Syllabus
Course Program

Computational methods

Specialty
113 - Applied mathematics

Institute
Institute of Computer Modelling, Applied Physics and Mathematics

Educational program
Applied Mathematics. Computer and Mathematical Modeling

Department
Mathematical Modeling and Intelligent Computing in Engineering (161)

Level of education
Bachelor's degree

Course type
Special (Professional), Mandatory

Semester
4

Language of instruction
English

Lecturers and course developers

Viktor Fedorov
Victor.Fedorov@khpi.edu.ua

Candidate of technical sciences, associate professor Author of 55 scientific publications, basic courses "Computational methods", "Theory of fluidity and strength", "Mathematical models of composite materials" Google Scholar: https://scholar.google.com/citations?user=xozYUyIAAAAJ&hl=uk SCOPUS: https://www.scopus.com/authid/detail.uri?authorId=56495691400 Orcid: https://orcid.org/0000-0002-4814-6768

More about the lecturer on the department's website

General information

Summary

This discipline provides methods that can be used to solve any problem in applied mathematics. They are an everyday tool of an engineer and a scientist and are a component of professional software complexes. Purpose and objectives of the disciplines The goal of studying the discipline is to acquire the ability to solve problems of applied mathematics using computer tools.

Course objectives and goals

Mastering knowledge of the theoretical foundations of computing methods, algorithms for solving typical problems of applied mathematics, acquiring skills and abilities to solve these problems by programming computer equipment.

Format of classes

Lectures, laboratory work, independent work, consultations, course work. The final control is an exam.

Competencies

ZK06. Ability to abstract thinking, analysis and synthesis.
FK01. Ability to use and adapt mathematical theories, methods and techniques to prove mathematical statements and theorems.
FK04. Ability to develop algorithms and data structures, software tools, and software documentation.
FK08. Ability to use modern programming and software testing technologies.
FK09. Ability to conduct mathematical and computer modeling, data analysis and processing, computational experiments, solving formalized problems using specialized software tools. Learning outcomes

Learning outcomes

PH02. To have basic principles and methods of mathematical, complex and functional analysis, linear algebra and number theory, analytical geometry, theory of differential equations, in particular partial differential equations, probability theory, mathematical statistics and random processes, numerical methods.
PH05. Be able to develop and use in practice algorithms related to approximation of functional dependencies, numerical differentiation and integration, solution of systems of algebraic, differential and integral equations, solution of boundary value problems, search for optimal solutions.
PH09. Build algorithms that are effective in terms of calculation accuracy, stability, speed, and system resource consumption for numerical research of mathematical models and solving practical problems.
PH13. To use specialized software products and software systems of computer mathematics in practical work.

Student workload

The total volume of the discipline is 150 hours. (5 ECTS credits): lectures – 32 hours, laboratory work – 32 hours, independent work – 86 hours.

Course prerequisites

The student must have knowledge and skills in mathematical analysis, linear algebra and differential equations.

Features of the course, teaching and learning methods, and technologies

The student must learn the theoretical material of the course, learn how to compile method algorithms and program them on a computer using modern software, solve individual tasks and complete course work.

Program of the course

Topics of the lectures

Topic 1. Introduction
Applied mathematics, computational mathematics, computer technology and engineering.

Topic 2. Error in calculations Concept of error, its origin, features of its estimates.

Topic 3. Approximation and interpolation of functions Approximation, its stages. Interpolation, linear and non-linear. Power interpolation: Newton's formula, Lagrange's formula. Quasi-linear interpolation: method of alignment. Spline interpolation (linear and cubic). Approximation by the method of least squares.

Topic 4. Differentiation of functions Polynomial and finite difference formulas for differentiation of functions. Error estimation and increasing the order of accuracy by Runge-Romberg formulas.

Topic 5. Integration of functions Numerical integration of functions by Newton-Cotes formulas: rectangles, trapezoids, Simpson. Formulas of higher order (Gauss and Markov). Special cases.

Topic 6. Systems of linear equations Gaussian method with selection of the main element. The method of running. The square root method. Calculation of the inverse matrix.

Topic 7. The problem of eigenvalues and matrix vectors Basic concepts and two directions of solving the problem: direct solution of the characteristic equation and reduction of the characteristic matrix to a special form.

