| UČNI NAČRT PREDMETA / COURSE SYLLABUS | |
|---|---|
| **Predmet:** | MODELIRANJE KEMIJSKIH SISTEMOV |
| **Course Title:** | MODELLING OF CHEMICAL SYSTEMS |

| Študijski program in stopnja<br>Study Programme and Level | Študijska smer<br>Study Field | Letnik<br>Academic Year | Semester<br>Semester |
|---|---|---|---|
| MAG Kemija, 2. stopnja | / | 2. | 4. |
| USP Chemistry, 2nd Cycle | / | 2nd | 4th |

**Vrsta predmeta / Course Type:** izbirni strokovni / Elective Professional

**Univerzitetna koda predmeta / University Course Code:** K2I22

| Predavanja<br>Lectures | Seminar<br>Seminar | Vaje<br>Tutorial | Klinične vaje<br>Work | Druge oblike študija | Samost. delo<br>Individual Work | ECTS |
|---|---|---|---|---|---|---|
| 30 | / | 45 LV | / | / | 75 | 5 |

**Nosilec predmeta / Lecturer:** izr. prof. Tomaž Urbič / Dr. Tomaž Urbič, Associate Professor

**Jeziki / Languages:**

| | |
|---|---|
| **Predavanja / Lectures:** | **slovenski / Slovenian** |
| **Vaje / Tutorial:** | **/** |

| Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti: | Prerequisites: |
|---|---|
| Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost. | The course has to be assigned to the student. |

| Vsebina: | Content (Syllabus outline): |
|---|---|
| Ponovitev osnov o programskih jezikih (fortran, c, phyton, java), ki se bodo predvidoma uporabljali za praktično delo na računalniku.<br>Statistične metode in pristopi pri obdelavi eksperimentalnih podatkov. Modeliranje podatkov (aproksimacija z nelinearnimi funkcijami). Filtriranje signalov in interpretacija (IR, NMR, masnih) spektrov (Fourierova transformacija in Fourierova analiza). Izračun časovnega poteka kemijskih reakcij (kemijska kinetika). Modeliranje dvoelektronskih sitemov v Hartree-Fockovem približku, primer helijevega atoma in vodikove molekule. Predstavitev in reševanje difuzijskih | Introduction in basics of computer programming (fortran, c, python, java) which will be used in practical work on computers.<br>Statistical methods for representation of experimental data. Modelling of data (fitting with non-linear functions). Filtering of signals and interpretation of (IR, NMR, mass) spectra (Fourier transform and Fourier analysis). Time dependence of chemical reactions (chemical kinetics). Modelling of two-electron systems with Hartree-Fock approximation (helium atom and hydrogen molecule). Numerical approximations for solving of partial differential equations (diffusion problems, flow of fluids and flow of heat). Lattice Boltymann method. Calculation of structure of fluids and solutions |

| | |
|---|---|
| problemov, pretakanja tekočin in toplotnih sistemov (numerično reševanje parcialnih diferencialnih enačb). Lattice Boltzmannova metoda. Določanje strukture tekočin in raztopin s pomočjo reševanja integralskih enačb. Modeliranje slučanih procesov. Numerično integriranje s pomočjo Monte Carlo metode in Monte Carlo simulacije preprostih tekočin (Metropolisov algoritem). Molekulska dinamika preprostih kemijskih sitemov. | by integral equation theory. Modelling of coincidental events. Numerical integration with Monte Carlo method and Monte Carlo simulation of simple fluids (Metropolis algorithm). Molecular dynamics of simple chemical systems. |

**Temeljna literatura in viri / Readings:**

-W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, Numerical Recipes in Fortran, Cambridge University Press, Cambridge, 1994. (20%)
-D. Frenkel, B. Smit, Understanding Molecular Simulation, Academic Press, San Diego, 1996. (10%)
-Priročniki za programske jezike.

