GHENT UNIVERSITY

Course Specifications

Valid in the academic year 2024-2025

Molecular Simulations of Biosystems (C002727)

Course size *(nominal values; actual values may depend on programme)*

Credits 3.0 **Study time 80 h**

Course offerings and teaching methods in academic year 2024-2025

A (semester 1)	English	Gent	seminar
			lecture

Lecturers in academic year 2024-2025

Verstraelen, Toon	WE05	lecturer-in-charge
Savvides, Savvas	WE10	co-lecturer

Offered in the following programmes in 2024-2025	crdts	offering
Master of Science in Teaching in Science and Technology(main subject Biochemistry and Biotechnology)	3	A
Master of Science in Biochemistry and Biotechnology	3	A
Exchange programme in Biochemistry and Biotechnology (master's level)	3	A

Teaching languages

English

Keywords

Proteins and DNA, molecular dynamics, force fields, multiscale modeling, QM/MM, PCA

Position of the course

The function of biological macromolecules is determined by their three-dimensional structure and dynamics. With molecular simulations, it is possible to calculate these microscopic properties and to link them to macroscopic variables, such as thermodynamic properties. Molecular modeling is increasingly used as a valuable tool by biologists and (bio)chemists. Due to the ever-increasing computer capabilities, these simulations have become accessible to end-users. In addition, simulations can often provide answers to fundamental scientific questions in a relatively inexpensive way, not requiring many (costly) chemical reactions or purifications. Within the academic world but also in the industry, modeling is frequently applied to biomolecules such as proteins, polynucleotides, pharmaceuticals, pesticides, etc.
Competence codes: Ma.WE.BB.1.1, Ma.WE.BB.1.3, Ma.WE.BB.2.1, Ma.WE.BB.2.4, Ma.WE.BB.2.6, Ma.WE.BB.3.2, Ma.WE.BB.3.5, Ma.WE.BB.4.3, Ma. WE.BB.6.1

Contents

In several lectures, the underlying principles are introduced of the techniques applied in the practical sessions; the aim is to understand, not to be able to reproduce. In addition, the lectures are structured entirely in function of the computational applications. In the practical sessions, conventional packages in the field will be used: VMD, NAMD, Gromacs, CP2K - all freely available for academic users.

1 Construction of a molecular model: the structure of a pdb file, visualization
2 Description of atomic/molecular interactions in biomolecular systems: classic (forcefields), quantummechanical (ab initio), semi-empirical
3 Multiscale approaches: QM/MM
4 Molecular dynamics: minimization, equilibration, annealing
5 Analysis of dynamics: energy contributions, RMSD, normal mode analysis, principal component analysis

Initial competences

Basic (bio)chemistry

Final competences

1 Understand and reproduce recent scientific literature, and implement these methods in own research.
2 Independently set up a computer simulation and perform a meaningful analysis.
3 Directly connect with the current research of different labs at home and abroad.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Seminar, Lecture

Study material

Type: Slides

Name: Molecular Simulations of Biosystems
Indicative price: Free or paid by faculty
Optional: no
Language : English
Number of Slides : 160
Available on Ufora : Yes
Online Available : Yes
Available in the Library : No
Available through Student Association : No

Type: Other

Name: OpenMM tutorial for the MSBS course
Indicative price: Free or paid by faculty
Optional: no
Language : English
Author : Jelle Vekeman en Toon Verstraelen
Available on Ufora : No
Online Available : Yes
Available in the Library : No
Available through Student Association : No
Usability and Lifetime within the Course Unit : not applicable
Usability and Lifetime within the Study Programme : intensive
Additional information: https://github.com/molmod/openmm-tutorial-msbs

References

Martin J. Field, “A Practical Introduction to the Simulation of Molecular Systems”, Cambrigde University Press Andreas Kukol, “Molecular Modeling of Proteins”, Humana Press

Course content-related study coaching

Guided computer exercises
Interactive support via Ufora

Assessment moments

end-of-term assessment

Examination methods in case of periodic assessment during the first examination period

Oral assessment, Assignment

Examination methods in case of periodic assessment during the second examination period

Oral assessment, Assignment

Examination methods in case of permanent assessment

Possibilities of retake in case of permanent assessment

not applicable

Extra information on the examination methods

Projects: a project-paper is required and the project is defended in a short oral presentation.

Calculation of the examination mark

100% project