230481 - COMBIO - Computational Biophysics

Coordinating unit: 230 - ETSETB - Barcelona School of Telecommunications Engineering
Teaching unit: 748 - FIS - Department of Physics
Academic year: 2019
Degree: BACHELOR'S DEGREE IN ENGINEERING PHYSICS (Syllabus 2011). (Teaching unit Optional)
ECTS credits: 6  
Teaching languages: English

Teaching staff

Coordinator: Alvarez Lacalle, Enrique
Others: Pons Rivero, Antonio Javier
         Pastor Satorras, Romualdo
         Alonso Muñoz, Sergio

Opening hours

Timetable: Students will be informed using atenea's webpage

Prior skills

- Basic knowledge of the human body obtained in ESO and Biophysics1.
- Knowledge of matlab or any other programming language (seen in MNC1)
- Knowledge of the main step/multistep algorithm to resolve ordinary differential equations, specially Runge-Kutta methods. (seen in MNC2)
- Knowledge and familiarity with the main concepts of ordinary differential equations and partial differential equations. (seen in MM2)
- Knowledge and familiarity with the basic concepts of bacteria, cell and the central dogma of biology (seen in BIOF2)
- Familiarity with the concepts of analytical mechanics related with phase space and dynamical attractors. (seen in MECF)

Requirements

Numerical and Computational Methods 2
Mecànica
Mètodes matemàtiques 2
Biophysics 2

Degree competences to which the subject contributes

Specific:

INF1. Understanding and mastery of computer programming, use of operative systems and computational tools (scientific software). Skills to implement numerical algorithms in languages of low (C, F90) and high (Matlab) level.

BIOC1. Ability to describe in general the structure of living things, from cellular to systemic level. Ability to analyze the constraints imposed by the physics laws to the development of biological systems, and the biological solutions to engineering problems.

BIOC2. Ability to analyze biological systems as complex systems.

INF2. Ability to solve problems in physics and engineering using fundamental numerical methods: experimental data processing, interpolation, roots of nonlinear equations, numerical linear algebra and optimization, quadrature and integration of differential equations, properly weighting their different aspects (accuracy, stability and efficiency or cost).

General:
Learning objectives of the subject

Once the student has finished the course he/she must be able to:

- Describe the four main methods of addressing spatio-temporal dynamics in extended systems used in physics: Compartmental models, iterative models, spatio-temporal models and network methods. This includes discerning which one is optimal for addressing the problem.

- Implement a random number generator in any given numerical simulation and know the Gillespie algorithm to code stochastic variables in time propagators. Implement extended nonlinear simulations with diffusion processes and different boundary conditions. Understand the concept of biological network, how to implement it numerically on a computer and how to obtain useful topological information of it. Learn how to implement realistic dynamical processes on top of networks.

- Define the basic dynamical interaction in a typical metabolic process and the kinetic reaction and network theory used to describe it. It must also be able to code a typical oscillatory genetic network and a typical signaling process. It must be able to describe briefly the general gene-protein network structure of the cell. It must be able to analyze the possible stochastic elements in a given biological system and implement it dynamics.
- Make linear stability analysis of pattern forming systems. Be able to solve linear and nonlinear initial value and boundary value problems using different numerical implementations analyzing its stability and accuracy. Understanding the dynamical features of reaction-diffusion-advection systems and to give different examples of pattern forming systems in Biology.

- Understand simple models of population dynamics and its relation to ecology, learning the different factors that can affect the growth and development of a population: spatio-temporal effects, effects of generational delays. At the same time, learn how to control possible chaotic effects in non-linear ecological models.

- Define the basic aspects of epidemiology and the relevant models that display the main features of realistic diseases. Understand the effects of a complex pattern of physical contacts in the spread of a biological disease.

Regarding the seminar series, students must be able to summarize any seminar presentation and be able to explain briefly three areas where biophysics approaches are presently top-edge.

