UNIVERSIDAD AUTÓNOMA DE MADRID

32526 - COMPUTATIONAL TECHNIQUES AND NUMERICAL ANALYSIS

Syllabus Information

Code - Course title: 32526 - COMPUTATIONAL TECHNIQUES AND NUMERICAL ANALYSIS

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional

Faculty: 104 - Facultad de Ciencias

Academic year: 2019/20

1.Course details

1.1.Content area

Computational Techniques and Numerical Calculations

1.2.Course nature

Compulsory

1.3.Course level

Máster (MECES 3)

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 1
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 1

1.5.Semester

Annual

1.6.ECTS Credit allotment

5.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no previous prerequisites.

1.9.Recommendations

There are no recommendations.

1.10.Minimum attendance requirement

Attendance is mandatory.

1.11.Faculty data

a. Subject's coordinator:
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- Department: Physical Chemistry

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e. Master's coordinators:
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- Sergio Díaz-Tendero: sergio.diaztendero@uam.es

1.12.Competences and learning outcomes

1.12.1.Competences

BASIC AND GENERAL COMPETENCES

CB6 – Students possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context.

CB7 - Students know how to apply the acquired knowledge and their problem solving capacity in new or little known environments within broader (or multidisciplinary) contexts related to their area of study.

CB8 - Students are able to integrate knowledge and face the complexity of making judgments from information that, incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and judgments.

CB9 - Students know how to communicate their conclusions and the knowledge and reasons that support them to specialized and non-specialized audiences in a clear and unambiguous way.

CB10 - Students possess the learning skills that allow them to continue studying in a way that will be self-directed or autonomous.

CG01 - 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.

CG02 - Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.

CROSS-COMPREHENSIVE COMPETENCES

CT01 - Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.

CT03 - 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.

SPECIFIC COMPETENCES

CE04 - 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.

CE13 - Students handle the most common programming techniques in physics and chemistry and are familiar with the essential computational tools in these areas.

CE14 – Students are able to develop efficient programs in FORTRAN in order to use such tools in their daily work.

1.12.2.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.

1.13.Course contents

Programming and Algorithms.

Fortran programming.

Matrix calculations.

Integrals.

Function optimization.

Multivariate analysis.

1.14.Course bibliography

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).

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	35
Independent study time	90

2.2.List of training activities

Activity	# hours
Lectures	20
Seminars	7

Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	8
Assessment activities	
Other	

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 .).

3.Evaluation procedures and weight of components in the final grade

3.1.Regular 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.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	70
Continuous assessment	30

3.2.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

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	70
Continuous assessment	30

4.Proposed workplan

Please, check the official schedule posted on the master website.