Grado en Ingeniería de Materiales

Department (School) / Departamento (Escuela)
Departamento de Ciencia de Materiales (ETSI Caminos Canales y Puertos)

Asignatura / Subject
Simulación en Ingeniería de Materiales
Simulation in Materials Engineering

ECTS	Type	Curso / Semestre	Idioma	Sylabus code	Subject Code
5	Compulsory	3 / 5	EN	04MI	45000123

Lecturers (Name)	Contact email	Office hours (Tutorials)
Javier Segurado	Javier.segurado@upm.es	Monday 12:00-14:00 and Tuesday 14-00 – 16:00
Álvaro Ridruejo	Alvaro.ridruejo@upm.es	Monday 12:00-14:00 and Tuesday 14-00 – 16:00
Javier LLorca	Javier.llorca@upm.es	Monday 12:00-14:00 and Wednesday 9:00– 11:00
Victor Rey de Pedraza	v.rey@upm.es	By appointment

El profesor que aparece en primer lugar es el coordinador de la asignatura

Criterio de evaluación

Continuum assessment.

- It will consist in the presentation of some exercise(s) that will be done as homework and two partial exams.
- The final mark for continuous assessment will be computed as 0.25*homework+0.75*partials
- Each partial exam will correspond to the corresponding halve of the subject content and both will have the same weight in the final mark
- Partial exams will consist on practical exercises that should be resolved with the aid of a personal computer (which each student should bring from home)
- The partial exams will be done during class time and the dates will be decided at the beginning of the subject
- The subject will be passed (no need of final exam) with average global score higher than 50%, and a minimum of 30% of score on each individual test.

Final assessment:

If the student does not pass the subject by continuum assessment, final exams can be done to pass the subject. In this case the mark of the subject will be exclusively the mark of the exam.

Regular Exam (January). The exam will cover the whole subject and only practical exercises with computer are to be solved. The homework and partials will not be considered if this exam is done and the final qualification will be the mark of the exam, that will be passed with an score higher tan 50%

Extraordinary Exam (July). This exam covers the whole subject and subject and only practical exercises with computer are to be solved. The homework and partials will not be considered if this exam is done and the final qualification will be the mark of the exam, that will be passed with an score higher tan 50%

Justification and Objectives

The objective of the subject is to provide to the students a basis to quantitatively solve, using computers, problems related to materials Engineering. To this aim, (1) an introduction to computer programming will be covered (using matlab/octave or python langauages) and (2) an overview of the main simulation techniques in materials engineering will be presented considering in all the cases its computational implementation.

The list of objectives is:

1) Learn the basis of computer programming (variables, loops, conditions, input/output) to allow the programing of basic algorithms and mathematical models in a standard programming code (i.e. matlab)

2) Learn the theory and implementation of the most common numerical techniques for linear algebra, the resolution of non-linear systems of equations and the numerical resolution of ordinary differential equations
3) Learn the basic aspects of Montecarlo type models including the generation of random numbers, statistical samples of a probability distributions, analysis of statistical data and some particular models as kinetic ;ontecarlo or random walk.
4) Learn the basic aspects of numerical simulation of partial differential equations with special emphasis in the Finite Element Method and its implementation.
6) Give a descriptive general view of the different simulation techniques available to solve other materials engineering problems: ab initio and molecular dynamics, computational thermodynamics, discrete dislocation dynamics, Mean field methods, etc...

Prerequisites

None

Previous knowledge of the student

Computer Science, Mathematical, Physical and Mechanical foundations of Materials Science
Mechanics of Materials I, II and III

Contents in coordination with other subjects

Mechanics of Materials I, II and III

Generic competencies

CG1, English communication skills
CG2, Team work capacity
CG3, Spoken and written communication
CG4, Usage of CIT
CG11, Responsibility and professional ethics

Specific competencies

CE2, Modelling the materials behaviour
CE5, Capacity of autonomous learning

Bibliography

- Slides of “Simulation in Material Science”
- Scientific computing with MATLAB and OCTAVE” A. Quarteroni and F. Saleri, Springler 2006 (Spanish version also available)
- “A first course in Finite Elements” Jacob Fish and Ted Belytschko, Wiley, 2007
- “Numerical Modeling in Materials Science and Engineering” Michel Rappaz, Michel Bellet, Michel Deville, Springer, 2002
- “Introduction to Computational Materials Science, Fundamentals to Applications” Richard LeSar, Cambridge University Press, 2013

Subject contents and time distribution

LM: Lesson at room, RP: Problems Resolution, LB: Laboratory,, TI: Individual Work, TG: Group Work, DB: Debate at Room, VI: Visits, EV: Exams, OT: Other procedures

Item	Contents	Code
	T0: Introduction	
0.1	Introduction to the subject. General description contents and subject	LM
	T1. Fundamentals of programming	

1.1	Introduction to programming: MATLAB and OCTAV	LM, RP, LB, TI
	T2. Systems of algebraical equations	
2.1	Linear systems of equations. LU decomposition and other methods	LM, RP
2.2	Non Linear systems of equations. Bisection method, Newton-Raphson, et	LM, RP
	Practical problems	LB
	T3. Ordinary Differential Equations.	LM, RP
3.1	First order linear Ordinary Differential equations: Euler methods	LM, RP
3.2	Systems of Ordinary Differential equations and higher order equations	LM, RP
	Practical problems	LM, RP
	T4. Probabilistic methods	
4.1	Random numbers	LM, RP
4.2	Monte Carlo simulation. An introduction	LM, RP
4.3	Random walk	LM, RP
4.4	Kinetic Monte Carlo	LM, RP
	Practical problems	LB
	T5. Partial Differential Equations: The Finite Element Method	
5.1	Introduction to the FEM method	LM, RP
5.2	The standard discrete system	LM, RP
5.3	Spatial discretization: Interpolation and Integration of functions	LM, RP
5.4	The finite element method. 1D and 3D formulation of elastic problem	LM, RP
	Programming of a 2D Matlab code for linear elasticity.	LB
	T6: Other Simulation techniques	
6.1	Ab initio methods, Computational thermodynamics, Phase field modeling	LM