1. PH701 Introduction to Molecular Simulations

Credit: 2-2-0-4 Approval: Approved in 2nd Senate

Prerequisite: Master-level courses in Physics/Chemistry

Students intended for: Ph.D.

Elective or Core: Elective Semester: Odd/Even

Course content:

- **Classical statistical mechanics**
- **Ensembles:** microcanonical, canonical, grand canonical ensembles ideal gas- harmonic oscillator – Spin Systems. Introduction to Stochastic process, Brownian Motion, Langevin equation, Fokker-Planck equation, Introduction to liquid state theory- pair distribution functions- structure factor-coherent and in-coherent scattering- Ornstein-Zernike correlation function Diffusion in a liquid-mean square displacement- self and collective van Hove correlation function – Intermediate scattering function and dynamics structure factor.
- **Programing in C and Fortran 95** - essential for programming in this course
- **Introduction of Monte Carlo methods:** Value of using MC method, Gaussian distribution from 1d random walk, Metrapolis algorithm for construction NVT ensemble, Implementation of ensemble using MC methods.
- **Proj 1**. Write a Monte Carlo simulation to simulate model liquid.
- **Introduction to Molecular dynamic simulations:** Molecular dynamics simulations, Numerical integration of linear differential equations, Leap-Frog algorithm, Velocity Verlet algorithm, Periodic boundary condition one, two and three dimensions.
- **Proj. 2** Write a MD simulation code for simple liquids and for a polymer chain connected by harmonic spring.
- **Introduction to Brownian and Lengevin dynamics simulations:** Simple Brownian dynamics algorithm without hydrodynamic interactions.Langevin dynamics simulations.
- **Proj. 3:** Write a Brownian dynamics code to simulate colloids in a solution and motion of single polymer chain.
- **Analysis data from simulations:** Computation of radial distribution function, Structure factor, Time series analysis, Mean square displacement.
- **Proj 4:** Using trajectories produced from the earlier simulation to compute: Radial distribution functions. Mean square displacement of center of mass and monomers for a polymer chain. Computation of stress, stress correlation function and viscosity.

Text & Reference Books:

Statistical Mechanics R. K. Pathria

Introduction stochastic process in physics and astronomy, Rev. Mod. Phys. 1 **15**(1943)

What is liquid? Understanding the state of matter, J. A. Barker and D. Henderson, Rev. Mod. Phys. 587 **48**(1976).

Theory of simple liquids by J. P. Hansen and I. R. McDonald

Statistical Mechanics by D. A. McQuarrie

Computer simulation of liquids by M. P. Allen and D. J. Tildesey

Understanding molecular simulation by DaanFrenkel

The art of molecular dynamics simulations by D. C. Rappaport

A guide to Monte Carlo simulations in statistical Physics by D. P. Landau and Kurt Binder