SUBHAJIT ROY

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EDUCATION

Physics,PhD *August 2022 - Present*
Petr Sulc's Lab, Arizona State University Current CGPA - 3.93/4
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

RESEARCH EXPERIENCE

- **Ph.D. research - Arizona State University- Professor Petr Sulc** *2022-Present*
  - Designed coarse grain DNA model using heterogeneous anharmonic oscillator and Patchy Particle using C++, CUDA.
  - Achieved 100 time computational speed up still maintaining underlying statistical features.
  - Accomplished self growth of DNA origami at 4C higher temperature and higher yield, guided by simulation.
  - Collaborated with experimental group to analyze DNA-PAINT data and deconvoluted complicated 3D origami geometry.
  - Improved resolution to 1nm and uncovered its dynamics using clusturing algorithm and statistical analysis.
  - Designed a high read out cryptography method with DNA origami using DNA-PAINT.
  - Developed new javascript based 3D viewing platform for non standard coarse grain models.
  - Contibuted to development of simulation engine oxDNA and its javascript viewer Oxview.
  - Setup and maintain linux HPC clusters with x86-64 and arm64-v8 cpus and nvidia gpus.
- **Master's Thesis - IIIT Hyderabad - Professor Deva Priyakumar** *2021-2022*
  - Generated 5000 protein ligand complexes using MD simulation
  - Calculated binding affinity and other important properties like polar, non-polar interaction, electrostatic interaction, Van Der Waal's interactions from the trajectory.
  - Docking results outperformed commonly used tools like Auto Dock Vina.
  - Trained the dataset on CNN models like OnionNet and obtained a Pearson's cofficient of 0.96 in a 10 fold validation.
- **Summer Project - DAE-CEBS - Professor Anand Hota** *2020-2021*
  - Generated and analyze images from GMRT Radio telescope and NASA SkyView.
  - Studies and classified various radio galaxies using wide spectrum data not only limited to radio or visible but IR,UV as well.
  - Real time data were also analysed targeted to gather more information about our Milky Way.
- **Summer Project - ISER Kolkata - Professor Neelanjana Sengupta** *2017-2020*
  - Established bio-chemical pathway to destabilised NS1 (Non Structural Domain) protein of ZIKA virus.
  - Different di-sulphide bonds in β ladder domain of NS1 protein were cleaved and simulated using NAMD.
  - Different parameters like conformational entropy, enthalphy, solvent accessible surface area, structural persistancy were used.
  - The above information could be used to design drug targed to ZIKA virus
- **Other Project during BS-MS - DAE-CEBS**
  - Studied micro controllers like Aurdino, STM32 and designed high altitude quadrocopter.
  - Designed uniform job distribution algorithm over multiple GPUS and CPU using OpenCL.

TECHNICAL SKILLS

Programming: Python, C++ (CUDA, OpenMP, MPI), Javascript (Babylon JS, Three JS), 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)
Linux: SLURM, Linux Kernel, Docker, Kubernet, Tinacore/EDK 2
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 Roy** et al. PLAS-5k: Dataset of Protein-Ligand Affinities from Molecular Dynamics for Machine Learning Applications. Sci Data 9, 548 (2022).
3. G. Bimananda M. Wisna, Daria Sukhareva, Jonathan Zhao, Deeksha Satyabola, Michael Matthies, **Subhajit Roy**, Petr Šulc, Hao Yan, Rizal F. Hariadia High-speed 3D DNA-PAINT and unsupervised clustering for unlocking 3D DNA origami cryptography bioRxiv 2023.08.29.555281

TEACHING EXPERIENCE

- **Teaching Assistance** for physics mechanics lab course on fall 2022,spring 2023 and spring 2024.
- **Graduate Research Assistance** on fall 2023.
- **Trained PhD students.**

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).

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.

EXTRA CURRICULAR ACTIVITIES

- Member of Biophysical Society student chapter, Arizona.