# Course guide
# 200247 - MODC - Computational Modelling

**Last modified:** 18/05/2024

**Unit in charge:** School of Mathematics and Statistics
**Teaching unit:** 751 - DECA - Department of Civil and Environmental Engineering.
749 - MAT - Department of Mathematics.

**Degree:** BACHELOR'S DEGREE IN MATHEMATICS (Syllabus 2009). (Optional subject).

**Academic year:** 2024 **ECTS Credits:** 6.0 **Languages:** Catalan

## LECTURER

**Coordinating lecturer:** SONIA FERNANDEZ MENDEZ

**Others:** Segon quadrimestre:
SONIA FERNANDEZ MENDEZ - M-A
JOSE JAVIER MUÑOZ ROMERO - M-A
PABLO SAEZ VIÑAS - M-A

## PRIOR SKILLS

Basic concepts in differential equations and calculus with differential operators.

## DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

**Specific:**
GM-CE2. CE-2. Solve problems in Mathematics, through basic calculation skills, taking in account tools availability and the constraints of time and resources.
GM-CE1. CE-1. Propose, analyze, validate and interpret simple models of real situations, using the mathematical tools most appropriate to the goals to be achieved.
GM-CE3. CE-3. Have the knowledge of specific programming languages and software.
GM-CE4. CE-4. Have the ability to use computational tools as an aid to mathematical processes.
GM-CE6. Ability to solve problems from academic, technical, financial and social fields through mathematical methods.

**Generical:**
GM-CB5. To have developed those learning skills necessary to undertake further interdisciplinary studies with a high degree of autonomy in scientific disciplines in which Mathematics have a significant role.
GM-CG1. CG-1. Show knowledge and proficiency in the use of mathematical language.
GM-CB4. CB-4. Have the ability to communicate their conclusions, and the knowledge and rationale underpinning these to specialist and non-specialist audiences clearly and unambiguously.
GM-CG2. CG-2. Construct rigorous proofs of some classical theorems in a variety of fields of Mathematics.
GM-CG3. CG-3. Have the ability to define new mathematical objects in terms of others already know and ability to use these objects in different contexts.
GM-CG4. CG-4. Translate into mathematical terms problems stated in non-mathematical language, and take advantage of this translation to solve them.
GM-CG6. CG-6 Detect deficiencies in their own knowledge and pass them through critical reflection and choice of the best action to extend this knowledge.

**Transversal:**
04 COE. EFFICIENT ORAL AND WRITTEN COMMUNICATION. Communicating verbally and in writing about learning outcomes, thought-building and decision-making. Taking part in debates about issues related to the own field of specialization.
05 TEQ. TEAMWORK. Being able to work as a team player, either as a member or as a leader. Contributing to projects pragmatically and responsibly, by reaching commitments in accordance to the resources that are available.
07 AAT. SELF-DIRECTED LEARNING. Detecting gaps in one's knowledge and overcoming them through critical self-appraisal. Choosing the best path for broadening one's knowledge.
01 EIN. ENTREPRENEURSHIP AND INNOVATION: Knowing about and understanding how businesses are run and the sciences that govern their activity. Having the ability to understand labor laws and how planning, industrial and marketing strategies, quality and profits relate to each other.
02 SCS. SUSTAINABILITY AND SOCIAL COMMITMENT. Being aware of and understanding the complexity of social and economic phenomena that characterize the welfare society. Having the ability to relate welfare to globalization and sustainability. Being able to make a balanced use of techniques, technology, the economy and sustainability.

## TEACHING METHODOLOGY

All material is available in English and, even though the main language is Catalan, lecturers are open to repeat the theoretical concepts in English for interchange students.

The mathematical models are derived in lectures, and numerically solved in computer laboratory. Assignments and some exercises will be partially developed in the classroom. Python intrisic functions will be used when possible, otherwise, lecturers will provide Python codes to be used and, sometimes, slightly modified.

## LEARNING OBJECTIVES OF THE SUBJECT

Experience in mathematical modelling, numerical solution with computers and analysis of results, through the solution of several particular problems of interest in engineering and applied sciences.

## STUDY LOAD

| Type | Hours | Percentage |
|---|---|---|
| Hours small group | 30,0 | 20.00 |
| Self study | 90,0 | 60.00 |
| Hours large group | 30,0 | 20.00 |

**Total learning time:** 150 h

## CONTENTS

### Verification and validation of computational models

**Description:**
Examples of computational models and the relevance of their validation (correspondence between model and real phenomena) and verification (quality assessment of the numerical solution) in computational modeling, and in laboratory experiments.

**Full-or-part-time:** 2h
Theory classes: 2h

## Modeling with Laplace operator

**Description:**
Mathematical modelling with the Laplace operator: heat equation, flow in a porous medium, potential flow, electrical potential. Derivation of the PDE and boundary conditions for each application (modelling). Basics on the numerical solution with the Finite Element Method (FEM): weak form, discretization, implementation in Python. Quality assessment of the numerical solution in particular realistic applications. Ttime integration for transient problems.

