ANX-PR/CL/001-01

LEARNING GUIDE

SUBJECT

43000602 - Modelado Y SimulaciÓn En Ciencia E IngenierÍa De Materiales

DEGREE PROGRAMME

04AN - Master Universitario En Ingenieria De Materiales

ACADEMIC YEAR & SEMESTER

2023/24 - Semester 1

Index

Learning guide

1. Description

1.1. Subject details

Name of the subject	43000602 - Modelado y Simulación en Ciencia e Ingeniería de Materiales
No of credits	6 ECTS
Type	Compulsory
Academic year ot the programme	First year
Semester of tuition	Semester 1
Tuition period	September-January
Tuition languages	English
Degree programme	04AN - Master Universitario en Ingenieria de Materiales
Centre	04 - Escuela Tecnica Superior De Ingenieros De Caminos, Canales Y Puertos
Academic year	2023-24

2. Faculty

2.1. Faculty members with subject teaching role

Name and surname	Office/Room	Email	Tutoring hours *
Alvaro Ridruejo Rodriguez		alvaro.ridruejo@upm.es	F - 17:00 - 18:00
Carlos Daniel Gonzalez Martinez		c.gonzalez@upm.es	F - 17:00 - 18:00
Fco. Javier Llorca Martinez		javier.llorca@upm.es	F - 17:00 - 18:00
Javier Segurado Escudero (Subject coordinator)		javier.segurado@upm.es	- -

* The tutoring schedule is indicative and subject to possible changes. Please check tutoring times with the faculty member in charge.

2.3. External faculty

Name and surname	Email	Institution
Valentin Vassilev	valentin.vassilev@imdea.org	IMDEA-Materiales
Damien Tourret	damien.tourret@imdea.org	IMDEA Materials Institute

3. Prior knowledge recommended to take the subject

3.1. Recommended (passed) subjects

The subject - recommended (passed), are not defined.

3.2. Other recommended learning outcomes

- Computer Science, Mathematical, Physical and Mechanical foundations of Materials Science, Themodynamics, Mechanics of Materials

4. Skills and learning outcomes *

4.1. Skills to be learned

CE1 - Capacidad para aplicar los fundamentos científicos del comportamiento físico y químico de los materiales para relacionar causalmente sus propiedades fundamentales físicas y químicas con su comportamiento macroscópico y el de los productos con ellos realizados / Ability to apply the scientific foundations of the physical and chemical behavior of materials to correlate their fundamental physical and chemical properties with their macroscopic behavior and that of the products made with them.

CE2 - Uso de equipos y técnicas experimentales de caracterización de materiales (micro y macroestructura, comportamientos mecánico, eléctrico, y óptico) para identificar y analizar los diversos tipos de materiales / Use of equipment and experimental techniques for the characterization of materials (micro and macrostructure, mechanical, electrical, and optical behavior) to identify and analyze the various types of materials.

CE4 - Autonomía para adquirir, analizar, actualizar y aplicar nuevos conocimientos, modelos y técnicas experimentales y numéricas en relación con la composición y estructura de los materiales, su caracterización física y química, sus procesos de fabricación, su utilización y aplicación científica y tecnológica, y su reciclado, reutilización y eliminación / Autonomy to acquire, analyze, update and apply new knowledge, models and experimental and numerical techniques related to the composition and structure of materials, their physical and

chemical characterization, their manufacturing processes, their use and scientific and technological application, and their recycling, reuse and disposal

CE7 - Manejo de herramientas de simulación numérica para diseño y análisis de materiales, desde la escala microscópica a la macroscópica / Management of numerical simulation tools for design and analysis of materials, from the microscopic to the macroscopic scale

CG1 - Uso de la lengua inglesa: Los alumnos son capaces de transmitir conocimientos y expresar ideas y argumentos de manera clara, rigurosa y convincente, tanto de forma oral como escrita, adaptándose a las características de la situación y de la audiencia / Use of the English Language: Students are able to transmit knowledge and express ideas and arguments in a clear, rigorous and convincing manner, both orally and in writing, adapting to the characteristics of the situation and the audience .

CG4 - Creatividad: Los alumnos son capaces de resolver de forma nueva, original y aportando valor, situaciones o problemas en el ámbito de la ingeniería de materiales / Creativity: Students are able to solve situations or problems in the field of materials engineering in a new, original way and adding value.

CG7 - Uso de las TIC: Los alumnos son capaces de aplicar conocimientos tecnológicos necesarios de manera que les permitan desenvolverse cómodamente y afrontar los retos que la sociedad les va a imponer en su quehacer profesional empleando la informática / Use of ICT: Students are able to apply the necessary technological knowledge in a way that allows them to function comfortably and face the challenges that society is going to impose on them in their professional work using computers.

