



Academic year	2016-17
Subject	11306 - Stochastic Simulation Methods
Group	Group 1, 1S
Teaching guide	B
Language	English

Subject identification

Subject	11306 - Stochastic Simulation Methods
Credits	1.44 de presencials (36 hours) 4.56 de no presencials (114 hours) 6 de totals (150 hours).
Group	Group 1, 1S (Campus Extens)
Teaching period	First semester
Teaching language	English

Professors

Lecturers	Horari d'atenció als alumnes					
	Starting time	Finishing time	Day	Start date	Finish date	Office
Pere Colet Rafecas	09:00	10:00	Tuesday	19/09/2016	31/01/2017	210
Raúl Toral Garcés rtg803@uib.es	You need to book a date with the professor in order to attend a tutorial.					

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 Advanced Physics and Applied Mathematics master.

Requirements

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

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

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



Generic

- * TG2: To acquire the capability to develop a research work in full: bibliographic search, subject development and elaboration of conclusions..
- * 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..
- * 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..

Basic

- * You may consult the basic competencies students will have to achieve by the end of the Master's degree at the following address: http://estudis.uib.cat/master/comp_basiques/

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 Dynamics and Hybrid Monte Carlo. Symplectic 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. Numerical integration of partial differential equations
Finite difference and pseudospectral methods. Extensions to stochastic partial differential equations.

Teaching methodology

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In-class work activities

Workload

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.

In-class work activities

Modality	Name	Typ. Grp.	Description	Hours
Theory classes	Lectures	Large group (G)	Explanation of theoretical concepts by the professor. Introduction to the use of the computational infrastructure and basic software (compilers and libraries). Solution by the professors of selected examples and exercises.	27
Practical classes	Public discussion of exercises	Large group (G)	Oral presentation by the students of assigned exercises.	9

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Distance education work activities

Modality	Name	Description	Hours
Individual self-study	Exercises assignments	The student has to solve assigned exercises and write down the solutions in a report.	45
Individual self-study	Solving an assigned long project	The student must solve the project and organize a presentation	24
Individual self-study	Understanding of theoretical concepts	Mastering of the theoretical techniques explained in the lectures	45

Specific risks and protective measures

The learning activities of this course do not entail specific health or safety risks for the students and therefore no special protective measures are needed.

Student learning assessment

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Public discussion of exercises

Modality	Practical classes
Technique	Papers and projects (non-retrievable)
Description	Oral presentation by the students of assigned exercises.
Assessment criteria	Oral presentation of assigned exercises.

The evaluation is based on the accuracy and quality of the presented work as well as the clarity in the oral exposition.

Final grade percentage: 30%

Exercises assignments

Modality	Individual self-study
Technique	Papers and projects (retrievable)
Description	The student has to solve assigned exercises and write down the solutions in a report.
Assessment criteria	The student has to solve assigned exercises and present the solutions in written form.

The evaluation is based on the accuracy and quality of the presented work

Final grade percentage: 30%

Solving an assigned long project

Modality	Individual self-study
Technique	Papers and projects (retrievable)
Description	The student must solve the project and organize a presentation
Assessment criteria	The student must solve an assigned long project.

The evaluation is based on the accuracy and quality of the presented work as well as the clarity in the oral exposition.

Final grade percentage: 40%

Resources, bibliography and additional documentation

Basic bibliography

- 1 - R. Toral, P. Colet, Stochastic Numerical Methods, Wiley-VCH (2014)
- 2 - M. Kalos and P. Whitlock, Monte-Carlo Methods, vol. 1: Basics (1986)
- 3 - A. Papoulis, Probability, Random Variables and Stochastic Processes. 4th edition McGraw-Hill (1984).
- 4 - 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).
- 5 - W.H. Press et al. Numerical Recipes, 3rd edition, Cambridge Univ. Press (2007), <http://www.nr.com/>

Complementary bibliography

- 1 - M.P Allen and D.J. Tildesley, Computer Simulation of Liquids, Clarendon Press (1987)
- 2 - G.R. Grimmett and D.R. Stirzaker, Probability and Random Processes, Oxford Science Pub. (1985).
- 3 - P.E Kloeden and E. Platen, Numerical Solution of Stochastic Differential Equations, Springer (1992).
- 4 - D. Heermann, Computer Simulation Methods in Theoretical Physics. Springer Verlag (1986).
- 5 - N.G. van Kampen, Stochastic Processes in Physics and Chemistry, 3rd. edition, North-Holland (2007).



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- 6 - R. Toral, Computational field theory and pattern formation, III Granada lectures in Computational Physics, P.L. Garrido, J. Marro, eds. Springer Lecture Notes in Physics, vol. 448, 3-65 (1995).
- 7 - M.E.J. Newman and G.T. Barkema, Monte Carlo Methods in Statistical Physics, Clarendon Press (1999).

Other resources

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

