

YALES2: modeling advances of interest for plasmas

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and many more at CORIA, LEGI, INRIA, SAFRAN TECH,
ARIANE GROUP, ONERA, ...

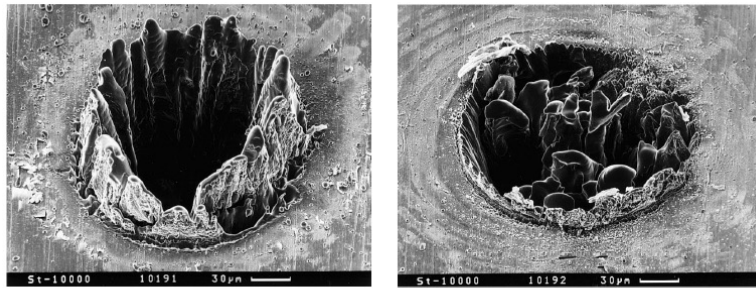
Presentation of the lecturer

- Vincent Moureau
 - Since 2009: **CNRS research director at CORIA**
 - Development of the finite-volume code YALES2
 - 2018: Grand prix of the French academy of science for aerospace & aeronautics engineering
 - Since 2016: scientific expert for SAFRAN TECH
 - 2008: combustion engineer at Turboméca, SAFRAN group
 - Design and modeling of combustion chambers in helicopter engines
 - 2006: post-doctoral fellowship at Stanford University, California
 - Modeling of premixed combustion and two-phase flows
 - 2004: PhD thesis at IFP – ECP
 - Large-eddy simulation of in-cylinder flows in piston engines
 - 2001: Ecole Centrale Paris – option Air & Espace
- Fields of expertise
 - Modeling of reacting and two-phase turbulent flows
 - Thermo-acoustic instabilities
 - Numerical methods and development of finite-volume codes
 - Aeronautical and automotive engines

Plasma flows from the modeling and simulation standpoint

Laser-induced plasma

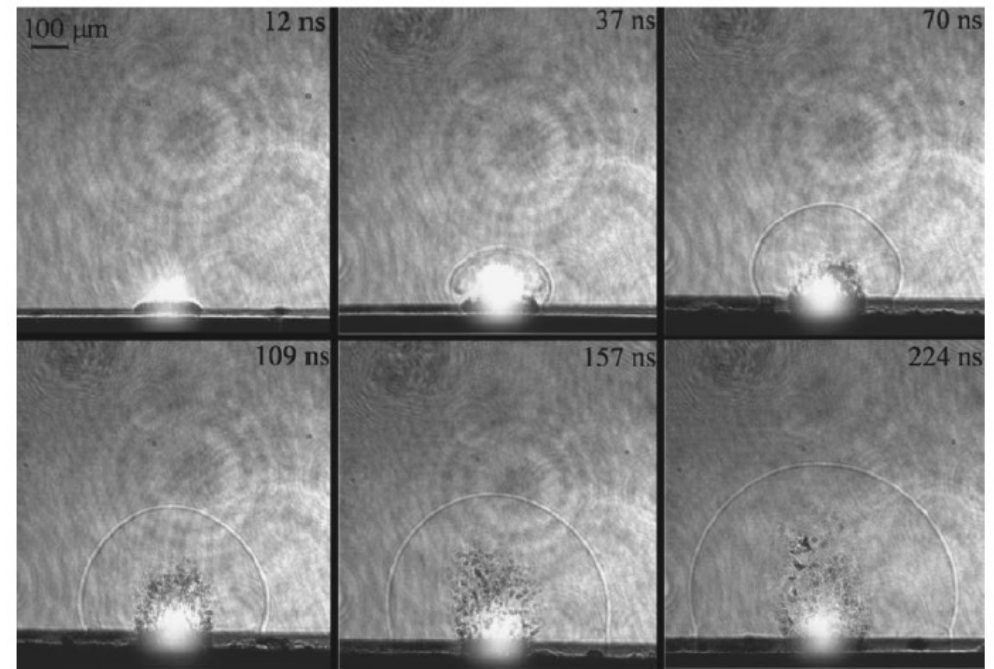
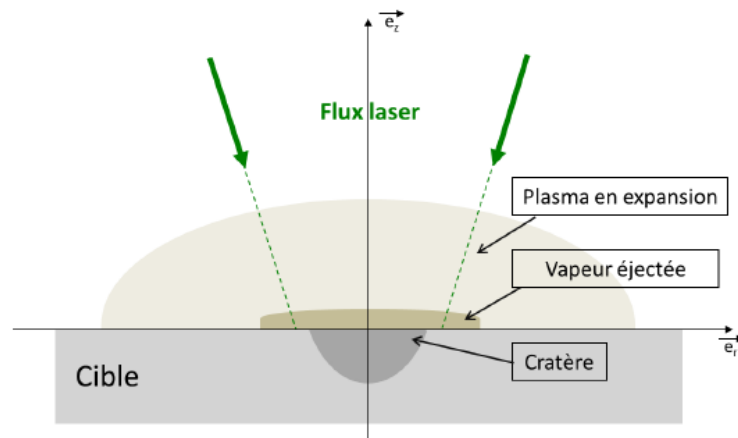
- Multiple phases, high-temperature and shocks



(a) Impulsion nanoseconde

(b) Impulsion picoseconde

Electron microscopy images of the surface of a steel sample



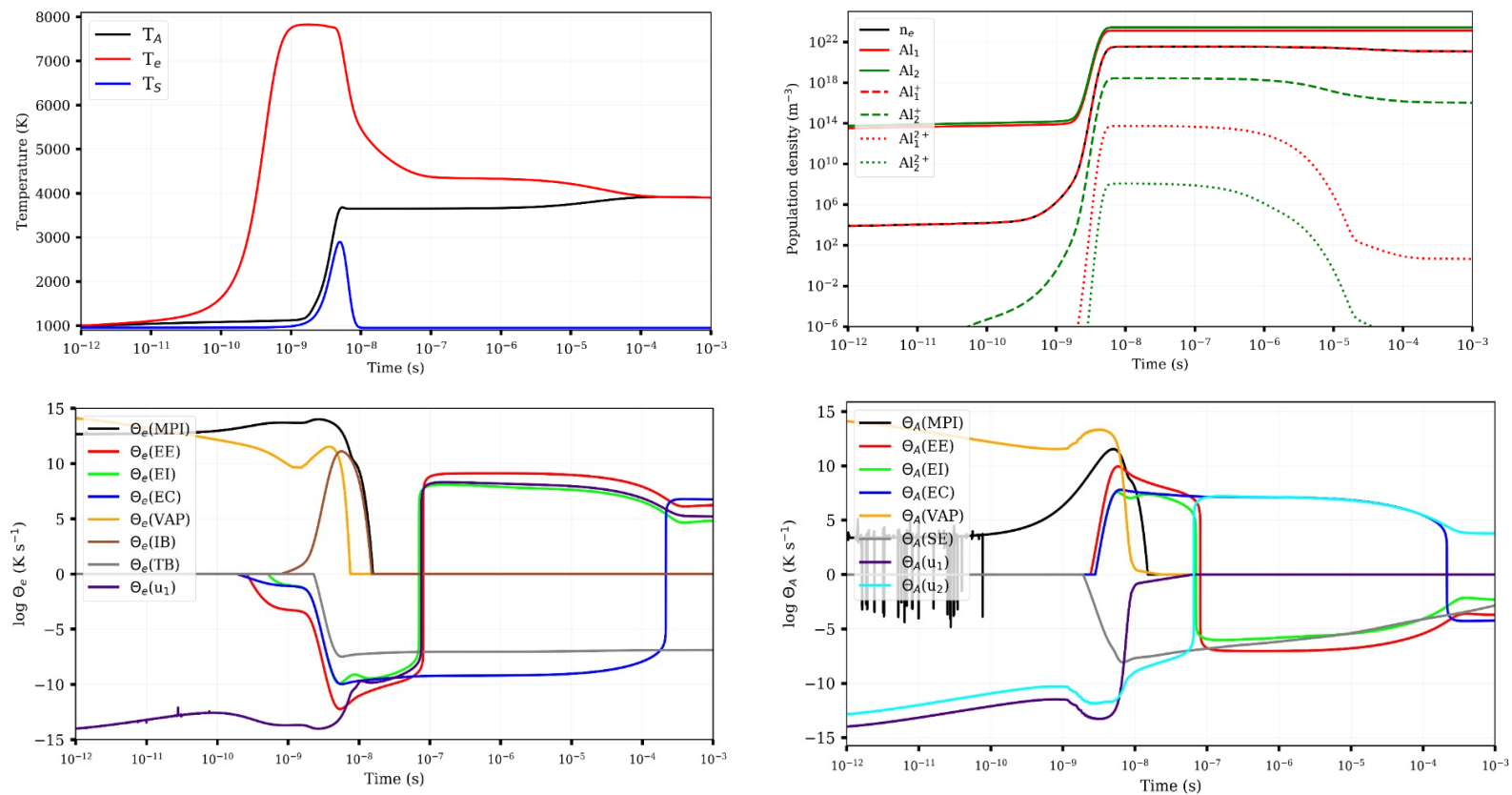
Formation and propagation of a shock wave and the progressive formation of Aluminium droplets

Courtesy A. Bultel, CORIA

Kinetics in out-of-equilibrium plasma

- Multiple species, ions, electrons and temperatures
- Many types of chemical reactions

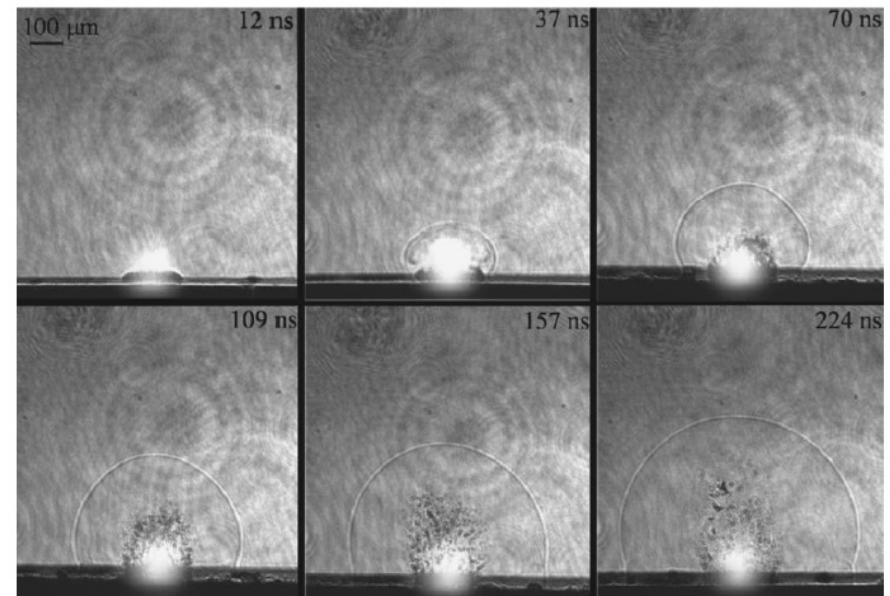
0-D simulation of laser-induced aluminum plasma



Courtesy Y. Bechane and V. Morel, CORIA

A summary of the simulation and modeling challenges

- Multi-regime
 - Laminar/turbulent/transitional flows
 - Subsonic / supersonic / hypersonic
 - Continuous/rarefied, ...
- Multi-physics
 - Complex thermodynamics
 - Complex transport
 - Reactive, non-equilibrium flows
 - Conjugate heat transfer
- Multi-scale
 - From meters to nanometers
 - From hours to nanosecond
- Complex geometries



Outline

- Context
 - Plasma flows from the modeling and simulation standpoint
- Numerical methods for Navier-Stokes type equations
 - Solving the compressible Navier-Stokes equations
 - Shocks
 - Solving the incompressible Navier-Stokes equations
- The **YALES2** project

Solving **compressible** Navier-Stokes equations

Mach number $Ma=u/c$

- Some applications have a **high Mach number**
 - Rocket engines, stato-reactors, supersonic planes, space shuttle...
- Or **moderate Mach number** with compressibility effects
 - Compressors, turbines, planes, ...
- Many daylife applications have a **low-Mach number**
 - Most burners (for flame anchoring...)
 - Industrial furnaces
 - Car engines
 - Aircraft/Helicopter combustors
 - Mixers, pipes, pumps, nuclear plants, wind-turbines, ...
- Be careful: some phenomena happen at low-Mach number but need compressibility to be explained
 - Acoustics
 - Combustion instabilities

Navier-Stokes Equations

- Conservative form with total energy E

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \nabla \cdot \tau$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) = -\nabla \cdot (P \mathbf{u}) + \nabla \cdot \lambda \nabla T + \nabla \cdot (\tau \mathbf{u})$$

- Thermal Equation of State

$$E = \frac{1}{2} u^2 + C_v T$$

- Mechanical Equation of State

$$P = \rho r T$$

Navier-Stokes Equations

- Variables in a vector $\mathbf{W}$ to simplify notations

$$\mathbf{W} = \begin{pmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{pmatrix}$$

$$\frac{\partial \mathbf{W}}{\partial t} + \nabla \cdot (\mathbf{F}_E + \mathbf{F}_V) = 0$$

- F_E : Euler Fluxes
- F_V : Viscous Fluxes

Euler Equations

- Conservative form with total energy E

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla P + \text{X}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E \mathbf{u}) = -\nabla \cdot (P \mathbf{u}) + \nabla \cdot \text{X} + \nabla \cdot \text{X}$$

- **HYPERBOLIC** equations
- ~~PARABOLIC~~ equations
- ~~ELLIPTIC~~ equations

Finding the waves from the 1D Euler equations

- Starting from the vector form:

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0$$

$$\mathbf{W} = \begin{pmatrix} \rho \\ \rho u \\ \rho E \end{pmatrix} \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ (\rho E + P)u \end{pmatrix}$$

$$P = \rho r T \quad \rho E = \frac{1}{2} \rho u^2 + \frac{P}{\bar{\gamma} - 1}$$

- Perform a linearization:

$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}}{\partial \mathbf{W}} \frac{\partial \mathbf{W}}{\partial x} = 0$$

Finding the waves from the 1D Euler equations

- Why???
$$\frac{\partial \mathbf{W}}{\partial t} + \frac{\partial \mathbf{F}}{\partial \mathbf{W}} \frac{\partial \mathbf{W}}{\partial x} = 0$$
- If lucky, the jacobian matrix is diagonal!
$$J = \frac{\partial \mathbf{F}}{\partial \mathbf{W}}$$
- This would mean that the components of $\mathbf{W}$ are independent
- They would be independent waves moving at given velocity
- If J is not diagonal, then the components of $\mathbf{W}$ are a mix of some waves that must be computed.
- How? **Diagonalisation** (which is just a change of basis...)
- Just rewrite the same equation with **nicer variables**...

Finding the waves from the 1D Euler equations

- For Euler equations, the Jacobian Matrix is:

$$\frac{\partial \mathbf{F}}{\partial \mathbf{W}} = \begin{pmatrix} 0 & 1 & 0 \\ -(3-\gamma)\frac{1}{2}u^2 & (3-\gamma)u & (\gamma-1) \\ -\gamma Eu + (\gamma-1)u^3 & \gamma E - \frac{3}{2}(\gamma-1)u^2 & \gamma u \end{pmatrix}$$

- We want to have **INDEPENDENT** variables → diagonalisation

$$\mathbf{V}_E^{-1} \frac{\partial \mathbf{W}}{\partial t} + \underbrace{\mathbf{V}_E^{-1} \frac{\partial \mathbf{F}}{\partial \mathbf{W}} \mathbf{V}_E}_{\text{diag}(\Lambda_E)} \mathbf{V}_E^{-1} \frac{\partial \mathbf{W}}{\partial x} = 0 \quad \Lambda_E = \begin{pmatrix} u+c \\ u-c \\ u \end{pmatrix}$$

$$\mathbf{V}_E^{-1} \partial \mathbf{W} \sim \begin{pmatrix} \rho c \partial u - \partial P \\ \rho c \partial u + \partial P \\ c^2 \partial \rho - \partial P \end{pmatrix} \begin{matrix} \swarrow \text{acoustics} \\ \swarrow \text{acoustics} \\ \longrightarrow \text{convection} \end{matrix}$$

What about 2D and 3D?

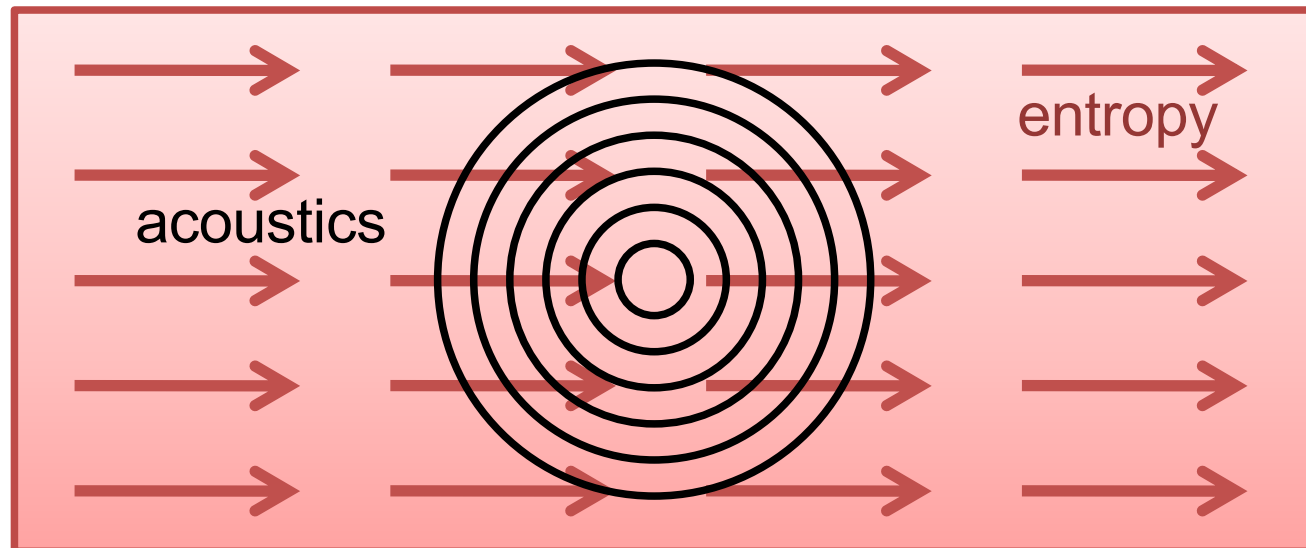
- Entropic transport is a 1st order hyperbolic problem

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0$$

- Acoustic is a 2nd order hyperbolic problem

$$\frac{\partial^2 \phi}{\partial t^2} - c^2 \nabla \cdot \nabla \phi = 0$$

- Consider someone throwing an object in a river:

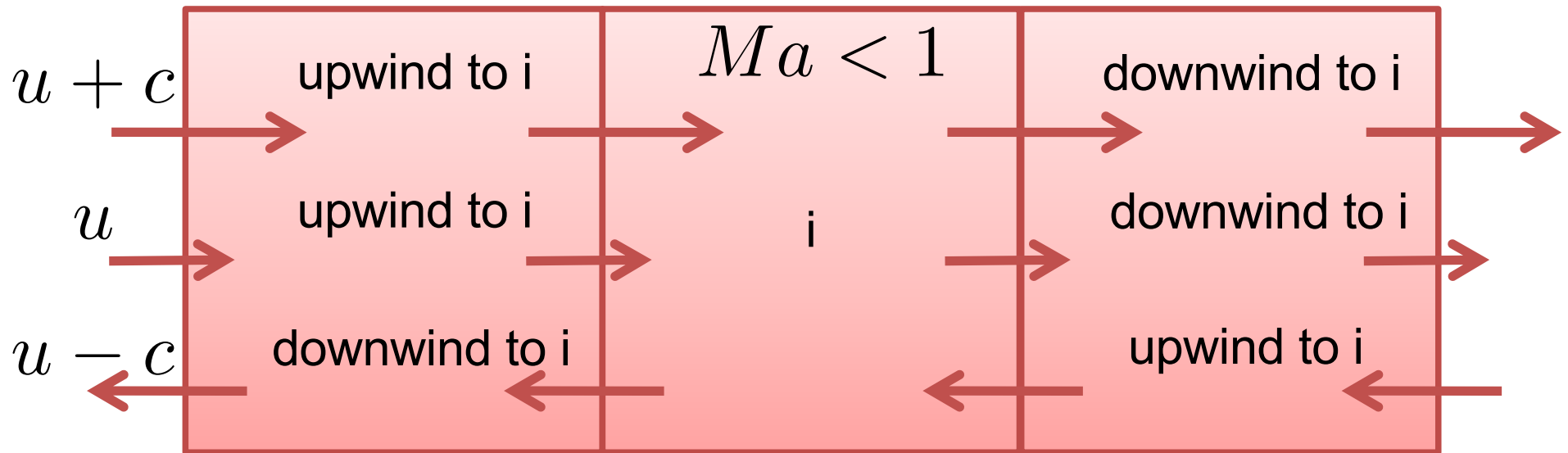


Explicit numerical methods and boundary conditions

- Classical numerical schemes can be used for time integration (RK3, RK4) but a CFL condition must be set for **ALL WAVES**:

$$CFL_{ac} = \frac{(|u| + c)\Delta t}{\Delta x}$$

- The spacial discretization is usually performed with **UPWIND** schemes. However, special attention must be paid to the direction of the characteristics!
- If $Ma < 1$, no boundary condition is a pure inlet or outlet!!!