CG8 - Resolución de problemas: Los estudiantes son capaces de reconocer, describir, organizar y analizar los elementos constitutivos de un problema para idear estrategias que permitan obtener, de forma razonada, una solución contrastada y acorde a ciertos criterios preestablecidos / Problem solving: Students are able to recognize, describe, organize and analyze the constitutive elements of a problem to devise strategies that allow obtaining, in a reasoned way, a contrasting solution and according to certain pre-established criteria.

4.2. Learning outcomes

RA27 - Conocer, comprender y saber aplicar los fundamentos científicos del comportamiento de los materiales

RA25 - Conocer, comprender y saber aplicar los fundamentos científicos del comportamiento de los materiales y la interrelación entre su estructura, propiedades, procesado y aplicaciones

RA26 - Saber utilizar y aplicar las técnicas y modelos matemáticos de simulación para predecir el comportamiento y evolución de los materiales. Saber evaluar su seguridad, durabilidad e integridad estructural y la de los componentes fabricados con ellos

RA24 - aber utilizar y aplicar las técnicas y modelos matemáticos de simulación para predecir el comportamiento y evolución de los materiales, en sus aspectos mecánico, electrónico, químico o biológico

* The Learning Guides should reflect the Skills and Learning Outcomes in the same way as indicated in the Degree Verification Memory. For this reason, they have not been translated into English and appear in Spanish.

5. Brief description of the subject and syllabus

5.1. Brief description of the subject

The objective of this subject is two fold:

1) To complete and uniform the level of the students in scientific programming, applied mathematics and simulation techniques. The students starting the master have different background, some of them have never study and use any programming language, while other are proficient in the use of programming and modeling tools as finite elements, etc. This subject is aimed at introducing these concepts to novel students and settle and widen them for the students with experience.

2) Provide an overview of the main simulations techniques and modelling strategies in Materials Science and Engineering.

The subject will cover a first part about methodology. This part will cover an introduction to programming in which a modern and open interpreted language, Python, will be introduced. This tool is highly demanded in the industry and has been chosen for its generality as a good tool for numerical methods but widely applied to other areas, specially data science and machine learning.Then different areas of applied maths will be reviewed and will show the methods and algorithms available to solve problems in those areas. Algebraical system of equations, ordinary

differential equations, optimization and partial differential equations are covered.

The second part of the subject cover different modeling and simulation techniques widely used in Materials Engineering, coverin: first principles simulations, computational thermodynamics, homogenization theory and an introduction to machine learning

The subject is though to be practical and the students will use their own laptop during the classes.

5.2. Syllabus

1. Introduction to materials modelling and simulation. Contents and evaluation.

2. Introduction to scientific programming: python

3. Numerical methods for model implementation

4. Fundamentals of first principles calculations. The DFT method. Practical information about crystallography and geometry optimization. Quantum Espresso. Examples of applications.

5. Computational thermodynamics. Thermodynamics and phase diagrams. Thermodynamic model and parameters. Calculation of phase diagrams. Case studies. Phase field modelling

6. Homogenization theory. Thermo-elastic constants of heterogeneous solids. Eshelby?s tensor. Mean-field approximations for finite concentrations. Extension to the nonlinear regime

7. Introduction to Machine Learning

8. Integrated Computational Materials Engineering

6. Schedule

6.1. Subject schedule*

Week	Classroom activities	Laboratory activities	Distant / On-line	Assessment activities
1	**T1: Introduction** Duration: 01:00 Lecture **T2: Introduction to scientific programming: python** Duration: 03:00 Lecture			
2	**T2: Introduction to scientific programming: python** Duration: 02:00 Problem-solving class **T3: Numerical methods** Duration: 02:00 Lecture			
3	**T3: Numerical methods** Duration: 03:00 Lecture **T3: Numerical methods** Duration: 01:00 Problem-solving class			
4	**T3: Numerical methods** Duration: 03:00 Lecture **T3: Numerical methods** Duration: 01:00 Lecture			
5	**T3: Numerical methods** Duration: 02:00 Lecture **T4: Fundamentals of first principles calculations** Duration: 02:00 Lecture			
6	**T4: Fundamentals of first principles calculations** Duration: 03:00 Lecture **T4: Fundamentals of first principles calculations** Duration: 01:00 Problem-solving class			**PROBLEM 1: Numerical methods** Individual work Continuous assessment and final examination Not Presential Duration: 00:00

7	**T4: Fundamentals of first principles calculations** Duration: 03:00 Lecture **T4: Fundamentals of first principles calculations** Duration: 01:00 Problem-solving class			
8	**T4: Fundamentals of first principles calculations** Duration: 02:00 Lecture **T5: Thermodynamics simulations** Duration: 02:00 Lecture			
9	**T5: Thermodynamics simulations** Duration: 03:00 Lecture **T5: Thermodynamics simulations** Duration: 01:00 Problem-solving class			**PROBLEM 2: Ab initio techniques** Individual work Continuous assessment and final examination Not Presential Duration: 00:00
10	**T5: Thermodynamics simulations** Duration: 03:00 Lecture **T5: Thermodynamics simulations** Duration: 01:00 Problem-solving class			
11	**T5: Thermodynamics simulations** Duration: 02:00 Lecture **T6: Micromechanics** Duration: 02:00 Lecture			
12	**T6: Micromechanics** Duration: 03:00 Lecture **T6: Micromechanics** Duration: 01:00 Problem-solving class			**PROBLEM 3: Thermodynamical simulations** Individual work Continuous assessment and final examination Not Presential Duration: 00:00
13	**T6: Micromechanics** Duration: 03:00 Lecture **T6: Micromechanics** Duration: 01:00 Problem-solving class			
14	**T7: Machine Learning** Duration: 02:00 Lecture **T7: Machine Learning** Duration: 02:00 Problem-solving class			

