciPy, scikit-learn), R, Java, C
- **Engineering Simulation:** VASP, LAMMPS, GROMACS, DFT, Molecular Dynamics, CG-Martini3, ORCA, MACE
- **HPC/Cloud Platforms:** MPI, AWS, GCP, Azure, Shell Scripting (SLURM/PBS), Flask, Firebase, Hadoop, BigData
- **Advanced Graduate Courses:** Parallel Computing (HPC), Density Functional Theory, Uncertainty Quantification, DoE, ML, DL
- **Process Informatics & Experimental Design:** Bayesian Optimization, Design of Exp., Pareto Frontier Analysis, Active Learning

EXPERIENCE

George W. Woodruff School of Mechanical Engineering (Atlanta, USA)   **MINED Group @ GT**
Graduate Research Assistant   *Aug 2021 to Present*
- Architected and published robust Foundation Model workflows for scientific domains, integrating physics-based constraints with deep learning to solve complex inverse problems. Developed interpretability methods for 3D convolutional architectures (Lean CNNs), analyzing feature activation maps to understand structure-property relationships in high-dimensional scientific data.
- Developed and published hybrid physics-AI models for multi-scale materials design, optimizing polymer physics in computational models, utilizing Uncertainty Quantification (UQ) and sensitivity analysis to correlate simulation data with experimental outputs.

Head Teaching Assistant (ME8813 & ME4853)   *Spring 2023 & Spring 2025*
- Instructed & graded classes of 100 graduate and UG students on ML Fundamentals for AI4Science applications (MSE/ME)

Multiscale Technologies Inc (Seattle, USA)   **R&D Team**
Data Science Manager & Materials Scientist Intern   *Jan 2024 to Sep 2024*
- Defined product strategy and executed the roadmap for AI-driven manufacturing solutions. Led cross-functional teams to deliver cost-saving tools for Fortune 100 clients, focusing on product lifecycle and ROI requirements.
- Deployed and published ML workflows that accelerated materials-selection for manufacturing clients, cutting R&D time by 80%.

Bhabha Atomic Research Centre (Mumbai, India)   **HP & SRPD**
Research Assistant (Advisor: Dr. Srikumar Banerjee & Dr. Brahmananda Chakraborty)   *May 2019 to Aug 2021*
- Theoretically discovered 3 distinct novel material systems for alternative fuels (Hydrogen Storage) using DFT & MD

Indian Institute of Technology (Bombay, India)   **IMaGen Lab**
Research Intern (Advisor: Dr. Alankar Alankar)   *July 2020 to Nov 2020*
- Workflows for predicting the mechanical properties of materials from composition using lower order ML models (RF, SVMs, etc.)

Indian Institute of Technology (Kharagpur, India)   **SRMSC Lab**
Research Intern (Advisor: Dr. Shibayan Roy)   *June 2020 to Oct 2020*
- Participated in a Phase-Field Modelling project involving DFT & MD Simulations (collab with Washington University at St. Louis)

Hindustan Aeronautics Limited (Bangalore, India)   **Foundry & Forge Division**
Project & Industrial Intern (Advisor: Soumya Mandi)   *May 2018 to July 2018*
- Deployed projects: (1) Led failure analysis investigations on casting defects, implementing process control measures that improved yield. (2) Applied Lean management principles to manufacturing quality control.

SELECTED RESEARCH

JOURNAL PUBLICATIONS

- **ML workflows for assisting in the treatment and removal of forever chemicals**
  P. Ray, A. Castillo, M. Kolel-Veetil, S.R. Kalidindi | Oct 2025
  Advanced Science | Under Review | Code
- **Unraveling the PFAS helix: A statistical approach**
  P. Ray, H. Cavalli, K.D. Tynes, G. Bizana, A. Castillo, S. Vyas, R. Siefert, S.R. Kalidindi, M. Kolel-Veetil | Sep 2025
  ACS Journal of Chemical Information and Modeling | Under Review | Code

- **Assessing the accuracy of Bayesian-optimized CGMD in predicting polymer miscibility**
  P. Ray, Y. Asoma, N. Vankireddy, A. P. Generale, M. Nakauchi, H. Lee, K. Yoshida, S.R. Kalidindi, Y. Okuno | Nov 2025
  RSC Chemical Science | Under Review
- **Refining Coarse-Grained Molecular Topologies: A Bayesian Optimization Approach**
  P. Ray, A. P. Generale, N. Vankireddy, Y. Asoma, M. Nakauchi, H. Lee, K. Yoshida, Y. Okuno, S.R. Kalidindi | July 2025
  npj Computational Materials | Volume 11 | Article 234
- **Lean CNNs for Mapping Electron Charge Density Fields to Material Properties**
  P. Ray, K. Choudhary, S.R. Kalidindi | January 2025
  Integrating Materials and Manufacturing Innovation | Volume 14 | Issue 1 | Pages 1-13 | Code

