

Academic Year/course: 2022/23

## 68459 - Modelling of Biological Systems

## Syllabus Information

Academic Year: 2022/23

**Subject:** 68459 - Modelling of Biological Systems **Faculty / School:** 100 - Facultad de Ciencias

Degree: 626 - Máster Universitario en Biofísica y Biotecnología Cuantitativa/Biophysics and Quantitative Biotechnology

**ECTS**: 6.0 **Year**: 01

**Semester:** Second semester **Subject Type:** Optional

Module:

## 1. General information

#### 1.1. Aims of the course

This course explains in detail the main theoretical and computational tools required to model biological systems. From this point of view it enlarges and deepens the description that the students received from "Systems and Synthetic Biology" and "Simulations of Biomolecules". It has been designed in order:

- To present the main theoretical/computational tools required to interpret the experimental data obtained during the study of biological systems.
- To present the dynamical and thermodynamic description of biological systems, focusing on the most relevant theories and equations.
- To introduce the most frequent models for the different scales and processes in the description of biological systems and the computational tools that allow to relate them with the experimental data.
- To provide the student with an educated criterion to choose the most suitable method to be used in each particular situation, and to be able to evaluate and criticize the results from an experiment or obtained from the Literature.

These objectives are relevant for Objective 3 "Good Health and Well-Being" of the Sustainable Development Goals of the UN 2030 Agenda (https://www.un.org/sustainabledevelopment/), so that the learning outcomes will provide students with skills to help reaching those goals.

## 1.2. Context and importance of this course in the degree

Together with the course "Biostatistics and Bioinformatics" and "Big Data in Biology", this course covers the most theoretical aspects of the program, and it is designed to provide the students interested in the theoretical and computational aspects of Biotechnology with the background required to begin a research career.

#### 1.3. Recommendations to take this course

It is convenient for the students to have a basic mathematical background in algebra and differential equations, and must have followed the obligatory courses of the first semester on "Simulations of Biomolecules" and "Systems and Synthetic Biology".

# 2. Learning goals

#### 2.1. Competences

#### **Basic and General**

- CG 01 To arrange, critically analyze, understand and synthesize information
- CG 02 To obtain information from different types of sources and evaluate their reliability
- CG 03 To learn efficiently through autonomous study and acquire a significant level of independence
- CG 04 To implement the acquired knowledge and solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to the study area
- CG 05 To formulate, analyze, evaluate and compare new or alternative solutions for different problems
- CG 06 To be able to work in multidisciplinary and international teams.
- CG 07 To be able to develop capacity for criticism and self-criticism.
- CB 6 To possess knowledge providing the grounds for the original development and implementation of ideas, often in a research context
- CB 7 The students know how to apply the acquired knowledge and their problem-solving ability to new, or little known, environments, within broader (or multidisciplinary) contexts related to their area of study
- CB 8 The students are able to integrate knowledge and face the complexity of providing opinions based on information that, being incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and opinions.
- CB 9 The students know how to communicate their conclusions and the latest knowledge and the fundamental tenets on which they are grounded to specialized and non-specialized audiences, in a clear and unambiguous way
- CB 10 The students have the learning skills that allow them to continue studying, largely self-directed or autonomous.

#### Transversal:

- CT 01 To properly manage both the available resources and time for solving a problem or developing a project
- CT~03 To transmit information orally, in written form or graphically, using the appropriate presentation tools and respecting the imposed time or space constraints.
- CT04 To communicate fluently in English (understanding scientific texts, writing reports, talks, colloquiums, etc.).

#### **Specific**

CE11 – To build and characterize theoretical models of a biological system, of different complexity, from experimental data, also assessing their scope and relevance to understand the system under study

CE12 – To develop simulations for the study of the dynamic, structural, and functional properties of the theoretical models describing a biological system (biomolecules, biological networks, etc.), using the most appropriate simulation algorithms for both the analysis and the interpretation of the results

## 2.2. Learning goals

At a general level, the main goal of the course is to provide the student with the ability to manage theoretical models and computational methods to describe a biological system. At the end of the course, he/she will be able to design a simulation of a biological system with the most adequate tools for each case. In more details, specific learning goals are:

- To know the theoretical / computational tools essential to rationalize the experimental data obtained in the study of biological systems.
- To know the fundamental aspects of both the dynamical and thermodynamical description of biological systems, the relevant theories and related equations.
- To know the most used models for the description of different scales and biological processes, and the simulation techniques that allow to relate the models with the experimental outcomes.
- To know how to select the most appropriate method for each particular case as well as critically
  evaluate the results obtained or found in the scientific literature.

#### 2.3. Importance of learning goals

Mastering theoretical and simulation techniques is a basic skill which is essential for a future career as a researcher within this field.

# 3. Assessment (1st and 2nd call)

### 3.1. Assessment tasks (description of tasks, marking system and assessment criteria)

- 1: (65% of the final grade). Continuous evaluation of the student's progress by direct interaction in the classroom, rewarding active participation during the lectures, with special care to the reports related to the practice sessions.
- 2: (10% of the final grade). Seminar on papers related to the topics studied.
- 3: (25% of the final grade) Written exam.

# 4. Methodology, learning tasks, syllabus and resources

#### 4.1. Methodological overview

The learning process designed for this course is based on a combination of lectures, exercises and practice sessions in the computer laboratory. The virtual platform Moodle will be used to distribute lecture notes, as well as to propose exercises and tests.

Students are expected to participate actively throughout the semester. We will promote the debate and the active participation of the students throughout all the activities

Students are guided into the preparation of a short seminar in order to train their organization and presentation skills.

### 4.2. Learning tasks

The course includes the following learning tasks:

- Lectures. The lecturer provides theorems and examples, organized according to the syllabus of the course.
- Practice sessions. Students can apply and consolidate the theoretical understanding by means of relevant examples and problems.
- Computer programming and simulations. They extend the scope of the classroom exercises to the cases where computations become too heavy.
- Assignments for the students interested in deepening their understanding in specific topics. Course material: Notes written by the teachers will be available on the course's Moodle page.

#### 4.3. Syllabus

The course will address the following topics:

- 1. Statistical mechanics models I: canonical and microcanonical ensembles.
- 2. Statistical mechanics models II: Coarse graining and force fields.
- 3. Statistical mechanics models III: Models of biopolymers.
- 4. Statistical mechanics models IV: Cooperativity and the Helix-Coil transition.
- 5. Statistical mechanics models V: DNA and Protein Models.
- 6. Stochastic models I: Brownian motion and diffusion.
- 7. Stochastic models II: Langevin and Fokker-Planck equations.
- 8. Stochastic models III: Chemical master equation and Gillespie algorithm.
- 9. Stochastic models IV: Kramers theory.
- 10. Simulation techniques: Monte Carlo methods and applications.
- 11. Introduction to Epidemics: Models and Methods in Networks and applications

#### 4.4. Course planning and calendar

The course takes place during the second semester of the academic year.

Lectures will be held in accordance with the official calendar, available at <a href="https://ciencias.unizar.es/calendario-y-horarios">https://ciencias.unizar.es/calendario-y-horarios</a>. Possible variations will be communicated through the Moodle page.

Homework and other assessment tests will be proposed to the students throughout the semester.

Examinations: There are two exam calls available; the student should refer to the official calendar (see link above) for more details.

# 4.5. Bibliography and recommended resources

http://psfunizar10.unizar.es/br13/egAsignaturas.php?codigo=68459