Name: Introduction to computational physics - 34057

Type: core **Semester:** 2nd

ECTS: 5

Periodicity: annual

Departments involved: Department of Structure and Constituents of Matter (UB)

Coordinator: Eugeni Graugés Pous

Professors: Mª Teresa Castán Vidal, Eugeni Graugés Pous, José Mª Fernández Varea

Language: Catalan / Spanish / English

Prerequisite: Basic knowledge of programming and numerical algorithms. This subject cannot be inscrired if it has previously been studied in the Degree of Physics.

Aims:

To introduce the student in the use of computational tools for the solution of simple problems in physics. The focus is on the practical work. It is intended to educated the attendee in the nature of computational approximations to analitically non-solvable problems, their degree of validity and explore possible improvements to fit the requirements of the soluction.

Syllabus:

Theoretical aspects:

1-Introduction

2-Programming languages and graphic tools

3-Iterative methods for finding roots

4-Interpolation methods

5-Random number generators

5.1 Aplication to Brownian dynamics

6-Numerical intergrations

6.1 Simpson and Gauss integration

6.2 Introduction to Monte Carlo integration

7-Finite differences method

7.1 Application to mechanics of few bodies: Runge-Kutta

7.2 Many body dynamics: Molecular dynamics

8-Methods for partial derivative equations

8.1 Application to transport phenomena: wave equation, Fourier equation

8.2 Application to quantum mechanics: Schrödinger equation, central potentials and interaction of radiation with matter.

9- Application to problems in electromagnetism

Practical work:

1- Numerical study of Van der Waals equation

2- Simulation of a Stern-Gerlach experiment

3- Exercices in Numerical integration

4- Molecular dynamics of a Lennard-Jones gas

5- Equation for a rocket to the moon

6- Brownian motion

7- One dimensional heat transport

8- Atomic structure

9- Phase space

10- Electron transport.

Method:

The course is structured as a series of activities that last for 13 weeks. On the one hand there are two weeky theoretical lectures (1h+1h) were the physical concepts and numerical methods needed for the practical work are presented. Some exercises are distributed at the end of the lectures. On the other hand the practical work is done during two sessions (1h+2h) each week. During the sessions, students work individually in front of the computer but guided by the tutor. Practical works are finished by the students as home work. After every practice, the student has to prepare a short written report.

The student is also asked to do a final individual work by its own, but supervised. The work should be related to some of the methods developed during the course. This work is presented orally at the end of the season.

Activity	Type	Hours	ECTS
Theoretical lectures	Classroom with the professor	2x13=26	1
Few exercises	Homework	13	0.5
Practical exercises	Computer classroom, tutor guided	3x11=33	1.3
Report preparation	Homework	33	1.3
Final individual work	Homework	24	0.9
Total			5

Evaluation:

Evaluation is continuous and is based on exercices risen from the theoretical classes (10%) and the written weekly reports for each practical work (90%).

To pass the subject, the students must attend the practices at the Computation LAB. If the student attends the practices, the evaluation can be continuous or unique.

Bibliography:

"A first course in computational physics", P.L.Devries, John Wiley & sons (1994)

"An introduction to computer simulation", M.M.Woolfson and G.J.Pert, Oxford University Press (1991)

"Numerical recipes in FORTRAN: the art of scientific computing" W.H.Press et al. , Cambridge University Press (1992).

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