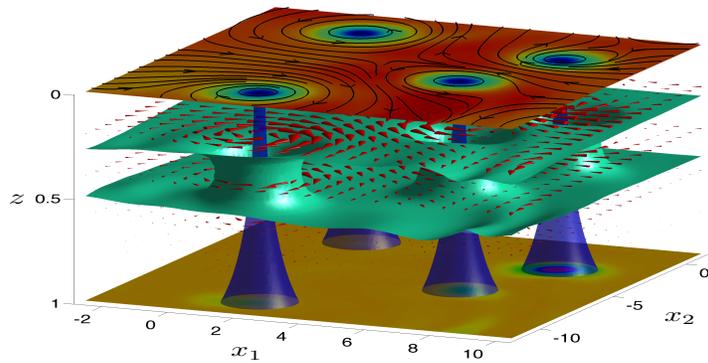


# Computational Fluid Dynamics (AC274)

Sauro Succi  
IAC-CNR Rome and IACS-Harvard

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Holographic turbulence (from A. Adams et al, Science, 2013)

# 1 Location and Timetable

Time: **Tue-Thu, 10-12 am**

Location: **Maxwell-Dworkin 223**

# 2 Course Description and Motivation

*Everything flows*, recites Heraclitus in 500 b.C., but ... how?

Two and half thousand years down the line, the question is still with us, with countless applications across all walks of science, industry and daily life, just think of water, air, blood, or oil...

In this Course, we shall learn how to provide quantitative answers to the fascinating question above, with the aid of mathematical models and computer programs. More precisely, we shall learn how to investigate the nature of flowing matter through dedicated computer simulations.

To this purpose, we shall begin with a general overview of the three main descriptions of **flowing matter**: *continuum fields (Macroscopic level)*, *atomistic particles (Microscopic level)* and *probability distribution functions (Mesoscopic level)*.

Computational fluid dynamics (CFD) is commonly associated with continuum mechanics, which surely offers a powerful representation of the physics of fluids. However, the picture is deeper and broader than that; in fact, modern science is increasingly concerned with flowing matter at micro and nanoscales, where the atomistic/molecular nature of the materials is fully exposed. This is why modern CFD must be informed on all three levels above.

Which one of three levels provides the most apt solution of a given problem, clearly depends on the nature of the specific problem at hand. In general, continuum mechanics holds at macroscopic scales, say from micrometers upwards, but no general rule exists to draw the line between the three levels; sometimes the continuum picture holds down to a few nanometers, sometimes it breaks down at micron scales, typically under the drive of large gradients and strong non-equilibrium effects.

In this Course, we shall familiarise with the main computational tools which permit to navigate across the above micro-meso-macro hierarchy.

### 3 Learning goals

The main goal of the course is to make the student acquainted with major theoretical and computational techniques for solving fluid dynamic problems at a continuum and mesoscale levels.

At the completion of the course, the student will be able to:

1. *Employ and develop concepts based on both the continuum and mesoscale description of flowing matter.*
2. *Read the current literature based on continuum and mesoscale approaches for various scientific and engineering applications involving complex fluids, such as turbulence, multiphase and soft matter flows.*
3. *Choose the most appropriate computational techniques for modeling problems in science and engineering that pertain to above mentioned fields.*
4. *Code the basic computational fluid methods for scientific and engineering applications across scales of motion*
5. *Appreciate the basic methodologies behind major commercial CFD codes*
6. *Contribute to science and engineering research projects involving complex flows*

## 4 Contents

The course consists of four main Parts.

In *Part I*, we shall expose the basic notions of the physics of fluids, covering the fundamental aspects of the Navier-Stokes equations of continuum fluid mechanics, the various flow regimes encountered in practical applications, including the long-standing problem of fluid turbulence. Honoring the idea that there is more to the physics of fluids than continuum mechanics, we shall expose the foundations of the kinetic theory of fluids, with special emphasis on the Boltzmann kinetic equation. After completing this Part, the student shall be acquainted with the basics of the physics of fluids, including its kinetic foundations, with no need of any prior knowledge of the subject.

In *Part II*, we shall cover the fundamentals of grid discretization of partial differential equations, with special focus on fluid transport phenomena. We shall cover the three main discretization methods: finite differences, elements and volumes. After completing this Part, the student will have acquired the basic tools for the numerical solution of partial differential equations, with no need of prior knowledge of the subject (some familiarity with coding will help for the completion of home assignments).

In *Part III*, we shall present the details of the numerical solution of the Navier-Stokes equations of continuum mechanics for compressible and incompressible flows. Lagrangian methods will also be discussed. This Part draws substantially on the notions developed in Part II and after completing it, the student shall be in a position to appreciate the basic methodologies behind commercial Computational Fluid Dynamics software.

Finally, in *Part IV*, we shall introduce mesoscale methods for complex fluid flows of particular relevance to soft matter applications. This includes both lattice kinetic (Boltzmann) and mesoparticle methods. After completing this Part, the student will be in a position to model basic micro and nanofluidic applications at the emerging interface between fluid mechanics and its allied disciplines, such as material science and biology.

- **Part I: Fluid Dynamics** (Lectures 1-5)

1. Fluids, Molecules and Probabilities (9/3)
2. The Navier-Stokes equations I: General (9/8)
3. The Navier-Stokes equations II: Topology (9/10)

4. The Navier-Stokes equations III: Turbulence (9/15)
  5. The Kinetic Theory of Fluids (9/17)
- **Part II: Grid Discretization Methods** (Lectures 6-11)
    1. Space discretization (9/22)
    2. Time discretization (9/24)
    3. *Guest Lecture: Population Dynamics in Biology* (9/29)  
**Break I: Thu Oct 1**
    4. Numerical Solution of Fluid Transport Equations (10/6)
    5. Finite Element Methods (10/8)
    6. Finite Volume Methods (10/13)
- **Part III: Computational Navier-Stokes** (Lectures 12-16)
    1. Compressible flows (10/15)
    2. Incompressible flows (10/20)
    3. Lagrangian methods (10/22)
    4. *Guest Lecture: Smoothed Particle Hydrodynamics* (10/27)  
**Break: Thu Oct 29**
    5. Flows with interfaces (11/3)
- **Part IV: Mesoscale Methods** (Lectures 17-22)
    1. Particles in Cell (11/5)
    2. Dissipative Particle Dynamics (11/10)
    3. Lattice Boltzmann I: Basics (11/12)
    4. Lattice Boltzmann II: Applications (11/17)
    5. Lattice Boltzmann III: Advanced (11/19)
    6. Farewell Lecture (11/24)
- **Exams** (Dec 14-15 TBF)

## 5 Basic References

1. J.H. Ferziger and M. Peric,  
*Computational Methods for Fluid Dynamics, Springer, (2002)*
2. R. Hockney, J. Eastwood,  
*Computer Simulations using Particles, C.R.C. Press, (1989)*
3. S. Succi,  
*The Lattice Boltzmann Equation for Fluid Dynamics and Beyond, Oxford U.P., (2001)*

Lecture notes will be available in the form of hard-copy powerpoint slides, enriched with a brief description of the main content of each lecture.

## 6 Pre-requisites

None, although some foreknowledge of numerical analysis and basic coding practices will help.

## 7 Grading policy

- Weekly assignments: 25%
- Break assignments: 25%
- Final Exam (Project): 50%

The final project may be related to an ongoing PhD thesis, on the *strict* condition that it represents original work. A brief selection of projects presented in the 2014 edition is available (see **Selected Final Projects from 2014**).