SYLLABUS

1. Information regarding the program

1.1 Higher education institution	Babeş-Bolyai University
1.2 Faculty	Faculty of Physics
1.3 Department	Doctoral School of Physics
1.4 Field of study	Physics
1.5 Study cycle	Doctorate
1.6 Study program / Qualification	Doctoral training/PhD in Physics

2. Course data

2.1 Name of discipline			Theoretical models and simulation methods in physics				
2.2 Teacher responsible for lectures			Prof.dr. Titus Beu, CS III.dr. Maria Ercsey-Ravasz, Prof. dr. Ladislau Nagy, Prof.dr. Zoltan Neda				
2.3 Teacher responsible for seminars			Prof.dr. Titus Beu, CS III.dr. Maria Ercsey-Ravasz, Prof. dr. Ladislau Nagy, Prof.dr. Zoltan Neda				
2.4 Year of study	I	**2.5 Semester**	I	**2.6 Type of evaluation**	E	**2.7 Course framework**	DS

3. Estimated total time of teaching activities (hours per semester)

3.1 Hours per week	3	Out of which: 3.2 Lectures	2	3.3 Seminars / Laboratory classes	1
3.4 Total hours in the curriculum	36	Out of which: 3.5 Lectures	24	3.6 Seminars / Laboratory classes	12
Allocation of study time:					**89**
Study supported by textbooks, other course materials, recommended bibliography and personal student notes					34
Additional learning activities in the library, on specialized online platforms and in the field					24
Preparation of seminars/laboratory classes, topics, papers, portfolios and essays					15
Tutoring					12
Examinations					4
Other activities: -					–

3.9 Total individual study hours	89
3.10 Total hours per semester	125
3.11 Number of ECTS credits	5

4. Prerequisites (if necessary)

4.1 Curriculum	Quantum mechanics, Statistical physics, Physics of atoms and molecules, Numerical methods, Calculus, Algebra, Probability theory
4.2 Competences	- Analytical thinking skills - Programming skills in Python, C/C++, Mathematica - Skills in using programming environments and graphical application

5. Conditions (where applicable)

5.1 Conducting lectures	Course hall, appropriate board, projector, dedicated software, computer
5.2 Conducting seminars/laboratory classes	Course hall, appropriate board, projector, dedicated software, computer network

6. Specific competences acquired

Professional competences	- Acquiring advanced concepts and models of molecular modeling. - Abilities to build molecular models and prepare input data for advanced numerical codes. - Ability to select appropriate models and options for complex simulations. - Correct use of quantum chemistry methods and appropriate models for calculating molecular properties - Correlation of theoretical and computational data with experimental ones - Communicating complex scientific ideas, the conclusions of experiments or the results of a scientific project. - Ability to obtain and support scientifically argued results; ability to develop scientific papers. - Use of scientific methods and models in narrow or interdisciplinary fields. - Advanced ability to plan and organize. - Operation with the principles of digital image data processing. Ability to analyze and synthesize data; the ability to model the effect of external factors on images. - Use and adaptation of software packages for data analysis and processing. Use of automated computer systems for processing and extracting data from 2D and 3D digital images, respectively. - Carrying out data processing experiments and evaluating their results based on existing theoretical models. Multi- and interdisciplinary way of thinking through biomedical applications.
Transversal competencies	- Modeling and analysis skills in an interdisciplinary context. - Competences in using high performance computing technology. - Carrying out professional tasks efficiently and responsibly, in compliance with the legislation and field-specific deontology. - The application, in the context of compliance with the legislation, of intellectual property rights (including technology transfer), of the product certification methodology, of the principles, norms and values of the code of professional ethics within its own rigorous, efficient and responsible work strategy. - Application of efficient work techniques in multidisciplinary team on various levels hierarchical. Identify roles and responsibilities in a team, apply techniques effective relationships, and work within the team. - Efficient use of information sources and communication and training resources professional, both in Romanian and English. - Demonstrate involvement in scientific activities, such as the development of specialized articles and studies. - To participate in scientific projects, compatible with the requirements of integration in European education and research.

7. Course objectives (based on the acquired competencies grid)

7.1 The general objective of the discipline	- Mastering physical models and advanced numerical methods for simulating the structural and dynamic properties of atomic, molecular, and other complex systems.
7.2 Specific objectives	- Developing an algorithmic thinking approach specific to numerical simulations. - Acquiring the ability to use advanced numerical methods and algorithms in complex simulation projects within the fields of computational physics, physical chemistry, materials science, network science and biophysics. - Familiarizing doctoral students with the most commonly used models of statistical and computational physics in interdisciplinary applications. - Encouraging interdisciplinary research. - Mastering the principles, methods, and computational techniques for calculating various molecular properties. - Efficient use of computational resources for molecular modeling. - Developing skills in calculating and analyzing atomic and molecular properties and digital information.

8. Content

8.1 Lectures	**Teaching methods**	**Comments**
1. Basics of molecular dynamics. Force field models. Molecular construction. Standard software codes.	Interactive lecture, Directed discussion, debate, Case-based learning, Just-in-time teaching	2 hours
2. Parametrization of molecular force fields 1. Application to the ethanol molecule. Adjustment of non-bonded interactions.		2 hours
3. Parametrization of molecular force fields 2. Optimization of bonded interactions. Construction of fluid systems. Molecular dynamic simulations in simple ensembles.		2 hours
4. Basics of graph theory: definitions, geodesic paths, metrics on graphs, centrality measures etc. Random walks on graphs. Large scale-structure of networks (small-world effect, scale-free networks).		2 hours
5. Random network models: Erdos-Renyi random graphs, Barabasi-Albert model, geometric random networks. Applications in neuroscience: structural and functional brain networks; the EDR network model.		2 hours
6. Optimization problems and algorithms. NP-hard problems. Examples from graph theory (Hamiltonian cycle, graph partitioning, community detection etc.).		2 hours
7. Models in atomic collision theory. Classical, semiclassical and quantum treatment.		2 hours
8. Comparison between the semiclassical and quantum treatment of ionization.		2 hours

9. Interference effects in the ionization of atoms and molecules by charged projectiles and laser pulses.		2 hours
10. The Monte-Carlo methods in Physics. Application and Methods. The study of spontaneous synchronization.		2 hours
11. Statistics of the Local Growth and Global Reset model. Applications to physical, sociological and economics models.		2 hours
12. Pattern formation and selection in grain-growth models. Modelling and simulations. The optimal clusterization model and the associated phase transition.		2 hours

8.2 Seminars / laboratory classes	**Teaching methods**	**Comments**
1. Construction of simple molecules and periodic fluid systems. Application to liquid ethanol.	Problem based learning, Project based learning, Inquiry guided learning, Experiential learning	1 hour
2. Parametrization of the non-bonded interactions of the ethanol molecule		1 hour
3. Simulations of liquid ethanol with the NAMD code. Basic measurements.		1 hour
4. Algorithms for calculating graph metrics. Shortest paths, centrality measures, clustering coefficient, triangular motifs, cliques etc.		1 hour
5. Methodology for analyzing real network data sets and comparing them to different random graph null models.		1 hour
6. Discussing some examples of optimization algorithms for the problems discussed.		1 hour
7. Examples for the use of classical, semiclassical and quantum treatment.		1 hour
8. The effect of the coherence width of the projectile in the fully differential ionization cross section.		1 hour
9. Interference in the ejected electron momentum spectrum in the ionization of hydrogen molecule.		1 hour
10. Use of the Monte-Carlo methods in different scientific models.		1 hour
11. The use of the LGGR model. Applications in different area of science.		1 hour
12. Grain-growth and pattern formation. Use of the optimal clusterization problem.		1 hour

Bibliography

1. Rapaport, D. C., The Art of Molecular Dynamics Simulation. Second Edition (Cambridge University Press, 2004).
2. M.E.J. Newman: Networks - an Introduction
3. A-L Barabasi: Network Science: http://barabasi.com/networksciencebook/
4. Eric D. Kolaczyk, *Statistical Analysis of Network Data* (Springer 2008).
5. A. Fornito, A. Zalesky, E. Bullmore: Fundamentals of Brain Network Analysis
6. Taylor, J.R., Scattering theory (Dover Publications, INC., 2006)
7. Newton, R.G., Scattering theory of waves and particles (Dover Publications, INC., 2002)

8. Borbély, S. et al, Photoelectron holography of atomic targets, Phys. Rev A 99, 013413 (2019)
9. Nagy, L. et al, The effect of projectile wave packet width on the fully differential ionization cross-sections, J Phys B 51, 144005 (2018)
10. Czipa, L. and Nagy, L., Two-center interference in the ionization of H2 by ion impact: Comparison of different models, Phys. Rev. A 95, 062709 (2017).
11. David P. Landau and Kurt Binder, A Guide to Monte Carlo Simulations in Statistical Physics, Cambridge Univ. Press, fourth Edition, 2015
12. T.S. Biro and Z. Neda, Unidirectional random growth with reset, Physica A: Statistical Mechanics and Applications, vol 499, 335 (2018)
13. K. Leung and Z. Neda, Pattern formation and selection in quasistatic fracture, Physical Review, vol 85, 664 (2000)

9. Aligning the contents of the discipline with the expectations of the epistemic community, representatives, professional associations and standard employers operating in the program field

The content of the discipline is in line with what is studied in other university centers in the country and abroad. In order to adapt to the requirements imposed by the labor market, the content of the discipline was harmonized with the requirements imposed by the specifics of postgraduate education, research institutes and the business environment.

10. Examination

Activity type	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Weight in the final grade
10.4 Lectures	Assessment of knowledge	Written report/project	75%
10.5 Seminars / laboratory classes	Activity during seminars	Discussions, answers to questions	25%
10.6 Minimum performance standard 50%			
Correct assessment of methods and models to be used to solve a particular problem. Proper use of computational techniques and available hardware and software resources.			

Signature of course coordinator	Signature of seminar coordinator
Prof. dr. Titus Beu	Prof. dr. Titus Beu
CS III dr. Maria Ercsey-Ravasz	CS III dr. Maria Ercsey-Ravasz
Prof. dr. Ladislau Nagy	Prof. dr. Ladislau Nagy
Prof. dr. Zoltan Neda	Prof. dr. Zoltan Neda

Date	Signature Head of department
21.09.2025	Prof. dr. Vasile Chiș