UNIVERSITAT POLITÈCNICA DE CATALUNYA BARCELONATECH

Course guide
295455 - 295TM122 - Computational Fluid Mechanics

Last modified: 02/10/2025

Unit in charge: Barcelona East School of Engineering
Teaching unit: 729 - MF - Department of Fluid Mechanics.

Degree: MASTER'S DEGREE IN MECHANICAL TECHNOLOGIES (Syllabus 2024). (Optional subject).

Academic year: 2025 **ECTS Credits:** 6.0 **Languages:** Spanish, English

LECTURER

Coordinating lecturer: LLUÍS JOFRE CRUANYES - FERNANDO GARCIA GONZALEZ

Others: Primer quadrimestre:
FRANCESCO CAPUANO - Grup: T1
FERNANDO GARCIA GONZALEZ - Grup: T1
LLUÍS JOFRE CRUANYES - Grup: T1

PRIOR SKILLS

Calculus. Partial differential equations.
Fluid mechanics, fluids engineering, thermodynamics, heat transfer.
Computer usage, notions of programming.

REQUIREMENTS

Advanced technologies in fluid science and engineering

LEARNING RESULTS

Knowledges:
K.01. Critically interpret the physical principles governing the behaviour of systems and advanced applications in the fields of mechanical design, manufacturing processes, strength of materials, fluid mechanics, thermodynamics and heat transfer.
K.08. Identify data analysis tools to characterise, synthesise, explain and predict the behaviour of physical systems in the field of mechanical engineering.
K.05. Identify emerging technologies, both in the mechanical domain and in the field of new information and communication technologies, that can be applied to mechanical engineering projects.
K.02. Identify the fundamental equations governing physical phenomena associated with complex problems in mechanical engineering.
K.07. Define appropriate analytical, experimental and/or computational models to study relevant problems in mechanical engineering.

Skills:
S.02. Correctly apply the analytical, computational and/or experimental techniques best suited to the analysis of a case or project in the mechanical field.
S.08. Integrate knowledge from different areas of the mechanical field in the design and development of projects, systems and engineering solutions.
S.05. Critically examine the results of the analysis of a process or product, taking into account the limitations of the techniques used.
S.03. Use advanced numerical simulation and virtual prototyping techniques to solve complex mechanical problems.
S.06. Efficiently manage information collected during analytical, numerical and/or experimental studies and automate its analysis to facilitate knowledge extraction.

Competences:
C.03. Manage the acquisition, structuring, analysis and visualisation of data and information in the mechanical field and critically evaluate the results of this process.
C.02. Work as part of a multidisciplinary team, whether as a team member or in a leadership role, to contribute to the development of projects with pragmatism and a sense of responsibility, undertaking commitments with due regard to the resources available.
C.05. Propose advanced scientific and technological solutions to complex industrial challenges in the field of mechanical engineering.

TEACHING METHODOLOGY

The hours of driven activities in large groups will be theoretical classes with an expository and participatory approach. The hours of activities directed in small groups will be devoted to the resolution of exercises and the development of computational tools and simulations (in computer rooms) using scientific software and programming languages. The hours of autonomous learning will be devoted to the study of theory, the solution of problems, the programming of flow solvers, and performing simulations of fluid flow problems.

LEARNING OBJECTIVES OF THE SUBJECT

- Learn to identify fluid mechanics problems whose solutions require computational approaches
- Understand the mathematical concepts and ideas behind the methods utilized
- Implement the corresponding methods using well-established programming languages
- Conduct thorough error analysis of the algorithms, including accuracy and stability
- Acquire expertise on the discrete solution and optimization of differential equations describing flow problems in science and engineering

STUDY LOAD

Type	Hours	Percentage
Hours large group	21,0	14.00
Self study	108,0	72.00
Hours small group	21,0	14.00

Total learning time: 150 h

CONTENTS

Numerical methods

Description:
Basic remarks. Numerical interpolation and differentiation based on Taylor series expansion. Truncation error: formal definition. Centered and asymmetric derivative formulas. Derivation of finite-difference formulas with arbitrary stencil and order of accuracy on uniform and non-uniform meshes. Matrix notation.
Boundary value problems. Numerical solution of 1D and 2D heat equation with Neumann, Dirichlet and Robin boundary conditions. Solution of linear systems: direct and iterative methods.
Initial value problems. Ordinary differential equations (ODEs): basic theoretical aspects. Numerical methods for ODEs: multi-stage (Runge-Kutta) and multi-step (Adams) schemes.
Partial differential equations (PDEs). Derivation of PDEs relevant to transport phenomena. The semi-discrete (or method of lines) approach. Numerical solution of unsteady advection-diffusion equations using finite-difference formulas and methods for ODEs for a variety of initial and boundary conditions.

