COURSE DATA

Data Subject	
Code	44985
Name	Advanced computational techniques
Cycle	Master's degree
ECTS Credits	6.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M	Faculty of Chemistry	2	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M	4 - Optativas de segundo	Optional

Coordination

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

SUMMARY

The subject Advanced Computer Techniques will be given by the University of Groningen in the format of an intensive course in November 2020. Due to the exceptional circumstances of covid19 all sessions will also be available in online format for all students who are unable to attend.

All course information is available on the website of the master: www.emtccm.org

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M

- 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 know the existence of advanced computational techniques such as instruction and data channeling, superscalar and multiscalar processors, chain operations, parallel platforms, etc.
- Students develop a critical thinking and reasoning and know how to communicate them in an egalitarian and non-sexist way both in oral and written form, in their own language and in a foreign language.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.

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

- Set up or recognize the Schrödinger equation for model systems in the presence of external conditions to solve it using computational techniques.
- To know how to use network-based High Performance Computation (HPC) facilities such as Grid or similar techniques.
- To know about some library of parallel computing routines and how to apply them to some kind of particular problems (e.g., magnetic systems).
- To know the basics of Quantum Computing applied to Theoretical Chemistry

DESCRIPTION OF CONTENTS

1. Grid Computing

2. Massive parallelization techniques: shared memory and distributed memory

3. Use of massively parallel mathematical libraries.

4. Quantum Computing

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	35,00	100
Tutorials	10,00	100
TOTAL	**45,00**	

TEACHING METHODOLOGY

Classes in computer science classroom:Teaching will be taught in a computer classroom. The classes, in two-hour sessions, will include a brief theoretical introduction, in which the teacher will explain the basic concepts and practical applications, and a practical part, in which the student will learn through the resolution of practical case.

Seminars:The Professor and the students will 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

Regular assessment

The final grade of the course will be based on:

- 60% Performance of a critical report on the practices carried out or exercises related to the subject.
- 40% Discussion in tutorials and/or seminars about the exercises, works or practices carried out in the subject.

Resit

The 100% of the mark will be the one obtained from the delivery of the exercises proposed by the teachers of the subject.

REFERENCES

Basic

- Se informará sobre el material de consulta para todas las asignaturas con la suficiente antelación en la página web del Curso Intensivo.
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- The teaching materials for all the subjects will be informed in advance on the website of the Intensive Course.