

**COURSE DATA****Data Subject**

Code	43991
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
2184 - Master's Degree in Theoretical Chemistry and Computational Modelling	Faculty of Chemistry	1	Annual
3156 - null		0	First term

Subject-matter

Degree	Subject-matter	Character
2184 - Master's Degree in Theoretical Chemistry and Computational Modelling	2 - Methods	Obligatory

Coordination

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

SUMMARY

English version is not available

PREVIOUS KNOWLEDGE**Relationship to other subjects of the same degree**

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

**Other requirements**

No pre-requisites

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)**2184 - Master's Degree in Theoretical Chemistry and Computational Modelling**

- 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.
- El estudiante es capaz de adaptarse a diferentes entornos culturales.
- El estudiante es capaz de resolver problemas y tomar decisiones.
- Skills in analysis and synthesis.
- Comprender los fundamentos teóricos y prácticos de técnicas con las que puede analizar la estructura electrónica, morfológica y estructural de un compuesto.
- 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.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

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.



DESCRIPTION OF CONTENTS

1. Numerical calculation and Programming

Programming and Algorithms.
FORTRAN programming.
Matrix calculations.
Integrals.
Function optimization and roots finding.
Multivariate analysis.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Tutorials	8,00	100
Seminars	7,00	100
Development of individual work	30,00	0
Study and independent work	40,00	0
Preparation of practical classes and problem	20,00	0
TOTAL	125,00	

TEACHING METHODOLOGY

Lecture classes in the computing lab: 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 (<http://www.uam.es/moodle>) will be used (uploading of teaching materials, utilization of work team strategies, wiki, blogs, e-mail, etc.).



EVALUATION

Ordinary assessment

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.

Extraordinary assessment

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 software: 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)

