Universitat Autònoma de Barcelona

2023/2024

Simulation of Nanometric Systems

Code: 103304
ECTS Credits: 6

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OT	4	2

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject. Please note that this information is provisional until 30 November 2023.

Teachers

Jordi Faraudo Gener

External teachers

Pol Febrer

Prerequisites

Interest for the use of computers in solving scientific problems.

Previous programming knowledge is not required, but it may be useful.

Objectives and Contextualisation

The objective of this course is to be able to use the main computational simulation methods applied to nanometric systems, and to know the possibilities and limitations of each technique. In particular, the specific objectives are: (a) to introduce the basics of programming and to know the general structure of the simulation codes in the most frequent scientific programming languages; (b) be able to understand the fundamental principles of electronic structure calculation, Monte Carlo methods and molecular dynamics algorithms and (c) use these computational methods in the study of nanotechnological and bionanotechnological systems.

Competences

- Adapt to new situations.
- Apply the concepts, principles, theories and fundamental facts of nanoscience and nanotechnology to solve problems of a quantitative or qualitative nature in the field of nanoscience and nanotechnology.
- Communicate clearly in English.
- Communicate orally and in writing in one's own language.
- Demonstrate knowledge of the concepts, principles, theories and fundamental facts related with nanoscience and nanotechnology.
- Interpret the data obtained by means of experimental measures, including the use of computer tools, identify and understand their meanings in relation to appropriate chemical, physical or biological theories.
- Lead and coordinate work groups.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
- Operate with a certain degree of autonomy.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse physical, chemical and biological problems in the field of nanoscience and nanotechnology and propose answers or suitable studies for their resolution, including when necessary the use of bibliographic sources.
- Recognise the terms used in the fields of physics, chemistry, biology, nanoscience and nanotechnology in the English language and use English effectively in writing and orally in all areas of work.
- Resolve problems and make decisions.
- Show motivation for quality.
- Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Learning Outcomes

1. Adapt to new situations.
2. Apply Monte Carlo techniques to solve problems in nanotechnology.
3. Apply the acquired theoretical contents to the explanation of experimental phenomena.
4. Apply the concepts of structured and object oriented programming to the development of programs for the simulation and computation of properties on a nanoscale.
5. Communicate clearly in English.
6. Communicate orally and in writing in one's own language.
7. Correctly analyse databases by means of statistical packages.
8. Correctly use archives and libraries of numerical methods to solve linear algebra problems in the simulation of nanometric systems.
9. Critically evaluate experimental results and deduce their meaning.
10. Draft reports on the subject in English.
11. Identify the different paradigms of nanoscale simulation (first principles, semi-empirical methods, continuum methods, molecular dynamics).
12. Identify the situations in which the different methodologies studied can help to resolve problematic situations and know how to select the best techniques.
13. Interpret discrepancies between theoretical and practical results (including simulation) found in measurements.
14. Interpret the capacities of a simulation program in accordance with the terms that the model incorporates and the derived effects.
15. Lead and coordinate work groups.
16. Learn autonomously.
17. Manage the organisation and planning of tasks.
18. Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
19. Operate with a certain degree of autonomy.
20. Perform bibliographic searches for scientific documents.
21. Present brief reports on the subject in English.

22. Propose creative ideas and solutions.
23. Reason in a critical manner
24. Recognise the correct terms for topics related to methodologies and experimentation in nanoscience and nanotechnology.
25. Recognise the range of applicability, both with regard to measurements of the system and the types of computable properties, of these simulation paradigms.
26. Resolve problems and make decisions.
27. Resolve problems with the help of the provided complementary bibliography.
28. Show motivation for quality.
29. Understand texts and bibliographies in English on each of the techniques, methodologies, tools and instruments in the subject area.
30. Use programs for first principle and molecular dynamic calculations.
31. Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Content

1. Introduction to scientific programming using python: use of scientific libraries. Numerical solution of models in r
2. Basic simulation algorithms in nanoscience: Monte Carlo method, Mol
3. Use of current scientific software to solve problems of nanoscience, na

Methodology

This is a practical subject, therefore the teaching method is mostly based on practical sessions in the computer labs, together with some lectures necessary to introduce the basic concepts and methods to be used in the computer lab. In the sessions we will encourage participation and discussion in class (including the possibility of quizzes during the sessions). The sessions will include introductory practice of the different methods, tutorials, computer exercises and a final practical synthesis project that will be carried out in the computer laboratory, which will have to be presented in class.

