Numerical Methods in Engineering Applications

Session #1
Finite Differences

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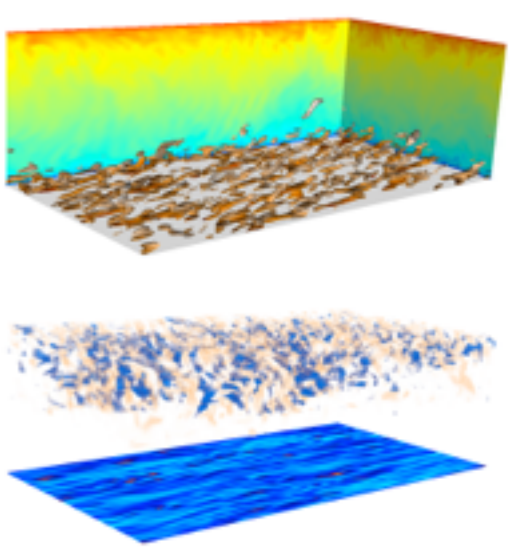
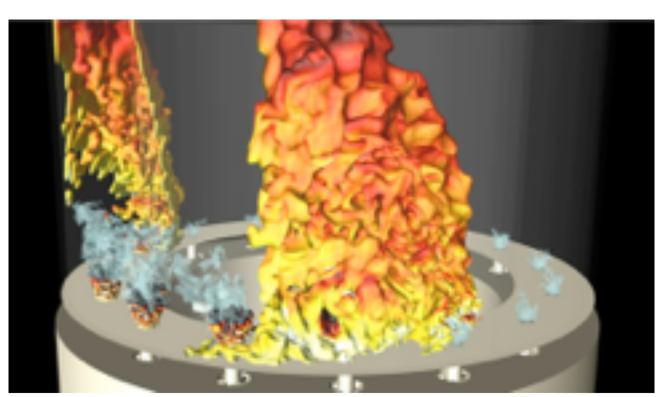
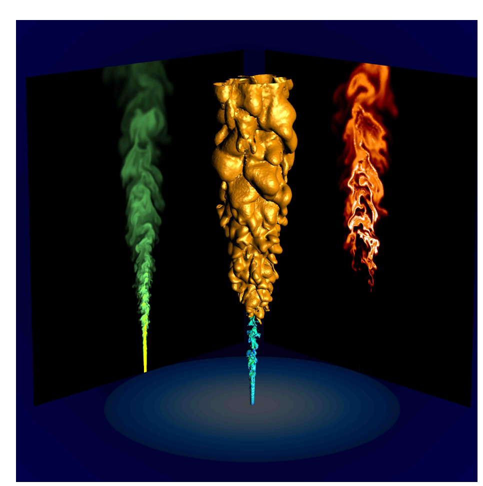
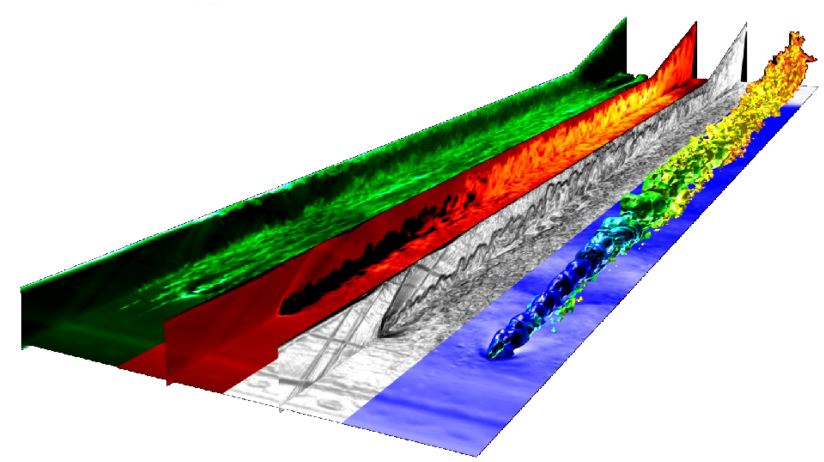
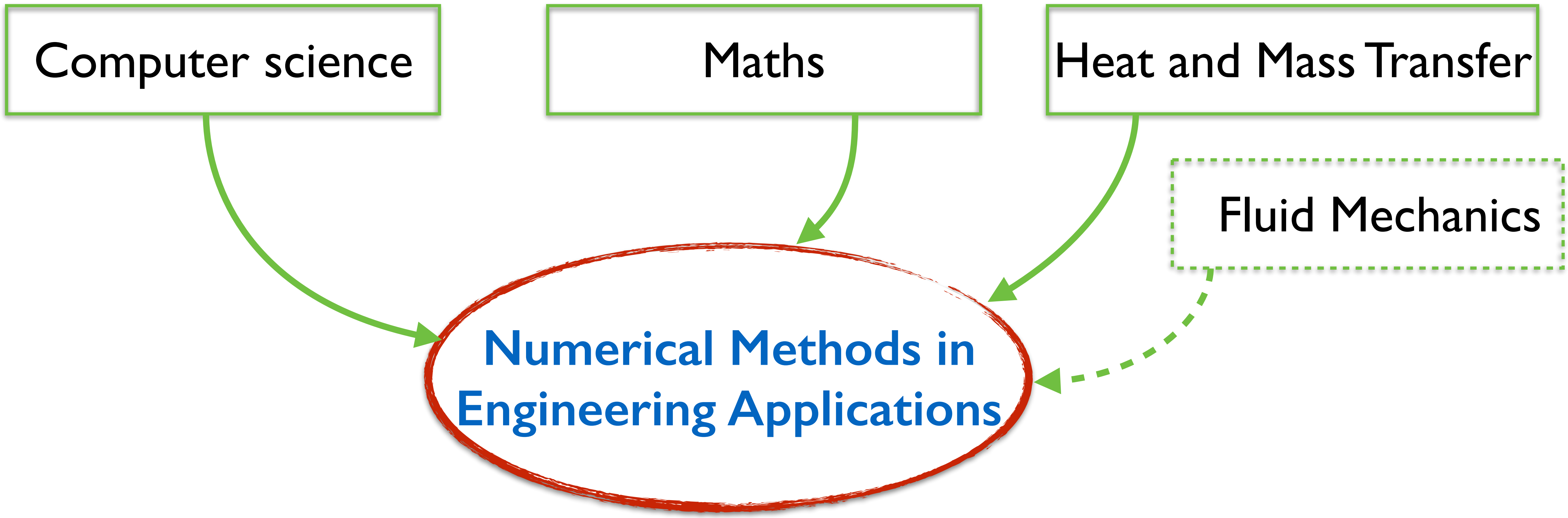





