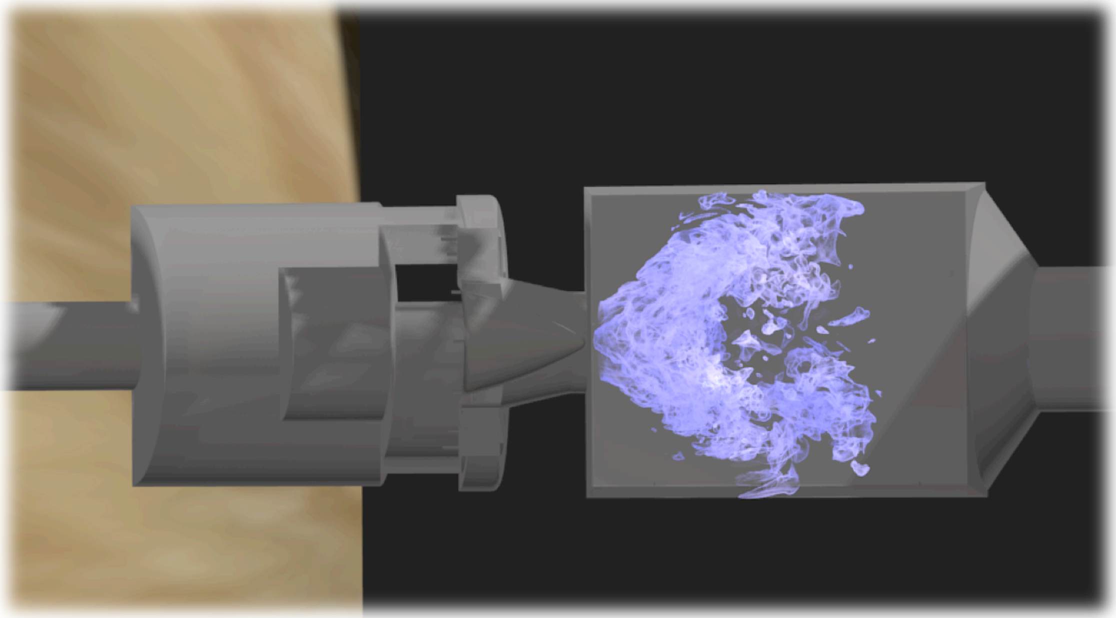
High Performance Computing for Large Scale Simulations of non-linear turbulent flows



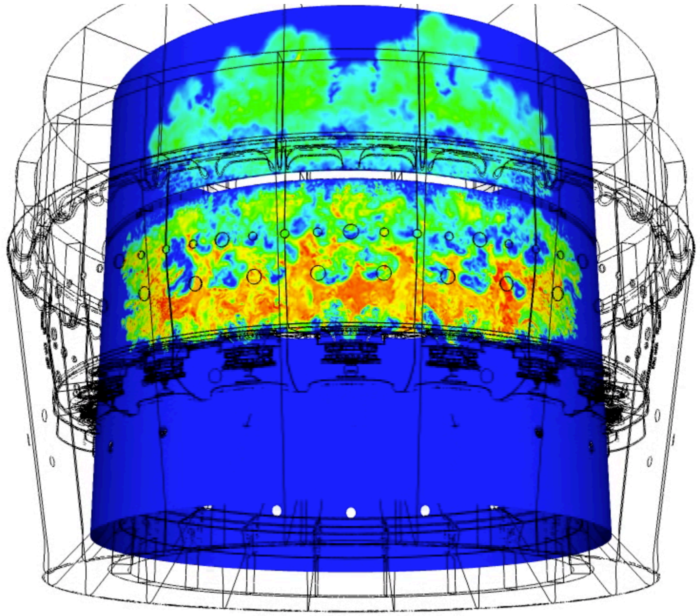
V. Moureau, G. Lartigue

CORIA, CNRS UMR 6614, University and INSA of Rouen

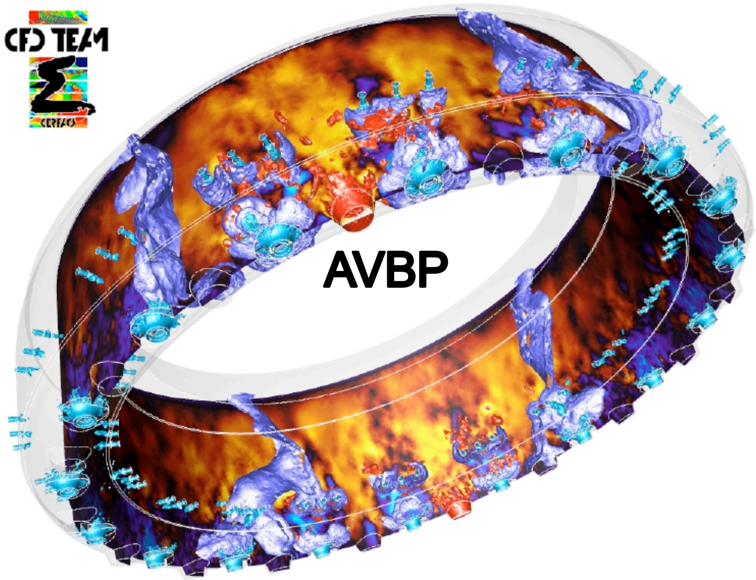
http://www.coria-cfd.fr

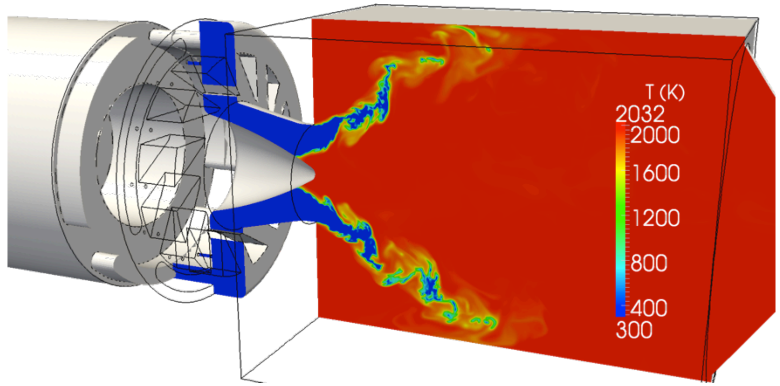
Context

- **Large-Eddy Simulation is coming of age for the prediction of combustor performances**
  - **Outlet temperature profile**
  - **Ignition / Relight**
  - **Blow-off / Extinction**
  - **Pollutant emissions**