Waves and boundary conditions

Courtesy Y. Bechane

Quizz on waves & boundary conditions

$$P = P_0 + dP$$

$$\rho = \rho_0$$

$$T = P/(r * \rho)$$

$$u = 0 \text{ m/s}$$

Outlets



9.0e+04 90100901509020090250903009035090400 9.0e+04
Pressure (Pa)



-1.4e+00 -1 -0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8 1 1.4e+00
Velocity (m/s)



1.0e+00 1.039 1.04 1.041 1.042 1.043 1.044 1.045 1.046 1.047 1.048 1.0e+00
Density (Kg/m3)



3.0e+02 300.5 301 301.5 302 302.5 303 3.0e+02
Temperature (K)

Quizz on waves & boundary conditions

$$P = P_0 + dP$$

$$\rho = \rho_0$$

$$T = P/(r * \rho)$$

$$u = 50 \text{ m/s}$$

Outlets



9.0e+04 90100901509020090250903009035090400 9.0e+04
Pressure (Pa)



4.9e+01 49 49.2 49.4 49.6 49.8 50 50.2 50.4 50.6 50.8 51 5.1e+01
Velocity (m/s)



1.0e+00 1.039 1.04 1.041 1.042 1.043 1.044 1.045 1.046 1.047 1.048 1.0e+00
Density (Kg/m3)



3.0e+02 300.5 301 301.5 302 302.5 303 3.0e+02
Temperature (K)

Quizz on waves & boundary conditions

$$\begin{aligned}P &= P_0 + dP \\ \rho &= \rho_0 + d\rho/c^2 \\ T &= P/(r * \rho) \\ u &= 0 \text{ m/s}\end{aligned}$$

Outlets



9.0e+04 90100901509020090250903009035090400 9.0e+04
Pressure (Pa)



-1.4e+00 -1 -0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8 1 1.4e+00
Velocity (m/s)



1.0e+00 1.039 1.04 1.041 1.042 1.043 1.044 1.045 1.046 1.047 1.048 1.0e+00
Density (Kg/m3)



3.0e+02 300.5 301 301.5 302 302.5 303 3.0e+02
Temperature (K)

Quizz on waves & boundary conditions

$$\begin{aligned}P &= P_0 + dP \\ \rho &= \rho_0 + d\rho/c^2 \\ T &= P/(r * \rho) \\ u &= 0 \text{ m/s}\end{aligned}$$

Walls



9.0e+04 90100901509020090250903009035090400 9.0e+04
Pressure (Pa)



-1.4e+00 -1 -0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8 1 1.4e+00
Velocity (m/s)



1.0e+00 1.039 1.04 1.041 1.042 1.043 1.044 1.045 1.046 1.047 1.048 1.0e+00
Density (Kg/m3)



3.0e+02 300.5 301 301.5 302 302.5 303 3.0e+02
Temperature (K)

Quizz on waves & boundary conditions

$$\begin{aligned}P &= P_0 + dP \\ \rho &= \rho_0 + d\rho/c^2 \\ T &= P/(r * \rho) \\ u &= 0 \text{ m/s}\end{aligned}$$

Walls Wave
Reflection coefficient = 0.2



9.0e+04 90100901509020090250903009035090400 9.0e+04
Pressure (Pa)



-1.4e+00 -1 -0.8 -0.6 -0.4 -0.2 0 0.2 0.4 0.6 0.8 1 1.4e+00
Velocity (m/s)



1.0e+00 1.039 1.04 1.041 1.042 1.043 1.044 1.045 1.046 1.047 1.048 1.0e+00
Density (Kg/m3)



3.0e+02 300.5 301 301.5 302 302.5 303 3.0e+02
Temperature (K)

Quizz on waves & boundary conditions

$$\begin{aligned}P &= P_0 + dP \\ \rho &= \rho_0 + d\rho/c^2 \\ T &= P/(r * \rho) \\ u &= u_0 + dP/(\rho * c)\end{aligned}$$

Outlets



9.0e+04 90200903009040090500906009070090800 9.1e+04
Pressure (Pa)



-1.4e+00 -1 -0.5 0 0.5 1 1.5 2 2.7e+00
Velocity (m/s)



1.0e+00 1.039 1.04 1.041 1.042 1.043 1.044 1.045 1.046 1.047 1.048 1.0e+00
Density (Kg/m3)

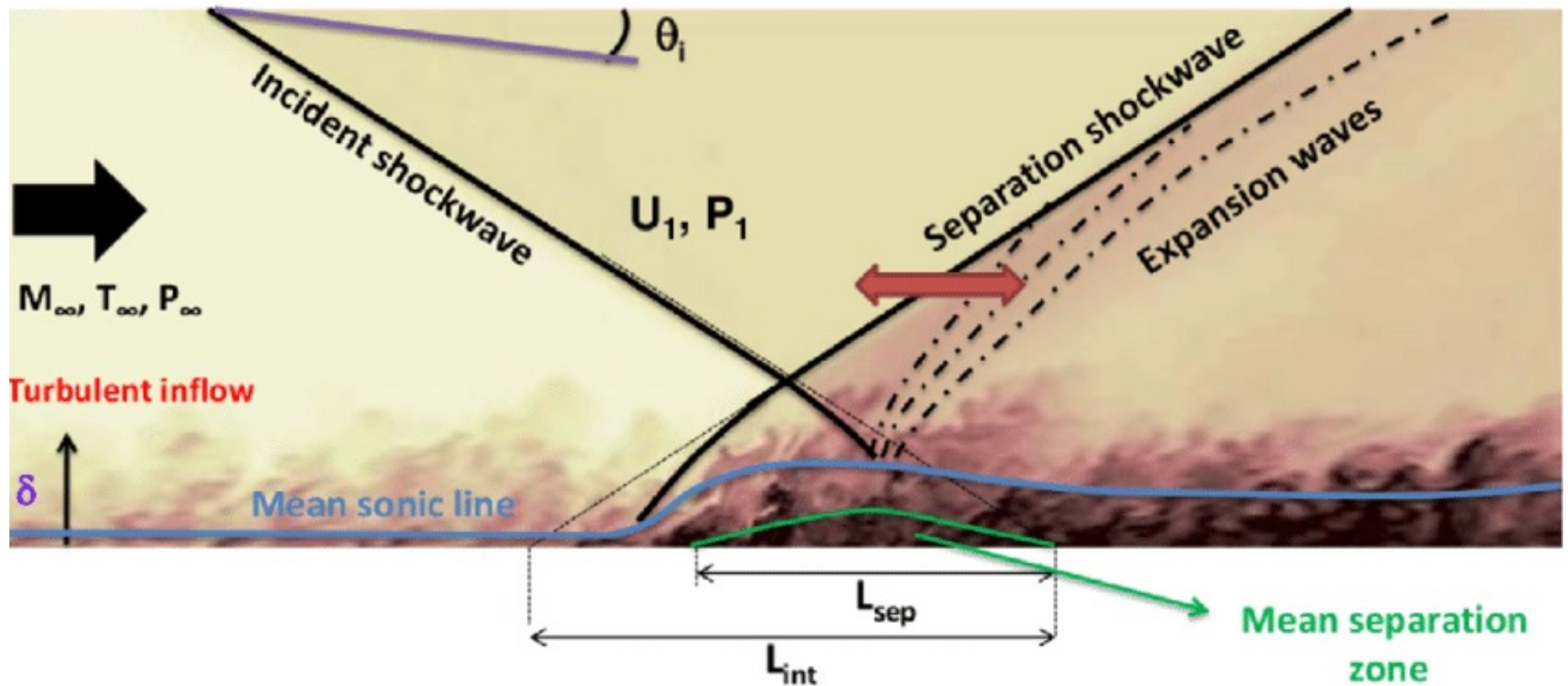


3.0e+02 300.5 301 301.5 302 302.5 303 3.0e+02
Temperature (K)

Shocks

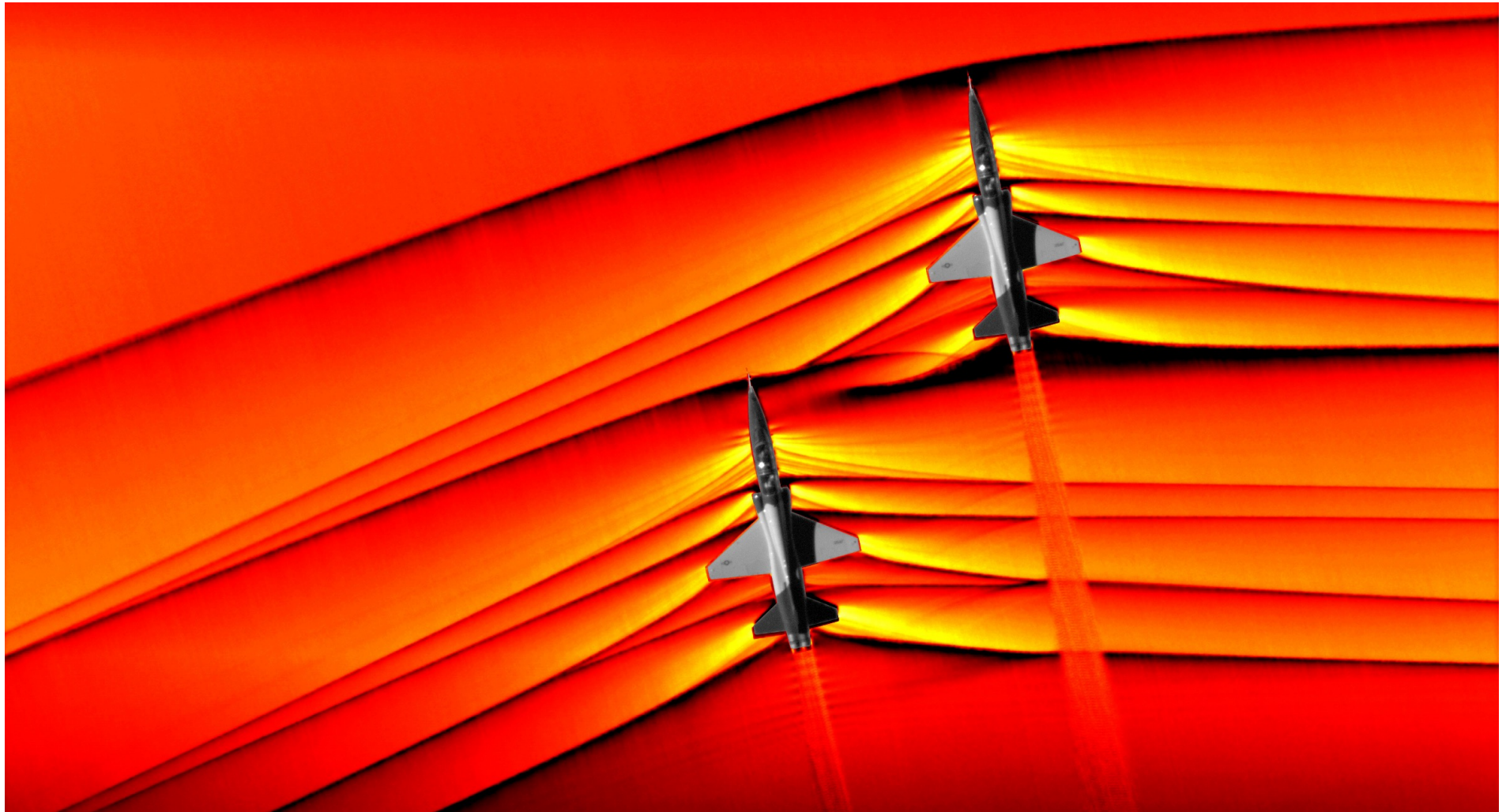
What can be described with Navier-Stokes equations?

- Shock / Boundary Layer Interaction



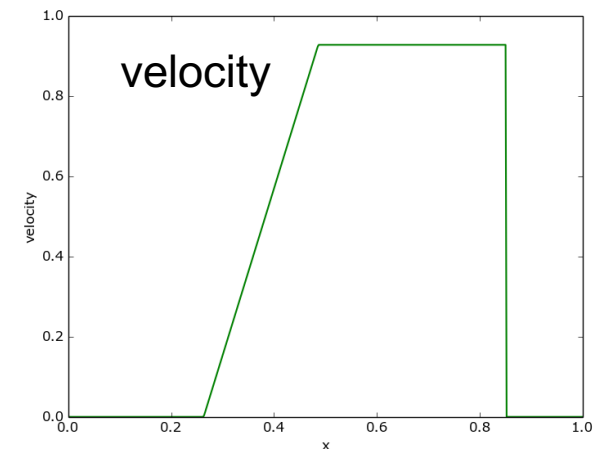
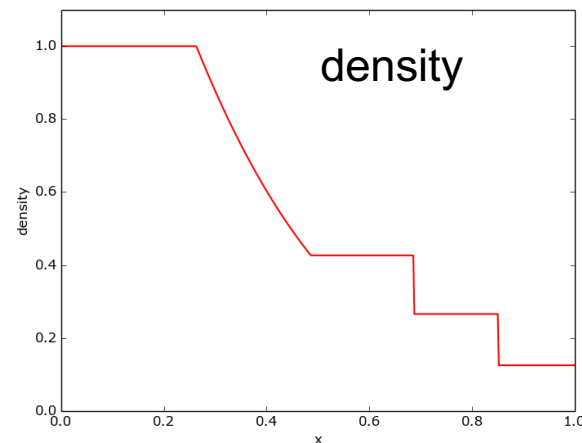
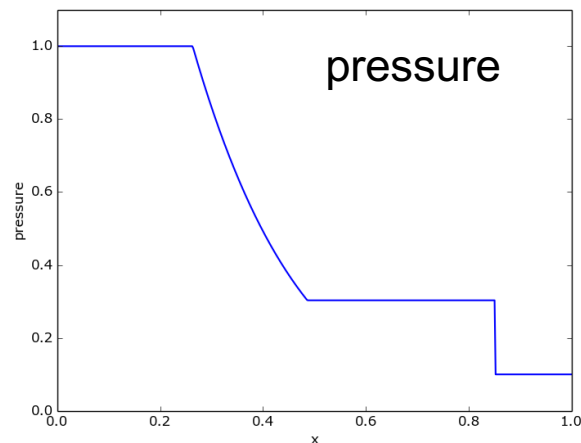
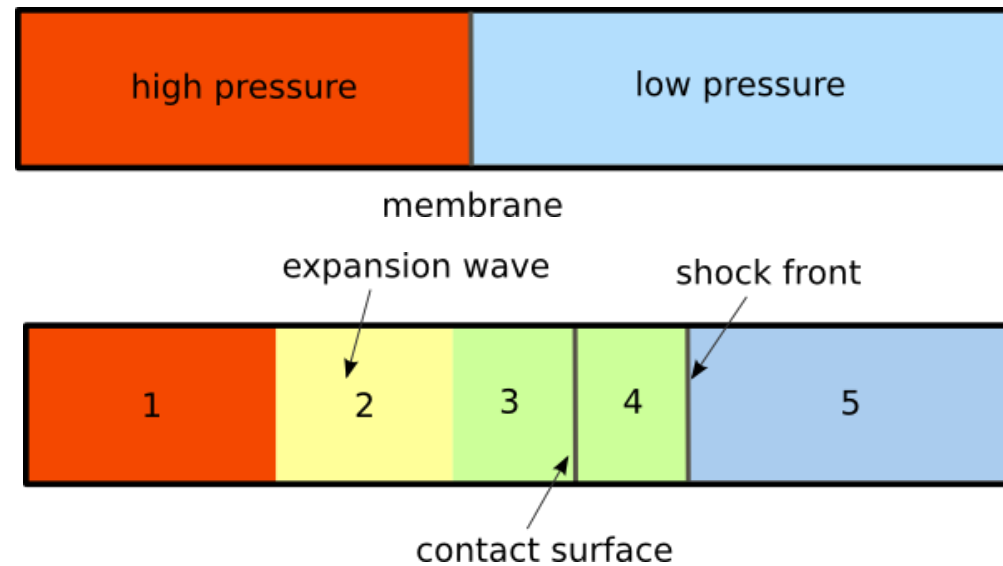
What can be described with Navier-Stokes equations?

- Shock waves around supersonic planes (NASA)



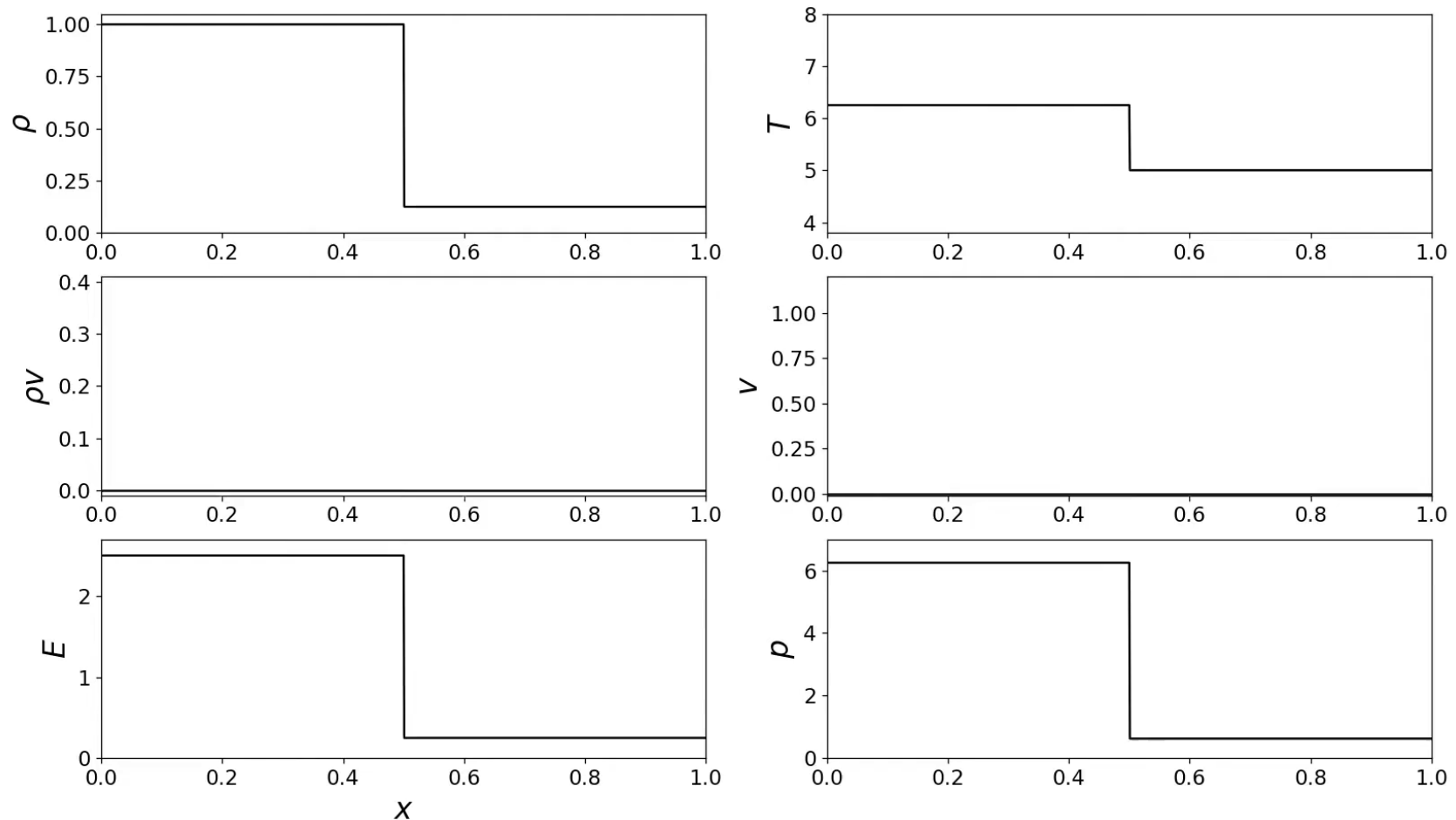
Riemann problem

- A good example: the Sod tube problem (courtesy Y. Bechane)



Riemann problem

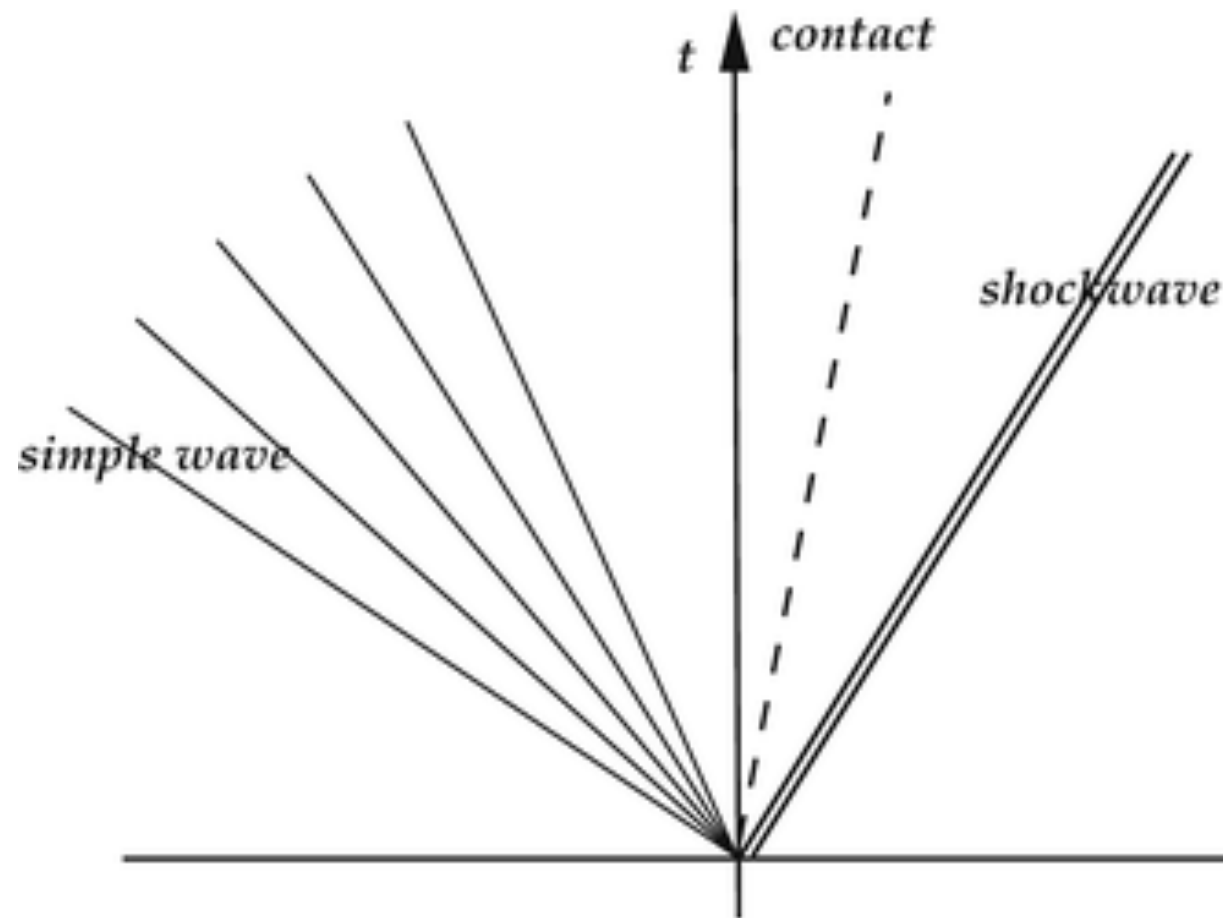
- A good example: the Sod tube problem



<https://www.youtube.com/watch?v=BYrhQ8oGT3Q>

Riemann problem

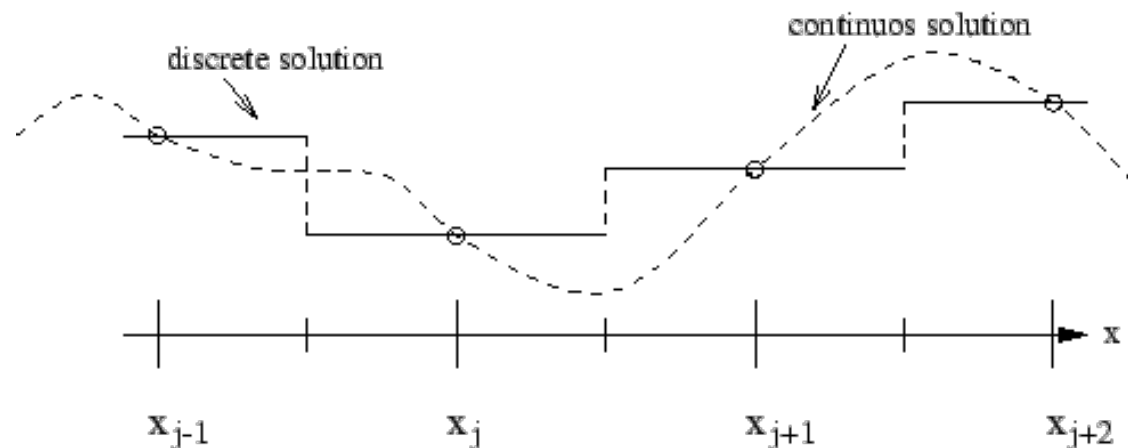
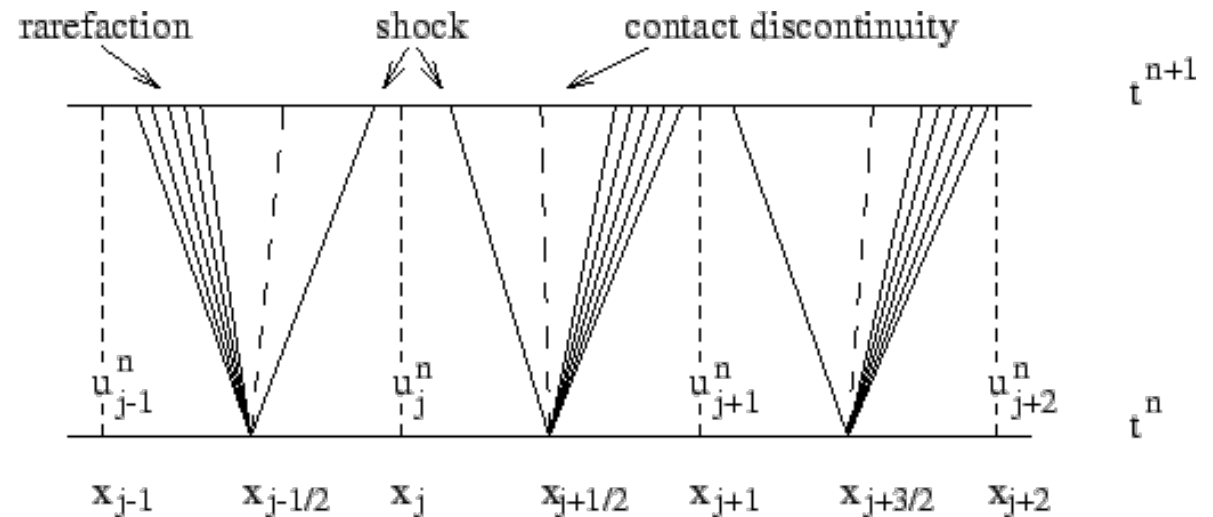
- Characteristics for the Sod tube problem



