IT- 773: Bimolecular Simulation; Theory and application (BioSimulation)

Pre-requisite: There is no strict pre-requisite but knowledge of mathematics, physics, chemistry up to class 12 is highly desirable.

Objective: To take the students at the fore-front of research in biomolecular simulation start from basics.

Syllabus:

- Introduction to computational structural biology (2 hrs)
- Review of protein structure (2 hrs)
- Basic thermodynamics and statistical mechanics (8 hrs) Molecular mechanics (2 hrs)
- Computer simulation (5 hrs)
- Free energy calculations (3 hrs)
- Protein structure prediction(2 hrs)
- Protein-ligand interaction (3 hrs)
- Enzyme catalysis (2 hrs)
- Advanced sampling techniques (3 hrs)
- Illustration using molecular modeling softwares (8 hrs).

Texts:

- A, Leach, *Molecular Modeling: Principles and Applications,* 2' edition, Addison-Wesley publications, 2001.
- D. Frenkel and B. Smit, *Understanding Molecular Simulation,* 2'' edition , Academic Press, 2001.
- Statistical Physics, F. Reif, Berkeley lecture series (volume 5). McGraw-Hill.

References:

- K. A. Dill and S. Bromberg, *Molecular driving forces: Statistical thermodynamics in Chemistry and Biology,* Garland Science, 2003.