MINISTRY OF EDUCATION AND SCIENCE OF UKRAINE
Ivan Franko National University of L'viv
Faculty of Applied Mathematics and Informatics
Department of Applied Mathematics

Approved
At the meeting
of the Department of Applied Mathematics
Faculty of Applied Mathematics and Informatics
Ivan Franko National University of L'viv
(Protocol No. 1 dated August 31, 2023)

Head of the Department Yuriy YASHCHUK

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Syllabus of the academic discipline "Optimization of Complex Systems (in English)" which is taught within the framework of the EPP "Applied Mathematics" Second (Master's) level of higher education for students specializing in 113 – Applied Mathematics

L'viv, 2023

Discipline name	**Optimization of complex systems**
Address where the discipline is taught	The main building of Ivan Franko National University of Lviv 1, Universytetska st., Lviv
The faculty and department under which the discipline is established	Faculty of Applied Mathematics and Informatics Department of Computational Mathematics
Field of knowledge, code and name of specialty	11 – mathematics and statistics 113 – applied mathematics
Teachers of the discipline	Shcherbatyy Mykhaylo Vasylovych, Candidate of Physical and Mathematical Sciences, Associate Professor of the Department of Computational Mathematics, Kukharskyy Vitaliy Mykhaylovych, Candidate of Physical and Mathematical Sciences, Associate Professor of the Department of Computational Mathematics, (laboratory classes)
Contact information of teachers	mykhaylo.shcherbatyy@lnu.edu.ua; https://ami.lnu.edu.ua/employee/shcherbatyy vitaliy.kukharskyy@lnu.edu.ua; https://ami.lnu.edu.ua/employee/kukharskyy Room 278, The main building of Ivan Franko National University of Lviv, 1, Universytetska st., Lviv
Consultations on issues of training in the discipline are taking place	Consultations on the day of lectures/laboratory sessions (by prior agreement).
Course page	https://ami.lnu.edu.ua/en/course/optimization-of-complex-systems-am-1-4
Information about the discipline	The discipline "Optimization of complex systems" is a mandatory discipline from specialty 113 - applied mathematics for the educational program "Applied Mathematics", which is taught in the 3rd semester in the amount of 3 credits (according to the European Credit Transfer System ECTS).
Brief abstract of the discipline	This course concerns optimization problems of complex systems, governed by ordinary differential equations and partial differential equations. Numerical methods for solution of optimization problems, which are based on direct and indirect approaches, are considered. Sensitivity analysis relations in discrete formulation that are obtained using various methods are presented. First-order necessary optimality conditions for finite-dimensional controls are obtained. A number of applications examples from different fields illustrate the material of this course.

Goal and objectives of the discipline	The **goal** and **objectives** of the discipline are to teach students: • formulate optimal control problems (optimization problems) for systems governed by ordinary differential equations (ODEs) and partial differential equations (PDEs); • write the necessary optimality conditions; • construct numerical schemes for solution of optimal control problems; • derive expressions of sensitivity analysis; • apply the capabilities of computer algebra systems (e.g., Matlab, Octave) to solve the optimization problems.
Literature for the discipline	**Basic literature** 1. F. Tröltzsch. *Optimal Control of Partial Differential Equations (Graduate Studies in Mathematics).* AMS, 2010. 2. M. Hinze, R. Pinnau, M. Ulbrich, S. Ulbrich. *Optimization with PDE Constraints.* Springer, 2009. 3. Reyes J.C. *Numerical PDE-Constrained Optimization*. Springer, 2015. *4.* Borzi A., *Modelling with Ordinary Differential Equations. A Comprehensive Approach.* CRC Press, 2020. *5.* Arora J.S., *Introduction to Optimum Design*. Elsevier Inc., 2017. **Additional literature** *6.* Choi K. K., Kim N. H. *Structural Sensitivity Analysis and Optimization 1. Linear Systems.* Springer, 2005. 7. Speyer J. L., Jacobson D. H., *Primer on optimal control theory*. SIAM, 2010. 8. Shcherbatyy M.V. *Sensitivity analysis for one-dimensional semilinear partial differential equations.* // Вісник Київського національного університету імені Тараса Шевченка, Серія: фізико-математичні науки. – 2017. – №2. – С. 157-164. 9. Наконечний О.Г. *Оптимальне керування та оцінювання в рівняннях із частинними похідними.: Навчальний посібник.* К.: ВПЦ "Київський університет", 2004. 10. Бейко І.В., Зінько П.М., Наконечний О.Г. *Задачі, методи і алгоритми оптимізації. Навчальний посібник.* Рівне, 2011. 11. MATLAB Homepage: http://www.mathworks.com/products/matlab/. 12. GNU Octave Homepage: http://www.gnu.org/software/octave/
Scope of the course	Total volume: 90 hours. Classroom classes: 32 hours, including 16 hours of lectures -and 16 hours of laboratory work. Independent work: 58 hours.
Expected learning outcomes	Upon completion of this course, the student will: ***Know:*** • Formulation of optimal control problems for systems with ODEs constraints and PDEs constraints; • numerical schemes for solution of optimal control problems with ODEs constraints and PDEs constraints. ***Be able to***: • formulate optimal control problems for systems with ODEs and equations PDEs constraints; write these problems in extended and reduced forms; • write first order necessary optimality conditions in discrete form; • construct numerical schemes for solution of optimal control problems; transform optimal control problem into nonlinear programming problem;