Topic 8. Nonlinear equations and their systems Methods of solving nonlinear equations: half division, simple iterations, Newton-Raphson, secant, parabola. The Newton-Raphson method of solving systems of nonlinear equations.

Topic 9. Initial problem for ordinary differential equations Taylor and Picard series methods. Euler's method. One-step methods (Runge-Kutta) of the second and fourth order of accuracy. Multi-step methods (Adams). Implicit methods (method of trapezoids).

Topic 10. Boundary value problem for ordinary differential equations Finite difference method. Reduction of the boundary value problem to initial ones. Analytical methods (collocations, Galerkin).

Topic 11. Evolutionary equations and their construction The role of evolutionary equations in modeling real processes. An explicit method of constructing evolutionary equations.

Topics of the workshops

Topic 1. Interpolation by Newton's and Lagrange's formulas

Topic 2. Cubic spline interpolation

Topic 3. Approximation by the method of least squares

Topic 4. Calculation of the derivative by the finite-difference formula

Topic 5. Integration by the trapezium method

Topic 6. Solving a system of linear equations by the Gaussian method with the selection of the main element

Topic 7. The problem of eigenvalues and matrix vectors

Topic 8. Solving a system of linear equations using the square root method

Topic 9. Solving a nonlinear equation by the method of half-division

Topic 10. Solving a nonlinear equation using the Newton-Raphson and secant methods

Topic 11. Solving a system of nonlinear equations using the Newton-Raphson method

Topic 12. Solving a nonlinear equation using the Newton-Raphson and secant methods

Topic 13. Solving the initial problem for the ordinary differential equation and their system by Euler's method

Topic 14. Solution of the initial problem for the ordinary differential equation and their system by the Runge-Kutta method of the second and fourth orders

Topic 15. Solution of the boundary value problem for an ordinary differential equation by the finite-difference method Independent work consists of the following components Elaboration of lecture material

.

Topics of the laboratory classes

Independent study of topics and issues that are not taught in lectures.

Self-study

Performance of course work Students choose any problem and method from the course program or beyond it as the topic of the course work. Content of the course work: formulation of the problem and method, algorithm for solving the problem in the form of a block diagram, computer program, test and substantive problems.

Course materials and recommended reading

1. Мусіяка О.А. Чисельні методи задач механіки. – Київ: Либідь 2004. – 240 с.
2. Фельдман Н.П., Петренко А.І., Дмітрієва О.А. Чисельні методи в інформатиці. – Київ: BHV, 2006. – 480 с.
4. Гончаров О. А., Васильєва Л. В., Юнда А. М. Чисельні методи розв'язання прикладних задач Навчальний посібник. Суми, Сумський державний університет 2020.
5. Fedorov V. Theory and methods of constructing equations for the evolutionary damageability of materials. International Journal of Damage Mechanics. Vol. 32, Iss. 10, pp. 1144–1163. DOI: 10.1177/10567895231191149.
6. Методичні указівки для виконання індивідуальних завдань з курсу "Чисельні методи"/ уклад. В.О. Федоров, С.В. Радіонова. – Харків: НТУ «ХПІ», 2021. – 32 с.

Assessment and grading

Criteria for assessment of student performance, and the final score structure

Timely and successful completion and completion of each laboratory work is estimated at 5 points. Timely and successful completion and completion of the coursework is estimated at 15 points. The answer to the exam is estimated at 10 points..

Grading scale

Total points	National	ECTS
90–100	Excellent	A
82–89	Good	B
75–81	Good	C
64–74	Satisfactory	D
60–63	Satisfactory	E
35–59	Unsatisfactory (requires additional learning)	FX
1–34	Unsatisfactory (requires repetition of the course)	F

Norms of academic integrity and course policy

The student must adhere to the Code of Ethics of Academic Relations and Integrity of NTU "KhPI": to demonstrate discipline, good manners, kindness, honesty, and responsibility. Conflict situations should be openly discussed in academic groups with a lecturer, and if it is impossible to resolve the conflict, they should be brought to the attention of the Institute's management.
Regulatory and legal documents related to the implementation of the principles of academic integrity at NTU "KhPI" are available on the website: http://blogs.kpi.kharkov.ua/v2/nv/akademichna-dobrochesnist/

Approval

Approved by | Date, signature | Head of the department

Alexey VODKA

Date, signature

Guarantor of the educational program
Gennadiy LVOV