WORKSHOP ON MOLECULAR MODELLING AND SIMULATION

Venue: Computer Laboratory, Department of Chemical Engineering, IIT Guwahati.

Details: Molecular modelling and simulation involves developing representations of physical systems at atomistic/molecular-level detail, and using such models to simulate (or mimic) physical processes/phenomena on a computer for studying properties of interest. Molecular simulations can also be used to calculate or predict properties and quantities that may be difficult to observe experimentally.

The workshop will introduce the field of molecular modelling and simulation to the participants through lecture, demonstration and hands-on session. In particular, the focus will be on classical molecular dynamics (MD) simulation technique. The simulations will be conducted and demonstrated using the open source software package LAMMPS. The software package VMD (also open source) will be used to visualize molecular models and simulation results.

The workshop will be conducted in two sessions. The first session will introduce preliminary concepts of molecular modelling and simulation and the MD simulation technique. This session will also feature demonstration of the LAMMPS package for setting up and running simple MD simulations. The second session will be hands-on where the participants will set up and run some MD simulations using LAMMPS.

Session I (10:00 to 13:00): Lecture + Demonstration

- Introduction to Molecular Modelling and Simulation
- Introduction to Molecular Dynamics Simulation
- Running Molecular Simulations using LAMMPS

Session II (14:00 to 17:00): Hands-on

- Energy Minimization/Geometry Optimization
- Molecular Dynamics Simulation of Simple System (e.g. pure gas or simple liquid)
- Molecular Dynamics Simulation of Complex System (e.g. polymers, porous solids)

The workshop will be introductory in scope, aimed at beginners in the field of molecular simulation. The objective of the workshop is to familiarize the participants with introductory concepts of molecular simulation so that they are equipped to learn advanced techniques on their own for applications to more complex systems. The expected outcome is that the participants should be able to conduct MD simulations using LAMMPS for calculating properties of interest.

Additional information on LAMMPS, including a detailed user manual, is available at the official website: http://lammps.sandia.gov/
Additional information on VMD is available at http://www.ks.uiuc.edu/Research/vmd/