PHY5002   Computer Simulations in Physics

Course Code	PHY5002	Semester	
Course Title	*Computer Simulation in Physics*		
Credits	3	Type	Elective

Course Outcome

This course in intended to give a hands-on training to students in using simulational techniques for research work in modern physics. Basically the very important models of monte-carlo and molecular dynamics are used to teach how the advanced simulational techniques are actually implemented. It is also the aim of the course to add research oriented work to be implemented individually so that the concepts are actually translated into practice.

Course Structure

Contents: (1) Random number generation. Simple sampling Monte Carlo methods: Percolation and random walk models. Importance sampling and Metropolis algorithm. Ising model, finite size scaling and application to phase transition. Quantum Monte Carlo methods. Introduction to polymers and Protein folding. (2) Molecular Dynamics: Verlett algorithm. MD for different ensembles. Application to simple systems. Melting transition. Quantum MD methods. (3) High performance computing and program development for parallel execution. (4) Practical implementation of these methods on computer.

Suggested Books

1. D.P.Landau and K.Binder, A Guide to Monte Carlo Simulation in Statistical Physics, Cambridge (2000)
2. M.P.Allen and D.J.Tildsley, Computer Simulation of Liquids, Oxford (1987)
3. N.J. Gordano and H. Nakanishi, Computational Physics, Addison Wesley (2005)