

IT-764: Stochastic Simulations in Biological Physics (SSBP)

Pre-requisites:

Must complete the semester one and at least credited the course on "Computational Biology & Bioinformatics".

Objective: This course will introduce students to stochastic simulation techniques as used in solving biological problems. Theory of stochastic processes will be briefly discussed along with the example of random walk problem. The basis of stochastic simulations will be rigorously elucidated using the method of master equations. This course will emphasize kinetic Monte Carlo simulations that are able to capture dynamical aspects, complex details in biological problems (such as spatial heterogeneity) and fluctuation effects. We plan to discuss stochastic modeling of important cellular (as mediated by gene regulatory networks and signal transduction networks) and immunological processes.

Syllabus:

1. Stochastic modeling approach to solve problems of biological and biomedical relevance (broad overview) (3+1 hours)
2. Introduction to stochastic processes Chapman-Kolmogorov formalism; Master equation (equations defined in probability space); Continuum limit and Fokker-Planck equation; Langevin equation (fast and slow time scales). Master equations for random walk problem and chemical kinetics Monte Carlo method to obtain solution of master equations (9+3 hours)
3. Stochastic simulation of the random walk problem (Statistical analysis of simulation data obtained from many parallel runs) Parallel computation based on task dependency. Kinetic Monte Carlo simulations, Metropolis Algorithm, rejection free algorithms (Gillespie's SSA) (9+3 hours)
4. Some basics of statistical mechanics, concept of ensembles, MC simulation in canonical ensemble, detailed balance in MC moves Kinetic Monte Carlo simulation that captures biological dynamics as well as spatial heterogeneity (simulation of receptor ligand binding and clustering); Langevin (Brownian) dynamics approach (9+3 hours)
5. Brief discussion of relevant biological applications and experiments. Kinetic Monte Carlo based in silico studies as a tool for mechanistic data analysis for biological / clinical data (such as NGS data): integration of big data with mechanistic models. Stochastic Modeling of Ligand-Receptor Binding process — applications to various two state biological problems. Research Projects. (12+4 hours)

Suggested readings:

Software: Programming and data analysis will be done in MATLAB or C/C++

Texts:

1. Stochastic Methods: A Handbook for the Natural and Social Sciences by C W Gardiner (Springer)
2. Theory and Applications of Monte Carlo simulations ed. By Victor Chan (InTech).

3. References:

1. Monte Carlo Simulations in Statistical Physics by K Binder and DW Heermann (Springer).
2. Understanding Molecular Simulation by D Frenkel and B Smit (Elsevier)
3. Essential Cell Biology by B Alberts, 13 Bray, K Hopkin, AD Johnson, J Lewis, M Raff, K Roberts, P Walter (Garland Science)