Akash Pallath

Graduate student in Chemical and Biomolecular Engineering

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University of Pennsylvania
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Education

University of Pennsylvania
Ph.D. in Chemical and Biomolecular Engineering *2019 - Present*
Advisor: Dr. Amish J. Patel

Indian Institute of Technology (IIT) Gandhinagar
B.Tech. in Chemical Engineering, minor in Computer Science and Engineering *2015 - 2019*
GPA: 8.91/10.0

Research Interests

Effects of hydration on protein structure, binding, and intermolecular interactions; enhanced sampling in molecular dynamics; high-performance computing; algorithm design; deep learning applications.

Research Experience

University of Pennsylvania *November 2019 – Present*
Developing and applying methods to computationally study the effects of hydration on protein structure and stability using enhanced molecular dynamics simulations.
Advisor: Dr. Amish J. Patel

California Institute of Technology *May 2018 – August 2018*
Performed molecular dynamics simulations and implemented algorithms to quantify vibrational mode contributions to the thermal conductivity of amorphous diamond.
Mentors: Dr. Austin J. Minnich, Dr. Jaeyun Moon

Indian Institute of Technology Gandhinagar *August 2017 – May 2019*
Studied fluctuations at Lennard-Jones solid-liquid interfaces using molecular dynamics, and implemented efficient Grand Canonical Monte Carlo simulation algorithms.
Mentor: Dr. Kaustubh S. Rane

Japan Advanced Institute of Science and Technology *June 2017 - July 2017*
Helped build a custom cluster using specialized proprietary network architecture, and designed benchmarks to measure Quantum Espresso performance improvements on the cluster.
Scholarship: MEXT Re-Inventing Japan Project FY 2017
Mentors: Dr. Ryo Maezono, Dr. Ken Qin

Indian Institute of Technology Gandhinagar *May 2016 - April 2017*
Designed fixed parameter tractable algorithms to solve NP-hard problems on structured approval ballots.
Mentor: Dr. Neeldhara Misra

Teaching Experience

Teaching Assistant, IIT Gandhinagar, India
ES112: Computing *Semester-I, 2018-19*
Instructor: Dr. Neeldhara Misra

HS202: Modern World History *Semester-II, 2017-18*
Instructor: Atul Singh

TEQIP Summer School on Algorithms *Summer 2016*
Instructors: Dr. Bireswar Das, Dr. Manoj Gupta, Dr. Neeldhara Misra,

Teaching Assistant, JAIST, Japan
Sakura Science Program Workshop for Undergraduates *Summer 2017*
Organizer: Maezono Lab, School of Information Science, JAIST

Technical Skills

Programming and scripting	Python, C++, MATLAB, Bash
Molecular simulation	GROMACS, VMD, MDAnalysis, LAMMPS
Machine learning	PyTorch, Scikit-learn
Software dev practices	Version control, unit testing, integration testing, documentation
Miscellaneous	Web development (HTML, CSS, JavaScript, PHP, Django), LaTeX, Git, ASPEN

Awards, Achievements, and Fellowships

PhD:
Distinction for outstanding performance on the PhD Qualifying Examination, Department of Chemical and Biomolecular Engineering, University of Pennsylvania *2020*
PhD Fellowship, Department of Chemical and Biomolecular Engineering, University of Pennsylvania *2019 - Present*

Undergraduate:
Summer Undergraduate Research Fellowship, Caltech [$6,275 stipend] *2018*
MEXT Re-Inventing Japan Project Fellowship [¥160,000 stipend] *2017*
Dean's List, IIT Gandhinagar *2015-16 (Sem-I,II), 2016-17 (Sem-I,II), 2017-18 (Sem-I)*
40^{th} place at the Coimbatore site, ACM-ICPC Asia Amritapuri Regionals *2016*
56^{th} place at the ACM-ICPC Asia Chennai Regionals *2016*
Travel grant to attend two ACM-ICPC Asia Regionals, IIT Gandhinagar *2016*

Training in Computational Science

Data-Driven Modeling and Probabilistic Scientific Computing*, Numerical Methods and Modeling*, Nature Inspired Computing†, Pattern Recognition and Machine Learning†, Topics in Complexity Science, Introduction to Computational Complexity Theory, Algorithm Analysis and Design, Data Structures.

Training in Chemical Engineering, Biology, and Physics

Macromolecular Biophysics*, Biotechnology Immunology Vaccines and COVID-19*, Advanced Chemical Kinetics and Reactor Design*, Advanced Molecular Thermodynamics*, Advanced Transport Phenomena*, Statistical Mechanics†, Condensed Matter Physics†, Process Synthesis and Design, Process Analysis and Simulation, Process Control, Process Dynamics and Control Lab, Separation Processes, Heat and Mass Transfer, Chemical Reaction Engineering, Mass Transfer and Reaction Engineering Lab, Chemical Engineering Thermodynamics, Heat Transfer and Thermodynamics Lab, Fluid Mechanics, Fluid Mechanics Lab.

Leadership

Co-organizer, Student Leadership Conclave, IIT Gandhinagar *2018, 2019*
Co-organized the first Student Leadership Conclave for discussion on academics and student governance with invited student representatives from 14 Indian Institutes of Technology. Chaired sessions in the second edition of the conclave.

Co-organizer, HackRush, IIT Gandhinagar *2018, 2019*
Co-organized IIT Gandhinagar's first hackathon and the second edition of the same.

Chief Election Commissioner, Election Commission, IIT Gandhinagar *2017 - 2018*
Lead a team of 8 members to organize and regulate an unprecedented 7 elections for student leadership positions. Worked with student governance to make electoral reforms and amendments to the Student Election Code of IIT Gandhinagar.

* Graduate course at Penn
† Graduate course at IIT