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
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Head of the Department Yashchuk Yu.O.

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Syllabus of the academic discipline "Optimization of Complex Systems" 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 (1 year, 9 months)

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, 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 Ihor.makar@lnu.edu.ua; https://ami.lnu.edu.ua/employee/makar-i-h 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-complex-systems (master, 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" (duration of training 1.9), which is taught in the 3rd semester in the amount of 6 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 and continuous formulation that are obtained using various methods are presented. First-order necessary optimality conditions for finite-dimensional and continuous 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. *6.* Quarteroni A. *Numerical Models for Differential Problems.* Springer, 2017. **Additional literature** *7.* Choi K. K., Kim N. H. *Structural Sensitivity Analysis and Optimization 1. Linear Systems.* Springer, 2005. 8. Speyer J. L., Jacobson D. H., *Primer on optimal control theory*. SIAM, 2010. 9. 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. 10. Наконечний О.Г. *Оптимальне керування та оцінювання в рівняннях із частинними похідними.: Навчальний посібник.* К.: ВПЦ "Київський університет", 2004. 11. Бейко І.В., Зінько П.М., Наконечний О.Г. *Задачі, методи і алгоритми оптимізації. Навчальний посібник.* Рівне, 2011. 12. MATLAB Homepage: http://www.mathworks.com/products/matlab/. 13. GNU Octave Homepage: http://www.gnu.org/software/octave/ 14. https://optpde.math.uni-hamburg.de/
Scope of the course	Total volume: 180 hours. Classroom classes: 64 hours, including 32 hours of lectures -and 32 hours of laboratory work. Independent work: 116 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 and continuous form; • construct numerical schemes for solution of optimal control problems; transform optimal control problem into nonlinear programming problem; • derive expressions of sensitivity analysis using different methods (direct differentiation method, adjoint method; discrete and continuous formulation); construct efficient algorithms for calculation of sensitivity coefficients. **The course provides the acquisition of the following competencies and program learning outcomes:** **Integral competence:** - Ability to solve research and/or innovative problems in the field of applied mathematics. **General competencies:** - GC01. Ability to think abstractly, analyze and synthesize. - GC02. Ability to apply knowledge in practical situations. - GC03. Ability to conduct research at the appropriate level. - GC04. The ability to search, process, and analyze information from various sources. - GC05. The ability for critical thinking and experimentation. - GC06. The ability to generate new ideas (creativity). - GC09. The ability to plan and manage time. - GC10. The ability to assess and ensure the quality of performed work. - GC11. Skills in using information and communication technologies. - GC12. The ability to work in an international context. - GC13. The ability to convey one's own knowledge to other individuals. **Professional Competencies of the Specialty (PC):** - PC01. The ability to develop a mathematical model based on conducted analysis. - SC04. The ability to construct a discrete analogue of a continuous model. - PC06. Writing program code in one of the programming languages to solve algorithmically complex problems. - PC07. Development of architecture and design of programs, utilizing necessary data structures. - SC08. Ability to debug computer programs with intricate logic. - SC09. Validation and verification of obtained results. - SC12. The ability to convey necessary professional information to others within any time constraints. **Program learning outcomes:** - PLO02. The ability to approximate a continuous problem with a finite-dimensional analogue. - PLO08. The ability to develop algorithms and software for solving optimal control problems using various approaches. - PLO09. The ability to combine algorithms and data structures to solve practical problems. - PLO10. The ability to analyze characteristics of practical problems and assess the effectiveness of potential solution methods. - PLO16. The skill to conduct scientific research and maintain accompanying documentation. - PLO17. The skill to present professional information in both oral and written forms under various constraints.
Keywords	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.
Course format	Face-to-face, remote Conducting lectures, laboratory sessions and consultations.
Topics	See below in the table Scheme of the course "Optimization of complex systems".
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; - Functional analysis; - Numerical Methods; - Computer algebra systems (e.g., Matlab, Octave) or numerical method libraries of other software products (e.g., NumPy for Python).
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: 12% of the semester grade; the maximum number of points is 14 (4 assignments; 3, 3, 2, 4 points properly); • individual assignments: 28% of the semester grade; maximum number of points 28 (4 assignments of 5, 5, 8, 10 points properly); • control measurements (modules): 10% of the semester grade; the maximum -number of points is 10 (1 module, 10 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 scored during testing and independent work are taken into account. At the same time, attendance of classes and the student's activity during practical 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 test or 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. 16. Differentiability in Banach spaces. Adjoint operators and adjoint functions. 17. Continuum sensitivity analysis. Direct differentiation method. Adjoint method. 18. Sensitivity analysis in initial value problems for ordinary differential equations (ODEs).

