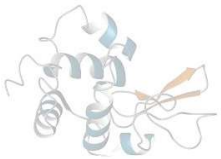
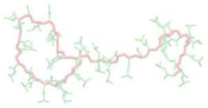


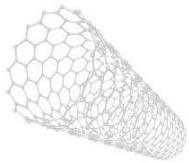


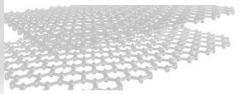
NEW INTER-DISCIPLINARY COURSE
SPRING SEMESTER 2018-19

Centre for Computational and Data Sciences (CCDS)

High Performance Computing and its Applications in Complex Physical Systems

Course Number: CD61004 Credits: 4 (3-1-0)





Objectives:
1.) To introduce the basic concepts related to HPC architecture and parallel computing
2.) To discuss various computational techniques for studying soft matter systems
3.) To apply these concepts for examining complex biomolecular/materials systems that generally require large-scale HPC platform with hybrid CPU-GPU architectures.

Target audience: Ph.D., M.Sc., M.Tech, Int. M.Sc. Students

Instructors: Dr. Divya Nayar (CD), Dr. Sandeep Kumar Reddy (CD), Prof. Sanjoy Bandyopadhyay (CY) , Dr. Somnath Roy (ME)

Key features: Hands-on sessions, tutorials, exposure to using hybrid CPU-GPU computing, practical knowledge and skills for using HPC environment, application to real-world problems in material science and biology.

Contents and Lecture Hours (L,T):

Component 1: Introduction to HPC architecture and parallel programming (11L, 4T)
- Basic architecture and organization: memory heirarchy, shared and distributed memory architectures, multiprocessor architecture
- Introduction to thread level parallelism
- Accelerators (GPU, Xeon-Phi)
- Performance prediction and evaluation
- Parallel programming/computing: Introduction to MPI/ OpenMP, basics of CUDA programming
- Optimizing cluster operation: Running jobs in HPC environment, job scheduler, cluster level load balancing

Component 2: Special methods for studying complex systems (15L, 4T)
- Basics of statistical mechanics
- Potential energy surface
- Introduction to molecular mechanics
- Simulation methods: Molecular Dynamics (MD), Monte Carlo (MC) simulations
- Enhanced sampling methods
- Coarse-grain modeling

Component 3: Applications to complex systems (14L, 6T)
- Open-source software: MD and MC simulation packages
- Parallelization in software: domain/spatial decomposition, distribution of nonbonded interactions, dynamic load balancing, multiprocessor communication
- Modeling of soft matter systems such as biomolecules, polymers, carbon nanostructures etc.
- Computation of thermodynamic, kinetic and mechanical properties of different complex systems

For further information, log on to ERP and look for course number CD61004
Contact : divya.nayar@iitkgp.ac.in, skreddy@iitkgp.ac.in