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- derive expressions of sensitivity analysis using different methods (direct differentiation method, adjoint method; discrete formulation); construct efficient algorithms for calculation of sensitivity coefficients.

The course provides the acquisition of the following competencies and program learning outcomes:

General competencies:

- GC1. Ability to think abstractly, analyze and synthesize.
- GC06. Ability to communicate in a foreign language on professional issues both orally and in writing.

Special competencies:

- SC1. Knowledge of the principles of construction and research of mathematical models, as well as numerical methods for their solution.
- SC2. Ability to develop and research mathematical models and methods for their solution.
- SC04. Ability to build a discrete analog of a continuous model.
- SC05. Ability to programmatically implement algorithms in one of the programming languages.
- SC07. Ability to debug computer programs with complex logic.
- SC09. Ability to increase the efficiency of computing schemes and algorithms.
- SC11. Ability to use the grammatical and stylistic aspects of a foreign language for scientific and professional purposes in the field of applied mathematics and IT..

Program learning outcomes:

- PLO 1. Demonstrate knowledge and understanding of approaches to the construction and research of mathematical models.
- PLO02. Apply, modify and investigate numerical methods for solving applied problems.
- PLO03. Develop and programmatically implement algorithms for solving applied problems..
- PLO04. Develop and programmatically implement algorithms for solving applied problems.
- PLO06. Determine the most effective method for solving a problem in terms of computational costs and accuracy of the results obtained.
- PLO13. Communicate fluently in a foreign language, both orally and in writing, when discussing professional issues and conducting research.