Objectives

- Numerical resolution of engineering problems
  - Fluid Mechanics
  - Species mass transfer
  - Heat transfer
  - Chemistry, ...
- Understanding of theoretical contents
- Practice (Python)

A synthesizing course…



… to solve practical cases

Computer science

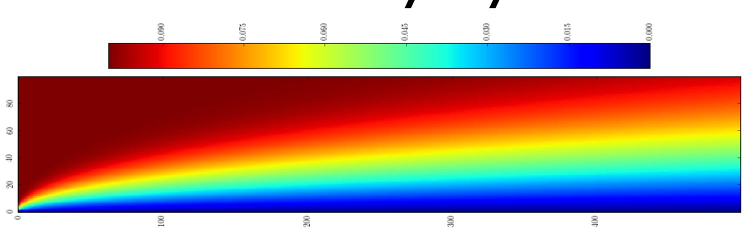
Maths

Heat and Mass Transfer

Fluid Mechanics

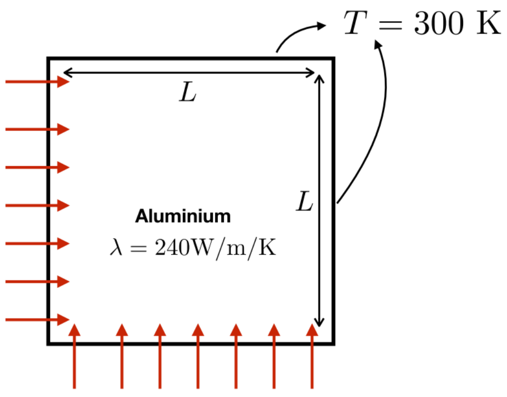
Numerical Methods in Engineering Applications

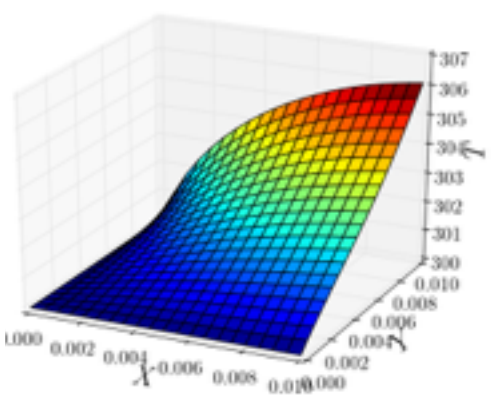
Boundary layer



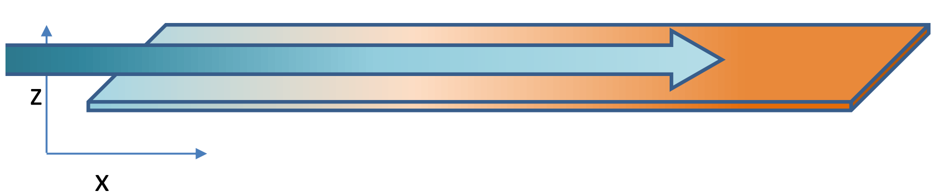
+ Numerical analysis
+ Numerical Efficiency
+ Physical analysis

