Course guide
820757 - MNTCM - Computational Methods in Energy Technology

Last modified: 16/05/2023

Unit in charge: Barcelona School of Industrial Engineering
Teaching unit: 724 - MMT - Department of Heat Engines.

Degree: ERASMUS MUNDUS MASTER'S DEGREE IN ENVIRONOMICAL PATHWAYS FOR SUSTAINABLE ENERGY SYSTEMS (Syllabus 2012). (Optional subject).
MASTER'S DEGREE IN ENERGY ENGINEERING (Syllabus 2013). (Optional subject).
MASTER'S DEGREE IN INDUSTRIAL ENGINEERING (Syllabus 2014). (Optional subject).
ERASMUS MUNDUS MASTER'S DEGREE IN DECENTRALISED SMART ENERGY SYSTEMS (DENSYS) (Syllabus 2020). (Optional subject).
MASTER'S DEGREE IN THERMAL ENGINEERING (Syllabus 2021). (Compulsory subject).
MASTER'S DEGREE IN ENERGY ENGINEERING (Syllabus 2022). (Optional subject).

Academic year: 2023 **ECTS Credits:** 5.0 **Languages:** English

LECTURER

Coordinating lecturer: Carlos-David Pérez-Segarra

Others: Xavier Trias

PRIOR SKILLS

Basic knowledge of fluid dynamics and heat transfer, as well as a programming language.

REQUIREMENTS

Knowledge equivalent to completion of the levelling course of the Master's

DEGREE COMPETENCES TO WHICH THE SUBJECT CONTRIBUTES

Specific:
CEMT-5. Employ technical and economic criteria to select the most appropriate thermal equipment for a given application, dimension thermal equipment and facilities, and recognise and evaluate the newest technological applications in the production, transportation, distribution, storage and use of thermal energy.

TEACHING METHODOLOGY

During the development of the course will use the following teaching methods:

Lecture or conference (EXP): presentation from teachers through lectures or by outsiders through invited lectures.
Participatory classes (parts): collective decision exercises, discussions and group dynamics with the teacher and other students in the classroom; Classroom presentation of an activity carried out individually or in small groups.
Presentations (PS): present in the classroom an activity conducted individually or in small groups (in person).
Theoretical and practical work directed (TD): completion of a classroom activity or theoretical/practical exercise, individually or in small groups with the teacher's guidance.
Project activity or reduced work scope (PR): Based Learning conducting individual or group of work of limited complexity or length, applying knowledge and presenting results.
Project or work of broader scope (PA): learning based on the design, planning and implementation of a group wide project or job complexity or length, applying and extending knowledge and writing a report poured approach this and the results and conclusions.
Activities Evaluation (EV).

LEARNING OBJECTIVES OF THE SUBJECT

Acquire basic training in the numerical solution of the governing equations of fluid dynamics and heat and mass transfer.
Acquiring a first practical experience in programming, verification and validation of CFD&HT codes (Computational Fluid Dynamics and Heat Transfer).
Become familiar with the use of CFD & HT code and acquire the ability to critically judge the quality (verification and validation of numerical solutions of the mathematical formulations used).

Learning Outcomes. At the end of the course, the student will have:
Consolidation of basic mathematical formulations of fluid dynamics and heat and mass transfer phenomena.
Knowledge of different numerical integration methodologies of the Navier-Stokes equations.
Introduction to the resolution of turbulent flows based on methods like RANS, LES and DNS.
Application of code verification techniques, verification and validation of numerical solutions of mathematical formulations.

STUDY LOAD

Type	Hours	Percentage
Hours small group	30,0	23.90
Self study	85,0	67.73
Guided activities	10,5	8.37

Total learning time: 125.5 h

CONTENTS

Introduction to numerical methods in fluid dynamics and heat and mass transfer

Description:
General approach to the problems involved in integrating the fluid dynamics and heat and mass transfer equations. General comments of the different methods of integration of equations (finite differences, finite volumes, finite elements, spectral methods, etc.)

Specific objectives:
Review of basic mathematical formulations in fluid dynamics and heat and mass transfer.
General outline of the various methods for integration of the Navier Stokes equations.

Related activities:
Lecture
Practical class
Reduced scope of work
Broad scope of work

Full-or-part-time: 23h 30m
Laboratory classes: 6h
Guided activities: 1h 30m
Self study : 16h

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Solving the equation of heat transfer by heat conduction in irregular domains. Steady and unsteady analysis.

Description:
Extension of the methodology explained in basic courses of heat and mass transfer, based on finite volume method and for structured mesh, orthogonal mesh and adaptable domain.
This topic will introduce blocking-off techniques for the treatment of complex geometries and unstructured meshes with non-orthogonal finite volume and variety of shapes (i.e. tetrahedra). Explanation of the techniques of data processing and connectivity tables.
At this stage solving equations systems of discretization is carried out with the methods already known of previous courses (Gauss-Seidel, line-by-line and sub/over relaxation techniques).

Specific objectives:
Numerical solution of the equations of heat transfer by conduction in irregular domains.
Review of the basic techniques of solving large systems of algebraic equations resulting from discretisation.

