



## Subject card

Subject name and code	Monte Carlo Methods, PG_00069102						
Field of study	Technical Physics						
Date of commencement of studies	February 2025		Academic year of realisation of subject		2025/2026		
Education level	second-cycle studies		Subject group		Specialty subject group		
Mode of study	Full-time studies		Mode of delivery		at the university		
Year of study	2		Language of instruction		Polish		
Semester of study	3		ECTS credits		2.0		
Learning profile	general academic profile		Assessment form		assessment		
Conducting unit	Division of Computational Chemical Physics -> Institute of Physics and Applied Computer Science -> Faculty of Applied Physics and Mathematics -> Wydział Politechniki Gdańskiej						
Name and surname of lecturer (lecturers)	Subject supervisor		dr hab. Jan Franz				
	Teachers		dr hab. Jan Franz				
Lesson types and methods of instruction	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	15.0	0.0	15.0	0.0	0.0	30
	E-learning hours included: 0.0						
	eNauczanie source addresses: Moodle ID: 1312 Metody Monte Carlo <a href="https://enauczanie.pg.edu.pl/2025/course/view.php?id=1312">https://enauczanie.pg.edu.pl/2025/course/view.php?id=1312</a>						
Learning activity and number of study hours	Learning activity	Participation in didactic classes included in study plan		Participation in consultation hours		Self-study	SUM
	Number of study hours	30		2.0		18.0	50
Subject objectives	The aim of the course is to provide students with a systematic introduction to Monte Carlo (MC) methods, with particular emphasis on their application in physical sciences. The course focuses on developing both conceptual understanding and practical skills in designing and analyzing MC simulations using Python. Key topics include random sampling techniques, variance reduction, Markov processes, convergence diagnostics, and statistical error estimation based on the central limit theorem. The course concludes with applications to transport phenomena and basic quantum systems, including Variational Monte Carlo and Path Integral Monte Carlo.						
Learning outcomes	Course outcome		Subject outcome		Method of verification		
	[K7_U07] has enhanced skill of preparing speeches in Polish and English, including presentation of own research results		is able to prepare a concise written report, in Polish or English, presenting the objectives, methodology, results, and interpretation of a Monte Carlo simulation.		[SU1] Assessment of task fulfilment		
	[K7_W02] has enhanced, theoretically-founded, detailed knowledge of selected field of physics, and sufficient knowledge of related fields of science or technology		demonstrates detailed and theoretically grounded knowledge of Monte Carlo methods in physics, including their use in modeling transport phenomena, stochastic processes, and quantum systems, as well as awareness of their applications in related scientific and technological fields.		[SW3] Assessment of knowledge contained in written work and projects		
	[K7_W03] has knowledge of current development paths and discoveries in the scope of physics and related fields of science and technology		is familiar with contemporary applications of Monte Carlo methods in physics, including particle transport and quantum simulations, and understands how these methods contribute to current developments in computational physics and related scientific disciplines.		[SW1] Assessment of factual knowledge		

