ANEXO I

Faculty Experimental Sciences

GENERAL SPECIFICATIONS

ACADEMIC YEAR 2022-23

BACHELOR'S DEGREE IN CHEMISTRY

Subject Data

Name:
QUÍMICA COMPUTACIONAL
English name:
COMPUTATIONAL CHEMISTRY

Code:	**Type:**
757509318	NON-MANDATORY

Hours:			
	Total	**In class**	**Out class**
Time distribution	75	30	45

ECTS:				
Standard group	**Small groups**			
	Classroom	**Lab**	**Practices**	**Computer classroom**
3		0	0	0

Departments:	**Knowledge areas:**
CIENCIAS INTEGRADAS	FÍSICA APLICADA
Year:	**Semester**
FOURTH	SECOND

TEACHING STAFF

Name:	**E-mail:**	**Telephone**
FRANCISCO PÉREZ BERNAL	FRANCISCO.PEREZ@DFAIE.UHU.ES	959219789

Others Data (Tutoring, schedule...)

Schedule:
Classes in the Physics Seminar Room (4th floor Experimental Sciences building)
Tuesday 12.00 – 14.00 (15 weeks)

Office Hours
Tuesday 10.00 – 12.00 and 16.00 – 18.00
Thursday 12.00 – 14.00

Students can arrange by mail office hours at other times and dates.

SPECIFIC INFORMATION OF THE COURSE

1. Contents description:

1.1 In English:

The present module aims to introduce students to some basic techniques for scientific programming and data analysis, working with free software apps in a GNU/Linux operating system environment. This is a very practical subject where students will carry out basic calculations, preferably in problems of molecular or atomic physics, though depending of their background the development of projects in other fields is also possible.

1.2 In Spanish:

Este curso presenta a los estudiantes una serie de técnicas básicas de programación científica, especialmente enfocada al análisis de datos, trabajando con aplicaciones de software libre en un entorno GNU/Linux. Es un curso eminentemente práctico con el fin de que los estudiantes sean capaces de desarrollar cálculos básicos, preferentemente en problemas de física atómica o molecular. Dependiendo de su formación, los estudiantes pueden desarrollar proyectos en otros campos.

2. Background:

2.1 Situation within the Degree:

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This course will provide to the students a basic introduction to programming, basic kowledge of GNU/Linux OS and the basic tools to perform calculations, treat results and present them effectively.

2.2 Recommendations

There are no prerequisites apart from the fact that students should bring their laptops with them to class. Students are expected to attend classes regularly and I highly encourage in-class participation. It can make a difference in the final grade.

3. Objectives (as result of teaching):

After completing this course students will be able to:

- demonstrate basic skills in GNU/Linux at the user and system administration level, with particular emphasis on a terminal approach rather than using GUI's.
- demonstrate basic user skills on several different applications of interest to chemists and scientists in general (e.g. LaTeX, Xmgrace, git, Inkscape etc.)
- apply basic programming skills using a modern language such as Fortran 90 or Python. Depending on students' background and interests, other programming languages, like Perl or GNU R, could be addressed.
- use the Python library pandas or GNU R for statistics and data treatment.
- apply the aforementioned tools to atomic or molecular physics problems or other scientific problems, in accordance with the student's background.

4. Skills to be acquired

4.1 Specific Skills:

C6 - Know the principles of quantum mechanics and their application in the description of the structure and properties of atoms and molecules.
Q2 - Ability to apply said knowledge to the resolution of qualitative and quantitative problems according to models previously developed.
Q5 - Competence to present, both in written and oral form, scientific material and argumentation to an audience specialized.
Q6 - Skill in handling and computer processing of chemical data and information.
P5 - . Interpretation of data from observations and measurements in the laboratory in terms of their significance and the theories that support it.

4.2 General, Basic or Transversal Skills:

BC1 - That students have demonstrated to possess knowledge and understand an area of study that starts from the base of general secondary education, and is usually found at a level that, while supported by advanced textbooks, it also includes some aspects that involve knowledge from the forefront of your field of study.
BC2 - That students know how to apply their knowledge to their work in a professional way and possess the competences that are usually demonstrated through the elaboration and defense of arguments and the resolution of problems within their area of study.
BC3 - That students have the ability to collect and interpret relevant data (normally within their area of study) to make judgments that include a reflection on relevant issues of a social, scientific, or ethical nature.
BC4 - That students can transmit information, ideas, problems and solutions to a public, specialized or not.
BC5 - That students have developed the learning skills necessary to undertake studies with a high degree of autonomy.

