Course guides
250337 - MODNUMER - Numerical Modelling

Last modified: 06/10/2020

Unit in charge: Barcelona School of Civil Engineering
Teaching unit: 751 - DECA - Department of Civil and Environmental Engineering.

Degree: BACHELOR'S DEGREE IN GEOLOGICAL ENGINEERING (Syllabus 2010). (Compulsory subject).

Academic year: 2020 **ECTS Credits:** 4.5 **Languages:** Catalan, Spanish, English

LECTURER

Coordinating lecturer: ALBERTO GARCIA GONZALEZ

Others: ALBERTO GARCIA GONZALEZ, ABEL GARGALLO PEIRO

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
4045. Deposit modelling
4056. Knowledge of basic numerical calculus as applied to engineering

Transversal:
588. SUSTAINABILITY AND SOCIAL COMMITMENT - Level 1. Analyzing the world¿s situation critically and systemically, while taking an interdisciplinary approach to sustainability and adhering to the principles of sustainable human development. Recognizing the social and environmental implications of a particular professional activity.
592. EFFICIENT ORAL AND WRITTEN COMMUNICATION - Level 2. Using strategies for preparing and giving oral presentations. Writing texts and documents whose content is coherent, well structured and free of spelling and grammatical errors.
596. TEAMWORK - Level 1. Working in a team and making positive contributions once the aims and group and individual responsibilities have been defined. Reaching joint decisions on the strategy to be followed.
599. EFFECTIVE USE OF INFORMATI0N RESOURCES - Level 3. Planning and using the information necessary for an academic assignment (a final thesis, for example) based on a critical appraisal of the information resources used.
602. SELF-DIRECTED LEARNING - Level 3. Applying the knowledge gained in completing a task according to its relevance and importance. Deciding how to carry out a task, the amount of time to be devoted to it and the most suitable information sources.
584. THIRD LANGUAGE. Learning a third language, preferably English, to a degree of oral and written fluency that fits in with the future needs of the graduates of each course.

TEACHING METHODOLOGY

The course consists of 3 hours per week of classroom activity (large size group).

The 1.3 hours in the large size groups are devoted to theoretical lectures, in which the teacher presents the basic concepts and topics of the subject, shows examples and solves exercises.

The rest of weekly hours devoted to laboratory practice.

Support material in the form of a detailed teaching plan is provided using the virtual campus ATENEA: content, program of learning and assessment activities conducted and literature.

LEARNING OBJECTIVES OF THE SUBJECT

Students will learn to formulate and program analytical models and numerical calculation models for design, planning and management; acquire the capacity to interpret results; and learn to apply these models to solve technological problems.

Upon completion of the course, students will be able to: 1. Use numerical analysis software to conduct sensitivity analyses of problems involving the solution of ordinary differential equations;
2. Use a partial differential equation to solve a boundary problem in a continuous medium, obtaining a numerical solution through finite difference (DF) or finite element methods (EF);
3. Use numerical techniques to solve engineering problems;
4. Analyse and solve deposit modelling problems.

Introduction to numerical modelling; Modelling in engineering; Conservation equations; Constitutive equations; Formulation of mathematical problems; Numerical simulation; Numerical solution of partial differential equations; Classification of methods; Difference operators; Convergence, stability and consistency of a difference scheme; Evolution problems: Diffusion, heat transfer, equilibrium; Eigenvalue problems: Introduction to the finite element method; Transport problems: Convection and convection-diffusion equations; Wave problems: Solution of ordinary differential equations; Solution of equations in partial derivatives: Finite differences and finite elements; Deposit modelling

STUDY LOAD

Type	Hours	Percentage
Hours large group	17,0	15.11
Hours small group	28,0	24.89
Self study	63,0	56.00
Guided activities	4,5	4.00

Total learning time: 112.5 h

CONTENTS

Ordinary Differential Equations (ODE)

Description:
Introduction to Ordinary Differential Equations (ODE). Initial value problems. Example: flow in porous media.
Introduction to Euler's method.
Domain discretization. Approximation of derivatives. Graphic interpretation. Implementation in a computer program. Examples.

