University of Gdańsk

Subject card

Subject name and code	Parallel programming in Python, PG_00117812		
Field of study	Chemistry		
Date of commencement of studies	October 2026	Academic year of realisation of subject	2026/2027
Education level	Master's studies	Subject group	Optional subject group
Mode of study	full-time studies	Mode of delivery	at the university
Year of study	1	Language of instruction	English
Semester of study	2	ECTS credits	2.0
Learning profile	academic	Assessment form	credit
Conducting unit	Faculty of Chemistry -> Rector		
Name and surname of lecturer (lecturers)	Subject supervisor	prof. dr hab. Cezary Czaplewski	
	Teachers		

Lesson types

Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
Number of study hours	0.0	0.0	30.0	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	5.0	15.0	50

Subject objectives

Introduction to parallel programming using MPI library in Python. Effectively design and conduct parallel computing.

Learning outcomes

Course outcome	Subject outcome	Method of verification
[CHEMMU2_W05] Has extended knowledge in the field of the specialisation studied.	Student recognizes and characterizes parallel computer architectures, differentiate parallel libraries and tools for parallel programming, knows function from MPI library	[SW2] presentation/project/paper/ report
[CHEMMU2_U02] Critically assesses the results of conducted, performed observations and theoretical calculations and discusses errors.	Student evaluates the usefulness of parallel programming to solve a given problem, runs parallel applications in batch and interactive mode, analyses parallel source codes, creates simple parallel codes using python with MPI library.	[SU2] presentation/project/paper/ report [SU8] observation of student's independent or team work
[CHEMMU2_K01] Knows the limitations of her/his own knowledge; understands the need for further education and can inspire other people to do so.	Develops the ability to work in a team.	[SK8] observation of student's independent or team work
[CHEMMU2_W06] Applies mathematics to the extent necessary to understand, describe and model chemical processes of medium complexity.	Applies parallel programming to selected computational chemistry topics	[SW2] presentation/project/paper/ report
[CHEMMU2_K06] Undertakes research tasks consciously and responsibly, understanding the social aspects of the practical application of the acquired knowledge and skills and the responsibility related to it.	The student learns the principles of safe, responsible and effective work on supercomputers in computing centers and on local computer clusters.	[SK8] observation of student's independent or team work

Subject contents	Parallel programming as an essential method in computational chemistry. Types of computer architectures used for parallel computing, shared and distributed memory. Scalability of parallel computing: Amdahl's law. Running parallel tasks on computing clusters - queuing systems. Parallel programs with the use of message passing interface (MPI) library. Initialization and termination of references to MPI libraries in Python programs. Point to point communication: safety and avoiding deadlock. Collective communication. Process groups and messengers. Intergroup communication. Data types and user operators in MPI. Virtual topologies. Libraries in MPI: rules of creation. Evaluation of the effectiveness of parallelization and profiling of parallel programs. MPI extensions (MPI2 and MPI3): MPI-IO, remote memory operations, dynamic process management.
Prerequisites and co-requisites	Introduction to Python programming Basis of calculus and linear algebra, ability to use the LINUX operating system

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
group project	51.0%	50.0%
reports	51.0%	50.0%

Recommended reading

Basic literature	W. Gropp, E. Lusk, A. Skjellum, Using MPI. Portable Parallel Programming with the Message-Passing Interface, The MIT Press, Cambridge, 1999. W. Gropp, E. Lusk, R. Thakur, Using MPI-2. Advanced Features of the Message-Passing Interface. The MIT Press, Cambridge, 1999. MPI for Python https://mpi4py.readthedocs.io/en/stable/
Supplementary literature	I. Foster, Designing and Building Parallel Programs, Addison Wesley, 1995 M. Snir, S. Otto, S. Huss-Lederman, D. Walker, J. Dongarra, MPI: the Complete Reference, The MIT Press, 1995
eResources addresses	

Example issues/ example questions/ tasks being completed	
Work placement	Not applicable

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