# Course guide
# 205609 - 205609 - Computational Fluid Mechanics

**Last modified:** 19/04/2023

**Unit in charge:** Terrassa School of Industrial, Aerospace and Audiovisual Engineering
**Teaching unit:** 729 - MF - Department of Fluid Mechanics.

**Degree:** MASTER'S DEGREE IN RESEARCH IN MECHANICAL ENGINEERING (Syllabus 2021). (Optional subject).

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

## LECTURER

**Coordinating lecturer:** LLUÍS JOFRE CRUANYES

**Others:**

## PRIOR SKILLS

Basic knowledge of programming languages, fluid mechanics and differential equations.

## REQUIREMENTS

## TEACHING METHODOLOGY

The teaching methodology will combine theoretical lectures, hands-on exercises, tutorial & seminars, and individual/group projects.

## LEARNING OBJECTIVES OF THE SUBJECT

Learn to identify 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, and acquire expertise on the discrete solution and optimization of differential equations describing multiphysics problems in science and engineering.

## STUDY LOAD

| Type | Hours | Percentage |
|---|---|---|
| Self study | 96,0 | 64.00 |
| Hours large group | 54,0 | 36.00 |

**Total learning time:** 150 h

## CONTENTS

### Topic 1: 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:** 44h
Theory classes: 16h
Self study : 28h

### Topic 2: Navier-Stokes Flow Solver

**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. Handling complex geometries: body-conforming approaches and the immersed boundary method. Alternatives to projection methods: SIMPLE and PISO algorithms.

**Full-or-part-time:** 44h
Theory classes: 16h
Self study : 28h

### Topic 3: 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:** 18h
Theory classes: 6h
Self study : 12h

**Topic 4: Computational Flow Physics**

**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. Dynamical indicators from time series (local, global, Poincaré sections). Case study: the two-dimensional lid-driven cavity problem.

**Full-or-part-time:** 44h
Theory classes: 16h
Self study : 28h

## GRADING SYSTEM

- Final project: connected to the solver developed & data analysis tools of topic 4; 35%; Start at week 8-10, evaluation at week 15.
- Oral exam/discussion: questions related to the project; 50%; evaluation at week 15.
- Activities: 1-D Burgers equation (comparison to analytical solution); 2 - 3 questions (L2-norm, total energy, etc); Evaluation during topic 2; 15%.

## BIBLIOGRAPHY

**Basic:**
- Vermeire, Brian C.; Pereira, Carlos A.;Karbasian, Hamidreza. Computational fluid dynamics: an open-source approach [on line]. Concordia: Concordia University, 2020 [Consultation: 25/01/2023]. Available on: https://users.encs.concordia.ca/~bvermeir/files/CFD%20-%20An%20Open-Source%20Approach.pdf.
- Moin, Parviz. Fundamentals of engineering numerical analysis. 2nd ed. Cambridge: Cambridge University Press, 2010. ISBN 9780521711234.
- Drazin, Philip G. Introduction to hydrodynamic stability. Cambridge, UK: Cambridge University Press, 2002. ISBN 0521009650.
- Ferziger, Joel H.; Peric, Milovan; Street, Robert L. Computational methods for fluid dynamics [on line]. 4th ed. Cham, Switzerland: Springer, 2020 [Consultation: 25/01/2023]. Available on: https://link-springer-com.recursos.biblioteca.upc.edu/book/10.1007/978-3-319-99693-6. ISBN 9783319996936.
- Hager, Georg; Wellein, Gerhard. Introduction to high performance computing for scientists and engineers [on line]. Boca Raton: CRC Press, 2011 [Consultation: 15/02/2023]. Available on: http://prdrklaina.weebly.com/uploads/5/7/7/3/5773421/introduction_to_high_performance_computing_for_scientists_and_engineers.pdf. ISBN 9781439811924.
- LeVeque, Randall J. Finite difference methods for ordinary and partial differential equations: steady-state and time-dependent problems [on line]. Philadelphia: Society for Industrial and Applied Mathematics, 2007 [Consultation: 10/02/2023]. Available on: https://faculty.washington.edu/rjl/fdmbook/. ISBN 9780898716290.

## RESOURCES

**Other resources:**
Access to in-house flow solvers written in Python and Matlab, and computing cluster.