Univerza v Mariboru

Fakulteta za naravoslovje in matematiko

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	**Metode biofizikalnega modeliranja**
Course title:	**Methods of biophysical modelling**

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
FIZIKA		**1**. ali 2.	**1., 2. ali 3.**
PHYSICS		1. or 2.	**1., 2. or 3.**

Vrsta predmeta / Course type	Izbirni za modula Biofizika 1, 2, 3 in Fizika 1, 2, 3
Univerzitetna koda predmeta / University course code:	

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Lab. vaje Laboratory work	Mentorstvo Mentorship	Samost. delo Individ. work	ECTS
7	**3**				**290**	**10**

Nosilec predmeta / Lecturer:	**Aleš Fajmut**
Jeziki / Languages: Predavanja / Lectures:	slovenski/Slovenian
Vaje / Tutorial:	

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

Vsebina:	**Content (Syllabus outline):**

Modeliranje molekularne dinamike:	Modelling of molecular dynamics:
- modeliranje na različnih velikostnih skalah (elektronska struktura, interakcije, medatomska polja sil, grobo zrnjenje)	- modelling on different scales (electron structure, interactions, inter-atomic fields of forces, rough fragmentation)
- simulacije molekulske dinamike, Langevinove in Brownove dinamike ter Monte Carlo simulacije	- simulation of molecular dynamics, Langevin's and Brown's dynamics and Monte Carlo simulations
- solvatacija/hidratacija biomolekul	- solvatation/hidratation of biomolecules
- računanje fizikalnih opazljivk iz računskih modelov	- calculation of physical observables from numerical models
Deterministične metode modeliranja celičnih procesov:	Deterministic methods in modelling cellular processes:
- modeliranje encimske kinetike in mrež biokemijskih reakcij	- modelling of enzyme kinetics and networks of biochemical reactions
- kontrolna analiza	- control analysis
- modeliranje prenosa signalov v celici	- modelling of signal transduction in the cell
- optimizacijske metode in določanje parametrov	- optimization methods and parameter estimation
- modeliranje fizioloških sistemov (srce, krvni obtok, izmenjava plinov, krčenje mišic, regulacija volumna celice…)	- modelling of physiological systems (heart, blood flow, gas exchange, muscle contraction, cell volume regulation…)
Stohastične metode modeliranja procesov v celici in tkivu:	Stochastic Methods for Modelling of Processes in Cells and Tissues:
- uvod: Brownovo gibanje, Langevinova enačba	- Introduction: Brownian motion, Langevin's equation
- predstavitev t.i. »birth-death« master enačbe na primeru Lotka-Volterra modela	- Presentation of birth-death master equation by using Lotka-Volterra model
- osnove Gillespievega algoritma za stohastično modeliranje celičnih procesov	- Basics of Gillespie's algorithm for stochastic modelling of cellular processes
- uporaba Gillespievega algoritma na primeru kalcijeve signalizacije	- Application of Gillespie's algorithm to the processes of calcium signaling

Temeljni literatura in viri / Readings:

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 in kompetence:	**Objectives and competences:**
Študenti poglobijo znanje s področja metod biofizikalnega modeliranja, optimiranja, neravnovesne 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:**
Znanje in razumevanje: Poglabljanje in nadgradnja interdisciplinarnih znanj s področij biofizikalnega modeliranja in metod statistične termodinamike ter aplikacij pri raziskovanju kompleksnih bioloških sistemov. Prenesljive/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:**
Način (pisni izpit, ustno izpraševanje, naloge, projekt)	**50%** **50%**	Type (examination, oral, coursework, project):

Ustni zagovor 3 projektne naloge		Oral exam 3 project assignments

Reference nosilca / Lecturer's references:

1. MBIKOU, Prisca, FAJMUT, Aleš, BRUMEN, Milan, ROUX, Etienne. Contribution of Rho kinase to the early phase of the calcium-contraction coupling in airway smooth muscle. *Experimental physiology*, ISSN 0958-0670, 2011, vol. 96, issue 2, str. 240-258, ilustr., doi: 10.1113/expphysiol.2010.054635. [COBISS.SI-ID 18009864]

2. DOBOVIŠEK, Andrej, FAJMUT, Aleš, BRUMEN, Milan. Role of expression of prostaglandin synthases 1 and 2 and leukotriene C [sub] 4 synthase in aspirin-intolerant asthma: a theoretical study. *Journal of pharmacokinetics and pharmacodynamics*, ISSN 1567-567X, 2011, vol. 38, no. 2, str. 261-278, doi: 10.1007/s10928-011-9192-6. [COBISS.SI-ID 18203144]

3. FAJMUT, Aleš, BRUMEN, Milan. MLC-kinase/phosphatase control of Ca[sup]2+ signal transduction in airway smooth muscles. *Journal of theoretical biology*, ISSN 0022-5193, 2008, vol. 252, no. 3, str. 474-481. http://dx.doi.org/10.1016/j.jtbi.2007.10.005, doi: 10.1016/j.jtbi.2007.10.005. [COBISS.SI-ID 15856392]

4. MBIKOU, Prisca, FAJMUT, Aleš, BRUMEN, Milan, ROUX, Etienne. Theoretical and experimental investigation of calcium-contraction coupling in airway smooth muscle. *Cell biochemistry and biophysics*, ISSN 1085-9195, 2006, vol. 46, no. 3, str. 233-251. http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?db=pubmed&cmd=Retrieve&dopt=AbstractPlus&list_uids=17272850&itool=iconabstr&query_hl=2&itool=pubmed_docsum. [COBISS.SI-ID 15168776]

5. FAJMUT, Aleš, JAGODIČ, Marko, BRUMEN, Milan. Mathematical modeling of the myosin light chain kinase activation. *Journal of chemical information and modeling*, ISSN 1549-9596. [Print ed.], 2005, [Vol.] 45, str. 1605-1609. [COBISS.SI-ID 14354184]