

## 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:** Prerequisites:

Vpis v letnik študija.

Enrollment into the program.

**Vsebina:**

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**Content (Syllabus outline):**

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**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 diferencialne enačbe: Langevin, Ornstein-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 – symplectic integrators
- efficient diagonalization of large and sparse matrices: Lanczos, 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, Ornstein-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.

**Temeljna literatura in viri / Readings:**

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- 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:**

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.

**Objectives and competences:**

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 kompleksnih 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 physics 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:**

Predavanja, vaje, individualne naloge, konzultacije

**Learning and teaching methods:**

Lectures, exercises, homework projects, consultations

**Načini ocenjevanja:**

Delež (v  
%) /  
Weight (in  
%)

**Assessment:**

<ul style="list-style-type: none"> <li>• Uspešna samostojna izdelava šestih dvotedenskih projektnih domačih nalog, predstavitev pri vajah in individualni zagovor</li> <li>• ocene: 1-5 (negativno), 6-10 (pozitivno) (po Statutu UL)</li> </ul>	<b>6 x 16.7%</b>	<ul style="list-style-type: none"> <li>▪ Successful individual completion of six biweekly project homeworks, their discussion in the class and individual defence with professor/assistant</li> <li>▪ grading: 1-5 (fail), 6-10 (pass) (according to the Statute of UL)</li> </ul>
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#### 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](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](#)]