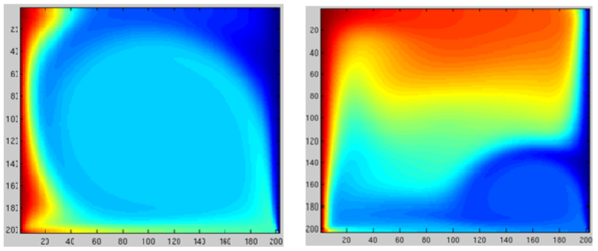
Maximum temperature



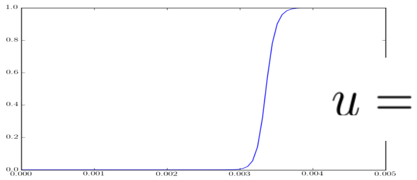


Transient heating



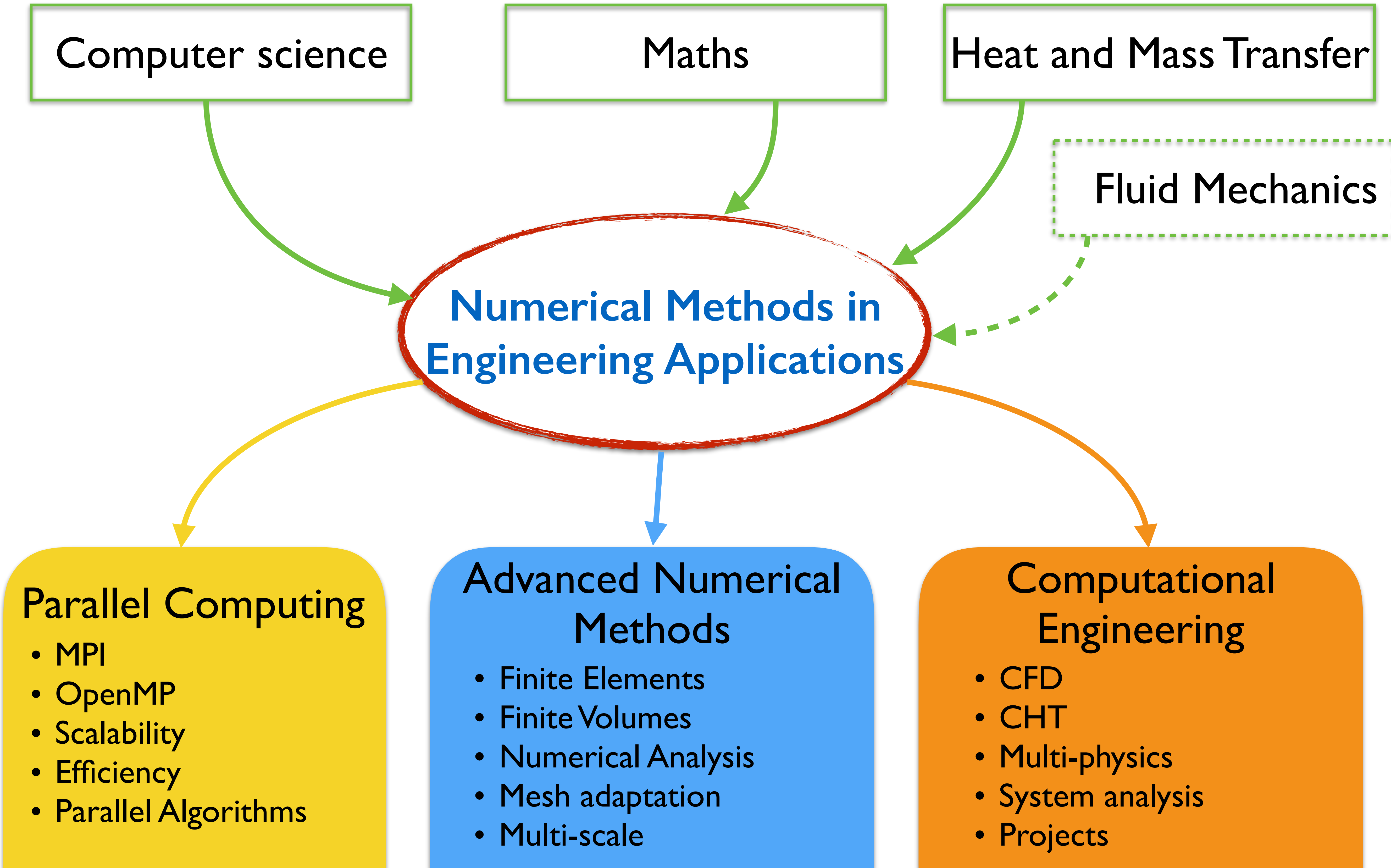


Flame speed



$u = 0.29 m.s^{-1}$

…and to go beyond



Course contents

Theoretical lecture
Problem-solving workshop

I. Basics on numerical approximations

- **Introduction and Finite Differences.**
- **Numerical solution of ordinary differential equations.**

II. Solving large linear equations systems: Applications to steady heat equation.

- **Elliptic PDE 1.**
- **Elliptic PDE 2.**

III. Methods for unsteady advection/diffusion problems

- **Hyperbolic and parabolic PDE: Explicit methods.**
- **Characterization of numerical errors.**
- **Hyperbolic and parabolic PDE: Implicit methods.**

IV. Towards computational fluid dynamics

- **Methodology in numerical computations.**
- **Incompressible Flow equations.**
- **Semi-Implicit method for incompressible flows.**
- **Final project on incompressible flow.**

Brilliant students

✔ Theoretical knowledge

✔ Not afraid to program
Welcome to the 21st century !

✔ Get practical answers
- Numerically sound and accurate
- Physically analyzed

65% of practice + projects

Evaluation

- 1 small project to hand out within a week
- 1 comprehensive mid-term project
- 1 small project to hand out within a week
- 1 comprehensive final project

Send slides and sources at each deadline

→ You will get some feed-back

Final deadline: send updated slides + final project

ECP+R
- 5 sessions
- Evaluation on the first 3 projects

Course contents

I. Basics on numerical approximations

- **Introduction and Finite Differences.**
- **Numerical solution of ordinary differential equations.** → Project #1

II. Solving large linear equations systems: Applications to steady heat equation.

- **Elliptic PDE 1.**
- **Elliptic PDE 2.** → Project #2

III. Methods for unsteady advection/diffusion problems

- **Hyperbolic and parabolic PDE: Explicit methods.** → Project #3
- **Characterization of numerical errors.**
- **Implicit methods for Parabolic PDE.**

IV. Towards computational fluid dynamics

- **Methodology in numerical computations.**
- **Incompressible Flow equations.**
- **Semi-Implicit method for incompressible flows.**
- **Final project on incompressible flow.** → Project #4

Numerical simulations in Engineering Applications

Characterize and improve systems

- Experimental investigation still unavoidable but can be extremely expansive
- It is not possible to measure everything everywhere

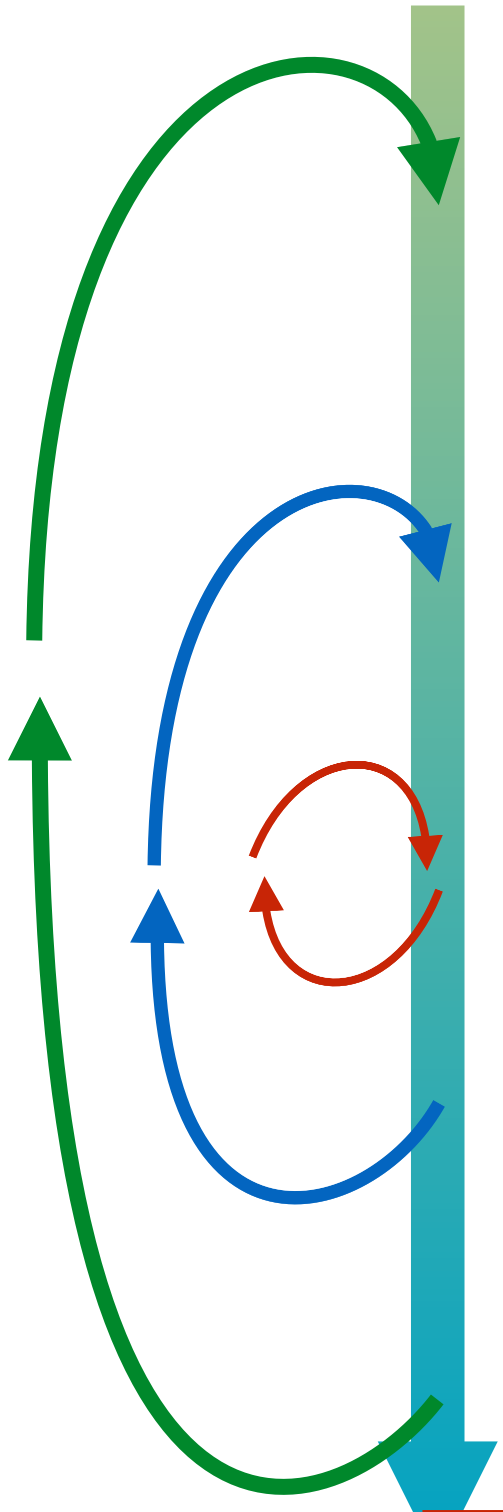
⟹ **Numerical simulations**

- Reduced cost even for the largest simulations compared to building prototypes
- All fields (u, v, w, T, Y_k) are available everywhere at each instant