CFD TEAM



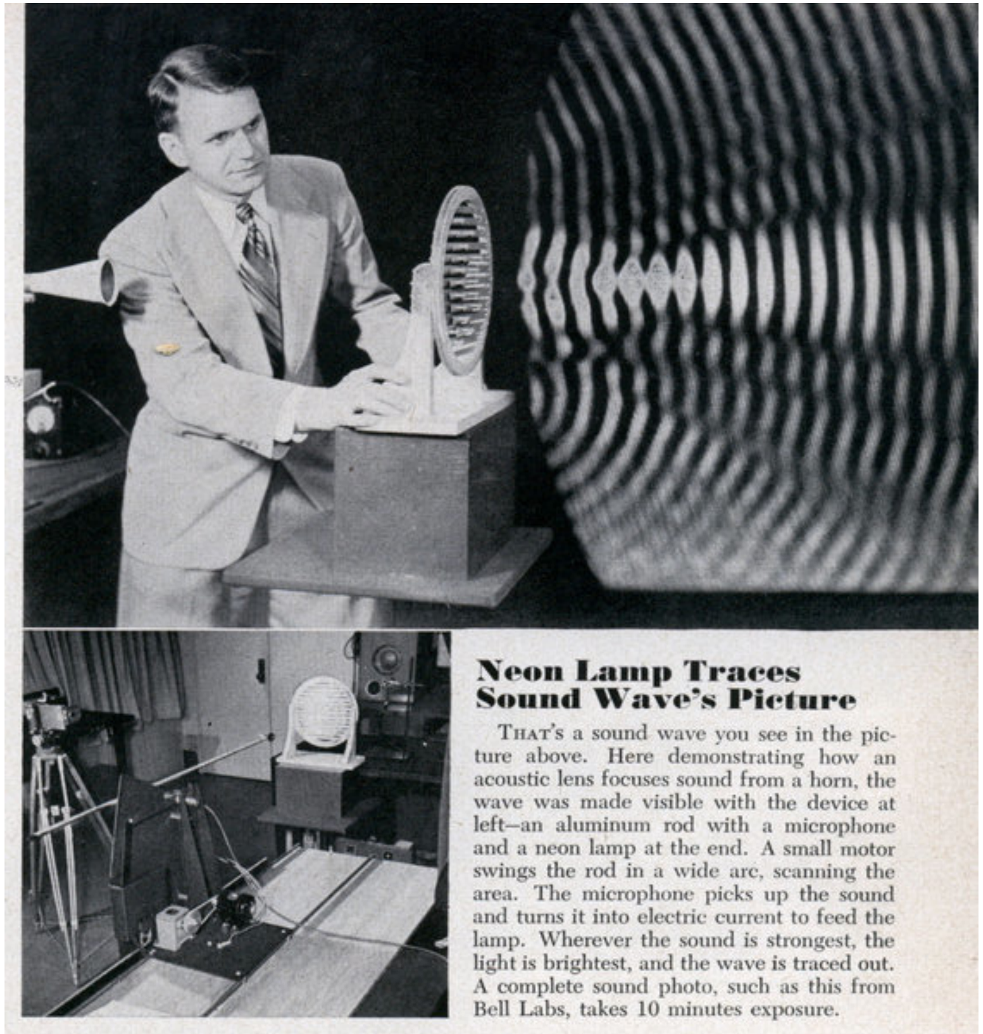


YALES2

- **But LES requires large meshes and a great deal of CPU power**

The choice of the governing equations

- If acoustics are at play, the fully compressible Navier-Stokes equations must be considered
- In many combustors, the Mach number may be considered “sufficiently” small
- In these cases, the low-Mach number expansion of the Navier-Stokes equations may be used instead



Neon Lamp Traces Sound Wave’s Picture

THAT’S a sound wave you see in the picture above. Here demonstrating how an acoustic lens focuses sound from a horn, the wave was made visible with the device at left—an aluminum rod with a microphone and a neon lamp at the end. A small motor swings the rod in a wide arc, scanning the area. The microphone picks up the sound and turns it into electric current to feed the lamp. Wherever the sound is strongest, the light is brightest, and the wave is traced out. A complete sound photo, such as this from Bell Labs, takes 10 minutes exposure.

Acoustic waves (Bell labs, 1950)

Variable density low-Mach number equations

- Equations

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

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

- Density is a prescribed data obtained from transported scalars
  - Tabulated chemistry: mixture fraction, progress variable, variances, …
  - Complex chemistry: species, enthalpy

- The dynamic pressure is obtained from a Poisson equation (Pierce and Moin, 2001)

$$\nabla \cdot \nabla \bar{P}^{n+1/2} = \frac{\bar{\rho}^{n+3/2} - \bar{\rho}^{n+1/2}}{\Delta t^2} + \frac{1}{\Delta t}\nabla \cdot (\bar{\rho}\tilde{\mathbf{u}}^{\star}) \quad \Longleftrightarrow \quad Ax = b$$

- *A* is sparse but may be as large as 10^{10}x10^{10} …

Outline

- Context
- High-performance linear solvers for low-Mach number codes
  - The optimized deflated preconditioned gradient algorithm
  - The YALES2 code
  - Massively parallel applications
- Application to the simulation of swirl burner dynamics
  - The PRECCINSTA burner
  - Extraction of large scale features
- Conclusions & perspectives