Roe P.L. (2015) Riemann Problem. In: Engquist B. (eds) Encyclopedia of Applied and Computational Mathematics. Springer, Berlin, Heidelberg.

Riemann solvers

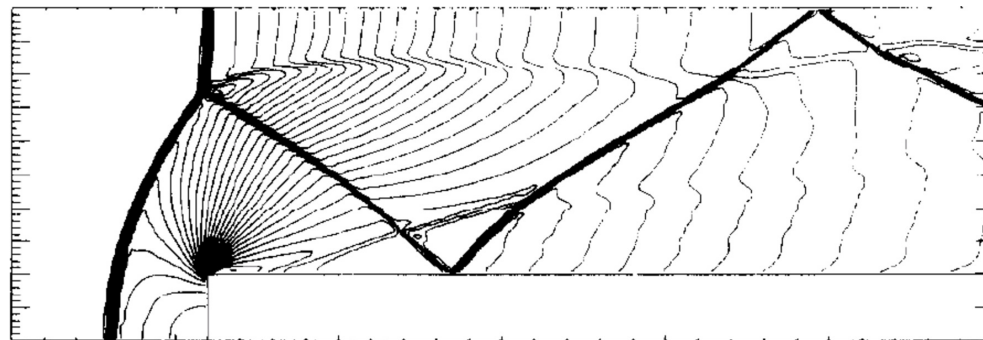
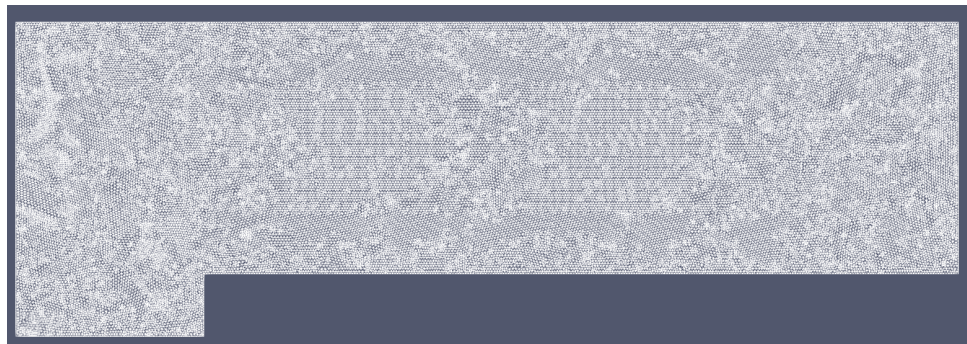
- Numerically, one can solve a Riemann problem at each interface
- Many options:
 - Godunov
 - HLL
 - HLLC
 - ...
- Enables to treat shocks and discontinuities
- Often very dissipative



Godunov's scheme: local solutions of Riemann problems

Application of Riemann solvers

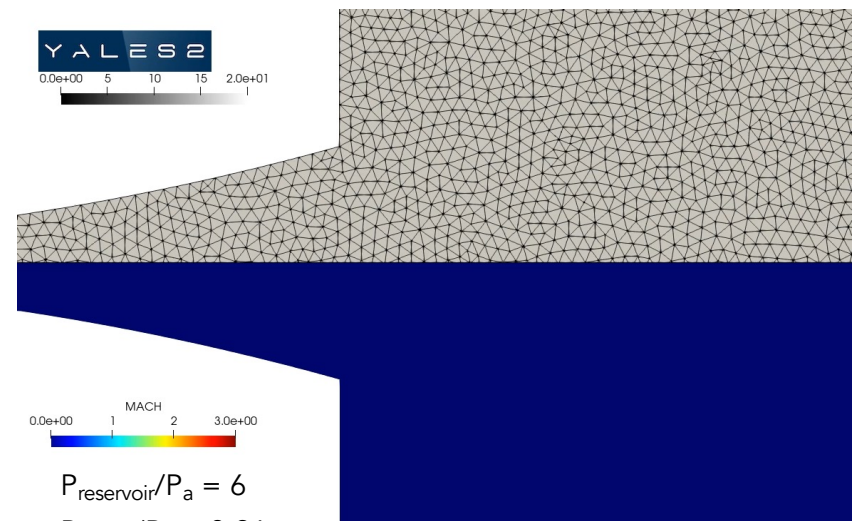
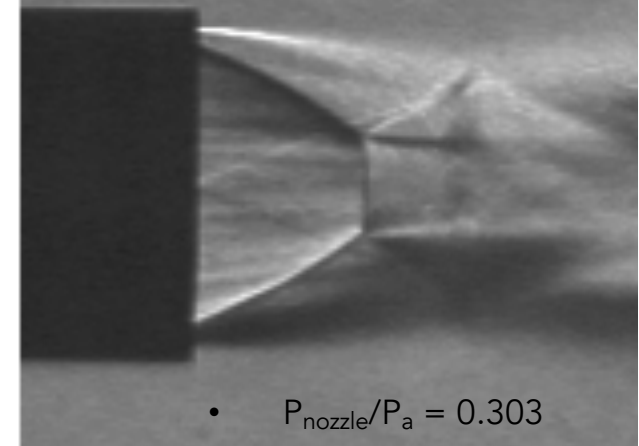
Supersonic step at Mach = 3.0



PPMLR, Woodward and Colella (JCP 1984)

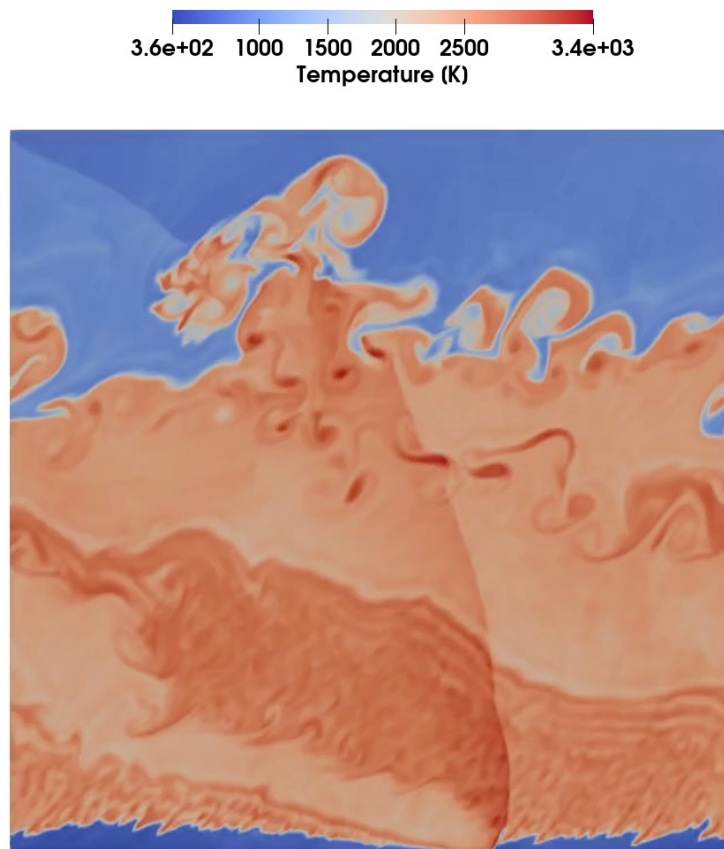
Laval nozzle

Zapryagaev et al. (report 2002)

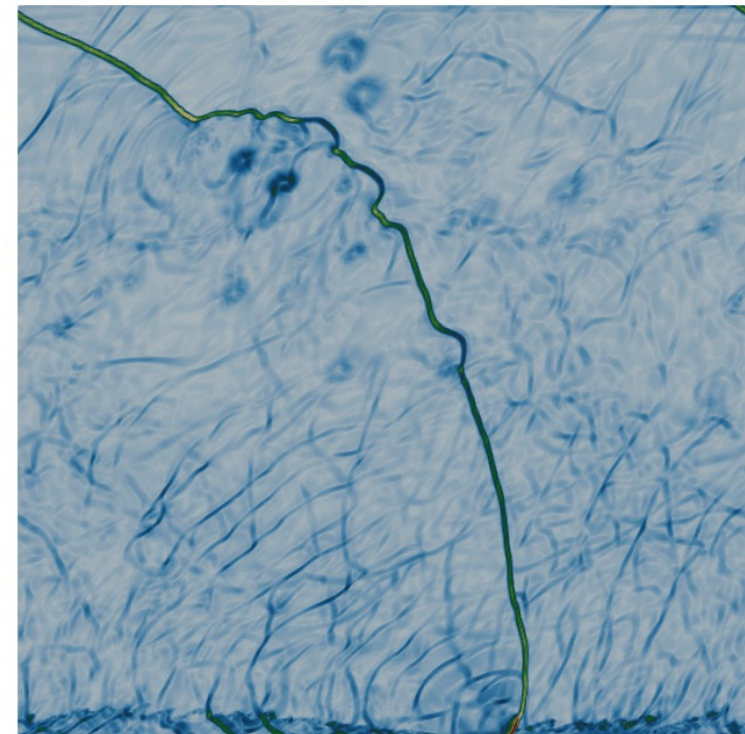


Application of Riemann solvers

2D H₂/air rotating detonation by Y. Bechane, CORIA

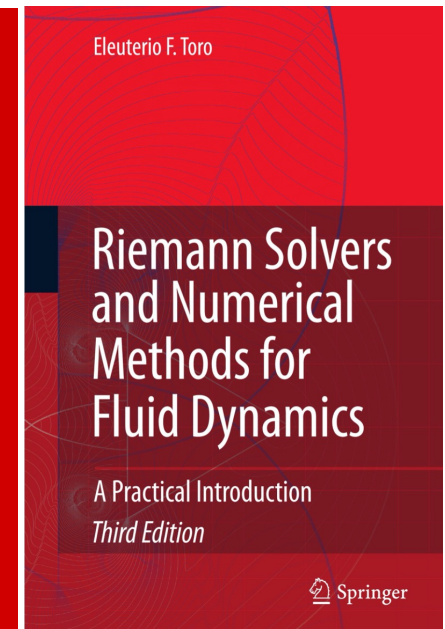
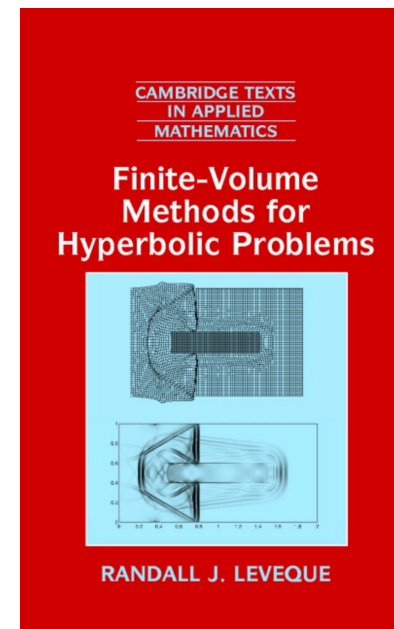


↑ H₂+air



Literature

- Useful links:
 - https://en.wikipedia.org/wiki/Riemann_problem
 - https://en.wikipedia.org/wiki/Roe_solver
 - https://en.wikipedia.org/wiki/Godunov%27s_scheme
- Books:
 - **Finite Volume Methods for Hyperbolic Problems** by Randall J. Leveque (Cambridge)
 - **Riemann Solvers and Numerical Methods for Fluid Dynamics** by Eleuterio F. Toro (Springer)
- Online Course:
 - Springel & Dullemond (Heidelberg)
http://www.ita.uni-heidelberg.de/~dullemond/lectures/num_fluid_2011/
 - François Dubois (CNAM)
<https://www.imo.universite-paris-saclay.fr/~fdubois/travaux/volumesfinis/volfi2k/dubois-volfi2k-hal-2011.pdf>



Solving **incompressible**
Navier-Stokes equations
(i.e. low-Mach number flows)

Low-Mach number asymptotics

- Reference and dimensionless variables / equations:

$$\frac{\partial \rho^*}{\partial t} + \nabla \cdot (\rho^* \mathbf{u}^*) = 0$$

$$\rho^* = \rho / \rho_\infty$$

$$\frac{\partial \rho^* \mathbf{u}^*}{\partial t} + \nabla \cdot (\rho^* \mathbf{u}^* \mathbf{u}^*) = -\frac{1}{M_\infty^2} \nabla P^*$$

$$\mathbf{u}^* = \mathbf{u} / \mathbf{u}_\infty$$

$$\frac{\partial \rho^* E^*}{\partial t} + \nabla \cdot (\rho^* E^* \mathbf{u}^*) = -\nabla \cdot (P^* \mathbf{u}^*)$$

$$E^* = E / c_\infty^2$$

$$P^* = \rho^* (\gamma - 1) \left(E^* - \frac{M_\infty^2}{2} \mathbf{u}^{*2} \right)$$

$$P^* = P / \rho_\infty c_\infty^2$$

- Perform an asymptotic development in Mach number (small parameter)

$$\rho^* = \rho_0^* + M_\infty \rho_1^* + M_\infty^2 \rho_2^* + \dots \quad E^* = E_0^* + M_\infty E_1^* + M_\infty^2 E_2^* + \dots$$

$$\mathbf{u}^* = \mathbf{u}_0^* + M_\infty \mathbf{u}_1^* + M_\infty^2 \mathbf{u}_2^* + \dots \quad P^* = P_0^* + M_\infty P_1^* + M_\infty^2 P_2^* + \dots$$

- Equations must be true at each power of Mach number!

Low-Mach number asymptotics

- Order $1/M_\infty^2$: The background pressure is constant **in space**

$$\nabla P_0 = 0$$

- Order $1/M_\infty$: no steady acoustics

$$\nabla P_1 = 0$$

- Order 1:
 - At each instant, density only depends on the local energy:

$$P_0 = \rho_0(\gamma - 1)E_0$$

- The velocity divergence is a function of the density only:

$$\nabla \cdot \mathbf{u}_0 = -\frac{1}{\rho_0} \frac{D\rho_0}{Dt}$$

- The pressure appearing in the momentum equation is **hydrodynamic**:

$$\frac{\partial \rho_0 \mathbf{u}_0}{\partial t} + \nabla \cdot (\rho_0 \mathbf{u}_0 \mathbf{u}_0) = -\nabla P_2$$

Projection of incompressible N.S. equations

- Solenoidal and irrotational parts of the velocity field are independent and can thus be solved separately.
- The projection method of Chorin (1968) is based on that decomposition.
- First, a prediction step advances the vortices.

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = 0$$

- This prediction is not exact and it introduces an (unwanted) irrotational field whose divergence is not zero.
- The correction step removes this part of the field

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} = -\frac{1}{\rho} \nabla P$$

$$\nabla \cdot \left(\frac{1}{\rho} \nabla P \right) = \frac{\nabla \cdot \mathbf{u}^*}{\Delta t}$$

Poisson Equation

- This is an **ELLIPTIC** equation
- The boundary conditions must also be taken into account...

Generalisation to variable density flows

- Pierce and Moin (2004) generalized the previous method to variable density flows (combustion...)
- Prediction

$$\frac{\rho \mathbf{u}^* - \rho \mathbf{u}^n}{\Delta t} + \nabla \cdot (\rho \mathbf{u}^{n+1/2} \mathbf{u}^{n+1/2}) = 0$$

- Correction

$$\frac{\rho \mathbf{u}^{n+1} - \rho \mathbf{u}^*}{\Delta t} = -\nabla P^{n+1/2}$$

Poisson Equation

$$\nabla \cdot \nabla P^{n+1/2} = \frac{\rho^{n+3/2} - \rho^{n+1/2}}{\Delta t^2} + \frac{1}{\Delta t} \nabla \cdot (\rho \mathbf{u}^*)$$

- The density must be provided through an Equation of State

Solving the Poisson Equation

$$\nabla \cdot \left(\frac{1}{\rho} \nabla P \right) = \frac{\nabla \cdot \mathbf{u}^*}{\Delta t}$$

- The Poisson equation is elliptic: very hard to solve...

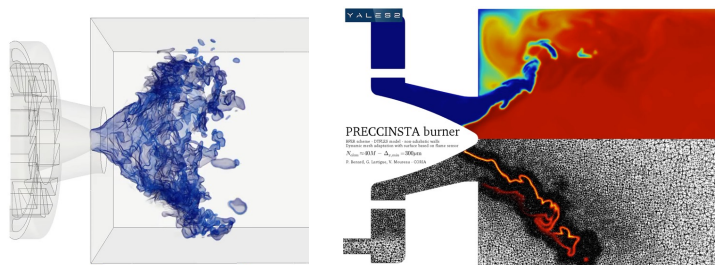
$$\frac{1}{\rho} \begin{pmatrix} \ddots & & & & \\ & \ddots & & & \\ & & 0 & 0 & 0 \\ & & \ddots & 0 & 0 \\ 0 & 1/\Delta x^2 & -2/\Delta x^2 & 1/\Delta x^2 & 0 \\ & 0 & 0 & \ddots & \ddots \\ & 0 & 0 & 0 & \ddots & \ddots \end{pmatrix} \begin{pmatrix} P_i \end{pmatrix} = \begin{pmatrix} \frac{\nabla \cdot \mathbf{u}^*}{\Delta t} \Big|_i \end{pmatrix}$$

- The A matrix is symmetric with non-dominant diagonal.
- Specific linear solvers must be used (PCG, MG, DPCG, ...)

