COURSE DATA

Data Subject	
Code	44988
Name	Computational chemistry programming project
Cycle	Master's degree
ECTS Credits	6.0
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	2	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	4 - Optativas de segundo	Optional

Coordination

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

SUMMARY

The aim of this course is to learn some basic programming and parallel programming techniques, which are relevant to many computational chemistry problems. During the class, the student will learn or reinforce their knowledge of a compiled programming language (typically Fortran or C++), and implement from scratch a basic (and perhaps more advanced) program for Lennard-Jones particle molecular dynamics simulations, as well as develop and test a parallel version of this code (using OpenMP or MPI).

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

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- 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 demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- Students are able to develop efficient programs in FORTRAN in order to use such tools in their daily work.
- Student are familiar with computational techniques which, based on mechanics and molecular dynamics, are the basis for designing molecules of interest in fields such as pharmacology, petrochemistry, etc.
- Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.
- 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 organized at work demonstrating that they know how to manage their time and resources.
- Students are able to generate new ideas based on their own decisions.

LEARNING OUTCOMES

English version is not available

WORKLOAD

ACTIVITY	Hours	% To be attended
Computer classroom practice	20,00	100
Tutorials	10,00	100
Theory classes	10,00	100
Seminars	5,00	100
TOTAL	45,00	

TEACHING METHODOLOGY

English version is not available

EVALUATION

Regular assessment

The final mark for the course will be based on: 20% final exam of the course and 80% corresponding to the delivery of a report of exercises proposed by the teacher.

Resit

The evaluation will be based on the delivery of a report with the proposed exercises.