SUBHAJIT ROY

Linkedin Subhajit-Roy-Partho Google Scholar me.subhajitroy1999@gmail.com Portfolio
1050 S Stanley Pl #P213, Tempe, AZ, 85281

SUMMARY

I am a highly motivated and ambitious graduate student passionately pushing the field of genetic materials to solve large scale self-assembly and related biophysical problems. Strong experienced in MD simulation and deep learning, big data, rich analysis skills in physical, chemical, statistical aspect of experimental data. Entrepreneurial plus independent research skills from framing new ideas, documenting in peer-reviewed journals and writing proposals for grants. Passionate about learning and implementing novel and challenging techniques that are advancing the science.

EDUCATION

Physics, PhD *August 2022 - Present*
Petr Sulc's Lab, Arizona State University Current CGPA - 3.94/4
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

TECHNICAL SKILLS

Programming: Python(Pytorch, TensorFlow,CuPy,Cython), C++ (CUDA, OpenMP, MPI), Javascript (Babylon JS, Three JS), FORTRAN, MATLAB Mathematica,Bash, Java, R, JS, C#, Lua

Software & Tools:
Simulation Platform: OxDNA,AMBER, NAMD, GROMACS,OpenMM,Ansys
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

MACHINE LEARNING EXPERIENCE

Skills: Pytorch, Tensorflow, CuPy, Transformer, CNN, Boltzmann Machines, Clustering, Molecular embedding, OpenCV

Ph.D. research - Arizona State University *2022-Present*
- Working on generation of equilibration conformation of DNA and RNA given the sequence using Scalable Interpolant Transformer with SE(3) ininvariant corrdinates.
- Improved resolution of DNA-PAINT to 1nm and deconvoluted complicated 3D origami geometry using clustering algorithms like DBSCAN.
- Uncovered the detailed dynamics using oxDNA simulation combined with ML algorithm.
- Fasten analysis of AFM images of DNA origami using openCV.

Master's Thesis - IIIT Hyderabad *2021-2022*
- Generated 5000 Protein Ligand complexes (PLAS 5k) with their binding affinity for ML training purpose.
- Generated a CNN model to train the database and obtained a Pearson's cofficient of 0.96 in a 10 fold validation.
- Outperformed conventional docking method in both accuracy and speed.

SIMULATION EXPERIENCE

Skills: Developer of oxDNA and oxView, AMBER MD, GROMACS, OpenMM, C++, CUDA, Force field development, Cython, DNA purification, AFM, DNA-PAINT, PCR

Ph.D. research - Arizona State University *2022-Present*
- Formulated the pathway of protein complex denaturation of proteins with help of DNA (PROTAC) using hybrid quantum-classical all atom simulation.
- Active developer of oxDNA and oxview, added features like non-singular mass, support for modern GPUs and ARM architecture.
- Improved the existing forcefield of patchy particle system to study crystal growth using DNA with improved dynamics.
- Developed coarse grain force field to simulate irregular origami shapes using rigid body physics and patchy particles.
- Speed up the simulation by 1000 times compared to oxDNA2 simulation using lesser particles and GPU compute (CUDA).
- Accomplished self growth of DNA origami crystal at 12C higher temperature and higher yield, guided by simulation.

- Devised a working design with DNA icosahedron and helix to form crystal with optical properties at visible wavelength.
- Formulated the pathway of protein complex denaturation of proteins with help of DNA using hybrid quantum-classical all atom simulation.
- Constructing a unified platform to simulate, analyse and host DNA origami and other nucleic acid structure in our clusters.
- Developed new babylon js based 3D viewing platform for non standard coarse grain models.
- Setup and maintain linux HPC clusters with x86-64 and arm64-v8 cpus and nvidia gpus.
- Experienced with experimental techniques like DNA gel electrophoresis, PCR, DNA-PAINT, AFM.

Master's Thesis - IIIT Hyderabad *2021-2022*

- Automatized all atom simulation of 5000 protein ligand complexes and extracted protein-ligand binding parameters like affinity, polar, non-polar interaction, electrostatic interaction, Van Der Waal's using MM-PBSA and MM-GBSA.
- Binding results outperformed Auto Dock Vina.

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

Skills: Micro-controller, Embedded C, NASA Skyview, Image Analysis, OpenCL

- 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.
- Studied micro controllers like Aurdino, STM32 and designed high altitude quadrocopter.
- Designed uniform job distribution algorithm over multiple GPUS and CPU using OpenCL.

PUBLICATION/PRE-PRINT

1. Rong Zheng, Abhay Prasad, Deeksha Satyabola, Yang Xu, **Subhajit Roy**, Yichen Yan, Petr Sulc, Hao Yan DNA-templated spatially controlled proteolysis targeting chimera for CyclinD1-CDK4/6 complex protein degradation.(Under Review JACS)
2. 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 Nature Com under review
3. 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).
4. 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.

TEACHING EXPERIENCE

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

AWARDS AND ACHIEVEMENTS

- **DST-INSPIRE (Innovation in Science Pursuit for Inspired Research) Fellowship**: offered to top 1% students after 12th grade to support students in India to pursue Ph.D.
- **Vijyoshi Science Camp-2018**: organized by KVPY, at IISC, bangalore.
- **Science Olympiad Silver zone**- 2014 (Gold Medalist National level).

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.

VOLUNTEER EXPERIENCE

- Member of Biophysical Society student chapter, Arizona.
- Presenter at Biodesign Open door, ASU Biophest 2024, Biosence Network ACP, ASU Homecoming, Biophest 2023.

- Represented ASU Physics Department at Luke Airforce Air-day 2024.
- Hosted multiple career conversation over coffee sessions, and BPS student chapter Image contest for calenders.