GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Modelling and simulation in nanotechnology, PG_00071034		
Field of study	Nanotechnology, Nanotechnology		
Date of commencement of studies	February 2027	Academic year of realisation of subject	2027/2028
Education level	second-cycle studies	Subject group	Obligatory subject group in the field of study 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	English
Semester of study	2	ECTS credits	2.0
Learning profile	general academic profile	Assessment form	assessment
Conducting unit	Division of Physics of Disordered Systems -> Institute of Nanotechnology and Materials Engineering -> Faculty of Applied Physics and Mathematics -> Faculties of Gdańsk University of Technology		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Jacek Dziedzic	
	Teachers	dr hab. inż. Jacek Dziedzic	

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	30.0	0.0	0.0	0.0	0.0	30

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	30	2.0	18.0	50

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, calculating macroscopic properties). Brief tour of more advanced concepts of MD (selected topics -- e.g. rigid molecules, shell model, constrained dynamics, thermostats, barostats, Ewald method).

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_W05] has in-depth knowledge of mathematical, numerical, and simulation methods - both classical and quantum - used in the modeling of nanostructures	The student possesses an advanced understanding of particle methods (molecular dynamics) and is aware of their limitations. They can position both classical and quantum methods within the broader landscape of computational techniques used at the nanoscale.	[SW1] Assessment of factual knowledge
[K7_W01] has broadened and well-structured knowledge in the field of materials science, including material fabrication or control of processes accompanying fabrication, with particular emphasis on materials and structures at the nanoscale.	The student understands the concepts of ordering and phase transitions. They possess broadened and well-structured knowledge of classical particle simulation methods in materials engineering at the atomic and nanoscale.	[SW1] Assessment of factual knowledge

<table>
<tr><td>Subject contents</td><td>Course content – lecture
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. Hockney's 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, AMOEBA. Polarizability and shell models (Cochran, Fincham). Constrained dynamics, formal approach, SHAKE, RATTLE, QSHAKE. NVT and NPT ensembles, primitive thermostats, ESM and CSM thermo- and barostats. Coulombic interactions in MD, Ewald method.</td></tr>
<tr><td>Prerequisites and co-requisites</td><td>The student is acquainted with Newtonian mechanics. The student knows the basics of the organization of matter. The student knows the basics of calculus and algebra.</td></tr>
<tr><td>Assessment methods and criteria</td><td><table>
<tr><th>Subject passing criteria</th><th>Passing threshold</th><th>Percentage of the final grade</th></tr>
<tr><td>Written assessment</td><td>50.0%</td><td>100.0%</td></tr>
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<tr><td>Recommended reading</td><td><table>
<tr><td>Basic literature</td><td>1. D.C. Rapaport, The Art of Molecular Dynamics Simulation, Cambridge University Press, 2004.
2. M.P. Allen, Introduction to Molecular Dynamics Simulation, Computational Soft Matter: From Synthetic Polymers to Proteins, Lecture Notes, Norbert Attig, Kurt Binder, Helmut Grubmuller, Kurt Kremer (Eds.), John von Neumann Institute for Computing, Julich, NIC Series, Vol. 23, ISBN 3-00-012641-4, pp. 1-28, 2004.
3. G. Ciccotti, S. Decherchi, S. Meloni, Foundations of molecular dynamics simulations: how and what, Riv. Nuovo Cim. 48, 194, Open Access, 2025. https://doi.org/10.1007/s40766-025-00065-4</td></tr>
<tr><td>Supplementary literature</td><td>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.</td></tr>
<tr><td>eResources addresses</td><td></td></tr>
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<tr><td>Example issues/ example questions/ tasks being completed</td><td>1. 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?
2. Describe Hockney's linked-cell method and Verlet neighbour list. What do these techniques allow? What are the advantages and disadvantages of both?
3. What is equilibration in MD simulations? What are the rules of thumb for performing equilibration?
4. What is the pair correlation function? How can it be calculated?
5. Draw the typical shape of the Lennard-Jones potential. What is its functional form? Describe the terms and symbols used.
6. Characterize the AMOEBA polarizable potential.
7. Briefly describe the Berendsen and Andersen thermostats.</td></tr>
<tr><td>Practical activites within the subject</td><td>Not applicable</td></tr>
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