High-performance linear solvers for low-Mach number codes

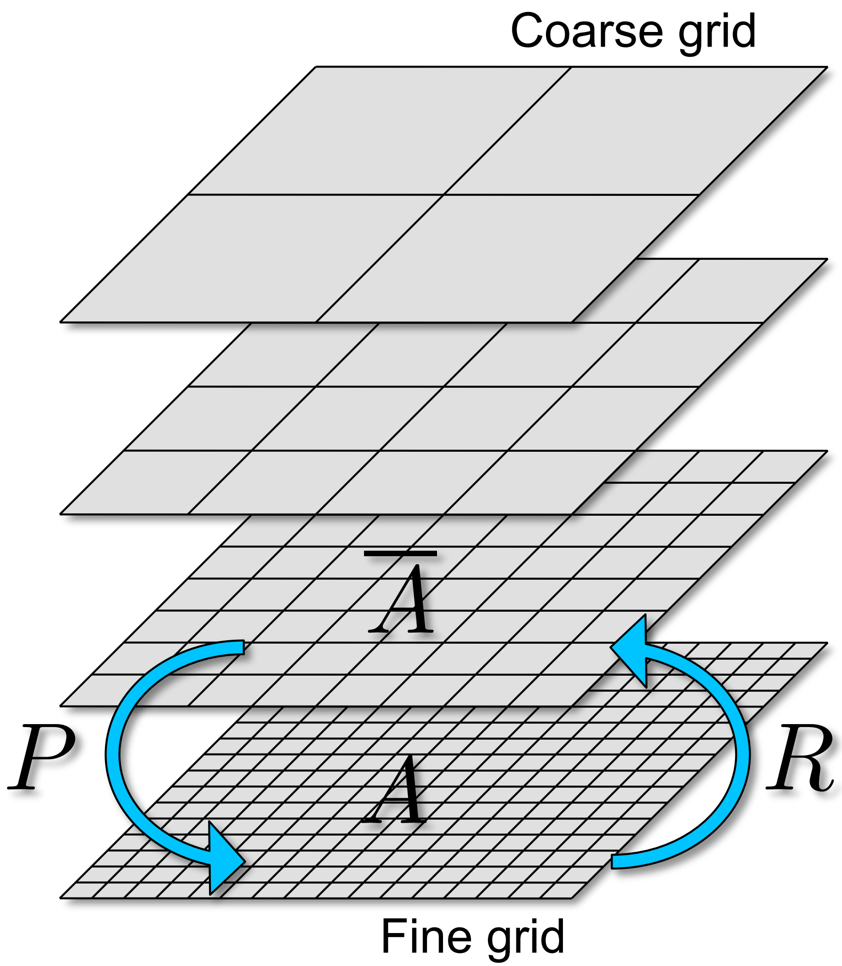
Multi-grid methods

- **Geometric/Algebraic multi-grid methods are based on nested grids**

$$\overline{A} = RAP$$

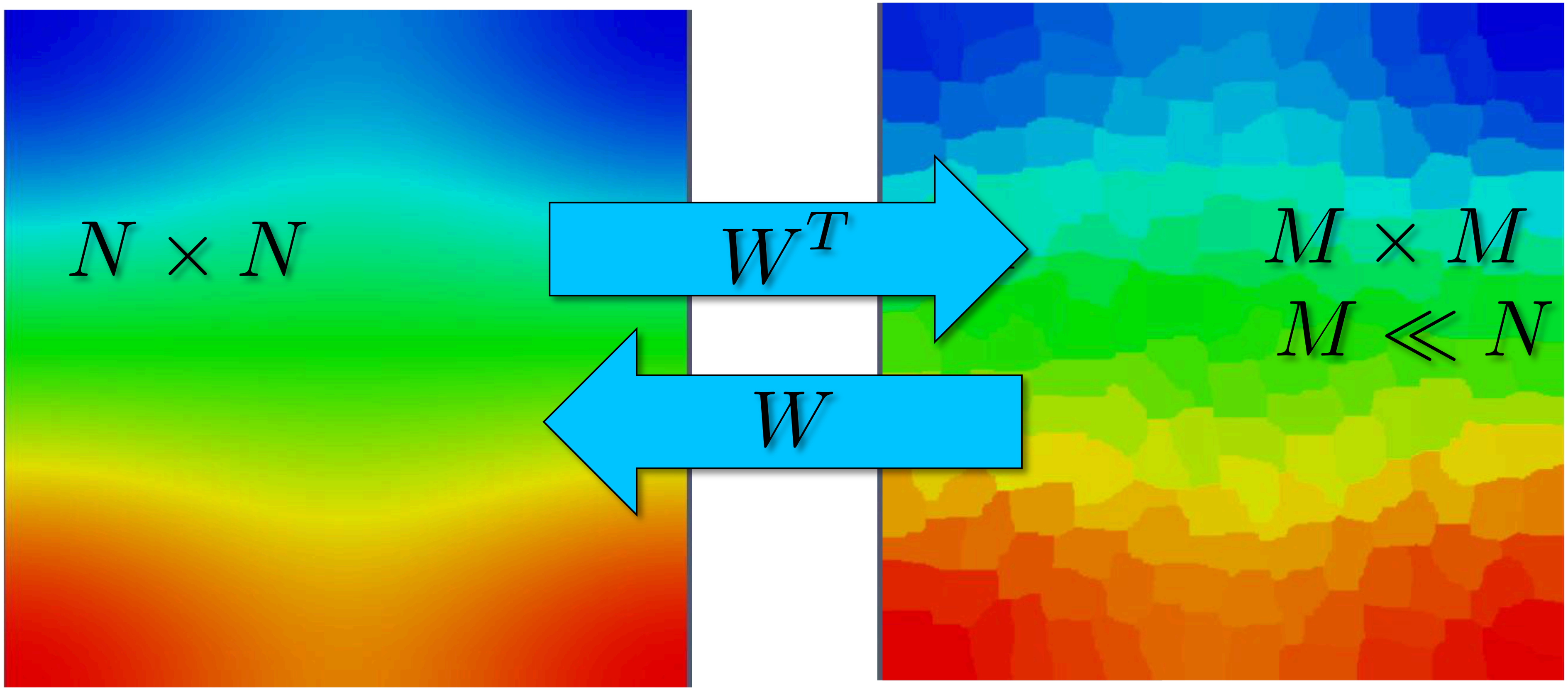
- **Low frequencies are solved efficiently on the coarse grids and high frequencies on the fine grids**

