GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	, PG_00058709					
Field of study	Nanotechnology					
Date of commencement of studies	February 2023		Academic year of realisation of subject		2023/2024	
Education level	second-cycle studies		Subject group		Optional subject group Subject group related to scientific research in the field of study	
Mode of study	Full-time studies		Mode of delivery		at the university	
Year of study	1		Language of instruction		Polish	
Semester of study	2		ECTS credits		5.0	
Learning profile	general academic profile		Assessment form		assessment	
Conducting unit	Instytut Nanotechnologii i Inżynierii Materiałowej -> Faculty of Applied Physics and Mathematics					
Name and surname of lecturer (lecturers)	Subject supervisor		dr inż. Szymon Winczewski			
	Teachers		dr inż. Szymon Winczewski			
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	30.0	0.0	30.0	0.0	0.0	60
	E-learning hours included: 0.0						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan		Participation in consultation hours	Self-study	SUM
	Number of study hours	60		5.0	60.0	125
Subject objectives	Discussion of particle methods in the context of modelling of nanoscale systems. Detailed description of the molecular dynamics method in theory (integration of equations of motion) and in practice (commonly used potentials, boundary conditions, starting a simulation, neighbourhood, cut-off radius). Brief tour of more advanced concepts of MD (selected topis -- e.g. rigid molecules, shell model, constrained dynamics, thermostats, barostats, Ewald method).					

Learning outcomes	see table below

Course outcome	Subject outcome	Method of verification
K7_W02	The student has acquired extended and well-ordered knowledge pertaining to classical simulation approaches to studying systems at the nanoscale, (s)he understands the basic principle, but also the most important nuances and limitations. (S)he is able to apply the molecular dynamics method to investigate uncomplicated systems on their own.	[SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects
K7_W05	The student has in-depth understanding of particle methods (molecular dynamics) and is aware of the methods' limitations. (S)he can position classical and quantum-based methods in the landscape of computational methods suitable for the nanoscale.	[SW1] Assessment of factual knowledge
K7_U03	The student is able to independently perform a molecular dynamics simulation using the LAMMPS package and to interpret the basic results.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task
K7_U06	The student is able to design and perform a simple simulation using the LAMMPS package, together with a critical analysis of obtained results, visualize the system's trajectory, prepare plots of key parameters of the simulation.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools [SU5] Assessment of ability to present the results of task

Subject contents

Main questions of modeling at the nanoscale. What is a particle? Dynamical equation.Classical and quantum-based methods, scaling of computational effort. The molecular dynamics method, its advantages and limitations. Conservation of energy in Newtonian mechanics. Phase space and trajectories. Periodic and mixed boundary conditions, minimum image convention, quasiinifinity, limitations of PBCs. Cut-off radius and its consequences. Hockneys linked cells and Verlet neighbour list. Initializing an MD simulation (positions, velocities), equilibration. Integration of the equations of motion. Verlet, leapfrog and predictor-corrector methods. Sources of error in integrating the equations of motion. Visualization in MD, calculating macroscopic observables (energy, temperature, virial, pressure, specific heat, RDF, ADF, S(k), MSD, D(T)). Potential and its relationship with force. General and particular forms of potentials. Selected potentials: LJ, soft- and hard-sphere, Born-Mayer, harmonic, Morse, Stillinger-Weber, Sutton-Chen, GAFF). Polarizability and shell models (Cochran, Fincham). Constrained dynamics, formal approach, SHAKE, RATTLE, QSHAKE. Rigid molecules in MD simulations, Euler angles, rotation matrix, vector transformations, quaternions. Coulombic interactions in MD, Ewald method. NVT and NPT ensembles, primitive thermostats, ESM and CSM thermo- and barostats. Hybrid (QM/MM) methods.

Prerequisites and co-requisites

The student is acquainted with Newtonian mechanics. The student knows the basics of organization ofmatter. The student knows the basics of calculus and algebra.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
hands-on computer lab	50.0%	50.0%
final test	50.0%	50.0%

Recommended reading

Basic literature	1. D.C. Rapaport, The Art of Molecular Dynamics Simulation, Cambridge University Press, 2004.

	Supplementary literature	1. D. Frenkel, Understanding Molecular Simulation, Academic Press, 2001. 2. M.P. Allen, D.J. Tildesley, Computer Simulation of Liquids, Clarendon Press, 1989. 3. V. Bulatov, W. Cai, Computer simulations of dislocations, Oxford University Press, 2006. 4. E.B. Tadmor, R.F. Miller, Modeling Materials, Cambridge University Press, 2011.
	eResources addresses	Adresy na platformie eNauczanie: Komputerowe modelowanie metodami cząstek - Moodle ID: 33884 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=33884
Example issues/ example questions/ tasks being completed	1. What are the typical system sizes and timescales for which molecular dynamics simulations are performed? Why arent continuum methods used for such systems? 2. What are the main differences between classical and quantum-based methods of computational analysis of nanoscale systems? 3. Briefly explain the principle of operation of the molecular dynamics method. 4. When is total energy conserved in an MD simulation and when is it not? 5. What are the main limitations of the molecular dynamics method? 6. Discuss the notion of periodic boundary conditions what are they, why are they used, what are their limitations and what difficulties are associated with their use? 7. Briefly describe the approaches for making MD simulations faster. 8. What is the potential cut-off radius? Why is it used? What difficulties does using a finite cut-off radius entail? 9. Describe Hockneys linked-cell method and Verlet neighbour list. What do these techniques allow? What are the advantages and disadvantages of both? 10. How would you generate starting positions and velocities for simulating a liquid with MD? 11. How would you generate starting positions and velocities for simulating a crystalline system with MD? 12. What skew start and how is it realized? 13. What is equilibration in MD simulations? What are the rules of thumb for performing equilibration? 14. Derive the Verlet integrator. 15. What are predictor-corrector approaches? What are their advantages compared to other integrators? 16. What is the pair correlation function? How can it be calculated? 17. Sketch typical shapes of pair correlation functions for a crystalline solid, a liquid and a gas. How does g(r) behave as r increases? 18. What additional information on a system can we gather having calculated its pair correlation function? How can we do that? 19. What is the mean-square displacement (MSD) in an MD simulation? How can we calculate it? What information does it hold? 20. What is the angular distribution function? Sketch its typical shape for various systems. 21. How can we calculate the self-diffusion coefficient in an MD simulation? What information does it hold? 22. What is a potential in an MD simulation? How is it related to the force acting on atom i? What is the general form of a potential used in practice? 23. Draw the typical shape of the Lennard-Jones potential. What is its functional form? Describe the terms and symbols used. What kinds of systems does this potential describe well? 24. Give the formula for the Lennard-Jones potential. What physical phenomena does each of its terms model? 25. Hard-sphere potential, Born-Mayer potential, harmonic potential, Morse potential describe selected three of these. 26. Compare the Stillinger-Weber and Sutton-Chen potentials. Which systems would you use them for? 27. Briefly characterize the GAFF potential. What effects does each of the terms in the potential model? 28. How is pressure calculated in MD simulations? Show a short derivation. 29. Describe the Ewald approach in detail. What is it used for? What kinds of systems is it applicable to? 30. What is constrained dynamics? Give examples when it would be useful. 31. Briefly describe the formal approach and the SHAKE approach to constrained dynamics. 32. Briefly describe the Berendsen and Andersen thermostats. 33. Describe the three general classes of approaches for keeping the temperature constant in MD simulations. 34. What are shell models? When are they used? Briefly compare the static Cochran shell model with thedynamic Fincham model.	
Work placement	Not applicable	