Course Title: High Performance Computing and its Applications in Complex Physical Systems

Course Number: CD61004 **Credits:** 3-1-0 **Dept:** CCDS

Time Slot: Tue 2.00-4.00 pm & Thu 11.00-1.00 pm (tentative)

Objective: This subject is primarily designed for students who would be working on applications that require basic understanding of the high performance computing (HPC) environment, but may not necessarily have a computer science background. The objective of the subject is to (1) Introduce the basic concepts related to HPC architecture and parallel computing; (2) To discuss various computational techniques for studying soft matter systems, and (3) To apply these concepts to examine complex biomolecular/materials systems that generally require large-scale HPC platform with hybrid CPU-GPU architectures. Hands-on tutorial sessions will provide an exposure to the students in using CPU and GPU based servers of a supercomputer (or local servers) to perform simulations and analysis of such complex systems. Upon attending the course, the students will be equipped with both theoretical and practical knowledge and skills of effectively using a large supercomputing platform and computational methods to solve and evaluate real-world problems in materials 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 non-bonded 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