ASHLIN JAMES PORUTHOOR

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EDUCATION

Doctor of Philosophy, Biophysics, University of Rochester (Anticipated) 2018 - 2023
Master of Science, Biophysics, University of Rochester 2018 - 2021
Master of Science, Physics, NIT Calicut 2016 - 2018
Bachelor of Science, Physics (Honors), St.Stephen's College, University of Delhi 2013 - 2016

SKILLS

Computational Biology and Structural Biology:
• All-Atom and Coarse-Grained Molecular Dynamics Simulations : (MD Engines) ◇ GROMACS ◇ OpenMM ◇ NAMD (MD Visualization) ◇ VMD ◇ PyMOL (Other MD Tools) ◇ MARTINI ◇ CHARMM-GUI • Free Energy Calculations using Enhanced Sampling : (Methods) ◇ Weighted Ensembleu ◇ Metadynamics ◇ Umbrella Sampling ◇ Thermodynamic Integration (Tools) ◇ WESTPA ◇ PLUMED • Alchemical and Geometrical Binding Free Energy Calculations : ◇ BFEE2 • Docking : ◇ Schrödinger Maestro Glide • Quantum Mechanics Calculations : ◇ VASP ◇ Gaussian • Membrane, Membrane - GPCR, Membrane - RNA modeling • Small Molecule Parameterization • Clustering • SVMs

Technical Expertise:
• Programming: Python, MATLAB, Fortran, C++, Bash • Others: Git - GitHub, Bitbucket, Jupyter Lab, AWS, MS Office Suite • System Biology Tools – Flux analysis and metabolic network reconstruction: COBRA, TIGER

RESEARCH EXPERIENCE

Grad Research Student June 2019 - Present
University of Rochester Medical Center, Grossfield Lab *Rochester, NY*

- Spearheaded a method development project in a field new to the lab. Created new directions for the project that demanded mentoring, collaborating, and training of grad and undergrad lab members
- Developed a computational pipeline to estimate the free energy landscape of phase separation in the lipid bilayers ◇ Analyzed > 40 TB data ◇ Coarse-Grained Modeling ◇ GROMACS ◇ Thermodynamics ◇ Enhanced Sampling
- Characterizing the effects of collective variable decisions on enhanced sampling outcomes by creating a protocol that gauges collective variables before, after, and during the enhanced runs ◇ Benchmarking ◇ Optimization
- Characterizing the effects of box size in MD simulations on the thermodynamics of phase-separating systems
- Equilibrium partitioning of lipopeptides between two co-existing phases. ◇ Peptide - Membrane modeling
- Using Machine Learning methods in the pipeline to effectively search and rank a better set of collective variables
- Improving the efficiency of free energy calculation by coupling replica-exchange to weighted ensemble dynamics
- Tracking Ultrafast dynamics of Rhodopsin upon light activation to interpret the XFEL experiments ◇ Analyzed > 10000 short All-Atom simulations ◇ NAMD ◇ Cross-functional collaboration ◇ Membrane - GPCR modeling

Computational Sciences Co-op Jan 2022 - June 2022
Moderna, Molecular Engineering and Modeling *Cambridge, MA*

- Studied RNA – lipid bilayer interactions with NAMD All-Atom Molecular Dynamics simulations in AWS EC2
- Studied RNA - small molecule interaction via docking and Molecular Dynamics. Proposed and implemented a python analysis suite for initial validation of binding pocket interactions and ligand conformational dynamics
- Investigated and benchmarked alchemical and geometrical routes for RNA - small molecule binding free energy calculations. Implemented a pipeline for test molecules that can be extended for a large ligand library screening
- Proposed and initiated an internal pilot project that involved cross-functional teams

Summer Research Fellow April 2018 - June 2018
JNCASR, Theoretical Sciences Unit *Bangalore, India*

- Studied the sensitivity of population dynamics of bacteria towards the nutrient environment using modeling and simulation. Modeled quorum sensing and chemotaxis behaviors and emulated racing conditions between them

Summer Research Fellow May 2017 - July 2017
JNCASR, Theoretical Sciences Unit *Bangalore, India*

- Conducted metabolic network reconstructions and flux balance analyses on constrained-based *in silico* yeast models. Studied the effect of various metabolites on the yeast growth rates upon network perturbations
- Integrated transcriptomic data into *in silico* models of *Plasmodium Falciparum* to emulate multiple malaria variants in southeast Asia to understand the rise of drug resistance using cross-functional efforts

OTHER RELEVANT EXPERIENCE

Moderna – Carnegie Mellon University, Artificial Intelligence (AI) – Academy Certification (2022): Internal training to educate and empower Moderna employees to integrate AI and ML solutions into their workflow

URBEST Trainee (2021 - Present) University of Rochester initiative to Broaden Experiences in Scientific Training for early career scientists. Training on leadership and management skills for scientists via coursework, panel discussions, informational interviews, career stories, mentoring, and other personalized programs

International Students and Scholars Advisory Board (ISSAB), University of Rochester (2022 - Present) Represent the international grad student community in the School of Medicine and Dentistry at UR Medical Center

Graduate Student Society, International student liaison (2022 - Present) Formed an internal student committee and conducting focus groups and panel discussions to enhance the international grad student experience

UR2 mentorship program (2020 - 2022) A program run by grad students to mentor and train first-generation undergrads and those from less privileged backgrounds on tools and resources for a research career

Teaching Assistant, BPH509 - Molecular Biophysics (2020) Instructed students in theoretical, experimental, and computational methods to study macromolecules. Topics include statistical mechanics, optical melting experiments, dynamic programming algorithms, molecular dynamics, protein folding, and isothermal titration calorimetry

Open source contributions (2020 - 2022) LOOS : A lightweight object-oriented structure analysis library for MD simulations. WESTPA : The Weighted Ensemble Simulation Toolkit with Parallelization and Analysis

General Secretary, Choreography Society, St.Stephen's College (2015 - 2016) Headed a 60+ dance crew with Indian classical and fusion choreography and production. One major and minor production each semester

SCHOLASTIC ACHIEVEMENTS

Biophysics Student Seminar Award, 2021 : For best student seminar based on popular votes

Graduate Women In Science Mentor-Up Winner, 2021 : University challenge to set and achieve multiple short-term personal and professional goals through mentoring-up and training

Neuman Travel Award, 2020, 2021 : To share and present the thesis research at academic conferences

Dr. K. Swaminathan Memorial Award, 2016 : For an excellent academic record and overall achievements in cultural activities during undergrad level, St. Stephen's College, University of Delhi, India

Top 1% of all the students who appeared at the Higher Secondary Examination, March **2013**. Nominated by Kerala State Higher Secondary Board for the Central Government Scholarship for higher education

INSPIRE SHE, 2013 -2018 : Five-year scholarship by the Department of Science and Technology, Government of India, based on an excellent performance at the higher secondary and undergrad level

INSPIRE AWARD, 2011 : For the outstanding academic performance at the high school level, from the Department of Science and Technology, Government of India