Course guide
230481 - COMBIO - Computational Biophysics

Last modified: 09/11/2022

Unit in charge: Barcelona School of Telecommunications Engineering
Teaching unit: 748 - FIS - Department of Physics.

Degree: **Academic year:** 2022 **ECTS Credits:** 6.0
Languages: English

LECTURER

Coordinating lecturer: Consultar aquí / See here: https://telecos.upc.edu/ca/estudis/curs-actual/professorat-responsables-coordinadors/responsables-assignatura

Others: Consultar aquí / See here: https://telecos.upc.edu/ca/estudis/curs-actual/professorat-responsables-coordinadors/professorat-assignat-idioma

PRIOR SKILLS

- 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 matemàtics 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).

Generical:
3. ABILITY TO IDENTIFY, FORMULATE, AND SOLVE PHYSICAL ENGINEERING PROBLEMS. Planning and solving physical engineering problems with initiative, making decisions and with creativity. Developing methods of analysis and problem solving in a systematic and creative way.

Transversal:
1. THIRD LANGUAGE. Learning a third language, preferably English, to a degree of oral and written fluency that fits in with the future needs of the graduates of each course.
2. SELF-DIRECTED LEARNING - Level 3. Applying the knowledge gained in completing a task according to its relevance and importance. Deciding how to carry out a task, the amount of time to be devoted to it and the most suitable information sources.
05 TEQ N1. TEAMWORK - Level 1. Working in a team and making positive contributions once the aims and group and individual responsibilities have been defined. Reaching joint decisions on the strategy to be followed.

TEACHING METHODOLOGY

The course will be centered in code-implementation classes and its theoretical and biological interpretation. Besides the normal classes, a few seminars showing examples of different types of modeling in biology will be given. During the course there will be basically two types of classes

-Theoretical classes will review and address definitions and frameworks in the area of computational sciences, math and biophysics. The basic structure of the class will be to expose the different concepts using blackboard, videos, and interactive resources.

-Practical classes where problems will be solved or discussed. Problems and codes will be set for home delivery.
One single class can be divided in theoretical and practical time if the topic at hand requires it.

Besides regular classes two different methodologies will be used:
-During the first week a special training program to code in python will be developed using the previous knowledge the students have in matlab.
-Seminar series will be arranged during the course. Professors will give seminars overviewing topics of computational biophysics which aren't addressed in the program so that students can overview more complex numerical methods and analysis.

All the resources will be published in the ATENEA website.

LEARNING OBJECTIVES OF THE SUBJECT

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

-Understand the syntax of python and be able to make basic programs including the simulation of dynamic systems in space and time

-Know and understand numerical tools using the Python programming language to solve physicla problems and represent visually data and information.

-Know how to use Python packages not included in the standard library

-Describe the main ways to approach the simulation of dynamic systems with spatial or positional components used in physics: Compartmental methods, extensive models with borders and network models. The student should be able to identify what is the best method to simulate a specific problem.

-Describe the main attractors and identify the main bifurcations of co-dimension 1. To be able to implement a computational decision using bifrucation theory.

-Understand the concept of limit cycle and chaotic attractor. Define the fundamental interactions in a metabolic process and their kinetic reactions. Be able to implement a genetic oscillating network and a typical cell signaling process. Analyze a biophysical problem in terms of its possible elements.

-Understand the concept of excitable system and its importance in the transmission of information.

-Understand the most fundamental models of population dynamics and their relationship with ecology, learning the different factors that affect the growth and development of populations: spatio-temporal, generational effects. Understand how population dynamics can affect their genetic variability.

-Define the fundamental aspects of epidemiology and the most relevant models that present its main characteristics of realistic disease spreading. Study the relevant parameters of an epidemic process and the observable ones. Understand the effects of the pattern of physical contacts on the spread of biological diseases.

-Define the concept of synchronization in dynamic systems. Understand its relevance in biology. Study simple synchronization models and understand their properties.

-Understand the importance of stochastic features in biophysical systems. Understand and know how to implement theoretically and numerically some stochastic methods relevant to the topics covered in this course.

-Do a linear stability analysis in a system with pattern formation. Be able to solve a linear and nonlinear boundary problem with initial conditions using different numerical implementations checking their stability and accuracy.

- Understand the dynamic behavior of reaction-diffusion-advection systems and give examples of the formation of structures in biology.

-Understand the limitations of linear stability and know some non-linear aspects of the formation of spatial and temporal structures such as the equations of amplitude or the interaction of modes.

As for the seminars, students should be able to summarize the seminars in one paragraph and write the basic outline of the research programs in two leading biophysics areas currently. They should also be able to briefly describe what simulation and computer tools are used in these fields.

STUDY LOAD

Type	Hours	Percentage
Self study	85,0	56.67
Hours large group	65,0	43.33

Total learning time: 150 h

CONTENTS

Intorduction to python

Description:
-Python programming structure and syntax.
-Fundamental functions of libraries

Related activities:
Periodic delivery

Full-or-part-time: 20h
Theory classes: 5h
Self study : 15h

Fundamentals of mathematical biology. Genes and decision making

Description:
- Basics of dynamical system: Attractors, bifurcations and nullclines
Introduction to ODE's. Fixed points and nullclines. Stability and bifurcations.
Linear stability analysis. Pitchfork and saddle-node bifurcation. Transcritical bifurcation. 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.

-Introduction to network theory. Gene regulatory networks.
Edges and vertices. Directed and undirected networks. Inhibitory and excitatory links. MM excitatoy/inhibtory terms. Decisions in cell genetic networks.

-Inhibitory and excitatory pathways.
Regulations. Simple gene regulation and expression. Excitability systems. Signal emission. Relevance of coding.