15	**T8: Multiscale and Multiphysical approaches** Duration: 02:00 Lecture **T8: Multiscale and Multiphysical approaches** Duration: 02:00 Problem-solving class			**PROBLEM 4: Micromechanics** Individual work Continuous assessment and final examination Not Presential Duration: 00:00
16				
17				**FINAL EXAM: ORAL PRESENTATION OF A PROBLEM** Individual presentation Continuous assessment and final examination Presential Duration: 01:00

Depending on the programme study plan, total values will be calculated according to the ECTS credit unit as 26/27 hours of student face-to-face contact and independent study time.

* The schedule is based on an a priori planning of the subject; it might be modified during the academic year, especially considering the COVID19 evolution.

7. Activities and assessment criteria

7.1. Assessment activities

7.1.1. Assessment

Week	Description	Modality	Type	Duration	Weight	Minimum grade	Evaluated skills
6	PROBLEM 1: Numerical methods	Individual work	No Presential	00:00	12.5%	/ 10	
9	PROBLEM 2: Ab initio techniques	Individual work	No Presential	00:00	12.5%	/ 10	
12	PROBLEM 3: Thermodynamical simulations	Individual work	No Presential	00:00	12.5%	/ 10	
15	PROBLEM 4: Micromechanics	Individual work	No Presential	00:00	12.5%	/ 10	
17	FINAL EXAM: ORAL PRESENTATION OF A PROBLEM	Individual presentation	Face-to-face	01:00	50%	/ 10	CE1 CG7 CG1 CE4 CE2 CE7 CG8 CG4

7.1.2. Global examination

Week	Description	Modality	Type	Duration	Weight	Minimum grade	Evaluated skills
6	PROBLEM 1: Numerical methods	Individual work	No Presential	00:00	12.5%	/ 10	
9	PROBLEM 2: Ab initio techniques	Individual work	No Presential	00:00	12.5%	/ 10	
12	PROBLEM 3: Thermodynamical simulations	Individual work	No Presential	00:00	12.5%	/ 10	
15	PROBLEM 4: Micromechanics	Individual work	No Presential	00:00	12.5%	/ 10	
17	FINAL EXAM: ORAL PRESENTATION OF A PROBLEM	Individual presentation	Face-to-face	01:00	50%	/ 10	CE1 CG7 CG1 CE4 CE2 CE7 CG8 CG4

7.1.3. Referred (re-sit) examination

No se ha definido la evaluación extraordinaria.

7.2. Assessment criteria

CONTINUOUS AND GLOBAL EVALUATION:

A) Individual exercises

- Each student will have to carry out a practical exercise corresponding to four parts of the subject:

  -Numerical methods

  -Ab initio technoques

  -computational thermodynamics

  -Homogenization theory.

-The result will be a short presentation for each problem detailing the simulation strategy, results and discussion will have to be submitted by e-mail (pdf format)

-Reports are mandatory to have access to the final exam. The weight of all the reports in 50%

If the reports have not been submitted, the student cannot attend the final oral exam.

B) Individual presentation

- Each student will present one of the exercises as an oral presentation with a discussion with the evaluators

8. Teaching resources

8.1. Teaching resources for the subject

Name	Type	Notes
Python Scripting for Computational Science, Hans Petter Langtangen, Python Scripting for Computational Science, Springer-Verlag Berlin Heidelberg, 2008	Bibliography	
?Introduction to computational Materials Science: fundamentals to applications?, Richard LeSar, Cambridge University Press, 2013.	Bibliography	
?Numerical modeling in Materials Science and Engineering? Michel Rappaz, Michel Bellet, Michel Deville, Springer, 2002.	Bibliography	
?Understanding molecular dynamics simulation. From algorithms to applications?, Daan Frenkel and Berend Smit, Academic Press, 2nd edition 2002.	Bibliography	
?A short introduction to basic aspects of continuum micromechanics?. Helmut J. Böhm, ILSB report 206, Vienna University of Technology, 2013.	Bibliography	
Notes in Moodle	Web resource	

Partial Differential Equations and the Finite Element Method, P. Solin, Partial Differential Equations and the Finite Element Method, John Wiley & Sons, 2004.	Bibliography	

9. Other information

9.1. Other information about the subject