



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 3. |
| PHYSICS | | 1. or 2. | 1., 2. or 3. |

Vrsta predmeta / Course type

Izbirni za modula Biofizika 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 |
|------------------------|--------------------|------------------|---------------------------------|--------------------------|----------------------------------|------|
| 5 | - | | | | 145 | 5 |

Nosilec predmeta / Lecturer: Victor Teboul, Samo Kralj

Jeziki / Languages:
Predavanja / Lectures: slovenski/Slovenian
Vaje / Tutorial:

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

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

Prerequisites:

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

Content (Syllabus outline):

- The physics behind the simulations. Advantages and drawbacks.
- The main simulation methods: Monte

- Carlo in molekularna dinamika.
- Principi naprednih simulacijskih metod (disipativna dinamika delcev, metoda zrnjenja, ograjenost...).
 - Statistika »surovih« rezultatov.
 - Naprednejše metode.
 - Primeri in aplikacije.

- 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.
- 6) 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.

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:

Predavanja in reševanje zastavljenih problemov.

Learning and teaching methods:

Lectures and solving of defined problems.

Načini ocenjevanja:

Način (pisni izpit, ustno izpraševanje, naloge, projekt)

Delež (v %) /

Weight (in %)

Assessment:

Type (examination, oral, coursework, project):

| | | |
|------------------------|--------------------------|----------------------|
| Seminar Ustni izpit | 50% 50% | Seminar Oral exam |
|------------------------|--------------------------|----------------------|

Reference nosilca / Lecturer's references:

1. A toy model mimicking cage effect, structural fluctuations and kinetic constraints in supercooled liquids, V. Teboul, *Journal of Chemical Physics*, 141, 194501 (2014).
2. S. Kralj, G. Cordoyiannis, D. Jesenek, A. Zidansek, G. Lahajnar, N. Novak, H. Amenitsch, Z. Kutnjak, Dimensional crossover and scaling behavior of a smectic liquid crystal confined to controlled-pore glass matrices, *Soft matter* 8, 2460 (2012).
3. Isomerization of azobenzene and the enhancement of dynamic heterogeneity in molecular glass-formers. V. Teboul, J.B. Accary, M. Chrysos, *Physical Review E*, 87, 032309 (2013)
4. RANJKESH SIAHKAL, Amid, AMBROŽIČ, Milan, KRALJ, Samo, SLUCKIN, T. J. Computational studies of history dependence in nematic liquid crystals in random environments. *Physical review. E, Statistical, nonlinear, and soft matter physics*, ISSN 1539-3755, 2014, vol. 89, iss. 2, str. 022504-1-022504-14, doi: 10.1103/PhysRevE.89.022504. [COBISS.SI-ID 20347912]
5. Time versus temperature rescaling for coarse grain molecular dynamics simulations, J.B. Accary, V. Teboul, *Journal of Chemical Physics*, 136, 094502 (2012)