Universitat de les Illes Balears

Teaching guide

Academic year	2012-13
Subject	10094 - Stochastic Simulation Methods
Group	Group 1, 1S
Teaching guide	B
Language	English

Subject identification

Subject	10094 - Stochastic Simulation Methods
Credits	1.2 in-class (30 hours) 3.8 distance (95 hours) 5 totals (125 hours).
Group	Group 1, 1S
Teaching period	1st semester
Teaching language	English

Lecturers

Lecturers	Timetable for student attention					
	Starting time	Finishing time	Day	Start date	Finish date	Office
Pere Colet Rafecas	There are no defined sessions					
Raúl Toral Garcés rtg803@uib.es	There are no defined sessions					

Degrees where the subject is taught

Degree	Character	Academic year	Studies
Master's Degree in Physics	Optional		Postgraduate degree
Master's Degree in Physics of Complex Systems	Optional		Postgraduate degree

Contextualisation

This is one of the compulsory courses of the Structural Module of the master of Physics of Complex Systems. It also belongs to the Master in Physics whithin the "Physics and Computation" basic module.

Requirements

At the subject advances, concepts needed in this course can be acquired in other courses of the Structural Module (Stochastic Processes, Cooperative and Critical Phenomena).

Date of publication: 04/07/2012

Recommendable

It is recommended that the student has a basic knowledge on probability theory and statistics, basic numerical integration (Simpson-type rules), numerical solution of differential equations (Euler and Runge-Kutta algorithms), and statistical physics (canonical distribution).

Skills

This course develops both specific and generic competences.

Specific

1. E2: Development and optimal application of numerical algorithms for the simulation of complex systems.
2. E6: To understand and to model processes subject to fluctuations.

Generic

1. TG2: To acquire the capability to develop a research work in full: bibliographic search, subject development and ellaboration of conclusions.
2. TG3: To be able to write in a clear and precise way the different steps of the research work and to present the results to an expert audience.
3. TG6: To develop the capability to understand and to apply knowledge of high performance computation and advanced numerical methods to the field of complex systems.

Content

Theme content

1. Concepts of probability and statistics.

   Random variables. Statistical description of data. Law of large numbers. Numerical calculation of basic estimators: average, variance, correlations, etc.

2. Monte Carlo integration.

   One dimensional problems: hit and miss method; sampling methods; variance reduction techniques; biased and unbiased estimators.

   Random number generation: congruential and feedback shift register generators. Non-uniform random number generation. Gaussian distribution. Discrete distributions. Rejection methods.

   Many variables problems: Metropolis et al. and Thermal Bath algorithms. Thermalization. Statistical errors.

3. Stochastic differential equations

   Basic algorithms for the numerical integration of stochastic differential equations (Euler-Maruyama, Milshtein and Heun). Colored noise.

4. Collective algorithms

   Swendsen and Wolff algorithms for Ising and Potts models.

Extrapolation techniques (Ferrenberg-Swendsen and multicanonical algorithms).

Molecular Dyamics and Hybrid Monte Carlo. Simplectic algorithms.

5. Applications to phase transitions
   Critical phenomena. Finite-size scaling analysis. Monte Carlo renormalization group.
6. Numerical simulation of master equations
   Rate equations. Gillespie algorithm.
7. Data ordering
   Quicksort. Ranking and indexing
8. Numerical integration of partial differential equations
   Finite difference and pseudospectral methods. Extensions to stochastic partial differential equations.

Teaching methodology

In-class work activities

Modality	Name	Typ.Gr.	Description
Theory classes	Theoretical lectures	Large group (G)	Explanation of theoretical concepts by the professor.
Practical classes	Hands-on sessions	Large group (G)	Introduction to the use of the computational infrastructure and basic software (compilers and libraries)
Assessment	Oral presentation	Large group (G)	Oral presentation to the whole class of an assigned problem

Distance education work activities

Modality	Name	Description
Individual self-study	Assignments	The student has to solve assigned exercises and present the solutions in written form.
Individual self-study	Preparation of the oral presentation	The student must solve the problem and organize a presentation
Individual self-study	Understanding of theoretical concepts	Mastering of the theoretical techniques explained in the lectures

Riscs especifics i mesures de protecció

Les activitats d'aprenentatge d'aquesta assignatura no comporten riscs específics per a la seguretat i salut de l'alumnat i, per tant, no cal adoptar mesures de protecció especials.

Workload estimate

Modality	Name	Hours	ECTS	%
In-class work activities		**30**	**1.2**	**24**
Theory classes	Theoretical lectures	25	1	20
Practical classes	Hands-on sessions	4.5	0.18	3.6
Assessment	Oral presentation	0.5	0.02	0.4
Distance education work activities		**95**	**3.8**	**76**
Individual self-study	Assignments	40	1.6	32
Individual self-study	Preparation of the oral presentation	25	1	20
Individual self-study	Understanding of theoretical concepts	30	1.2	24
	Total	**125**	**5**	**100**

At the beginning of the semester a schedule of the subject will be made available to students through the UIBdigital platform. The schedule shall at least include the dates when the continuing assessment tests will be conducted and the hand-in dates for the assignments. In addition, the lecturer shall inform students as to whether the subject work plan will be carried out through the schedule or through another way included in the Campus Extens platform.

Student learning assessment

Oral presentation

Modality	Assessment
Technique	Papers and projects **(Non-recoverable)**
Description	Oral presentation to the whole class of an assigned problem
Assessment criteria	Accuracy and quality of the presented work as well as the clarity in the oral exposition

Percentage of final qualification: 50% following path A

Assignments

Modality	Individual self-study
Technique	Papers and projects **(Non-recoverable)**
Description	The student has to solve assigned exercises and present the solutions in written form.
Assessment criteria	Accuracy and quality of the presented work

Percentage of final qualification: 50% following path A

Resources, bibliography and additional documentation

Basic bibliography

- M. Kalosand P. Whitlock, Monte-Carlo Methods, vol. 1: Basics (1986).
- P.E Kloeden and E. Platen, Numerical Solution of Stochastic Differential Equations, Springer (1992).
-A. Papoulis, Probability, Random Variables and Stochastic Processes. 4th edition McGraw-Hill (1984).
-M. San Miguel and R. Toral, Stochastic effects in physical systems, Instabilities and Nonequilibrium Structures VI, eds. E. Tirapegui, J. Martínez and R. Tiemann, Kluwer Academic Publishers 35-130 (2000).
-W.H. Press et al. Numerical Recipes, 3rd edition, Cambridge Univ. Press (2007).

Complementary bibliography

- M.P Allen and D.J. Tildesley, Computer Simulation of Liquids, Clarendon Press (1987)
- G.R. Grimmett and D.R. Stirzaker, Probability and Random Processes, Oxford Science Pub. (1985).
- D. Heermann, Computer Simulation Methods in Theoretical Physics. Springer Verlag (1986).
- N.G. van Kampen, Stochastic Processes in Physics and Chemistry, 3rd. edition, North-Holland (2007).
- D.E. Knuth, The Art of Scientific Programming. Vol.1: Semi-numerical Algorithms, Addison-Wesley (1981).
- J. Marro and P.L Garrido, eds. Third Granada Lectures in Computational Physics. Springer (1995).

Other resources

The lecture notes, presentations and other additional material will be available at the master's webpage.