- **Some issues of multi-grids**
  - This structure has to fit in the chosen domain decomposition method
  - The coarse grids require a lot of parallel communications for a small amount of work
  - Hard to perform for unstructured meshes



The Deflated Preconditioned Conjugate Gradient
(Nicolaides 1987, Vermolen et al. 2002, Tang et al. 2011)

- The principle is very close to the one of algebraic multi-grids

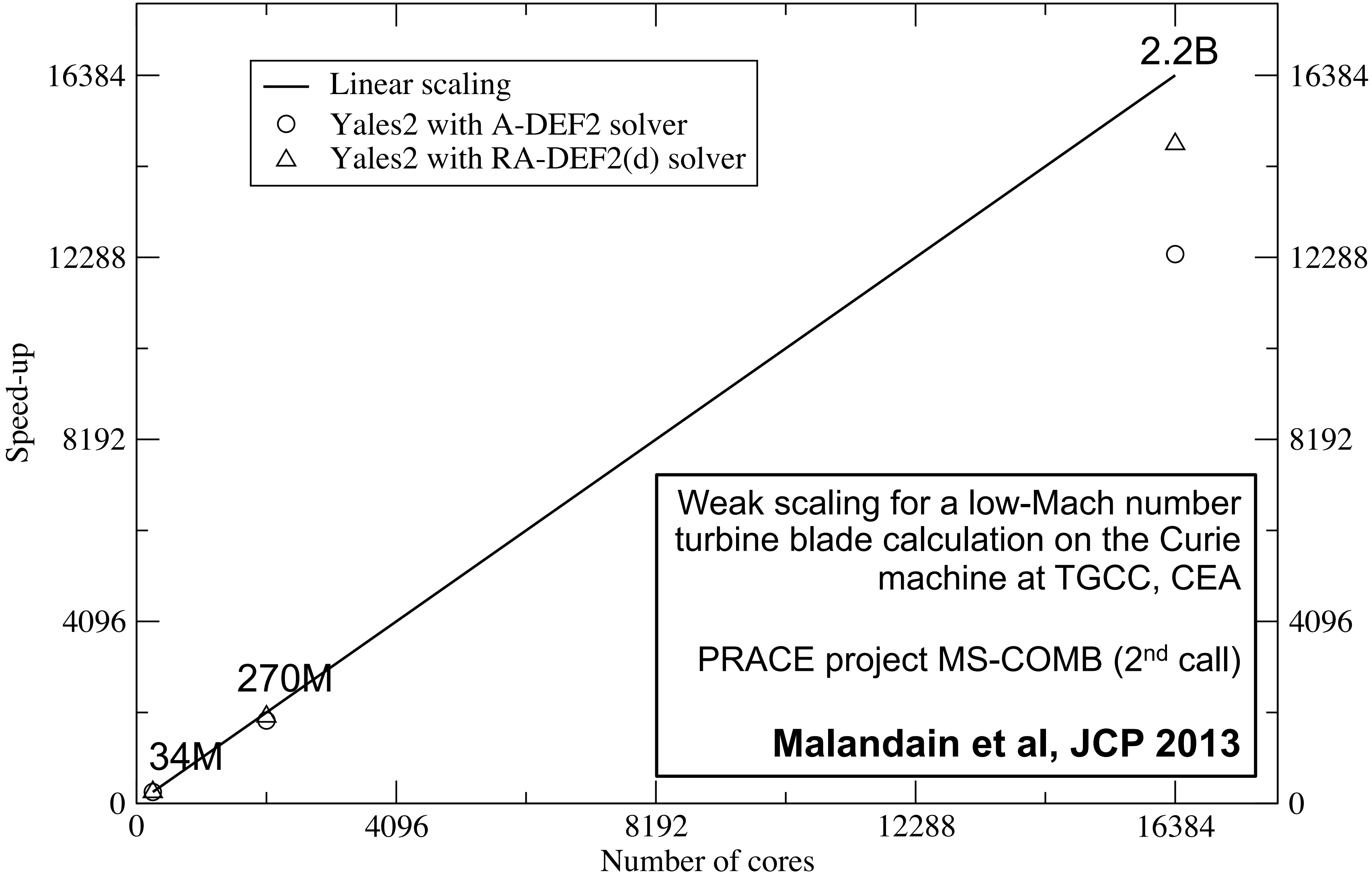


- The PCG preconditioning is based on a projection operator

$$P = I - W\hat{A}^{-1}W^T A \qquad \hat{A} = W^T A W$$

Optimized deflated PCG (DPCG)

- Combining improved residual recycling (Fischer 1998) and an optimal stopping criterion on the coarse grid allows to further reduce the communication cost



