

PRANOY RAY

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CAREER OBJECTIVE

Interdisciplinary Data Scientist with a PhD and 4+ years of experience leveraging machine learning, Bayesian optimization, and statistical modeling to solve complex, high-dimensional problems. Proven track record of delivering scalable engineering solutions and driving ROI for Fortune 100 clients. Expert in translating complex data into actionable business insights for non-tech stakeholders.

EDUCATION

- Ph.D: Mechanical Engineering, Georgia Institute of Technology - Atlanta, USA (*expected May 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

- **Applied Statistics & Process Informatics:** Bayesian Optimization, Gaussian Processes (GPyTorch, BoTorch), Active Learning, Uncertainty Quantification (UQ), Pareto Frontier Analysis, Design of Experiments (DoE), Failure Modes & Effects Analysis (FMEA).
- **Machine Learning & Gen. AI:** PyTorch, Neural Networks, Computer Vision (CNN), Autoencoders, Normalizing Flows, Scikit-learn.
- **Programming, HPC & Cloud:** Python, R, C, Java, MPI, AWS, GCP, Azure, SLURM/PBS, Flask, Shell Scripting.
- **Data Visualization & Management:** Matplotlib, Seaborn, Tableau, PowerBI, Google BigQuery, Firebase, SQL, Spark, Hadoop.

RESEARCH & INTERNSHIP EXPERIENCES

George W. Woodruff School of Mechanical Engineering (Atlanta, USA)

Graduate Data Scientist

MINED Group @ GT

Aug 2021 to Present

- Developed Computer Vision and Deep Learning pipelines (PyTorch) to solve inverse optimization problems. Built robust models using Uncertainty Quantification (UQ) to handle noise in large-scale datasets, improving prediction accuracy by 40%.
- Partnered with cross-functional engineering teams to define product metrics and KPIs for manufacturing efficiency. Conducted exploratory data analysis (EDA) on process telemetry, identifying key drivers of yield loss and improving system reliability.
- LLM-Driven Workflow Automation: Designed and deployed Generative AI models to automate feature extraction from unstructured technical data, directly improving the throughput of the research pipeline.

Head Teaching Assistant (ME8813 & ME4853)

Spring 2023 & Spring 2025

- Translated complex ML concepts and process optimization for large datasets, into accessible lectures for 100+ students with varying technical backgrounds, demonstrating strong ability to communicate technical insights to non-experts.

Multiscale Technologies Inc (Seattle, USA)

Data Science Manager & Materials Scientist Intern

R&D Team

Jan 2024 to Sep 2024

- Defined product strategy and executed the roadmap for semiconductor manufacturing process optimization (SMPO) solutions
- Led cross-functional teams to deliver and deploy high-fidelity cost-saving tools for Fortune 100 clients, focusing on product life-cycle and ROI requirements. 10+ digital twins developed, and results published in scientific journals.

Bhabha Atomic Research Centre (Mumbai, India)

Research Assistant (Advisor: [Dr. Srikumar Banerjee](#) & [Dr. Brahmananda Chakraborty](#))

May 2019 to Aug 2021

- Theoretically discovered & published 3 distinct novel material systems for alternative fuels (Hydrogen Storage) using DFT & AIMD

Indian Institute of Technology (IIT) 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 (IIT) 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

- Led and deployed projects on shop floors: (1) Led failure analysis investigations on casting defects, implementing process control measures that improved yield. (2) Applied Lean management principles to manufacturing quality control.

LEADERSHIP & COMMUNITY SERVICES

- Board Member: Emerging Leaders Advisory Board @GT (2025-2026)
- Internal VP: Mechanical Engg Grad Association (MEGA) @GT (2023-2024)
- Peer Reviewer: Springer Nature, Journal of Materials, Chemical Papers (since 2023)
- Peer Reviewer: ICLR 2026, NeurIPS 2025, CVPR 2025, PEARC 2025, SciPy Conference (2023, 2024, 2025), GT UGRS 2025

HONORS & AWARDS

- **Woodruff School Fellow** (2025): GWW School of Mechanical Engineering, GeorgiaTech (Atlanta, GA, USA)
- **TMS Standout Article** (2025): Highlighted by TMS Editors as a standout 2025 publication for novel work on Lean CNNs.
- **Novelis Graduate Scholar** (2024): Novelis Innovation Hub & [Novelis Inc.](#) (Kennesaw, GA, USA)

- Featured in: [GTRI News](#) as a top scholar advancing sustainability, circularity, and AI-driven materials discovery.
- **EII Fellow (2022)**: TokyoTech & Strategic Energy Institute @GT (Honolulu, HI, USA)
 - Invited Scholar: Selected by [GT Strategic Energy Institute](#) for the 2nd Energy & Informatics Forum.
- **CMS3 Fellow (2022)**: NSF + Texas A&M University (College Station, TX, USA)
- **The Telegraph (India) (2018)**: Featured in "Backyard Startups" for launching the bootstrapped venture #JustHashtags.

KEY DATA SCIENCE PROJECTS

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
[Angewandte Chemie \(Under Review\)](#)
- **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
[ChemRxiv preprint](#) | [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 Technical 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

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
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Dr. Manoj Kolel-Veetil (manoj.k.kolel-veetil.civ@us.navy.mil)
Research Scientist, Chemistry Division
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Dr. Brahmananda Chakraborty (brahma@barc.gov)
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