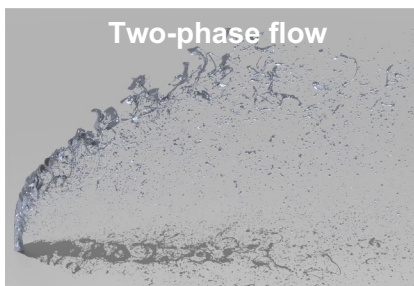
The YALES2 project

A multi-physics & High-Fidelity platform for complex flows

Gaseous combustion



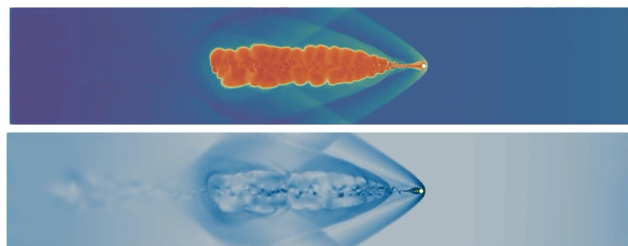
Two-phase flow



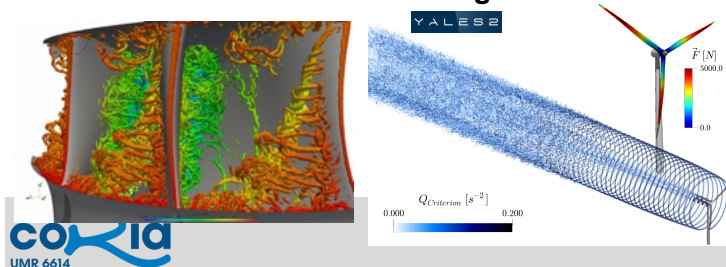
Spray combustion



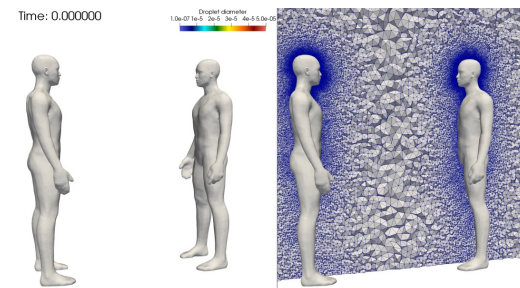
Safety



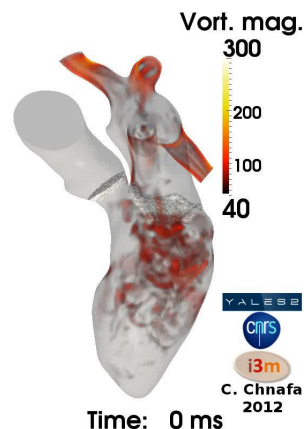
Renewable energies



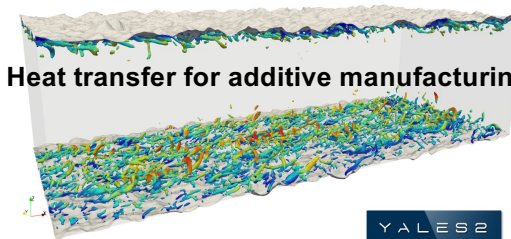
Aerosol dispersion



Bio-mechanics



Heat transfer for additive manufacturing



Sloshing in tanks



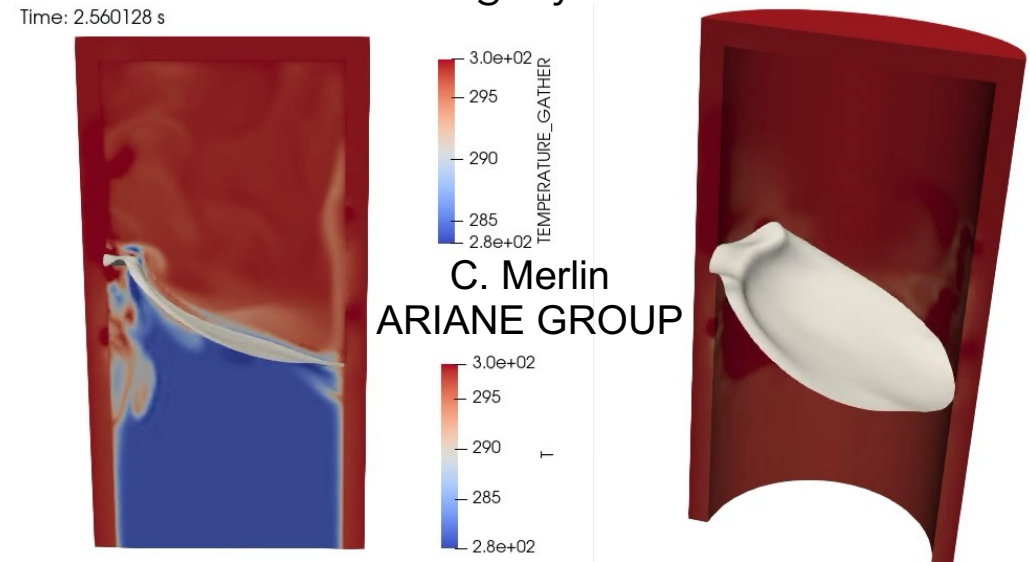
- Developed by CORIA, the French Combustion Community and others
- 600+ researchers/engineers trained at CORIA since 2009
- 300+ articles (Google Scholar)

Context: HiFi CFD in aeronautical and aerospace industry

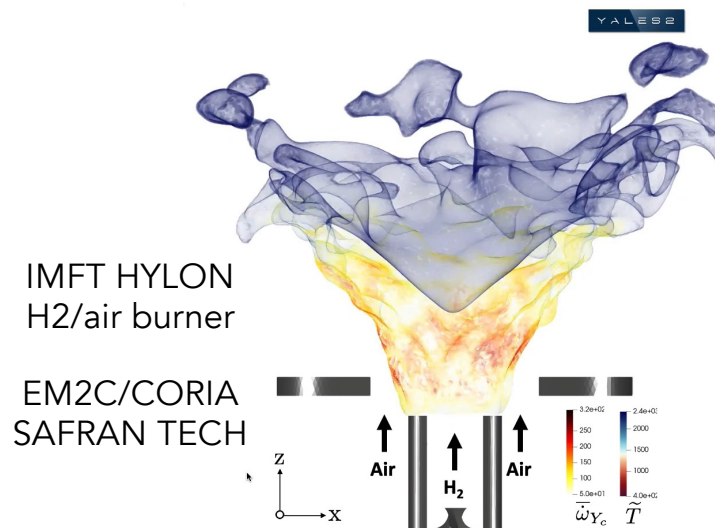
Pressure swirl atomizer



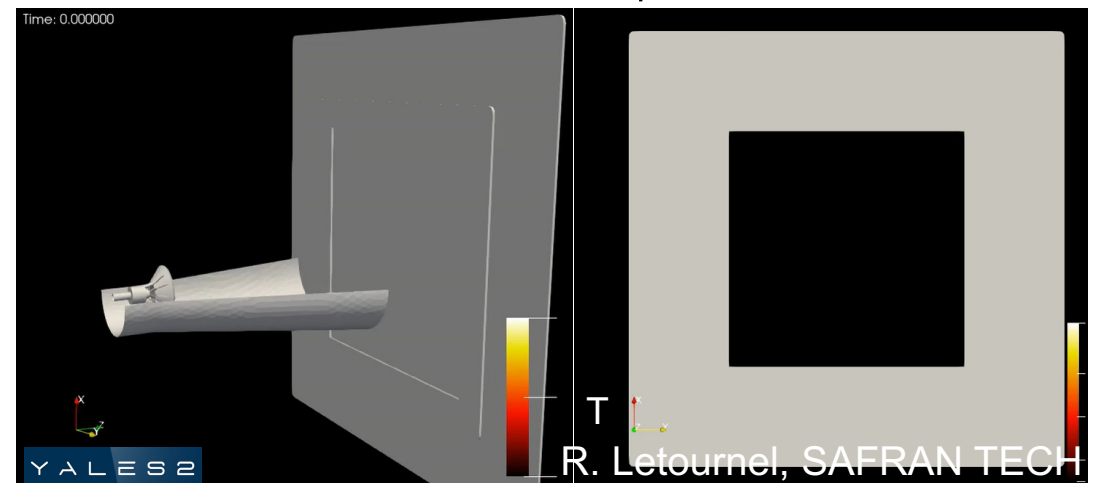
Sloshing cryo-tanks



H2 combustion



Fire resistance of composite materials



The YALES2 objectives

- 1) **Fast, agile and open** development for **innovation**
- 2) **High-performance computing** for **multi-physics & multi-scale** problems
- 3) **Large documentation** resources and **test cases** for minimal training.
Everyone can contribute !
- 4) **Fast industrialization** even for 10'000+ core simulations

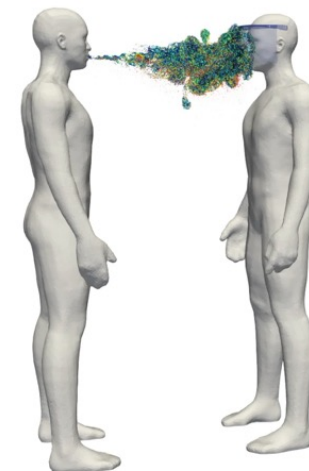


As fast as possible

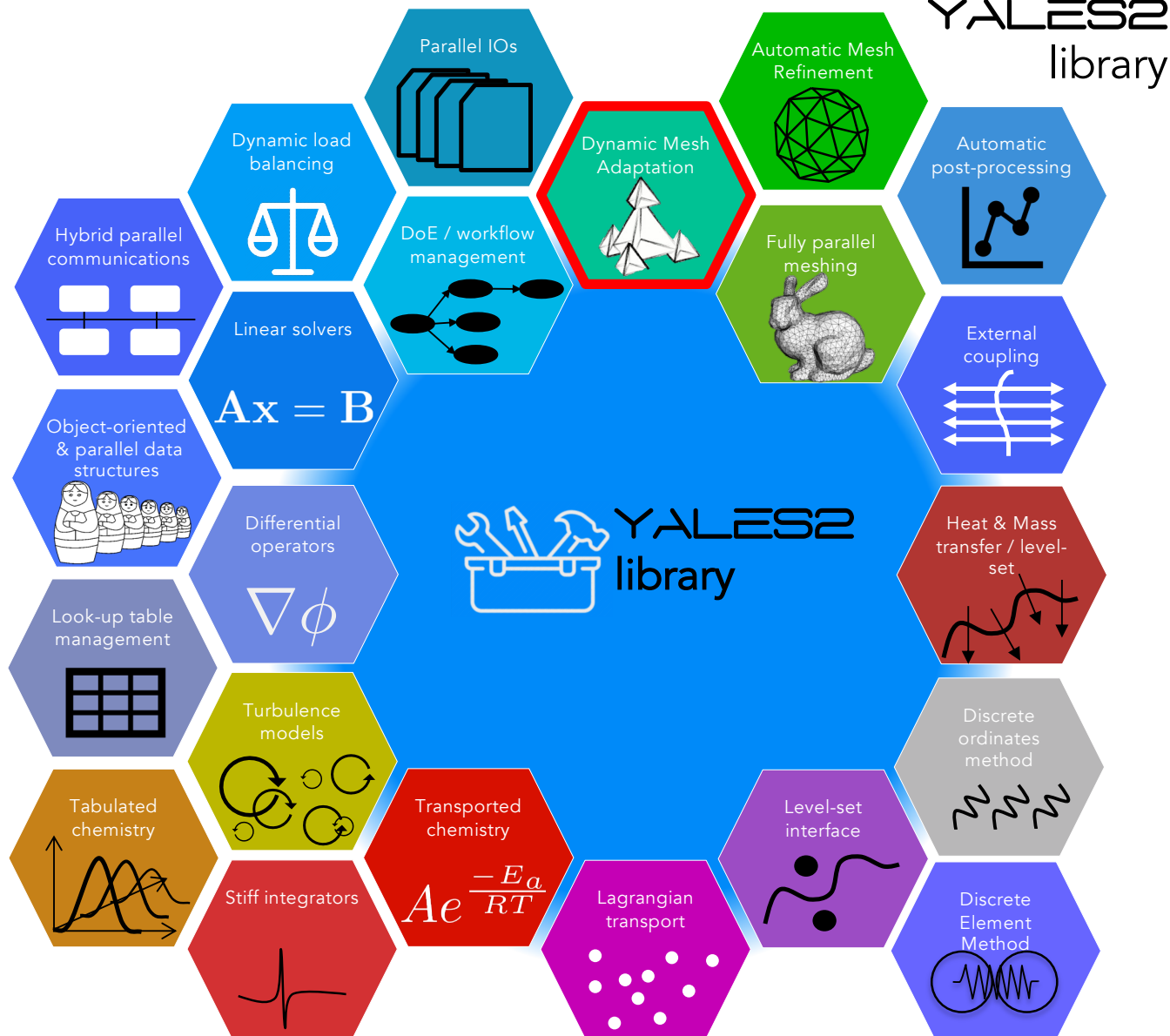


ime: 0.400098

Droplet diameter
1.0e-07 1e-5 2e-5 3e-5 4e-5 5.0e-05



A modular CFD platform



YALES2 45 solvers



ICS

Incompressible at constant density



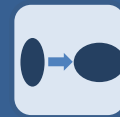
VDS

Incompressible at variable density



SPS

Spray with level-set and ghost-fluid method



ALE

Arbitrary Lagrangian Eulerian



MFS

Explicit compressible Multifluid method



ECS

Explicit compressible with shock capturing



HTS

Heat transfer



MHD

Magneto-hydro-dyn



SMS+FSI

Structural mech.



ACS

Acoustics



YALES2

features



High fidelity



Multiphysics



High performance

CORIA commitments to the YALES2 community

Training

- General training sessions: 3-4/year
- Two-phase flow training sessions: 1x/year
 - Tutorials: many/year
- Integrated in the INSA of Rouen curriculum
- 700 people trained
- 25% from industry

Events & dissemination

- Extreme CFD workshop: 1x/year
- YACKATHON: 2x/year
- Participation to HPC projects: CVT GENCI and H2020 CoEC



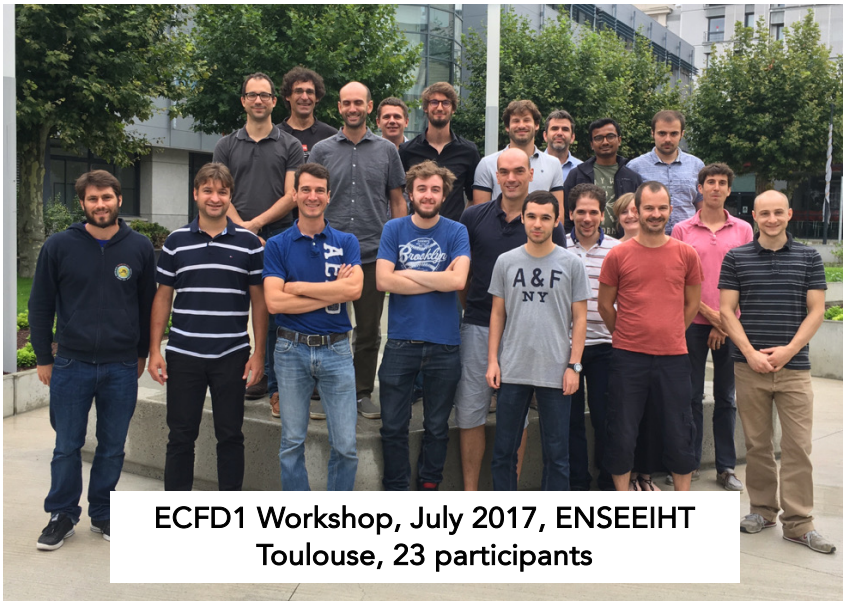
Support

- YALES2 users meetings: 2x/year
- Management of yales2.coria-cfd.fr: gitlab + centralized documentation
 - Dedicated contracts with industrial partners
- Support for submission of EuroHPC projects

Training: more than 700 persons trained since 2009



The Extreme CFD workshop



ECFD1 Workshop, July 2017, ENSEEIHT
Toulouse, 23 participants



Extreme CFD workshop & hackathon GENCI
Du 26 au 31 Janvier 2020
Au Centre Escandille, à Autrans, en France



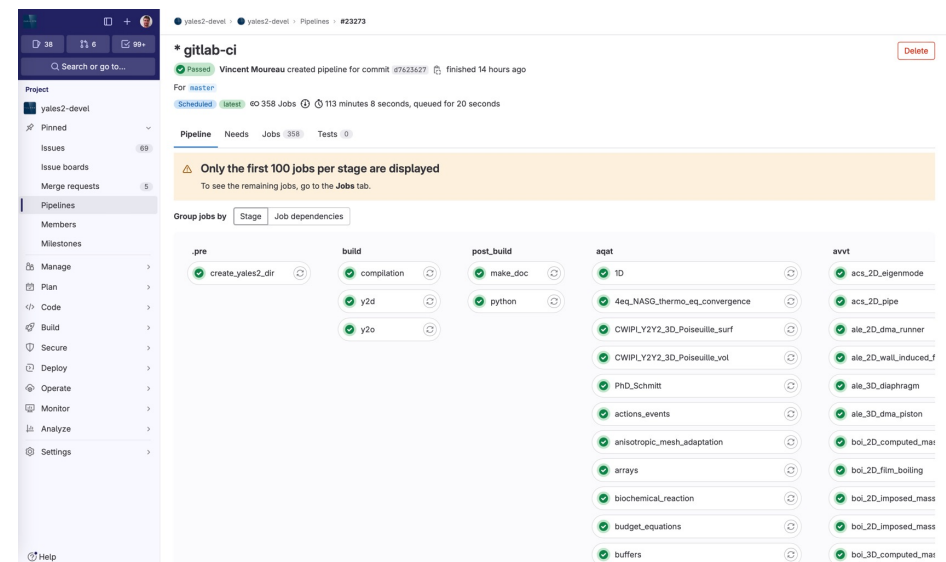
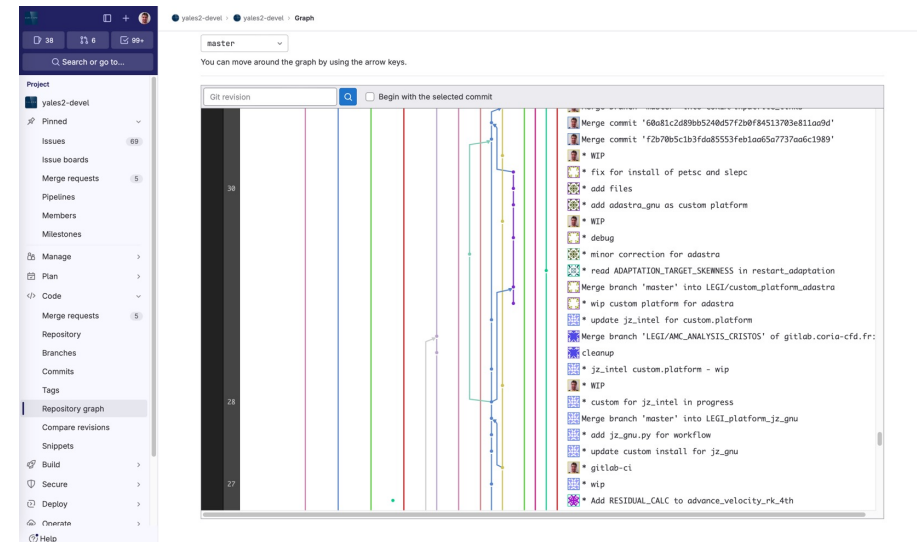
Thanks to Christophe and all the admin staff !



Support & agile development: coria-cfd.fr

- Dedicated forge since 2010
 - gitlab.coria-cfd.fr
 - mattermost.coria-cfd.fr
 - y2training.coria.fr
 - yales2.coria-cfd.fr & sphinx
 - Available from Irene, Topaze, Adastra, ...
 - Full access to the community
- Key figures for YALES2
 - 20 major releases
 - **1.2M object-oriented F2008 lines**
 - 30 000+ commits
 - **15+ commits per day**
 - 300+ active branches
 - 2 000+ merge requests
 - 120+ contributors
 - 600+ project members

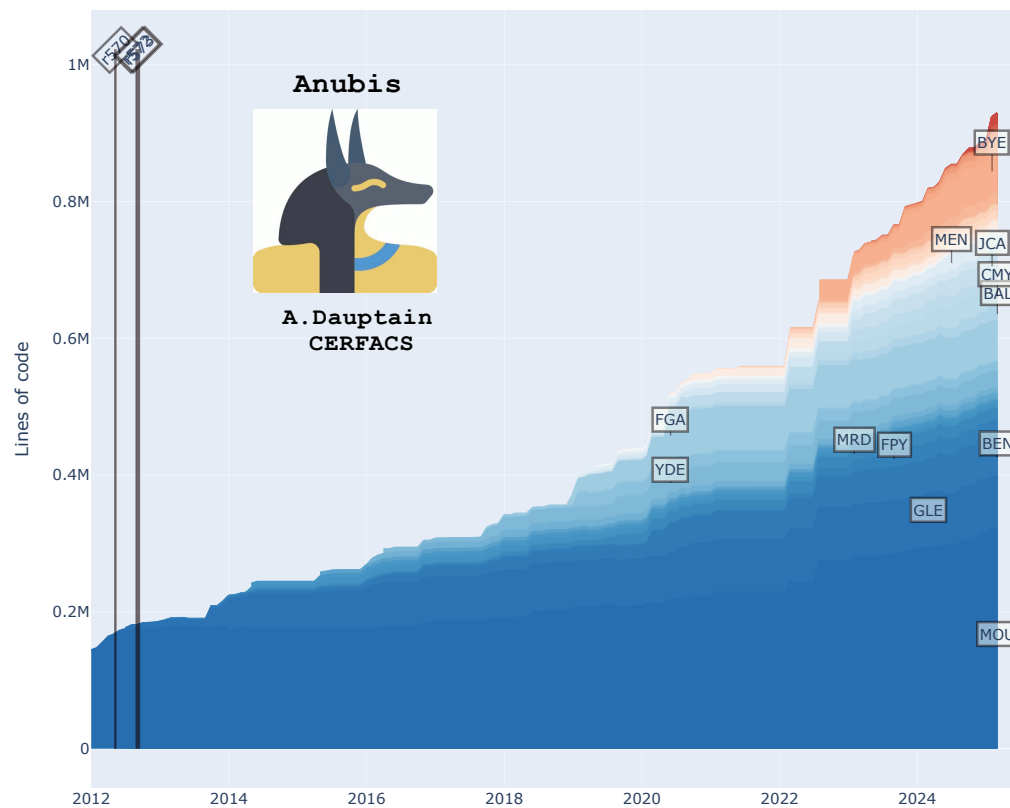
Thanks to Alexandre, Ghislain & Jérôme !



