

Two days Hands-on Workshop on High Performance Computing in Bioinformatics

Venue: Centre for Computational and Data Sciences, J C Bose Annex, IIT Kharagpur

Date: 10th - 11th February 2024

Time	Events	
9:00 – 9:30	Welcome and Introduction	
9:30 – 18:00	Day (1)	
	Speaker	Title
9:30 – 10:30	Speaker 1: <i>Saugata Hazra</i>	
10:30 – 11:00	Tea Break	
11:00 – 12:30	Speaker 2: <i>Sabyashachi Mishra</i>	Quantum Mechanics in Biomolecular Simulations
12:30 – 13:30	Lunch Break	
14:00 – 15:30	Speaker 3: <i>Pralay Mitra</i>	High-performance Parallel Programming in Protein Docking and Design
15:30 – 16:30	<i>Hands-on CD-HIT</i>	
16:30 – 17:00	Tea Break	
17:00 – 18:00	Speaker 4: <i>Srayanta Mukherjee</i>	Super Charging Traditional Bioinformatics Problem with Deep Learning and AI
9:00 – 17:00	Day(2)	
	Speaker	Title
9:00 – 10:00	Speaker 5: <i>Sudipta Dutta</i>	Valley-polarization in noncentrosymmetric systems
10:00 – 13:00	<i>Hands-on Molecular Dynamics Simulation</i>	
13:00 – 14:00	Lunch Break	
14:00 – 17:00	<i>Hands-on Molecular Docking</i>	