COURSE SYLLABUS

Academic Year: 2020/2021

Identification and characteristics of the course				
Code	401922	ECTS Credits		6
Course title (English)	Computational Statistical Physics			
Course title (Spanish)	Física Estadística Computacional			
Degree programs	Master on Simulation in Science and Engineering			
Faculty/School	Industrial Engineering School			
Semester	2	Course type (compulsory/optional)	Optional	
Module	Optional			
Subject matter	Simulation in Science			
Lecturer/s				
Name	Room	E-mail		Web page
Juan Jesús Ruiz Lorenzo	B.202	ruiz@unex.es	www.eweb.unex.es/eweb/fisteor/juan/	
Juan José Meléndez Martínez	A.007	melendez@unex.es	http://materiales.unex.es/miembros/personal/jj-melendez/Index.html	
Subject Area	Theoretical Physics & Condensed Matter Physics			
Department	Physics			
Coordinator (Only if there is more than one lecturer)	Juan José Meléndez Martínez			

Competencies (see table in https://goo.gl/BJxjVH)[1*]

Basic Competencies	Tick if needed	Generic Competencies	Tick if needed	Transverse Competencies	Tick if needed	Specific Competencies	Tick if needed	Optional Specific Competencies	Tick if needed
CB6	X	CG1	X	CT1	X	CE1		CEO1	X
CB7	X	CG2	X	CT2	X	CE2		CEO2	
CB8	X	CG3	X	CT3	X	CE3		CEO3	
CB9	X	CG4	X	CT4	X	CE4		CEO4	X
CB10	X	CG5	X	CT5	X	CE5		CEO5	
		CG6	X	CT6	X	CE6		CEO6	
		CG7	X	CT7	X	CE7		CEO7	X
				CT8	X	CE8		CEO8	X
				CT9				CEO9	X
				CT10					

[1] *The sections concerning competencies, course outline, teaching activities, teaching methodology, learning outcomes and assessment methods must conform to those included in the ANECA verified document of the degree program.

Contents

Course outline*

Monte Carlo numerical simulations in Statistical Physics. Metropolis and Heat Bath algorithms. Cluster methods. Methods for vectorial models. Molecular Dynamics simulations; hybrid Monte Carlo methods. Molecular Dynamics in several ensembles: Molecular Dynamics at constante temperatura and pressure.

Course contents

Title of unit 1: **Monte Carlo simulations** (10 hours)
Contents of unit 1:

- 1.1 Introduction of the Statistical Physics of magnetic models.
- 1.2 Static Monte Carlo methods.
- 1.3 Dynamic Monte Carlo methods.
- 1.4 Algorithms for the Ising model.
- 1.5 Algorithms for the Heisenberg model.
- 1.6 Clusters methods.
- 1.7 Applications.

Practical lessons: Simulation of the Ising model in one and two dimensions. Simulation of the three dimensional Ising model using a cluster algorithm. Simulation of the three dimensional Heiseneberg model using the Heat-Bath methods and using a cluster algorithm. (10 horas)

Title of unit 2: **Data Analysis** (4 hours)
Contents of unit 2:
2.1 Introduction.
2.2 Computation of the exponential and integrated autocorrelation times.
2.3 Error computation: Jack-Knife and Boostrap methods.
2.4 Spectral density method.
2.5 Applications.

Practical lessons: Computation of exponential and integrated autocorrelation times for different observables: scaling. Characterization of the phase transition in the Ising and Heisenberg models in three dimensions. (5 horas)

Title of unit 3: **Molecular Dynamics simulations** (14 hours)
Contents of unit 3:

- 3.1 Fundamentals of C language. Plotting, statistical methods, optimization libraries.
- 3.2 Fundamentals of Condensed Matter Physics and Statistical Physics regarding Molecular Dynamics.
- 3.3 Molecular Dynamics of hard particles: sorting algorithms and selection of number lists (quicksort, heapsort, mergesort and timsort).
- 3.4 Structural characterization: radial distribution function, order parameters, orientation ordering. Voronoi diagrams and symmetry breaking.
- 3.5 Dynamical characterization: Microscopic state, distribution function and its properties. Macroscopic state: mean fields and transpor properties (diffusivity, viscosity, thermal conductivity).