Comment: the material employed in class (software, papers, manuals) corresponds to actual scientific material used by the scientific community which is typically in English only.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Computer Lab practical sessions	20	0.8	1, 7, 4, 3, 16, 9, 29, 6, 28, 20, 17, 12, 13, 14, 15, 18, 19, 22, 23, 24, 10, 27, 26, 31, 8, 30
Master Classes (Theory) and discussion sessions	14	0.56	1, 2, 16, 29, 5, 6, 28, 20, 11, 12, 13, 14, 18, 19, 22, 23, 25, 24, 10, 27, 26
Tutorials	18	0.72	1, 7, 4, 16, 29, 6, 28, 20, 17, 12, 18, 19, 22, 23, 24, 10, 27, 26, 31, 8, 30

Type: Autonomous			
Assigments (readings, exercices and reports), individual project work	54	2.16	1, 4, 3, 2, 16, 9, 29, 6, 28, 21, 20, 17, 11, 12, 13, 14, 18, 19, 22, 23, 25, 24, 10, 27, 26, 8, 30

Assessment

A continuous evaluation will be carried out using the following instruments:

a) Compulsory computer lab practicals with delivery of a report (LB). (20%)

b) Exercises or problems (PB) related to the basic concepts exposed in the sessions. (20%)

c) Participation in discussions and "quizzes" in theoretical sessions (Q) (20%)

d) Final project (PJ) that includes both the delivery of the work carried out and an oral presentation. (40%)

The continuous evaluation activities have the objective of evaluating the daily follow-up of the subject and therefore, as in the case of computer lab practicals, they are not subject to retake.

In the event that a minimum of 2/3 of the practices (LB) are not completed or the final work (PJ) is not submitted, the final grade will be "NON-ASSESSABLE".

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Computer Lab reports	20%	10	0.4	7, 4, 3, 9, 29, 6, 17, 12, 13, 19, 22, 24, 10, 27, 26, 31, 8, 30
Final project	40%	20	0.8	1, 7, 4, 3, 2, 16, 9, 5, 28, 21, 20, 17, 11, 12, 13, 14, 15, 18, 19, 22, 23, 25, 24, 27, 26, 31, 8, 30
Problems and exercises	20%	10	0.4	16, 29, 6, 28, 20, 13, 19, 22, 23, 27, 26
Quizzes and questions and participation in discussions	20%	4	0.16	3, 6, 28, 11, 13, 14, 25

Bibliography

1) "Understanding Molecular Simulation"

Daan Frenkel and Berend Smit, Academic Press, 2n edition 2002, 3rd Edition 2023

https://bibcercador.uab.cat/permalink/34CSUC_UAB/1c3utr0/cdi_askewsholts_vlebooks_9780080519982

2) "Simulating the Physical World: Hierarchical Modeling from Quantum Mechanics to Fluid Dynamics"

Berendsen, Herman J. C. (Cambridge University Press, 2007)

https://bibcercador.uab.cat/permalink/34CSUC_UAB/1c3utr0/cdi_skillsoft_books24x7_bke00023160

3) "Molecular Modelling Basics"

Jan H. Hensen, CRC Press, 2010

http://molecularmodelingbasics.blogspot.com/

Software

Visual Molecular Dynamics (VMD) https://www.ks.uiuc.edu/Research/vmd/

NAnoscale Molecular Dynamics (NAMD) https://www.ks.uiuc.edu/Research/namd/

Spanish Initiative for Electronic Simulations with Thousands of Atoms - SIESTA https://siesta-project.org/siesta/

Python software available at GitHub: https://github.com/jfaraudo