… **but** the numerical model must be

- Efficient to be affordable
- Numerically accurate to make sure the discretization errors are controlled
- Validated to verify the physical representation of the system

Methodology

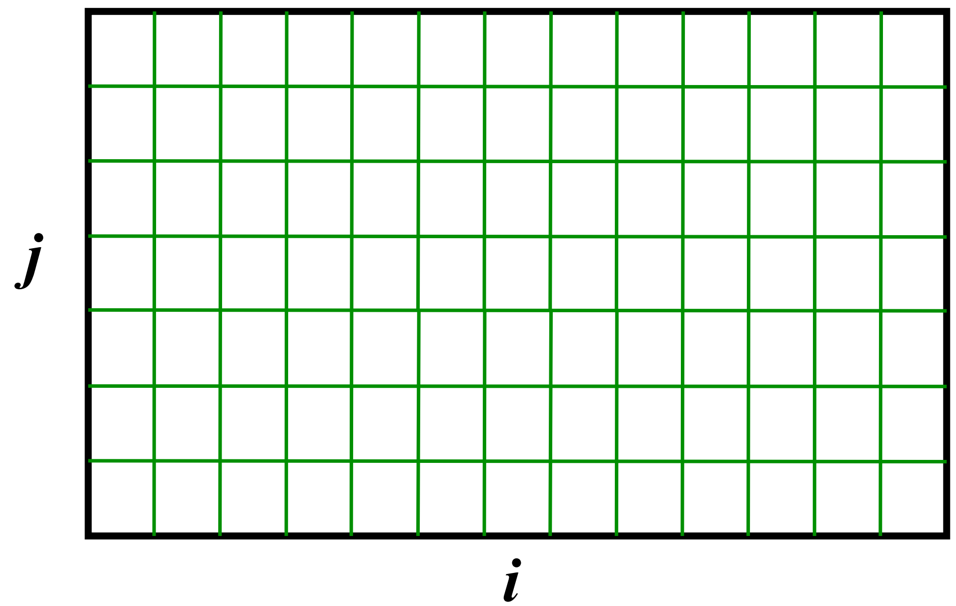


- Set the physical problem
- Formalization: Equations and Hypotheses
- Simplifications, symmetries
- Discretization (structures, unstructured mesh)
- Boundary conditions. Initial conditions.
- **Numerical resolution** (finite differences, finite volumes, finite elements, ...)
- Characterization of numerical error (accuracy of the numerical scheme, mesh convergence/adaptation)
- Data post-processing
- Model validation, Verification of hypotheses

