UAB Universitat Autònoma de Barcelona

Modelling and Simulation of Biosystems.

2020/2021

Code: 100919
ECTS Credits: 6

Degree	Type	Year	Semester
2500253 Biotechnology	OT	4	0

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

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Use of Languages

Principal working language: catalan (cat)

Some groups entirely in English: No

Some groups entirely in Catalan: Yes

Some groups entirely in Spanish: No

Prerequisites

To have fundamental knowledge of algebra, differential and integral calculus, chemistry and biochemistry.

Be able to read English scientific literature.

Be able to use basic office software (word, Excel,...)

Basic knowledge in computer programming is an advantage

Oral and written basic knowledge of Catalan language is necessary

Objectives and Contextualisation

Computer simulation of real systems is a well-developed field of science especially in engineering areas, in physics or in chemistry. In biotechnology and in generally in biological sciences, its application was initially limited. In this context classical simulation approaches reproduce the behavior of microorganisms and enzymes in bioreactor. But the real impact of computer simulation in biotechnology results as a consequence on one side, due to the accumulation of knowledge about the isolated operation of components of biological systems and on the other side from the experimental observation that the components of a biological entity, such as a cell, operate in an autonomous and coordinated manner as an integrated system. Thus the biological system can be seen as a network of networks (metabolic, genetic, signal transduction,..) operating in a coordinated manner. This way, to understand the operation of even one of the simplest of those systems, is not possible without the perspective of its operation as an integrated system. The operation as a system results in the emergence of key properties, non-existing in any of its isolated parts but fundamental for the successful operation of the system. This new vision has resulted in the emergence of the field of Systems Biology. Biological systems computer simulation has been key in the development of systems biology, together with the increasing accumulation of knowledge on the operation of biological systems in public databases and the wide spread and cheap availability of computing power. By means of computer simulation it is made evident the different behaviors obtained depending on the individual properties of the components, their interconnections as well as the operational conditions.

In this context the course intends to introduce the student in the basic approximations and methodologies to simulate the behavior of a biological system in a computer. From the bioreactor as an experimental system to the examples of simulation of different types of networks (metabolic, genetic, signal transduction,..) in different operational modes (steady state, dynamic,..). As a global objective it is intended that the student has a firsthand experience on the differences and relevance of the behavior of a system as an integrated 'whole' in opposition to the isolated characteristics of its components, as well as the information derived from the different operational modes and therefore the requirements for their study.

As the main goal is to offer the student firsthand experience on biological systems simulation, the course has a high practical content. Thus the student will use either a programming environment, such as Matlab, to understand the basic procedures by means of simple examples, as well as using more specific simulation software for biological systems (SBW, COPASI, ...) in examples of higher complexity.

The different subjects are introduced gradually, from the basic concepts towards the description of systems of increasing complexity. In a way such that the student can understand the need to study biological systems as integrated entities in the context of the new biotechnology of the XXI century.

Competences

- Display an integrated vision of an R&D&I process, from the discovery of the basic knowledge and the development of applications to market launch, and apply the main concepts of organisation and management to a biotechnological process.
- Learn new knowledge and techniques autonomously.
- Read specialised texts both in English and ones own language.
- Search for and manage information from various sources.
- Search for, obtain and interpret information from the principal databases on biology, bibliography and patents and use basic bioinformatic tools.
- Think in an integrated manner and approach problems from different perspectives.
- Use ICT for communication, information searching, data processing and calculations.
- Use the fundamental principles of mathematics, physics and chemistry to understand, develop and evaluate a biotechnological process.

Learning Outcomes

1. Describe mathematically the behaviour of a biotechnological system based on the information available in the bibliography or in databases.
2. Describe the behaviour of a biotechnological system of moderate complexity.
3. Learn new knowledge and techniques autonomously.
4. Read specialised texts both in English and ones own language.
5. Search for and manage information from various sources.
6. Simulate the behaviour of a biotechnological process under different conditions.
7. Think in an integrated manner and approach problems from different perspectives.
8. Use ICT for communication, information searching, data processing and calculations.

Content

Unless the requirements enforced by the health authorities demand a prioritization or reduction of contents, the course will include:

1. Introduction. Models and systems
    1. Model. Definition, advantages, necessity
    2. Approximations to systems modelling
    3. Characteristics of systems
    4. Phases in the modelling process
    5. Components and types of models.
2. Review of fundamental concepts and modelling
    1. Balance equations and structure.
    2. Kinetics and thermodynamics
3. Dynamics of simple systems

    1. Bioreactor and biocatalyst systems
    2. Simple metabolic systems
    3. Basics of systems dynamics
4. Systems in steady state
    1. Bioreactor and biocatalyst systems
    2. Metabolic networks. Elementary modes.
    3. Optimization of systems in steady state.
    4. Systems sensitivity analysis. Metabolic control analysis
6. Simulation examples
    1. Metabolic networks
    2. Gene networks.
    3. Signal transduction networks

Methodology

The proposed teaching methodology may experience some modifications depending on the restrictions to face-to-face activities enforced by health authorities.

The methodology is heavily based on the student's work guided by the mentorship of the faculty members. In this context, and according with the objectives of the course, the different activities proposed can be grouped into theoretical classes, practical classes, autonomous work or individual tutor appoinments.

