UAB
Universitat Autònoma de Barcelona

From Microscopic to Macroscopic Modelling

Code: 45560
Credits: 6

2026/2027

Degree programme	Type	Course
Modelling for Science and Engineering	OP	1

Contact lecturer

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Teaching staff

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Group languages

You can consult this information at the end of the document.

Prerequisites

A solid foundation in physics and mathematics is required. It is recommended that students have previously completed courses such as multivariable calculus, ordinary and partial differential equations, introduction to probability theory, and statistical mechanics.

Objectives

The main objective of this course is to introduce students to the mathematical modelling of physical phenomena (as well as chemical, biological, and social phenomena) at different spatial and temporal scales, as well as to the connections between these scales.

The course aims to provide criteria for determining when a description is more appropriate in deterministic or stochastic terms, and how to choose the characteristic scales and the most suitable level of detail for each problem. It will also address the study of emergent phenomena arising from microscopic models and the relationship between microscopic processes and observable macroscopic phenomenology.

In addition, the course will introduce several numerical and simulation tools for solving mathematical models, including finite difference and finite element methods. Therefore, one of the objectives is for students to acquire the necessary skills to formulate, analyse, and simulate complex models in different scientific contexts.

Learning outcomes

- CA12 (Communicate to an expert audience the results obtained from the analysis of problems based on stochastic processes and partial differential equations.) Communicate to an expert audience the results obtained from the analysis of problems based on stochastic processes and partial differential equations.
- CA13 (Develop models based on partial differential equations to solve specific practical problems.) Develop models based on partial differential equations to solve specific practical problems.
- CA14 (Develop modelling studies and stochastic analysis to analyse real datasets.) Develop modelling studies and stochastic analysis to analyse real datasets.
- KA11 (Recognise the main types of platforms and computer tools to implement partial differential equations.) Recognise the main types of platforms and computer tools to implement partial differential equations.
- KA12 (Identify the levels of description of stochastic processes and the main mathematical techniques associated with each of them.) Identify the levels of description of stochastic processes and the main mathematical techniques associated with each of them.
- SA12 (Implement specific partial differential equations in software, including the appropriate meshing techniques and boundary conditions.) Implement specific partial differential equations in software, including the appropriate meshing techniques and boundary conditions.
- SA13 (Establish relationships between the different levels of description of stochastic processes.) Establish relationships between the different levels of description of stochastic processes.
- SA14 (Associate the solutions and results of partial differential equations with the properties of the corresponding physical and natural systems that they represent.) Associate the solutions and results of partial differential equations with the properties of the corresponding physical and natural systems that they represent.

Contents

Part I. Foundations of Multiscale Modelling (12h)

- Deterministic microscopic modelling.
- Stochastic microscopic modelling.
- Probabilistic descriptions: master equation and Fokker-Planck equation.
- Deterministic macroscopic modelling.

Part II. Examples of Physical Modelling (16h)

- Models of magnetism and spin dynamics: Ising model, Landau-Lifshitz-Gilbert (LLG) equation, Thiele equation, and introduction to field theories and their numerical solution.
- Electronic transport: Boltzmann transport equation (BTE), Ohm's law, and numerical methods for solving the BTE using Monte Carlo simulations and finite element tools (COMSOL).

Part III. Interdisciplinary Examples (6h)

- Social dynamics and epidemiology: SIR/COVID models, comparison between agent-based models and population models.
- Financial modelling: random walk and geometric Brownian motion (GBM).
- Thermal transport: molecular dynamics (MD) and kinetic constrained models (KCM).

Part IV. Final Assessment (4h)

- Development of a group project on a free topic related to the modelling and simulation of complex systems.

Learning activities and methodology

Title	Hours	ECTS	Learning outcomes
Study and homework	50	2	KA11, SA12, SA14
Teaching classes	39	1.56	CA13, CA14, KA12, SA13
Solving questions	9	0.36	CA12

The course methodology combines lectures with practical sessions (both in class and at home) aimed at the application and consolidation of the concepts introduced throughout the course.

Note: 15 minutes of one class, within the schedule established by the faculty/degree program, will be reserved for students to complete the teaching performance and course/module evaluation surveys.

In this course, the use of Artificial Intelligence (AI) technologies is permitted as an integral part of the development of assignments, provided that the final result reflects a significant contribution from the student in terms of analysis and personal reflection. Students must clearly identify which parts have been generated using this technology, specify the tools used, and include a critical reflection on how these tools have influenced both the process and the final outcome of the activity. Failure to disclose the use of AI will be considered a breach of academic integrity and may result in a penalty to the assignment grade or more serious sanctions in cases of greater severity.

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	Weight	Hours	ECTS	Learning outcomes
Homework	30	50	2	CA12, CA13, CA14, KA11, KA12, SA12, SA13, SA14
Exam	70	2	0.08	CA13, CA14, KA12, SA13, SA14

The assessment of the course will be based on practical activities and projects related to the contents covered during the course. The final grade will be distributed as follows:

- Individual assignment for Part I (20%)
- Exercises and problems related to the foundations of microscopic and macroscopic modelling.
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- Individual assignment for Part II (20%)
- Development of one of the modelling examples proposed in the course, chosen by the student.

- Final group project (60%)
- The final project will consist of the study, modelling, and simulation of a problem related to the contents of the course.
- Written project report: 30%
- Oral presentation and project defense: 30%

Bibliography

Basic:

- V. Méndez, D. Campos, F. Bartumeus. *Stochastic Foundations in Movement Ecology,* Springer-Verlag, 2014
- C. W. Gardiner. *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences*. Springer-Verlag, Berlin, 1990
- H. Risken. *The Fokker-Planck Equation: Methods of Solution and Applications*. Springer, Berlin, 1989
- C. Cercignani. *The Boltzmann Equation and Its Applications*. Springer-Verlag, 1988
- L.J.S. Allen, *An Introduction to Stochastic Processes with Applications to Biology*. Chapman & Hall/CRC, Boca Ratón. 2011
- R. Toral, P. Colet. *Stochastic Numerical Methods*. Wiley-VCH, 2014

Complimentary:

- N. van Kampen, *Stochastic Processes in Physics and Chemistry*, Third Edition (North-Holland Personal Library) 2007
- A. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford University Press, 1994
- K. Huang. *Statistical Mechanics*. Wiley, 1987
- D. J. T. Sumpter. *Collective Animal Behavior*. Princeton University Press, 2010
- N.C. Petroni. *Probability and Stochastic Processes for Physicists*. Springer-Verlag, 2020
- N. Lanchier. *Stochastic Modelling*. Springer-Verlag, 2017

Software

The practical activities of the course will be carried out using different programming languages, such as C++, Python, and R, among others, depending on the requirements of each problem.

Course groups and languages

The information provided is provisional until November 30. After this date, you will be able to consult the language of each group through this link. To access the information, you will need to enter the course CODE

Type of teaching	Group	Language	Semester	Shift
(TEm) Theory (master)	1	English	first semester	afternoon