ORAL PRESENTATIONS/CONFERENCE TALKS

- **Statistical quantification of helicity in linear PFAS**
  P.Ray, H.Cavalli, et. al. | March 2026 | **ACS Spring, Atlanta, GA, USA**
- **(INVITED) Lean CNNs for materials discovery using electron charge density fields**
  P.Ray, S.R. Kalidindi | October 2025 | Host: Prof. Stefano Sanvito | **Trinity College, Dublin, Ireland**
- **Structure-aware Bayesian optimization for efficient design of disordered CCAs**
  P.Ray, S.R. Kalidindi | October 2025 | **SES Annual Techinical Meeting, Atlanta, GA, USA**
- **(INVITED) Bayesian frameworks for advanced materials design at the atomistic scale**
  P.Ray, S.R. Kalidindi | October 2024 | **Novelis' Global Research and Technology Center, Kennesaw, GA, USA**
- **(INVITED) Bayesian optimization of Coarse-Grained topologies: Applications to common polymers**
  P.Ray, A.P. Generale, et. al. | October 2024 | **TMS Fall Meeting, Pittsburgh, PA, USA**
- **(INVITED) Feature engineering of electron charge density fields for building AI/ML models to predict material properties**
  P.Ray, S.R. Kalidindi | December 2022 | **2nd Energy & Informatics International Forum, Oahu, HI, USA**

SELECTED AWARDS & ACCOLADES

- **Woodruff School Fellow** (2025): GWW School of Mechanical Engineering, GeorgiaTech (Atlanta, GA, USA)
- **Novelis Graduate Scholar** (2024): Novelis Innovation Hub & Novelis Inc (Kennesaw, GA, USA)
  - *Featured in:* GTRI News based on the scholarship awarded by Novelis Inc. (world's largest aluminium rolling & recycling) as a top scholar conducting research in aspects of sustainability (de-carbonization), techno-economics of circularity, high-throughput materials discovery, & AI/data science in materials/manufacturing/supply chains.
- **EIIF Fellow** (2022): TokyoTech & Strategic Energy Institute @GT (Honolulu, HI, USA)
  - *Invited Scholar:* GT Strategic Energy Institute covering us at the 2nd Energy & Informatics Forum.
- **CMS3 Fellow** (2022): NSF + Texas A&M University (College Station, TX, USA)

Other "selected" Media & Press

- **TMS Standout Article** (2025): Journal article on Lean CNNs highlighted by TMS Editors as a standout article for 2025.
- **The Telegraph (India)** (2018): Featured in "Backyard Startups" regarding the launch of #JustHashtags without VC assistance.

SERVICES TO THE SCIENTIFIC COMMUNITY

Academic:

- Reviewer & Committee Member: SciPy Conference (2023, 2024, 2025)
- Peer Reviewer (AI4Mat): NeurIPS 2025, CVPR 2025, PEARC 2025
- Peer Reviewer: Springer Nature, Journal of Materials, Chemical Papers (since 2023)
- Session Chair & Reviewer: GT Undergraduate Research Symposium (2025)

Leadership:

- Board Member: Emerging Leaders Advisory Board @GT (2025-2026)
- Internal VP: Mechanical Engg Grad Association (MEGA) @GT (2023-2024)
- President: Entrepreneurship Development Cell, NIT Durgapur, India (2016-2020)
- Treasurer: Strokes (Art & Photography Club), NIT Durgapur, India (2017-2020)

REFERENCES

Dr. Surya R. Kalidindi (surya.kalidindi@me.gatech.edu)
Regents' Professor, Rae S. and Frank H. Neely Chair
Mechanical Engineering, Georgia Institute of Technology
Atlanta, GA, USA 30332

Dr. Brahmananda Chakraborty (brahma@barc.gov)
Scientist G, HP&SRPD, Bhabha Atomic Research Center
Associate Professor, Homi Bhabha National Institute
Mumbai, MH, India 400085

Dr. Manoj Kolel-Veetil (manoj.k.kolel-veetil.civ@us.navy.mil)
Research Scientist, Chemistry Division
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Associate Professor, Georgia Institute of Technology
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