DOCTORAL (PHD) STUDIES

COURSE UNIT DESCRIPTION

Course unit title	Scientific areas	Faculty	Institute, department
Numerical modeling	Informatics (N 009)	Faculty of Mathematics and Informatics	Institute of Computer Science, Department of Computational and Data Modeling

Study method	Number of credits	Study method	Number of credits
Lectures		Consultations	2
Individual works	3	Seminars	2 (spring semester)

Summary

The aim of the course unit is to understand the concepts and phenomena typical for numerical (computer) modeling, to get acquainted with the fields of application. Learn to apply and program various numerical simulation algorithms, create and develop applied modeling tasks, perform expert research of such tasks. Practical part of the project – the implementation of the project related to the computer modeling of biosensor (more detailed information is given below). Developing the project, you will need to go deep into many topics of numerical modeling, to understand their interrelationships.

Course unit content – breakdown of the topics:

- Principles of numerical modeling, examples of the simplest numerical algorithms illustrating these principles.
- Errors, estimation and analysis.
- Monte Carlo methods, generating pseudo-random numbers and evaluation of their quality
- Polynomial and spline interpolation and approximation.
- Numerical differentiation and integration.
- Spectral methods, fast Fourier transform.
- Algorithms for solving scalar nonlinear equations.
- Linear and nonlinear dynamical systems and spatial evolutionary differential models: linear differential models and their applications; examples of nonlinear differential models. Boundary and initial conditions in differential models.
- Principles of algorithm construction for differential models, difference schemes for common types of differential equations, double-layer and multi-layered schemes, weighted schemes, economical difference schemes.
- Numerical modeling of nonlinear spatial evolutionary models, difference equations, basic structure of algorithm.
- The importance of linear algebra solvers for modeling nonlinear differential problems, direct and iterative methods for solving difference equations.
- Algorithm and its computer implementation validating, test task creation, algorithm reliability control strategies.
- Approximation order, convergence and stability of an algorithm, conservative algorithms. Explicit and implicit algorithms, their advantages and disadvantages.

- An example of the application of numerical modeling – computer modeling of biosensor: structure of an electrochemical biosensor and a biochemical reaction scheme; mathematical models and numerical algorithms for solving it; numerical experiments and their results.

Before taking course unit theory exam (during which one will need to answer the questions from the list of topics provided), one project must be completed (implemented on a computer and defended during the seminar). The topics to choose (one of two):

1. Computer modeling of biosensor, taking into account *S* (substrate), *P* (product), *E* (enzyme) and *EP* (enzyme-product complex) kinetics (methodological material for the implementation of the project is provided in the main literature reference [4], chapters 1–3).
2. Computer modeling of biosensor, taking into account *S* (substrate) and *P* (product) kinetics (methodological material for the implementation of the project is provided in the main literature reference [4], chapters 4–6).

To get the final grade for the course unit, one must complete and defend the project (50% of the final grade) and demonstrate the knowledge of the theory during the examination (50% of the final grade).

Main literature
1. G. Dahlquist and Å. Björck. Numerical Methods in Scientific Computing: Volume 1. SIAM, 2008.
2. R. Čiegis. Diferencialinių lygčių skaitiniai sprendimo metodai (in Lithuanian). VGTU leidykla "Technika", 2003.
3. R. Baronas, F. Ivanauskas and J. Kulys. Mathematical Modeling of Biosensors. Second edition. Springer, 2021.
4. T. Meškauskas. Computer modeling of biosensor: methodological material for projects (in Lithuanian). 2018. http://mif.vu.lt/~meska/projektai/Kompiuterinis_Biojutiklio_Modeliavimas.pdf

Lecturer(s) (name, surname)	Science degree	Main publications
Tadas Meškauskas	dr.	http://elaba.mb.vu.lt/mif/?aut=Tadas+Meškauskas
Romas Baronas	dr.	http://elaba.mb.vu.lt/mif/?aut=Romas+Baronas
Linas Bukauskas	dr.	http://elaba.mb.vu.lt/mif/?aut=Linas+Bukauskas