# UNIVERSITAT POLITÈCNICA DE CATALUNYA
## BARCELONATECH

# Course guide
# 295455 - 295TM122 - Computational Fluid Mechanics

**Last modified:** 18/03/2024

| | |
|---|---|
| **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:** 2024   **ECTS Credits:** 6.0   **Languages:** Spanish, English

## LECTURER

| | |
|---|---|
| **Coordinating lecturer:** | Garcia Gonzalez, Fernando<br>Jofre Cruanyes, Lluís |
| **Others:** | Capuano, Francesco |

## 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

## 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.