Univerza v Mariboru

Fakulteta za naravoslovje in matematiko

UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	**Simulacijske metode v fiziki kondenzirane snovi**
Course title:	**Simulation methods in condensed matter physics**

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
FIZIKA		1. ali 2.	**1., 2. ali 4.**
PHYSICS		1. or 2.	**1., 2. or 4.**

Vrsta predmeta / Course type: Izbirni za vse module

Univerzitetna koda predmeta / University course code:

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Lab. vaje Laboratory work	Mentorstvo Mentorship	Samost. delo Individ. work	ECTS
15					**165**	**6**

Nosilec predmeta / Lecturer: **Victor Teboul**

Jeziki / Languages:		
	Predavanja / Lectures:	angleško/English
	Vaje / Tutorial:	

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

Predznanje klasične fizike, moderne fizike, osnovnih numeričnih metod, matematičnih metod v fiziki.

Prerequisits:

Pre-knowledge of classical physics, modern physics, basic numerical methods, and mathematical methods in physics.

Vsebina:

- Fizikalne osnove simulacij. Prednosti in slabosti.
- Poglavitne simulacijske metode: Monte Carlo in molekularna dinamika.
- Principi naprednih simulacijskih metod (disipativna dinamika delcev, metoda zrnjenja, ograjenost...).

Content (Syllabus outline):

- The physics behind the simulations. Advantages and drawbacks.
- The main simulation methods: Monte Carlo and Molecular Dynamics.
- Principles of advanced simulations methods (dissipative particle dynamics. coarse graining, confinement, ...).
- Statistics from the raw results.

• Statistika »surovih« rezultatov. • Naprednejše metode. • Primeri in aplikacije.	• More advanced technics. • Examples and applications.

Temeljni literatura in viri / Readings:

1) M.P. Allen and D.J. Tildesley, Computer simulation of liquids, Clarendon Press, Oxford, 1994.
2) M. Griebel, S. Knapek, G. Zumbusch, Numerical Simulation in Molecular Dynamics, Springer, Berlin 2007.
3) D. Frenkel, B. Smit, Understanding Molecular Simulation, Academic Press, San Diego 1996.
4) D.P. Landau, K. Binder, A guide to Monte Carlo simulations in Statistical Physics, Cambridge University Press, Cambridge, 2000.
5) Molecular modelling: Principles and applications, A. Leach, Pearson, 2001.
6) Introduction to modern statistical mechanics, D. Chandler, Oxford University Press, Oxford 1987.

Cilji in kompetence:	**Objectives and competences:**
Študenti pridobijo napredna znanja s področja simulacij v fiziki kondenzirane materije.	Students acquire advanced knowledge on simulations in condensed matter physics.

Predvideni študijski rezultati:

Znanje in razumevanje: Razumevanje simulacijskega modeliranja različnih fizikalnih problemov. Pridobitev naprednih znanj na področju računalniških metodologij za reševanje fizikalnih problemov. Prenesljive/ključne spretnosti in drugi atributi: Reševanje problemov z numeričnimi metodami.	Knowledge and understanding: Understanding of simulation modeling of various problems in physics. Knowledge of computational methodologies for physics problem solving. Transferable/Key Skills and other attributes: Solving of problems with numerical methods.

Metode poučevanja in učenja:	**Learning and teaching methods:**
Predavanja in reševanje zastavljenih problemov.	Lectures and solving of defined problems.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Način (pisni izpit, ustno izpraševanje, naloge, projekt)		Type (examination, oral, coursework, project):
Seminar	**50%**	Seminar
Ustni izpit	**50%**	Oral exam

Reference nosilca / Lecturer's references:

1. Taamalli SoniaHafedh BelmabroukVo Van HoangVictor Teboul, How do packing defects modify the cooperative motions in supercooled liquids? Apr 2017, Chemical Physics

2. Taamalli SoniaJulia HindsSam Vincent MigirditchVictor Teboul, Enhanced diffusion in finite-size simulations of a fragile diatomic glass former, Nov 2016, Physical Review E

3. Ciobotarescu SimonaNicolae HurducVictor Teboul, How does the motion of the surrounding molecules depend on the shape of a folding molecular motor? May 2016, Physical Chemistry Chemical Physics

4. A toy model mimicking cage effect, structural fluctuations and kinetic constraints in supercooled liquids, V. Teboul, Journal of Chemical Physics, **141**, 194501 (2014).

5. Induced cooperative motions in a medium driven at the nanoscale: Searching for an optimum excitation period, V. Teboul, J.B. Accary, Physical Review E , **89**, 012303 (2014).