**Full-or-part-time:** 13h
Theory classes: 13h

## Simulation of actin flow in cells

**Description:**
Modelling of actin flow in a living cell: transient convection-diffusion-reaction equation. Boundary conditions. FEM discretization and stabilization techniques for convection-dominated problems. Analysis of the effect of actin flow in the cell migration. Visit https://www.youtube.com/watch?v=xtpaymWR22E

**Full-or-part-time:** 15h
Theory classes: 15h

## Transport of pollutants

**Description:**
This point focuses on the mathematical modeling and numerical solution of a particular pollutant transport problem: an activated carbon (AC) filter https://www.youtube.com/watch?v=2tWOzebxil8&t=1s

Mathematical modeling of adsorption and desorption in an AC particle and semi-analytical approximation with polynomials of degree 2 in the radius of the particle, implementation in Python and analysis of the results and effect of material parameters.
Mathematical modeling of the transport of the pollutant inside the filter, without AC (convection-diffusion) and with AC (convection-diffusion-reaction) Numerical solution, for a filter with 1D simplification, with the method of finite differences and analysis of the results and effect of material parameters.
Introduction to the Finite Volume method (FV) for transport problems.
Computational modeling of a 2D filter: potential flow to calculate the velocity field and solution with MEF, and solution of the convection-reaction equation with FV.
Other applications of mathematical modeling of pollutant transport https://www.youtube.com/watch?v=LsVQj8fiflU

**Full-or-part-time:** 15h
Theory classes: 15h

## Simulation of particle systems

**Description:**
Modelling of the interaction between particles with an associated potential. Simulation of systems with different scales: chain configurations of particles (https://www.youtube.com/watch?v=_dQJBBklpQQ) or molecules (https://www.youtube.com/watch?v=ILFEqKl3sm4), monolayer cell systems o multibody systems, as an approach to the simulation of systems with large number of particles (http://sbel.wisc.edu/Animations). Statement of the ODEs system and numerical solution. Analysis of stability properties of time-integration algorithms. Extension to problems with constraints (volume conservation, contact, etc). Solution of optimal control problems

**Full-or-part-time:** 15h
Theory classes: 15h

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## GRADING SYSTEM

80% continuous assessment (exercises, assignments) + 20% exam

## BIBLIOGRAPHY


**Basic:**

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- Griebel, Michael; Zumbusch, Gerhard W; Knapek, Stephan. Numerical simulation in molecular dynamics : numerics, algorithms, parallelization, applications [on line]. Springer Berlin Heidelberg, 2007 [Consultation: 20/06/2023]. Available on: https://link-springer-com.recursos.biblioteca.upc.edu/book/10.1007/978-3-540-68095-6. ISBN 3540680950.
- Quarteroni, Alfio. Numerical models for differential problems [on line]. Milano: Springer Milan, 2009 [Consultation: 20/06/2023]. Available on: https://link-springer-com.recursos.biblioteca.upc.edu/book/10.1007/978-88-470-1071-0. ISBN 9786613562357.
- Donea, Jean M; Huerta, Antonio. Finite element methods for flow problems [on line]. Chichester: John Wiley & Sons, cop. 2003 [Consultation: 20/06/2023]. Available on: https://onlinelibrary-wiley-com.recursos.biblioteca.upc.edu/doi/book/10.1002/0470013826. ISBN 0471496669.
- Rodríguez-Ferran, A., Sarrate, J. and Huerta, A.. "Numerical modelling of void inclusions in porous media". International Journal for Numerical Methods in Engineering [on line]. 2004 [Consultation: 20/06/2023]. Available on: https://onlinelibrary-wiley-com.recursos.biblioteca.upc.edu/loi/10970207.- Mogilner, A. ; Edelstein-Keshet, L. "Regulation of actin dynamics in rapidly moving cells: a quantitative analysis.". Biophysical Journal [on line]. [Consultation: 20/06/2023]. Available on: https://www-sciencedirect-com.recursos.biblioteca.upc.edu/journal/biophysical-journal.- Pollard, TD ; Cooper, JA. "Actin, a central player in cell shape and movement.". Science [on line]. doi: 10.1126/science.1175862 [Consultation: 20/06/2023]. Available on: https://www-science-org.recursos.biblioteca.upc.edu/loi/science.- Pérez-Foguet, A.; Casoni , E.; Huerta, A. "Dimensionless analysis of HSDM and application to simulation of breakthrough curves of highly adsorbent porous media.". Journal of environmental engineering (ASCE) [on line]. 10.1061/(ASCE)EE.1943-7870.0000665 [Consultation: 20/06/2023]. Available on: http://hdl.handle.net/2117/26352.