

BIO-692

Symmetry and Conservation in the Cell

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Cursus	Sem.	Type
Computational and Quantitative Biology		Obl.
Neuroscience		Opt.

Language of teaching	English
Credits	3
Session	
Exam	Multiple
Workload	90h
Hours	61
Courses	21
Exercises	40
Number of positions	20

Frequency

Every 2 years

Remark

Next time: Spring 2025

Summary

This course shows students how the physical principles of conservation, symmetry, and locality influence the dynamics of living organisms at the molecular and cellular level. Computer simulations are used to explore examples of cellular dynamics and phase transitions.

Content

Learning outcomes: Justify selected molecular simulation techniques for simulating cellular processes; solve simplified dynamical models relevant to a cell; explain how symmetry affects cellular dynamics

This course aims to show how the principles of symmetry and conservation are used by a cell in carrying out its functions. We will examine selected cellular structures and dynamical processes and construct computational models of them that are solved analytically, numerically or with computer simulations. The importance of dimensionality is illustrated by examining random walks in 1, 2 and 3 dimensions and two-dimensional fluid membranes that surround many cellular organelles and form the plasma membrane. The symmetry of a system usually changes when passing through a phase transition, and it is increasingly accepted that cells manipulate the phase behaviour of intrinsically-disordered proteins in the cytoplasm to create membraneless organelles. These organelles, which are also referred to as biomolecular condensates, carry out vital functions for the cell, but are also implicated in neurodegenerative diseases such as Alzheimer's disease. They are three-dimensional, fluid networks formed by a process of liquid-liquid phase separation, and exhibit quite distinct structures and dynamics that are controlled by the thermodynamic properties of their constituent proteins within the crowded environment of the cytosol. We will construct models of IDPs and use simulations to quantitatively connect the structural properties of IDPs to the physical chemical properties of the condensates. Computer simulations are used to explore model systems in homework problems and a semester project. The primary goal of the course is to show students how nature uses symmetry and conservation to achieve specific cellular goals, and to understand how computer simulations can be used to study these processes.

Course content:

Overview of the biophysics of a cell on different length scales: a "day in the life of a cell"

Mathematical models in 1d: Random Walks and Langevin equations

Scaling laws for polymers, self-avoiding and phantom polymers, entropic spring, stiff asymmetric filaments and filament self-assembly and growth

Overview of computer simulations, fundamentals, coarse-graining, and simulations on multiple scales

Mathematical models in 2d: membranes, formation, material properties, and endo- and exocytosis

Molecular self-assembly on an axis from irreversible to reversible

Mathematical models in 3d: Biomolecular condensates - a new phase of cellular matter

As part of the exercises and project, students will be expected to solve simplified models of diffusion processes in a cell using differential equations; set up and run a Dissipative Particle Dynamics simulation (the executable code and sample input files for modification will be provided), analyse the simulation output and present it in the form of time-averaged

observables with an error estimation, and as time series plots. A report of their chosen semester project in the form of a scientific paper is the major deliverable of the course.

Note

Students are expected to watch the lecture videos in their own time. Class time will be for reviewing the slides and doing exercise/project work.

Keywords

Simulation, coarse-grained, membrane, organelle, lipid, nanoparticle, protein, symmetry, mathematical modelling

Learning Prerequisites**Required courses**

BIO-205, MATH-106, PHYS-10

Recommended courses

BIO-205, MATH-106, PHYS-101
CS-111

Resources**Moodle Link**

- <https://go.epfl.ch/BIO-692>