JT305: Advanced Computational Methods
Credits: Ph. D. 3:0
January - April 2020 Semester

Instructor: Srikanth Sastry
Jawaharlal Nehru Centre for Advanced Scientific Research
Jakkur, Bengaluru,560064
sastry@jncasr.ac.in
Teaching Assistant: Yagyik Goswami
yagyikg@jncasr.ac.in
Course URL : $http://www.jncasr.ac.in/sastry/jt305_2020$

Course Ouline

Class Times: Mon, Wed 2:00 PM – 3:30 PM (Tutorials 4:00 - 5:30 PM)

Venue: Seminar Hall II, College Bldg Ground Floor, JNCASR

Tutorial Venue: CCMS Classroom, College Bldg II floor, JNCASR

Course Structure

The lectures will cover the following topics.

1 Statistical Mechanics - Basic Concepts

2 The Monte Carlo method for sampling and importance sampling.

3 Monte Carlo simulation of lattice and off-lattice systems.

4 Molecular dynamics simulations - basic principles

5 Molecular dynamics simulations in various ensembles

6 Analysis of data: Statistics, Error Estimation

7 Tools for computation: (Introduction and tutorials for some of..) Scripts (python, awk..), visualization, parallelization, GROMACS, LAMMPS, mathematica, matlab.

8 Histogram Methods

9 Free Energy Methods

10 Optimization, Biased and Accelerated Sampling

11 Special Topic: Rare Events

12 Special Topic: Nonequilibrium Molecular Dynamics

Lectures will cover concepts and algorithms, and tutorial sessions will provide hands-on instruction. Two special topics (rare events and nonequilibrium molecular dynamics) will be covered in detail (six lectures each). *Exercise* problems will be gone over in detail in the tutorials, and broad guidance will be given for *assignment* problems.

Prerequisites: Prior knowledge of statistical mechanics and familiarity with a programming language. Anybody willing to pick up the relevant background (the discussion in the course is in principle self contained), and programming skills along the way can also attend.

Evaluation: Grading will be based on solutions to homework assignments and oral presentation of solutions assigned to each student, and of a course project chosen by the student in consulation with the instructor.

Reference Books:

1. "Understanding Molecular Simulation" by D. Frenkel and B. Smit (Academic Press)
2. "Computer Simulation of Liquids" by M. P. Allen and D. Tildesley (Oxford University Press)
3. "Nonequilibrium Molecular Dynamics" by B. D. Todd and P. J. Daivis (Cambridge University Press)