Practical lessons: Development of a general Molecular Dynamics algorithm (4 hours). Development of algorithms to compute transport coefficients (6 hours). Characterization of structural changes in crystalline solids. (5 hours).

Educational activities *

Student workload (hours per lesson)		Lectures	Practical sessions				Monitoring activity	Homework
Unit	**Total**	**L**	**HI**	**LAB**	**COM**	**SEM**	**SGT**	**PS**
1	40	10	0	0	10	0	0	20
2	29	4	0	0	5	0	0	20
3	49	14	0	0	15	0	0	20
Assessment 2**	32	2	0	0	0	0	0	30
TOTAL ECTS	150	30	0	0	30	0	0	90

L: Lectures (100 students)
HI: Hospital internships (7 students)
LAB: Lab sessions or field practice (15 students)
COM: Computer room or language laboratory practice (30 students)
SEM: Problem-solving classes, seminars or case studies (40 students)
SGT: Scheduled group tutorials (educational monitoring, ECTS type tutorials)
PS: Personal study, individual or group work and reading of bibliography

Note: This course belongs to the internationalization program PALEX_Intermedio. Consequently, 25% of the lectures (final exam excluded) will be given in English. This represents 7 hours.

Teaching Methodology*

Among the different methodologies described in the degree syllabus, the following ones will be used in the course:

Teaching methodologies	Tick as indicated
1. Lectures.	X
2. Workshops with suitable methodology	X
3. Problem solving in the class	X
4. Practical work in environments with specialized equipment (labs, computer rooms, fieldwork).	X
5. Technical visits to installations.	
6. Elaboration and analysis (by groups or individually) of memoirs, exercises, case studies, on the skills and contents (theoretical and practical) related to the course.	X
7. Exams, defense of assignments, etc., oral or written, individually or in groups.	X
8. Student study. Individual preparation and analysis of texts, cases, problems, etc.	X
9. Development of communication skills (oral, written, multimedia).	X
10. Out-of-class learning based on the link between academic education and professional or entrepreneurial experiences.	
11. Tutored and supervised learning in order to detect, by a student-tutor interaction, potential problems in the education process. This will also allow assessing the learning outcome out of class and programming activities such as the master thesis.	

The theoretical fundamentals of the course concepts will be presented in the **lectures**.
The basic tools for programming the algorithms will be explained in the **computer sessions**.

[2] **Insert as many rows as necessary. For instance, you can include one row for a partial exam and another for the final exam.

The **tutored projects** will consist in the solution by means of the course tools of more realistic and relevant problems than those considered in the computer sessions.

Learning outcomes *

To know and be able to implement numerical simulations in Statistical Physics for the study and resolution of particular scientific problems.

Assessment methods *

Assessment criteria

CE1. Command of the theoretical contents of the course.
This is related to the competencies CB6, CB7, CB8, CB10, CG1, CG4, CG5, CT1, CT4, CT7, CEO4, CE08, CE09.

CE2. Ability to apply the acquired theoretical knowledge to the solution of real problems.
This is related to the competencies CB6, CB7, CB8, CG2, CG3, CG4, CG5, CG6, CG7, CT1, CT2, CT4, CT5, CT6, CT7, CT8, CEO4, CEO8, CE09.

CE3. Command of the computational tools related to the course.
This is related to the competencies CG2, CG3, CG6, CG7, CT5, CT6, CEO4, CE07, CE09.

CE4. Ability to communicate knowledge with the appropriate technical language (oral or written) within the field of artificial intelligence.
This is related to the competencies CB8, CB9, CG4, CG5, CT3, CT4, CT5, CT7, CT8.

