200247 - MODC - Computational Modelling

Coordinating unit: 200 - FME - School of Mathematics and Statistics
Teaching unit: 749 - MAT - Department of Mathematics
751 - DECA - Department of Civil and Environmental Engineering

Academic year: 2018
Degree: BACHELOR'S DEGREE IN MATHEMATICS (Syllabus 2009). (Teaching unit Optional)
ECTS credits: 6
Teaching languages: English

Teaching staff

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

Opening hours

Timetable: Send an e-mail to the lecturer to arrange a meeting, or ask after lectures.

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 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>Total learning time: 150h</th>
<th>Hours large group: 30h</th>
<th>20.00%</th>
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<tbody>
<tr>
<td></td>
<td>Hours medium group: 0h</td>
<td>0.00%</td>
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<tr>
<td></td>
<td>Hours small group: 30h</td>
<td>20.00%</td>
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<td></td>
<td>Guided activities: 0h</td>
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<td>Self study: 90h</td>
<td>60.00%</td>
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## Content

<table>
<thead>
<tr>
<th>Verification and validation of computational models</th>
<th>Learning time: 2h</th>
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<tbody>
<tr>
<td></td>
<td>Theory classes: 2h</td>
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**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.

<table>
<thead>
<tr>
<th>Simulation of particle systems</th>
<th>Learning time: 15h</th>
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<tbody>
<tr>
<td></td>
<td>Theory classes: 15h</td>
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**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=lLFEqK13sm4), 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). Analysis of systems with change of neighbours.

<table>
<thead>
<tr>
<th>The Laplace operator in computational modelling</th>
<th>Learning time: 13h</th>
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<tr>
<td></td>
<td>Theory classes: 13h</td>
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**Description:**

<table>
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<tr>
<th>FEM for the simulation of actin flow in cells</th>
<th>Learning time: 15h</th>
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<tr>
<td></td>
<td>Theory classes: 15h</td>
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**Description:**
**Transport of pollutants**

<table>
<thead>
<tr>
<th>Learning time</th>
<th>15h</th>
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</thead>
<tbody>
<tr>
<td>Theory classes</td>
<td>15h</td>
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</table>

**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 Galerkin methods for problems with sharp fronts.

**Qualification system**
50% continuous assessment (exercises, assignments, oral presentations) + 50% exam

**Bibliography**

**Basic:**


**Others resources:**

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 Galerkin methods for problems with sharp fronts.