UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet	Napredne numerične metode
Course name	Advanced numerical methods

Študijski program in stopnja Study program and level	Študijska smer Study field	Letnik Academic year	Semester Semester
Fizika in Astrofizika II. stopnja	Fizika trdne snovi	1	/
Physics and Astrophysics II. level	Solid state physics	1	/

Vrsta predmeta / Course type	obvezni / mandatory
Univerzitetna koda predmeta / University course code	2FTS03

Predavanja Lectures	Seminar Seminar	Sem. vaje Tutorial	Lab. vaje Lab. work	Teren. vaje Field work	Samost. delo Indiv. work	ECTS
30	/	30	/	/	210	9

Nosilec predmeta / Lecturer	Doc. dr. Luigi Giacomazzi	
Jeziki / Languages	**Predavanja / Lectures**	slovenščina / English
	Vaje / Tutorial	slovenščina / English

Pogoji za opravljanje študijskih obveznosti	Prerequisites
Računalniško programiranje	Computer programming

Vsebina	Syllabus outline
Uvod - Sistem linearnih enačb - Sistem linearnih diferencialnih enačb - Minimizacija - Iskanje prevoja - Diagonalizacija - Konsistenčna rešitev - Iskanje parametrov funkcij - Filtriranje Molekulsko modeliranje - Rešitve enačbe gibanja, Verletov algoritm - Robni pogoji - NVE - NVT, nastavitve začetne hitrosti in kontrola temperature - NPE	Introduction -System of linear equations -System of linear differential equations -Minimization -Saddle points search -Diagonalization -Self-Consistent equation -Fittings -Filtering Molecular Modeling -Solution of the Equation of Motion, the VERLET algorithm -Boundary conditions -NVE -NVT, intialization of velocities and temperature control -NPE

1D veriga harmonskih oscilatorjev - diskretizacija enačbe gibanja - dinamika z fiksnimi robnimi pogoji ali periodičnimi robnimi pogoji - nihajni načini 3D model s klasičnim opisom sil in peridočnimi robnimi pogoji (p.r.p.) - diskretizacija enačbe gibanja - dinamika z p.r.p. in NVE in NVT - difuzijski koeficient - Parska korelacijska funkcija in strukturni faktor	1D-Chain of harmonic oscillators -Discretization of the equation of motion -dynamics with Fixed borders or periodic boundary conditions -Vibrational modes 3D modeling with classical force-fields and periodic boundary conditions -Discretization of the equation of motion -Dynamics with PBC in NVE and NVT -Diffusion coefficient -Pair-correlation functions and structure factor

Temeljni literatura in viri / Basic readings
Introduction to numerical Methods, Jeffrey R. Chasnov, Honkong University for Science and Technology. Molecular Modelling: Principles and applications, Dr. Andrew Leach, Prentice Hall (2001).

Cilji in kompetence	**Objectives and competences**
Cilj predmeta je študente soočiti z izbranimi numeričnimi temami, ki so aktualne za njihov študij fizike trdne snovi. Študenti bodo dobili znanje priprave in izvedbe izračunov iz področja molekulskih simulacij, ki jih bodo s pomočjo nosilca predmeta združili v izboljšano in poglobljeno razumevanje problematike. Osnovni cilj predmeta je usposobiti študente za samostojno delo z numeričnimi metodami na vseh glavnih področjih matematične fizike. Na osnovi pridobljenih znanj bodo znali kritično izbrati primerne metode za numerične probleme, ki jih bodo srečali v praksi.	The objective of the course is to face students with selected numerical topics that are relevant for their studies in solid state physics. Students will acquire specialized knowledge from the construction from scratch of a complete molecular dynamic code. With the help of the course principal, they will transform this knowledge into an improved and in-depth understanding. The primary goal of this course is to prepare students for independent work with numerical methods in all major areas of mathematical physics. On the basis of attained knowledge they will be competent to choose the correct methods in order to tackle numerical problems that they will encounter in practice.

Predvideni študijski rezultati	**Intended learning outcomes**
Znanje in razumevanje: Slušatelji se bodo naučili samostojnega razvoja in uporabe različnih numeričnih metod. Sami bodo razvili programe, ki implementirajo numerične metode, opisane v vsebini predmeta. S temi numeričnimi metodami bodo razrešili dane probleme. Na osnovi rešitev teh problemov bodo kritično	Students will learn independent development and use of various numerical methods. They will develop their own codes that implement given numerical approaches, described in the syllabus. Using these numerical methods they will tackle given problems. On the basis of the solutions of these problems, they will critically evaluate the

ocenili implementirane numerične metode. Tako bodo osvojili razumevanje za natančnost, stabilnost in računsko zahtevnost različnih numeričnih pristopov.	implemented numerical methods. In this way, they will attain understanding of accuracy, stability and computational complexity demands of various numerical approaches.

Metode poučevanja in učenja	**Learning and teaching methods**
- predavanja, vaje, domače naloge	- lectures, tutorial, homework

Načini ocenjevanja	**Utež / Weight (%)**	**Assessment**
- domače naloge - pisni izpit - ustni izpit	33 33 34	- homework - written exam - oral exam

Reference nosilca / references of the course principal
Dr. Luigi Giacomazzi je docent za področje fizike na Univerzi v Novi Gorici. Luigi Giacomazzi is an assistant professor of physics at the University of Nova Gorica.