BIOENG-455 Computational cell biology

Shillcock Julian Charles

Cursus	Sem.	Type
Computational biology minor	H	Opt.
Life Sciences Engineering	MA1, MA3	Opt.
Minor in life sciences engineering	H	Opt.

Language of teaching	English
Credits	4
Session	Winter
Semester	Fall
Exam	During the semester
Workload	120h
Weeks	14
Hours	**4 weekly**
Courses	2 weekly
Exercises	2 weekly
Number of positions	

Summary

Computer modeling is used to study dynamic phenomena in cell biology. This course shows how to identify mathematical features of cell biology mechanisms and use numerical algorithms to model their behavior.

Content

- Characteristics of a cell, scales of life
- Macromolecules in the mammalian cell
- Intermolecular forces and cellular compartments
- Diffusion and entropic forces in the cell
- Thermodynamics at human and cellular scales
- Phases and phase transitions in cells
- Computer simulations of cellular dynamics
- Coarse-Grained simulations because the world is more than atoms
- Dissipative Particle Dynamics
- Membraneless organelles - a new phase of cellular material

Keywords

Cell Biology, Soft Matter, Thermodynamics, Diffusion, Random walks, Self-Assembly, Differential equations, Numerical algorithms, Computer simulations, Dissipative Particle Dynamics, Protein Aggregation, Biomolecular Condensates

Learning Prerequisites

Required courses

Phys-101
Math-106
Bio-205

Recommended courses

CS-111

Important concepts to start the course

Students should have a basic knowledge of cellular anatomy, calculus and ordinary differential equations, probability and statistics, mechanics and thermodynamics. They will be required to write short programmes using a programming language of their choice (python, matlab, C, C++, etc) to solve mathematical problems relevant to the topics in the course. A Dissipative Paricle Dynamics simulation code is provided (https://github.com/Osprey-DPD/osprey-dpd), which forms the basis of the project, and students should be familiar with running programmes from the command line. A laptop or access to a computer on which the student can execute their own programmes is mandatory for this course.

Learning Outcomes

By the end of the course, the student must be able to:

- Describe selected cellular structures and dynamical mechanisms
- Choose a numerical technique for simulating models of cellular dynamics
- Create a programme to solve numerical problems
- Justify using a specific simulation technique for a cell dynamical problem
- Explore effects of changing parameters in a simulation
- Estimate the accuracy of a model or simulation
- Explain the similarities and differences between different simulation methods
- Perform a set of DPD simulations of a chosen complex fluid

Transversal skills

- Demonstrate a capacity for creativity.
- Plan and carry out activities in a way which makes optimal use of available time and other resources.
- Write a scientific or technical report.
- Continue to work through difficulties or initial failure to find optimal solutions.

Teaching methods

Lectures
Exercises
Tests
Journal club
Semester project

Expected student activities

Attending lectures, completing in-class tests, writing short programmes to solve mathematical models, selecting and working in collaboration on a simulation-based semester project, presenting a paper in a journal club, writing a scientific report summarising the semester project

Assessment methods

DPD simulation project and report - 50%
2 x Homework exercises on numerical modelling / simulations - 15%
3 x in class / take home tests - 30%
Journal club presentation - 5%

Supervision

Office hours	No
Assistants	Yes
Forum	Yes

Resources

Notes/Handbook

User Guide to the Dissipative Particle Dynamics simulation code is provided

Moodle Link

- https://go.epfl.ch/BIOENG-455