SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	**Babes-Bolyai University**
1.2 Faculty	**Physics**
1.3 Department	**Physics**
1.4 Field of study	**Physics**
1.5 Study cycle	**Master**
1.6 Study programme / Qualification	**Common semester of all master programmes**

2. Information regarding the discipline

2.1 Name of the discipline	**Computational methods in physics**						
2.2 Course coordinator	**Jarai-Szabo Ferenc / Emil Vinteler**						
2.3 Seminar coordinator	**Jarai-Szabo Ferenc / Emil Vinteler**						
2.4. Year of study	1	2.5 Semester	1	2.6. Type of evaluation	E	2.7 Type of discipline	Fundamental

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

3.1 Hours per week	3	Of which: 3.2 course	2	3.3 seminar/laboratory	1
3.4 Total hours in the curriculum	42	Of which: 3.5 course	28	3.6 seminar/laboratory	14
Time allotment:					hours
Learning using manual, course support, bibliography, course notes					21
Additional documentation (in libraries, on electronic platforms, field documentation)					14
Preparation for seminars/labs, homework, papers, portfolios and essays					30
Tutorship					4
Evaluations					5
Other activities:					

3.7 Total individual study hours	74
3.8 Total hours per semester	125
3.9 Number of ECTS credits	5

4. Prerequisites (if necessary)

4.1. curriculum	
4.2. competencies	knowledge of basic algorithms, basic programming competences

5. Conditions (if necessary)

5.1. for the course	
5.2. for the seminar /lab activities	

6. Specific competencies acquired

Specific competences	• Using in-depth knowledge of physics, mathematics, and programming in various multi- and inter-disciplinary fields. • Applying computational methods to understand complex scientific phenomena. • Independently apply the achieved knowledge to define and formulate research problems in the computational chemistry and physics fields, use information retrieval, data collection, experiment and/or computer methods to solve such problems. • Advanced skills in modeling molecular systems, statistical and solid-state physics systems using computers. • Ability to critically analyse and evaluate scientific models.
Transversal competences	• Accomplishment of professional tasks in an effective and responsible manner, in compliance with the field-specific legislation and code of ethics. • Ability to work in projects, and also to plan and lead projects. • Effective use of information sources, as well as communication and professional-assisted training resources in both mother tongue and English.

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

7.1 General objective of the discipline	• Students should acquire basic knowledge about modern computational modeling techniques and their applications.
7.2 Specific objective of the discipline	• Students will understand theories used in the calculation of the electronic structure of molecules and the approximations on which they are based. • They should be familiar with approximations made in understanding the molecular mechanics, semiempirical, ab-initio and DFT methods and their use for the calculation of various molecular properties. • Students should have theoretical and practical skills in using random number generators for simulating physics problems. • They should have the basic knowledge of the Monte Carlo simulation technique and its application in statistical and solid state physics problems.

8. Content

8.1 Course	Teaching methods	Remarks
Introduction to Computational Molecular Physics. What is computational physics? Computational molecular physics applications History of computing in molecular physics.	oral presentation	
Molecular Mechanics. Force fields. Energy minimization. Geometry optimization. Molecular mechanics examples	oral presentation, demonstration	
Conformation Searching Potential energy surfaces. Systematic methods. Monte Carlo methods. Molecular Dynamics methods. Conformation searching examples	oral presentation, examples	
Molecular Orbital Methods Quantum mechanics background. Hartree-Fock equations. Electron correlation. Basis sets	oral presentation	
Additional Quantum-based Methods Semi-empirical methods. Density functional theory. Molecular Orbital Applications	oral presentation, examples	
Molecular Dynamics Methods Newton's equations. Verlet algorithm. Practical aspects. MD examples	oral presentation, demonstration, examples	
Applications of Computational Molecular Physics	oral presentation, example movies	
Introduction to Monte Carlo methods Computational modeling examples. Basic MC algorithms, problem solving.	oral presentation, example movies	
The random walk Introducing the problem. Analytical solution in 1D. Generalization in higher dimensions. Monte Carlo approach.	oral presentation, demonstration	
Random number generators Random number generation. Pseudo random number generators. RNG tests. Basic transformations.	oral presentation, method demonstration	
Monte Carlo integration methods The hit or miss method and average sampling methods. Calculating the PI value by MC simulations. The error of the MC integration. Importance sampling. The Metropolis algorithm.	oral presentation, demonstration, examples	
Theoretical background of of the MC algorithms Basic MC approaches. The detailed balance. The Metropolis random walk algorithm.	oral presentation, demonstration,	
Monte Carlo methods in statistical physics The Daemon algorithm for an ideal gas. Averages in statistical physics. MC sampling approaches. Metroplis Monte Carlo algorithm with Boltzmann statistics.	oral presentation, example codes and movies	
Interdisciplinary applications.	oral presentation, example movies	

Bibliography

1. Christopher J. Cramer, Essentials of Computational Chemistry, 2nd Ed., John Wiley & Sons, Hoboken, NJ, 2004.

2. H. Gould and J. Tobochnik Introduction to Computer Simulation Methods and applications in physics (Addison-Wesley, 1996)

3. Werner Krauth. Introduction to Monte Carlo algorithms.. summer school in Beg-Rohu (France) and Budapest1996, 2006, https://cel.archives-ouvertes.fr/cel-00092936

4. Werner Krauth, Four lectures on computational statistical physics, https://arxiv.org/abs/0901.2496v1

8.2 Laboratory	Teaching methods	Remarks
Molecular geometry specification; Cartezian coordinates; Z-matrix formalism; Molecular mechanics	Avogadro program	
Conformal searching; Tinker program; HF method, basis sets; DFT method, semiempirical methods	GaussView/Gaussian program	
Molecular dynamics; Applications of Computational Molecular Physics	Tinker and VMD program	
Computer simulation approaches of basic interdisciplinary problems	c/c++ programming	
Monte Carlo simulation of the random walk.	c/c++ programming, gnuplot	
Monte Carlo calculation of the PI value, Simple Monte Carlo integration methods	c/c++ programming, gnuplot	
Metropolis Monte Carlo simulation of the Ising model	c/c++ programming, gnuplot	

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 is consistent with courses of similar content from other foreign academic centers. To adapt to the demands of the labor market, the content of the discipline has been harmonized with the requirements of the pre-university education, research institutes and the business environment.

10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	Knowledge, understanding and capacity of application of the computational molecular physics	Written exam	30
	Knowledge, understanding and capacity of application of the Monte Carlo methods	Written exam	30
10.5 Seminar/lab activities	Homework, activity, project (computational molecular physics)	Problem solving, project elaboration	20
	Homework, activity, project (Monte Carlo simulation methods)	Problem solving, project elaboration	20
10.6 Minimum performance standards			
Homework assignments will come from textbook problems, and will be turned in every 3 weeks. Completing and understanding the homework assignments is essential to performing well on the exams and mastering this challenging subject.			

Date ……………………

Signature of course coordinator ……………………………………

Signature of laboratory coordinator ………………………………………

Date of approval ……………………………………

Signature of the head of department ……………………………………