UNIVERSITÀ DEGLI STUDI DI BARI ALDO MORO

DIPARTIMENTO INTERUNIVERSITARIO DI FISICA

General information		
Academic subject	Molecular Dynamics	
Degree course	Physics (LM)	
Academic Year	2022/2023	
European Credit Transfer and Accumulation System (ECTS)	3	
Language	English	
Academic calendar (starting and ending date)	1° semester of second year (dates and timetable to choose via email with interested students)	
Attendance	Highly suggested	

Professor/ Lecturer	
Name and Surname	Antonio Suma
E-mail	antonio.suma@uniba.it
Telephone	
Department and address	*Physics department, room R10*
Virtual headquarters (Microsoft Teams code)	
Tutoring (time and day)	Wednesday, from 16:00 to 18:00 previous appointment via e-mail

Syllabus	
Learning Objectives	Extensive knowledge of main molecular dynamics simulation techniques, and knowledge of numerical implementation of these techniques
Course prerequisites	Newtonian dynamics, statistical mechanics
Contents	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. 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.
Books and bibliography	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.
Additional materials	

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

Teaching strategy	Frontal teaching, tutorials using the computer

Expected learning outcomes	
Knowledge and understanding on:	○ Main techniques to simulate different physical systems which follow Newton's equations using the computer ○ Distinguish which technique is needed in order to sample each ensemble (microcanonical, canonical, isobaric)
Applying knowledge and understanding on:	○ Knowing how to implement programs in the Linux environment to simulate, analyze and visualize simple molecular systems
Soft skills	• **Making informed judgments and choices** ○ 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** ○ Informatic competences related to process and analyze data, ○ Present the topics considered using an adequate scientific language • **Capacities to continue learning** ○ Build more complex programs in the Linux environment. ○ Study individually more advanced molecular dynamics simulation techniques

Assessment and feedback	
Methods of assessment	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 systems, the results found by simulating this systems. The arguments can be chosen from the suggested books or from scientific articles, and must be agreed-upon with the lecturer.
Evaluation 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
Criteria for assessment and attribution of the final mark	The final mark is out of thirty
Additional information	