

## SYLLABUS

### 1. Information about the study programme

|                                            |                                      |
|--------------------------------------------|--------------------------------------|
| <b>1.1 Institution of higher education</b> | West University of Timisoara         |
| <b>1.2 Faculty</b>                         | Physics and Mathematics              |
| <b>1.3 Department of</b>                   | Physics                              |
| <b>1.4 Field of study</b>                  | Physics                              |
| <b>1.5 Study cycle</b>                     | Master                               |
| <b>1.6 Study programme</b>                 | Advanced research methods in physics |

### 2. Information about the subject/discipline

|                                |                                                    |                     |   |                               |                |                               |           |
|--------------------------------|----------------------------------------------------|---------------------|---|-------------------------------|----------------|-------------------------------|-----------|
| <b>2.1 Name</b>                | Advanced methods in computational physics ARMP2304 |                     |   |                               |                |                               |           |
| <b>2.2 Course coordinator</b>  | Lect. dr. Alexandra Popescu                        |                     |   |                               |                |                               |           |
| <b>2.3 Seminar coordinator</b> | Lect. dr. Alexandra Popescu                        |                     |   |                               |                |                               |           |
| <b>2.4 Year of study</b>       | II                                                 | <b>2.5 Semester</b> | 1 | <b>2.6 Type of assessment</b> | E <sup>1</sup> | <b>2.7 Type of discipline</b> | DS<br>DOP |

### 3. Total estimated time (hours of teaching per semester)<sup>2</sup>

|                                                                            |            |                   |           |                               |              |
|----------------------------------------------------------------------------|------------|-------------------|-----------|-------------------------------|--------------|
| <b>3.1 Number of hours per week</b>                                        | <b>3</b>   | <b>3.2 course</b> | <b>2</b>  | <b>3.3 seminar/laboratory</b> | <b>1</b>     |
| <b>3.4 Total hours in the curriculum</b>                                   | <b>42</b>  | <b>3.5 course</b> | <b>28</b> | <b>3.6 seminar/laboratory</b> | <b>14</b>    |
| <b>Distribution of time:</b>                                               |            |                   |           |                               | <b>hours</b> |
| Study based on Instructions, course materials, bibliography and notes      |            |                   |           |                               | <b>60</b>    |
| Additional documentation library, specialized electronic platforms / field |            |                   |           |                               | <b>45</b>    |
| Training seminars / laboratories, homework, essays, portfolios and essays  |            |                   |           |                               | <b>18</b>    |
| Tutoring                                                                   |            |                   |           |                               |              |
| Examinations <sup>3</sup>                                                  |            |                   |           |                               | <b>10</b>    |
| Other activities                                                           |            |                   |           |                               |              |
| <b>3.7 Total hours of individual study</b>                                 | <b>123</b> |                   |           |                               |              |
| <b>3.8 Total hours per semester<sup>4</sup></b>                            | <b>175</b> |                   |           |                               |              |
| <b>3.9 Number of credits</b>                                               | <b>7</b>   |                   |           |                               |              |

<sup>1</sup> According to article 37, paragraph (1) of the Higher Education Law no. 199/2023, with subsequent amendments and additions, "the academic success of a student during a study program is determined by verifying the acquisition of the expected learning outcomes through exam-type evaluations and evaluation throughout the semester".

<sup>2</sup> The total number of contact hours and individual study hours will be aligned with the number of credits allocated to the course. One credit corresponds to a total between 25 and 30 hours of teaching activities and individual study. At the level of academic departments may establish, by discipline categories, the exact equivalence between one credit and the number of hours.

<sup>3</sup> The hours corresponding to examinations are added only to the point 3.8 – The total hours per semester, not to be added to the point 3.7 – Total hours of individual study.

<sup>4</sup> Total hours per semester = total hours in the curriculum + total hours of individual study + hours allocated to examinations.