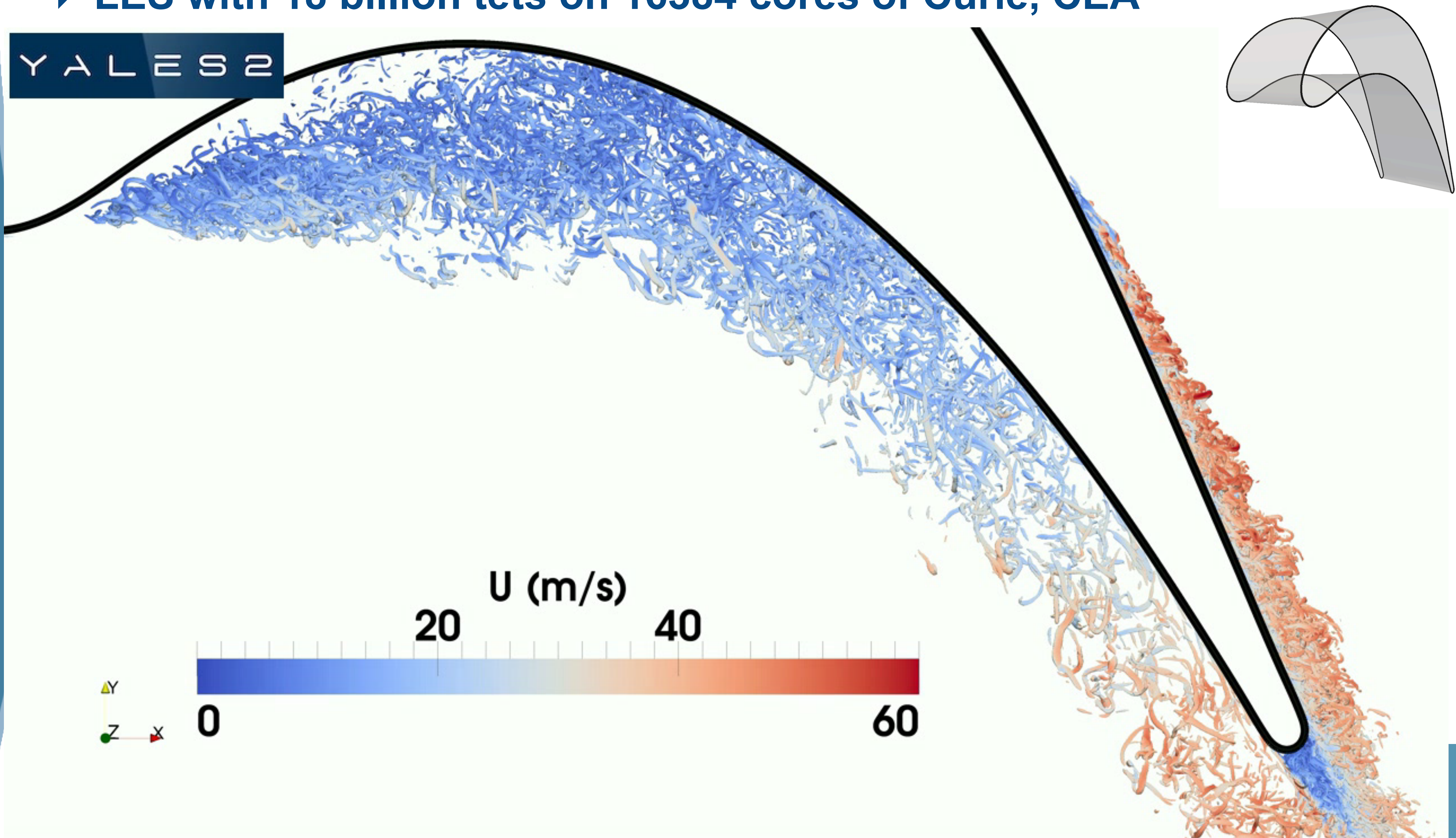
- **YALES2 is an unstructured low-Mach number code for the DNS and LES of reacting two-phase flows in complex geometries. It solves the unsteady 3D Navier-Stokes equations**

- **It is used by more than 80 people in labs and in the industry**
  - **SUCCESS scientific group (http://success.coria-cfd.fr)**
    - CORIA, I3M, LEGI, EM2C, IMFT, CERFACS, IFP-EN, LMA
  - **Other labs: ULB, LOMC, …**
  - **Industry: SAFRAN, SOLVAY, GDF-SUEZ, …**