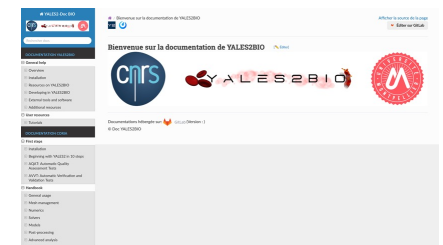
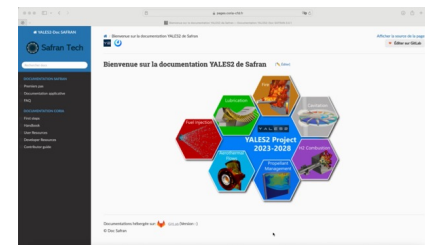
Development dynamics in the community

- **YALES2** Moore's law: the number of commits doubles every 2 years

	2022.10 vs 2023.10	2023.10 vs 2024.10	2024.10 vs 2025.10
Commits	2 725	3 633	5 073
Modified lines	291 513	323 326	412 398
Contributors	37	40	50



Strongly helped by the involvement of all labs



The YALES2 solvers



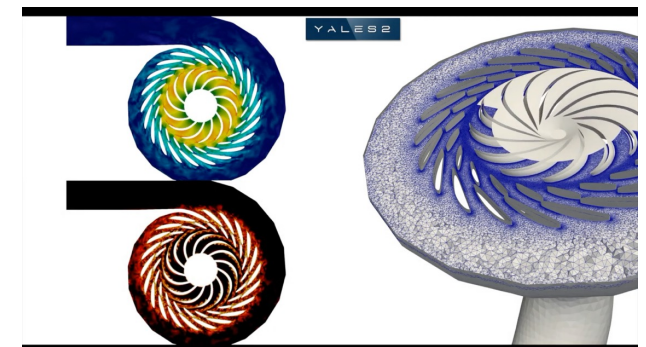
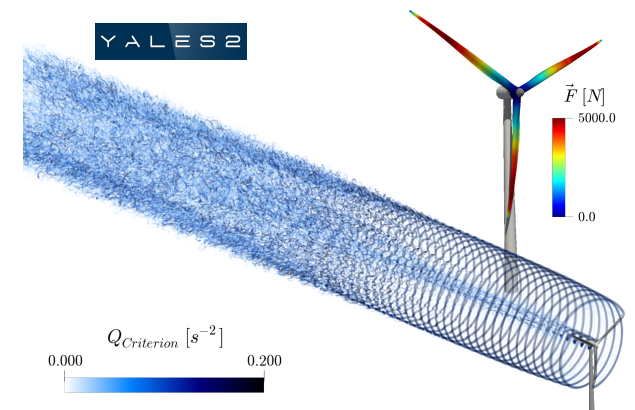
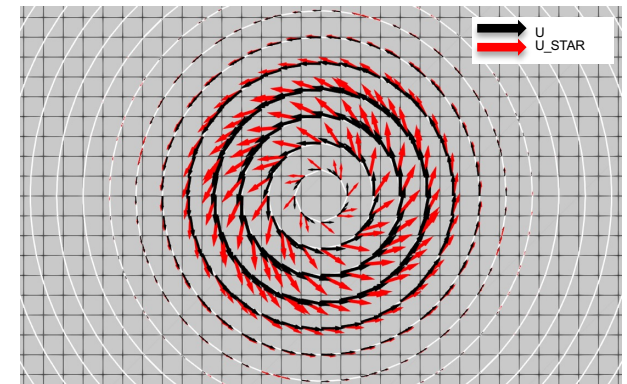
- Low-Mach projection method (Chorin)
- Prediction

$$\frac{\mathbf{u}^* - \mathbf{u}^n}{\Delta t} + \nabla \cdot \mathbf{u}\mathbf{u} = \nabla \cdot \boldsymbol{\tau}$$

- Correction

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} = -\frac{1}{\rho} \nabla P \quad \nabla \cdot \left(\frac{1}{\rho} \nabla P \right) = \frac{\nabla \cdot \mathbf{u}^*}{\Delta t}$$

- Explicit or implicit time advancement
 - TFV4A, RK, BDF, ...
- Highly-efficient linear solvers
 - DPCG, PCG, GMRES, ...
- Lagrangian point particle model
- Scalar transport
- Turbulence models
 - LES: Dynamic Smagorinsky, WALE, SIGMA
 - RANS & U-RANS: k-epsilon, k-omega
 - PANS





- Mass conservation:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} = \bar{S}_\rho$$

- Momentum conservation:

$$\frac{\partial \bar{\rho} \tilde{u}_j}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_i} = -\frac{\partial \bar{P}}{\partial x_j} + \frac{\partial \bar{\tau}_{ij}}{\partial x_i} + \frac{\partial \bar{\tau}_{SGS}}{\partial x_i} + \bar{\rho} \tilde{f}_i$$

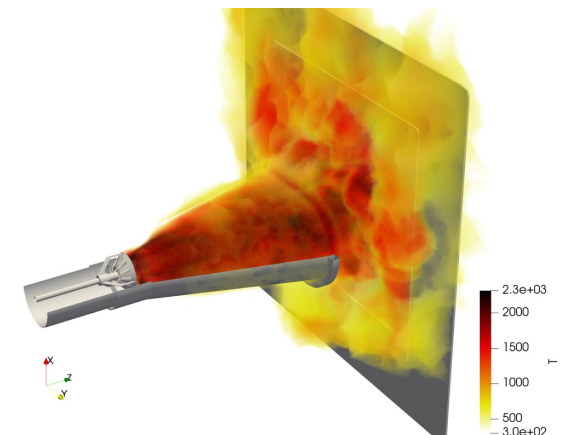
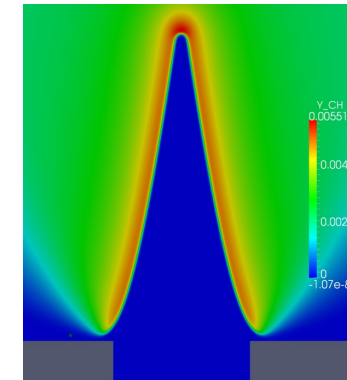
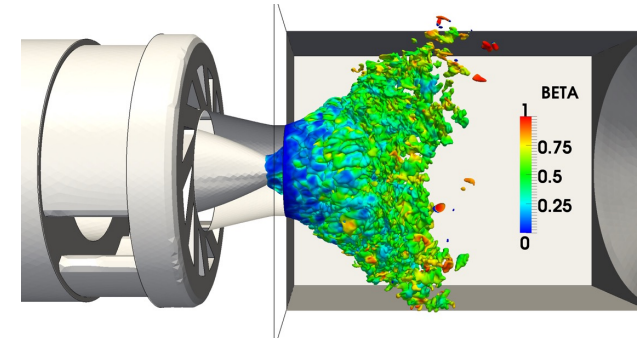
- Sensible enthalpy conservation (finite-rate chemistry)

$$\frac{\partial \bar{\rho} \tilde{h}_s}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{h}_s}{\partial x_i} = -\frac{\partial \bar{Q}'_i}{\partial x_i} + \frac{D\bar{P}}{Dt} + \frac{\partial}{\partial x_i} (-\bar{\rho} \tilde{V}_h \tilde{h}_s) + \bar{\omega}_T + \bar{S}_{h_s}$$

- Low-Mach projection method
- Lagrangian point particle model
- Combustion models

- Finite-rate chemistry: TFLES, VOM
- Tabulated chemistry: PCM-FPI, FTACLES, TFLES-FPI

[1] P. Bénard et al. – 2015
[2] L. Boulet - 2018



■ Radiative Transfer Equation in spectral space:

$$\frac{dI_\nu(\mathbf{r}, \mathbf{s})}{ds} = \underbrace{-\kappa_\nu(\mathbf{r})I_\nu(\mathbf{r}, \mathbf{s})}_{\text{Absorption}} + \underbrace{\kappa_\nu(\mathbf{r})I_{b,\nu}(\mathbf{r})}_{\text{Emission}}$$

■ Full spectrum SNB Correlated-k (FS-SNB-Ck)

- Includes CO₂, H₂O, CO & CH₄ species
- 7-point quadrature method Gauss-Lobato

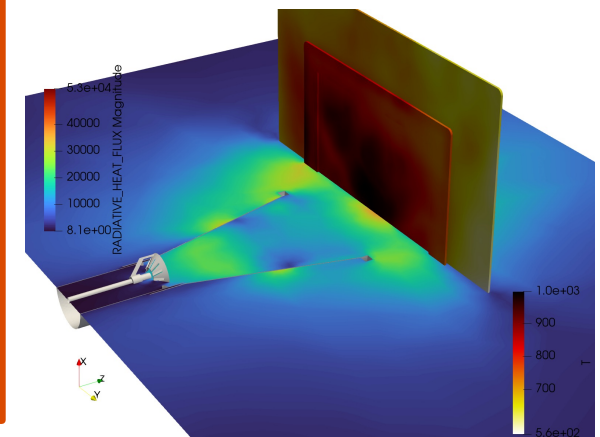
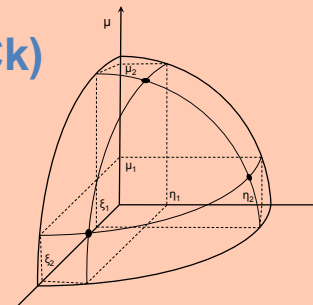
■ Discrete Order Method

- Spatial resolution relies on angular quadrature
- 3D-S4 quadrature with 24 angular points

■ High performance

- Domain decomposition
- BICGStab(2) linear solver

- [1] Goody (1989). J. Quant. Spectro. & Radiative Transfer
 [2] Lacis & Oinas (1991). J. Geophysical Research
 [3] Liu (2000). Int. J. Heat Mass Transfer
 [4] Rivière & Soufiani (2012). Int. J. Heat Mass Transfer





- Heat transfer in the solid
 - Solving of the unsteady heat equation with an implicit FV method

- Thermal conduction equation

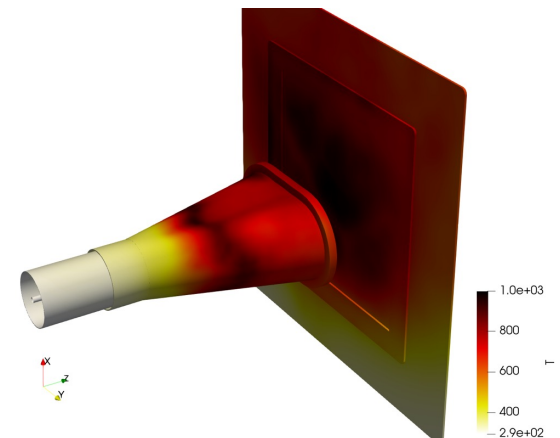
$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\lambda \nabla T) \rightarrow \frac{\partial T}{\partial t} = \nabla \cdot (D_{th} \nabla T)$$

- Discretization with Cranck-Nicolson scheme

Fourier number : $\Delta t = \frac{Fo \Delta x^2}{D_{th}}$

- Wall treatment

Dirichlet , Neumann, Robin conditions



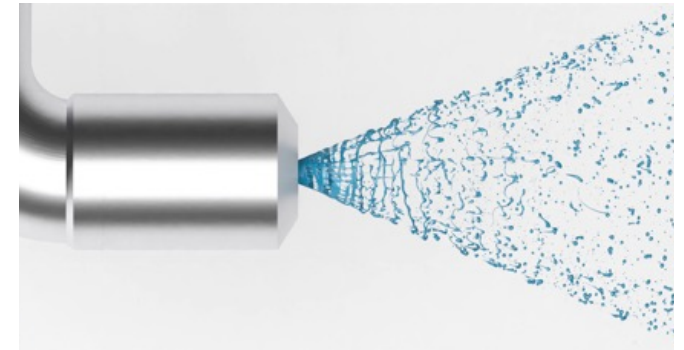
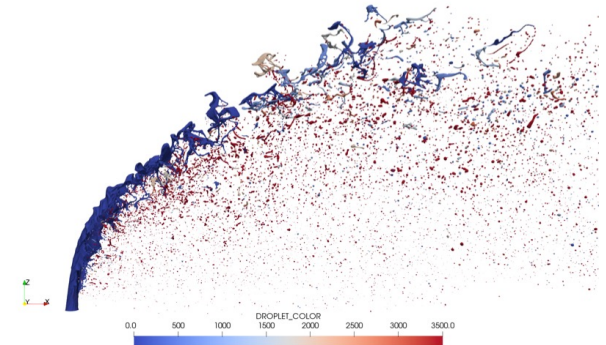


- **Low-Mach projection method from ICS**

$$\frac{\partial u}{\partial t} + \nabla \cdot (uu) = -\frac{1}{\rho} \nabla P + \frac{1}{\rho} \nabla \cdot \tau$$

$$[P]_{\Gamma} = \sigma \kappa + 2[\mu]_{\Gamma} n^t \cdot \nabla u \cdot n$$

- **Interface capturing**
 - Accurate Conservative Level Set
 - Algebraic VOF (under development)
- **Surface tension models**
 - Ghost-Fluid Method (GFM)
 - Continuum Surface Force (CSF)
- **Coupling with Lagrangian point force model**
- **Dedicated mesh adaptation algorithms**
- **Static/dynamic contact angles**



Phase Change Solver - PCS

- Based on spray solver (SPS)

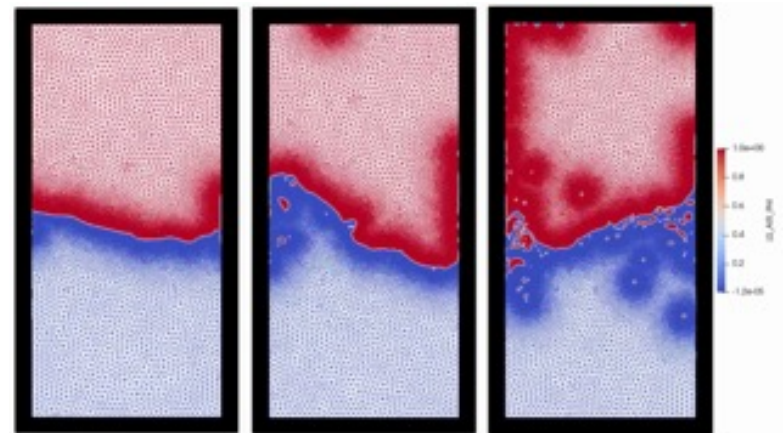
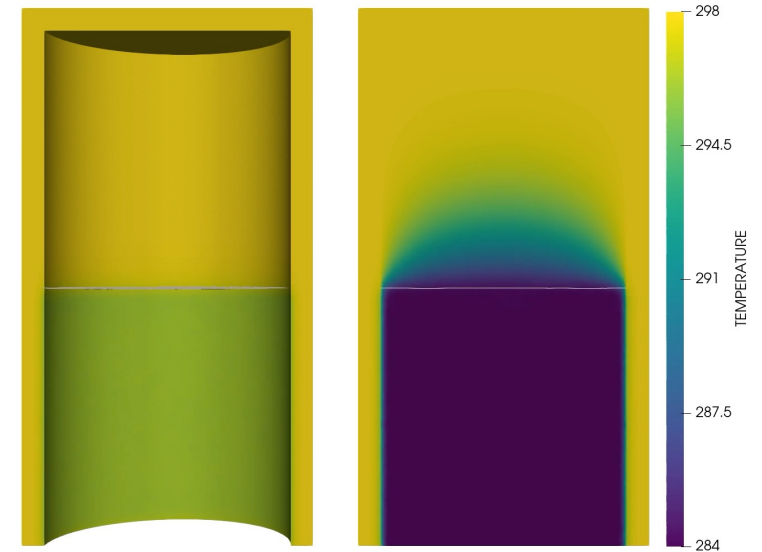
- Interface capturing
 - ACLS

- Two-fluid transport

$$\frac{\partial \bar{\rho}_l \bar{\phi}_l \tilde{H}_l}{\partial t} + \nabla \cdot (\bar{\rho}_l \tilde{u} \bar{\phi}_l \tilde{H}_l) = \nabla \cdot (\lambda_l \bar{\phi}_l \nabla T_l) - \lambda_l \nabla T_l \cdot \nabla \bar{\phi}_l + \dot{m}_{cond} \tilde{H}_l(T_{sat}) \vec{n}_l \cdot \nabla \bar{\phi}_l$$

$$\frac{\partial \bar{\rho}_g \bar{\phi}_g \tilde{H}_g}{\partial t} + \nabla \cdot (\bar{\rho}_g \tilde{u} \bar{\phi}_g \tilde{H}_g) = \nabla \cdot (\lambda_g \bar{\phi}_g \nabla T_g) - \lambda_g \nabla T_g \cdot \nabla \bar{\phi}_g - \dot{m}_{cond} \tilde{H}_g(T_{sat}) \vec{n}_g \cdot \nabla \bar{\phi}_g$$

- Phase change models
- Thermodynamics
 - NASA
 - NIST tables





- **Mass/momentum/energy conservation**

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho Y_k \vec{u}) = S_k$$
$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u} + P \vec{I}) = S_m$$
$$\frac{\partial \rho E}{\partial t} + \nabla \cdot ((\rho E + P) \vec{u}) = S_e + S_{e_c}$$

- **High-order schemes**

- TFV2A, TFV4A, 4th-order V4

- **Shock capturing schemes**

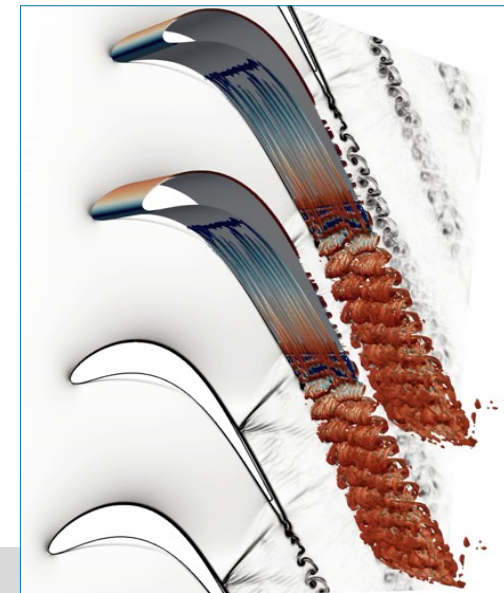
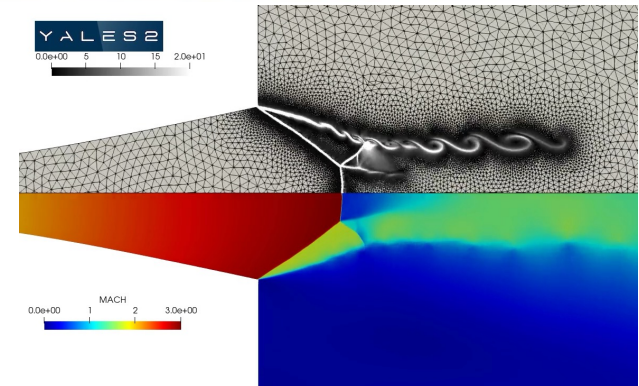
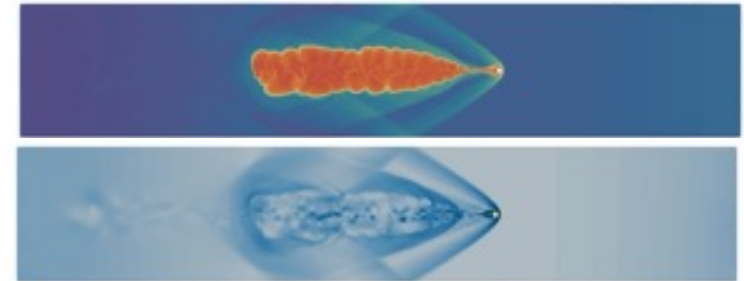
- Time integration: RK, HLLC, SLAU, SLAU2
- Space integration: 4TH, 2nd-order MUSCL
- V4 gradient reconstruction [Dervieux et al.]

- **Combustion models from VDS**

- Tabulated chemistry models (with TTC)
- Finite-rate chemistry models

- **Pressure gradient scaling for low-Mach number**

- **Coupled to ALE**



4-equation model

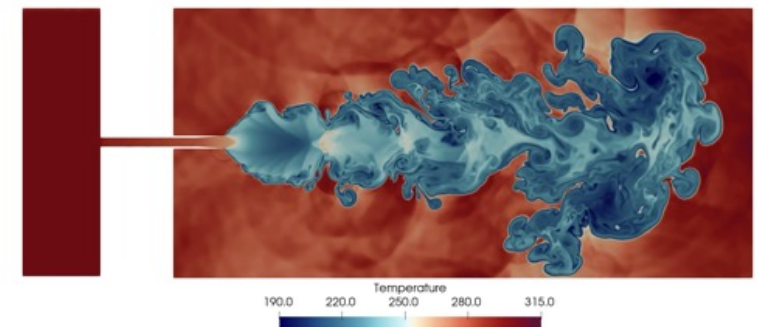
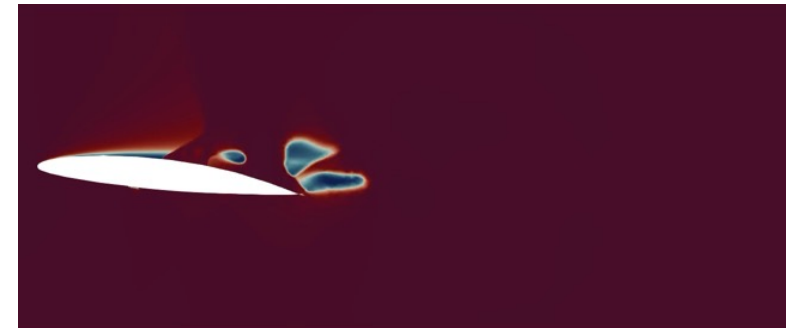
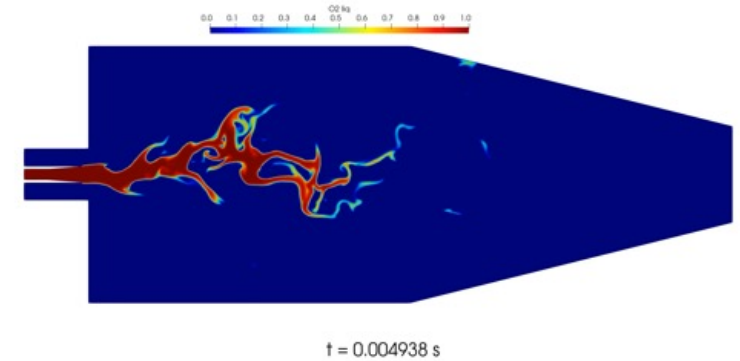
$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u} + P \vec{I}) = 0$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot ((\rho E + P) \vec{u}) = 0$$

$$\frac{\partial \rho Y_{k,l}}{\partial t} + \nabla \cdot (\rho Y_{k,l} \vec{u}) = 0$$

$$\frac{\partial \rho Y_{k,g}}{\partial t} + \nabla \cdot (\rho Y_{k,g} \vec{u}) = 0$$

- Exact thermodynamic equilibrium
- NASG equation-of-state
- ECS time integrations + Pressure gradient scaling
- Coupled to ALE



- DEM/CFD model
- Gas phase

$$\frac{\partial}{\partial t} (\varepsilon \bar{\rho}) + \nabla \cdot (\varepsilon \bar{\rho} \tilde{\mathbf{u}}) = 0$$

$$\frac{\partial}{\partial t} (\varepsilon \bar{\rho} \tilde{\mathbf{u}}) + \nabla \cdot (\varepsilon \bar{\rho} \tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}) = -\nabla \bar{P} + \nabla \cdot (\varepsilon \bar{\tau}) + \varepsilon \bar{\rho} \mathbf{g} + \bar{\mathbf{F}}_{p \rightarrow f}$$

$$\frac{\partial}{\partial t} (\varepsilon \bar{\rho} \tilde{h}_s) + \nabla \cdot (\varepsilon \bar{\rho} \tilde{\mathbf{u}} \tilde{h}_s) = \nabla \cdot \left(\frac{\mu_t}{Pr_t} \nabla \tilde{h}_s \right) + \frac{dP_0}{dt} + \nabla \cdot (\varepsilon \lambda \nabla \tilde{T}) + \varepsilon \bar{\omega}_T + \bar{Q}_{p \rightarrow f}$$

$$\frac{\partial}{\partial t} (\varepsilon \bar{\rho} \tilde{Y}_k) + \nabla \cdot (\varepsilon \bar{\rho} \tilde{\mathbf{u}} \tilde{Y}_k) = \nabla \cdot \left(\frac{\mu_t}{Sc_{k,t}} \nabla \tilde{Y}_k \right) + \nabla \cdot (\varepsilon \bar{\rho} D_k \nabla \tilde{Y}_k) + \varepsilon \bar{\omega}_k$$