Local and global error. Order of convergence. Possible improvements.
Propose, implement and compare the different variations of Euler methods. Analyse their properties. Examples.
Introduction to the family of Runge-Kutta methods. RK1, RK2, RK3, RK4.
Application to case studies. Computational cost comparison.
Initial value problem. Examples.
Examples of initial value problems. Introduction and boundary problems. Shooting method.
Computer lab: shooting method

Specific objectives:
Brief introduction to the subject.
Basics on modeling, theory and practical examples.
To know some applications of ODEs.
To understand conceptually what is the discretization of the domain and its relation to the approximation of the derivatives.
To understand the Euler method.
To have basic knowledge of its computer implementation.
Understand the concepts of local and global errors.
To understand the consequences of evaluating numerical derivatives in different ways.
To know the development and properties of Runge-Kutta methods.
To acquire, from practice, an idea of the numerical properties of the different methods.
To know how to convert a higher-order ODE into a system of first order ODEs.
To understand what is an initial value problem and what is a boundary value problem.

To understand how to use the shooting method for boundary value problems.

Full-or-part-time: 33h 36m
Theory classes: 4h
Laboratory classes: 10h
Self study : 19h 36m

Partial Differential Equations - Finite Differences

Description:
Physical and mathematical classification. Boundary conditions. Discretization of differential operators.
Taylor Series. Forward, centered and backward differences. Order. Higher derivatives. Partial derivatives. Computer exercises.
1D diffusion problem. Dirichlet boundary conditions. Discretization. Approximation of derivatives. Explicit method (FTCS). Matrix formulation.
Examples, implementation and stability.
1D diffusion problem. Dirichlet boundary conditions. Discretization. Implicit method (BTCS). Matrix formulation.
Examples, implementation stability. 1D diffusion problem. Dirichlet boundary conditions. Stability.
1D diffusion problem. Dirichlet boundary conditions. Discretization. Crank-Nicolson method. Matrix formulation.
Examples, implementation and stability.

Specific objectives:
To demonstrate an ability to analyze, represent and interpret various engineering problems that require solving PDEs.
To demonstrate knowledge and understanding of: identification and classification of second order PDEs, from a mathematical and physical point of view, the meaning of the boundary conditions,
the dimensionless form of initial or boundary value problems (in particular "heat"),

First and second order difference operators,
To understand and to solve diffusion problems by finite differences explicit in time.
To understand the concept of stability.
To acquire basic ideas on the implementation of the FTCS method.
To understand and to solve diffusion problems by implicit finite differences.
To acquire basic ideas on the implementation and use of the BTCS method.To know their stability and convergence properties.
To understand and being able to solve a diffusion problem using finite elements and Crank-Nicolson for the time discretization.
To acquire basic notions on the implementation and use of the Crank-Nicolson method. To know their properties: stability, convergence, etc..

Full-or-part-time: 28h 47m
Theory classes: 4h
Laboratory classes: 8h
Self study : 16h 47m

Partial Differential Equations - Finite Elements

Description:
Introduction to FEM. Strong and weak forms. Weighted residuals. Discretización.Piecewise interpolation. Integral approximation. Elementary matrices. Assembly. Reference elements. Shape functions. Isoparametric transformation.
Continued
Basic syntax. Meshing.
Continued
Boundary conditions. Poisson Problem

Specific objectives:
To know FEM applications in engineering.
To being able to determine the weak form for elliptic problems with Dirichlet, Neumann or Robin boundary conditions.
To being able to describe the various numerical aspects of FEM: discretization / approximation, integration, assembly, equation solving, ...
To know Castem environment and syntax.
Learn how to use basic meshing tools.
To solve a parabolic problem using Castem.

