COURSE SYLLABUS

1. Information of the program

1.1 Higher Education Institution	”Babeş-Bolyai” University Cluj-Napoca
1.2 Faculty	Physics
1.3 Department	Biomolecular Physics
1.4 Domain of Studies	Physics
1.5 Cycle of studies	Master
1.6 Program	Biofizica si Fizica moleculara

2. Information on the subject

2.1 Subject		**Introduction to Molecular Dynamics Simulations**					
2.2 Instructor		Prof. Dr. Titus Beu					
2.3 Seminar instructor		Prof. Dr. Titus Beu					
2.4 Laboratory instructor		Prof. Dr. Titus Beu					
2.5 Year of study	I	2.6 Semester	II	2.7 Evaluation	E	2.8 Type of subject	DA

3. Allotted time (hours per semester)

3.1 No. of weekly hours	4	From which:			
3.2 Course	2	3.3 Seminar	0	3.4 Laboratory	2
3.5 Total no. of hours	56	From which:			
3.6 Course	28	3.7Seminar		3.8 Laboratory	28

Distribution of allotted time:	Hours
Study based on textbook, bibliography, and notes	14
Additional documentation in the library, on specialized electronic platforms, and on the field	7
Preparation of seminars / laboratories, assignments, papers, portfolios, and essays	28
Tutoring	3
Examinations	3
Other activities:	–

3.9 Total no. of hours for individual study	70
3.10 Total no. of hours per semester	126
3.11 No. of credits	6

4. Prerequisites

4.1 Curriculum related	•
4.2 Competencies	• Knowledge of C/C++ programming.

5. Infrastructure

5.1 For course teaching	• Video Projector
5.2 For seminar teaching	• Video Projector
5.3 For laboratory teaching	• Video Projector, computer network

6. Specific competencies acquired

Professional competencies	• Students will acquire the basic concepts and techniques, the numeric formalism and specific molecular dynamics simulation and will be able to solve the fundamental problems of Physics. • Students will develop skills to use numerical methods and simulation of advanced physics and condensed. • Students will acquire skills of application of numerical methods and simulation in concrete fields of physics, chemistry or Biophysics. • Students will develop the ability to identify and use adequate laws and the physical principles in a given context. • Students will become familiar with solving physics problems under conditions imposed, by using statistical and numerical methods. • Students will be acquainted with the interdisciplinary approach of some topics in the field of physics.
Transversal competencies	• Students will assimilate interdisciplinary knowledge. • Students will acquire analytical work skills with complex theoretical formalisms and individual documentation. • Students will acquire group work skills, arguing ways to solve problems and identifying optimal solutions. • Students will develop their spirit of competition and team spirit. • Achieving professional tasks in an efficient and responsible manner with respect to the field-specific deontology legislation under qualified assistance. Apply efficient and responsible work strategies, punctuality, seriousness and personal responsibility based on the principles, norms and values of the professional ethics code. Implementation of intellectual property rights (including technology transfer), product certification methodology, principles, norms and values of the Code of Professional Ethics in the context of law enforcement, within its rigorous, efficient and responsible work strategy.

7. Discipline objectives (based on the specific competencies acquired grid)

7.1 Overall objective of the discipline	• Familiarity with the modern numerical methods used for the structural and dynamic simulation of atomic and molecular systems.
7.2 Specific objectives	• Implement a range of numerical algorithms efficiently in a modern scientific computing programming language.

8. Course contents

8.1 Course	Teaching methods	Comments
1. INTRODUCTION. Computer experiments. Ensemble averages and time averages. Molecular dynamics. Relationship of MD statistical mechanics, Monte Carlo method and statistical mechanics.	Conversation, debate, case studies	[1] C1.pdf
2. BASIC PROGRAMMING TECHNIQUES IN C. Integrated C/C++ development environments. Functions and parameters. Pointers and variable argument lists. Passing arguments to functions. Dynamic array allocation.	Conversation, debate, case studies	[1] C2.pdf
3. ELEMENTS OF SCIENTIFIC GRAPHICS. Plotting Functions in C/C++ and Python. Plotting functions of one variable. Histograms.	Conversation, debate, case studies	[1] C3.pdf
4. ORDINARY DIFFERENTIAL EQUATIONS. Transforming higher-order ODEs into systems o first order ODEs. Taylor series expansion method. Euler's method (method of polygonal lines). Implementation and examples.	Conversation, debate, case studies	[1] C4.pdf
5. BASICS OF MOLECULAR DYNAMICS. Equations of motion for MD simulations. Potential derivatives and forces. Van der Waals potentials. Bonded potentials. Time integration methods: Euler, Verlet, Leap Frog, Velocity Verlet, Gear predictor-corector	Conversation, debate, case studies.	[1] C5.pdf
6. MD program. Program structure. Protein Data Bank, PDB format. Using include files.	Conversation, debate, case studies	[1] C6.pdf
7. SIMULATING SIMPLE FLUIDS. Thermodynamic properties. Periodic boundary conditions. Initial configuration. Thermostats and barostats. Applications.	Conversation, debate, case studies	[1] C7.pdf
8. MEASUREMENTS. Statistical analysis. Velocity	Conversation,	[1] C8.pdf

