BIO-692 **Symmetry and Conservation in the Cell**

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Cursus	Sem.	Type
Neuroscience		Obl.

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

Frequency

Every year

Remark

Sping 2017

Summary

This course aims to show 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 processes illustrating these principles.

Content

This course aims to show students how the physical principles of conservation, symmetry and locality influence the dynamics of living organisms at the molecular and cellular level. We start with simple equations that embody a physical principle and compare them with experiments on cells or model systems. The importance of the local environment on dynamics at the molecular scale is introduced, and its influence on typical molecular-scale motions explored, including particle diffusion, the forces between particles in various media, and self-assembly of molecules into larger aggregates. Symmetric and asymmetric random processes are explored in 1, 2 and 3 dimensions, and the combined effects of symmetry, in the sense of invariance under an operation, and mass conservation, or the re-use of a limited amount of matter, are shown to constrain how molecular aggregates assemble, stabilise or disassemble. Computer simulations of simple model systems are used as examples for exploration in problems and a semester project. The primary goal of the course is to show students how nature takes advantage of symmetry and conservation, or selectively breaks them, to achieve specific cellular goals, and to understand how computer simulations can be used to study these processes.
Lecture 1 - Overview of the biophysics of a cell at different length scales: a “day in the life of a cell”
Lecture 2 - Constructing mathematical models, Random Walks (RW) in 1, 2 and 3 dimensions.
Lecture 3 - RW part 2, Langevin equation and diffusion processes in the cell
Lecture 4 - RW part 3, scaling laws for polymers, self-avoiding versus phantom polymers, entropic spring, stiff asymmetric filaments and filament self-assembly and growth
Lecture 5 - Linear RW model of neurite growth, branched polymers as models of neurons
Lecture 6 - Self-assembly in the cell; oil droplet coarsening, vesicle self-assembly, crowding effects on diffusion and reactions in cells
Lecture 7 - Overview of computer simulations relevant to molecular processes in the cell
Lecture 8 - Computer Simulation fundamentals: initial config, BCs, PBCs, observables, statistics, and errors
Lecture 9 - Computer Simulations, part 2, simulating different scales in a cell, Atomistic MD, mesoscopic DPD, BD, MC, what does each type of simulation get right at what cost?
Lecture 10 - Membranes, influence of lipid molecular shape and symmetry on self-assembly
Lecture 11 - Membranes part 2, fluid and solid membranes
Lecture 12 - Membranes part 3, not only a barrier, Litster theory of pore formation, pore shape fluctuations at reduced line tension, localised pore formation in vesicle fusion, endocytosis and exocytosis
Lecture 13 - Harnessing symmetry in cellular processes: why do lipids have two hydrocarbon tails? Nanoparticles and their interactions with membranes

Lecture 14 - Project presentations
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.
Learning Outcomes -
Choose and justify which molecular simulation techniques are suitable for simulating selected cellular processes; solve simplified dynamical models relevant to a cell; and explain how the symmetry of molecules and aggregates influences cellular properties

Note

Because of the limited size of the class, please sign up by contacting edne@epfl.ch

Keywords

Membrane, organelle, lipid, vesicle, nanoparticle, diffusion equations, simulation, molecular shape, symmetry, random walk

Learning Prerequisites

Required courses

BIO-205, MATH-106, PHYS-101

Recommended courses

CS-111