Full-or-part-time: 43h 30m
Theory classes: 6h
Laboratory classes: 6h
Guided activities: 1h 30m
Self study : 30h

Numerical solution Navier-Stokes equations

Description:
Introduction. General overview of a Computational Fluid Dynamics (CFD) process: mesh generation, solution, post-processing; examples. Basic properties of Navier-Stokes equations. The incompressible flow model. The role of pressure, initial and boundary conditions.
Discretization of incompressible N-S. The pressure Poisson equation and projection methods. Chorin-Temam fractional step method. Layout of variables: collocated and staggered arrangement. The "Harlow-Welch" staggering. Implementation of boundary conditions. Development of a numerical code in primitive variables using a second-order staggered scheme and the projection method. A simple example: the lid-driven cavity problem.
Other topics. Towards multiscale flow problems: the modified wavenumber analysis and the issue of non-linear stability. Remarks on the concept of discrete energy conservation. Remarks on the compressible Navier-Stokes equations and related numerical schemes. Alternatives to projection methods: SIMPLE and PISO algorithms.

Full-or-part-time: 43h 30m
Theory classes: 6h
Laboratory classes: 6h
Guided activities: 1h 30m
Self study : 30h

High performance computing

Description:
Modern processors & data access. Introduction to parallel computing (what, why, how). Parallel computer memory architectures: shared, distributed, hybrid shared-distributed. Fundamentals of parallelization: strong and weak scalability, parallel efficiency, load balance, parallel overheads.
Shared-memory parallel programming (OpenMP). General characteristics. Uniform & Non-Uniform Memory Access (UMA/NUMA). Introduction to OpenMP. Case study: OpenMP-parallel Jacobi algorithm.
Distributed-memory parallel programming (MPI). General characteristics. Messages and point-to-point communication & Nonblocking point-to-point communication. Introduction to MPI. Case study: MPI-parallel Jacobi algorithm.
Hybrid architectures & accelerators (OpenACC). Exascale computing & hybrid architectures. Acceleration strategies. Introduction to OpenACC. Case study: OpenACC-accelerated Jacobi algorithm.

Full-or-part-time: 19h 30m
Theory classes: 3h
Laboratory classes: 3h
Guided activities: 1h 30m
Self study : 12h

Computational flow analysis

Description:
Computational experiments. Basic definitions, historical notes and different approaches (theoretical, experimental, computational), application to hydrodynamic instabilities and turbulence.
Analysis of flow regimes. Base flow of a Navier-Stokes problem. Types of bifurcations (Hopf, pitchfork, saddle-node). Linear stability analysis. Overview of numerical techniques. Case study: the two-dimensional lid-driven cavity problem.
Tools for time-dependent flows. Types of time dependent flows (base, quasi-periodic, chaos). Qualitative measures of the flow. Modal flow analysis (POD, DMD). Dynamical indicators from time series (local, global, Poincaré sections). Case study: the two-dimensional lid-driven cavity problem.

Full-or-part-time: 43h 30m
Theory classes: 6h
Laboratory classes: 6h
Guided activities: 1h 30m
Self study : 30h

GRADING SYSTEM

20% Computational exercices/activities
35% Course project
45% Final exam

Final project: connected to the solver developed & data analysis tools, 35%; evaluation at week 15.
Final exam: questions related to the theory presented and activities; 50%.
Activities: 1-D Burgers equation (comparison to analytical solution); 2 - 3 questions (L2-norm, total energy, etc); Evaluation during topic 2; 15%

BIBLIOGRAPHY

Basic:
- LeVeque, Randall J. Finite difference methods for ordinary and partial differential equations : steady-state and time-dependent problems [on line]. Philadelphia, PA: SIAM, Society for Industrial and Applied Mathematics, 2007 [Consultation: 18/09/2024]. Available on: https://faculty.washington.edu/rjl/fdmbook/. ISBN 9780898716290.
- Ferziger, Joel H.; Peric, Milovan; Street, Robert L. Computational Methods for Fluid Dynamics. Fourth edition. Cham: Springer, [2019]. ISBN 9783319996912.
- Hager, Georg; Wellein, Gerhard. Introduction to high performance computing for scientists and engineers. Boca Raton, FL: CRC Press, cop. 2011. ISBN 9781439811924.
- Drazin, P. G. Introduction to hydrodynamic stability. Cambridge, UK [etc.]: Cambridge University Press, 2002. ISBN 9780521009652.