distribution. Equilibrium – the Boltzmann H-function. Radial distribution function. Diffusion coefficients.	debate, case studies	
9. VIBRATIONAL SPECTRA OF CLUSTERS. Autocorrelation functions. Velocity correlation function. Power spectrum of velocity correlation function. Discrete Fourier transform. Discrete cosine transform. Efficient implementation of cosine transform	Conversation, debate, case studies	[1] C9.pdf
10. SPECIAL NUMERICAL TECHNIQUES. Neighbor-list methods. Ewald sum. P3M method.	Conversation, debate, case studies	[1] C10.pdf
11. RIGID-BODY DYNAMICS. Modeling options for molecules. Site-site interaction models. Placing a molecular model in the system of principal axes. Euler angles. Equations of motion for rigid molecules. Quaternions. Equations of motion for rigid molecules using quaternions	Conversation, debate, case studies	[1] C11.pdf
12. NON-ORTHOGONAL TIGHT-BINDING MD. Sp3 and sp2 Hybridization. Basic formulation. TB parametrization	Conversation, debate, case studies	[1] C12.pdf
13. PARALLEL NUMERICAL INTEGRATION. Shared Memory Parallel: OpenMP.	Conversation, debate, case studies	[7]

Bibliography: [1] T.A. Beu, "Molecular dynamics simulations", http://phys.ubbcluj.ro/~tbeu/courses.htm (Intranet Universitatea "Babeş-Bolyai", Cluj-Napoca, 2000).
[2] D.C. Rapaport, "The Art of Molecular Dynamics Simulation" (Cambridge University Press, Cambridge, 1995).
[3] M.P. Allen, D.J. Tildsley, "Computer Simulation of Liquids" (Oxford University Press, Oxford, 1987).
[4] H. Gould, J. Tobochnik, "An Introduction to Computer Simulation Methods" (Addison-Wesley Publishing Company, Reading, MA, 1996).
[5] T.A. Beu, "Calcul numeric în C, Ediția a II-a" (Grupul MicroInformatica, Editura Albastră, Cluj-Napoca, 2004).
[6] T.A. Beu, "Numerical methods for physicists", http://phys.ubbcluj.ro/~tbeu/courses.htm (Intranet Universitatea "Babeş-Bolyai", Cluj-Napoca, 2000).
[7] The OpenMP® API specification for parallel programming, http://openmp.org/wp/resources/#Tutorials

8.2 Seminar / laboratory	Teaching methods	Comments
1. INTRODUCTION. Computer experiments. Ensemble	Conversation, debate, case	[1] C1.pdf