	19. AM of sensitivity analysis for quadratic elliptic control problems and quadratic parabolic control problems. 20. A Lagrangian-based view of the adjoint approach. Lagrangian approach in initial value problems for ordinary differential equations (ODEs). 21. Iterative solution of the optimal control problem (sensitivity approach, Lagrangian approach). 22. Second order sufficient optimality conditions.
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	Assign ment, 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, Independent work	[1-5]	2 3	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). Examples of the use of appropriate solvers for solving finite-dimensional optimal design problems).*	Laboratory Independent work	[1-5], [11], [12]	2 3	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, Independent work	[4], [7], [1-3], [9]	2 3	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 Independent work	[4], [7], [11], [12]	2 4	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, Independent work	[1-3]	2 3	1 week
	Topic 3. Optimization problems for PDEs of elliptic type and PDEs of parabolic type.	Laboratory Independent work	[1-3]	2 3	1 week

	(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.***				
4	**Topic 4.** The scheme of solving optimization problems. Direct and indirect methods. *(Formulation of optimal control problem as nonlinear programming problem (NPP). Optimization methods for solution of NPP (line search methods, trust region methods).*	Lecture, Independent work	[1], [3], [5], [7]	2 4	1 week
	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 Independent work	[4], [5], [7], [10-12]	2 6	2 weeks
5	**Topic 5.** Necessary optimality conditions (finite-dimensional case). Lagrange function. Karush-Kuhn-Tucker conditions.	Lecture, Independent work	[1], [3], [5], [10]	2 5	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*	Laboratory Independent work	[1], [3], [5], [10-12]	2 5	1 week

	finite-dimensional controls. Program structure). ***Homework assignment 3.***				
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, Independent work	[1], [5], [6], [8]	2 3	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 Independent work	[3-4], [7], [11-12]	2 4	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, Independent work	[1-3], [6], [8]	2 6	1 week
	Topic 7. Control measurement (module)	Laboratory	[1], [6], [8]	2	4 weeks
8	**Topic 8.** Necessary conditions optimality based on Lagrangian for elliptic systems. Finite dimensional case of control function.	Lecture, Independent work	[1-3], [5], [10]	2 3	1 week
	Topic 8. Algorithms for solving the optimal control problem based on the Lagrangian.	Laboratory Independent work	[1], [3]	2 3	1 week
9	**Topic 9.** Differentiability in Banach spaces. Adjoint operators and adjoint functions.	Lecture, Independent work	[1-3], [5], [6]	2 3	1 week

	Topic 9. Differentiability of functionals in optimal control problems. Adjoint operators and adjoint functions. (*Systems of ordinary differential equations (ODEs) and equations of elliptic and parabolic partial derivatives).*	Laboratory Independent work	[1], [3]	2 3	1 week
10	**Topic 10.** Continuum sensitivity analysis (SA). Direct differentiation method (DDM). Adjoint Method (AM).	Lecture, Independent work	[1-3], [6-8], [14]	2 4	1 week
	Topic 10. A general approach to obtaining sensitivity analysis *expressions (conjugate operators, direct differentiation method, adjoint method, comparison of methods).*	Laboratory Independent work	[1-3], [6-8],	2 4	1 week
11	Topic 11. Sensitivity analysis in initial value problems for ODEs. The direct differentiation method. The method of adjoint functions.	Lecture, Independent work	[4], [6]	2 3	1 week
	Topic 11. Derivation of sensitivity analysis relationships in initial value problems for ODEs. ***Individual assignment 3.***	Laboratory Independent work	[4], [6]	2 5	2 week
12	**Topic 12.** AM of sensitivity analysis for quadratic elliptic control problems with distributed control.	Lecture, Independent work	[1-3], [14]	2 3	1 week
	Topic 12. Derivation of sensitivity analysis relationships for equations of elliptic and parabolic types *(two-dimensional equations in spatial coordinates).* ***Homework assignment 4.***	Laboratory Independent work	[1-3], [6], [14]	2 5	1 week
13	**Topic 13.** Sensitivity analysis using the adjoint method based on the	Lecture,	[1-3], [6-7], [14]	2 4	1 week

	Lagrangian. Application of the Lagrangian to optimal control problems for ODEs.	Independent work			
	Topic 13. Scheme of computing sensitivity coefficients in ODEs and their utilization in optimization algorithms. ***Individual assignment 4.***	Laboratory Independent work	[3], [6]	2 4	3 weeki
14	**Topic 14.** Necessary optimality conditions based on the Lagrangian. Solving optimal control problems based on the Lagrangian.	Lecture, Independent work	[1-3], [6]	2 4	1 week
	Topic 14. Derivation of relationships for sensitivity coefficients based on the Lagrangian in the case of elliptic type systems (two-dimensional equations in spatial coordinates).	Laboratory Independent work	[1-3], [6], [14]	2 4	1 week
15	**Topic 15.** Iterative solution of the optimal control problem (sensitivity approach, Lagrangian approach).	Lecture, Independent work	[1-3], [6]	2 3	1 week
	Topic 15. Derivation of relationships for sensitivity coefficients based on the Lagrangian in the case of parabolic type systems (two-dimensional equations in spatial coordinates).	Laboratory Independent work	[1-3], [14]	2 3	1 week
16	**Topic 16.** Second order sufficient optimality conditions.	Lecture, Independent work	[1-3], [6]	2 6	1 week
	Topic 16. Discussion of results obtained through various approaches to solving optimal control problems. Summary and conclusion.	Laboratory	[1-3], [6]	2	1 week