- 4-way coupling for particles

$$m_p \frac{d\mathbf{u}_p}{dt} = \mathbf{F}_D + \mathbf{F}_G + \mathbf{F}_C$$

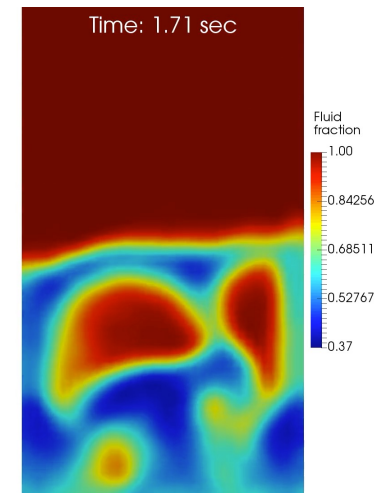
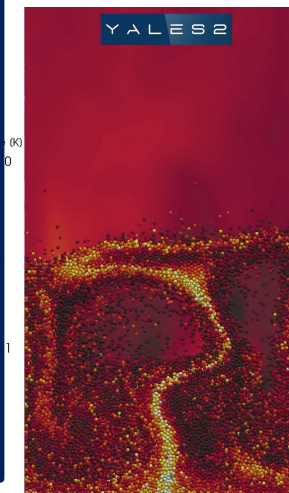
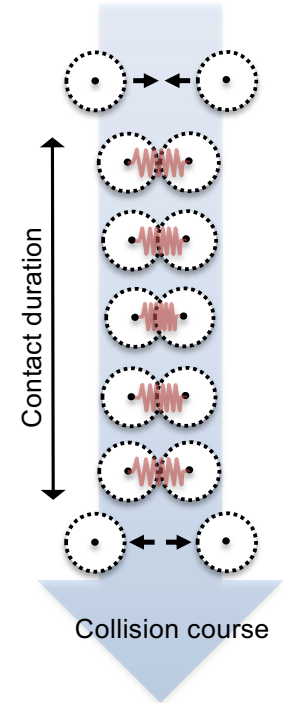
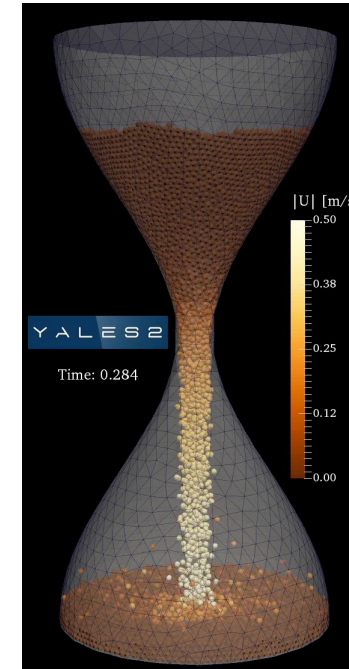
Newton's second law

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p$$

$$I_p \frac{d\boldsymbol{\omega}_p}{dt} = \mathcal{M}_C + \mathcal{M}_D + \mathcal{M}_R$$

Heat transfer : $m_p C_{p_p} \frac{dT_p}{dt} = Q$

- Soft sphere model for collisions

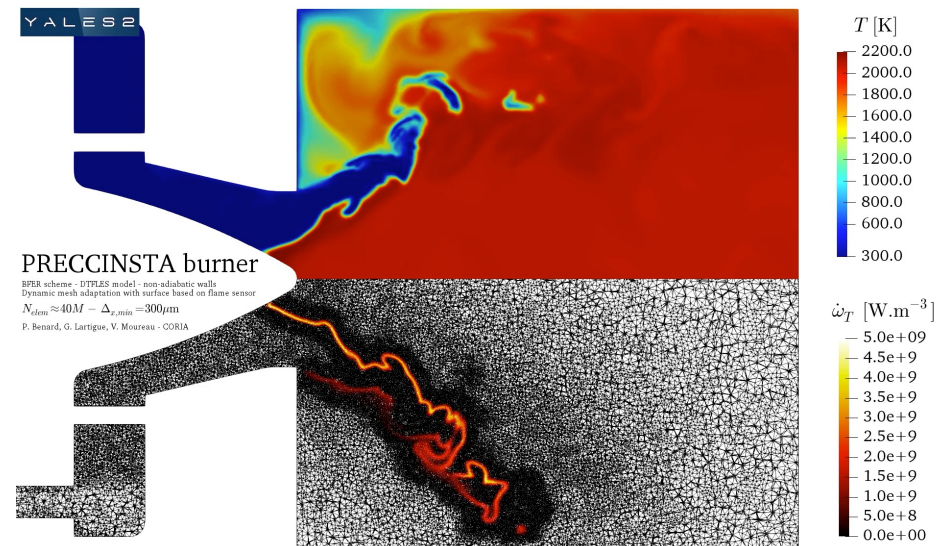


Dealing with multi-scale flows

HP-dynamic adaptation

Adaptive simulations

- H-adaptation
 - Topological changes of the mesh
 - MMG: <https://www.mmgtools.org>

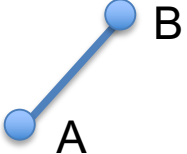


- P-adaptation
 - Discretization order change [1]

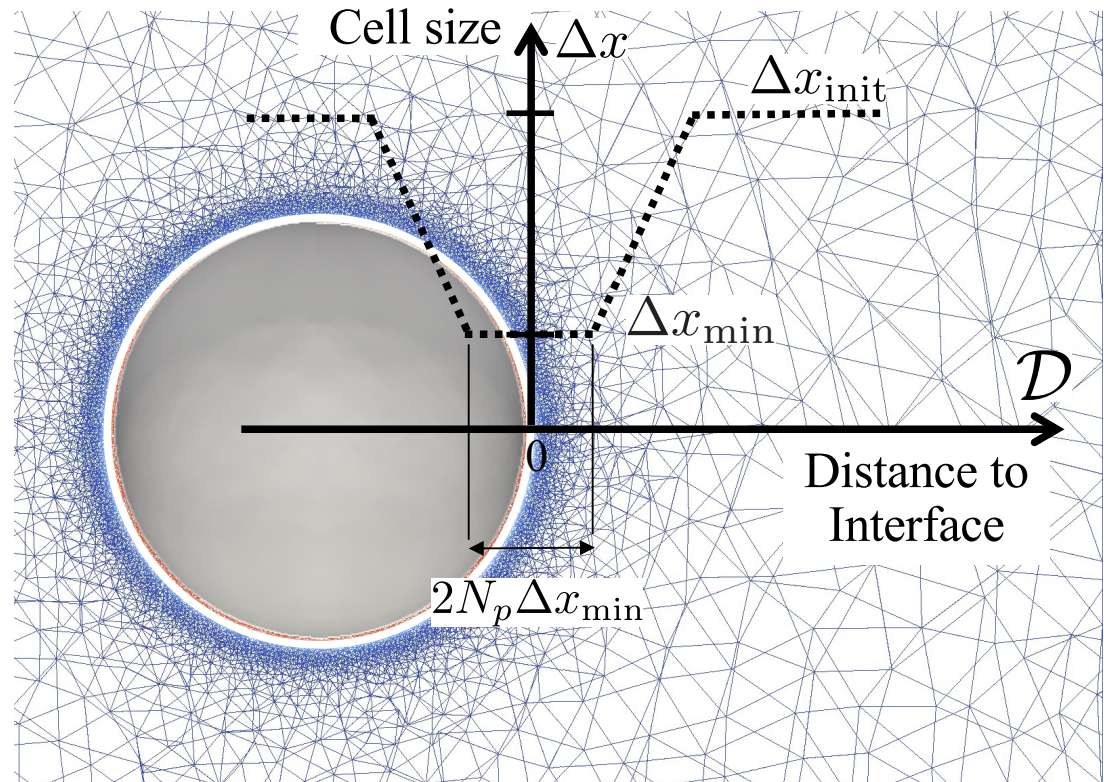


- HP-adaptation
 - Combination of both

H-adaptation: Mesh metric definition

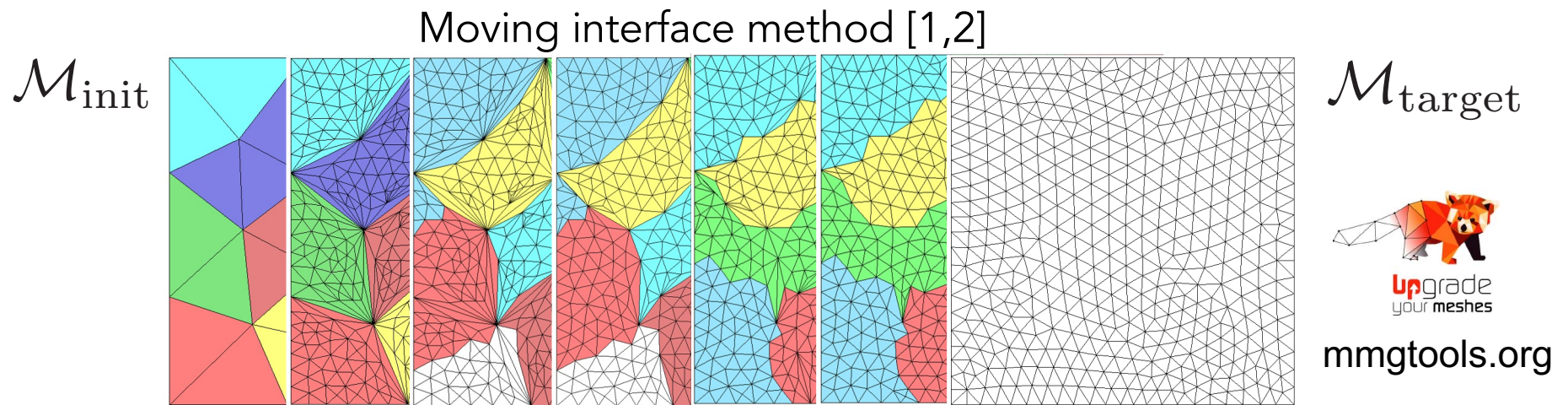
- A continuous metric is defined [1,2] $L_{\mathcal{M}}(AB) = \int_A^B \sqrt{\mathcal{M}(s)} ds$ 
- The isotropic metric is linked to the local cell size $\mathcal{M}(x_i) \simeq 1/\Delta x_i^2$

- Example of cell size distribution to track a gas/liquid interface
- Remeshing is triggered by the interface going out of a protected region (CFL-like condition)

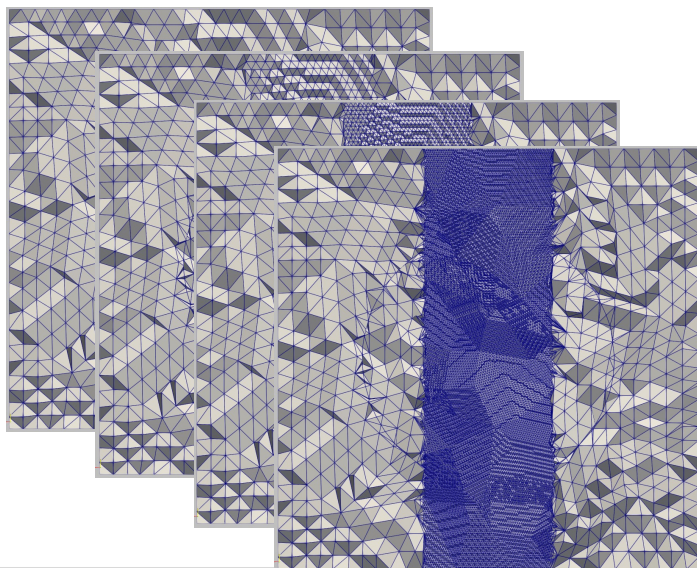


H-adaptation: High Performance Computing

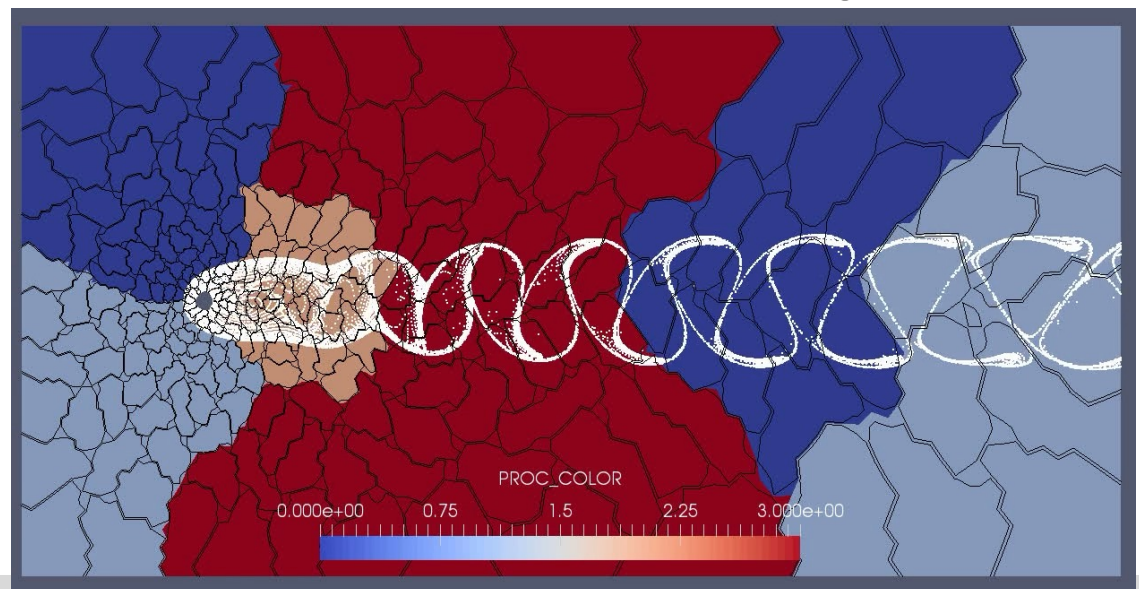
- A combination of several kernels



Parallel edge-cutting

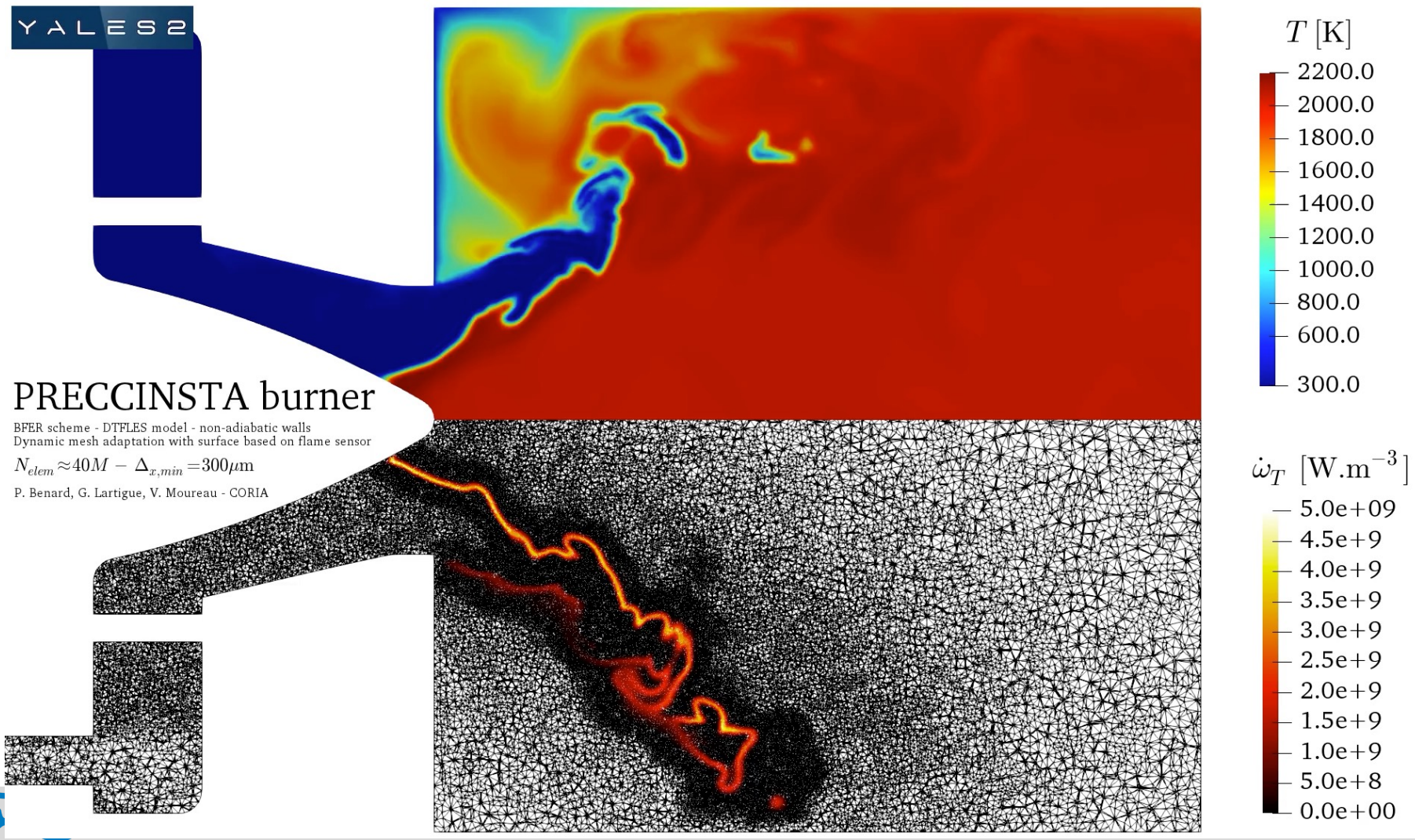


Parallel load-balancing



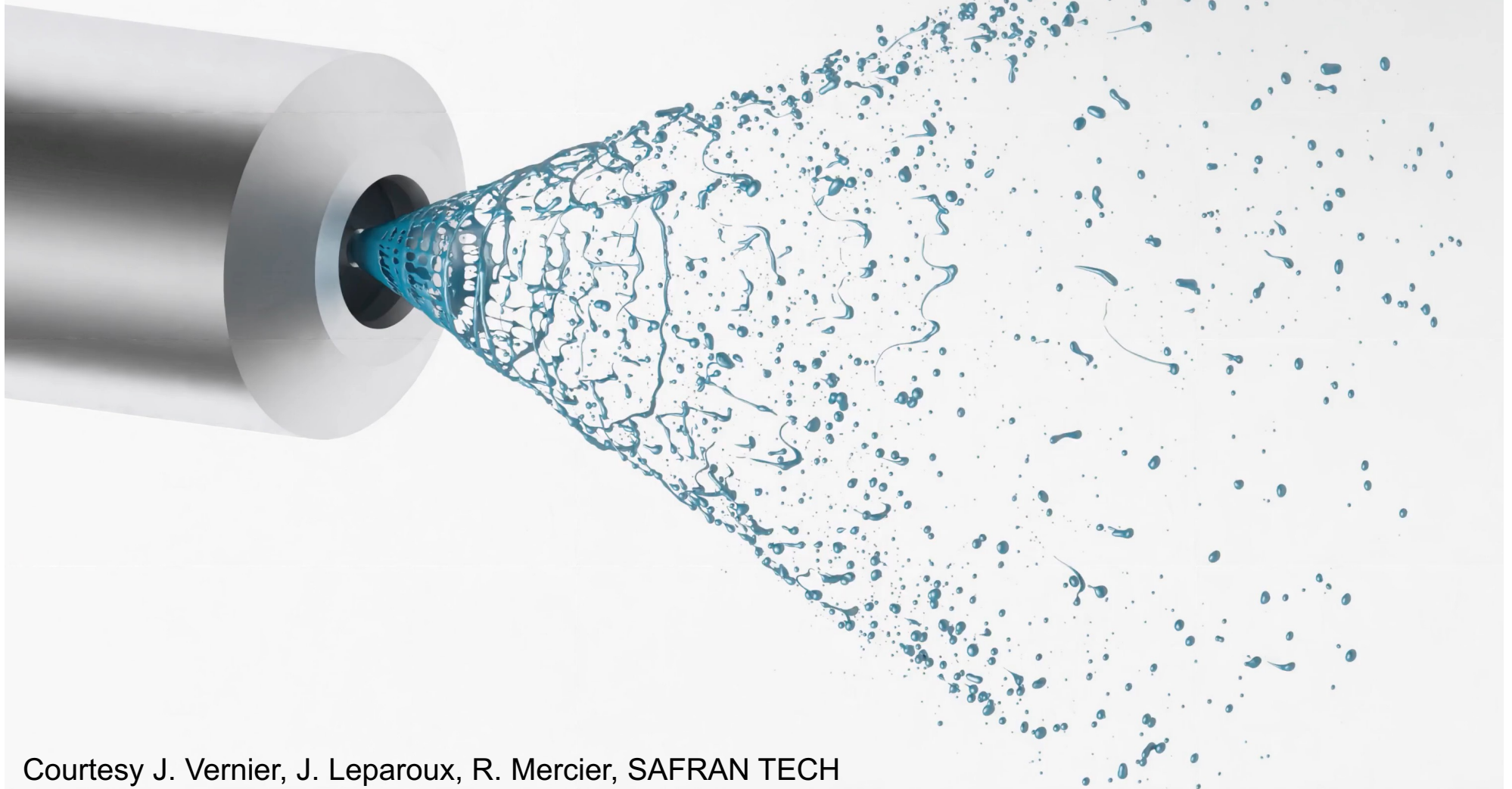
H-adaptation: Application to the PRECCINSTA burner

- ▶ Volume/surface adaptation with MMG5.3 and YALES2 2018.11
- ▶ Metric definition based on a calculated progress variable gradient
- ▶ Same resolution as 110M (300 microns) but with 38M cells: **global x3 speed-up**



H-adaptation: Application to primary atomization

- Pressure swirl atomizer
 - 390M elements, 2176 cores, $\Delta x = 10 \mu\text{m}$ at interface