averages and time averages. Molecular dynamics. Relationship of MD statistical mechanics, Monte Carlo method and statistical mechanics.	studies.	
2. BASIC PROGRAMMING TECHNIQUES IN C. Integrated C/C++ development environments. Functions and parameters. Pointers and variable argument lists. Passing arguments to functions. Dynamic array allocation.	Conversation, debate, case studies.	[1] C2.pdf
3. ELEMENTS OF SCIENTIFIC GRAPHICS. Plotting Functions in C/C++ and Python. Plotting functions of one variable. Histograms.	Conversation, debate, case studies.	[1] C3.pdf
4. ORDINARY DIFFERENTIAL EQUATIONS. Transforming higher-order ODEs into systems o first order ODEs. Taylor series expansion method. Euler's method (method of polygonal lines). Implementation and examples.	Conversation, debate, case studies.	[1] C4.pdf
5. BASICS OF MOLECULAR DYNAMICS. Equations of motion for MD simulations. Potential derivatives and forces. Van der Waals potentials. Bonded potentials. Time integration methods: Euler, Verlet, Leap Frog, Velocity Verlet, Gear predictor-corector	Conversation, debate, case studies.	[1] C5.pdf
6. MD program. Program structure. Protein Data Bank, PDB format. Using include files.	Conversation, debate, case studies.	[1] C6.pdf
7. SIMULATING SIMPLE FLUIDS. Thermodynamic properties. Periodic boundary conditions. Initial configuration. Thermostats and barostats. Applications.	Conversation, debate, case studies.	[1] C7.pdf
8. MEASUREMENTS. Statistical analysis. Velocity distribution. Equilibrium – the Boltzmann H-function. Radial distribution function. Diffusion coefficients.	Conversation, debate, case studies.	[1] C8.pdf
9. VIBRATIONAL SPECTRA OF CLUSTERS. Autocorrelation functions. Velocity correlation function. Power spectrum of velocity correlation function. Discrete Fourier transform. Discrete cosine transform. Efficient implementation of cosine transform	Conversation, debate, case studies.	[1] C9.pdf
10. SPECIAL NUMERICAL TECHNIQUES. Neighbor-list methods. Ewald sum. P3M method.	Conversation, debate, case studies.	[1] C10.pdf

11.RIGID-BODY DYNAMICS. Modeling options for molecules. Site-site interaction models. Placing a molecular model in the system of principal axes. Euler angles. Equations of motion for rigid molecules. Quaternions. Equations of motion for rigid molecules using quaternions	Conversation, debate, case studies.	[1] C11.pdf
12.NON-ORTHOGONAL TIGHT-BINDING MD. Sp3 and sp2 Hybridization. Basic formulation. TB parametrization	Conversation, debate, case studies.	[1] C12.pdf
13.PARALLEL NUMERICAL INTEGRATION. Shared Memory Parallel: OpenMP.	Conversation, debate, case studies.	[7]

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[1] T.A. Beu, "Molecular dynamics simulations", http://phys.ubbcluj.ro/~tbeu/courses.htm (Intranet Universitatea "Babeş-Bolyai", Cluj-Napoca, 2000).
[2] D.C. Rapaport, "The Art of Molecular Dynamics Simulation" (Cambridge University Press, Cambridge, 1995).
[3] M.P. Allen, D.J. Tildsley, "Computer Simulation of Liquids" (Oxford University Press, Oxford, 1987).
[4] H. Gould, J. Tobochnik, "An Introduction to Computer Simulation Methods" (Addison-Wesley Publishing Company, Reading, MA, 1996).
[5] T.A. Beu, "Calcul numeric în C, Ediția a II-a" (Grupul MicroInformatica, Editura Albastră, Cluj-Napoca, 2004).
[6] T.A. Beu, "Numerical methods for physicists", http://phys.ubbcluj.ro/~tbeu/courses.htm (Intranet Universitatea "Babeş-Bolyai", Cluj-Napoca, 2000).
[7] The OpenMP® API specification for parallel programming, http://openmp.org/wp/resources/#Tutorials

8.3 Laboratory	Teaching methods	Comments

Bibliography:

9. Correlating the contents of the discipline with the expectations of the epistemic community, of professional associations and of representative employers in the field of the program.

- The informational content and the formative character of the course are compatible with the practices of the main universities in the country and prestigious universities abroad.
- In order to increase the chances of graduates (in research, industry or education) to take on the labor market, the course presents, besides classical fundamental themes and topical themes, with direct applicability.
- In order to adapt to the demands imposed by the labor market, the content of the discipline has been harmonized with the requirements of the pre-university education, research institutes and the business.

10. Assessment

Type of activity	10.1 Assessment criteria	10.2 Assessment methods	10.3 Percentage of the final grade
10.4 Course	Intermediary evaluations (1)	Written exam	10%
10.5 Seminar	Activity during seminars	Seminar activity	25%
10.6 Laboratory			25%
10.7 Minimum performance standards			

- Seminar attendance is mandatory in a proportion of at least 75%
- Minimum grade: 5/10 for the intermediary evaluations and written exam.
- Final exam 40%.

Course holder signature	Seminar holder signature	Laboratory holder signature
Prof. Dr. Titus Beu		

Date	Date of departmental approval	Head of department signature
01.05.2018	31.05.2018	