School on Understanding Molecular Simulations: Theory and Applications (UMS 2010)

List of Lectures and Tutorials:
The workshop will consist of 90 minute lectures, tutorials and computer tutorials. There will be two sessions every morning and two in the afternoon.

L1 Statistical Mechanics: Concept of phase space and ensembles. Canonical, microcanonical and grandcanonical ensembles, Ideal and Interacting systems, Equilibrium averages, Correlation functions, fluctuations, fluctuation-dissipation theorem, Markov Processes, Stationarity, Ergodicity, Deterministic and Stochastic dynamics. (2 lectures + 2 Tutorials)

L2 Principles of Monte Carlo Simulations: Markov Processes, transition rates, detailed balance, stationary probability distributions, random numbers, metropolis algorithm, equilibration and production, Monte Carlo simulation of molecular dynamics. (2 Lectures + 1 Tutorial + 1 Computer Tutorial)

L3 Principles of Molecular Dynamics: Classical Molecular Dynamics, Interatomic interactions, trajectories, Equations of motion, Verlet and velocity Verlet algorithms, simulation cell, periodic boundary conditions, constrained molecular dynamics, microcanonical ensemble averages, extension to other ensembles, Nose-Hoover thermostats, other thermostats, grand canonical ensembles. (2 Lectures + 1 Tutorial + 1 Computer Tutorial)

L4 Interaction Potentials: Model Potentials for atomic systems, hard spheres, Lennard-Jones potentials, intermolecular potentials, force-fields, potentials for water, biological systems. (1 Lecture + 1 Tutorial)

L5 Advanced Monte Carlo Methods: Solid on Solid model, Kinetic Monte Carlo, Rejection Free methods, Cluster moves, Biased Monte Carlo methods.(2 Lectures + 2 Computer Tutorials)

L6 Advanced Molecular Dynamics: Car–Parrinello molecular dynamics simulations, blue–moon ensemble, umbrella sampling, and metadynamics (2 Lectures

+ 2 Computer Tutorials)

L7 Applications: Biological systems, Solids and surfaces Classical force–fields, protein–simulation, periodic–density functional theory and its applications in simulating bulk solids and surfaces, phase–transitions. (2 Lectures + 2 Computer Tutorials)

L8 Data Analysis: Equilibrium averages, time correlation functions, transport coefficients, averages and error estimates, relaxation processes, free energy calculations, reaction rates. (2 Lectures + 1 Tutorial + 1 Computer Tutorial)

L9 Programming Methods: Popular Numerical methods, mathematical libraries, programming tips, data storage and analysis. (1 Lecture + 1 Computer Tutorial)

L10 Parallelization : High–performance computing, Programming using Message Passing Interface (MPI) and OpenMP (2 Lecture + 2 Computer Tutorials)

L11 Future of Molecular Simulations: Simulation of reactions, large scale systems and rare events, new computational paradigms, storage and analysis of large data sets. (2 Lecture)

ACADEMIC TIMETABLE:

Date	09.00-10.30	11.00-12.30	14.00-15.30	16.00-17.30
03/11	ARR	ARR	ARR	ARR
04/11	L1	T1	L2	T1
05/11	L2	T2	L2	CT2
06/11	L3	T3	L3	CT3
07/11	L4	T4	L5	CT5
08/11	L5	CT5	L6	CT6
09/11	L6	CT6	L7	CT7
10/11	L7	CT7	L8	T8
11/11	L8	CT8	L9	CT9
12/11	L10	CT10	L10	CT10
13/11	L11	L11	DEP	DEP

10.30-11.00 : Tea Break
12:30-14.00 : Lunch Break

15.30-16.00 : Tea Break
L = Lecture, T = Tutorial, CT = Computer Tutorial
Lecture numbers are in accordance with Annexure-I.
ARR = Arrival, DEP= Departure