Stampare su carta intestata del CdS

General information	
Academic subject	***Molecular Dynamics***
Degree course	*Physics (LM)*
Academic Year	*2021/2022*
European Credit Transfer and Accumulation System (ECTS)	3
Language	*English*
Academic calendar (starting and ending date)	*2021/2022*
Attendance	*Highly suggested*

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

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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

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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	