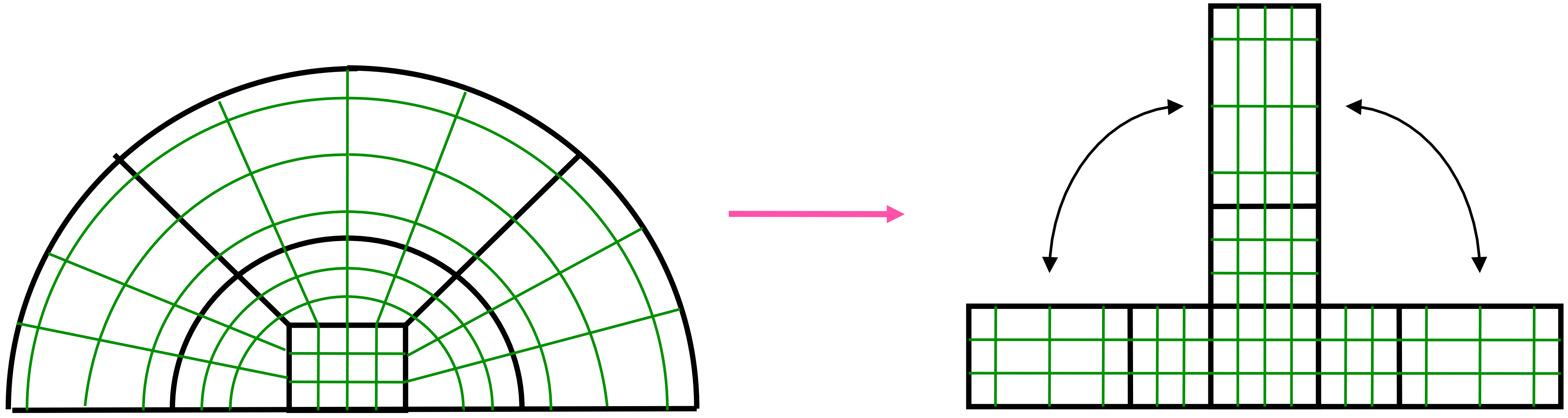
The problem answer

Meshes

Structured

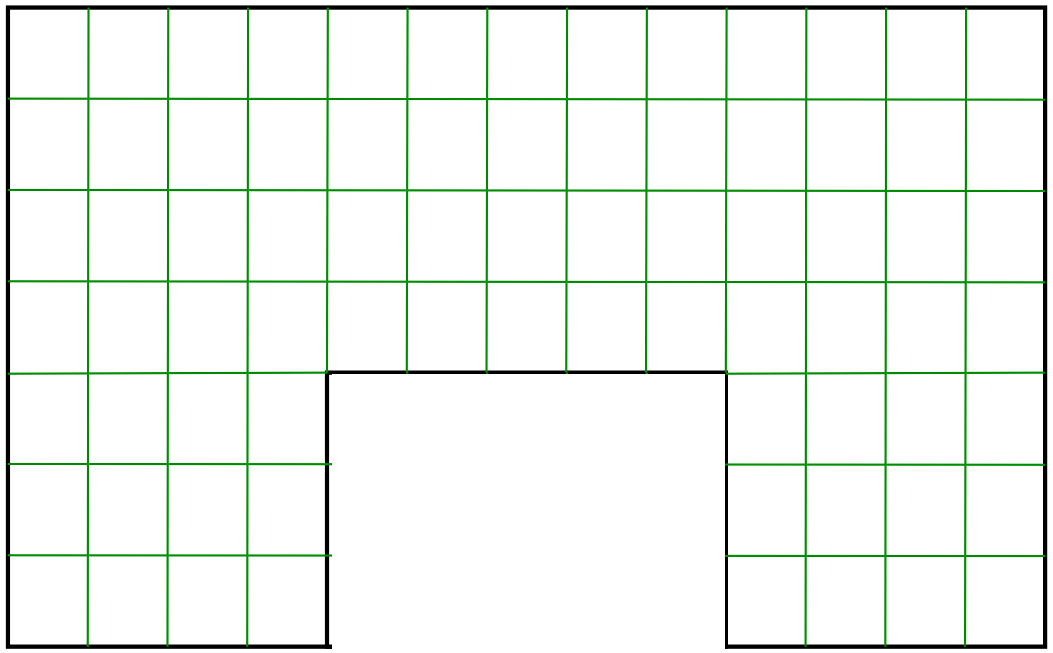


Multi-block Structured

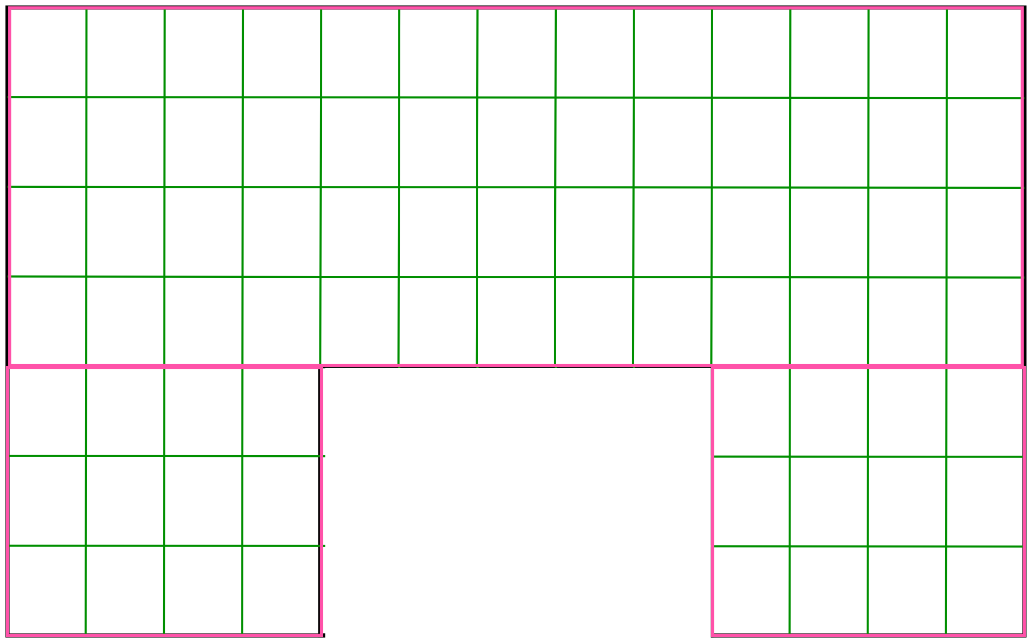


Meshes

Unstructured

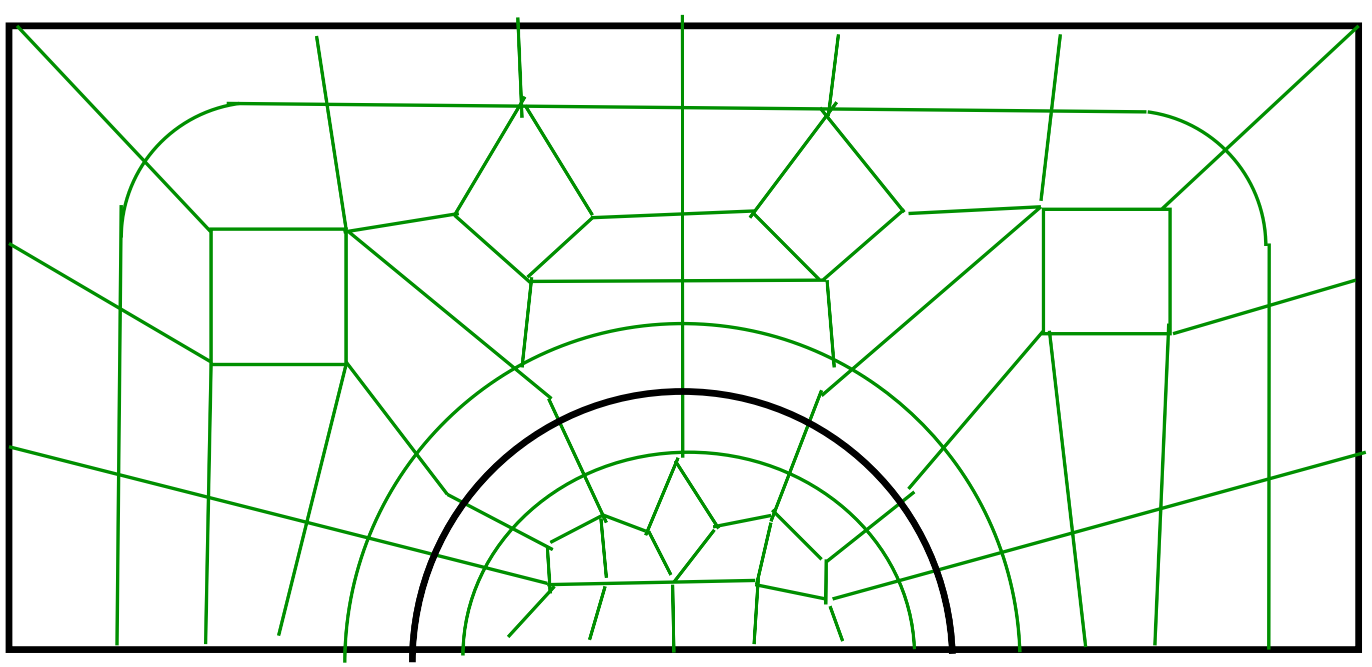


Multi-block Structured

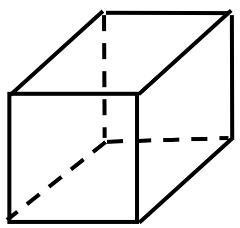


