Course guide
200247 - MODC - Computational Modelling

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 into 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.

General:
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 intrinsic 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

<table>
<thead>
<tr>
<th>Type</th>
<th>Hours</th>
<th>Percentage</th>
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</thead>
<tbody>
<tr>
<td>Hours small group</td>
<td>30,0</td>
<td>20.00</td>
</tr>
<tr>
<td>Self study</td>
<td>90,0</td>
<td>60.00</td>
</tr>
<tr>
<td>Hours large group</td>
<td>30,0</td>
<td>20.00</td>
</tr>
</tbody>
</table>

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=_dQJBKiIpQQ) or molecules (https://www.youtube.com/watch?v=ILFeqKhJ3sm4), monolayer cell systems or 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:**

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

### FEM for the simulation of actin flow in cells

**Description:**

**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=LsVQj8fiU. 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=2tWOZebxiIl&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 Galerkin methods for problems with sharp fronts.

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

### GRADING SYSTEM

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

Basic: