SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	Babes-Bolyai University
1.2 Faculty	Physics
1.3 Department	Biomolecular Physics
1.4 Field of study	Physics
1.5 Study cycle	Master
1.6 Study programme / Qualification	Computational Physics

2. Information regarding the discipline

2.1 Name of the discipline				Simulation of spectra			
2.2 Course coordinator				Lect. dr. Crăciun Cora			
2.3 Laboratory coordinator				Lect. dr. Crăciun Cora			
2.4. Year of study	I	2.5 Semester	2	2.6. Type of evaluation	E	2.7 Type of discipline	DA

3. Total estimated time (hours/semester of didactic activities)

3.1 Hours per week	4	Of which: 3.2 course	2	3.3 laboratory	2
3.4 Total hours in the curriculum	56	Of which: 3.5 course	28	3.6 laboratory	28
3.7 Number of ECTS credits					5

4. Prerequisites (if necessary) (next)

4.1. curriculum	• Linear Algebra, Quantum Mechanics
4.2. competencies	• Computer programming

5. Conditions (if necessary)

5.1. for the course	• Computer room (computers, blackboard)
5.2. for the seminar /lab activities	• Computer room (computers, blackboard)

6. Specific competencies acquired

Professional	**C1.** Numerical modelling of spin systems' interaction with magnetic fields and electromagnetic radiation. **C2.** Critical assessment of existent methods for spectra simulation. **C3.** Development of computer programs for spectra simulation.
Transversal	**CT1.** Development of a project (planning, documentation, software development, presentation).

7. Objectives of the discipline (outcome of the acquired competencies)

7.1 General objective of the discipline	• Acquiring notions about the existent numerical methods of spectra simulation.
7.2 Specific objective of the discipline	• Understanding, assessment, and testing of different methods for spectra simulation. • Development of a programming project based on the acquired knowledge.

8. Content

8.1 Course	Teaching methods	Remarks
Learning the Octave language	Lecture, discussion, demonstration on the computer	
Numerical methods for spectra simulation: Fourier Transform, convolution, interpolation		
Theoretical description of magnetic resonance spectra (classical description, quantum mechanical description)		
Spin Hamiltonian. Matrix form		
Determination of energy levels using Perturbation theory		
Determination of energy levels using eigenvectors and eigenvalues methods		
Resonance magnetic fields		
Magnetic resonance spectra: signals' intensity and line shape		
Simulation of polycrystalline magnetic resonance spectra: spectral intensity, spherical grids		
Simulation of polycrystalline magnetic resonance spectra: the projection method		
Simulation of polycrystalline magnetic resonance spectra using homotopy		
Polycrystalline magnetic resonance spectra: g-strain		
Product operators		
Pulse magnetic resonance		

Bibliography:

1. C. Crăciun, Modelarea spectrelor de Rezonanţă Electronică de Spin in unda continua, Ed. Napoca Star, 2009.
2. J. A. Weil, J. R. Bolton, J. E. Wertz, Electron Paramagnetic Resonance Theory and Practical Applications, Wiley, 1994.
3. C. Cohen-Tannoudji, B. Diu, F. Laloe, Quantum Mechanics, Wiley-VCH, 1997.
4. B. H. Bransden, C. J. Joachain, Quantum mechanics, Pearson Education, 2000.
5. https://www.easyspin.org/
6. S. Stoll, Spectral simulations in solid-state electron paramagnetic resonance, PhD thesis, ETH Zürich, 2003.
7. D.W. Alderman, M.S. Solum, D.M. Grant, J. Chem. Phys. 84, 3717-3725 (1986).
8. http://www-keeler.ch.cam.ac.uk/lectures/understanding/chapter_6.pdf

8.2 Laboratory	Teaching methods	
Learning the Octave language	Individual discussion and assessment	
Cubic splines interpolation		
Quantum mechanical description of magnetic resonance spectra. Transition probability between the energy levels		

Spin Hamiltonian. Matrix form		
Determination of energy levels using eigenvectors and eigenvalues methods		
Resonance magnetic fields.		
Convolution of stick spectra with given lineshapes.		
Simulation of continuous wave polycrystalline magnetic resonance spectra.		
The projection method.		
Product operators.		
Bibliography: the same as for the course, articles, web resources 1. https://www.gnu.org/software/octave/ 2. http://www-mdp.eng.cam.ac.uk/web/CD/engapps/octave/octavetut.pdf 3. http://ais.informatik.uni-freiburg.de/teaching/ws11/robotics2/exercise/OctaveExercise.pdf		

9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program

The content of the discipline agrees with current research in spectra simulation. The discipline has an applied character, showing how theoretical concepts are used for simulation of experimental spectra. The course and the laboratory aims to improve the students' programming skills, which contributes to their professional development.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	Understanding and use of acquired knowledge for solving specific problems.	Written exam	40%
10.5 Laboratory	Activity and homework	Addressed topics	40%
	Project	Project development.	20%
10.6 Minimum performance standards			
➢ Understanding the methods presented at the course and laboratory. ➢ Developing a project of medium complexity.			

Date	Signature of course coordinator	Signature of laboratory coordinator
19.11.2021	Lect. dr. Crăciun Cora	Lect. dr. Crăciun Cora

Date of approval	Signature of the head of department