GDAŃSK UNIVERSITY
OF TECHNOLOGY

Subject card

Subject name and code	Monte Carlo Methods, PG_00069102		
Field of study	Technical Physics		
Date of commencement of studies	February 2027	Academic year of realisation of subject	2027/2028
Education level	second-cycle studies	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 -> Faculties of Gdańsk University of Technology	
Name and surname of lecturer (lecturers)	Subject supervisor	dr hab. Jan Franz
	Teachers	dr hab. Jan Franz

Lesson types	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						

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

Subject contents

Course content – lecture
Part I Fundamentals

1. Lecture: Introduction to Monte Carlo (MC) methods, history, applications.
Lab: First steps in Python (print, loops, lists, simple plots).

2. Lecture: Random numbers: uniform, normal, pseudo-random generators.
Lab: Generate random numbers, histograms, sanity checks of distributions.

3. Lecture: Probability and statistics: expectation, variance, central limit theorem (CLT).
Lab: Dice-roll simulations; compute mean, variance, confidence intervals.

4. Lecture: Monte Carlo integration, error estimation.
Lab: Estimate PI by sampling; compare with simple numerical quadrature.

5. Lecture: Variance reduction: importance sampling, stratified sampling.
Lab: Integrate simple functions using importance sampling.

Part II Stochastic Models in Physics

6. Lecture: Random walks and diffusion.
Lab: Simulate 1D/2D random walks; visualize trajectories and mean-square displacement.

7. Lecture: Particle transport in matter: scattering, absorption, mean free path.
Lab: Photon transport through a slab; tally transmission/absorption with error bars.

8. Lecture: Markov chains and equilibrium distributions.
Lab: Simulate a finite-state Markov chain; verify stationary distribution.

9. Lecture: Metropolis algorithm in statistical physics.
Lab: Ising model (1D or 2D) with Metropolis updates; magnetization versus temperature.

10. Lecture: Error analysis and convergence, autocorrelation in Markov chains.
Lab: Convergence and autocorrelation study on Ising observables.

Part III Quantum Methods & Applications

11. Lecture: Variational Monte Carlo (VMC): trial wavefunctions and expectation values.
Lab: VMC for hydrogen ground state (very simple Gaussian trial).

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.

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.

14. Lecture: Applications outside physics: finance, biology, engineering (gentle survey).
Lab: Simulation outside physics (for example, from finance, biology, or engineering).

15. Lecture: Summary and outlook.
Lab: Open problems and explorations.

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
Programming task	50.0%	50.0%
Quizzes	50.0%	50.0%

Recommended reading

Basic literature

1. K. Binder, Monte Carlo simulation in statistical physics : an introduction, Springer, Berlin, 1997.
2. D. C. Joy, Monte Carlo modeling for electron microscopy and microanalysis, Oxford University Press, New York, 1995.
3. O. N. Vassiliev, Monte Carlo Methods for Radiation Transport, Springer Nature, Cham, Switzerland, 2017.
4. W. Schattke, R. Diez Muino, Quantum Monte-Carlo programming : for atoms, molecules, clusters, and solids, Wiley-VCH, Weinheim an der Bergstrasse, Germany, 2013.

	Supplementary literature	1. W. Krauth, Statistical Mechanics: Algorithms and Computations, Oxford University Press, Oxford, 2006. 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. 3. I. H. Hutchinson, A Student's Guide to Numerical Methods, Cambridge University Press, Cambridge, 2015. 4. J. Seco, F. Verhaegen (editors), Monte Carlo Techniques in Radiation Therapy, CRC Press, Boca Raton, FL, 2016.
	eResources addresses	
Example issues/ example questions/ tasks being completed	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? 2. Compare plain Monte Carlo integration and importance sampling. Under what conditions does importance sampling provide a significant advantage? Illustrate with a brief example. 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. N = 10, 50, 100, 500, 1000) and estimate the mean square displacement as a function of N. Plot the results and verify the expected linear scaling.	
Practical activites within the subject	Not applicable	