UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH

Course guide
200247 - MODC - Computational Modelling

Last modified: 01/06/2023

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: 2023 **ECTS Credits:** 6.0 **Languages:** English

LECTURER

Coordinating lecturer: SONIA FERNANDEZ MENDEZ

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

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

Lectures, solution of exercises and computer laboratory sessions. Lectures will be taught in English unless all students and the lecturer agree on another language.

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

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=lLFEqKl3sm4), 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

The Laplace operator in computational modelling

Description:
Mathematical modelling with the Laplace operator and applications: 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 Matlab. Quality assessment of the numerical solution. Solution of particular problems with real-life application. Discretization and time integration for transient problems.

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

FEM for the 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:
Numerical solution of a problem of transport of pollutants in air, see https://www.youtube.com/watch?v=LsVQj8fiflU. Computational modelling of activated carbon (AC) filters: air flow in the filter, adsorption and desorption in AC grain, coupled convection-diffusion-(non-linear)reaction problem for filter bulk scale, see https://www.youtube.com/watch?v=2tWOzebxil8&t=1s. Application to the design of an AC filter for a car: effect of air chambers, interior walls, etc. Introduction to Finite Volumes and Discontinuous Garlerkin methods for problems with sharp fronts.

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

GRADING SYSTEM

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

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BIBLIOGRAPHY

Basic:

- 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.- 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.

- 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.- Hairer, E; Lubich, Christian; Wanner, Gerhard. Geometric numerical integration structure-preserving algorithms for ordinary differential equations [on line]. Springer, 2006 [Consultation: 20/06/2023]. Available on: https://link-springer-com.recursos.biblioteca.upc.edu/book/10.1007/3-540-30666-8. ISBN 9786610610600.

- 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.

- 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.