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<tr><td>Keywords</td><td>Optimal control problem, optimization criterion, control function, set of admissible controls, optimal design problem, parameter identification problem, reduced form of the optimization problem; direct and indirect methods for solving optimization problems, necessary optimality conditions (Karush-Kuhn-Tucker conditions), sensitivity analysis, sensitivity coefficients, direct differentiation method, adjoint method.</td></tr>
<tr><td>Course format</td><td>Face-to-face
Conducting lectures, laboratory sessions and consultations.</td></tr>
<tr><td>Topics</td><td>See below in the table Scheme of the course "Optimization of complex systems".</td></tr>
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Final control, form	Exam
Prerequisites	To study this course, students need basic knowledge of the following courses: Mathematical Analysis; Linear algebra; Optimization methods; Differential equations; Equations of mathematical physics; Numerical Methods; Computer algebra systems (e.g., Matlab, Octave) or numerical method libraries of other software products (e.g., NumPy for Python). Also, to study this course, students require knowledge of the courses: - Methods of functional analysis in applied scientific research; - Foreign language for professional orientation.
Teaching methods -and techniques that will be used during the teaching of the course	Presentations, lectures, laboratory materials Homework and individual assignments
Required equipment	Computer with one of the computer algebra systems (Matlab, Octave) or a software product with available libraries of numerical methods for solving systems of ordinary differential equations, partial differential equations, and optimization methods.
Evaluation criteria -(separately for each type of educational activity)	The assessment is carried out on a 100-point scale. Points are awarded according to the following ratio: • homework assignments: 14% of the semester grade; the maximum number of points is 14 (3 assignments; 5, 5, 4 points properly); • individual assignments: 24% of the semester grade; maximum number of points 24 (2 assignments of 12 points each); • module: 12% of the semester grade; the maximum -number of points is 12 (1 module, 12 points); A total of 50 points during the semester. Exam: 50 points. **Academic Integrity**: Students' works are expected to be their own original research or reasoning. Lack of references to used sources, fabrication of sources, plagiarism, interference in the work of other students are, but are not limited to, examples of possible -academic dishonesty. The detection of signs of academic dishonesty in a student-'s written work is a reason for its rejection by -the teacher, regardless of the scale of plagiarism or deception. **Attending classes** is an important part of learning. All students are expected to attend all lectures and laboratory sessions of the course. Students must inform the teacher about the impossibility to attend classes. In any case, students are obliged to adhere to the deadlines -set for homework and individual assignments provided by the course. **Literature.** All literature that students cannot find on their own will be provided by the teacher for educational purposes only, without the right to transfer it to third parties. Students are also encouraged to use other literature and sources that are not among the recommended ones.

	Scoring policy. Points obtained on individual and homework assignments and module are taken into account. At the same time, attendance of classes and the student's activity during laboratory sessions must be taken into account; inadmissibility of absences and lateness to classes; using a mobile phone, tablet or other mobile -devices during class for purposes not related to education; plagiarism; untimely performance of the assigned task, etc. Any form of breach of academic integrity will not be tolerated.
Questions for the exam.	1. Introduction and examples of optimization problems. 2. Formulation of Optimization Problem. Reduced formulation 3. Optimization problems for ODEs. 4. Optimization problems for PDEs of elliptic type. 5. Optimization problems for PDEs of parabolic type. 6. Parameter identification problems. 7. The scheme of solving optimization problems. Direct and indirect methods (first discretize - then optimize; first optimize - then discretize). 8. Formulation of optimal control problem (OCP) as nonlinear programming problem 9. Classification of optimization methods (line search methods, trust region methods). 10. Necessary optimality conditions (Lagrangian, Karush-Kuhn Tucker conditions). Finite dimensional case. 11. Optimization problems with equality and inequality constraints. 12. Formulation of sensitivity analysis (SA) problems. Metods of SA (finite dimensional case of control function). Direct differentiation method. Adjoint method. 13. Sensitivity analysis for boundary value problem of ordinary differential equation. Finite dimensional case of control function. 14. Sensitivity analysis in optimal control problems of elliptic systems. 15. Necessary conditions optimality based on Lagrangian for elliptic systems. Finite dimensional case of control function.
Poll	An evaluation questionnaire for the purpose of assessing the quality of the course will be provided upon completion -of the course.

Scheme of the course ***"Optimization of complex systems"***

Week	**Topic, plan, short theses**	**Form of activity (class)**	**Literature, Internet resources**	**Assignment, hours**	**Deadline**
1	**Topic 1.** Introduction and examples of optimization problems. General formulation of optimization problems *(The main components of optimization problems. Reduced formulation of optimization problems).*	Lecture (2 hours)	[1-5]	Elaboration of lecture material (3 hours)	1 week
	Topic 1. Formulation of problems of optimization of complex systems. Extended and reduced formulation. *(Optimal control problems, optimal design problems. The main steps in formulating an optimization problem. Examples of optimization problems. Solvers of computer mathematics systems (for example, Matlab/Octave) for solving nonlinear programming problems (NPP)).*	Laboratory (2 hours	[1-5], [11], [12]	Examples of the use of appropriate solvers for solving finite-dimensional optimal design problems (3 hours)	1 week
2	**Topic 2.** Formulation of optimization problems for systems of ordinary differential equations (ODEs). Formulation of optimization problems for systems of elliptic type. *(Integral, local, and point type characteristics. Reduced formulation of optimal control problems. Examples of optimal control problems for ODEs and PDEs of elliptic type).*	Lecture (2 hours)	[4], [7] [1-3], [9]	Elaboration of lecture material (3 hours)	1 week