Meshes

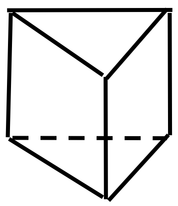
Unstructured

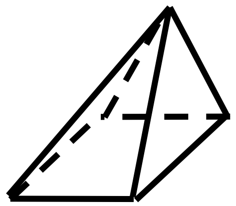


Hexa



Prisme (wedge)

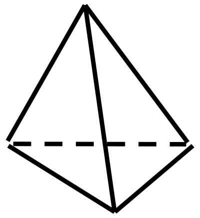




Pyramide

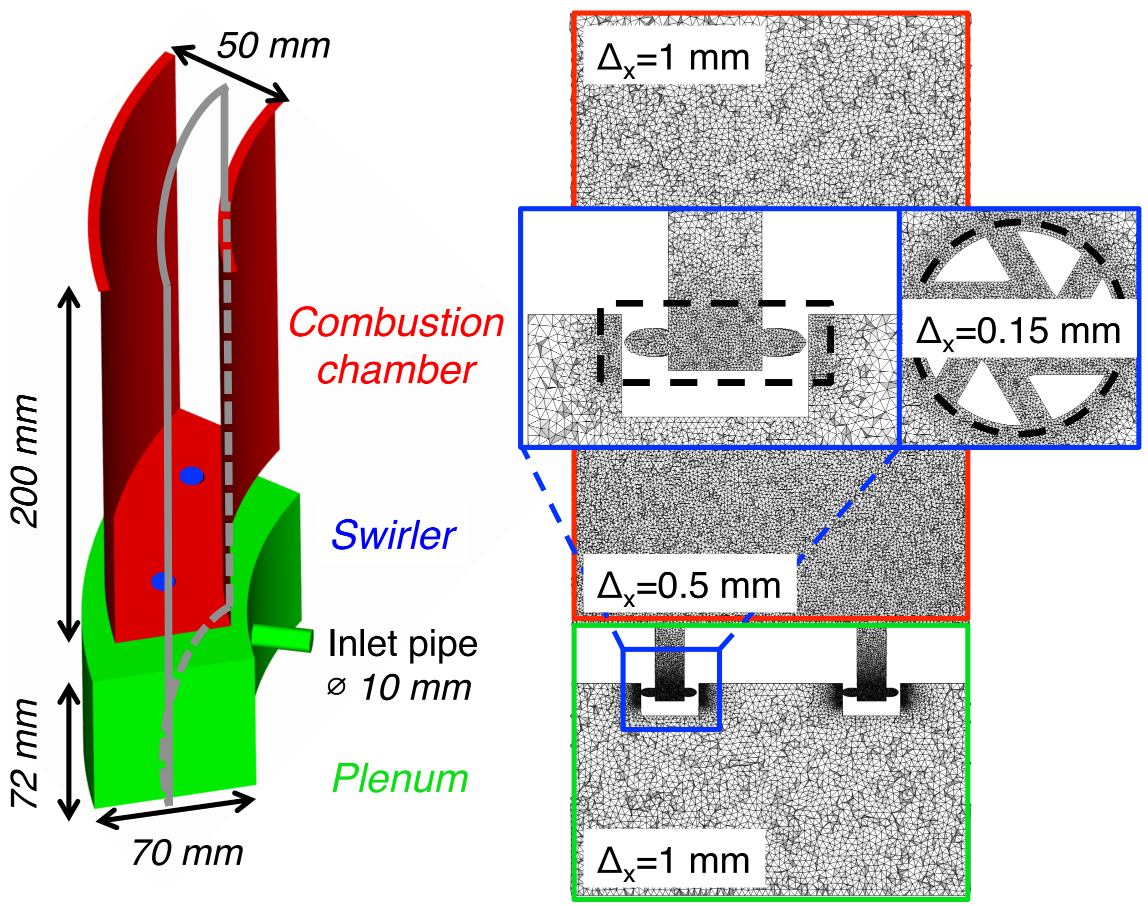
(transition conforme

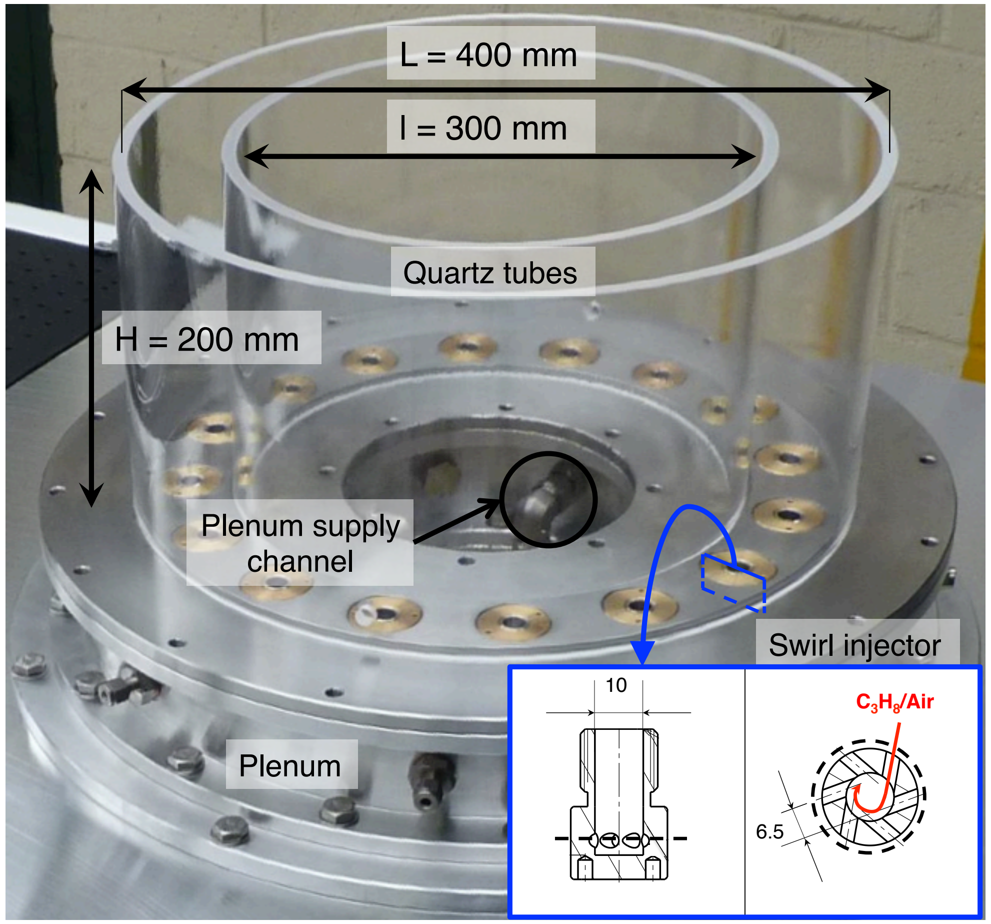
Hexa / Tétra)



