Course title: Computer Modeling of Physics Phenomena and Simulations of Material Properties

Instructor(s): Milentije D. Luković, Vanja V. Luković

Course status: elective

ECTS credits: 10

Prerequisites: none

Course objective

Acquiring knowledge of, and methods for, the use of computers in simulations of physical phenomena and in data processing, through the use of the Wolfram Mathematica and Origin software packages. Familiarization with contemporary approaches to modeling in the field of materials science. Training students to independently formulate and implement physical models, as well as to critically analyze and interpret the obtained results.

Learning outcomes

Mastering the theoretical and practical knowledge of applying computers and artificial intelligence methods in simulations of physical phenomena. Mastering the methods of computational modeling, numerical analysis, visualization and data processing. The ability to apply the acquired knowledge to the simulation of the properties of modern materials and to independent research work.

Course content

Theoretical instruction

The significance and role of computers in solving real physical problems through the formulation and implementation of computer models of physical systems. Numerical methods for representation, analysis and calculation in the Wolfram Mathematica and Origin software packages. Deterministic systems and stochastic processes. The Monte Carlo method and tomographic methods. Analysis, processing and simulation of physical phenomena. Machine learning and artificial intelligence methods in the analysis and modeling of physical systems and material properties. Application of computational methods in the study of the structural, electronic, magnetic, piezoelectric, optical, mechanical, thermal and other properties of materials.

Practical instruction.

Part of the instruction is carried out through independent research work on the application of the Mathematica and Origin software tools to selected physical phenomena. The study research work includes the analysis of relevant scientific literature, the planning and realization of numerical experiments, as well as the processing, analysis and interpretation of the obtained results. Preparation of a scientific paper in the scientific field to which the topic of the doctoral dissertation belongs.

Recommended literature

[1] P. T. Tam, *A Physicist's Guide to Mathematica*, 2nd ed., Academic press, 2008.

[2] M. Luković, *Zbirka rešenih zadataka iz Fizike korišćenjem aplikacija u programskom paketu Mathematica* [Collection of Solved Physics Problems Using Applications in the Mathematica Software Package], Faculty of Technical Sciences Čačak, University of Kragujevac, 2023.

[3] J. G. Lee, *Computational Materials Science: An Introduction*, CRC Press, 2017.

[4] A. M. Ovrutsky, A. S. Prokhoda, *Computational Materials Science: Surfaces, Interfaces, Crystallization*, Elsevier, 2014.

[5] J. Dojčilović, *Fizika čvrstog stanja [Solid State Physics]*, Faculty of Physics, University of Belgrade, Belgrade, 2007.

[6] M. O. Steinhauser, S. Hiermaier, *A Review of Computational Methods in Materials Science: Examples from Shock-Wave and Polymer Physics*, International Journal of Molecular Sciences, vol. 10, no. 12, pp. 5135–5216, 2009.

Number of active teaching hours: 7	**Theoretical instruction: 5**	**Practical instruction: 2**

Teaching methods

Interactive lectures, consultations, study and research work.

Assessment (maximum 100 points)

Activity during lectures (discussion of selected topics): 20

Presentation of the completed project assignment: 30

Oral exam: 50