	Topic 2. Formulation of optimal control problems for ODEs. Selection of control functions, system characteristics, optimization criterion. *(Solvers of computer algebra systems (for example, Matlab/Octave) for solving ODEs. Calculation characteristics of the systems under consideration using control functions and solutions of analysis problem analysis (state functions)).* ***Homework assignment 1.***	Laboratory (2 hours	[4], [7], [11], [12]	Fulfillment of homework assignment 1 (4 hours)	1 week
3	**Topic 3.** Optimization problems for PDEs of parabolic type. Parameter identification problems. *(Integral, local, and point type characteristics.* *Reduced formulation of optimal control problems.* *Examples of optimal control problems for PDEs of parabolic type).*	Lecture (2 hours)	[1-3]	Elaboration of lecture material (3 hours)	1 week
	Topic 3. Optimization problems for PDEs of elliptic type and PDEs of parabolic type. *(Integral, local, and point type characteristics. Reduced formulation of optimal control problems. Optimal control problems and optimal design problems. Examples of optimal control problems).* ***Homework assignment 2.***	Laboratory (2 hours	[1-3]	Fulfillment of homework assignment 2 (3 hours)	1 week
4	**Topic 4.** The scheme of solving optimization problems. Direct and indirect methods. *(Formulation of optimal control problem as nonlinear programming problem*	Lecture (2 hours)	[1], [3], [5], [7]	Elaboration of lecture material (4 hours)	1 week

	(NPP). Optimization methods for solution of NPP (line search methods, trust region methods).				
	Topic 4. Development of algorithm for solving optimal control problems for ODEs *(approximation of the control function, transformation of the optimization problem into a nonlinear programming problem, solving the obtained problem using solvers of computer algebra systems for solving direct and nonlinear programming problems).* ***Individual assignment 1.***	Laboratory (2 hours	[4], [5], [7], [10-12]	Fulfillment of individual assignment 1 (8 hours)	2 weeks
5	**Topic 5.** Necessary optimality conditions (finite-dimensional case). Lagrange function. Karush-Kuhn-Tucker conditions.	Lecture (2 hours)	[1], [3], [5], [10]	Elaboration of lecture material (5 hours)	1 week
	Topic 5. Necessary optimality conditions for optimization problems with equality and inequality constraints. *(Solution scheme for optimization problems using necessary optimality conditions in the case of finite-dimensional controls. Program structure).* ***Homework assignment 3.***	Laboratory (2 hours	[1], [3], [5], [10-12]	Fulfillment of homework assignment 2 (3 hours)	1 week
6	**Topic 6.** Formulation of sensitivity analysis (SA) problems. Methods of SA (finite dimensional case of control function). Sensitivity analysis for boundary value problem of ordinary differential equation (finite dimensional case of control function). *(Finite diference method, Direct differentiation method, Adjoint method.)*	Lecture (2 hours)	[1], [5], [6], [8]	Elaboration of lecture material (3 hours)	1 week

	Topic 6. Software implementation of optimization algorithm for solving the optimal control problem of ODEs *(constraints on the control function and state function).* ***Individual Assignment 2.***	Laboratory (2 hours	[3-4], [7], [11-12]	Fulfillment of individual assignment 2 (7 hours)	2 weeks
7	**Topic 7.** Sensitivity analysis for PDEs of elliptic types Finite dimensional case. *(Approximation of control and state functions. Direct differentiation method, Adjoint method.)*	Lecture (2 hours)	[1-3], [6], [8]	Elaboration of lecture material (5 hours)	1 week
	Topic 7. Module.	Laboratory (2 hours	[1], [6], [8]		During the class
8	**Topic 8.** Necessary conditions optimality based on Lagrangian for elliptic systems. Finite dimensional case of control function.	Lecture (2 hours)	[1-3], [5], [10]	Elaboration of lecture material (4 hours)	1 week
	Topic 8. Evaluation of the individual task 2. Analysis of the results. Summarizing the conclusions.	Laboratory (2 hours	[1], [3]		During the class