UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

Course guides
250402 - MODELNUM - Numerical Modelling

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

Degree: MASTER'S DEGREE IN CIVIL ENGINEERING (PROFESSIONAL TRACK) (Syllabus 2012). (Compulsory subject).

Academic year: 2020 **ECTS Credits:** 9.0 **Languages:** English

LECTURER

Coordinating lecturer: JOSE SARRATE RAMOS

Others: ALBERTO GARCIA GONZALEZ, ABEL GARGALLO PEIRO, DAVID MODESTO GALENDE, JOSE SARRATE RAMOS

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
8198. The ability to address and solve advanced mathematical problems in engineering, from the scope and context of the problem to its statement and implementation in a computer program. In particular, the ability to formulate, program and apply advanced analytical and numerical calculation models to the design, planning and management of a project, as well as the ability to interpret the results obtained in the of civil engineering.

Transversal:
8562. EFFECTIVE USE OF INFORMATION RESOURCES: Managing the acquisition, structuring, analysis and display of data and information in the chosen area of specialisation and critically assessing the results obtained.

8563. FOREIGN LANGUAGE: Achieving a level of spoken and written proficiency in a foreign language, preferably English, that meets the needs of the profession and the labour market.

TEACHING METHODOLOGY

Taught module delivery: fifteen weeks of teaching, coursework and self-study. Apart from the 6 hours per week in the classroom, self-study must last an average of 9 hours per week.

At least a half of the classroom hours are devoted to work in small groups (computer laboratory, problem solving, etc.)

LEARNING OBJECTIVES OF THE SUBJECT

Students will acquire an understanding of partial differential equations in mathematical physics and develop the skills to analyse and solve mathematical problems in engineering that involve these concepts. They will learn to formulate and program analytical models and numerical calculations models for design, planning and management, and to interpret the results of these models in engineering contexts.

Upon completion of the course, students will be able to:

Apply partial differential equations to engineering problems in continuous media;
Use basic software to program and obtain numerical results for complex solutions;
Analyse and solve complex boundary and initial value problems in multiple dimensions in simple geometric conditions;
Use a range of techniques including parametric analysis to evaluate the solutions found;
Use numerical analysis software to conduct sensitivity analyses of problems involving the solution of ordinary differential equations;
Use partial differential equations to solve boundary problems in a continuous medium, obtaining a numerical solution through finite difference or finite element methods;
Use numerical techniques to solve modelling problems in engineering.

Divergence theorem, Green's theorem and Stokes' theorem; Partial differential equations, existence and uniqueness of solutions, stability; Types of equations and analytical solutions in specific engineering problems; History of numerical models and their application to engineering; Numerical modelling in engineering; Number storage, algorithms and error analysis; Numerical methods for the determination of zeros of functions; Solution of systems of equations using direct numerical methods and basic interactive methods; Numerical methods for the solution of nonlinear systems of equations; Eigenvalue problems: Functional approximation; Numerical quadrature; Solution of partial different equations: Finite differences and finite elements.

Intended Learning Outcomes:
1.- To demonstrate a knowledge and understanding of: the fundamentals of the behaviour and numerical approximation of differential equations; functional approximation; truncation error and solution error; consistency, stability and convergence; direct and iterative solution of linear systems of equations and eigenvalue problems.

2.- To demonstrate an ability to (thinking skills): understand and formulate basic numerical procedures and solve illustrative problems; identify the proper methods for the corresponding problem.

3.- To demonstrate an ability to (practical skills): understand practical implications of behaviour of numerical methods and solutions; logically formulate numerical methods for solution by computer with a programming language (Matlab or Octave).

4.- To demonstrate an ability to (key skills): study independently; use library resources; use a personal computer for basic programming; effectively take notes and manage working time.

STUDY LOAD

Type	Hours	Percentage
Theory classes	27,0	12.00
Guided activities	3,0	1.33
Practical classes	9,0	4.00
Laboratory classes	42,0	18.67
Self study	144,0	64.00

Total learning time: 225 h

CONTENTS

1.- Basics on modeling, programming and error

Description:
Introduction to programming in MATLAB or OCTAVE.
Basics and definition of error (absolute, relative, rounding, truncation, significant figures) and its propagation.

Specific objectives:
Ability to develop simple programs in MATLAB or OCTAVE
Knowledge and understanding of the representation of integers and a real numbers in a computer.
Understanding the basics on errors and how they affect numerical computations.

