

## Foundations and Applications of Molecular Dynamics (C004662)

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

**Credits 3.0**

**Study time 80 h**

**Course offerings in academic year 2026-2027**

A (semester 1)

English

Gent

**Lecturers in academic year 2026-2027**

Verstraelen, Toon

WE05

lecturer-in-charge

**Offered in the following programmes in 2026-2027**

Master of Science in Teaching in Science and Technology(main subject Biochemistry and Biotechnology)

crdts

offering

3

A

Master of Science in Bioinformatics(main subject Systems Biology)

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**

Molecular Dynamics, Force Field Models, Machine Learning Potentials, Uncertainty Quantifications, Macromolecules, Proteins, Molecular Liquids, Interfaces, Equilibrium and Non-Equilibrium Dynamics, High-Performance Computing

**Position of the course**

The properties of molecular systems are fundamentally determined by their 3D structure and their dynamics at the atomic scale. Molecular dynamics simulations provide a powerful computational platform to calculate these microscopic properties and establish their connection to experimentally observable macroscopic variables, such as thermodynamic, transport, and mechanical properties. With ever-increasing computational capabilities and the advent of machine learning potentials, molecular dynamics has evolved into an indispensable tool across chemistry, solid-state science, physics and biology.

Molecular dynamics simulations enable researchers to address fundamental scientific questions in a cost-effective manner, complementary to experimental research. These simulations provide atomic-level insights that are difficult to obtain experimentally, such as interfacial phenomena, non-equilibrium transport processes, and rare events. Within both academia and industry, molecular dynamics is routinely applied to diverse systems including proteins, biomolecules, pharmaceuticals, molecular liquids, electrolytes, battery materials, lubricants, catalysts, porous materials, 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**

The theory lectures will provide students with a broad overview of molecular dynamics methodology, starting from its foundations in (statistical) physics. A key ingredient in these simulations is the model used to compute interatomic forces, of which two main categories will be discussed: classical force fields and machine learning potentials. The theory will also emphasize the post-processing of molecular dynamics simulations to extract meaningful equilibrium and non-equilibrium properties. During the practical sessions, students will gain hands-on experience with high-performance computing and well-established open-source

simulation tools, including OpenMM and Jupyter Notebooks. The practical sessions will emphasize basic skills to ensure the validity of simulations performed, including the following:

- 1 Construction of a molecular model from one or multiple initial structure files.
  - 2 Specification of the model for the interatomic forces.
  - 3 Energy minimization and molecular dynamics simulations in different thermodynamic ensembles.
  - 4 Post-processing of molecular dynamics trajectories: assessment of equilibration and convergence, extraction of equilibrium and non-equilibrium properties.
- Students carry out their calculations at the VSC Tier-2 high performance cluster at Ghent University.

#### **Initial competences**

Basic (bio)chemistry and Python programming

#### **Final competences**

- 1 Understand and reproduce basic molecular dynamics simulations in recent scientific literature, and implement these methods in own research.
- 2 Understand the foundations of molecular dynamics simulations and the algorithms used to post-process the resulting trajectory data.
- 3 Independently set up a computer simulation and perform a meaningful analysis.
- 4 Connect simulation outcomes 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**

Lecture, Independent work

#### **Extra information on the teaching methods**

The theory lessons are given in the form of lectures. Tutorials consist of solving computational projects under supervision and independently, in which the theory is applied.

Lecture recordings will be made available, provided that the designated lecture room is equipped with the necessary high-quality recording equipment.

#### **Study material**

Type: Slides

Name: Foundations and Applications of Molecular Dynamics

Indicative price: Free or paid by faculty

Optional: no

Language : English

Number of Slides : 200

Available on Ufora : Yes

Online Available : Yes

Available in the Library : No

Available through Student Association : No

Type: Software

Name: OpenMM tutorial for the course

Indicative price: Free or paid by faculty

Optional: no

Online Available : Yes

Available in the Library : No

Available through Student Association : No

Usability and Lifetime within the Course Unit : intensive

Usability and Lifetime within the Study Programme : intensive

#### **References**

- Martin J. Field, "A Practical Introduction to the Simulation of Molecular Systems", Cambridge University Press
- Andreas Kukol, "Molecular Modeling of Proteins", Humana Press
- Daan Frenkel & Berend Smit, "Understanding Molecular Simulation", Academic

Press

#### **Course content-related study coaching**

- Solving computational projects under supervision. Possibility to ask questions before, during and after the lesson, and online.
- Guidance, supervision and feedback on the project assignment

#### **Assessment moments**

end-of-term and continuous assessment

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

Oral assessment

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

Oral assessment

#### **Examination methods in case of permanent assessment**

Presentation, Assignment

#### **Possibilities of retake in case of permanent assessment**

examination during the second examination period is possible

#### **Extra information on the examination methods**

- The project assignment (continuous assessment) is an opportunity for students to apply the skills from the course to a topic of interest, e.g. related to an ongoing thesis. The outcome of the project is defended during the semester and primarily evaluates final competences 1, 3 and 4.
- The oral exam (end-of-term evaluation) is closed-book with written preparation. This exam will mainly evaluate final competence 2.

#### **Calculation of the examination mark**

60% project assignment, 40% theory exam.

Students who eschew periodical and/or permanent evaluations for this course unit may be failed by the examiner.

#### **Facilities for Working Students**

No additional facilities