Course Code	BIO506		
Course Name	Stochastic Simulations in Systems Biology and Biophysics		
Credits	4		
Course Offered to	UG/PG		
Course Description	This course will introduce students to stochastic simulations as used in solving biological probelms. It will emphasize kinetic Monte Carlo simulations that are able to capture dynamical aspects (such as in cellular phenotype generation), complex details in biological problems (such as spatial heterogeneity) and fluctuation effects. We plan to discuss stochastic modeling of important cellular (as mediated by regulatory networks) and immunological processes and biomedical applications.		
	Pre-requisites		
Pre-requisite (Mandatory)	**Pre-requisite (Desirable)**	**Pre-requiste (Other)**	
Intro to Math Bio (BIO303/503) coursework	Some familiarity with thermodynamics (coursework in biology will be helpful).	None	
*Please insert more rows if required			
	Post Conditions		
CO1	**CO2**	**CO3**	**CO4**
1. An ability to explain biological applications, concepts, and tools / techniques of stochastic (Monte Carlo) simulations	2. Basic knowledge of constructing a stochastic computational model utilizing biological data	3.An ability to design kinetic Monte Carlo study of cellular processes and plan statistical data analysis 3	4. Some proficiency in correlating stochastic simulation results with kinetic/longitudinal biological data
	Weekly Lecture Plan		
Week Number	**Lecture Topic**	**COs Met**	**Assignments/Lab/Tutorial**
Week 1	Stochastic (Monte Carlo) simulation approach to (i) solve problems of biological and biomedical relevance and (ii) analyze kinetic/longitudinal biological data (broad overview) Brief introduction to the immune system (innate and adaptive immunity)	CO1	
Week 2	Monte Carlo and other simulation approaches (length and time scales in a problem); Monte Carlo simulations can capture complex details of a biological process and fluctuations Kinetic Monte Carlo simulations, rejection free algorithms (Gillespie's SSA)	CO1, CO3	HW assignment / Project work based on kinetic Monte Carlo simulation of post-mitochondrial cell death activation module and statistical data analysis (biological / biomdeical relevance related to neural cell apoptosis)
Week 3	Stochastic simulation of random walk problems in biology (Statistical analysis of simulation data obtained from many parallel runs). Parallel computation based on task dependency Some basics of statistical mechanics, concept of ensembles, MC simulation in canonical ensemble, detailed balance in MC moves	CO1, CO3	
Week 4	Stochastic modeling of immunological problems Kinetic Monte Carlo simulation that captures biological dynamics as well as spatial heterogeneity (simulation of receptor ligand binding and clustering)	CO1, CO2, CO3	
Week 5	Apoptosis as a immune mechanism for eliminating DNA damaged cells; cell-to-cell stochastic variability in apoptotic cell death signaling and phenotype generation (dynamic bistability) Type 1/Type 2 pathway choice problem in apoptosis biology (application to network/systems based therapies in the context of cancer and degenerative disorders)	CO1, CO2, CO3, CO4	
Week 6	Introduction to cellular regulatory networks (gene regulatory networks and signal transduction networks) Kinetic Monte Carlo simulation as a tool to carry out single cell biology in silico (mechanisms for cellular phenotype generation); role of stochastic fluctuations (noise) in important cellular processes	CO1, CO3, CO4	
Week 7	Brief discussion of relevant biological experiments (including single cell experiments such as FISH, microfluidics based pscWGA) Kinetic Monte Carlo based in silico studies as a tool for mechanistic data analysis for kinetic/longitudinal biological and/or clinical data (such as NGS data); integration of big data with mechanistic models	CO1, CO4	
Week 8	Introduction to theoretical formalism of 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)	CO1	HW assignment: Exact (analytical) solution of master equations and correlate to solutions obtained from Monte Carlo simulations
Week 9	Master equations for random walk problem and chemical kinetics Monte Carlo method to obtain solution of master equations Direct numerical solution of master equations (comparison with stochastic simulation approach)	CO1	
Week 10	Study of affinity discrimination and self/non-self discrimination in adaptive immune cells (B and T lymphocytes)	CO1, CO2, CO3, CO4	HW assignment based on kinetic Monte Carlo simulation of immune receptor-ligand binding and affinity discrimination
Week 11	The problem of affinity discrimination and affinity maturation in B lymphocytes (basis of adaptive immunity) Key role of receptor clustering (spatial heterogeneity) in immune cell activation and immune response: lipid rafts and immunological synapses; Hybrid kinetic Monte Carlo simulations	CO1,CO2,CO3,CO4	
Week 12	Immunological basis of diseases and disease sub-type classification	CO1,CO4	
Week13	Biomedical applications of computational studies of immunological problems (infectious / autoimmune diseases, cancer, vaccine design)	CO1	
*Please insert more rows if required			
	Assessment Plan		
Type of Evaluation	**% Contribution in Grade**		
HW assignments / Project work	50		
Midsem exam	30		
Endsem exam	20		
*Please insert more row for other type of Evaluation			
	Resource Material		
Type	**Title**		
Textbook	1. Stochastic Methods: A Handbook for the Natural and Social Sciences by C W Gardiner (Springer)		
Textbook	2. Theory and Applications of Monte Carlo simulations ed. By Victor Chan (InTech). http://www.intechopen.com/books/theory-and-applications-of-monte-carlo-simulations		