EPFL

BIOENG-455

# Computational cell biology

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

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|---|---|
| Contact language | English |
| Credits | 4 |
| Session | Winter |
| Semester | Fall |
| Exam | During the semester |
| Workload | 120h |
| Weeks | 14 |
| **Hours** | **4 weekly** |
| Lecture | 2 weekly |
| Exercises | 2 weekly |
| **Number of positions** | |


## Summary

Computer modelling is increasingly used to study dynamic phenomena in cell biology. This course shows how to identify common mathematical features in cell biological mechanisms, and become proficient in selecting numerical algorithms to model them and predict their behaviour.


## Content

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


## Keywords

Cell Biology, Soft Matter, Thermodynamics, 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 applying a simulation technique to a problem
- Explore consequences of parameter changes on model results
- Estimate the accuracy of a numerical routine
- Explain the common elements in different simulation types
- Perform a series of DPD simulations of a complex fluid
- Organize the data produced by a series of simulations

## 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.

## 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 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 and simulation data management - 15%
3 x in class tests - 30%
Journal club presentation - 5%

## Resources

### Bibliography

Biological Physics, Philip Nelson, W. H. Freeman and Co. New York, USA, 2014

Molecular Biology of the Cell, Bruce Alberts, et al., 2nd ed., Garland Publ. Inc. New York and London, 1989

### Ressources en bibliothèque

- Molecular Biology of the Cell, Bruce Alberts,
- Biological Physics, Philip Nelson

### Notes/Handbook

User Guide to the Dissipative Particle Dynamics simulation code is provided

### Moodle Link

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