Related activities:
Lecture
Practical class
Reduced scope of work
Broad scope of work

Full-or-part-time: 24h 30m
Laboratory classes: 6h
Guided activities: 2h 30m
Self study : 16h

Solving convection-diffusion equations.

Description:
Unlike the equations presented on the topic before, here comes the generic form of the transport equations with convective terms. Explains the different techniques of integration of the equation and accuracy problems (numerical diffusion) and/or convergence (stability) that can appear according to the scheme. Different benchmark problems with given velocity fields are proposed (i.e. inclined uniform flow, Smith-Hutton problem, etc.).

Specific objectives:
Presentation of the convection-diffusion equation (generic transport equation) and the method of numerical integration.
Presentation of different schemes for the convective term.
Introducing different benchmark cases for the verification of the codes developed by the students.

Related activities:
Lecture
Practical class
Practical work
Reduced scope of work

Full-or-part-time: 25h 30m
Laboratory classes: 6h
Guided activities: 3h 30m
Self study : 16h

Technical verification of codes and numerical solutions and review of the most appropriate solvers.

Description:
This topic addresses two fundamental aspects in the methodology of the numerical solution. The first concerns the verification of the code and verification of numerical solutions. The second concerns the solution techniques for large systems of algebraic equations.
Regarding the first point, we present different techniques for verification of codes, such as comparison with known analytical solution of simplified cases, verification of global mass balance, momentum and / or energy, creation of ad hoc numerical solutions (known as MMS or Method of Manufactured Solutions). Once the code is sufficiently verified, some techniques will be explained to ensure the quality of the numerical solution (i.e. the results can not be conditional on the generated mesh discretization or numerical parameters used or the number of significant digits (precision-used for the computer).
In the second part iterative solvers are presented (Gauss-Seidel or line-by-line). In particular, preconditioner for Krylov methods (CG, GMRES, BiCGSTAB) and multimesh-multilevel methods. In 3D cases with a periodic direction, Fourier diagonalisation methods are explained.

Specific objectives:
Presentation of techniques for code verification and verification techniques of numerical solutions.
Presentation of new solvers more efficient for the treatment of large algebraic equations systems resulting from the discretisation of the convection-diffusion equations.

Related activities:
Lecture
Practical class
Practical work
Reduced scope of work

Full-or-part-time: 26h
Laboratory classes: 6h
Guided activities: 4h
Self study : 16h

Solving the Navier-Stokes equations.

Description:
Description of the issues to solve these equations, from a physical and numerical point of view. Different properties are discussed about the conservation of the discretisation equations and how these properties are introduced in the numerical treatment. The methodology is explained based on techniques such as explicit and spectro-consistent discretisation schemes. The global algorithm is based on the Fractional-step method. Different benchmark cases are proposed (driven cavity, differentially cavity, backward-facing step, etc.). This approach allows students to address situations of turbulent flows with standard models like DNS (Direct Numerical Simulation) and LES (Large Eddy Simulation). We discuss phenomenological aspects related to turbulence (energy cascade, filtering equations, initial and boundary conditions) and statistical treatment of data.

Specific objectives:
Methodology for solving the Navier-Stokes equations (partial differential equations system like the convection-diffusion euqations , nonlinear and strongly coupled).
Introducing different benchmark cases for verification of the codes developed by the students.
Introduction to turbulence and numerical techniques based on DNS and LES models.

Related activities:
Lecture
Practical class
Reduced scope of work
Broad scope of work

Full-or-part-time: 25h 30m
Laboratory classes: 6h
Guided activities: 3h 30m
Self study : 16h

ACTIVITIES

Lectures

Description:
Methodology in a big group. Presentation of the content of the course following a expository and participatory class model. The material is organized into different groups according to the content of the subject.

Specific objectives:
At the end of this activity, students should be able to master the knowledge, consolidate and apply them correctly to various technical problems. Moreover, being a techno course, the lectures should serve as a basis for the development of other more technical subjects related to the thermal field as Refrigeration, Solar energy and Heat Engines.

Material:
Bibliography. Teacher's notes.

Delivery:
This activity is evaluated along with the second activity (problems) by course work and tests.

Full-or-part-time: 20h
Laboratory classes: 15h
Self study: 5h

Practical classes

Description:
Methodology for large and medium groups. On each topic, there will be some problems in class, so the students will get the necessary guidelines to carry out this resolution: simplifying assumption, numerical approach, numerical solution, discussion of the results.

Specific objectives:
At the end of this activity, students should be able to apply theoretical knowledge to solve different kinds of problems. Given the methodology the student should be able to:
1. - Understand and analyze the problem statement.
2. - Set up and develop a solution scheme.
3. - Solve the problem using equations with a suitable resolution algorithm.
4. - Critically interpret the results.

Material:
Bibliography. Teacher's notes

Delivery:
This activity is evaluated in conjunction with activity 1 (theory) through course work and tests.

