SUBHAJIT ROY

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1050 S Stanley Pl #P213, Tempe, AZ, 85281

EDUCATION

Physics,PhD *August 2022 - Present*
Petr Sulc's Lab, Arizona State University Current CGPA - 4/4
Computational design and analysis of genetic materials,focusing on self-assembly.

Physics,Integrated BS-MS *August 2017 - July 2022*
UM-DAE-Centre For Excellence In Basic Sciences Current CGPA - 7.3/10
PLAS-5k binding affinity database and retrosynthesis prediction usig Deep Learning, Prof Deva Priyakumar,IIIT Hydrabad
Entropic theoretical study of β ladder domain of Zika Virus

Senior Secondary Education *April 2015 - May 2017*
D.A.V. Public School, Rupnarayanpur Score - 84.6%

Secondary Education *March 2015*
Burnpur Riverside School, Chittranjan CGPA - 10/10

RESEARCH EXPERIENCE

- **Coarse Grain DNA Origami Model** *2022-Present*
  Designing a coarse grain representation of DNA origami using heterogeneous anharmonic oscillator and Patchy Particle model reducing computational time by 100times still maintaining underlying statistical features using oxDNA with vanilla C
- **Seeding DNA Origami Growth** *2022-Present*
  Achieved higher yield and self growth of DNA origami crystals using pre-assembled origami particles experimentally, guided by simulation prediction.
- **DNA-PAINT data analysis via oxDNA prediction** *2022-2023*
  Collaborated with experimental group to help them analyse their experimental data generated using DNA-PAINT and de-convolute complicated 3D geometry of the origami used in the experiment. This analysis even improved the resolution to approximately 1nm and shed light on its dynamics.
- **PLAS-5k Database** *2021-2022*
  Created 5000 protein ligand complex database using MD simulation in aqueous environment and reported various important properties like polar, non-polar interaction, electrostatic interaction, Van Darwall's interaction. Results out performed commonly used docking tool Auto Dock Vina, and strongly believe that this would be highly helpful to ML studies related to protein-lingand complexes and docking.
- **Potential destabilizing hotspot in the β ladder domain of ZIKA** *2017-2020*
  Established bio-chemical pathway to destabilise one of the essential protein of ZIKA virus by cleaving di-sulphide bond in the β ladder domain of NS1 protein, which is responsible for its growth and infection via surface attachement and many other essential functions. This was concluded using extensive thermodynamics study.
- **Observational Radio Astronomy** *2019-2020*
  Generated images from GMRT Radio telescope and NASA SkyView data query. Studied and classified radio galaxies using wide-spectrum data. Also anlaysed real time Milky Way data from PICTOR telescope.
- **Heterogeneous computing with multiple GPU and CPU using Raspberry Pis** *2018-2019*
  Achieved heterogeneous computing capabilities using openCL and MPI with multiple GPUs and CPU spread across 8 Raspberry Pis. Designed an algorithm that was able uniformly distribute GPU jobs over LAN.

TECHNICAL SKILLS

Programming: Python, C++ (including CUDA and MPI), FORTRAN, MATHLAB, Bash, Java, R, JS, C#, Lua
Software & Tools: **Simulation Platform:** NAMD, GROMACS,Amber20,OpenMM,OxDNA
Visualizing Software : VMD, UCSF Chimera, Pymol, OxDNA-viewer(Oxview)
Non-Accademic Platforms: Gatsby(React) JS, Laravel, Lumen, NodesJs Backend, Unity Android(Java), React Native, Flutter(Android and IOS)
Others: Tensorflow, Keras, PyTorch, Embedded C (Arduino and STM32), Raspberry PI

PUBLICATION/PRE-PRINT

1. Roy P, Roy S, Sengupta N. Disulfide Reduction Allosterically Destabilizes the β-Ladder Subdomain Assembly within the NS1 Dimer of ZIKV. Biophys J. 2020 Oct 20;119(8):1525-1537.
2. Korlepara, D.B., Vasavi, C.S., Jeurkar, S. , Pal, Pradeep, Roy, Subhajit et al. PLAS-5k: Dataset of Protein-Ligand Affinities from Molecular Dynamics for Machine Learning Applications. Sci Data 9, 548 (2022).
3. High-speed 3D DNA-PAINT and unsupervised clustering for unlocking 3D DNA origami cryptography G. Bimananda M. Wisna, Daria Sukhareva, Jonathan Zhao, Deeksha Satyabola, Michael Matthies, Subhajit Roy, Petr Šulc, Hao Yan, Rizal F. Hariadia bioRxiv 2023.08.29.555281

AWARDS AND ACHIEVEMENTS

- Recipient of DST-INSPIRE fellowship under SHE schemes (2017-2022)
- Vijyoshi Science Camp-2018 organized by KVPY, at IISC, bangalore.
- Science Olympiad Silver zone- 2014 (Gold Medalist).

CONFERENCES AND WORKSHOP ATTENDED

- Journal of Physical Chemistry Workshop, at IISER Kolkata, June, 2018.
- AWS World Summit Online 2020, 13th May.
- Science Leadership Workshop – 2020.
- Big Data 2020, Centre For Mathematical Sciences and Applications, Harvard University.