

# Ameya Daigavane

70 Willow Street, Apt. #3, Cambridge, MA 02141  
Phone: +1-(857)5077253

Email: ameya.d.98@gmail.com  
Website: <https://ameya98.github.io>

## 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** South San Francisco, CA  
*Mentor: Dr. Bodhi P. Vani* May 2025 - August 2025
  - Working on accelerating free energy perturbation calculations using machine-learned potentials.
- Research Intern - Prescient Design** South San Francisco, CA  
*Mentor: Dr. Joseph Kleinhenz* May 2024 - August 2024
  - Designed JAMUN, a new 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<sup>2</sup>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 – 61 <sup>st</sup> in India among 4000+ teams . . . . .	2019
ACM ICPC Kanpur Regionals – 18 <sup>th</sup> in India among 200+ teams . . . . .	2019
OzCHI Student Design Challenge – Honorable Mention (Top 5) . . . . .	2019
Analyze This – Outstanding Performer – 55 <sup>th</sup> in India among 2000+ teams . . . . .	2017
KVPY Science Scholarship – SA Stream – 156 <sup>th</sup> in India . . . . .	2015
FIITJEE Talent Reward Examination – 1 <sup>st</sup> in India . . . . .	2014
Regional Mathematics Olympiad – 1 <sup>st</sup> in state . . . . .	2014