

Group Teaching guide Language 2014-15 11306 - Stochastic Simulation Methods Group 1, 1S A English

Subject identification

| Subject Credits | 11306 - Stochastic Simulation Methods1.44 de presencials (36 hours) 4.56 de no presencials (114 hours) 6 de totals (150 hours). |
|--------------------|--|
| Group | Group 1, 1S (Campus Extens) |
| Teaching period | 1st semester |
| Teaching language | English |

Professors

| Lecturers | | Horari d'atenció als alumnes | | | | |
|------------------------------------|-----------------------|------------------------------|------------|-------------|--------------------|--|
| | Starting time Finishi | ng time Day | Start date | Finish date | Office | |
| Pere Colet Rafecas | 09:30h 10: | 30h Thursday | 25/09/2014 | 18/12/2014 | IFISC-210 | |
| Raúl Toral Garcés rtg803@uib.es | 11:00h 12: | 00h Monday | 01/09/2014 | 15/07/2015 | 212 Edi. Instituts | |

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).

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..



Group Teaching guide Language 2014-15 11306 - Stochastic Simulation Methods Group 1, 1S A English

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: <u>http://estudis.uib.cat/master/comp_basiques/</u>

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.
- Numerical integration of partial differential equations
 Finite difference and pseudospectral methods. Extensions to stochastic partial differential
 equations.

Teaching methodology

2 / 5

Date of publication: 30/07/2014



Group Teaching guide Language 2014-15 11306 - Stochastic Simulation Methods Group 1, 1S A English

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 | Theoretical lectures | Large group (G) | Explanation of theoretical concepts by the professor. | 30 |
| Practical classes | Hands-on sesscions | Large group (G) | Introduction to the use of the computational infrastructure and basic software (compilers and libraries) | e 5.5 |
| Assessment | Public discussion of an exercise | Large group (G) | Oral presentation to the whole class of an assigned problem | 0.5 |

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.

Distance education work activities

| Modality | Name | Description | Hours |
|---------------------------|--------------------------------------|--|-------|
| Individual self- study | Assignements | The student has to solve assigned exercises and present the solutions in written form. | 48 |
| Individual self- study | Solving an assigned long problem | The student must solve the problem and organize a presentation | 36 |
| Individual self- study | Understading of theoretical concepts | Mastering of the theoretical techniques explained in the lectures | 30 |

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

4

Date of publication: 30/07/2014

3/5



Group Teaching guide Language 2014-15 11306 - Stochastic Simulation Methods Group 1, 1S A English

Public discussion of an exercise

| Modality | Assessment |
|---------------------|---|
| Technique | Papers and projects (non-retrievable) |
| Description | Oral presentation to the whole class of an assigned problem |
| Assessment criteria | Oral presentation to the whole class of an assigned problem. |
| | The avaluation is based on the accuracy and quality of the presented work as well as the clarity in the oral exposition |

Final grade percentage: 10%

Assignements

| Modality | Individual self-study |
|---------------------|--|
| Technique | Papers and projects (non-retrievable) |
| Description | The student has to solve assigned exercises and present the solutions in written form. |
| Assessment criteria | The student has to solve assigned exercises and present the solutions in written form. |
| | The avaluation is based on the accuracy and quality of the presented work |

Final grade percentage: 40%

Solving an assigned long problem

| Modality | Individual self-study |
|---------------------|---|
| Technique | Papers and projects (non-retrievable) |
| Description | The student must solve the problem and organize a presentation |
| Assessment criteria | The student must solve an assigned long problem. |
| | The avaluation is based on the accuracy and quality of the presented work |

Final grade percentage: 50%

Resources, bibliography and additional documentation

Basic bibliography

4

- 1 R. Toral, P. Colet, Stochastic Numerical Methods, Wiley-VCH (2014)
- 2 M. Kalosand 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
- 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)

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).

Date of publication: 30/07/2014



Academic year Subject Group Teaching guide Language 2014-15 11306 - Stochastic Simulation Methods Group 1, 1S A English

6 - 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.

5/5

4