Univerza v Mariboru
University of Maribor

FAKULTETA za NARAVOSLOVJE in MATEMATIKO
FACULTY OF NATURAL SCIENCE and MATHEMATICS

UČNI NAČRT PREDMETA / SUBJECT SPECIFICATION

Predmet:	Metode biofizikalnega modeliranja
Subject Title:	Methods of biophysical modelling

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
20	20		10		**250**	**10**

Nosilec predmeta / Lecturer: Franci Merzel, Aleš Fajmut

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

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	**Prerequisites:**
Ni posebnih zahtev.	No special prerequisites.

Vsebina:

Modeliranje molekularne dinamike:
- modeliranje na različnih velikostnih skalah (elektronska struktura, interakcije, medatomska polja sil, grobo zrnjenje)
- simulacije molekulske dinamike, Langevinove in Brownove dinamike ter Monte Carlo simulacije
- solvatacija/hidratacija biomolekul
- računanje fizikalnih opazljivk iz računskih modelov

Deterministične metode modeliranja celičnih procesov:
- modeliranje encimske kinetike in mrež biokemijskih reakcij
- kontrolna analiza
- modeliranje prenosa signalov v celici
- optimizacijske metode in določanje parametrov
- modeliranje fizioloških sistemov (srce, krvni obtok, izmenjava plinov, krčenje mišic, regulacija volumna celice…)

Stohastične metode modeliranja procesov v celici in tkivu:
- uvod: Brownovo gibanje, Langevinova enačba
- predstavitev t.i. »birth-death« master enačbe na primeru Lotka-Volterra modela
- osnove Gillespievega algoritma za stohastično modeliranje celičnih procesov
- uporaba Gillespievega algoritma na primeru kalcijeve signalizacije

Content (Syllabus outline):

Modelling of molecular dynamics:
- modelling on different scales (electron structure, interactions, inter-atomic fields of forces, rough fragmentation)
- simulation of molecular dynamics, Langevin’s and Brown’s dynamics and Monte Carlo simulations
- solvatation/hidratation of biomolecules
- calculation of physical observables from numerical models

Deterministic methods in modelling cellular processes:
- modelling of enzyme kinetics and networks of biochemical reactions
- control analysis
- modelling of signal transduction in the cell
- optimization methods and parameter estimation
- modelling of physiological systems (heart, blood flow, gas exchange, muscle contraction, cell volume regulation…)

Stochastic Methods for Modelling of Processes in Cells and Tissues:
- Introduction: Brownian motion, Langevin's equation
- Presentation of birth-death master equation by using Lotka-Volterra model
- Basics of Gillespie’s algorithm for stochastic modelling of cellular processes
- Application of Gillespie’s algorithm to the processes of

	calcium signalling

Temeljni literatura in viri / Textbook:

1. G.W. Gardiner, Handbook of Stochastic Methods, Springer, Hidelberg, 1997.
2. D.T. Gillespie, A general method for numerically simulating the stochastic time evolution of coupled chemical reactions. *J. Comput. Phys.* **22** (1976) 403–434.
3. R. Heinrich, S. Schuster: The Regulation of Cellular Systems, Chapman and Hall, New York 1996
4. E. Klipp, R. Herwig, A. Kowald, C. Wierling, H. Lehrach, Systems biology in practice, Wiley-vch, 2005, Weinheim
5. F.C. Hoppensteadt, C.S. Peskin, Modelling and simulation in medicine and the life science, Springer, 2002, New York
6. J. Keener, J. Sneyd, Mathematical Physiology, Springer, 1998, New York
7. A. R. Leach, Molecular Modelling: Principles and Applications, Prentice Hall, 2001.
8. D. Frenkel, B. Smit, Understanding Molecular Simulation: From Algorithms to Applications, Academic Press, 2002.

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

Cilji:	**Objectives:**
Študenti poglobijo znanje s področja metod biofizikalnega modeliranja, optimiranja, neravnosvesne termodinamike, reakcij in difuzije. Razumejo povezanost matematično-fizikalnih znanj ter znanj o raziskovanih bioloških sistemih. Spoznajo najnovejše raziskave in delo raziskovalnih skupin na tem področju v regiji.	Students acquire advanced knowledge on methods of biophysical modelling, optimization, nonequilibrium thermodynamics, reactions and diffusion. Students understand the connection between mathematical-physical skills and knowledge about biological systems. Students get familiar with up-to-date research work and research teams working in that field in the region.

Predvideni študijski rezultati:	**Intended learning outcomes:**
Znanja in razumevanja: Poglabljanje in nadgradnja interdisciplinarnih znanj s področij biofizikalnega modeliranja in metod statistične termodinamike ter aplikacij pri raziskovanju kompleksnih bioloških sistemov. Prenosljive/ključne spretnosti in drugi atributi: Reševanje interdisciplinarnih problemov v bioloških vedah z matematično-fizikalnimi orodji, numeričnimi metodami, univerzalnosti v fiziki in celosten pristop k reševanju biofizikalnih problemov.	Knowledge and Understanding: Gaining additional knowledge and upgrading interdisciplinary approach in the fields of biophysical modeling and statistical thermodynamics in exploration of complex biological systems. Transferable/Key Skills and other attributes: Solving interdisciplinary problems in biology sciences with mathematical-physical tools, numerical methods, universalities in physics and gained global approach on solving a biophysical problem.

Metode poučevanja in učenja:	**Learning and teaching methods:**
Predavanja in študij metod za analizo bio-relevantnih primerov	Lectures and study of methods for analysis of bio-relevant examples

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Ustni zagovor	**50**	Oral exam
3 projektne naloge	**50**	3 project assignments