GDAŃSK UNIVERSITY OF TECHNOLOGY

Subject card

Subject name and code	Modelling of Biological Systems, PG_00040972		
Field of study	Biomedical Engineering, Biomedical Engineering, Biomedical Engineering		
Date of commencement of studies	October 2022	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	2	Language of instruction	Polish
Semester of study	4	ECTS credits	3.0
Learning profile	general academic profile	Assessment form	exam
Conducting unit	Instytut Fizyki i Informatyki Stosowanej -> Faculty of Applied Physics and Mathematics		
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. inż. Marta Łabuda	
	Teachers	dr hab. inż. Marta Łabuda	

Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	0.0	30.0	0.0	45
	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	45	5.0	25.0	75

Subject objectives	Students will be introduced to the definitions and computational methods used to perform of the simulations of the structure and properties of the complex systems of biological interest, from biomolecules, proteins, DNA bases and more complex biological systems. Students will be introduced to the numerical methods used in the description of physical phenomena and understanding of the processes in the biological systems. Students will gain the knowledge of the chosen modelling methods and thechniques allowing their use in practise, particularly in biophysics, biochemistry and medicine.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[K7_U01] can apply mathematical knowledge to formulate and solve complex and non-typical problems related to the field of study by:n- appropriate selection of source information and its critical analysis, synthesis, creative interpretation and presentation,n- application of appropriate methods and toolsn	The student is aware of applications of chosen methods and apply them in the area of science and medicine. Student can perform simple calculations and simulations by means of the computational packages introduced in the lecture. Student can use the computational tools and interfaces for chosen biological systems. Student can use and search data in the databases and use the internet as a tool for search useful information.	[SU1] Assessment of task fulfilment [SU2] Assessment of ability to analyse information [SU4] Assessment of ability to use methods and tools
[K7_K01] is ready to create and develop models of proper behaviour in the work and life environment; undertake initiatives; critically evaluate actions of their own, teams and organisations they are part of; lead a group and take responsibility for its actions; responsibly perform professional roles taking into account changing social needs, including:n - developing the achievements of the profession,n- observing and developing rules of professional ethics and acting to comply to these rulesn	The student knows the theoretical aspects and basic definitions and theorems which concern the molecular physics and quantum mechanical calculations.Student can perform simple calculations by means of the computational packages introduced in the lecture.	[SK3] Assessment of ability to organize work [SK5] Assessment of ability to solve problems that arise in practice [SK2] Assessment of progress of work
[K7_W01] Knows and understands, to an increased extent, mathematics to the extent necessary to formulate and solve complex issues related to the field of study.	The student is aware of applications of chosen methods and apply them in the area of science and medicine.	[SW1] Assessment of factual knowledge [SW2] Assessment of knowledge contained in presentation [SW3] Assessment of knowledge contained in written work and projects

Subject contents

Computer modeling of physical processes taking place in nature. Software packages for studying of the properties of molecules, eg ORCA, MOLPRO. Characteristics, similarities and differences; technical limitations; errors, interpretation and visualization of results. Analysis of molecular dynamics simulation results, incorporation of experimental information into calculations, structures from NMR spectra. Modeling of structure and dynamics in large biological complexes, e.g. DNA. Visualization of structures and chemical properties of biomolecules. The most commonly used graphical interfaces. 3D graphics. The role of modeling methods in the analysis of complex biological systems. Databases of molecular structures. Modeling in medicine as a challenge for computational theories and methodologies. Modeling of physiological systems, e.g. the dynamics of blood flow in the heart muscle. Investigation of the influence of tissue blood supply on temperature stabilization. Nature-inspired computer algorithms. Information processing in the body. The nervous system as a cybernetic system. Neural networks and other artificial intelligence systems for medicine.

Prerequisites and co-requisites

Interest in mechanisms and processes taking place in biological systems and in modelling tools and methods.

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
Project	50.0%	60.0%
Project presentation	50.0%	40.0%

Recommended reading	Basic literature	Teaching materials in the form of the lectures given in on-line presentations Łabuda M. "Modelowanie układów biologicznych" (unpublished) Tadeusiewicz R, collective work, " Inżynieria biomedyczna" AGH 2008 Leach A., Molecular Modelling: Principles and applications Longman 1996 Schlick T., Molecular Modeling and Simulation Springer 2002 Jensen F.,Introduction to Computational Chemistry, Academic Press 2007 Peskin C.S., McQueen D.M., A three dimensional computational method for blood flow in the heart, J. Comput. Phys., 81, 1989, s. 372405.
	Supplementary literature	Homepages of the tools and packages used in the course.
	eResources addresses	Adresy na platformie eNauczanie:
Example issues/ example questions/ tasks being completed	1. Modeling of the dialysis therapy 2. Neural networks and other artificial intelligence algorithms for medicine 3. Modelling of carbohydrates metabolism	
Work placement	Not applicable	