SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	**Babeş Bolyai University**
1.2 Faculty	**Faculty of Mathematics and Computer Science**
1.3 Department	**Department of Computer Science**
1.4 Field of Study	**Computer Science**
1.5 Study Cycle	**Master**
1.6 Study Programme/Qualifications	**High Performance Computing and Big Data Analytics**

2. Information regarding the discipline

2.1 Name of the discipline			Stochastic Simulation Methods with Interdisciplinary Applications				
2.2 Course coordinator			Prof. Dr. Zoltán Néda				
2.3 Seminar coordinator							
2.4 Laboratory coordinator			Prof. Dr. Zoltán Néda				
2.5 year of study	2	**2.6 semester**	4	**2.7 Type of evaluation**	E	**2.8 Type of Discipline**	Opt.

3. Timpul total estimat (ore pe semestru al activităţilor didactice)

3.1 Hours per week		**Of which:**			
3.2 course	3	**3.3 seminar**		**3.4 laboratory**	2
3.5 Total hours in the curriculum		**Din care:**			
3.6 course		**3.7 seminar**		**3.8 laboratory**	

Time allotment:	**ore**
Learning using manual, course support, bibliography, course notes	42
Additional documentation (in libraries, on electronic platforms, field documentation)	14
Preparation for seminars/labs, homework, papers, portfolios and essays	42
Tutorship	3
Evaluations	4
Other activities:	–

3.9 Total individual study hours	105
3.10 Total hours per semester	161
3.11 Number of ECTS credits	7

4. Prerequisities

4.1 curriculum	Statistical Physics, C Programming, Elements of Probability Theory and Mathematical Statistics
4.2 competencies	Logical thinking, interdisciplinay thinking, communication abilities in English, active participation at the courses and laboratories

5. Conditions

5.1 for the course	Video projector, blackboard
5.2 for the seminars	
5.3 for lab activities	Computers with Linux operating system, Vidoe projector

6. Specific competencies acquired

Professional	**C1.** Capacities for analyzing and synthetizing physical data, capacities for modelling complex phenomena **C2.** Working and mastering with software packages for analyzing and processing experimental data. Using C , Python and Mathematica software for modelling complex phenomena. Capacities for using information technologies in describing complex phenomena from physics, biology, chemistry and social sciences. Advanced programming techniques. **C3.** Trans- and Interdisciplinary thinking. **C4.** Planning and Performing computer experiments for validating physical models. Abilities for making high performance computations in physics. Capacieties for writing computer codes and running them on modern supercomputers. **C5.** Communicating efficiently modern scientific ideas. Presenting in a professional manner results of a research or scientific projects. Capacities for writing scientific publications, to interact and have a scientific debate with Editors and Referees. omunicarea ideilor științifice complexe, a concluziilor experimentelor sau a rezultatelor unui proiect științific. Capacities for arguing and defeneding scientific views and ideas.
Transversal	**CT1.** To deal with professional duties efficiently and in a responsible manner, keeping in mind the laws and scientific ethics. Being responsible for the published scientific results and taking all actions for their proper use. **CT2.** Working in an Interdisciplinar environment respecting the professional hierarchy. Having initiative, new ideas and approaches to classical problems. Promoting the dialogue, cooperation and positive attitude in a group. Respecting multicultural environment and helping the others. **CT3.** Efficient use of information tehnology tools and presentation methods in English. Learning and applying autoevaluation methods, f or keeping the professional training up to date, in agreement with the deminds of the market.

7. Objectives of the discipline

7.1 General objective of the discipline	- a rigorous introduction in MC simulation methods, oriented on interdisciplinary applications.
7.2 Specific objective of the discipline	- mastering stohastic simulation methods and physical modelling - learning to approach modern problems in an interdisciplinary manner - using classical models of physics in approaching interdisciplinary problems. - advance programming in C and C++ - an introduction to scientific research

8. Content

8.1 Course	**Teaching methods**	**Observations**
Computer simulation techniques – an overview	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-role of Monte Carlo (MC) simulations in physics - Monte Carlo simulations versus Molecular Dynamics (MD) methods - the interdisciplinar applicability of the MC methods

Examples of MC simulations	Problem formulation Presentation Demonstartations Software packages Discutions Movies	- detailed discussion of two examples of MC simulations: simple random walk, phase transition in a sociological system,
Random number generators	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-generating uniformly distributed random numbers -generating random numbers distributed according to an arbitrary distribution -generating random numbers with a normal distribution -testing the random number genrators
Elements of Statistical Physics, Stochastic Processes and Critical Phenomena	Problem formulation Presentation Demonstartations Software packages Discutions Movies	- overview of basic thermodynamics, statistical physics, stochastic processes and critical phenomena knowledge, needed for the course
Brownian dynamics	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-Langevin equation -implementing Brownian dyanimcs -examples
Monte Carlo integration	Problem formulation Presentation Demonstartations Software packages Discutions Movies	- straightforward sampling -reducing the error: important sampling -advantages of important sampling for high dimensional integrals
The Ising model	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-history of the Ising model -phase transition in the Ising model -exact solution in 1D -mean-field solution -critical behavior -known and unknown issues
Metropolis and Glauber MC for the Ising model	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-important sampling and Markov chains for statistical physics integrals -detailed balance -Metropolis method -Glauber method -application for the ising model
The BKL or kinetic MC method	Problem formulation Presentation Demonstartations Software packages Discutions Movies	- problems with the Metropolis and Glauber methods - noniform time-update - grain-growth - kinetic MC techniques and interdisciplinary applications