Related activities:
Home work periodic deliveries.

Full-or-part-time: 38h
Theory classes: 18h
Self study : 20h

Dynamical processes in biology. Population dynamics, epidemiology, and ecology

Description:
- Introduction to population dynamics: Discrete time versus continuous time models. One species and two species models. Effects of age and population structure. Introduction to population genetics.

- Dynamics of infectious diseases: Compartmental models of disease propagation, from the simple to the realistic. The epidemic threshold. Effects of population structure. Epidemiological forecasting. Herd immunity and vaccination. More complex models of disease propagation.

- Synchronization phenomena in biology: Definition of synchronization. Empirical observations of synchronization in biology, from fireflies to collective motion. Models of synchronization.

Related activities:
Home work periodic deliveries

Full-or-part-time: 45h
Theory classes: 20h
Self study : 25h

Extended systems in biology. Brain activty and morphogenesis.

Description:
- Stochastic processes. Neuronal description. Spatial and Time scales in biological models. The example of the brain: neurons and networks. Markov Processes. Langevin and Fokker-Planck Equations and their numerical implementation.

- Stability and Nonlinear dynamics in extended systems. Linear stability analysis of nonlinear systems. The Turing Mechanism and other examples of biological reaction-diffusion-advection pattern formation systems. Numerical implementation of these type of equations. Numerical stability and accuracy of these implementations. Limitations of the linear stability analysis and non-linear extensions of linear models.

- Patterns and Waves in the Brain. Mesoscopic description of the brain tissue. Formation of patterns and waves in neuroscience.

Full-or-part-time: 45h
Theory classes: 20h
Self study : 25h

Seminar series

Description:
Examples of models outside the topics of the course.

Full-or-part-time: 2h
Practical classes: 2h

ACTIVITIES

Periodic homework deliveries

Description:
Teachers will raise issues that will put in context with the syllabus. These problems can be simple to solve in class or more complicated where they are solved part by class and part at home. In these problems both clearly guided mathematical and computational tools were used in order to understand specific points and problems of importance.

Specific objectives:
Guide the student through the key features and problems of the subject at hand

Material:
Delivery and/or discussion of the problem set-up in class

Delivery:
Delivery of the solution of the problem indicated to be finished or done at home.

Full-or-part-time: 45h
Practical classes: 15h
Self study: 30h

Final Project

Description:
This project consists on developing a simulation of a relatively complex biophysical system. Students will work in pairs (notnecessarily) and learn the fundamentals of the biophysical system, will decide how to address a simulation of the system and willuse the numerical algorithms learnt in class (or in autonomous learning) to implement it. The code written by the students willhave one of two aims: simulate numerically a full biophysical system or understand via simulations a particular feature of thesame. The student will have to test the code modularly. Once the code is up and running, they will comment and comment it andproceed to use it to attain the desired goal. The project will end with a short report of the work done according to givenguidelines

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

Material:
Project gudielines or guide

Delivery:
Solutions to the questions or problems indicated in the exam

Full-or-part-time: 33h
Theory classes: 3h
Self study: 30h

GRADING SYSTEM

The evaluation will consist of periodic deliverables that might need coding to solve typical problems using mathematical or computational analysis (HE). There will also be a final project where a code in pairs will be developed in python and an individual report (PF) will be prepared.
The grade will be obtained from the following formula
0.5*PF+0.5*HE

EXAMINATION RULES.

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

BIBLIOGRAPHY

Basic:
- Gries, P.; Campbell, J.; Montojo, J. Practical programming : an introduction to computer science using Python 3. 2nd ed. The Pragmatic Bookshelf, 2013. ISBN 9781937785451.
- DiStefano, J. Dynamic system biology modeling and simulation. Elsevier, 2013. ISBN 9780124104112.
- Ingalls, B.P. Mathematical Modeling in Systems Biology [on line]. Cambridge, MA: MIT, 2013 [Consultation: 15/04/2020]. Available on: https://ebookcentral.proquest.com/lib/upcatalunya-ebooks/detail.action?docID=3339638. ISBN 9780262018883.
- Barrat, A.; Barthelemy, M.; Vespignani, A. Dynamical processes on complex networks. Cambridge: Cambridge University Press, 2008. ISBN 9780521879507.

Complementary:
- Murray, J.D. Mathematical biology, vol. 1 [on line]. 3rd. ed. Springer, 2002 [Consultation: 09/07/2014]. Available on: http://link.springer.com/book/10.1007/b98868. ISBN 9780387952239.
- Kriete, A.; Elis. R. Computational Systems biology: from molecular mechanism to diseases [on line]. 2nd. ed. Amsterdam: Elsevier, 2014 [Consultation: 15/04/2020]. Available on:

https://ebookcentral.proquest.com/lib/upcatalunya-ebooks/detail.action?docID=1574921. ISBN 9780124059269.
- Brauer, F.; Castillo-Chavez, C. Mathematical models in population biology and epidemiology [on line]. 2nd. ed. New York: Springer, 2012 [Consultation: 15/04/2020]. Available on: https://doi.org/10.1007/978-1-4614-1686-9. ISBN 9781461416869.
- Murray, J.D. Mathematical biology, vol. 2 [on line]. 3rd. ed. Springer, 2003 [Consultation: 15/04/2020]. Available on: http://link.springer.com/book/10.1007/b98869. ISBN 9780387952284.

RESOURCES

Computer material:
- Curs a atenea.. Web resources in atenea

Hyperlink:
- The virtual heart. http://thevirtualheart.org/- Human Brain Project. https://www.humanbrainproject.eu/es/discover/the-project/overview