Approved in 45th BoA Meeting (18-02-22)

Course number : BE506
Course Name : Biological Modelling and Simulation
Credit Distribution : 2-0-2-3
Prerequisite :Understanding Biotechnology and its applications (IC136), and Bioinformatics (BE304), Computational Biology (BE505), or with permission of the instructor.
Intended for : Core for Integrated Dual Degree Bioengineering students with Specialisation in Computational Bioengineering, elective for other B.Tech and Mtech students, Elective for other UG, PG
Mutual Exclusion : None

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1. Preamble:

The course is intended to teach students how to reason about developing formal mathematical models of biological systems that are amenable to computational analysis. The course will broadly cover useful models, algorithms, and theoretical analysis tools normally used for biological systems in numerous subfields of biology. The course topics provide a general framework for learning how to formulate mathematical models of biological systems, what techniques are available to work with these models, and how to fit the models to particular systems. The course will include practical sessions for the students to help them master some of the advanced techniques from hands-on experience. The course will cover the following broad topics:

2. Course Modules with quantitative lecture hours: (28 hours)

A. Modelling biomolecular structure, interactions and dynamics using atomistic simulations (13 hours) ***(Dr. D. Mohanty, NII)***

Introduction to Molecular Modelling, Molecular Mechanics (MM) Forcefields & empirical energy functions, Potential energy surface & Energy minimization algorithms, Molecular dynamics (MD), Explicit solvent simulations & Water models, Calculation of energy (E), temperature (T), Pressure (P) and Volume (V). Temperature control by velocity scaling and coupling to heat bath, Equilibration vs Production Dynamics, MD at higher temperatures for enhanced sampling & Simulated Annealing, Analysis of MD trajectories by Principal Component Analysis (PCA) and essential dynamics, MD Simulations in membrane environment, Calculation of Free Energy changes from explicit solvent MD by Free Energy Perturbation (FEP) approach, Monte Carlo (MC) Simulations, Atomistic vs coarse-grained dynamics.

B. Systems Biology & Biological Networks (2 hours) ***(Prof James Gomes, IIT Delhi)***

C. Simulation of cellular subsystems (11 hours)

Simulation & Analysis of Biochemical Network Models (3 Hours) ***(Prof James Gomes, IIT Delhi)***

Simulation of Genome-Scale Metabolic (GSM) Networks, Flux-Balance Analysis (FBA) & Constraint based models (5 Hours) ***(Dr. Karthik Raman, IIT Chennai)***

Introduction to Boolean Network Modeling of Gene Regulation (2 hours) ***(Dr D. Mohanty, NII)***

D. Population models (3 hours) ***(Dr. Tulika P Srivastava, IIT Mandi)***

Lab Course content: (28 hours)

The below mentioned 10 topics will be covered over the 14 weeks:

A. **Atomistic Simulations 12 hours** ***(Dr. D. Mohanty & Tulika P. Srivastava)***

1. Visualization and analysis of 3D structures of bomolecules and Model building.
2. Energy minimization.
3. Molecular Dynamics Simulation of a Protein using GROMACS.
4. Analysis of MD trajectory & Principal Component Analysis (PCA) of MD trajectory.
5. Calculation of Free Energy (solvation of methane or amino acids in water) using explicit water simulations.
6. MD simulations of a Protein-Ligand complex.
7. MD simulation of a model transmembrane peptides in lipid bilayers.

B. Analysis of biological networks 3 hours

1. Visualization of biological networks and calculation of network parameters using Cytoscape.

C. Simulation of cellular subsystems 8 hours

1. Simulation & Analysis of biochemical network models using differential equations (COPASI).

2. Flux Balance Analysis using COBRA Tool for simulation of genome scale metabolic networks: Applications to central metabolism of *E. coli*.

D. Population models 5 hour

1. Predator-Prey Simulation
2. Modeling spread of infectious disease: COVID19.

3. Text books:

1. **Molecular Modelling. Principles and Applications (2nd Edition) by Andrew R. Leach (**ISBN 978-0582382107).
2. **An Introduction to Computational Systems Biology Systems-Level Modelling of Cellular Networks**. *By* *Karthik Raman* (ISBN 9781138597327 Published May 31, 2021 by Chapman and Hall/CRC).

4. References:

1. Dynamics of Proteins & Nucleic Acids (JA McCammon & SC Harvey) Cambridge University Press online ISBN 9781139167864.

5. Similarity Content declaration with existing courses:

S. No.	Course Code	Similarity Content	Approx. % of Content
1	BY504	Constraint based flux analysis.	15%

6. Justification of new course proposal if cumulative similarity content is >30%: Not Applicable