Divyesh Mistry

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Professional Summary

Computational materials scientist with 5+ years of experience in multiscale modeling, high-performance computing, and simulation-driven research for aerospace and defense applications. Specialized in molecular dynamics, discrete dislocation dynamics, and integrated computational materials engineering (ICME), with significant expertise in metallic alloys and high-temperature ceramics. Proficient in Python, C++, LAMMPS, ABAQUS, and parallel programming (MPI/OpenMP), with a proven track record in developing atomistic and continuum-level models to study material behavior under extreme conditions. Successfully contributed to DRDO- and DMRL-funded projects focused on high-strain-rate materials, composite modeling, and dislocation dynamics.

Core Competencies

Programming & HPC	Python, C++, MATLAB, Shell scripting (Bash), OpenMP, MPI, Git, GitHub
Modeling & Simulation Tools	LAMMPS, ATOMSK, OVITO, NEPER, Ansys, ABAQUS, AutoCAD, LaTeX, Gnuplot
Data Science & Visualization	pandas, NumPy, SciPy, scikit-learn, Matplotlib
Experimental Techniques	Split Hopkinson Pressure Bar (SHPB), Resin Film Infusion (RFI)
Operating Systems	Linux (Ubuntu), macOS, Windows
Languages	Fluent in English, Hindi, and Gujarati (reading, writing, speaking)

Experience

Jan 2025 – Present — **Junior Research Fellow (JRF)**, *IIT Bombay*, *Aerospace Engineering*, *Mumbai*
- Leading DRDO-funded project on constitutive modeling of shape memory alloy (SMA) composites under ballistic conditions.
- Developed Resin Film Infusion (RFI) protocols to optimize curing and eliminate resin delamination and brittle fracture.
- Validated strain-rate dependent material behavior using Split Hopkinson Pressure Bar (SHPB) and high-speed data acquisition systems.

Jan 2024 – July 2025 — **Independent Researcher (Ph.D. Project)**, *IIT Bombay*, *Aerospace Engineering*, *Mumbai*
- Investigating dislocation avalanche and plastic instability phenomena in metals using in-house 2D discrete dislocation dynamics (DDD) simulations.
- Developed a modular solver in C++ with boundary condition and interaction modeling.

Jun 2019 – Jun 2025 — **Ph.D. Research Scholar**, *IIT Bombay*, *Aerospace Engineering*, *Mumbai*
- Designed multiscale models to study dislocation–microstructure interactions in Ni-based superalloys, with focus on prior particle boundaries (PPBs) and γ/γ' phases.
- Automated simulation workflows using LAMMPS, Atomsk, Python, and Bash for high-throughput HPC analysis.
- Collaborated with DMRL to investigate microstructure evolution in metal additive manufacturing contexts.

Jan 2019 – Dec 2023 — **Teaching Assistant**, *IIT Bombay*, *Aerospace Engineering*, *Mumbai*
- Supported undergraduate and postgraduate instruction in Continuum Mechanics, Finite Element Methods, Multiscale Modeling, and Data Analysis.
- Assisted with lab sessions, project mentoring, and simulation assignments.

Jun 2016 – Dec 2018 — **Assistant Professor**, *CMR Institute of Technology*, *Mechanical Engineering*, *Bangalore*
- Delivered courses in FEM and Experimental Stress Analysis; conducted CAD/design lab workshops.
- Organized applied workshops on MATLAB, Python, and ANSYS; contributed to academic program development.

Jun 2014 – Jul 2016 — **Teaching Assistant & M.Tech. Researcher**, *IIT Kharagpur*, *Mechanical Engineering*, *Kharagpur*
- Developed mesh-free numerical model for static analysis of smart composite beams.
- Assisted in teaching/labs for Vibration Analysis, FEM, and Tribology.
- Validated research model using FEM outputs from ANSYS and ABAQUS.