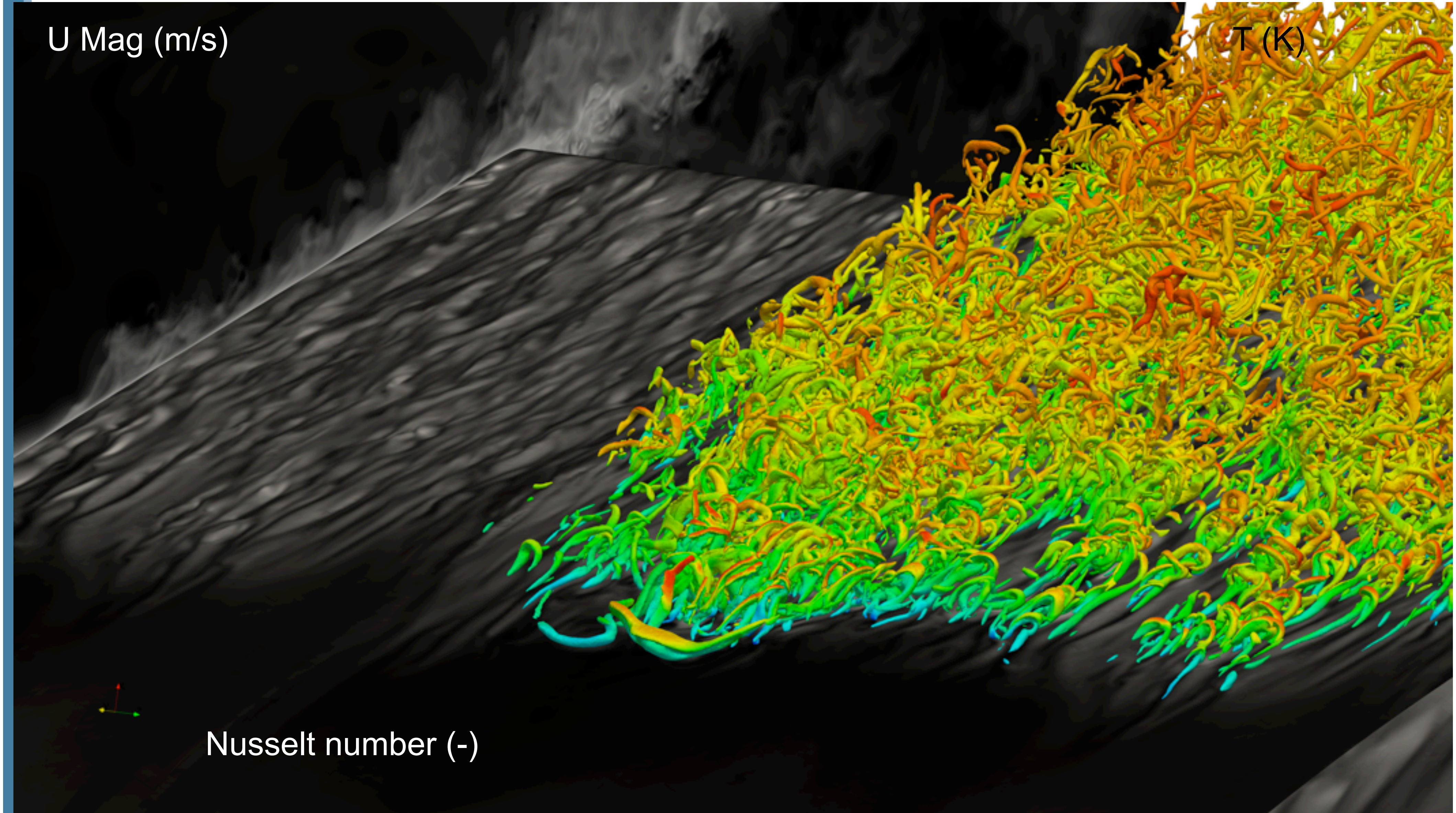
- **Awards**
  - **2011 IBM faculty award**
  - **3rd of the Bull-Joseph Fourier prize in 2009**
  - **Principal investigator of 2 PRACE proposals**

Extreme case: smallest resolved vortices in the LES of heat transfer on a low-Mach turbine blade

- T7.2 blade, Re = 150 000, 5.8% inlet turbulence
- LES with 18 billion tets on 16384 cores of Curie, CEA

