UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	Višje računske metode
Course title:	Advanced computational physics

Študijski program in stopnja Study programme and level	**Študijska smer Study field**	**Letnik Academic year**	**Semester Semester**
Univerzitetni študijski program 2.stopnje Fizika	Fizika	**2**	**drugi**
Second cycle academic study program Physics	Physics	**2**	**second**

Vrsta predmeta / Course type	obvezni predmet/compulsory course

Univerzitetna koda predmeta / University course code:	???

Predavanja Lectures	**Seminar Seminar**	**Vaje Tutorial**	**Klinične vaje work**	**Druge oblike študija**	**Samost. delo Individ. work**	**ECTS**
45		**45**			**150**	**8**

Nosilec predmeta / Lecturer:	prof. dr. Tomaž Prosen

Jeziki / Languages:	**Predavanja / Lectures:**	**Slovensko/Slovene**
	Vaje / Tutorial:	**Slovensko/Slovene**

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

Vpis v letnik študija.	Enrollment into the program.

Vsebina:

Content (Syllabus outline):

Kvantna fizika: • simulacije časovnega razvoja v kvantni mehaniki, “split-step” (Suzuki-Trotter) razcepi unitarnih operatorjev – simplektični integratorji, • učinkovite diagonalizacijske metode za velike, redke matrike: Lanczos, Arnoldi, • osnovni ensembli slučajnih matrik in statistično modeliranje kompleksnih kvantnih sistemov, • metoda gostotnih funkcionalov. **Statistična fizika (klasična in kvantna):** • časovni razvoj klasičnih statistično-mehanskih sistemov, primeri simulacije "molekularne dinamike", • modeliranje toplotnih kopeli in stohastične differencalne enačbe: Langevin, Ohrnstein-Uhlenbeckovi procesi, • metode Monte-Carlo, detajlno ravnovesje in simulirano ohlajanje. primeri: klasični spinski sistemi, • kvantni Monte-Carlo, preprost primeri, Feynmanov pot-integral • numerične metode renormalizacijske grupe (NRG, DMRG), primeri: časovna relaksacija in termalizacija • variacijske metode v bazi stanj matričnih produktov, kvantna prepletenost, ploščinski zakoni, entropije in simulabilnost.	**Quantum physics:** • simulation of time evolution in quantum mechanics, “split-step” (Suzuki-Trotter) decompositions of unitary operators – simplectic integrators • efficient diagonalization of large and sparse matrices: Lancoz, Arnoldi • basic concepts of random matrix theory and modelling of complex quantum systems, • density functional theory (DFT). **Statistična fizika (klasična in kvantna):** • time evolution of classical statistical-mechanical systems, “molecular dynamics” simulations, • modelling of heat baths and stochastic differential equations: Langevin, Ohrnstein-Uhlenbeck processes, • Monte-Carlo methods, detailed balance and simulated annealing. examples: classical spin systems, • Quantum Monte-Carlo, simple examples, Feynman path-integral • numerical renormalization group methods (NRG, DMRG), examples: quantum spin chains, relaxation and thermalization • variational methods in matrix-product basis, area-laws, quantum entanglement, simulability.

Temeljni literatura in viri / Readings:

- W. G. Hoover, Computational Statistical Mechanics, (Elsevier 1991),
- J. P. Sethna, Entropy, Order Parameters and Complexity (Oxford UP, 2006),
- Quantum Simulations of Complex Many-Body Systems: From theory to algorithms (Lecture notes, ur. J. Grotendorst, D. Marx in A. Muramatsu), NIC Series, Vol 10 (2002).
- U. Schollwoeck, The density-matrix renormalization group in the age of matrix product states, Annals of Physics 326 , 96-192 (2011)

Cilji in kompetence:	**Objectives and competences:**
Študent naj bi se seznanil z nekaterimi najosnovnejšimi in uporabnimi state-of-the-art numeričnimi metodami in algoritmi za simulacijo sistemov z nekaj ali mnogo interagirajočimi prostostnimi stopnjami v statistični in/ali kvantni fiziki.	Student should master some of the most basic and useful state-of-the art computational methods for simulation of simple (single particle, or linear), and complex (many particle, or non-linear) quantum or classical statistical systems.

