Ameya Daigavane

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Education

- **Massachusetts Institute of Technology** — Cambridge, MA
  PhD in Electrical Engineering and Computer Science (GPA 5.0/5.0) — 2022-Current
  - Research Assistant in the Atomic Architects group led by Prof. Tess Smidt.

- **Indian Institute of Technology, Guwahati** — Guwahati, India
  B.Tech in Computer Science and Engineering (GPA 9.38/10.0) — 2016-2020

Experience

- **Research Intern - Prescient Design, Genentech** — South San Francisco, CA
  Mentor: Dr. Bodhi P. Vani — May 2025 - August 2025
  - Worked on accelerating free energy perturbation calculations using machine-learned potentials.

- **Research Intern - Prescient Design, Genentech** — South San Francisco, CA
  Mentor: Dr. Joseph Kleinhenz — May 2024 - August 2024
  - Designed JAMUN, a fast transferable sampler for 3D conformations of peptides.

- **Pre-Doctoral Researcher - Google Research** — Bangalore, India
  Mentors: Dr. Gaurav Aggarwal and Dr. Prateek Jain — September 2020 - August 2022
  - Designed node-level differentially-private graph neural networks.
  - Developed interactive visualization tools for microplate experiments.

- **Research Intern - NASA, Jet Propulsion Laboratory** — Pasadena, CA
  Mentor: Dr. Gary Doran — June 2020 - August 2020
  - Designed, prototyped and assessed radiation sensitivity of time-series anomaly detection methods in a flight system setting.

- **Research Intern - NASA, Jet Propulsion Laboratory** — Pasadena, CA
  Mentor: Dr. Kiri Wagstaff — May 2019 - July 2019
  - Developed unsupervised algorithms for onboard event detection in time-series data for the Plasma Instrument for Magnetic Sounding on the upcoming Europa Clipper mission.

Publications

- **Matching the Optimal Denoiser in Point Cloud Diffusion with (Improved) Rotational Alignment**
  Ameya Daigavane*, YuQing Xie*, Bodhi P. Vani, Saeed Saremi, Joseph Kleinhenz, Tess Smidt.
  Presented at MoML 2025. Longer version under review.

- **JAMUN: Bridging Smoothed Molecular Dynamics and Score-Based Learning for Conformational Ensembles**
  Ameya Daigavane*, Bodhi P. Vani*, Darcy Davidson, Saeed Saremi, Joshua Rackers and Joseph Kleinhenz.
  Published at NeurIPS, 2025. Presented at GenBio at ICML, 2025 and AIDrugX at NeurIPS, 2024.
  Contributed talk at Conformational Ensembles, 2025.

- **The Price of Freedom: Exploring Tradeoffs between Expressivity and Computational Efficiency in Equivariant Tensor Products**
  YuQing Xie, Ameya Daigavane, Mit Kotak and Tess Smidt.
  Published at ICML, 2025. Presented at GRaM at ICLR, 2024.

- **EquiJump: Protein Dynamics Simulation via SO(3)-Equivariant Stochastic Interpolants**
  Allan dos Santos Costa, Ilan Mitnikov, Franco Pellegrini, Ameya Daigavane, Mario Geiger, Zhonglin Cao, Karsten Kreis, Tess Smidt, Emine Kucukbenli and Joseph Jacobson.
  Accepted for oral presentation at GEM at ICLR, 2025.

- **Symphony: Symmetry-Equivariant Point-Centered Spherical Harmonics for Molecule Generation**
  Ameya Daigavane, Song Kim, Mario Geiger, and Tess Smidt.
  Published at ICLR, 2024.

- **Unsupervised Detection of Magnetic Field Boundary Crossings From Plasma Spectrometer Data**
  Ameya Daigavane, Kiri Wagstaff, Gary Doran, Corey Cochrane, Caitriona Jackman, and Abigail Rymer.
  Published at Computers and Geosciences, 2022. Invited talk at ML for Planetary Science and Space Physics and ML in Heliophysics.

- **Resource Consumption and Radiation Tolerance Assessment for Data Analysis Algorithms Onboard Spacecraft**
  Gary Doran, Ameya Daigavane, and Kiri Wagstaff.
  Published at IEEE Transactions on Aerospace and Electronic Systems, 2022.

- **Integrating Deep Learning and Unbiased Automated High-Content Screening to Identify Complex Disease Signatures in Human Fibroblasts**
  Lauren Schiff, et al.
  Published at Nature Communications, 2022.

- **Node-Level Differentially Private Graph Neural Networks**
  Ameya Daigavane, Gagan Madan, Aditya Sinha, Abhradeep Thakurta, Gaurav Aggarwal, and Prateek Jain.
  Accepted for oral presentation at PAIR^{2}Struct at ICLR, 2022.

- **Understanding Convolutions on Graphs**
  Ameya Daigavane, Balaraman Ravindran, and Gaurav Aggarwal.
  Published at Distill, 2021.

- **Detection of Environment Transitions in Time Series Data for Responsive Science**
  Ameya Daigavane, Kiri Wagstaff, Gary Doran, Corey Cochrane, Caitriona Jackman, and Abigail Rymer.
  Accepted for oral presentation at MiLeTS at KDD, 2020.

Awards and Honours

NSF Graduate Research Fellowship Award	2023
MIT SERC Scholar Award	2022
ACM SIGBED Scholars Award – One of three awardees	2020
ACM SIGKDD Student Registration Award	2020
Caltech Summer Undergraduate Research Fellowship (SURF) Award	2019
ACM ICPC Qualifiers – 61st in India among 4000+ teams	2019
ACM ICPC Kanpur Regionals – 18th in India among 200+ teams	2019
OzCHI Student Design Challenge – Honorable Mention (Top 5)	2019
Analyze This – Outstanding Performer – 55th in India among 2000+ teams	2017
KVPY Science Scholarship – SA Stream – 156th in India	2015
FIITJEE Talent Reward Examination – 1st in India	2014
Regional Mathematics Olympiad – 1st in state	2014