tétrahèdre

Example: Large Eddy Simulation of Light-Round





Example: Large Edd Simulation of Light-Round

Parall

+ Combustion, Fluid Dynamics, Turbulence, …

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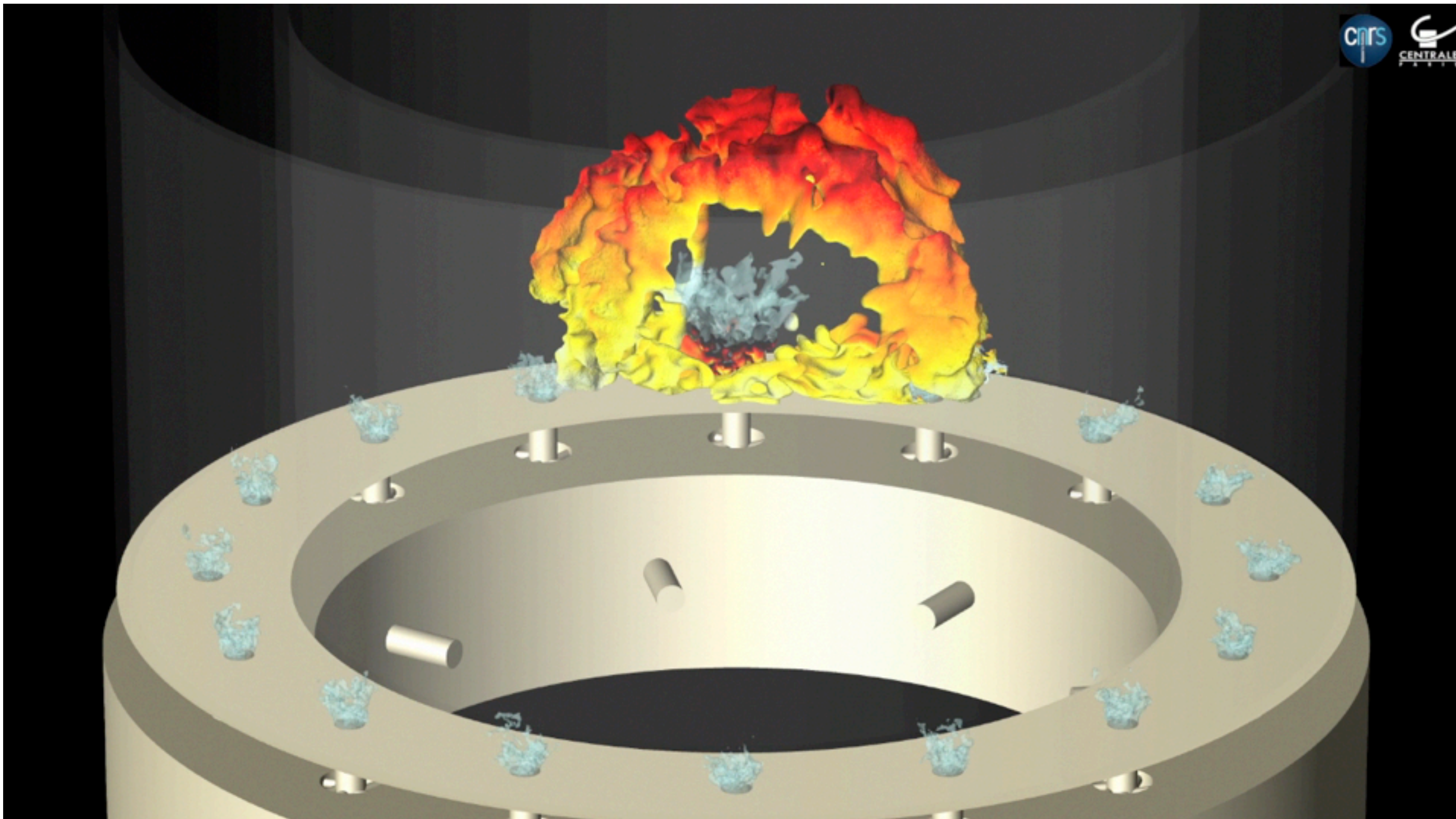

Partial Differential Equations (PDE)

Laplace

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

Poisson

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = S$$

Unsteady Heat Equation

$$\frac{\partial T}{\partial t} = a\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$

Advection

$$\frac{\partial c}{\partial t} + u_0 \frac{\partial c}{\partial x} = 0$$

Stokes

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial y^2}$$

Wave Equation

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0$$

ODE

$$\frac{dY_k}{dt} = \frac{\dot{\omega}_k}{\rho}$$

General Equations (Energetics applications)