Courtesy J. Vernier, J. Leparoux, R. Mercier, SAFRAN TECH

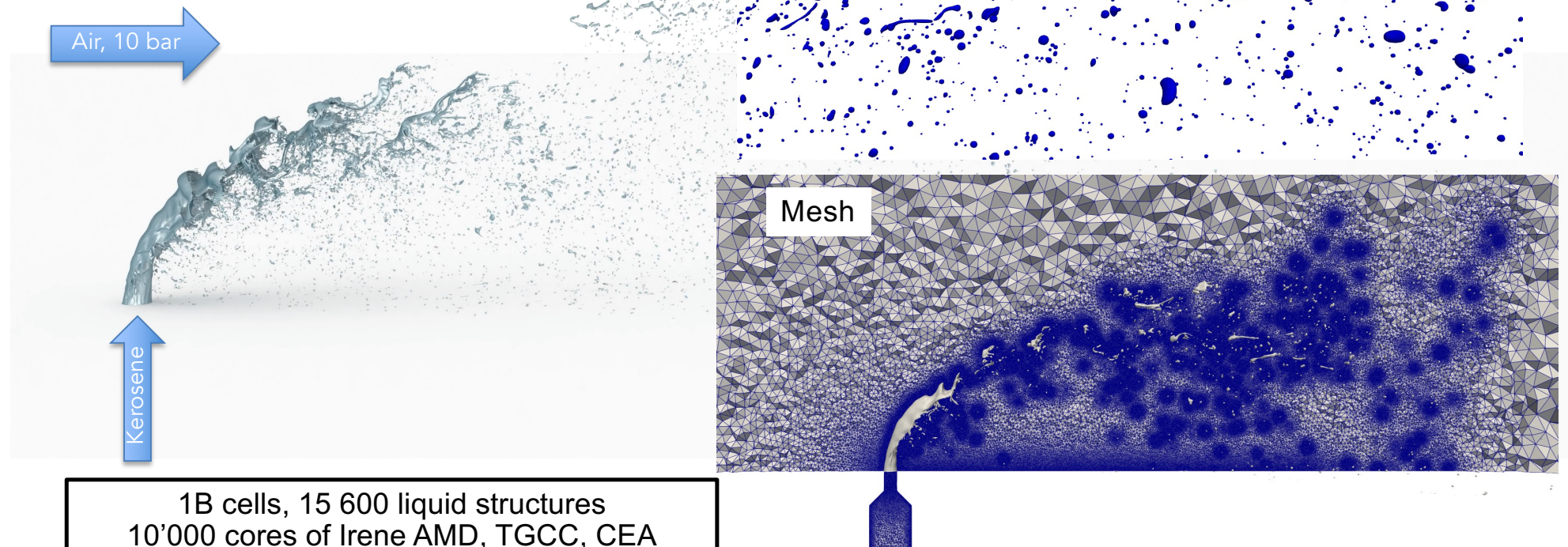
H-adaptation: DLR jet-in-cross-flow [1]

- Liquid jet in cross flow

$$\Delta x_{\min} = 10\mu\text{m}$$

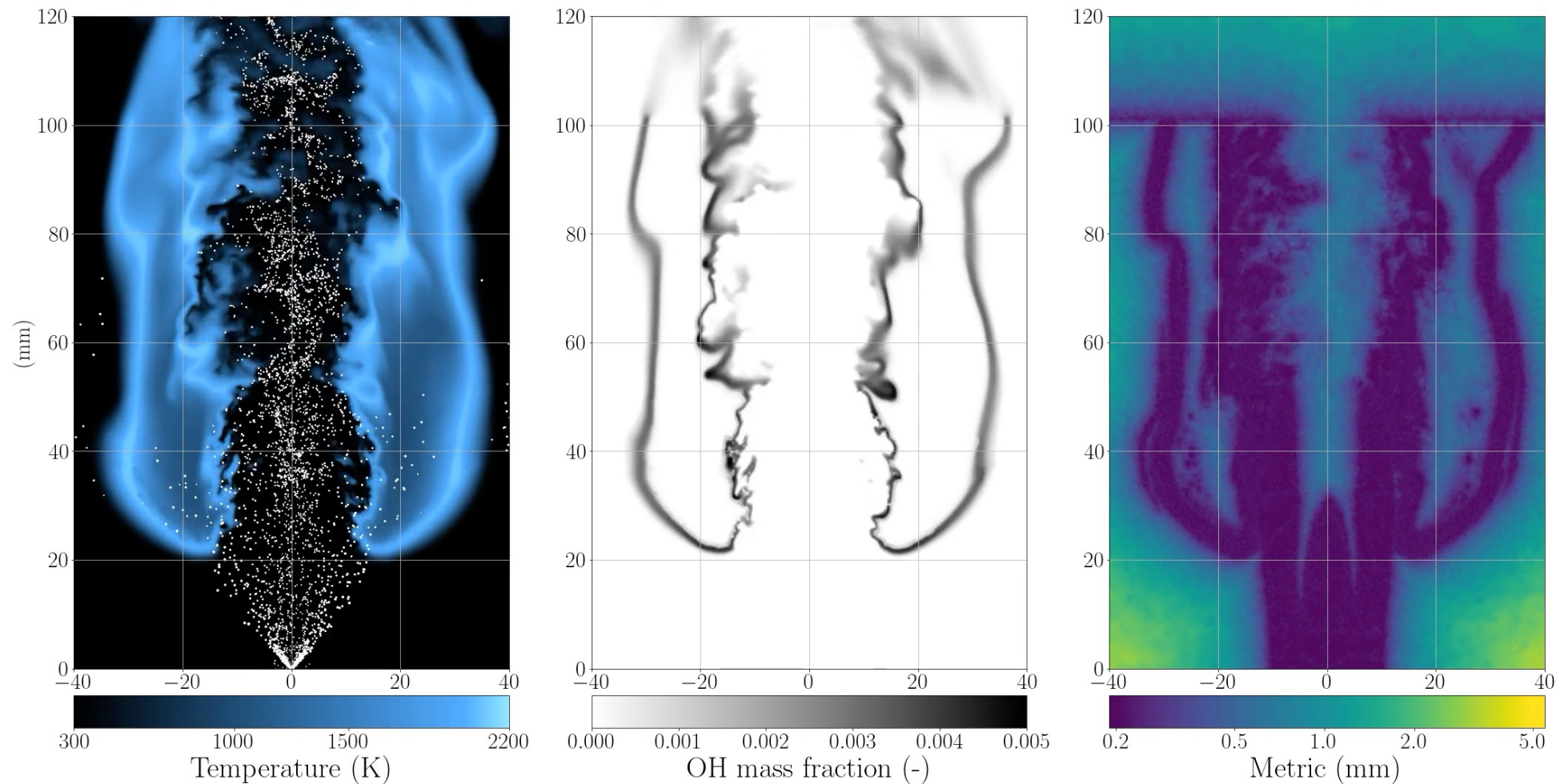
$$\text{We}_g = \frac{\rho_g u_g^2 d_{\text{inj}}}{\sigma} = 1470$$

$$\text{q} = \frac{\rho_l u_l^2}{\rho_g u_g^2} = 6$$



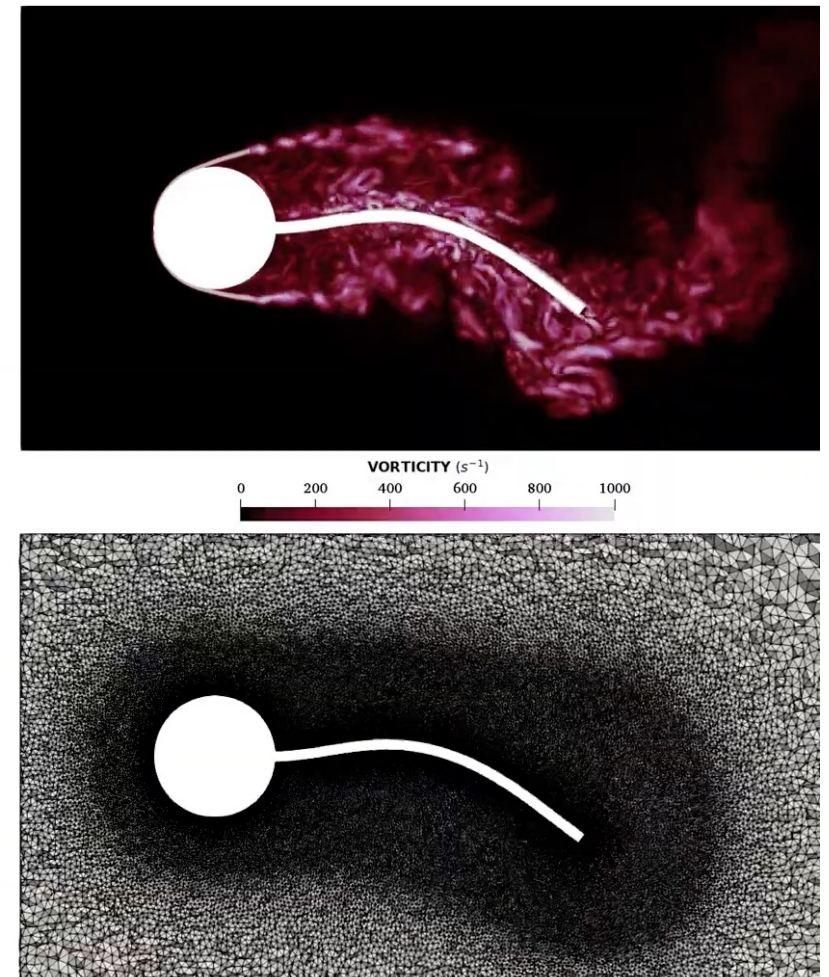
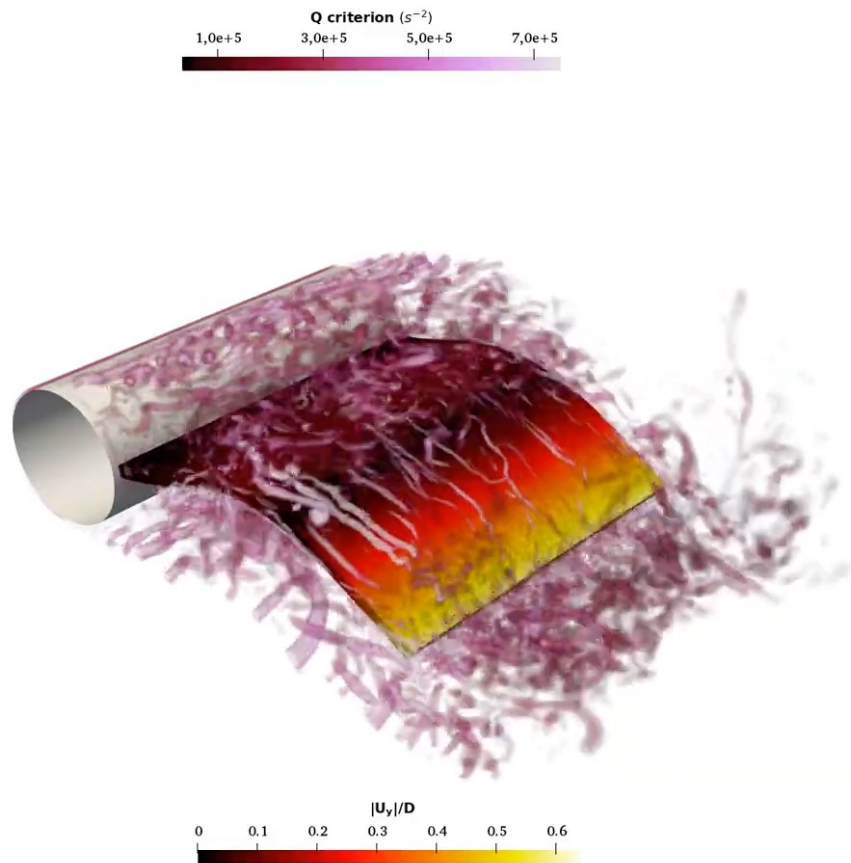
Spray combustion in the CRSB burner

- N-heptane spray burner
- Experimental data: <https://crsb.coria-cfd.fr>



Fluid/struct. int. with LEGI (T. Fabbri, G. Balarac)

- DYNEOL ANR project
- Structural mechanics solver (SMS) + incompressible solver (ICS)
- 3D Turek case [1] with dynamic mesh adaptation



YALES2

P-adaptation: Pair-based Finite-Volume Formalism

- Discrete Finite-Volume conservative Navier-Stokes equations on unstructured meshes

$$\frac{\bar{\mathbf{U}}_i^{n+1} - \bar{\mathbf{U}}_i^n}{\Delta t} + \frac{1}{V_i} \sum_{j=1}^{Neighbors} \mathbf{F}_{ij} \cdot d\mathbf{A}_{ij} = 0$$

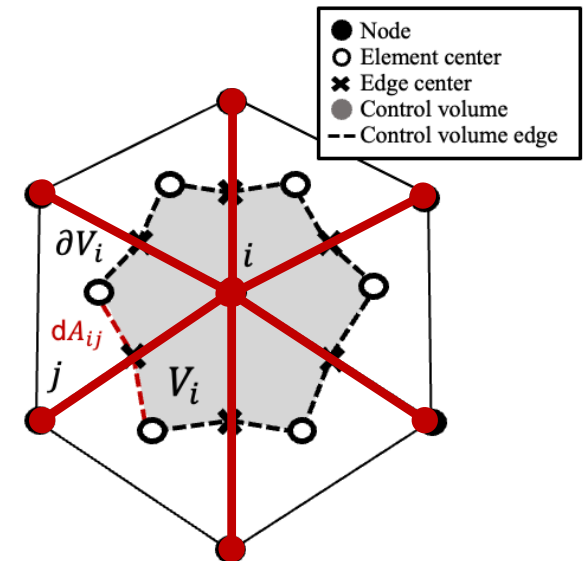
2D barycentric control volume

- Pair-based flux estimation

$$\mathbf{F}_{ij} = f(\bar{\mathbf{U}}_i, \bar{\mathbf{U}}_j, \dots)$$

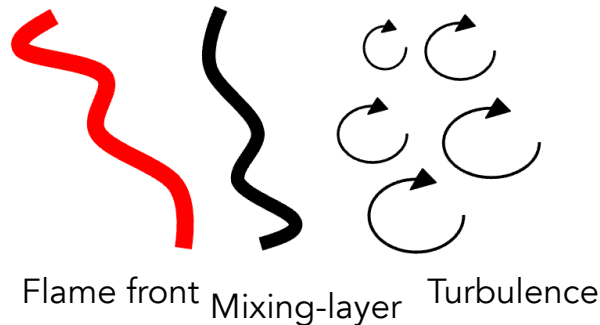
1-D independent flux estimations

- Pair-based schemes can be:
 - Central transport: Kinetic-energy conserving [1]
 - Central diffusion: Necessarily dissipative
 - Upwind transport: Maximum principle preserving [2]
 - Higher-order: k-exact [3]



P-adaptation: Pair-based Finite-Volume numerical schemes

How to compute the flux $\mathbf{F}_{i+\frac{1}{2}}$ at face ?



Continuous phenomenon

Taylor expansion (continuity hypothesis)

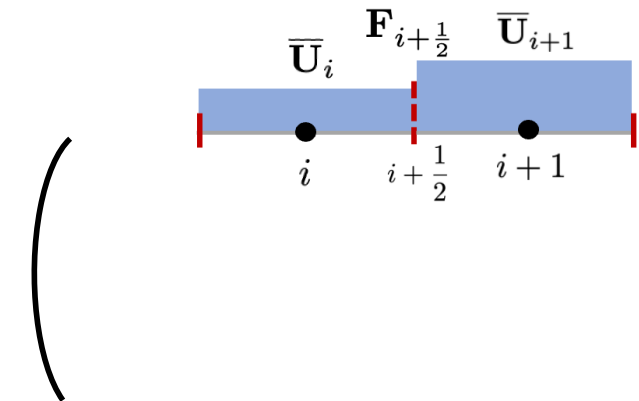
- Polynomial approximation of $\mathbf{U}_{i+\frac{1}{2}} = f(\bar{\mathbf{U}}_i, \bar{\mathbf{U}}_{i+1}, \dots)$
- Compute $\mathbf{F}_{i+\frac{1}{2}} = F(\mathbf{U}_{i+\frac{1}{2}})$

Advantages:

- High order (4th-order in YALES2)
- Non-dissipative

Drawbacks:

- Not Total variation diminishing (TVD)
- Not robust to high gradient (Gibbs problem)



Shock wave or gas/liquid interface

Discontinuous phenomenon

Solving a Riemann problem

- Godunov schemes
- V4 reconstruction [1]

Advantages:

- Total variation diminishing (TVD)
- Robust to high gradient

Drawbacks:

- Low order
- Dissipative

HP-adaptation: how to choose metric H and order P?

- Two main strategies

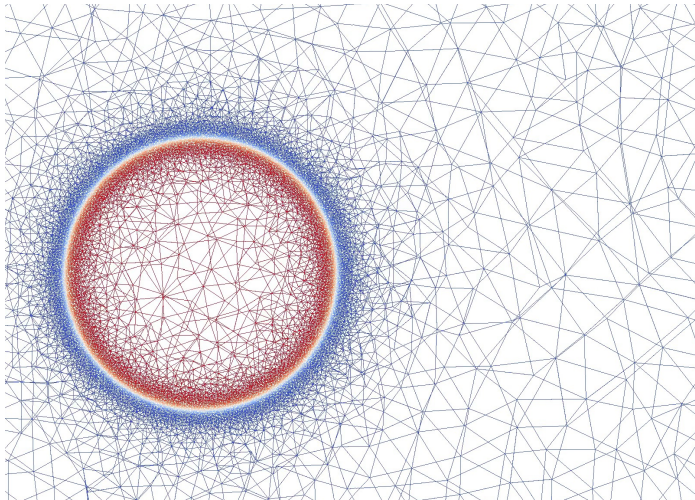
User-defined

- Order P and metric H are chosen by the user

Physics-based criteria

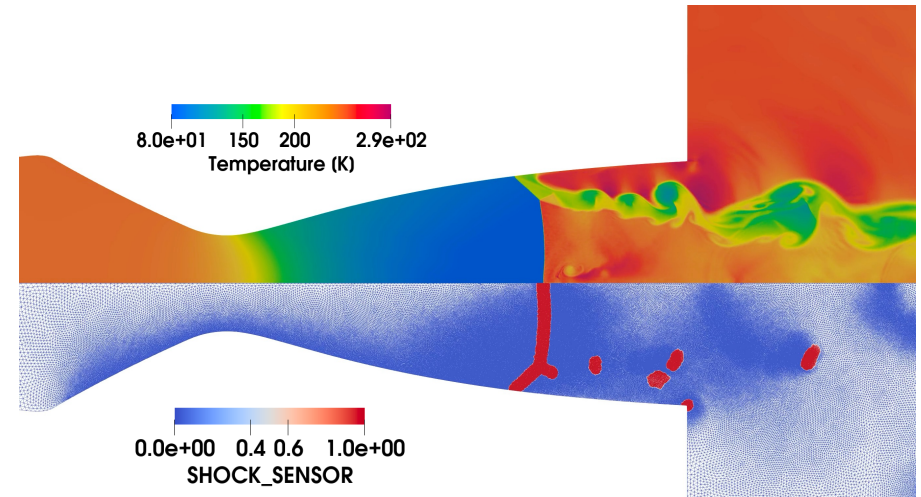
- Flow and turbulence criteria
 - (QC1, QC2, QC3) [1,2,3]
- Combustion criteria (S2R3)

Example: Based on a transported variable



Droplet convection with level-set

Example: Using a shock sensor



2D-axis nozzle symmetric simulation

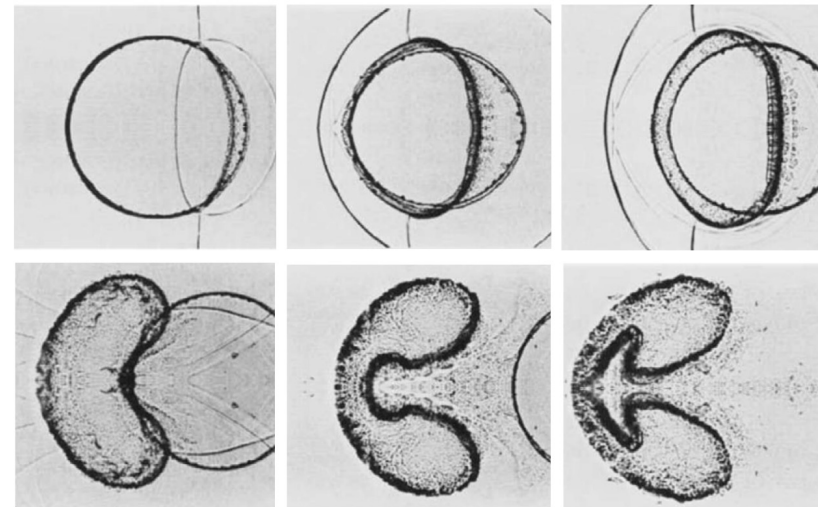
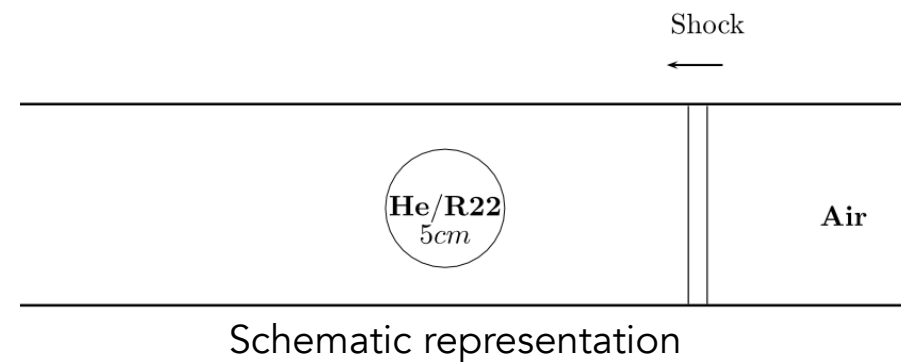
HP-adaptation: Simulation of shock bubble interaction

Numerical set-up

- **ECS** : Explicit compressible solver
- **Time discretisation**: TFV2A 2-step, 2nd order
- **Space discretisation** :
 - Central 4th order scheme
 - HLLC + MUSCL shock capturing scheme.
 - P-adaptation (*shock sensor [1]*)
- **Mesh adaptation** (H-adaptation)