GC1 - Capacity for analysis and synthesis.
GC3 - Oral and written communication.
GC6 - Information management capacity.
GC7 - Problem solving.
GC9 - Teamwork.
GC12 - Autonomous learning.
GC14 - Critical reasoning.
GC18 - Sensitivity towards environmental issues.
GC20 - Use of the Internet as a means of communication and as a source of information.

TC1 - That students have developed and demonstrated learning skills and knowledge from their field of study, being able to apply them in their work, assessing relevant data to make judgments of topics of various kinds, being able to transmit them to both a specialized and non-specialized audience.

5. Training Activities and Teaching Methods

5.1 Training Activities:

- Expository method (lecture).
- Exercise, rehearse and put into practice with their computers the methods characteristic of the discipline.
- Autonomous Learning.
- Cooperative learning.
- Personalized attention to students.
- All classes will be practical and the students will work with their computers in them.

5.2 Teaching Methods::

- Expository method (lectures).
- Audiovisual exhibitions.
- invited conferences.
- Organization of seminars, workshops or debates.
- Autonomous Learning.
- Cooperative learning.
- Personalized attention to students.

5.3 Development and Justification:

The module development is done in such a way that the student gets first acquainted with the GNU/Linux OS from a CLI (Command Line Interface) approach. Simultaneously, they are introduced to a modern version control system as GIT. Once this has been achieved, the way is paved to introduce a programming language (either Python, Fortran, or other) and basic scientific programming techniques. Finally, students apply the concepts learnt to a project of their interest. All the subject is practical and the students work in class with their computers, using a virtual machine to have access to the GNU/Linux OS.

6. Detailed Contents

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1.- Basic user and admin concepts in GNU/Linux. 7 hours

2.- Introduction to scientific programming. 10 hours

3.- Basic calculations. Application to problems of interest. 8 hours

4.- Scientific Applications in GNU/Linux. 5 hours

7. Bibliography

7.1 Basic Bibliography:

Wes McKinney. Python for Data Analysis. Ed. O'Reilly. 2013.
Python notes (Francisco Pérez Bernal, https://curropb.gitbook.io/python-notes/)

7.2 Additional Bibliography:

David B. Cook. Handbook of Computational Chemistry. Ed. Dover 2005.
Stephen J. Chapman. Fortran 95-2003 for Scientists and Engineers. Ed. Mc Graw-Hill 2008.
Michael Metcalf. Modern Fortran Explained. Ed. Oxford University Press 2011.
Peter F. Bernath. Spectra of Atoms and Molecules. Ed. Oxford University Press. 2005.

Students can find in the Moodle site for this course many links to documents and other material of interest for the different topics treated.

8. Systems and Assessment Criteria

8.1 System for Assessment:

- Evaluation of exercises in the Moodle platform.
- Writing of a final project memory.
- Slides and defense of the final project memory.

8.2 Assessment Criteria and Marks:

8.2.1 Examinations Convocatory I

The final grade will be computed as the sum of the following components:

20% Moodle Assignments on GNU/Linux

30% Moodle Assignments on Python

10% Moodle Assignments on Git and LaTeX

20% Student final project memory.

20% Student presentation of the memory of his final project in the classroom.

No minimal grading in the items is required

Those students that have not properly followed the course or those that choose to have a single assessment will sit a final exam. The final exam will be the only component of the grade and it will consist on some practical exercises on the different topics covered in the course.

8.2.2 Examinations Convocatory II

A final exam will be the only component of the grade and it will consist on some practical exercises on the different topics covered in the course.

8.2.3 Examinations Convocatory III

A final exam will be the only component of the grade and it will consist on some practical exercises on the different topics covered in the course.

8.2.4 Extraordinary Convocatory

A final exam will be the only component of the grade and it will consist on some practical exercises on the different topics covered in the course.

8.3 Single Final Evaluation:

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A final exam will be the only component of the grade and it will consist on some practical exercises on the different topics covered in the course.