Assessment activities

Among the assessment activities described in the degree syllabus, the following ones will be used in the course (with the indicated weights):

	Range established in the degree memoir	Ordinary call	Extraordinary call	Global assessment (*)
1. Exams (Final and/or partial).	40%–70%(1) 0%–40%(2) 0%(3)	20 %	20 %	20 %
2. Resolution and delivery of activities (cases, problems, reports, projects, etc.), individually and/or in groups.	0%–40%(1) 40%–80%(2) 0%(3)	70 %	70 %	80 %
3. Attendance and achievement in classes, practices and other face-to-face activities.	0%–20%(1,2) 0%–20%(2) 0%(3)	10 %	10 %	---
4. Presentation and defense of projects and reports.	0%(1) 0%(2) 100%(3)			

(*) The student will communicate in the first three weeks of each semester to the instructor, in writing, the type of assessment chosen. The instructor will then inform the Degree Quality Commission. In the absence of communication, it will be understood that the student chooses continuous assessment. Once the type of assessment has been chosen, the student will not be able to change in the ordinary call for that semester and will abide by the evaluation regulations for the extraordinary call.

(1) Courses of the subject *Mathematical foundations* (*Numerical methods, Differential equations*, and *Statistical treatment of data*).

(2) Rest of courses.

(3) Master thesis.

Description of the assessment activities

The student will develop program codes in practical classes whose results will be presented in a report. The evaluation of this report will make 30% of the grade of the course (Recoverable 30%). The student will develop one or more program codes, depending on their length and difficulty, where one or more practical cases will be solved using the techniques studied in the course. A report will be presented with the results obtained. This will represent 40% of the grade for the course (Recoverable 40%).
There will be a theoretical-practical exam at the end of the course, which will represent 20% of the grade for the course (Recoverable 20%).

The global assessment will take place the same day assigned to the final exam of each call by the School of Industrial Engineering. It will consist of the following tests:

- A theoretical-practical exam. This will make 20% of the grade.
- The student must present a report with the results obtained in the resolution of several practical cases similar to those carried out in the practical classes. It will represent 30% of the grade.
- The student must also present a report with the results obtained in solving one or more (depending on their difficulty and length) practical cases using the techniques studied during the course. These practical cases will be similar to those proposed to the rest of students throughout the course. It will represent 50% of the grade.

The practical cases will be assigned to the student when he/she expresses his/her decision to opt for the global assessment.

Note: This subject belongs to the PALEx-intermedio program. Therefore, the students will be able to present the different projects and practices, as well as the exam, in English or in Spanish.

Bibliography (basic and complementary)

Basic

- D. P. Landau, K. Binder, A Guide to Monte Carlo Simulations in Statistical Physics (Cambridge, New York, 2000).
- D. E. Knuth, Seminumerical Algorithms, Vol. 2 from "The Art of Computer Programming" (Addison-Wesley, New York 1998).
- A. D. Sokal in Functional Integrations: Basics and Applications (1996 Cargese Summer School). C. DeWitt-Morette, P. Cartier y A. Folacci, eds. (Plenum, New York, 1997).
- W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery, Numerical Recipes Third Edition, (Cambridge University Press, 2007).
- D. C. Rapaport, The Art of Molecular Dynamics Simulation, (Cambridge University Press, 2007).
- D. E. Knuth, Sorting and Searching, Vol. 3, 2nd edition, of "The Art of Computer Programming" (Addison-Wesley, New York 1998).
- T. Schwager, T. Pöschel, Computational Granular Dynamics : Models and Algorithms (Springer 2005).
- M. Griebel, S. Knapek, G. Zumbusch, *Numerical simulation in Molecular Dynamics.* Springer-Verlag, 2007.

Complementary

- D. J. Amit and V. Martín-Mayor*, Field Theory, the Renormalization Group and Critical Phenomena* (World Scientific, Singapur, 2005).

- P. M. Chaikin, T. C. Lubensky, *Principles of condensed matter physics*, (Cambridge University Press, 2006).

Other resources and complementary materials

See
www.unex.es/eweb/fisteor/juan/
and
http://materiales.unex.es/miembros/personal/jj-melendez/Index.html