#### 4. Prerequisites (where applicable)

|                          |                                                                                                                                                                                       |
|--------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>4.1 of curriculum</b> | <ul style="list-style-type: none"> <li>Algorithms and programming</li> <li>Introduction in programming</li> <li>Computational physics (undergraduate level)</li> </ul>                |
| <b>4.2 of skills</b>     | <ul style="list-style-type: none"> <li>General skills: the ability to gain general basic knowledge; proper usage of computer science terminology; basic programming skills</li> </ul> |

#### 5. Conditions (where applicable)

|                            |                                                                     |
|----------------------------|---------------------------------------------------------------------|
| <b>5.1 for the course</b>  | Laptop/workstation with a working compiler for C, C++, Fortran etc. |
| <b>5.2 for the seminar</b> |                                                                     |

#### 6. Discipline objectives - expected learning outcomes which contribute to the completion and passing the discipline

|                                    |                                                                                                                                                                                                                                                  |
|------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Knowledge</b>                   | 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                                                        |
| <b>Skills</b>                      | The ability to use modelling software to solve numerical problems in the field of physics                                                                                                                                                        |
| <b>Responsibility and autonomy</b> | <ul style="list-style-type: none"> <li>Development of a multi- and interdisciplinary way of thinking</li> <li>Efficient usage of information sources and communication resources both in Romanian and in a foreign language (English)</li> </ul> |

#### 7. Contents

The platform through which the course materials in electronic format and other learning/bibliographic resources can be accessed: Google Classroom

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

**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                                                                                                      | Teaching methods                                                    | Comments                                                                                                                                                                                                                       |
|-------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1. 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 notes, 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. |
| 2. Monte Carlo methods. Ising model                                                                               |                                                                     |                                                                                                                                                                                                                                |
| 3. Monte Carlo simulation of a Lennard Jones system                                                               |                                                                     |                                                                                                                                                                                                                                |
| 4. Molecular Dynamics. Diffusion. Static and dynamic properties of the Lennard Jones fluid.                       |                                                                     |                                                                                                                                                                                                                                |
| 5. Molecular Dynamics simplified simulation of the orbit of Halley’s Comet.                                       |                                                                     |                                                                                                                                                                                                                                |
| 6. Computational fluid dynamics. 1D convection-diffusion equation with Dirichlet boundary conditions at both ends |                                                                     |                                                                                                                                                                                                                                |
| 7. Computational fluid dynamics. Numerical diffusion                                                              |                                                                     |                                                                                                                                                                                                                                |
| Bibliography: lecture notes                                                                                       |                                                                     |                                                                                                                                                                                                                                |

**8. Corroboration of the course contents with the epistemic expectations of the community representative, professional associations and representative employers of the programme itself**

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. Use of tools based on generative artificial intelligence

To complete the laboratory tasks the students are allowed to use generative AI tools for checking the consistency of the programs written based on the discussed algorithms.

Each student will specify, in a statement written separately for each assignment, according to the model in Annex 3 of the [Regulation on the use of generative artificial intelligence in the educational process at UVT](#), the tool they used, how it was used, and the part of the assignment in which it was used.

## 10. Evaluation

| Type of activity                                     | 10.1 Evaluation criteria                                             | 10.2 Evaluation methods                                                     | 10.3 Percentage of the final mark |
|------------------------------------------------------|----------------------------------------------------------------------|-----------------------------------------------------------------------------|-----------------------------------|
| 10.4 Course                                          | The assimilation level of the gained knowledge                       | Individual project (based on topics discussed during lectures + tutorials). | 100 %                             |
| 10.5 Seminar                                         | Capacity of solving specific problems and implementing an algorithm. |                                                                             |                                   |
| 10.6 Minimum performance standards                   |                                                                      |                                                                             |                                   |
| Presenting an algorithm with its associated program. |                                                                      |                                                                             |                                   |

**Date of submission:**  
16.09.2026

**Titular of the course:** Lect. Dr. Alexandra Popescu  
Signature: 

**Date of approval in department:**

**Seminary titular:** Lect. Dr. Alexandra Popescu  
Signature: 

**HEAD OF THE DEPARTMENT:**  
Conf. Dr. Nicoleta Ștefu