Cluster MC methods	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-crtitical slowing down -dynamic exponent -Swendsen and Wang algorithm -Wolf algorithm
The histogram MC method and the microcanonical MC method	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-fluctuation of the energy and magnetization -determining relevant quantities at different temperatures - the demon algorithm - determining the temperature of the microcanonical simulation
Quantum Monte Carlo methods	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-elements of quantum statistics -quantum statistical models -the Trotter-Suzuki transformation -QMC method for 1D interacting fermions
MC simulation of Frustrated Systems	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-spin-glasses -NP hard and NP complete problems -simulated annealing -extremal optimization -other heuristic methods
Interdisciplinary application of the MC methods	Problem formulation Presentation Demonstartations Software packages Discutions Movies	-applications in materials science, biophysics, economics, sociology and biology.

Bibliography

1. Z. Neda : Stochastic simulations in physics with interdisciplinary applications, http://www.phys.ubbcluj.ro/~zneda/edu/mc.htm

2. Z. Neda: Stochasztikus szimulacios modszerek a fizikaban (Erdelyi Tankonyvtanacs, 1998). accesibil in numar mare la biblioteca Facultăţii de Fizică

3. H. Gould and J. Tobochnik Introduction to Computer Simulation Methods and applications in physics (Addison-Wesley, 1996). Accesibil pentru studenţi pe pagina de web a cursului în format PDF.

4.A. MacKinnon: Computational Physics online course (http://b.sst.ph.ic.ac.uk/~angus/Lectures/compphys/compphys.html)

5.F. Bagnoli: Introduction to Cellular Automata (cond-mat/9810012; http:arxiv.org, 1998)

6.David Landau and Kurt Binder: A guide to Monte Carlo Simulations in Statistical Physics, Cambridge Univ. Press, 2004 (disponibil la titular curs)

8.3 Laboratory	**Teaching methods**	**Observations**
- Organization aspects - The C programming language, some basic	Explanations Presentations Discussions Problem formulation	[1] coresponding links

facts - Linux operational system, some basic facts	Individual work Programming	
- research projects - scientific papers that will be discussed - computational study of the random walk	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- programming the projects and presentations - computational study of phase transition in a two-state interacting systems	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- working of pseudo-random number generators -testing the pseudo-random number generators	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- generating random numbers with non-uniform distribution - discussing novel scientific works related to Monte Carlo methods	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- studying the Brownian dynamics - studying stohastic resonance with molecular dynamics - discussing novel scientific works related to Monte Carlo methods	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- The Monte Carlo integration with straightforward and important sampling - calculating the number PI with MC methods. - individual discussions with the students on their chosen research projects.	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- computational study of the 2D and 3D Ising	Explanations Presentations	[1] coresponding links and programs in

model. - discussing novel scientific works related to Monte Carlo methods - individual discussions with the students on their chosen research projects.	Discussions Problem formulation Individual work Programming	C
- finite size effects in the MC studies of the Ising model. - discussing novel scientific works related to Monte Carlo methods. - individual discussions with the students on their chosen research project.	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- simulating the Potts model with q states at low temperatures (the BKL Monte Carlo method) - simulationg the dynamics of atoms deposited on surfaces. - discussing novel scientific works related to Monte Carlo methods. - individual discussions with the students on their chosen research project.	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- studying 2D and 3D Ising models with the Swendsen and Wang and Wolf dynamics. -discussing novel scientific works related to Monte Carlo methods. - individual discussions with the students on their chosen research project.	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
- Studying 2D and 3D Ising problems with the histogram MC method. The microcanonical MC method. - discussing novel scientific works related to Monte Carlo methods. - individual discussions with the students on their chosen research project.	Explanations Presentations Discussions Problem formulation Individual work Programming	[1] coresponding links and programs in C
Presentation of individual research projects (I)	Presentations	
Presentation of individual research projects(II)	Presentations	
References 1. Z. Neda : Stochastic simulations in physics with interdisciplinary applications,		

http://www.phys.ubbcluj.ro/~zneda/edu/mc.htm

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 syllabus and the studied material is in agreement with similar courses from other universities in Romania and abroad. For helping the integration with the deminds of the work-force market, the syllabus was harmonized with the deminds of the pre-university and university educations, of those of research institutes and the business sector.

10. Evaluation

Type of activity	**10.1 Evaluation criteria**	**10.2 Evaluation method**	**10.3 Percent in the final grade**
10.4 Course	knowledge of the tought material	Exam	55%
	application of the tought material		
10.5 Seminar			
10.6 Laboratory	Solving the proposed exercises	Colloquium	25%
	Realization degree and presentation of the research project	Colloquium	20%
10.7 Minimal performance standard			
Understanding the methods presented at the course and laboratory. Addressing the laboratory requirements in proportion of at least 75%. Successful Developing a project of medium complexity.			

Signature of course coordinator Prof. Dr. Neda Zoltan	Signature of seminar coordinator	Signature of laboratory coordinator Lect. Dr. Zsolt Lazar
Date 12.01.2014	Date of approval	Signature head of Department