Subject contents	<p>Part I Fundamentals</p> <p>1. Lecture: Introduction to Monte Carlo (MC) methods, history, applications. Lab: First steps in Python (print, loops, lists, simple plots).</p> <p>2. Lecture: Random numbers: uniform, normal, pseudo-random generators. Lab: Generate random numbers, histograms, sanity checks of distributions.</p> <p>3. Lecture: Probability and statistics: expectation, variance, central limit theorem (CLT). Lab: Dice-roll simulations; compute mean, variance, confidence intervals.</p> <p>4. Lecture: Monte Carlo integration, error estimation. Lab: Estimate PI by sampling; compare with simple numerical quadrature.</p> <p>5. Lecture: Variance reduction: importance sampling, stratified sampling. Lab: Integrate simple functions using importance sampling.</p> <p>Part II Stochastic Models in Physics</p> <p>6. Lecture: Random walks and diffusion. Lab: Simulate 1D/2D random walks; visualize trajectories and mean-square displacement.</p> <p>7. Lecture: Particle transport in matter: scattering, absorption, mean free path. Lab: Photon transport through a slab; tally transmission/absorption with error bars.</p> <p>8. Lecture: Markov chains and equilibrium distributions. Lab: Simulate a finite-state Markov chain; verify stationary distribution.</p> <p>9. Lecture: Metropolis algorithm in statistical physics. Lab: Ising model (1D or 2D) with Metropolis updates; magnetization versus temperature.</p> <p>10. Lecture: Error analysis and convergence, autocorrelation in Markov chains. Lab: Convergence and autocorrelation study on Ising observables.</p> <p>Part III Quantum Methods &amp; Applications</p> <p>11. Lecture: Variational Monte Carlo (VMC): trial wavefunctions and expectation values. Lab: VMC for hydrogen ground state (very simple Gaussian trial).</p> <p>12. Lecture: Path Integral Monte Carlo (PIMC) I: discretized paths, bead-chain (ring-polymer) model. Lab: Build bead-chain for the harmonic oscillator; histogram bead positions.</p> <p>13. Lecture: Path Integral Monte Carlo (PIMC) II: observables and simple applications. Lab: Extend PIMC simulation: estimation of energy or other basic observables; compare with analytical results.</p> <p>14. Lecture: Applications outside physics: finance, biology, engineering (gentle survey). Lab: Simulation outside physics (for example, from finance, biology, or engineering).</p> <p>15. Lecture: Summary and outlook. Lab: Open problems and explorations.</p>		
Prerequisites and co-requisites	Knowledge of the basics of classical mechanics and quantum mechanics.		
Assessment methods and criteria	Subject passing criteria	Passing threshold	Percentage of the final grade
	Quizzes	50.0%	50.0%
	Programming task	50.0%	50.0%
Recommended reading	<p>Basic literature</p> <ol style="list-style-type: none"> <li>1. K. Binder, Monte Carlo simulation in statistical physics : an introduction, Springer, Berlin, 1997.</li> <li>2. D. C. Joy, Monte Carlo modeling for electron microscopy and microanalysis, Oxford University Press, New York, 1995.</li> <li>3. O. N. Vassiliev, Monte Carlo Methods for Radiation Transport, Springer Nature, Cham, Switzerland, 2017.</li> <li>4. W. Schattke, R. Diez Muino, Quantum Monte-Carlo programming : for atoms, molecules, clusters, and solids, Wiley-VCH, Weinheim an der Bergstrasse, Germany, 2013.</li> </ol>		

	Supplementary literature	<ol style="list-style-type: none"> <li>1. W. Krauth, Statistical Mechanics: Algorithms and Computations, Oxford University Press, Oxford, 2006.</li> <li>2. M. Dapor, Transport of Energetic Electrons in Solids: Computer Simulation with Applications to Materials Analysis and Characterization (third edition), Springer Tracts in Modern Physics 271, Springer Nature, Cham, Switzerland, 2020.</li> <li>3. I. H. Hutchinson, A Student's Guide to Numerical Methods, Cambridge University Press, Cambridge, 2015.</li> <li>4. J. Seco, F. Verhaegen (editors), Monte Carlo Techniques in Radiation Therapy, CRC Press, Boca Raton, FL, 2016.</li> </ol>
	eResources addresses	
Example issues/ example questions/ tasks being completed	<ol style="list-style-type: none"> <li>1. Explain how a random walk can be used to model diffusion. Derive the expected relationship between the mean square displacement and the number of steps. What assumptions are required for this scaling law to hold?</li> <li>2. Compare plain Monte Carlo integration and importance sampling. Under what conditions does importance sampling provide a significant advantage? Illustrate with a brief example.</li> <li>3. Simulate a two-dimensional random walk for a large number of particles. For each particle, record the squared displacement after a given number of steps. Repeat the simulation for increasing numbers of steps (e.g. <math>N = 10, 50, 100, 500, 1000</math>) and estimate the mean square displacement as a function of <math>N</math>. Plot the results and verify the expected linear scaling.</li> </ol>	
Work placement	Not applicable	

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