Full-or-part-time: 20h
Laboratory classes: 15h
Self study: 5h

Guided activities

Description:
Students must do theoretical and practical exercises. The works consist of solving little problems, of which the initial data can be the results of a laboratory experiment or data given by the teacher. The structure to be followed:
Preparation of the practical work by a manual.
Groups of 2 or 3 people with a maximum of 2 hours.
Discussion of results and of the problems that have arisen during the exercise.
Completion of a report about the exercise with the respective results, questions and conclusions. This report will be evaluated along with the completion of the practice.

Specific objectives:
Consolidate the knowledge acquired in theory and practice classes.

Material:
Bibliography. Teacher's notes

Delivery:
Reports will follow the guidelines given in class.

Full-or-part-time: 17h
Guided activities: 12h
Self study: 5h

Reduced scope work

Description:
Resolution up two problems based on situations posed by the teacher.

Specific objectives:
Consolidate the knowledge acquired in theory and practice classes.

Material:
Bibliography. Teacher's notes

Delivery:
There will be a report following the guidelines given in class.

Full-or-part-time: 25h
Self study: 25h

Broad scope work

Description:
Solving a problem-based situation posed by the teacher or the student.

Specific objectives:
Expand and consolidate the knowledge acquired in theory and practice classes.

Material:
Bibliography. Teacher's notes

Delivery:
There will be a report following the guidelines given in class.

Full-or-part-time: 40h
Self study: 40h

Written tests

Description:
Development testing knowledge of the subject content 1 and 2. Includes theoretical and development issues.

Specific objectives:
Show the level of knowledge achieved in theoretical activities and problems.

Material:
Bibliography. Teacher's notes

Delivery:
The exams will be developed and delivered freely with the statement duly completed with the data required.

Full-or-part-time: 3h
Guided activities: 3h

GRADING SYSTEM

Midterm exam: 20%
Final exam: 35%
Works developed individually or in groups throughout the course: 45%

EXAMINATION RULES.

Students must follow the instructions explained in class and contained in the file with the activities to develop in practice. As a result of these activities, the student must submit a report (preferably in pdf format) to the teacher, following his instructions and deadline for each activity. The assessment will involve both its accomplishment, as well as their defense.
Practices:
Practical exercises can begin during the class schedule planned for this activity and will be completed (if necessary) as autonomous activity, following the instructions given in class. The results of practical exercises will be given to the teacher by following the instructions given in class. The evaluation of the practice can lead to both its implementation, as well as their defense.
Exams:
There will be a final exam for the course. Students must complete both theoretical questions and problems related to theoretical and practical content of the course.
Reviews and/or claims with reference to the exams are conducted according to the dates and times established in the academic calendar.

BIBLIOGRAPHY

Basic:
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- Roache, Patrick J. Fundamentals of computational fluid dynamics. Albuquerque, New Mexico: Hermosa, cop. 1998. ISBN 0913478091.
- Incropera, Frank Paul; DeWitt, David P. Fundamentos de transferencia de calor. 4a ed. México [etc.]: Prentice Hall, cop. 1999. ISBN 9701701704.
- Patankar, Suhas V. Numerical heat transfer and fluid flow [on line]. Washington : New York: Hemisphere ; McGraw-Hill, cop. 1980 [Consultation: 16/11/2022]. Available on: https://www-taylorfrancis-com.recursos.biblioteca.upc.edu/books/mono/10.1201/9781482234213/numerical-heat-transfer-fluid-flow-suhas-patankar. ISBN 0070487405.
- Ferziger, Joel H. [et al.]. Computational methods for fluid dynamics [on line]. 4th ed. Cham: Springer, 2019 [Consultation: 16/11/2022]. Available on: https://link-springer-com.recursos.biblioteca.upc.edu/book/10.1007/978-3-319-99693-6. ISBN 9783319996912.

Complementary:

- Bradshaw, P. An Introduction to turbulence and its measurement [on line]. Oxford ; New York: Pergamon Press, 1971 [Consultation: 27/05/2020]. Available on: https://ebookcentral.proquest.com/lib/upcatalunya-ebooks/detail.action?docID=1828885. ISBN 080166202.
- Roache, Patrick J. Verification and validation in computational science and engineering. New Mexico: Hermosa Publishers, cop. 1998. ISBN 0913478083.
- Pope, S. B. Turbulent flows. Repr. with corr. Cambridge [etc.]: Cambridge University Press, 2000. ISBN 0521591252.
- Wei Shyy, H.S. [et al.]. Computational fluid dynamics with moving boundaries [on line]. Mineola, N.Y.: Dover, 2007 [Consultation: 16/11/2022]. Available on: https://web-p-ebscohost-com.recursos.biblioteca.upc.edu/ehost/ebookviewer/ebook?sid=f13f1c0b-4ce9-4371-a078-3b07f2f00a5a%40redis&vid=0&format=EK. ISBN 9780486135557.
- Libby, Paul A. An introduction to turbulence. Bristol, PA: Taylor & Frances, cop. 1996. ISBN 1560321008.

RESOURCES

Audiovisual material:
- Material audiovisual. Slides, proposed problems to be used in class.

Computer material:
- Notes. Notes made by professors of the subject.