UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	Napredne numerične metode v fiziki
Course title:	Advanced numerical methods in Physics

Študijski program in stopnja Study programme and level	Študijska smer Study field	Letnik Academic year	Semester Semester
Fizika 2. st.		1	2
Physics 2nd degree		1	2

Vrsta predmeta / Course type izbirni/ optional

Univerzitetna koda predmeta / University course code:

Predavanja Lectures	Seminar Seminar	Sem. vaje Tutorial	Lab. vaje Laboratory work	Teren. vaje Field work	Samost. delo Individ. work	ECTS
45	0	15	60	0	180	**10**

Nosilec predmeta / Lecturer: Jure dobnikar

Jeziki / Languages:	
Predavanja / Lectures:	slovenski/Slovenian in/and angleški/English
Vaje / Tutorial:	slovenski/Slovenian in/and angleški/English

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

Priporočljivo je predznanje, ki se ga pridobi pri predmetih:
- Numerične metode v fiziki
- Modelska fizika

Prerequisits:

Knowledge about topics included in the following subjects is recomended:
- Numerical methods in physics
- Physical modeling

Vsebina:

- programski jeziki in orodja (Fortran, C, Matlab, Mathematica, razni paketi za simulacije)
- programiranje paralelnih računalnikov
- analiza in vizualizacija podatkov (obdelava podatkov, Fourier-jeva transformacija, statistične metode, izdelava diagramov in poročil)
- Monte Carlo, molekularna dinamika in stohastične metode simulacije
- Nelinearni sistemi: od integrabilnosti do kaosa
- Modeliranje bioloških sistemov
- Faze in fazni prehodi
- Numerična hidrodinamika in disipativni sistemi
- Numerična kvantna mehanika
- Modeliranje molekul in makromolekul
- Numerično reševanje navadnih in parcialnih diferencialnih enačb

Content (Syllabus outline):

- Programming languages and tools (Fortran, C++, Matlab, Mathematica and various simulation packages)
- Paralel programming
- Data analysis and visualization (data manipulation, Fourier transform, statistical methods, creating diagrams and reports)
- Monte Carlo, molecular dynamics and stochastic simulation methods
- Nonlinear systems: from integrability to chaos
- Modeling of biological systems
- Phases and phase transitions
- Numerical hydrodynamics and dissipative systems
- Numerical quantum mechanics
- Molecular and macromolecular modeling
- Numerical methods for ordinary and partial differential equations

Temeljni literatura in viri / Readings:

1. D. Frenkel, B.J.Smit, Understanding Molecular Simulation,Elsevier, 2002
2. M.P. Allen, D.J. Tildesley, Computer Simulation of Liquids,Oxford, 1989
3. W.H. Press indr.: Numerical Recipes in C, Cambridge University Press, 1994
4. Z. Bohte: Numerične metode. Ljubljana: DMFA,1985,
5. F. J. Vesely: Computational Physics, An Introduction, Plenum Press, 1994
6. Duane C. Hanselman, Bruce L. Littlefield: Mastering Matlab 7, Prentice Hall, 2004

Cilji in kompetence:

- Podati pregled programskih jezikov in orodij
- Poudariti pomen obdelave in predstavitve podatkov
- Podati osnove modernih numeričnih metod, ki se uporabljajo pri znanstvenoraziskovalnem delu
- Predelati primere uporabe metod na fizikalnih problemih

Objectives and competences:

- Overview: programming languages and tools
- Data presentation and manipulation
- Modern numerical techniques used in research
- Examples of application of the methods on physical problems

Predvideni študijski rezultati:

Znanje in razumevanje:

- Numerične metode za reševanje diferencialnih enačb
- Pregled metod numerične simulacije
- Pararelno programiranje
- Programski jeziki in orodja

Prenesljive/ključne spretnosti in drugi atributi:

- numerično reševanje parcialnih in navadnih diferencialnih enačb
- numerične simulacije
- opis fizikalnega modela, numerično reševanje in predstavitev rezultatov
- samostojno pregledovanje znanstvene literature in predstavitev seminarja

Intended learning outcomes:

Knowledge and Understanding:

- Numerical methods for differential equation solving
- Knowledge about the methods of numerical simulation
- Paralel programming
- Programming languages and tools

Transferable/Key Skills and other attributes:

- Numerical solving of ordinary and partial differential equations
- numerical simulations
- Physical model, numerical solution and presentation of the results
- Independent literature search and presentation of seminars

Metode poučevanja in učenja:

- Predavanja
- Naloge
- Seminarji
- Vaje

Learning and teaching methods:

- Lectures
- Coursework
- Seminars
- Excersises

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Ustni izpit	25	Oral exam
Seminar	25	Seminar
Naloge	50	Coursework

Reference nosilca / Lecturer's references:

KANDUČ, Matej, DOBNIKAR, Jure, PODGORNIK, Rudolf. Counterion-mediated electrostatic interactions between helical molecules. *Soft matter*, 2009, issue 5, vol. 5, str. 868-877, doi: 10.1039/b811795k. [COBISS.SI-ID 2149988]

TRIZAC, Emmanuel, EL SHAWISH, Samir, DOBNIKAR, Jure. Dimeric and dipolar ground state orders in colloidal molecular crystals. *An. Acad. Bras. Cienc.*, 2010, vol. 82, no. 1, str. 87-94. [COBISS.SI-ID23483687]

EL SHAWISH, Samir, DOBNIKAR, Jure, TRIZAC, Emmanuel. Colloidal ionic complexes on periodic substrates : ground-state configurations and pattern switching. *Phys. rev., E Stat. nonlinear soft matter*

phys. (Print), 2011, vol. 83, no. 4, str. 041403-1-041403-10. [COBISS.SI-ID 24653095]

MATTHÄUS, Franziska, MOMMER, Mario S., CURK, Tine, DOBNIKAR, Jure. On the origin and characteristics of noise-induced Lévy Walks of E. Coli. *PLoS one*, 2011, vol. 6, no. 4, str. e18623-1-e18623-8.http://www.plosone.org/article/info:doi/10.1371/journal.pone.0018623. [COBISS.SI-ID 25045031]

CURK, Tine, HOOGH, Anouk de, MARTINEZ-VERACOECHEA, Francisco J., EISER, Erika, FRENKEL, Daan, DOBNIKAR, Jure, LEUNISSEN, Mirjam E. Layering, freezing, and re-entrant melting of hard spheres in soft confinement. *Phys. rev., E Stat. nonlinear soft matter phys. (Online)*. [Online ed.], 2012, vol. 85, iss. 2, str. 021502-1-021502-5. http://link.aps.org/doi/10.1103/PhysRevE.85.021502, doi:10.1103/PhysRevE.85.021502. [COBISS.SI-ID 518221081]