Finally, students must perform a project where they develop a code to show expertise in one particular biophysics problem. At the end of this project, students must be able to show that they can understand the physiology or structure of a given biophysical problem in order to properly simulate it. They must be able to structure a code and clarify its different subroutines checking that the code works correctly and, if possible, perform simulations to draw conclusions about the problem or about future improvements of the code.

### Study load

<table>
<thead>
<tr>
<th>Total learning time: 150h</th>
<th>Hours large group:</th>
<th>65h</th>
<th>43.33%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Self study:</td>
<td>85h</td>
<td></td>
<td>56.67%</td>
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</tbody>
</table>
### Content

#### Introduction

**Learning time:** 45h
- Theory classes: 5h
- Self study: 40h

**Description:**
- System biology. Introduction and general approach.

- Introduction to python language: basic commands.

- Basic data processing in python.
  Managing of data sets to obtain relevant statistical descriptions. Reading and writing numerical data. Analysis, linear and non-linear regression of empirical data. Efficient graphical representation.

**Related activities:**
- Presentación AV1

#### Non-extended dynamical systems. Genetic networks.

**Learning time:** 36h
- Theory classes: 14h
- Practical classes: 6h
- Self study: 16h

**Description:**
- Introduction to ODE’s. Fixed points and nullclines.
  High order differential equations and ODE’s. Fixed points in one-dimensional systems. Generalization. Oscillation and periodicity in two-dimensional system. Nullclines in two-dimensional systems.

- Slaving and freezing conditions. Applications to cell reactions.
  Simulation of different time scales. Long time scales and freezing variables. Fast time scales and slaving. Optimal time steps in Euler methods.


- Stochastic modeling: Random number generator. Application to cell signaling.
### Spatially extended systems. Pattern formation in biology

**Description:**
- Introduction to Pattern formation


**Description:**
- Introduction to networks and their implementation.
Planning of activities

### AV1: Main project: Numerical simulation of a biophysical system.

**Hours:** 43h  
Guided activities: 3h  
Self study: 40h

**Description:**  
This project consists on developing a simulation of a relatively complex biophysical system. Students will work in pairs (not necessarily) and learn the fundamentals of the biophysical system, will decide how to address a simulation of the system and will use the numerical algorithms learnt in class (or in autonomous learning) to implement it. The code written by the students will have one of two aims: simulate numerically a full biophysical system or understand via simulations a particular feature of the same. The student will have to test the code modularly. Once the code is up and running, they will comment and comment it and proceed to use it to attain the desired goal. The project will end with a short report of the work done according to given guidelines.

**Support materials:**  
The general structure of the project will be given to the student together with bibliographic support and notes if necessary. The main structure of the code will be developed with the support of a tutor if necessary.

**Descriptions of the assignments due and their relation to the assessment:**  
Commented and documented code (up to 500 lines of code +100 in comments with one page documentation).  
Standard brief report with abstract, introduction, implemented model, code tests and results with conclusion (maximum 4 pages).  
Evaluation 40% of the total grade

**Specific objectives:**  
Students should develop a project with the aim of applying the different numerical techniques and theoretical knowledge explained during the course. When necessary, students may need to study a new numerical technique specifically useful for the project. All this means the student must learn autonomously, plan and focus in order to reach a clear goal. This would allow the students to consolidate the knowledge of the course, develop the ability to solve new problems and communicate this knowledge clearly and efficiently.

Qualification system

The students' evaluation will consist on grading the work done in class and at home through handed-in homework (HE), and the formal evaluation of the project (PE). There will not be a mid-term exam nor a final exam. The final mark will be given by:

0.6*HE+0.4*PE
Regulations for carrying out activities

All activities are compulsory. Any report or project which is not delivered or presented will have a grade of zero.

Bibliography

Basic:


Complementary:


Others resources:

Hyperlink

- The virtual heart
  http://thevirtualheart.org/

- Human Brain Project
  https://www.humanbrainproject.eu/es/discover/the-project/overview

Computer material

- Curs a atenea.
  Web resources in atenea