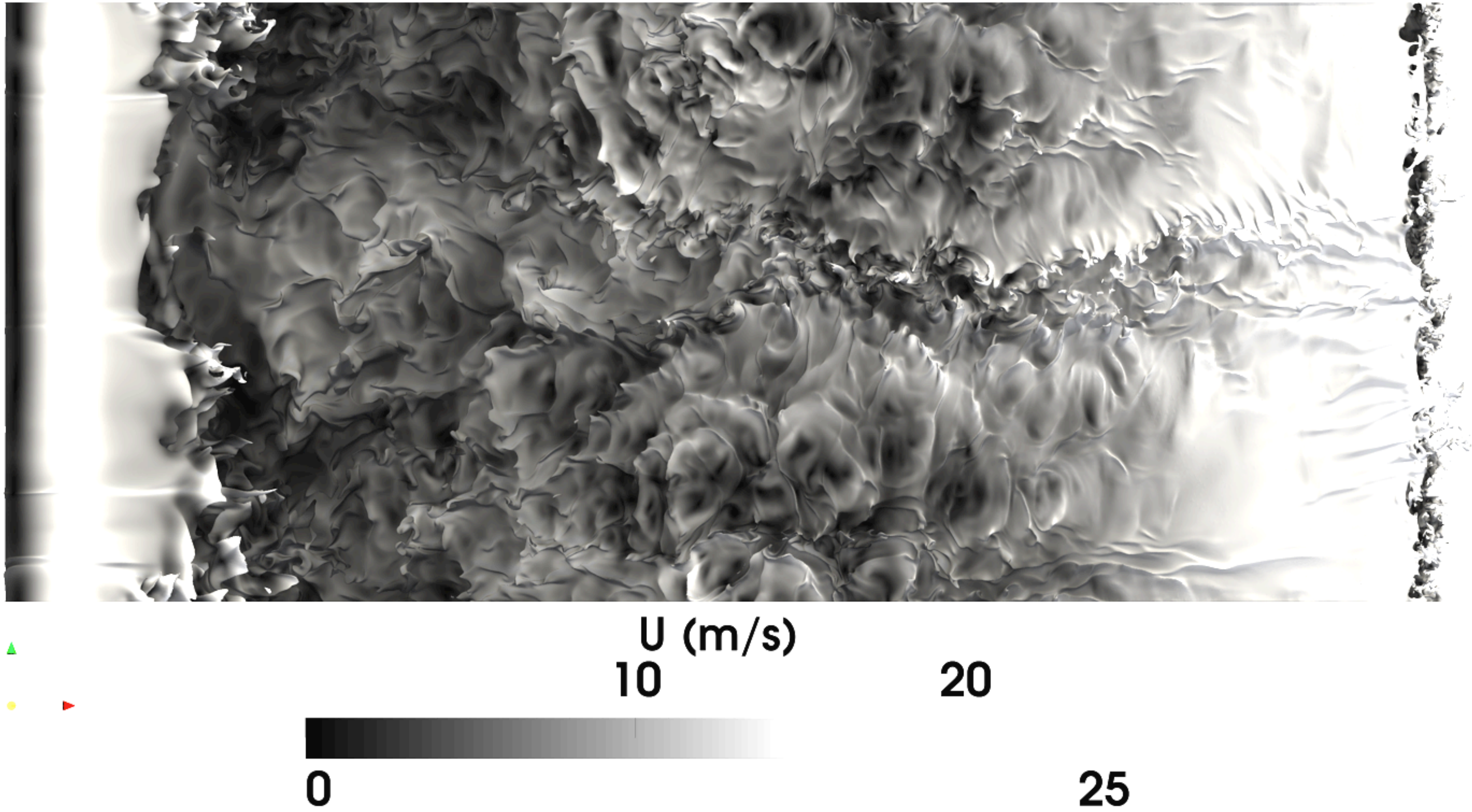


LES of heat transfer on a low-Mach turbine blade



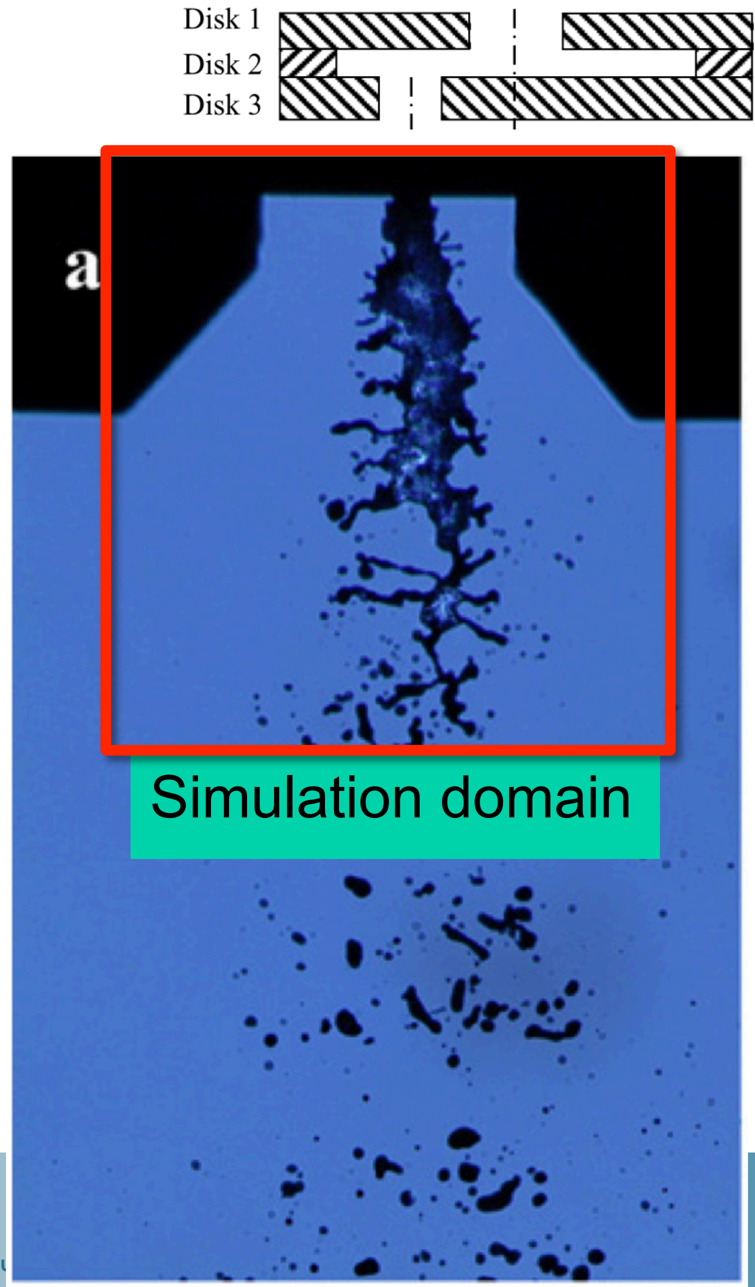
LES of heat transfer on a low-Mach turbine blade

- Study of local heat transfer



Simulation of primary atomization

- **Triple disk injector from Grout et al. 2007**
  - Water and air experiment
  - Complex injector geometry
  - Re = 3653
  - We_L = 1061
  - Injector outlet = 180 μm