Full-or-part-time: 24h
Laboratory classes: 10h
Self study : 14h

2.- Introduction to FEM

Description:
Equilibrium (solid mechanics, soils ...), evolution (structural dynamics, heat, consolidation, traffic, pollutants ...) and eigenvalue problems (structural vibration, acoustics ...).
Mathematical and physical classification of PDEs
Obtaining the weak form: for the mechanical problem (principle of virtual work) and the Laplace problem (weighted residuals)
Sectional interpolation
Discretization of the weak form
Calculation of integrals
Elementary matrices and assembly
Solving an equilibrium problem using the FEM

Specific objectives:
To demonstrate an ability to analyze, represent and interpret several engineering problems that require solving PDEs.
To demonstrate knowledge and understanding of:
- the identification and classification of second order PDEs, from a mathematical and physical point of view,
- the meaning of the boundary conditions.

To understand the use of FEM as a tool to solve engineering problems.
To be able to determine the weak form for elliptic problems with Dirichlet, Neumann or Robin boundary conditions.
To demonstrate knowledge and understanding of the various numerical aspects of MEF: discretization / approximation, integration, assembly, system solving, ...
Ability to deduce the weak form of an equilibrium problem.
Ability to use the FEM for solving equilibrium problems.

Full-or-part-time: 24h
Theory classes: 4h
Practical classes: 2h
Laboratory classes: 4h
Self study : 14h

3.- Systems of linear equations

Description:
Classification and definitions.
Factorization methods: Crout and Cholesky
Iterative methods, conjugate gradient (analogy with minimization problem, maximum descent, conjugate gradient algorithm, properties)

Practical problems of systems of equations: storage, condition number, preconditioning
Solving linear systems using different methods and preconditioners.

Specific objectives:
To demonstrate knowledge and understanding of:
- the classification of methods for solving systems of linear equations,
- the range of applicability of each method and its computational advantages and disadvantages,
- the detailed analysis of the conjugate gradient method and how to implement it properly.

To demonstrate knowledge and understanding of the basic practical aspects on: renumbering, condition number, preconditioners, significant digits, convergence criteria.
To demonstrate an ability to implement the methods of resolution presented.
To demonstrate an ability to identify the practical influence the condition number, preconditioners ...

Full-or-part-time: 24h
Theory classes: 4h
Practical classes: 2h
Laboratory classes: 4h
Self study : 14h

4.- Roots of functions and nonlinear systems

Description:
Basics of iterative methods: consistency, linear convergence, superlinear or order p, convergence rate, asymptotic factor.
Methods: Newton, secant, Whittaker.
Introduction to non-linear systems: functional iteration, direct iteration, Picard method, Newton-Raphson method.

Practical problems of convergence analysis and influence of rounding errors.

Specific objectives:
To demonstrate knowledge and understanding of:
- iterative schemes and their inherent differences with finite operations methods,
- the properties, advantages and disadvantages of standard iterative schemes,
- the basic extensions to systems of equations.
Ability to choose the most appropriate method.

To demonstrate an ability to analyze, represent and interpret the results of iterative methods.

Full-or-part-time: 14h 23m
Theory classes: 4h
Practical classes: 1h
Laboratory classes: 1h
Self study : 8h 23m

Test #1

Description:
Test #1 solution

Full-or-part-time: 7h 11m
Laboratory classes: 3h
Self study : 4h 11m

5.- Interpolation and approximation

Description:
General approach: type and criteria for functional approximation
Polynomial interpolation
Least squares
Splines

To analyze a data set and discuss, approximate it using several approximation methods and discuss the results.

Specific objectives:
To demonstrate knowledge and understanding of:
- the criteria and types of functional approximation and their advantages and disadvantages,
- Lagrange interpolation and its error and an ability to use it,
- the least squares problem, namely to deduce the normal equations and understand the approximation orthogonality,
- splines.

To demonstrate an ability to use and code some intrinsic functions to approximate a data set.

Full-or-part-time: 14h 23m
Theory classes: 3h
Laboratory classes: 3h
Self study : 8h 23m

6.- Numerical integration

Description:
General approach, eg with trapezoidal rule
Definition of order of a quadrature
Quadrature classification
Newton-Cotes formulas
Gauss quadrature
Composite formulae
An example of numerical integration: FEM
Analyze and discuss convergence of the following quadratures:
- Newton-Cotes and Gauss-Legendre as the number of integration points increases,
- composite formulae as the number of intervals increases.

Specific objectives:
To demonstrate knowledge and understanding of:
- The basis of numerical integration,
- The classification of quadratures,
- The basis of the Newton-Cotes and Gaussian quadratures,
- The composite quadratures and their advantages and disadvantages.