Full-or-part-time: 19h 12m
Theory classes: 4h
Laboratory classes: 4h
Self study : 11h 12m

UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

Optimization

Description:
Linear programming. Examples. Standard form. Feasible region. Simplex method.
Lab exercises
Simple version of the simplex algorithm.
opt

Specific objectives:
To know, identify, classify and state an optimization problem.
To solve a linear optimization problem using Matlab.
To understand the basic ideas on the simplex method.

Full-or-part-time: 14h 23m
Theory classes: 5h
Laboratory classes: 1h
Self study : 8h 23m

Evaluation

Full-or-part-time: 12h
Laboratory classes: 5h
Self study : 7h

GRADING SYSTEM

The subject will be evaluated using two factors: * Work in class (class work, CW), to be done individually or in small teams depending on the particular objectives of each work. * Two exams (T1 and T2), which are strictly individual and not eliminatory. 1. The work in class (CW) will include, among others: * Programming / solving problems in Matlab in the computer classroom. * The resolution of problems in class. The voluntary participation in class will be valued positively. 2. The contents of the T1 and T2 exams will be in accordance with all the subject taught since the beginning of the course. - The T1 exam will be done approximately halfway through the semester and will enter the subject taught so far. - The T2 exam will be a final exam, where the complete subject taught throughout the course will enter. Both exams will be in computer rooms, where Matlab will be another tool for the resolution of the exercises. The final exam marks (EF) will be obtained by following the formula: EF = max (0.3 * T1 + 0.7 * T2, T2) if T1 greater than or equal to 2 over 10 EF = 0.3 * T1 + 0.7 * T2 if T1 <2 out of 10 That is, it will be the maximum between the grade obtained by the calculation (0.3 * T1 + 0.7 * T2) or the grade of the final exam T2. To be eligible for this scoring criterion, the student must have obtained a minimum score of 2 out of 10 in T1, otherwise the EF mark will necessarily be obtained by calculating EF = 0.3 * T1 + 0.7 * T2. During the first 5 days of the semester from the presentation of the subject may be requested, through the official criteria and procedures, changes or readjusting dates of exams already scheduled (T1 and T2) for reasons such as field trips from other subjects (but always of the same course to which this subject belongs). Both in these cases and those more particular and extraordinary, the applications must be duly documented by the students and finally approved by the head of studies. 3. The final grade of the subject is obtained according to: Endnote = CW ^ (3/10) * EF ^ (7/10)

EXAMINATION RULES.

Good Practices and Behavior Academic dishonesty (including, among others, plagiarism and falsification of results) will be severely punished, in accordance with current academic regulations: any act of this nature implies a final grade of 0 in The subject. Criteria for admission to reevaluation: Students suspended in the ordinary evaluation will have the option to perform a re-evaluation test. Students who have already passed it will not be able to take the re-evaluation test of the subject. In the same way, students who have not presented the exams of the ordinary evaluation will not be able to take the re-evaluation test of the subject. The maximum score in the case of taking the re-evaluation test will be five (5.0). The non-attendance of a student summoned to the re-evaluation test, held during the period established, may not lead to the performance of another test with a later date.

BIBLIOGRAPHY

Basic:

- Ames, W.F. Numerical methods for partial differential equations. 3th ed. Boston: Academic Press, 1992. ISBN 012056761X.
- Hoffman, J.D. Numerical methods for engineers and scientists. 2nd ed. rev. and exp. New York: Marcel Dekker, 2001. ISBN 0824704436.
- Isaacson, E.; Keller, H.B. Analysis of numerical methods. New York: Dover, 1994. ISBN 0486680290.
- Fletcher, R. Practical methods of optimization. 2nd ed. Chichester: John Wiley and Sons, 1987. ISBN 0471915475.
- Zienkiewicz, O.C.; Morgan, K. Finite elements and approximation. New York, [NY]: John Wiley and Sons, 1983. ISBN 0471982407.