VNIVERSITAT DE VALÈNCIA

Course Guide
44973 Computational techniques and numerical calculation

COURSE DATA

Data Subject	
Code	44973
Name	Computational techniques and numerical calculation
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	2 - Métodos	Obligatory

Coordination

Name	Department
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	315 - Physical Chemistry

SUMMARY

The goal of this subject is to introduce the most usual programming techniques in physics and chemistry. The student will learn the essential computational tools and will learn to create efficient programs using the FORTRAN programming language.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

OUTCOMES

2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Students are able to foster, in academic and professional contexts, technological and scientific progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) The principles of equal opportunities and universal accessibility for persons with disabilities, and c) the values of a culture of peace and democratic values.
- Students handle the most common programming techniques in physics and chemistry and are familiar with the essential computational tools in these areas.
- Students are able to develop efficient programs in FORTRAN in order to use such tools in their daily work.
- Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- Students have the ability of analyze and synthesize in such a way that they can understand, interpret and evaluate the relevant information by assuming with responsibility their own learning or, in the future, the identification of professional exits and employment fields.
- Students understand the theoretical and practical bases of computational techniques with which they can analyze the electronic, morphological and structural structure of a compound and interpret the results adequately.

LEARNING OUTCOMES

To introduce the most usual programming techniques in physics and chemistry. The student will learn the essential computational tools and will learn to create efficient programs using the FORTRAN programming language.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Tutorials	8,00	100
Seminars	7,00	100
TOTAL	**35,00**	

TEACHING METHODOLOGY

Lecture classes in the computing lab: The Professor will deliver face-to-face, or, online video lectures about the theoretical contents of the course during two-hour sessions. Teaching will be done in a computer lab, Two hours lectures will include an introduction, a theory to introduce the basic concepts and practical work. Student will learn through practicing. During the practical sessions the student will develop his own programs

Online Seminars: After the lecturing period, online seminars between the Professor and the students will be arranged at the *virtual classroom* in order to discuss the results being obtained, the potential problems and difficulties in using the various methodologies as well as to supervise the preparation of the required reports.

Tutoring sessions: The professor can organize either individual or group tutoring sessions about particular topics and questions raised by students.

Network teaching: All the tools available at the Moodle website (https://posgrado.uam.es) will be used (uploading of teaching materials, utilization of work team strategies, wiki, blogs, e-mail, etc .).

EVALUATION

The knowledge acquired by the student will be evaluated along the course. The educational model to follow will emphasize a continuous effort and advance in training and learning.

The final student mark will be based on exercises that must be done during the course.

The next criteria will be followed for assessment of student exercises:

- 60% from the student report,
- 40% from discussions between the student and professor in tutoring sessions and seminars.

Resit

The student will have to face a final exam, including both theory and practical exercises.

The student mark will be obtained from:

- 70% from the final exam,
- 30% from the individual work

REFERENCES

Basic

- Química Teórica y Computacional. J.Andrés y J.Bertrán, Eds. Publ Univ.Jaime I (Castellón) 2000.

Ingeniería del sofware: Diseño estructurado. J.A. Calco Manzasno y L.Fernández Sanz. Univ. Politécnica de Madrid (Madrid) 1995.

Structured FORTRAN-77 for Engineers and Scientists, D.M. Etter. Addison Wesley Longman (Menlo Park) 1977.

S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Numerical Recipes in Fortran (second edition, Univ. Press, Cambridge, 2003).

A. R. Krommer and C. W. Ueberhuber, Numerical integration on Advance Computer Systems (Springer-Verlag Berlín, Heidelberg, 1994).

P. J. Davis and P. Rabinowitz, Methods of Numerical Integration (second edition, Academic Press, Inc., London, 1984).

C. A. Floudas and P. M. Pardalos, Optimization in Computational Chemistry and Molecular Biology Local and Global Approaches (Springer, 1st edition, 2000).