Predvideni študijski rezultati:	**Intended learning outcomes:**

Znanje in razumevanje Obvladovanje zahtevnejših numeričnih metod in pristopov za simulacijo sistemov z velikim številom prostostnih stopenj v statistični in kvantni fiziki. **Uporaba** Pridobljeno znanje naj bi študent znal uporabljati predvsem pri teoretičnem modeliranju in računalniškem simuliranju kompleksmih sistemov v fiziki. **Refleksija** Študent naj bi pridobil občutek kaj je možno učinkovito simulirati z računalnikom in kaj ne. **Prenosljive spretnosti - niso vezane le na en predmet** Metode in vsebine se neposredno navezujejo na (neravnovesno) statistično fiziko, teorijo dinamičnih sistemov, teorijo trdne snovi in višjo kvantno mehaniko.	**Knowledge and understanding:** Mastering of advanced numerical methods and approaches to simulations of systems with many degrees of freedom in statistical and quantum physics. **Application:** Student should know how to apply the new knowledge in theoretical modelling and computer simulations of complex systems in physics **Reflection:** Student should get a feeling for what is possible to simulate efficiently in pysics and what not. **Transferable skills:** The methods and contents of the course have links to, or require some prior knowledge from courses on: statistical physics, theory of dynamical systems, solid state physics and advanced quantum mechanics.

Metode poučevanja in učenja:	**Learning and teaching methods:**
Predavanja, vaje, individualne naloge, konzultacije	Lectures, exercises, homework projects, consultations

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**

• Uspešna samostojna izdelava šestih dvotedenskih projektnih domačih nalog, predstavitev pri vajah in individualni zagovor • ocene: 1-5 (negativno), 6-10 (pozitivno) (po Statutu UL)	**6 x 16.7%**	▪ Sucessful individual completion of six biweekly project homeworks, their discussion in the class and individual defence with professor/ assistant ▪ grading: 1-5 (fail), 6-10 (pass) (according to the Statute of UL)

Reference nosilca / Lecturer's references:

Prof. dr. Tomaž Prosen

1) GORIN, Thomas, PROSEN, Tomaž, SELIGMAN, Thomas H., ŽNIDARIČ, Marko. Dynamics of Loschmidt echoes and fidelity decay. *Physics reports*, ISSN 0370-1573. [Print ed.], 2006, 435, nos. 2-5, str.3-156. [COBISS.SI-ID 1972068]
2) PROSEN, Tomaž, ŽNIDARIČ, Marko. Matrix product simulations of non-equilibrium steady states of quantum spin chains. *Journal of statistical mechanics*, ISSN 1742-5468, 2009, no. 2, str. P02035-1-P02035-19, doi: 10.1088/1742-5468/2009/02/P02035. [COBISS.SI-ID 2150756]
3) PROSEN, Tomaž. Open XXZ spin chain : nonequilibrium steady state and strict bound on ballistic transport. *Physical review letters*, ISSN 0031-9007. [Print ed.], 2011, vol. 106, issue 21, str. 217206-1-217206-4, doi: 10.1103/PhysRevLett.106.217206. [COBISS.SI-ID 2347108]
4) ILIEVSKI, Enej, PROSEN, Tomaž. Thermodynamic bounds on Drude weights in terms of almost-conserved quantities. *Communications in Mathematical Physics*, ISSN 0010-3616, 2013, vol. 318, no. 3, str. 809-830. http://download.springer.com/static/pdf/48/art%253A10.1007%252Fs00220-012-1599-4. pdf?auth66=1363681672_5113fee186b3d7c9c4df4b1c6a129545&ext=.pdf. [COBISS.SI-ID 2535524]
5) PROSEN, Tomaž. Exact nonequilibrium steady state of an open Hubbard chain. *Physical review letters*, ISSN 0031-9007. [Print ed.], 2014, vol. 112, iss. 3, str. 030603-1-030603-5. http://prl.aps.org/abstract/PRL/v112/i3/e030603. [COBISS.SI-ID 2636644]