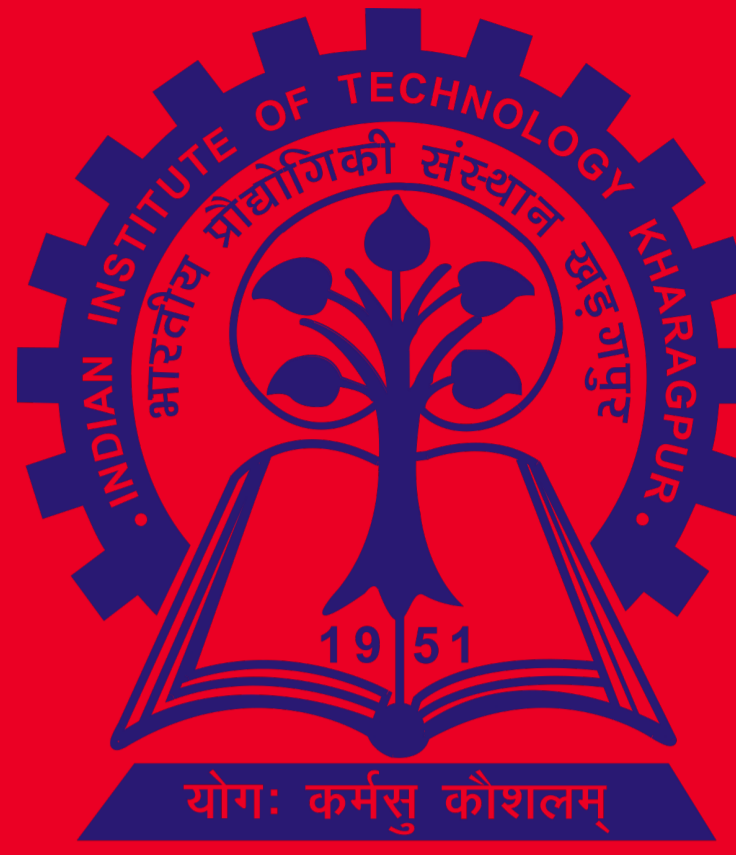


Two days Hands-on Workshop on High Performance Computing in Bioinformatics

February 10-11, 2024, IIT Kharagpur, India

Jointly organized by

National Supercomputing Mission (NSM) Nodal Center, Indian Institute of Technology Kharagpur, India



Objective and Scope

Explore the frontier of Computational Biology and Bioinformatics in this hands-on workshop. The workshop offers practical insights and essential skills vital for conducting cutting-edge research in Computational Biology and Bioinformatics.

Advance Your Research: Acquire skills at the forefront of bioinformatics, empowering you to conduct advanced research in computational biology.

Practical Application: Translate theoretical knowledge into practical expertise through immersive hands-on activities.

Interdisciplinary Learning: Bridge biology and computer science, fostering an interdisciplinary approach to problem-solving.

Networking Opportunities: Connect with experts and peers in the field, building valuable professional connections.



ParamShakti Facility at IIT Kharagpur

Who can apply?

Join us in unlocking the potential of computational techniques in unraveling the mysteries of biological systems.

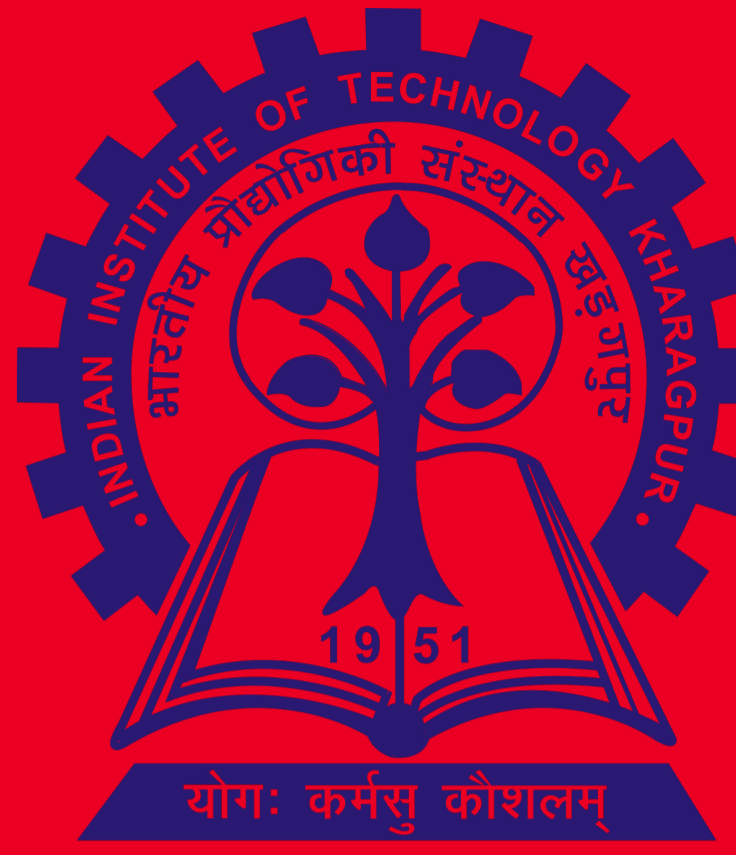
Explore computational techniques in this specialized workshop designed for researchers, students, and professionals interested in Computational Biology and Bioinformatics. Gain expertise in simulating biomolecular dynamics, Quantum Mechanics in Biomolecular Simulations, mastering molecular docking, protein engineering, and acquiring skills in clustering and data reduction. Don't miss the chance to enhance your computational biology skills and contribute to groundbreaking discoveries in the biological sciences.