To demonstrate an ability to:
- Define a quadrature if the integration points are given,
- Use Newton-Cotes and Gaussian quadratures, choosing the correct one in terms of accuracy and computational cost,
- Use composite quadratures.

To demonstrate an ability to apply all the concepts of numerical integration to the FEM.
To demonstrate an ability to implement an algorithm for numerical integration.
To demonstrate an ability to implement an algorithm for composite formulae.

Full-or-part-time: 16h 48m
Theory classes: 3h
Practical classes: 1h
Laboratory classes: 3h
Self study : 9h 48m

Test #2

Description:
Test #2 solution

Full-or-part-time: 7h 11m
Laboratory classes: 3h
Self study : 4h 11m

7.- Modeling with ODEs

Description:
General approach: reduction to first order, initial value (IVP), boundary value (BVP) or eigenvalue problem, existence and uniqueness theorem.
Methods based on the approximation of the derivative: Euler,
backward Euler.
Truncation error, consistency, local and global error, order, absolute stability.
Single step methods (Runge-Kutta) methods: second and fourth order.
Prediction-correction methods.

Modelling and numerical resolution of an engineering problem governed by ODEs.

Specific objectives:
Understand the concept of well-posed initial value problems (IVP).
Ability to identify and classify a problem of ODEs (in any order and dimension).
Ability to rewrite high-order ODEs as a system of first order ODEs.
Ability to identify Initial Value Problems (IVP) and Boundary Problem (BP).
Understand the concepts of convergence, order of convergence and absolute stability.
Knowledge of the basic properties of Runge- Kutta methods. Understand the general form and be able to apply them. Ability to identify explicit, semi-implicit and implicit methods.
To demonstrate an ability to model an engineering problem as a system of ODEs.
To demonstrate an ability to use a library for the numerical solution of ODEs.

Full-or-part-time: 19h 12m
Theory classes: 3h
Laboratory classes: 5h
Self study : 11h 12m

8.- Modeling with PDEs

Description:
Finite element method for elliptic problems: boundary conditions, organization of the calculations, concepts of accuracy and numerical efficiency.
Dynamic problems: mass, stiffness and damping matrices; Newmark method; concepts of stability and time accuracy
Hyperbolic problems of structural dynamics
Solving a dynamic problem.

Specific objectives:
To demonstrate knowledge and understanding of:
- the dimensionless form of initial or boundary value problems (in particular "heat"),
- the basics of the FEM: weak form, boundary conditions, integration, types of matrices, algorithm,
- the concepts of precision in FEM (elliptic) and how to identify problems and propose solutions,
- FEM problems in structural dynamics,
- the concept of stability (conditional and unconditional), versus temporal precision and to distinguish between explicit and implicit methods.
To demonstrate knowledge and understanding of:
- the fundamental features of dynamic problems,
- the use of Newmark's method for solving dynamic problems.
To demonstrate an ability to program Newmark's method and analyze its behavior

Full-or-part-time: 28h 47m
Theory classes: 6h
Practical classes: 2h
Laboratory classes: 4h
Self study : 16h 47m

Test #3

Description:
Test #3 solution

Full-or-part-time: 7h 11m
Laboratory classes: 3h
Self study : 4h 11m

GRADING SYSTEM

1. The module is graded with the following elements:
* Class work (CW), to be carried out either individually or in teams.
* A course project (CP), to be carried out in teams.
* Two tests (T1 and T2), which are strictly individual.

2. Class work (CW) refers, among others, to:
* Exercises in the classroom.
* Assignments in the computer room.
* Participation in class.

3. The course project (CP) is a small project in computational engineering, to be presented in two different formats: a report and a poster.

4. Tests T1 and T2 will cover all the topics presented from the beginning of the module.

5. Academic dishonesty (including, among others, communication during tests, plagiarism and falsification of results) will be severely punished, in accordance with current academic regulations: any such act will imply a final mark of 0 in the module.

6. The final mark for the module is obtained as

Mark = (0.5*T1+0.5*T2)^0.6 * (0.5*CW+0.5*CP)^0.4

EXAMINATION RULES.

Will be discussed in class.

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- Quarteroni A.; Saleri, F.; Gervasio, P. Scientific computing with MATLAB and Octave. 3rd ed. Heidelberg: Springer-Verlag, 2010. ISBN 9783642124297.

Complementary:
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- Shampine L.F. Numerical solution of ordinary differential equations. CRC Press, 1994. ISBN 0412051516.
- Stoer, J.; Bulirsch, R. Introduction to numerical analysis. Springer-Verlag, 2002. ISBN 9781441930064.
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