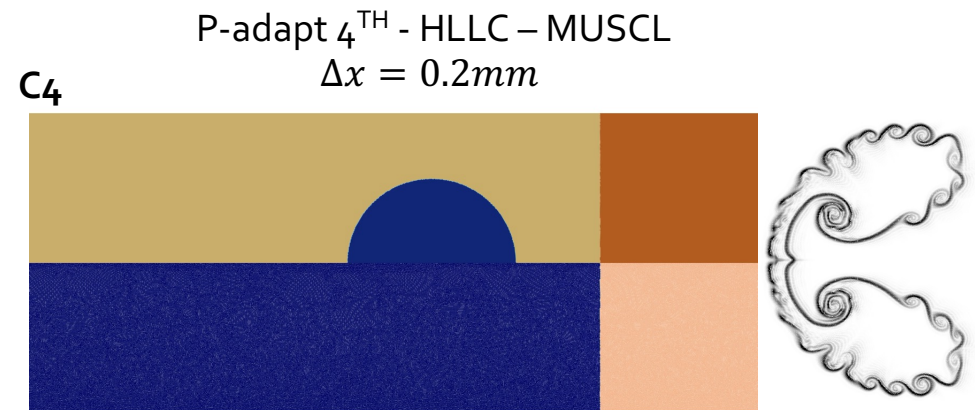
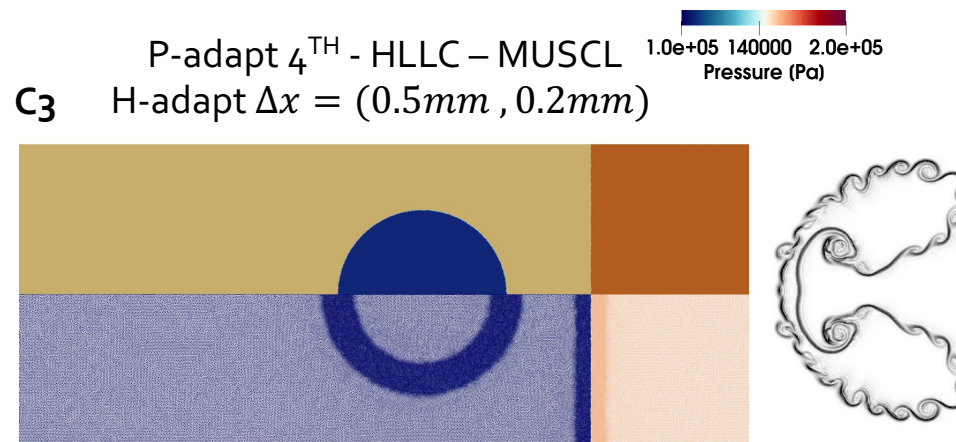
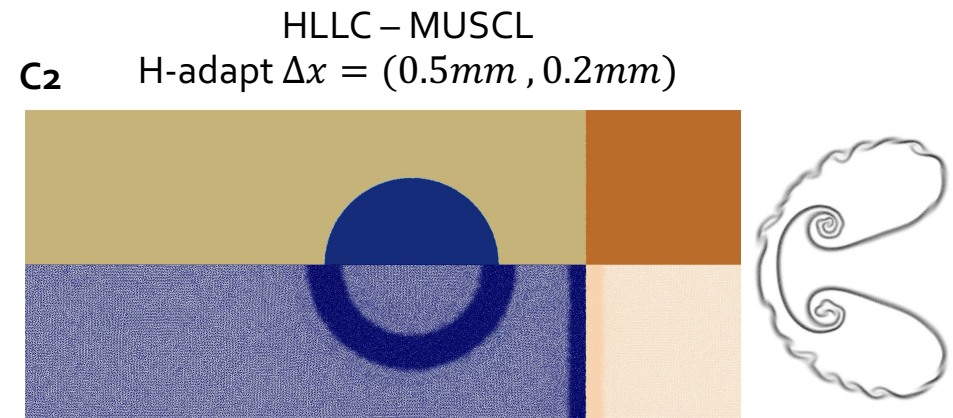
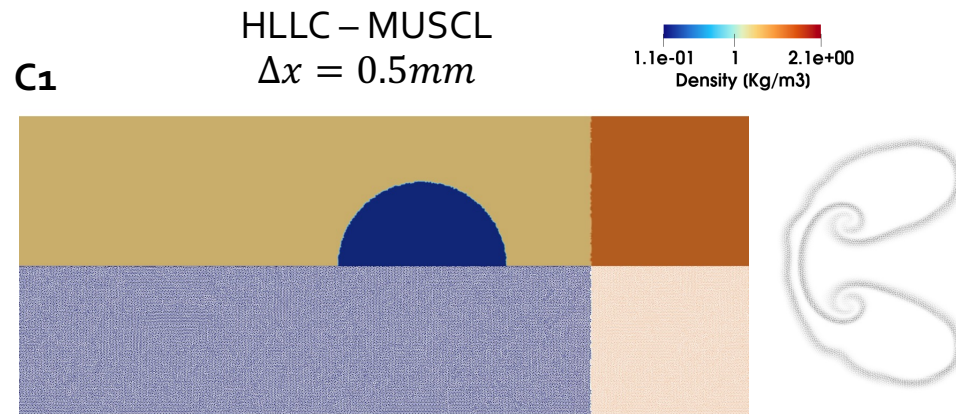
Boundary conditions

- **Walls** : No-slip
- **Inlet** : Velocity – Temperature (NSCBC)
- **Outlet** : Static Pressure

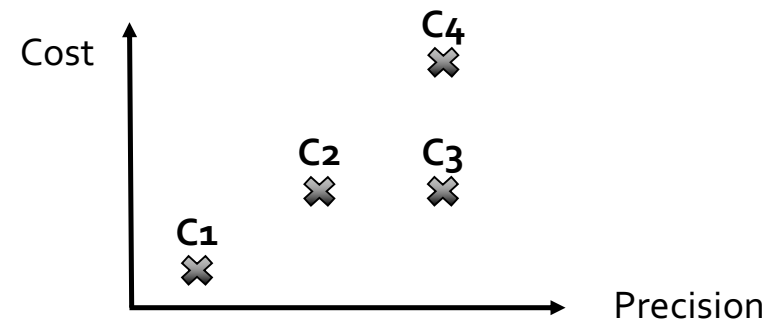


Schlieren images [2]

HP-adaptation: Simulation of shock bubble interaction

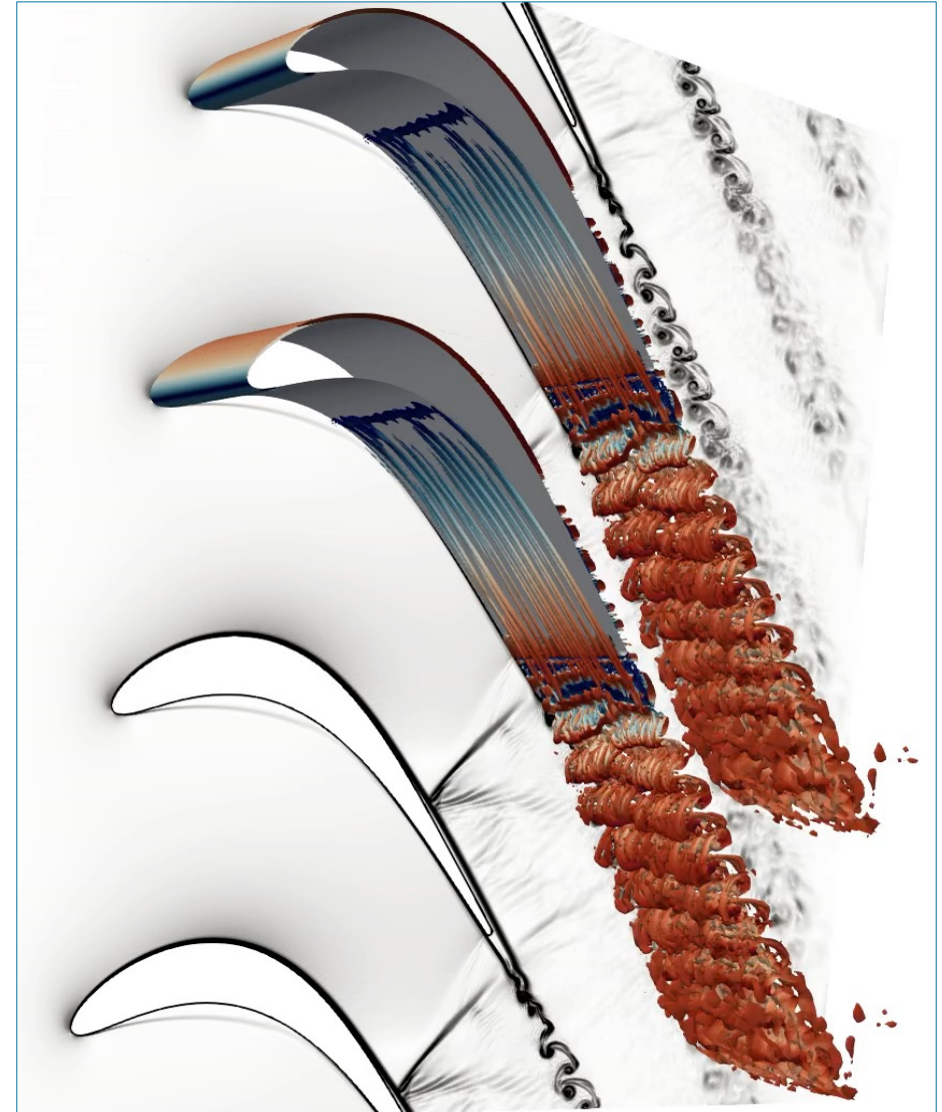
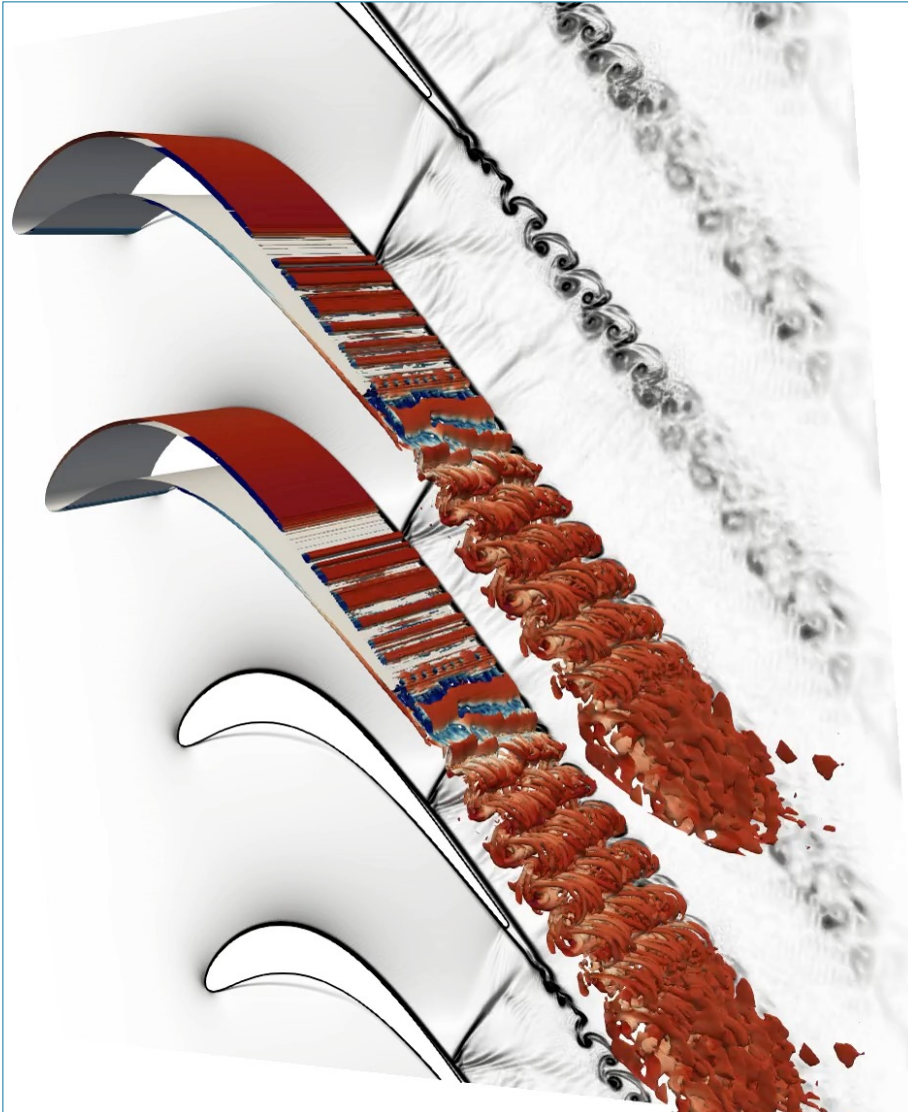


Case	Turnaround (10 Proc)
C1	6 min -15 sec
C2	20 minutes - 8 sec
C3	20 minutes – 17 sec
C4	54 minutes – 26 sec



HP-adaptation: LES of High-Speed low-pressure turbine

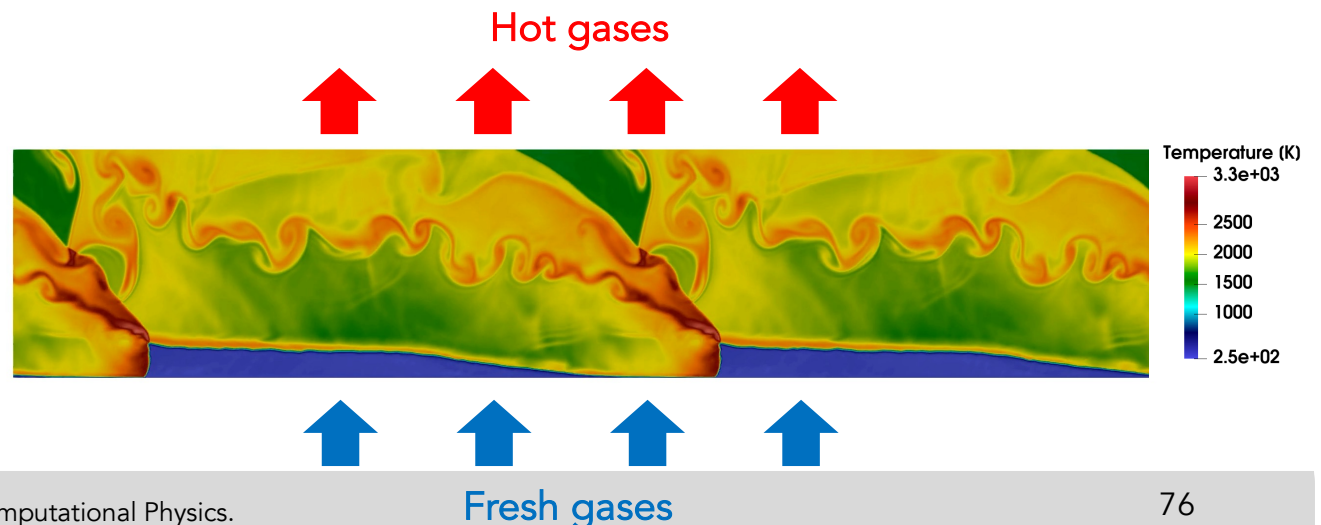
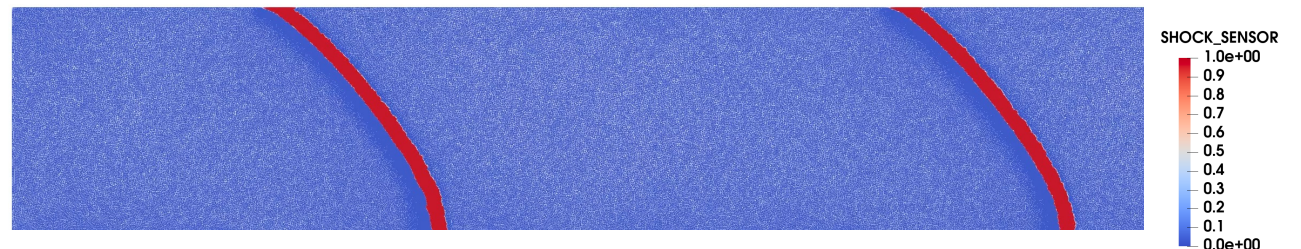
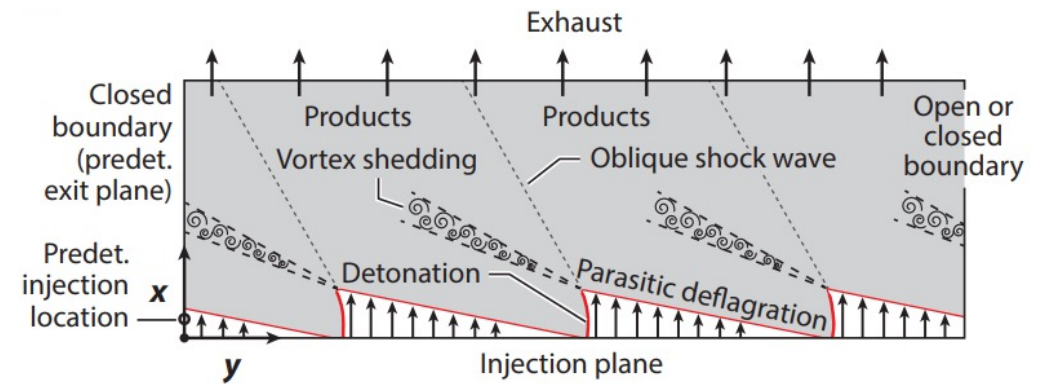
3D flows $Q = \frac{1}{2}(\Omega_{ij}\Omega_{ij} - S_{ij}S_{ij})$ $M_{2,is} = 0.95$



HP-adaptation: Rotative Detonation Combustion

Numerical set-up

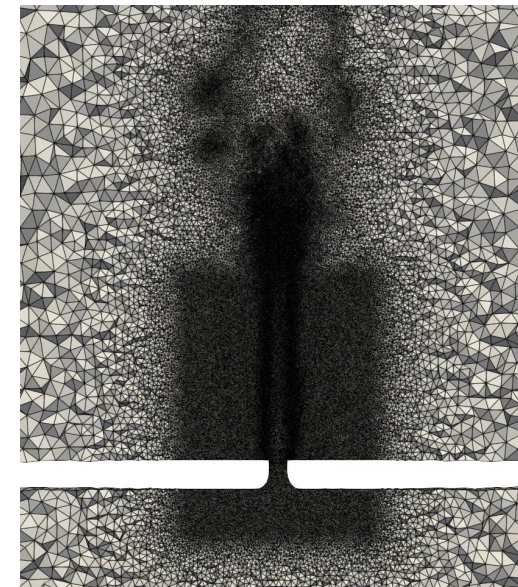
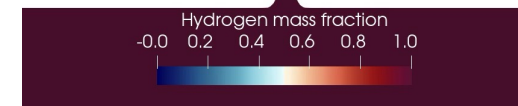
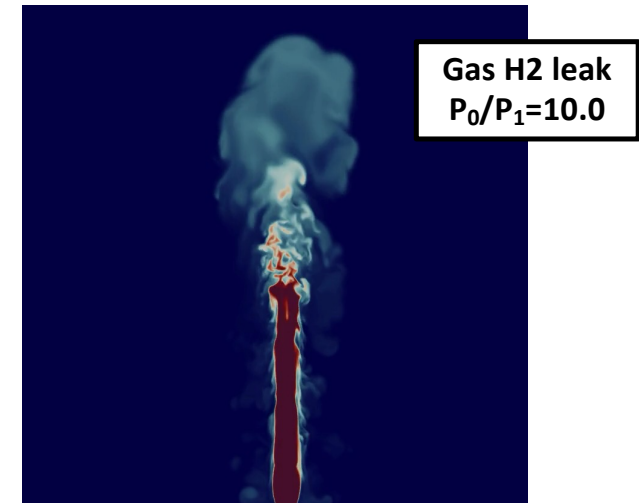
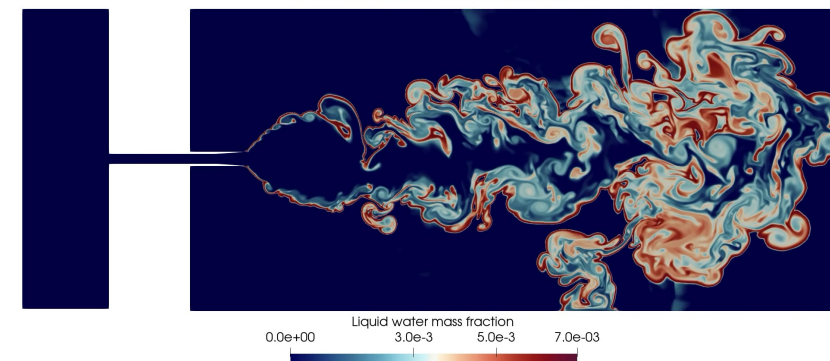
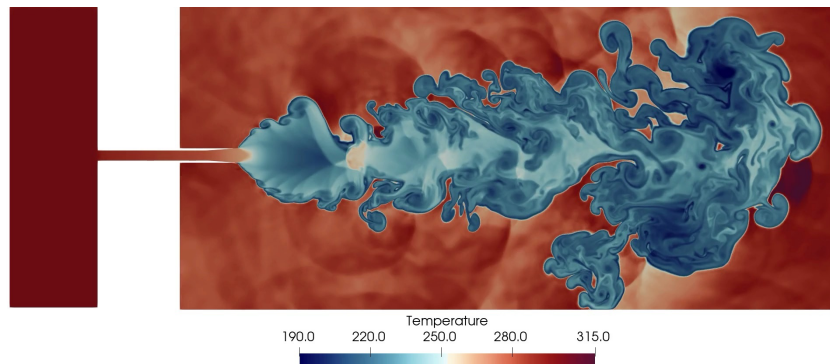
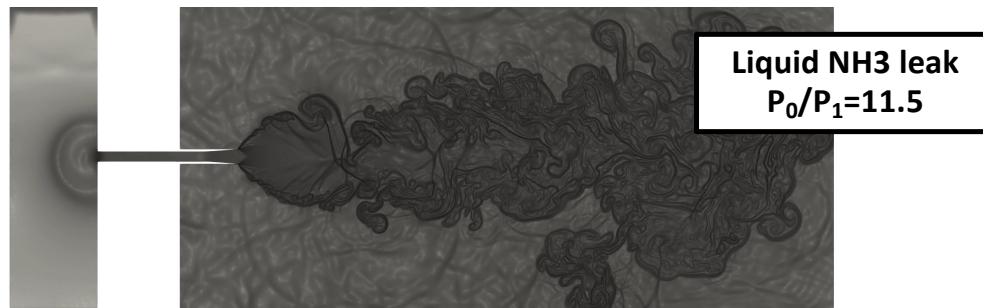
- **ECS** : Explicit compressible solver
- **Space discretisation** :
 - Central 4th order scheme
 - SLAU2 + MUSCL shock capturing
 - HP-adaptation (*shock sensor* [1])
- **Kinetic scheme** :
 - H2-air mechanism
(5 species, 3 reactions)



Courtesy of Said Taieb
SAFRAN TECH

HP-adaptation: high-pressure leakage flows

- Multi-fluid solver: 4-equation model
- NASG equation-of-state



Conclusions

Conclusions & perspectives

- Proposed methodology
 - Pair-based Finite-Volume scheme adaptation (P) and mesh-adaptation (H) method for the simulation of fronts and interfaces
- The scheme adaptation (P) involves using:
 - High-order non-dissipative centered scheme in smooth regions
 - Low-order positive Godunov-MUSCL scheme in high gradients regions
 - Discontinuity sensors
- Dynamic mesh adaptation (H) near areas of significant variation to enhance resolution and minimize numerical errors.
- Demonstrated for
 - Compressible flows with shocks
 - Incompressible flows
 - Combustion / detonation
 - More to come...

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- YALES2 community
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