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, and should be familiar with running programmes from the command line (or within matlab or ipython). 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

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%
Numerical modelling of chosen cellular functions - 20%
4 x class tests - 20%
Journal club presentation - 10%

Resources
Bibliography
Notes/Handbook
User Guide to the Dissipative Particle Dynamics simulation code is provided