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

February 10-11, 2024, IIT Kharagpur, India

Jointly organized by

National Supercomputing Mission (NSM) Nodal Center, Indian Institute of Technology Kharagpur, India



SPEAKER

Name – Dr. Saugata Hazra
Affiliation – Department of Biosciences and Biotechnology, IIT Roorkee
Expertise – Studying Antimicrobial Drug Resistance, Structural Biology, Protein crystallography, Structure-based drug development



SPEAKER

Name – Dr. Sabyashachi Mishra
Affiliation – Department of Chemistry, IIT Kharagpur
Expertise – Quantum Computing in Chemistry, Enzyme Catalysis with QM/MM Approach, Multi-scale Simulations of Biochemical Systems



SPEAKER

Name – Dr. Sudipta Dutta
Affiliation – Department of Physics, IISER Tirupati
Expertise – Theoretical condensed matter, Strongly correlated systems, Atomically thin nanomaterials, Mesoscopic transport



SPEAKER

Name – Dr. Pralay Mitra
Affiliation – Department of Computer Science and Engineering, IIT Kharagpur
Expertise – Investigate Cancer Progression, Designing High-throughput Techniques for Drug Discovery, Computational Protein Engineering, Biomarker discovery



SPEAKER

Name – Dr. Srayanta Mukherjee
Affiliation – Lead Data Scientist, BCGX-AI Institute, Basel, Switzerland
Expertise – Stochastic simulations including replica exchange, simulated annealing and Monte Carlo, molecular dynamics, QM/MM, stokesian and Brownian dynamics



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

February 10-11, 2024, IIT Kharagpur, India

Jointly organized by

National Supercomputing Mission (NSM) Nodal Center, Indian Institute of Technology Kharagpur, India



Saturday, 10 February, 2024

- 09:00 – 09:30 Welcome and Introduction
- 09:30 – 10:30 TBA Saugata Hazra
- 11:00 – 12:30 Quantum Mechanics in Biomolecular Simulations Sabyashachi Mishra
- 12:30 – 13:30 Lunch Break
- 14:00 – 17:00 Hands-on Molecular Dynamics Simulation
- 17:00 – 18:00 Super charging traditional bioinformatics problem deep learning and AI Srayanta Mukherjee

Sunday, 11 February, 2024

- 09:00 – 10:00 TBA Sudipta Dutta
- 10:30 – 12:00 High-performance Parallel programming in protein docking and design Pralay Mitra
- 12:00 – 13:00 Hands-on CD-HIT
- 13:00 – 14:00 Lunch Break
- 14:00 – 17:00 Hands-on Autodock

Important Information

- Venue: Center for Computational and Data Sciences, J.C Bose Annexe, Ramanujan Complex, IIT Kharagpur
- Registration fees: INR 600/- (non-refundable) (Free for IIT Kharagpur Students)
- Registration link: <https://forms.gle/nSLQKLj3Qh88H4NYA>
- Last date of Registration: 4th February 2024 till 5 P.M
- The student needs to carry their laptop for the hands-on session.
- Selected outstation students will be provided accommodation during the workshop.
- Participants must have a fundamental understanding of Linux and proficiency in Python and R programming.
- If you have any questions or doubts, feel free to reach out. ccdsoffi@ccds.iitkgp.ac.in
- Due to limited physical capacity, the sessions will be conducted in a hybrid mode. Fill out the Google form with your preference.