| **Cilji in kompetence:** | **Objectives and Competences:** |
|---|---|
| *Cilj* predmeta je študentom predstaviti metode za numerično reševanje matematičnih problemov, na katere lahko naleti pri vsakdanjem delu na področju znanosti, tehnike.<br>*Kompetence:* Pri predmetu naj bi dobil študent teoretično podlago in praktične izkušnje za samostojno reševanje matematičnih problemov, na katere naleti pri vsakodnevnem delu na različnih področij znanosti in tehnike s posebnim poudarkom na kemijo. | Goal: To understand basic numerical methods for solving of mathematical problems which scientists can find in everyday work in science and technology.<br>Competence: Students will get theoretical and practical experience to independently solve mathematical problems which can be found at everyday work in different field of science and technology with emphasis on chemistry. |

| **Predvideni študijski rezultati:** | **Intended Learning Outcomes:** |
|---|---|
| <u>Znanje in razumevanje</u><br>Predmet je namenjen seznanjanju z osnovnimi metodami za reševanje numeričnih problemov v naravoslovju in tehniki s posebnim poudarkom na kemiji. Študent se nauči identificirati problem, ga razčleniti in potem rešiti s pomočjo računalniškega programa. | <u>Knowledge and Comprehension</u><br>Goal of the subject is to acquaint students with basic methods for solving numerical problems in science and technology with emphases on chemistry. Student will learn how to identify problem, examine it and later solve it with help of computer program. |
| <u>Uporaba</u><br>Uporabnost pridobljenega znanja je zelo široka in nikakor ni omejena samo na fizikalno kemijo oziroma kemijo. Študent se je sposoben spoprijeti skoraj z vsakim numeričnim problemom, na katerega naleti | <u>Application</u><br>Usefulness of gained knowledge is very general and goes beyond physical chemistry and chemistry. Student gets knowledge that he can use to solve any kind of numerical problem he might find during the study and later in any kind |

| | |
|---|---|
| med študijem ali pozneje, neodvisno od področja znanosti. | of field of science. |
| Refleksija<br>Študent pridobi občutek, da se je sposoben lotiti poljubnega problema in si pri tem pomagati z računalniškimi programi. | Analysis<br>Student gets the feeling that he is capable of solving any kind of problem with help of computer programming. |
| Prenosljive spretnosti<br>Spretnosti in znanje, ki si ga študent pridobi pri predmetu, so v največji meri splošne in prenosljive, uporabne na vseh področjih znanosti in tehnike, kjer si lahko pri reševanju problemov pomaga z računalnikom. | Skill-transference Ability<br>Knowledge and experience are general and can be used in all areas of science and technology, where one can find problems that can be solved with help of computer. |

| **Metode poučevanja in učenja:** | **Learning and Teaching Methods:** |
|---|---|
| Predavanja, seminarji, praktične vaje na računalniku. | Lectures, seminars and practical work on computers. |

| **Načini ocenjevanja:** | Delež (v %) / Weight (in %) | **Assessment:** |
|---|---|---|
| - projekt<br>- seminarske in domače naloge<br>Ocene: 6-10 (pozitivno), 1-5 (negativno) ob upoštevanju Statuta UL in fakultetnih pravil. | **50**<br>**50** | - final project<br>- seminars and homeworks<br>Grades: 6-10 (pozitive), 1-5 (negative) |

**Reference nosilca / Lecturer's references:**

- URBIČ, Tomaž, VLACHY, Vojko, KALYUZHNYI, Yu. V., SOUTHALL, N. T., DILL, K. A. A two dimensional model of water : theory and computer simulations. J. chem. phys., February 2000, vol. 112, no. 6, str. 2843-2848.
- URBIČ, Tomaž, BEŠTER-ROGAČ, Marija, JAMNIK, Andrej, STARE, Jernej. Small-angle x-ray scattering functions of rodlike polyelectrolytes in aqueous solutions. Acta chim. slov.. [Tiskana izd.], September 2001, vol. 48, 343-352.
- URBIČ, Tomaž, VLACHY, Vojko, KALYUZHNYI, Yu. V., DILL, K. A. Orientation-dependent integral equation theory for a two-dimensional model of water. J. chem. phys., 2003, 118, 5516-5525.