COURSE OF STUDY *Physics (LM-17)*

ACADEMIC YEAR *2024-2025*

ACADEMIC SUBJECT *Molecular Dynamics*

General information	
Year of the course	1st
Academic calendar (starting and ending date)	2nd semester: March - May 2025
Credits (CFU/ECTS):	3
SSD	FIS/07
Language	English
Mode of attendance	Recommended, not compulsory

Professor/ Lecturer	
Name and Surname	Antonio Suma
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Telephone	0805443214
Department and address	Physics department, room 10 at ground floor
Virtual room	
Office Hours (and modalities: e.g., by appointment, on line, etc.)	In person or online previous appointment via e-mail

Work schedule			
Hours			
Total	Lectures	Hands-on (laboratory, workshops, working groups, seminars, field trips)	Out-of-class study hours/ Self-study hours
75	16	15	44
CFU/ECTS			
3	2	1	

Learning Objectives	Extensive knowledge of main molecular dynamics simulation techniques, and knowledge of numerical implementation of these techniques
Course prerequisites	Newtonian dynamics, statistical mechanics

Teaching strategies	Frontal teaching, tutorials using the computer
Expected learning outcomes in terms of	
Knowledge and understanding on:	o Main techniques to simulate different physical systems which follow Newton's equations using the computer o Distinguish which technique is needed in order to sample each ensemble (microcanonical, canonical, isobaric)
Applying knowledge and understanding on:	o Knowing how to implement programs in the Linux environment to simulate, analyze and visualize simple molecular systems
Soft skills	● *Making informed judgments and choices* o Understanding which are the typical problems that arise from modelling and implementing codes of molecular dynamics systems, included problems related with sampling and with the choice of the sampling technique. ● *Communicating knowledge and understanding* o Informatic competences related to process and analyze data,

	○ Present the topics considered using an adequate scientific language ● *Capacities to continue learning* ○ Buil more complex programs in the Linux environment. ○ Study individually more advanced molecular dynamics simulation techniques
Syllabus	
Content knowledge	Introduction to molecular dynamics simulations. Basics of Newtonian dynamics and harmonic oscillator. Sampling microcanonical ensemble: Verlet, Leap-Frog, Velocity Verlet, Liouville equation and Trotter splitting. Sampling canonical ensemble: Monte Carlo, balance and detailed balance, Metropolis rule, velocity rescaling, Berendsen thermostat, Andersen thermostat, Langevin thermostat, Nosé-Hoover thermostat, stochastic velocity rescaling. Limits on the choice of timestep, multiple timestepping (RESPA), rigid bonds, shake. Sampling isobaric ensemble: Andersen and Monte Carlo barostat, pressure estimator. Periodic boundary conditions, origin of different force terms, neighbors list (Verlet and linked cell list methods), reduced units. Rare events and enhanced sampling methods. Free energy estimations and errors. Umbrella Sampling. Weighted histogram analysis method. Metadynamics. Tutorials on the use of BASH, AWK, Gnuplot and LAMMPS, to write simple molecular dynamics and Monte Carlo codes, analysis codes and to visualize data.
Texts and readings	D. Frenkel, B. Smit, Understanding Molecular Simulation, Academic Press, 2001. M . P. Allen, D. J. Tildesley, Computer Simulation of Liquids, OUP Oxford, 2017. M. E. Tuckermann, Statistical mechanics: theory and molecular simulation, Oxford Graduate Texts, 2010.
Notes, additional materials	
Repository	

Assessment	
Assessment methods	Oral presentation of a topic related to the course. The topic can be a different technique from the ones presented during the lessons, a molecular system, the results found by simulating these systems. The arguments can be chosen from the suggested books or from scientific articles, and must be agreed-upon with the lecturer.
Assessment criteria	● *Knowledge and understanding* ○ Capacity to describe the topic ○ Capacity to answer to comprehension question related to the techniques/results presented ● *Applying knowledge and understanding* ○ Capacity to understand how the techniques described are numerically implemented ● *Autonomy of judgment* ○ Have a critical assessment of the topic presented ● *Communication skills* ○ quality of presentation ○ competence in the lexicon used ● *Capacities to continue learning* ○ Understanding the general context of the argument
Final exam and grading criteria	The final mark is out of thirty.
Further information	

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