The different class typologies used can be described as follows:

Theory classes: Where all the necessary basic concepts will be provided as necessary to allow a proper autonomous learning step. IT resources (slides, .ppt, .pdf, simulations,…) used in class will be available to the student through the Moodle virtual platform.

Practical computer classes: Most of the learning outcomes of the course will be acquired via the practical classes using a computer. On the one side one objective is learning to use appropriated software for the simulation of biological systems. To this purpose the student will perform practical computer simulation exercises allowing the student to see the model implementation as well as the evolution of its behavior in different conditions. One of the main objectives will be to gain a deeper understanding of the behavior of a biological system and understand that this knowledge cannot be gained knowing the isolated behavior of its parts. The exercises will consist in the programming and simulation of example models corresponding to metabolic, genetic, signal transduction or other complex networks using the proper software for each case. The practical simulation classes will be performed in the computer rooms as scheduled in the course calendar. For each practical class a guide for the practical work will be available at the Moodle virtual campus for the course. While performing the exercises the student will keep the corresponding computer files inhis own virtual portfolio. Once the class will be finished the student will deliver the required files through the Moodle virtual campus as described ineach practical class guide. This will also serve as a register for each student's personal work. Some of the delivered exercises will be graded and given a mark. Which particular exercises are graded will be specified in the corresponding practical class guides. It is mandatory to be present in all practical classes. Should a student no be able to fulfill such requirement without proper documented justification it will be penalized as detailed in the corresponding evaluation section.

Simulation (team) work: Besides the above mentioned activities, the students will present a simulation work alone or in small group (2, 3 or 4 people) based on a computer simulation research paper. The paper can be selected from a list proposed by the teacher or alternatively proposed previously by the group and agreed with the teacher.

Individual tutor appointments: individual tutor appointments can be arranged with the professor to clarify concepts or any other course issues as well as to receive other advice such as available information resources.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Individual tutor appointments	4	0.16	8, 2, 1, 6
Practical computer classes	36	1.44	3, 8, 2, 1, 7, 6
Theory classes	14	0.56	8, 2, 1, 6
Type: Autonomous			
Personal computer simulation practice	36	1.44	3, 8, 5, 1, 4, 7
Simulation (team) work	30	1.2	3, 8, 5, 2, 1, 4, 7, 6
Study	30	1.2	3, 8, 5, 4

Assessment

Student's assessment may experience some modifications depending on the restrictions to face-to-face activities enforced by health authorities.

Course assessment will be performed in the following way

Activity A. Delivery of practical computer class results (25%): During the course the student will deliver through the Moodle virtual campus, the computer files resulting from the practical computer work as described in the corresponding practical class guide document. The delivery is compulsory. Failure in the delivery at the proper time will result in a penalty proportional to the number of course deliveries.

Activity B. Simulation (team) work (30%). It will correspond to the grade obtained in the delivered (team) simulation work.

Activity C. Graded exercises (45%): It will be the average of the marks received for the graded exercises. At present time it can be foreseen that the graded exercises will be included in the practical computer class results corresponding to practical classes 3, 6, 9 and 12. Nevertheless the graded practical exercises will be clearly identified in the corresponding practical class guide.

Final grade: It will be calculated as the weighted average of the practical computer class results (25%), Group simulation work (30%) and Graded exercises (45%). To allow for such weighted average it is necessary to have a minimum average grade of 3.8 in the Graded exercises.

Remedial exam (100%). In case the weighted average obtained using the above procedure would not be equal or higher to 5, the student can take a remedial exam. In this case, the final mark obtained will be the one obtained in this exam. This exam will also be open to students who failed to pass the course in previous editions of the course.

The minimum grade mark necessary to pass the course is 5.

Other issues:

Not Evaluable: Any student notattending to two thirds (2/3) of the graded activities, will be qualified as 'Not Evaluable'. Also, any student not attending to at least 50% ofthe practical classes will be qualified as 'Not evaluable'.

Dates: The dates of delivery of practical exercises or simulation (group) work will be informed thorough the Moodle virtual campus and may be changed for addaptation to previously unforeseen events. This communication method will also be used to inform of any change in the schedule or planned activities as it is considered the main communicaiton method between the student and the faculty members.

Plagiarism: Irrespective of any other measure that may be adopted, and according to the actual academic regulations, any irregular action committed by a student resulting in a variation of the result of any evaluation activity, will receive a qualification of zero. Therefore, to copy or let any other one to copy, during a test, an exercise or a practical activity will result in its failure. Should this activity be necessary to pass the course, the complete course will not be passed. Any activity qualified this way cannot be recovered. Therefore the complete course will be failed without the opportunity to pass it during the same semester.

Grading of the previously enrolled students: Once the student has been enrolled in the course for more than one year, grading of the course will be done in a final exam. Grading using the A, B and C activities is possible but has to be previously agreed with the professor at the beginning of the course (joan.albiol@uab.cat). That is before 8 days after the beginning of the course.

Honors Grade (MH): it is a personal decision of the faculty team responsible of the course to give a final honors grade. According to UAB regulations it can be given to students with a final mark equal or higher than 9. The maximum number of Honors that can be given is limited to 5% of the students enrolled in the course.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Delivery of practical computer class results (activity A)	25	0	0	8, 2, 1, 7, 6
Graded exercises (activity C)	45	0	0	8, 2, 1, 7, 6
Simulation (team) work (activity B)	30	0	0	3, 8, 5, 2, 1, 4, 7, 6

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