- Fluid Mechanics + Heat Transfer+ Mass Transfer:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

$$\rho \frac{\partial v_i}{\partial t} + \rho v_j \frac{\partial v_i}{\partial x_j} = \rho g_i - \frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p v_j \frac{\partial v_i}{\partial x_j} = \frac{\partial p}{\partial t} + v_j \frac{\partial p}{\partial x_j} + \tau_{ij} \frac{\partial v_i}{\partial x_j} + \dot{\Omega} - \frac{\partial q_j}{\partial x_j} - \sum_{k=1}^{N} h_k \dot{\omega}_k + \sum_{k=1}^{N} \rho V_{k,j} Y_k c_{pk} \frac{\partial T}{\partial x_j}$$

$$\rho \frac{\partial Y_k}{\partial t} + \rho v_j \frac{\partial Y_k}{\partial x_j} = -\frac{\partial}{\partial x_j}\left(\rho V_{k,j} Y_k\right) + \dot{\omega}_k$$

General conservative form of the equations

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F}(\mathbf{U}, \nabla \mathbf{U}) = \mathbf{S}$$

- Fluid Mechanics + Heat Transfer+ Mass Transfer

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho v_1 \\ \rho v_2 \\ \rho v_3 \\ \rho(e + \frac{1}{2} v_i v_i) \\ \rho Y_1 \\ \vdots \\ \rho Y_N \end{pmatrix} \qquad \mathbf{F} = \begin{pmatrix} \\ \\ \\ \\ \vdots \\ \\ \\ . \end{pmatrix} \qquad \mathbf{S} = \begin{pmatrix} 0 \\ \rho g_1 \\ \rho g_2 \\ \rho g_3 \\ \mathbb{P} \\ \dot{\omega}_1 \\ \vdots \\ \dot{\omega}_N \end{pmatrix}$$

PDE Classification

- **Order-1 PDE**

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{U}}{\partial x} = \mathbf{S}$$

A Eigenvalues	PDE Type
Complex (non-real)	Elliptic
Real	Hyperbolic
Complex and real	Hybrid
Rank(A) < n	Parabolic

PDE Classification

- **Order-2 PDE**

$$\sum_{i,j} a_{ij} \frac{\partial^2 \mathbf{U}}{\partial x_i \partial x_j} = 0 \Longrightarrow \sum_{i,j} a_{ij} X_i X_j = 0$$

Type of the PDE hyperplane ⇒ Type of the PDE

Example : $A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} = 0 \Longrightarrow AX^2 + BXY + CY^2 = 0$

$\Delta = B^2 - 4AC$	PDE Type
$\Delta < 0$	Elliptique
$\Delta = 0$	Parabolique
$\Delta > 0$	Hyperbolique

More details: See C. Hirshc's Numerical Computation of Internal & External Flows

Physical definition

- **Hyperbolic**
  - Purely propagative wave solutions exits
  - Ex: advection
- **Parabolic**
  - Only one type of wave solutions : damped waves
  - Ex: Unsteady diffusion
- **Elliptic**
  - No wave solutions
  - Ex: Steady Diffusion

Nomenclature for order 1 and 2 denotes the same physics

Elliptic/Parabolic/Hyperbolic

- **Elliptic**
  - No notion of propagation of physical information
  - Solution at a point depends on the whole field, and reciprocally.
  - Requires BCs on the entire domain border
- **Parabolic**
  - Propagation of information along one preferred direction
  - Solution at a point depends on a half-space domain
  - Requires an "initial condition"
  - Requires BCs for directions different from the preferred one
- **Hyperbolic**
  - Propagation of information at finite speed along one or several directions
  - Solution at a point depends on a region delimited by the PDE characteristics
  - Requires an "initial condition"
  - Requires BCs only where information is incoming

2D Euler equations, steady, isentropic

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0$$

Mass conservation

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{1}{\rho}\frac{\partial p}{\partial x} = 0$$

Momentum along x-axis

$$u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{1}{\rho}\frac{\partial p}{\partial y} = 0$$

Momentum along y-axis

$$p = k\rho^{\gamma} \qquad \frac{\partial p}{\partial x} = c^2 \frac{\partial \rho}{\partial x} \qquad \frac{\partial p}{\partial y} = c^2 \frac{\partial \rho}{\partial y}$$

Isentropic

2D Euler equations, steady, isentropic

$$A\frac{\partial U}{\partial x} + B\frac{\partial U}{\partial y} = 0$$

$$U = \begin{pmatrix} u \\ v \\ Logp \end{pmatrix}$$

$$A = \begin{bmatrix} u & 0 & c^2/\gamma \\ 0 & u & 0 \\ \gamma & 0 & u \end{bmatrix}$$

$$B = \begin{bmatrix} v & 0 & 0 \\ 0 & v & c^2/\gamma \\ 0 & \gamma & v \end{bmatrix}$$

2D Euler equations, steady, isentropic

$$\frac{\partial U}{\partial x} + M\frac{\partial U}{\partial y} = 0$$

$$M = A^{-1}B = \frac{1}{u^2 - c^2}\begin{bmatrix} uv & -c^2 & -vc^2/\gamma \\ 0 & \frac{v}{u}\left(u^2 - c^2\right) & \frac{c^2}{u\gamma}\left(u^2 - c^2\right) \\ -v\gamma & u\gamma & uv \end{bmatrix}$$

M Eigenvalues : $\lambda_1 = \frac{v}{u}$ $\qquad \lambda_2 = \frac{uv}{u^2 - c^2} \pm \frac{c^2}{u^2 - c^2}\sqrt{Mach^2 - 1}$

Euler 2D, stationnaire, isentropique

M Eigenvalues : $\lambda_1 = \dfrac{v}{u}$ $\qquad \lambda_2 = \dfrac{uv}{u^2 - c^2} \pm \dfrac{c^2}{u^2 - c^2}\sqrt{Mach^2 - 1}$

If Mach<1 Hybrid: Elliptic-Hyperbolic

If Mach=1 Parabolic

If Mach>1 Hyperbolic

Numerical discretization

- The real solution is approximated by a discrete solution
  => Finite number of degrees of freedom to represent the solution

- The numerical solution is governed by a discrete “PDE” where derivative operators are discretized

- **Finite Differences**: The solution values are stored at the mesh nodes.

  Taylor series

- **Finite Volumes:** The cell-averaged value is stored

  Conversation equation integrated on the cell

- **Finite Elements** : Expansion on basis functions

  Variational Formulation

Unstructured Mesh