Course guide
230464 - MNC2 - Numerical and Computational Methods 2

Last modified: 25/05/2023

Unit in charge: Barcelona School of Telecommunications Engineering
Teaching unit: 748 - FIS - Department of Physics.

Degree: BACHELOR'S DEGREE IN ENGINEERING PHYSICS (Syllabus 2011). (Compulsory subject).

Academic year: 2023 **ECTS Credits:** 6.0 **Languages:** English

LECTURER

Coordinating lecturer: Consultar aquí / See here:
https://telecos.upc.edu/ca/estudis/curs-actual/professorat-responsables-coordinadors/responsables-assignatura

Others: Consultar aquí / See here:
https://telecos.upc.edu/ca/estudis/curs-actual/professorat-responsables-coordinadors/professorat-assignat-idioma

PRIOR SKILLS

C1) Mathematics: knowledge of linear algebra, differential calculus / integral in Rn, ordinary differential equations.

C2) Programming: Basic knowledge of Matlab / Octave and programming tools with high performance scientific calculators (HP48, 49 50 or similar).

C3) Numerical methods: polynomial interpolation, solution methods of nonlinear approaches (1 variable), derivation / integration number (1 variable)

REQUIREMENTS

R1) Numerical and Computational Methods 1
Linear Algebra
Calculus 1/2
Mathematical Methods 1/2

R2) Knowledge of Analytical Mechanics / Fluids

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
3. Ability to select numerical and optimization methods suitable for solving physical and engineering problems. Ability to apply the knowledge of numerical algorithms and optimization.
1. Understanding and mastery of computer programming, use of operative systems and computational tools (scientific software). Skills to implement numerical algorithms in languages of low (C, F90) and high (Matlab) level.
2. Ability to solve problems in physics and engineering using fundamental numerical methods: experimental data processing, interpolation, roots of nonlinear equations, numerical linear algebra and optimization, quadrature and integration of differential equations, properly weighting their different aspects (accuracy, stability and efficiency or cost).

Generical:

5. ABILITY TO IDENTIFY, FORMULATE, AND SOLVE PHYSICAL ENGINEERING PROBLEMS. Planning and solving physical engineering problems with initiative, making decisions and with creativity. Developing methods of analysis and problem solving in a systematic and creative way.

Transversal:

3. 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.
4. SELF-DIRECTED LEARNING - Level 2: Completing set tasks based on the guidelines set by lecturers. Devoting the time needed to complete each task, including personal contributions and expanding on the recommended information sources.
2. EFFECTIVE USE OF INFORMATI0N RESOURCES - Level 2. Designing and executing a good strategy for advanced searches using specialized information resources, once the various parts of an academic document have been identified and bibliographical references provided. Choosing suitable information based on its relevance and quality.
1. 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.

TEACHING METHODOLOGY

Lectures (2.6 ECTS): presentation of theoretical concepts and their applications
in problem solving. Practicals: resolution of specific problems with computer
(Individual / team). Tutorials.

LEARNING OBJECTIVES OF THE SUBJECT

To be able of numerically formulating problems arising in physics and engineering and implementing robust and accurate algorithms for their solution.

STUDY LOAD

Type	Hours	Percentage
Hours large group	39,0	26.00
Hours small group	26,0	17.33
Self study	85,0	56.67

Total learning time: 150 h

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CONTENTS

1. Numerical Linear Algebra and Systems of Nonlinear Equation

Description:
1.1 Direct linear solvers (I): Gauss Elimination (GEM) and LU factorization.
1.2 Direct linear solvers (II): PA=LU factorization and partial pivoting.
1.3 QR factorization (I): Orthogonal matrices, Householder re
flectors.
1.4 QR factorization (II): Least squares problem.
1.5 Conditioning: Matrix norms, condition numbers and sensitivity of linear systems.
1.6 Gram-Schmidt orthonormalization: Numerical instability of GS and Reorthogonalized-GS.
1.7 Iterative Krylov Methods (I): Richardson iteration and Krylov subspaces.
1.8 Iterative Krylov Methods (II): GMRES and Arnoldi iteration.
1.9 Systems of Nonlinear Equations (I): Newton's method.
1.10 Systems of Nonlinear Equations (II): Parameter-dependent systems and arc-length continuation.

Full-or-part-time: 73h
Theory classes: 19h
Laboratory classes: 11h
Guided activities: 1h
Self study : 42h

2. Approximation Theory

Description:
2.1 Least Squares Problem in Functional spaces.
2.2 Generalized Fourier Series.
2.3 Bounded domains (Legendre and Chebychev polynomials).
2.4 Periodic domains (Fourier trigonometric polynomials and DFT).
2.5 Applications (I): Fourier-Chebychev-Legendre diferentiation matrices.
2.6 Applications (II): Computation of boundary value problems.
2.7 Applications (III): Computation of eigenfunctions and spectra of Sturm-Liouville problems.

Full-or-part-time: 41h
Theory classes: 10h
Laboratory classes: 9h
Guided activities: 1h
Self study : 21h

3. Ordinary Differential Equations (Initial Value Problems)

Description:
3.1 Introduction: Cauchy-Picard Theorem, existence and uniqueness of solutions to IVP.
3.2 Linear multistep formulas (I): Characteristic polynomials, local truncation error and order of accuracy. Adams formulas and Curtiss-Hirschfelder BDF methods.
3.3 Linear multistep formulas (II): Stability and convergence of LMSF. Dahlquist's First Stability barrier.
3.4 Linear multistep formulas (III): A-stability, Dahlquist's Second Stability barrier. Explicit Runge-Kutta methods.

Full-or-part-time: 36h
Theory classes: 10h
Laboratory classes: 4h
Guided activities: 1h
Self study : 21h

GRADING SYSTEM

1. Mid-semester exam (PE) : weight 30% of the total.

2. Final Exam (FE) of all course content: weight 50% - 80% of the
total mark, depending on maximization criteria.

3. Evaluation computing laboratory practicals P: weight 20% of the total.

COURSE GRADE = 0.8 x max{ EF , 0.7x EF + 0.3 x EP } + 0.2 x P

BIBLIOGRAPHY

Basic:
- Kincaid, D; Cheney, E. W. Numerical analysis: mathematics of scientific computing. 3th ed. Pacific Grove [etc.]: Brooks/Cole, 2002. ISBN 0534389058.
- Griffiths, D.H, Desmond J.. Numerical Methods for Ordinary Differential Equations : Initial Value Problems [on line]. 1. London: Springer-Verlag, 2010 [Consultation: 15/07/2020]. Available on: http://dx.doi.org/10.1007/978-0-85729-148-6. ISBN 9780857291486.
- Meseguer, A. Fundamentals of numerical mathematics for physicists and engineers [on line]. Hoboken, NJ: John Wiley & Sons, 2020 [Consultation: 15/07/2020]. Available on: https://onlinelibrary.wiley.com/doi/book/10.1002/9781119425762. ISBN 9781119425762.

Complementary:
- Quarteroni, A.; Saleri, F.; Sacco, R. Numerical mathematics [on line]. 2nd ed. New York ; Barcelona [etc.]: Springer, 2007 [Consultation: 25/09/2018]. Available on: https://link.springer.com/book/10.1007/b98885. ISBN 9783540346586.
- Watkins, D. S. Fundamentals of matrix computations. 3rd ed. Hoboken: Wiley, 2010. ISBN 9780470528334.