## BASIC DETAILS:

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|---|---|
| **Subject:** | MATEMÁTICA COMPUTACIONAL Y SIMULACIÓN |
| **Id.:** | 33286 |
| **Programme:** | GRADUADO EN BIOINFORMÁTICA. PLAN 2019 (BOE 06/02/2019) |
| **Module:** | MATEMÁTICAS |
| **Subject type:** | OBLIGATORIA |

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|---|---|---|---|
| **Year:** | 2 | **Teaching period:** | Primer Cuatrimestre |
| **Credits:** | 6 | **Total hours:** | 150 |
| **Classroom activities:** | 62 | **Individual study:** | 88 |
| **Main teaching language:** | Inglés | **Secondary teaching language:** | Castellano |
| **Lecturer:** | | **Email:** | |

## PRESENTATION:

This subject explains the principles of mathematical modeling and simulation. It provides definitions and illustrative examples of the important concepts as well as an overview of the main types of mathematical models. This subject is mainly focused on the mechanistic (process-oriented) models. These models are developed using ordinary and partial differential equation models (ODE and PDE respectively). This subject will cover how to solve simple models and and how to implement them to be solved by the computer.

## PROFESSIONAL COMPETENCES ACQUIRED IN THE SUBJECT:

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| **General programme competences** | G01 | Use learning strategies autonomously for their application in the continuous improvement of professional practice. |
| | G02 | Perform the analysis and synthesis of problems of their professional activity and apply them in similar environments. |
| | G05 | Communicate professional topics in Spanish and / or English both orally and in writing. |
| | G07 | Choose between different complex models of knowledge to solve problems. |
| | G08 | Recognise the role of the scientific method in the generation of knowledge and its applicability to a professional environment. |
| | G09 | Apply information and communication technologies in the professional field. |
| | G10 | Apply creativity, independence of thought, self-criticism and autonomy in the professional practice. |
| **Specific programme competences** | E01 | Solve mathematical problems that may arise in bioinformatics, by integrating the knowledge acquired in algebra, geometry, differential and integral calculus, optimisation and numerical methods. |
| | E03 | Apply the fundamental concepts of mathematics, logic, algorithmics and computational complexity to solve problems specific to bioinformatics. |
| **Learning outcomes** | R01 | Explain the mathematical models that can be described by Ordinary Differential Equations. |
| | R02 | Solve systems of ordinary differential equations with initial values or contour problem. |
| | R03 | Resolve contour problems for parabolic equations. |
| | R04 | Choose the most appropriate technique for solving a system of differential equations. |

## PRE-REQUISITES:

The only mathematical prerequisites are some calculus and linear algebra

## SUBJECT PROGRAMME:

### Subject contents:

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| **1 - Introduction** |
|   1.1 - Principles of Mathematical Modeling |
|   1.2 - Phenomenological models |
|   1.3 - Mechanistic models |
| **2 - Ordinary differential equations** |
|   2.1 - ODE Models |

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|---|---|
| 2.2 - Initial value problems and boundary problems | |
| 2.3 - Fitting ODE's to Data | |
| 2.4 - Numerical solution | |
| **3 - Equations in partial derivatives** | |
| 3.1 - Contour problems for parabolic equations | |
| 3.2 - Contour problems for hyperbolic equations | |
| 3.3 - Numerical solution | |

Subject planning could be modified due unforeseen circumstances (group performance, availability of resources, changes to academic calendar etc.) and should not, therefore, be considered to be definitive.


**TEACHING AND LEARNING METHODOLOGIES AND ACTIVITIES:**

**Teaching and learning methodologies and activities applied:**

**Theory Sessions**: Lectures will be used to explain the basis of the different chapters. Wherever possible, explanations will be accompanied by images, text or sounds to be used as practical examples and discussion topics. During the sessions, the lecturer will propouse activities or to look for information out of the class and he will resolve doubts.

**Practical Sessions**:During practice, students will use problem-based learning methodological strategy. The student will have the slides of all the chapters of the course. They should be able to expand it with the content explained in class and other bibliographic resources.

The lecturer will be available to students during the tutorial schedule to help them in all matters concerning the course. On request, group tutorials may be programmed to control the work of the group. The course requires a significant effort by the student. The concepts explained in one chapter will be used in the followings.

**Student work load:**

| Teaching mode | Teaching methods | Estimated hours |
|---|---|---|
| **Classroom activities** | Master classes | 29 |
| | Other theory activities | 10 |
| | Practical exercises | 14 |
| | Practical work, exercises, problem-solving etc. | 5 |
| | Assessment activities | 4 |
| **Individual study** | Tutorials | 5 |
| | Individual study | 29 |
| | Individual coursework preparation | 20 |
| | Group cousework preparation | 24 |
| | Project work | 10 |
| | **Total hours:** | 150 |


**ASSESSMENT SCHEME:**

**Calculation of final mark:**

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|---|---|---|
| Written tests: | 50 | % |
| Individual coursework: | 30 | % |
| Group coursework: | 20 | % |
| **TOTAL** | 100 | % |

*Las observaciones específicas sobre el sistema de evaluación serán comunicadas por escrito a los alumnos al inicio de la materia.

**BIBLIOGRAPHY AND DOCUMENTATION:**

**Basic bibliography:**

VELTEN, Kai. Mathematical modeling and simulation. Introduction for Scientists and Engineers. Wiley, 2009. ISBN: 978-3-527-40758-8

INGALLS, Brian. Mathematical Modelling in Systems Biology: An Introduction. University of Waterloo

**Recommended bibliography:**

ATKINSON, Kendall E.; HAN, Weimin; STEWART, David. Numerical Solution of Ordinary Differential Equations. John Wiley & Sons, Inc, 2009. ISBN: 9781118164495

ILIEV, O.P.; MARGENOV, S.D.; MINEV, P.D.; VASSILEVSKI, P.S.; ZIKATANOV, L.T. Numerical Solution of Partial Differential Equations: Theory, Algorithms, and Their Applications. Springer 2013. ISBN: 978-1-4614-7171-4

**Recommended websites:**

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|---|---|
| Mathematical Modelling in Systems Biology: An Introduction. | https://www.math.uwaterloo.ca/~bingalls/MMSB/ |
| CellML | www.cellml.org |

\* Guía Docente sujeta a modificaciones