Education

Jan 2019 – July 2025 Indian Institute of Technology - Bombay, Mumbai, India

Doctorate, Aerospace Engineering
Thesis : Multiscale Modeling of Prior Particle Boundaries in Nickel-based Superalloys
CGPA : 9.36/10 *Funding :* MHRD Teaching Assistantship through Project
Key Subjects : Multiscale Modeling, Continuum Mechanics, HPC, FEM, Scientific Visualization
Advisors : Prof. Amuthan A. Ramabathiran, Prof. P. J. Guruprasad

Jun 2014 – Jul 2016 Indian Institute of Technology - Kharagpur, West Bengal, India

M.Tech., Mechanical Engineering (Mechanical System Design)
Thesis : A Mesh-Free Model for Static Analysis of Smart Composite Beams
CGPA : 8.85/10 *Funding :* MHRD GATE Fellowship
Key Subjects : Solid Mechanics, Fracture Mechanics, FEM, Composites, Elasticity, Vibration
Advisor : Prof. Manas Chandra Ray

Dec 2013 The Aeronautical Society of India, New Delhi

B.E., Aeronautical Engineering (Aero Mechanical)
Key Subjects : Aircraft Structures, Aerodynamics, Propulsion, Stability & Control, Solid/Fluid Mechanics

Publications and Conference Proceedings

[1] Mistry D. A., & Ramabathiran, A. A., *Size-Dependent Power Laws for Edge Dislocations in Nickel Superalloys : A Molecular Dynamics Study*, *Computational Materials Science*, (Accepted July 11, 2025). arXiv preprint : doi.org/10.48550/arXiv.2504.16409

[2] Mistry D. A., Tawqeer N. Tak, & Guruprasad, P. J., *Studying Dislocation–Prior Particle Boundary Interactions in Ni-Based Superalloys Using Polycrystalline Discrete Dislocation Dynamics*. Submitted.

[3] Mistry D. A., Tawqeer N. Tak, & Guruprasad, P. J., *Polycrystalline Discrete Dislocation Dynamics of Ni-Based Superalloys : Interactions with Prior Particle Boundaries and Second Phases Using Atomistically Informed Inputs*. Manuscript under preparation.

[4] Mistry D. A., Tawqeer N. Tak, & Guruprasad, P. J., *Hierarchical Multiscale Modeling of Plasticity in Ni-Based Superalloys : The Combined Role of Prior Particle Boundaries and Second Phases*. To be presented at the *14th International Symposium on Plasticity and Impact Mechanics (IMPLAST 2025)*, October 12–16, 2025, IIT Roorkee, India.

[5] Mistry, D., Guruprasad, P. J., & Ramabathiran, A. A., *An Atomistically Informed Discrete Dislocation Dynamics Study of Prior Particle Boundaries in Ni-Based Superalloys*, *17th Conference on Computational Plasticity (COMPLAS)*, September 5–7, 2023, Barcelona, Spain.

Certifications

Jan 2020 **Using Python for Research**, edX, HarvardX, Harvard University.
Aug 2020 **The Unix Workbench**, Coursera, Johns Hopkins University.
Aug 2020 **Material Behavior**, Coursera, Georgia Institute of Technology.
May 2018 **A Hands-on Introduction to Engineering Simulations**, edX, CornellX, Cornell University.

Positions of Responsibility

June 2021 – July 2022 **Department Placement Coordinator (DPC)**, *Department of Aerospace Engineering, IIT Bombay*

Awards, Achievements, and Honorable Mentions

2013 **Permanent Membership** : Awarded permanent membership as an **Associate Member** at the **Aeronautical Society of India**

2014 ★ **All India Rank 69** : Achieved in the Graduate Aptitude Test in Engineering (GATE)

2019 MHRD Teaching Assistantship Through Project : Awarded by the **Industrial Research and Consultancy Centre (IRCC)**

2023 IIT Bombay Travel Grant : Awarded to attend the international conference *COMPLAS 2023*, Spain

2025 Institution of Eminence Funds, IIT Bombay : Awarded to attend the international conference *TMS 2025*, USA

2025 **Membership** : Member of The Minerals, Metals & Materials Society (TMS), USA