

## Simulation Techniques

Code: 43440  
ECTS Credits: 6

**2025/2026**

Degree	Type	Year
Advanced Nanoscience and Nanotechnology	OT	0

### Contact

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### Teachers

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### Teaching groups languages

You can view this information at the [end](#) of this document.

### Prerequisites

Basic notions of quantum mechanics will be required for the ab-initio part of the course.

### Objectives and Contextualisation

Introduction to the use of software devoted to the calculation of physical and chemical properties at the nanoscale, and overview of the underlying formalisms.

### Competences

- Communicate and justify conclusions clearly and unambiguously to both specialised and non-specialised audiences.
- Continue the learning process, to a large extent autonomously
- Identify the characterisation and analysis techniques typically adopted in nanotechnology and know the principles behind these, within one's specialisation.
- Seek out information in the scientific literature using appropriate channels, and use this information to formulate and contextualise a research topic.
- Show expertise in using scientific terminology and explaining research results in the context of scientific production, in order to understand and interact effectively with other professionals.

- Solve problems in new or little-known situations within broader (or multidisciplinary) contexts related to the field of study.

## Learning Outcomes

1. Analyse the underlying complexity and the computational limits of the different methods for solving the model's descriptive equations.
2. Communicate and justify conclusions clearly and unambiguously to both specialised and non-specialised audiences.
3. Continue the learning process, to a large extent autonomously
4. Identify the equations governing Newtonian molecular dynamics, the electronic transport of first principles and structural dynamics.
5. Identify the most appropriate computational technique for the problem addressed.
6. Interpret the capacities of a simulation technique and its fundamental limitations on the basis of the terms that the model incorporates.
7. Seek out information in the scientific literature using appropriate channels, and use this information to formulate and contextualise a research topic.
8. Show expertise in using scientific terminology and explaining research results in the context of scientific production, in order to understand and interact effectively with other professionals.
9. Solve problems in new or little-known situations within broader (or multidisciplinary) contexts related to the field of study.
10. Use computational techniques efficiently to study scientific problems relating to materials at the nanoscale.
11. Use simulation tools self-sufficiently to gain greater understanding in experimental situations.

## Content

- Brief introduction to Linux.
- Ab-initio methods for electronic transport: Density functional theory. Kohn-Sham equations. Plane waves and quasi-atomic orbitals. Foundations of ballistic transport. Non-equilibrium Green's functions. Getting transmission coefficients with TRANSIESTA - practical sessions: transport through a molecule and graphene nanoribbons.
- Molecular Dynamics with classical force fields: Micro/Macro canonical collectivities, thermostats. Intermolecular forces. Force fields for biological systems. Lammps code - practical sessions: water through a carbon nanotube, and antigen-antibody binding.
- Continuum models: Equations of continuity: mass, momentum, energy. Diffusion, heat conductions, fluids, elasticity. k.p formalism. Elmer Multiphysics code - practical sessions: vibrations in Si nanowires, and flexing of a Si bridge due to thermal dilatation.

## Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Traditional lecture	15	0.6	1, 5, 4, 6, 9, 10
Type: Supervised			
Tutorials	22	0.88	1, 4, 6, 3, 11, 10
Type: Autonomous			

About 2/5 of the lectures will be traditional lectures, and the remaining 3/5 will be practical sessions using the different software packages. Out-of-class activities will include reading of journal articles, and carrying out small works/simulations expanding what has been explained in class.

Traditional lectures and practical sessions may be online depending on the public health status at the time.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

## Assessment

### Continuous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Attendance and participation in class	5%-10%	0	0	8, 2
Exposition of a paper	10%-15%	5	0.2	1, 7, 8, 5, 6, 2, 3
Lab reports - Continuum methods	25%-30%	20	0.8	1, 7, 8, 5, 4, 6, 9, 2, 3, 11, 10
Lab reports - First principles	30%-35%	25	1	1, 7, 8, 5, 4, 6, 9, 2, 3, 11, 10
Lab reports - Molecular Dynamics	20%-25%	20	0.8	1, 7, 8, 5, 4, 6, 9, 2, 3, 11, 10

A final exam may be required in very specific cases.

The single evaluation system will not apply to this module.

## Bibliography

J. M. Thijssen. Computational Physics (Cambridge University Press, 1999)

R. M. Martin. Electronic Structure: Basic Theory and Practical Methods (Cambridge University Press, 2004).

S. Datta, Electronic transport in mesoscopic systems (Cambridge University Press, 1995)

D. C. Rapaport, The Art of Molecular Dynamics Simulations (Cambridge University Press, 1995)

D. Frenkel, B. Smit, Understanding Molecular Simulations: from algorithms to applications, Academic Press (1996).

O.C. Zienkiewicz, R.L. Taylor and J.Z. Zhu, The Finite Element Method: Its Basis and Fundamentals (6th Ed, Elsevier Butterworth-Heinemann, 2005) Sections 3.1-3.3

## Software

A computer configured for ssh access to remote machines with graphical capabilities will be needed. Help will be offered for configuration.

## Groups and Languages

Please note that this information is provisional until 30 November 2025. You can check it through this [link](#). To consult the language you will need to enter the CODE of the subject.

Name	Group	Language	Semester	Turn
(PLABm) Practical laboratories (master)	1	English	first semester	afternoon
(TEm) Theory (master)	1	English	first semester	afternoon