MB 211 Jan 3:1

Multiscale Theory and Simulations of Biomolecular Systems

Instructor

Anand Srivastava
Email: anand@iisc.ac.in

Teaching Assistant

Email:

Department: Molecular Biophsyics Unit

Course Time: Tues

Lecture venue:

Detailed Course Page:

Announcements

Brief description of the course

Theoretical and computational aspects of various advance sampling and free energy calculation methods.

Prerequisites

Basic knowledge in statistical mechanics, thermodynamics and molecular simulation (and/or basic exposure to biomolecule conformations) Working knowledge of any one molecular dynamics tool.

Syllabus

Theoretical and computational aspects of various advance sampling and free energy calculation methods (maximum work theorem, Jarzinsky equality, umbrella sampling, replica exchange, metadynamics, markov state model, etc). Continuum representation of solvent and calculation of electrostatics and non-electrostatics component of solvation free energy. Method development and application of multiscale coarse-graining methods such as force-matching, elastic network models, Inverse-Boltzmaanâ€™s method and relative entropy methods.

Course outcomes

Advance methods in molecular modeling

Grading policy

30% assignment, 30% workshop, 40% project

Assignments

Resources

a. Michael P. Allen and Dominic J. Tidesley, Computer Simulation of Liquids (Oxford Science Publications), 1981

b. Andrew Leach, Molecular Modeling: Principles and Application (Princet Hall), 2001.

c. Christophe Chipot (Ed.) and Andrew Pohorille (Ed.), Free Energy Calculations (Springer), 2008

d. Gregory A. Voth (Ed.), Coarse-Graining of Condensed Phase and Biomolecular Systems (CRC Press), 2008

e. Mark Tuckerman, Statistical Mechanics: Theory and Molecular Simulation (Oxford Graduate Texts), 2010

f. Ken Dill and Sarina Bromberg, Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics, and Nanoscience (Taylor and Francis), 2010

g. Gregory R. Bowman (Ed.), Vijay S. Pande (Ed.) and Frank NoÃ© (Ed.), An Introduction to Markov State Models and Their Application to Long Timescale Molecular Simulation: Advances in Experimental Medicine and Biology (Springer), 2013