Last update: 06-05-2019

230486 - SIMCON - Computer Simulation of Condensed Matter

Coordinating unit: 230 - ETSETB - Barcelona School of Telecommunications Engineering
Teaching unit: 748 - FIS - Department of Physics
Academic year: 2019
Degree: BACHELOR'S DEGREE IN ENGINEERING PHYSICS (Syllabus 2011). (Teaching unit Optional)
ECTS credits: 6 Teaching languages: English

Teaching staff

Coordinator: ELVIRA GUARDIA MANUEL

Others: JORDI MARTÍ RABASSA

Opening hours

Timetable: To be determined

Prior skills

Individual and team working procedures
Ability to work with graphical data (representation, visualization)
Ability to analyze data and interpreting results
Proficiency in programming in a high level language (C, FORTRAN, Java, etc.).

Requirements

Specific previous topics: Statistical Physics, Thermodynamics, Quantum Physics, Numerical and Computational Methods (1 and 2)
Topics to be studied simultaneously: none

Degree competences to which the subject contributes

Specific:

1. Knowledge of the structure of matter and its properties at molecular and atomic level. Ability to analyze the behavior of materials, electronics and biophysical systems, and the interaction between radiation and matter.
2. Understanding and mastery of computer programming, use of operative systems and computational tools (scientific software). Skills to implement numerical algorithms in languages of low (C, F90) and high (Matlab) level.
3. Knowledge of the scientific method and its applications in physics and engineering. Ability to formulate hypotheses and make critical analysis of scientific problems in the field of physics and engineering. Ability to relate the physical reality with their mathematical models and vice versa.

Generical:

4. ABILITY TO IDENTIFY, FORMULATE, AND SOLVE PHYSICAL ENGINEERING PROBLEMS. Planning and solving physical engineering problems with initiative, making decisions and with creativity. Developing methods of analysis and problem solving in a systematic and creative way.

Transversal:

6. THIRD LANGUAGE. Learning a third language, preferably English, to a degree of oral and written fluency that fits in with the future needs of the graduates of each course.
5. SELF-DIRECTED LEARNING - Level 3. Applying the knowledge gained in completing a task according to its relevance and importance. Deciding how to carry out a task, the amount of time to be devoted to it and the most suitable information sources.
7. TEAMWORK - Level 3. Managing and making work groups effective. Resolving possible conflicts, valuing working

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with others, assessing the effectiveness of a team and presenting the final results.

Teaching methodology

Lectures
Classes of problems and exercises
Practical computer exercises
Educational seminars

Learning objectives of the subject

Topic: Computational modeling and simulation of physical systems at the microscopic level (solids, liquids, gases)
Understanding by students of the main theoretical aspects and most important computational simulation techniques
Students should be able to create their own simulation codes (Monte Carlo, Molecular Dynamics)
Students should be able to use powerful simulation packages and its application to modeling and simulation of systems with a high degree of realism.

Study load

Total learning time: 150h	Hours large group:	65h	43.33%
	Self study:	85h	56.67%

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Content

Modeling and simulation. Introduction.

Learning time: 8h

Theory classes: 3h
Self study : 5h

Description:
Introduction to simulation methods and modeling of physical systems at the microscopic scale
Topics:
1. Models and force fields
2. Simulation methodologies
3. Basics of FORTRAN programming language and of LINUX operating system

Related activities:
Lectures

Specific objectives:
Give general ideas of the section. Introduction to the course

Molecular Dynamics

Learning time: 43h

Theory classes: 12h
Laboratory classes: 8h
Self study : 23h

Description:
Molecular Dynamics technique is able to generate trajectories of Newtonian particles in a classical system and study the structure and temporal dynamics of the system.
Topics:
1. Solving the equations of motion numerically
- Equations of motion
- Finite Difference Methods: Euler, Verlet, Leapfrog, Runge-Kutta and predictor-corrector algorithm
2. Simulating a system of N particles
- Energy and forces
- Periodic boundary conditions
- Short-range forces and minimum image method
- Long-range interactions: Ewald and particle mesh Ewald methods, reaction field
- Thermostats and barostats
3. Introduction to quantum methods
- Basics of Density Functional Theory, "ab initio" methods and Car-Parrinello Molecular Dynamics.

Related activities:
Programming and use of codes of classical MD

Specific objectives:
Understanding the concept of molecular dynamics (MD).
Understanding the main tools needed to create a classical MD simulation.
Study the calculation of properties of the system.
See the main elements of the simulation of quantum systems.

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Monte Carlo method

Learning time: 35h

Theory classes: 10h
Laboratory classes: 7h
Self study : 18h

Description:
The technique of Monte Carlo simulation is based on simulating reality through the study of a statistical sample that has been generated completely at random.
Topics:
1. Monte Carlo simulation of discrete systems: the Ising model
2. Monte Carlo simulation of continuous systems
- Basics: Metropolis algorithm. Detailed balance
- Monte Carlo statistical ensembles: canonical and beyond
- Re-scaling and finite size phase transitions
- Quantum Monte Carlo methods

Related activities:
Programming and use of codes of classical MC

Specific objectives:
Understanding the concept of Monte Carlo simulation (MC).
Understanding the main tools needed to generate random numbers and sampling of a classical system.
Study calculating system properties.

Applications of simulation to realistic systems

Learning time: 64h

Theory classes: 6h
Laboratory classes: 15h
Guided activities: 3h
Self study : 40h

Description:
See the techniques described in previous chapters applied to systems with a high degree of realism.
Topics:
1. Hard Condensed Matter:
- Nanomaterials: carbon nanotubes, graphene
- Defects in Solids
- Interfaces and confined fluids: silica pores
2. Soft Condensed Matter:
- Polymers
- Biomembranes: lipids and cholesterol in aqueous ionic solution

Related activities:
Practical exercises on computer simulation

Specific objectives:
Sophisticated simulations developed with specific tools.
Analyze results of microscopic properties: structure (distribution functions, orientation and molecular bonds) and dynamics (diffusion, spectra).
Visualizing the system and generating animations.

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Qualification system

Theoretical questions: 20% of final grade,
Practices with computer: 40% of final grade,
Presentation of personal work (MD or MC project code) in class: 40% of final grade.
Final grade = 0.2*questions + 0.4*practices + 0.4*project
Students who fail a grade greater than or equal to 3 (and a maximum of two subjects) are eligible for re-evaluation, which
will consist of an examination on all contents of the topic. Practical exercises not re-evaluated.

Regulations for carrying out activities

Presentation of practical work in the classroom with computer equipment

Bibliography

Basic:

Frenkel, D.; Smit, B. Understanding molecular simulation. London: Academic Press, 2002. ISBN 0122673514.

Gould, H.; Tobochnik, J.; Christian, W. Introduction to Computer Simulation Methods: application to Physical Systems. 3rd. ed. Addison-Wesley, 2006. ISBN 0805377581.

Thijssen,J.M. Computational physics. 2nd. ed. Cambridge University Press, 2007. ISBN 9780521833462.

Others resources:

Computer material

Codis de simulació

Molecular Dynamics and Monte Carlo codes