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

Molecular Simulations and Modeling:
• 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 sensitivity of population dynamics of bacteria towards the nutrient enviroment using modeling and simulation. Modeled quorum sensing and chemotaxis behaviors, and emulated racing condition between them

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

- Conducted metabolic network reconstructions and flux balance analyis 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 south east Asia to understand the rise of drug resistantance 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 personalised 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 previleged 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

OTHERS

- Sample bullet point.