



Univerza v Mariboru

Fakulteta za naravoslovje  
in matematiko

### UČNI NAČRT PREDMETA / COURSE SYLLABUS

<b>Predmet:</b>	<b>Simulacijske metode v fiziki kondenzirane snovi</b>
<b>Course title:</b>	<b>Simulation methods in condensed matter physics</b>

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
FIZIKA, 3. stopnja		1. ali 2.	1., 2. ali 4.
PHYSICS, 3 <sup>rd</sup> cycle		1. or 2.	1., 2. or 4.

**Vrsta predmeta / Course type**

Izbirni za vse module/ Optional for all  
modules

**Univerzitetna koda predmeta / University course code:**

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje work	Druge oblike študija	Samost. delo Individ. work	ECTS
15					165	6

**Nosilec predmeta / Lecturer:**

Victor Teboul

**Jeziki /**

**Languages:**

**Predavanja /**

**Lectures:**

angleško/English

**Vaje / Tutorial:**

angleško/English

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

Pogojev ni.

Priporočljiva znanja so: predznanje klasične fizike, moderne fizike, osnovnih numeričnih metod, matematičnih metod v fiziki.

**Prerequisites:**

None.

Recommended is knowledge of classical physics, modern physics, basic numerical methods, and mathematical methods in physics.

**Vsebina:**

**Content (Syllabus outline):**

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

Primeri in aplikacije.

- 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.
- 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.
- Introduction to modern statistical mechanics, D. Chandler, Oxford University Press, Oxford 1987.

### Cilji in kompetence:

Študenti pridobijo napredna znanja s področja simulacij v fiziki kondenzirane materije.

### Objectives and competences:

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.

Prenosljive/ključne spretnosti in drugi atributi:

Reševanje problemov z numeričnimi metodami.

### Intended learning outcomes:

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.

Delež (v %) /

**Načini ocenjevanja:**

Weight (in %) **Assessment:**

Seminar.

**50%**

Seminar.

Ustni izpit.

**50%**

Oral exam.

**Reference nosilca / Lecturer's references:**

Teboul, V. (2023). Dynamic phase transition induced by active molecules in a supercooled liquid. *Physical Review E*, 108(2), 024605 <https://doi.org/10.1103/PhysRevE.108.024605>

V Teboul, S. Ciobotarescu. Orientation of motion of a flat folding nano-swimmer in soft matter. *Physical Chemistry Chemical Physics* 14 (2021) DOI <https://doi.org/10.1039/D1CP00136A>

V Teboul, G Rajonson, Temperature dependence of the violation of Purcell's theorem experienced by a folding molecular motor. *Physical Chemistry Chemical Physics* 21 (5), 2472-2479 (2019)