Univerza v Mariboru
University of Maribor

FAKULTETA za NARAVOSLOVJE in MATEMATIKO
FACULTY OF NATURAL SCIENCE and MATHEMATICS

UČNI NAČRT PREDMETA / SUBJECT SPECIFICATION	
Predmet:	Atomistične simulacije biomolekul
Subject Title:	Atomistic simulations of biomolecules

Študijski program Study programme	Študijska smer Study field	Letnik Year	Semester Semester
FIZIKA PHYSICS		1 ali 2	**1 ali 2**

Univerzitetna koda predmeta / University subject code:

Predavanja Lectures	Seminar Seminar	Sem. vaje Tutorial	Lab. vaje Labor work	Teren. vaje Field work	Samost. delo Individ. work	ECTS
30	**20**				**250**	**10**

Nosilec predmeta / Lecturer: Franci Merzel

Jeziki / Languages:	
Predavanja / Lecture:	slovenski/Slovenian in/and angleški s slovenskim prevodom/English with translation in Slovenian
Vaje / Tutorial:	

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:

Ni posebnih zahtev.

Prerequisits:

No special prerequisites.

Vsebina:

- Opis kvantnih in klasičnih prostostnih stopenj ter inerakcij pri biomolekularnih sistemih
- Simulacije različnih statističnomehanskih porazdelitev
- Napredne metode in algoritmi za simulacije
- Struktura, dinamika in funkcija biomolekul
- Analiza normalnih načinov nihanja
- Povezava z glavnimi eksperimentalnimi tehnikami za določanje strukture (rentgenska kristalografija, NMR spektroskopija) in dinamike (IR in nevtronska spektroskopija)
- Računanje proste energije pri biokemijskih procesih (vezava ligandov)
- Problem zvijanja proteinov
- Simulacije agregacije polipeptidov

Content (Syllabus outline):

- Description of quantum and classical degrees of freedom and corresponding interactions in biomolecular systems
- Simulating various statistical-mechanical ensambles
- Advanced simulation methods and algorithms
- Structure, dynamics and function of biomolecules
- Normal mode analysis
- Simulation methods versus experimental techniques for structure determination (X-ray crystallography, NMR) and for studying dynamics (light and neutron spectroscopy)
- Calculating free energies in biochemical processes (ligand binding)
- Protein folding problem
- Simulating polypeptide aggregation

Temeljni literatura in viri / Textbook:

1) A. R. Leach, Molecular Modelling: Principles and Applications, Prentice Hall, 2001.

2) D. Frenkel, B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 2002.

3) M. Daune, Molecular biophysics: Structures in motion, Oxford, University Press, 1999.

Cilji:

Objectives:

Študenti poglobijo znanje s področja modeliranja v molekularni biofiziki. Študenti so sposobni uporabiti metode molekularnega modeliranja pri konkretnih problemih iz molekularne biofizike. Spoznajo pomembnost povezanosti računalniških simulacij z eksperimentalnimi metodami. Spoznajo najnovejše raziskave in delo raziskovalnih skupin na tem področju po svetu in v regiji.	Students acquire advanced knowledge in the field of modeling in molecular biophysics. Students are able to apply methods of molecular modeling to solve various problems in molecular biophysics. They learn about the importance of the link between computer simulations and experimental methods. Students get familiar with up-to-date research work and research teams working in that field in the region and worldwide.

Predvideni študijski rezultati:	**Intended learning outcomes:**
Znanja in razumevanja: Poglobljeno razumevanje in sposobnost formulacije problemov iz molekularne biofizike na atomskem nivoju ter njihovo reševanje s sodobnimi računalniškimi metodami. Prenosljive/ključne spretnosti in drugi atributi: Sposobnost razvoja in uporabe izvirnih znanstvenih rešitev pri konstruiranju matematičnih modelov molekularne biofizike ter njihova predstavitev v mednarodni znanstveni periodiki.	Knowledge and Understanding: Deeper understanding of - and abilities to formulate - problems in molecular biophysics on atomic-detail level and solving these problems using modern computational methods. Transferable/Key Skills and other attributes: Skills for development and implementation of original scientific solutions in constructing mathematical models of molecular biophysics. Presentation of acquired knowledge and research results in international scientific journals.

Metode poučevanja in učenja:	**Learning and teaching methods:**
Predavanja, seminar in izdelava samostojnih raziskovalnih/seminarskih nalog.	Lectures, seminar and work out of individual research-seminars.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Seminarska naloga	**50**	Coursework
Ustni izpit	**50**	Oral exam