COURSE INFORMATION

COMPUTATIONAL CHEMISTRY -- INTRODUCTION TO SCIENTIFIC PROGRAMMING

Code number: 757509318(T1) (English Total)
Degree in Chemistry
Minor in Chemistry
Academic Year: 2018-2019
Elective course. 4th year
Second semester: 3 credits
Tentative Schedule:
Classes start in the second half of the semester: Mo and Tu 10:00-11:30.
Classroom: Integrated Sciences Department seminar room. Experimental Sciences Building, fourth floor, red doors module.

TEACHING STAFF

Prof.: Francisco Pérez Bernal
Department: Integrated Sciences (Departamento de Ciencias Integradas)
Office: M1 P4-07 (Experimental Sciences building, red doors)
Phone: +34 959 219789
E-mail: francisco.perez@dfaie.uhu.es
Office hours: Tu 16.00-18.00, We 12:00-14.00, 16:00-18:00

Students are welcomed to come to my office during office hours or by email appointment to discuss homework problems or any other aspect of the course.

SYLLABUS

1. DESCRIPTION

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 structure, though depending of their background the development of applications in other fields is also possible.

2. PREREQUISITES

There are no prerequisites apart from the fact that students should bring their laptops with them to class. The required software will be installed in their own computers. 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/LEARNING OUTCOMES

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 GNU R or the Python library pandas for statistics and data treatment.
- apply the aforementioned tools to atomic or molecular structure problems or other scientific problems, in accordance with the student's background.

4. Teaching Methodology

Classes will be mainly practical and students will follow the different activities with their laptops. Intensive use of Moodle is expected, where most of the documentation and links of interest can be found. Students will also find in Moodle exercise assignments for the different items explained in class.

5. Contents

1.- Basic user and admin concepts in GNU/Linux. 5 hours

2.- Introduction to scientific programming. 7 hours

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

4.- Scientific Applications in GNU/Linux. 3 hours

6. Bibliography

Basic references

Stephen J. Chapman. *Fortran 95-2003 for Scientists and Engineers*. Ed. Mc Graw-Hill 2008.

Wes McKinney. *Python for Data Analysis*. Ed. O'Reilly. 2013.

David B. Cook. *Handbook of Computational Chemistry*. Ed. Dover 2005.

Complementary references

Michael Metcalf. *Modern Fortran Explained*. Ed. Oxford University Press 2011.

Peter F. Bernath. *Spectra of Atoms and Molecules*. Ed. Oxford University Press. 2005.

Jeffrey I. Steinfeld. *Molecules and Radiation.* Ed. Dover. 2005.

A basic set of notes for FORTRAN 90 are also provided (Check Basic_Fortran90_notes). A large number of documents and links are provided in Moodle.

7. Assessment

Grading breakdown

Coursework and exercises	65%
Student Presentation	15%
Final assignment	20%

Exam 100% (Only for those students who fail the standard assessment above.)

Final results will be given in terms of a numerical scale between 0 and 10 (including tenths), with the corresponding qualitative ratings below:

- ≤4.9: Fail (D)
- 5.0 - 6.9: Pass (C)
- 7.0 - 8.9: Pass with Merit (B)
- 9.0 - 10: Distinction (A)

The total number of distinctions cannot exceed 5% of the students enrolled in the subject in the academic year (unless the number of students enrolled is lower to 20, in which case one distinction can be awarded).