Universitat de les Illes Balears

# Syllabus

## Subject

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|---|---|
| **Subject / Group** | 11306 - Stochastic Simulation Methods / 1 |
| **Degree** | Master's Degree in Physics of Complex Systems<br>Master's Degree in Advanced Physics and Applied Mathematics |
| **Credits** | 6 |
| **Period** | First semester |
| **Language of instruction** | English |

### Professors

| Lecturers | Office hours for students | | | | | |
|---|---|---|---|---|---|---|
| | **Starting time** | **Finishing time** | **Day** | **Start date** | **End date** | **Office / Building** |
| Raúl Toral Garcés *(Responsible)* rtg803@uib.es | 09:30 | 11:00 | Monday | 03/09/2018 | 31/07/2019 | IFISC, despatx 212 |
| Pere Colet Rafecas | 09:30 | 11:00 | Monday | 01/09/2018 | 31/07/2019 | Despatx 210, Edifici Instituts Universitaris de Recerca. IFISC |

## Context

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.

In all areas of science, there are situations in which the description of the system under study requires the consideration of probability theory. There are many examples of this intrinsic randomness, from the production of complex molecules inside the cell, to the stock market dynamics and many others in different disciplines. That does not mean that a mathematical description of the system is not possible, but that an element of randomness has to be introduced in the theory from the very beginning. Despite the general belief that physical theories are always deterministic and predictive, the truth is that Statistical and Nonlinear Physics is a well established discipline that incorporates randomness in the description of a physical system at a very fundamental level. Since the pioneering works of Ludwig Boltzmann, Albert Einstein, Paul Langevin and many others, it has become clear that macroscopic laws can emerge from a probabilistic framework that takes into account the unavoidable elements of randomness, arising from our lack of knowledge of the exact microscopic description, including all forces between particles and their initial conditions. After more than a century and a half of expertise, we have learnt that beyond the predictions of the average values of the outcome of an experiment, the fluctuations around the mean values and the probability distribution of the possible outcomes bear much information about the microscopic mechanisms that underlie the process under scrutiny. In these cases, a deterministic analysis of the occurring processes may be inadequate or lacking of the relevant information sought. In this context, Master and Langevin equations are extensively used mathematical tools to deal with such situations. In this course, we present the main numerical techniques for Monte Carlo



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integration, Master and Langevin equations with emphasis on the applications to Statistical and Non Linear Physics problems.

## Requirements

As the subject advances, some concepts needed in this course will be acquired in other courses of the Structural Module (mainly *Stochastic Processes* and *Cooperative and Critical Phenomena*). The course teaches algorithms but does not provide teaching on programing lenguages. While the proficiency in scientific programing (preferably fortran, C++, python) is not a formal requirement at the beginning of the course, the student must adquire this proficiency by the time assignments are given.

### Recommended

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

### 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

### Range of topics

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.

6. Numerical simulation of master equations.
   Rate equations. The first reaction method and the residence time (Gillespie) algorithm.

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

## Teaching methodology

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 (1.44 credits, 36 hours)

| Modality | Name | Typ. Grp. | Description | Hours |
|---|---|---|---|---|
| Theory classes | Lectures | Large group (G) | Explanation of theoretical concepts by the professor and exposition by the professor and discussion with the students of selected case studies. | 33 |
| Practical classes | Oral presentation of an assigned long project | Large group (G) | The student must present orally the results of the assigned long project. | 3 |

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### Distance education tasks (4.56 credits, 114 hours)

| Modality | Name | Description | Hours |
|---|---|---|---|
| Individual self-study | Exercises assignements | The student has to solve assigned exercises and write down the solutions in a report. | 35 |
| Individual self-study | Understading of theoretical concepts | Mastering of the theoretical techniques explained in the lectures | 34 |
| Individual self-study | Solving an assigned long project | The student must solve the project and organize an oral presentation and a written report. | 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

### Frau en elements d'avaluació

In accordance with article 33 of Academic regulations, "regardless of the disciplinary procedure that may be followed against the offending student, the demonstrably fraudulent performance of any of the evaluation elements included in the teaching guides of the subjects will lead, at the discretion of the teacher, a undervaluation in the qualification that may involve the qualification of "suspense 0" in the annual evaluation of the subject".

#### Oral presentation of an assigned long project

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|---|---|
| Modality | Practical classes |
| Technique | Papers and projects **(retrievable)** |
| Description | The student must present orally the results of the assigned long project. |
| Assessment criteria | Quality and clarity of the oral presentation and the answers to the questions by the professor and the other students. |

Final grade percentage: 30%with a minimum grade of 4

### Exercises assignements

| | |
|---|---|
| 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.<br><br>The evaluation is based on the accuracy and quality of the presented work |

Final grade percentage: 40%with a minimum grade of 4

### Solving an assigned long project

| | |
|---|---|
| Modality | Individual self-study |
| Technique | Papers and projects **(retrievable)** |
| Description | The student must solve the project and organize an oral presentation and a written report. |
| Assessment criteria | The student must solve an assigned long project, write a report and prepare an oral presentation.<br><br>The avaluation is based on the accuracy and quality of the work as well as the submitted report. |

Final grade percentage: 30%with a minimum grade of 4

## Resources, bibliography and additional documentation

Besides the slides and notes of the course that will be made available to students through UIB's Aula Digital, we recommend the following bibliography:

### 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).
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 UIB's Aula Digital