COURSE CONTENT

1. Information about the program

1.1 Organization	West University of Timisoara
1.2 Faculty	Physics and Mathematics
1.3 Department	Physics
1.4 Field of study	Physics
1.5 Level	Master
1.6 Study program/qualification	**Advanced research methods in physics** / according to COR: physicist (211101); teacher (233001); research assistant (248102); analyst (213101);

2. Course information

2.1 Title				**Advanced methods in computational physics ARMP2304**			
2.2 Course instructor				dr. Sergiu BUSUIOC			
2.3 Laboratory/Seminar instructor				dr. Sergiu BUSUIOC			
2.4 Year of study	II	2.5 Semester	1	2.6 Type of evaluation	E	2.7 Course type	DOP

3. Study time distribution (teaching hours per semester)

3.1 No. of hours/week	3	In which: 3.2 course	1	3.3 seminar/laboratory	2
3.4 Total hours in the educational plan	42	In which: 3.5 course	14	3.6 seminar/laboratory	28

Time distribution:	hours
Study of lecture notes, bibliography or notes	55
Additional documentation in the library, electronic specialty platforms/ field	40
Seminar / laboratory preparations, homework, portfolio and essays	13
Tutoring	
Exams	
Other activities	

3.7 Total hours of individual study	**108**
3.8 Total hours in a semester	**150**
3.9 Number of credits	**6**

4. Prerequisites (if it is the case)

4.1 curriculum	● Algorithms and programming ● Introduction in programming ● Computational physics (undergraduate level)
4.2 skills	● General skills: the ability to gain general basic knowledge; proper usage of computer science terminology; basic programming skills

5. Requirements (if it is the case)

5.1 for the course	Laptop with a working compiler for C, C++, Fortran etc.
5.2 for the seminar/laboratory	

6. Course objectives - expected learning outcomes that contribute to the training and passing of the course

Knowledge	After successful completion of this course students can represent problems of various areas of application simplified, by means of mathematical models, describe and simulate numerically
Abilities	The ability to use modelling software to solve numerical problems in the field of physics
Responsibility and autonomy	• Development of a multi- and interdisciplinary way of thinking • Efficient usage of information sources and communication resources both in Romanian and in a foreign language (English)

7. Content

7.1 Course	Teaching methods	Observations
1. Monte Carlo methods and statistical physics.	lecture, conversation, exemplification	Bibliographic resources [1]-[3]
2. Monte Carlo importance sampling. Simple sampling. Biased sampling (2h)		Bibliographic resources [1]-[3]
3. Monte Carlo Translational moves. Orientational moves.		Bibliographic resources [1]-[3]
4. MC methods and random numbers		Bibliographic resources [1]-[3]
5. Molecular dynamics. Basic steps in bulling a MD program. Forces computation and integration of motion equations		Bibliographic resources [1]-[3]
6. Molecular dynamics. Integration of the Newton's equation of motion. Verlet algorithm and predictor-corrector scheme. (2h)		Bibliographic resource [4]
7. MD. Integration of the Newton's equation of motion. Leapfrog scheme and Velocity-Stormer-Verlet method. (2h)		Bibliographic resource [5]

8. Computational fluid dynamics. Basic steps for numerical methods (mathematical model, numerical grid, discretization approaches)		Bibliographic resource [5]
9. Finite difference methods in fluid dynamics. Approximation of first and second derivative of PDEs. Boundary conditions		Bibliographic resource [5]
10. Finite Volume Methods in fluid dynamics. Approximations of surface and volume integrals		Bibliographic resource [5]
11. Fluid dynamics. Lattice Boltzmann method		Bibliographic resource [6]

Minimal bibliography:

1. K. Binder, D.W. Heermann – Monte Carlo Simulation in Statistical Physics. An introduction. Springer, 2002
2. D. Frenkel, B. Smit – Understanding Molecular Simulation. From Algorithms to Applications, Academic Press, 2002
3. M. E. J Newman, G. T. Barkema – Monte Carlo Methods in Statistical Physics, Claredon Press, Oxford, 1998
4. M. Griebel, S. Knapek, G. Zumbusch – Numerical Simulation in Molecular Dynamics. Numerics, Algorithms, Parallelization, Applications, Springer 2007
5. J. H. Ferziger, M. Peric, R. L. Street – Computational Methods for Fluid Dynamics, Springer 2020
6. Krüger, T., Kusumaatmaja, H., Kuzmin, A., Shardt, O., Silva, G., Viggen, E.M., 2017. The lattice Boltzmann method. Springer International Publishing 10 (978-3).

7.2 Seminar / laboratory	Teaching methods	Observations
Monte Carlo methods and statistical physics – Random walk; Non-reversal random walk; Self-avoiding random walk	Conversation and individual work under the guidance of the lecturer	The students, using the lecture note, will discuss with the lecturer about the algorithms of the numerical methods. Using a language program (C, C++, Fortran etc.) the students will write programs based on the algorithms.
Monte Carlo methods. Ising model		
Monte Carlo simulation of a Lennard Jones system		
Molecular Dynamics. Diffusion. Static and dynamic properties of the Lennard Jones fluid.		
Molecular Dynamics simplified simulation of the orbit of Halley's Comet.		
Computational fluid dynamics. 1D convection-diffusion equation with Dirichlet		

boundary conditions at both ends		
Computational fluid dynamics. Numerical diffusion		
Bibliography: lecture notes		

8. Corroborating the contents of the discipline with the expectations of the representatives of the epistemic community, professional associations and representative employers in the field related to the program

The computation physics course comes as a complement for the theoretical and experimental physics courses offering a future physicist an increased ability to understand the physical phenomena and to offer a numerical solution for solving specific physics problems.

9. Evaluation

Activity	9.1 Evaluation criteria	9.2 Evaluation methods	9.3 Percentage of the final mark
9.4 Course	The assimilation level of the gained knowledge	Individual project (based on topics discussed during lectures + tutorials).	100%
9.5 Seminar / laboratory	Capacity of solving specific problems and implementing an algorithm.		
9.6 Minimum performance standards			
• Presenting an algorithm with its associated program.			

Data completării
15.09.2025

Titular de disciplină
Dr. Sergiu BUSUIOC

[redacted]

Data avizării în departament
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Director de departament
Conf. Univ. Dr. Nicoleta ȘTEFU