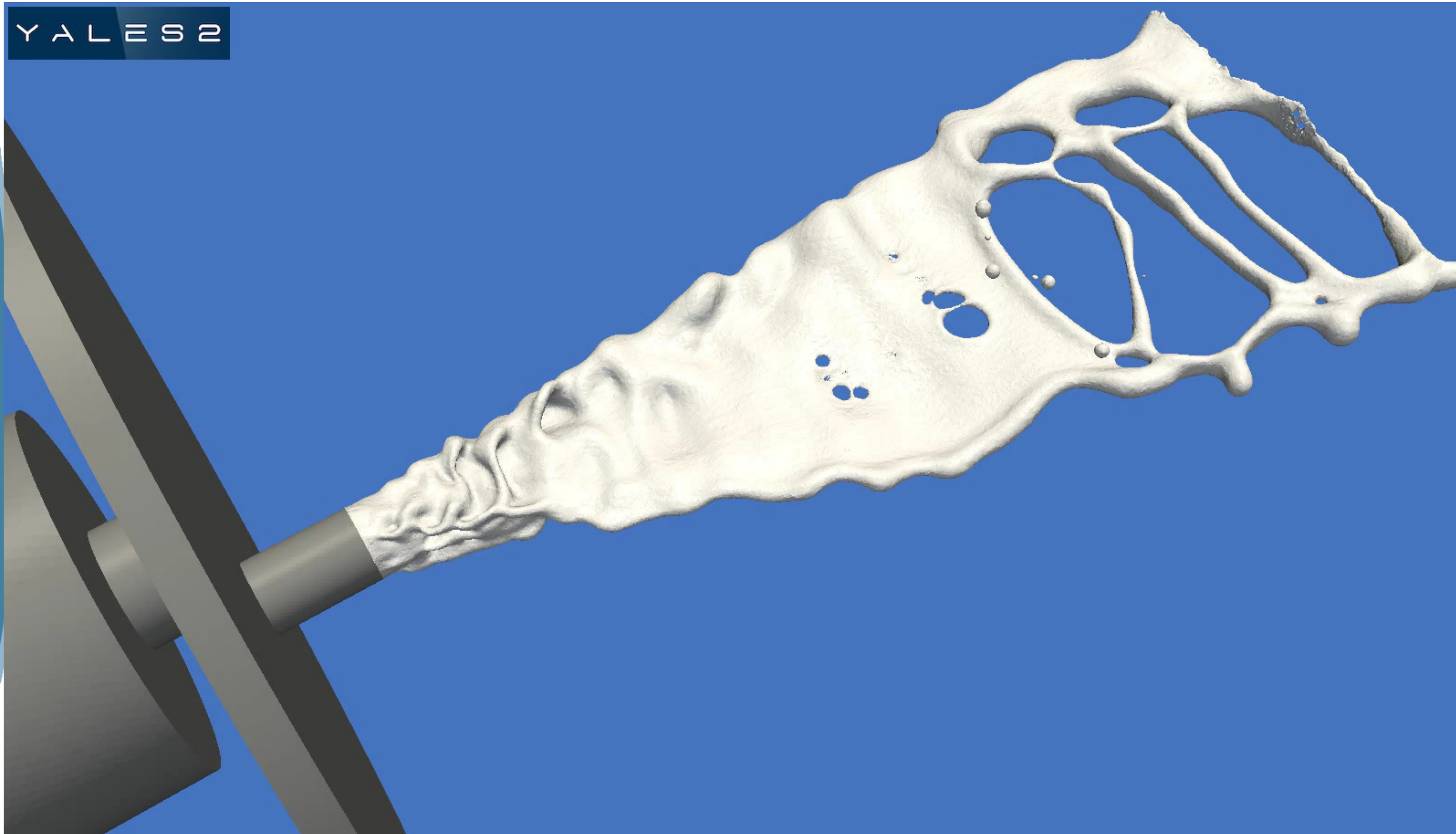
- **Badly conditioned Poisson equation**

$$\nabla \cdot \frac{1}{\rho} \nabla P = RHS$$

- **CPU hours from the X-VAMPA PRACE project (5th call)**

The triple disk injector: fine calculations

- Mesh: 1.6B cells with a cell size of 2.5 μm, 8192 cores (Curie,CEA)
- The optimized DPCG solver is 71.9% faster than the classical DPCG

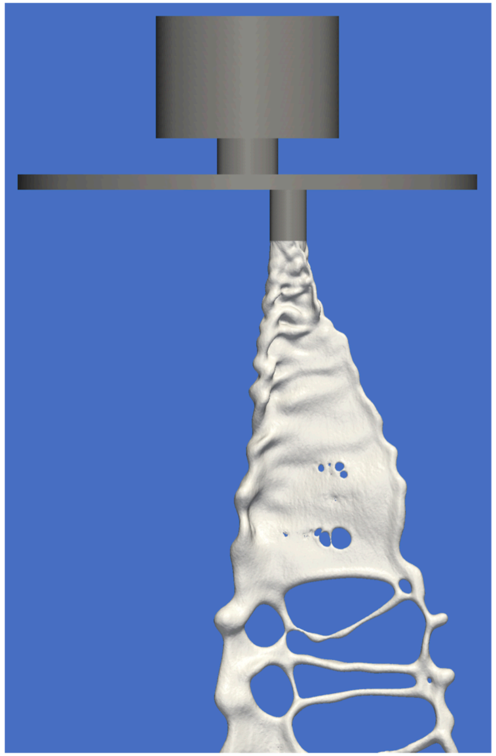


The triple disk injector: mesh refinement study

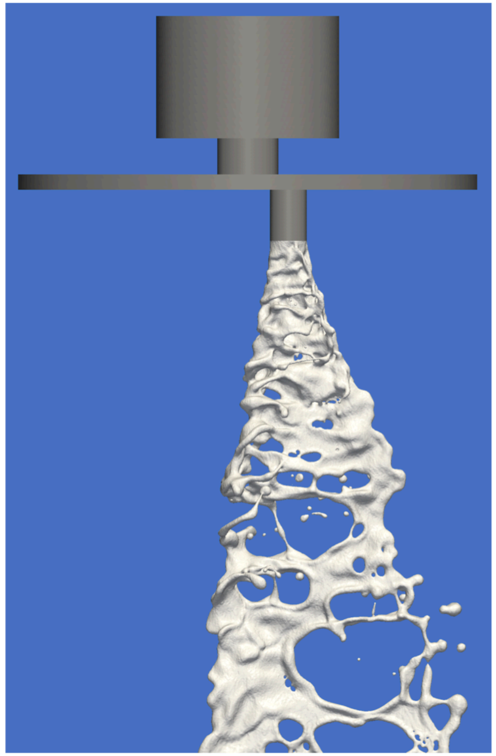
- **Primary atomization is highly non-linear and requires very fine mesh resolution in order to capture the instabilities at the basis of the jet that are responsible for the break-up**

25M tets, Δx = 10 μm

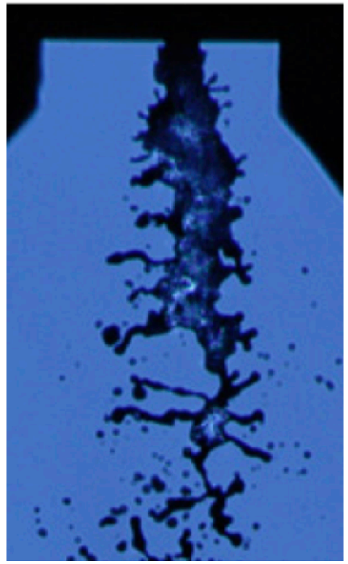
200M tets, Δx = 5 μm



1.6B tets, Δx = 2.5 μm

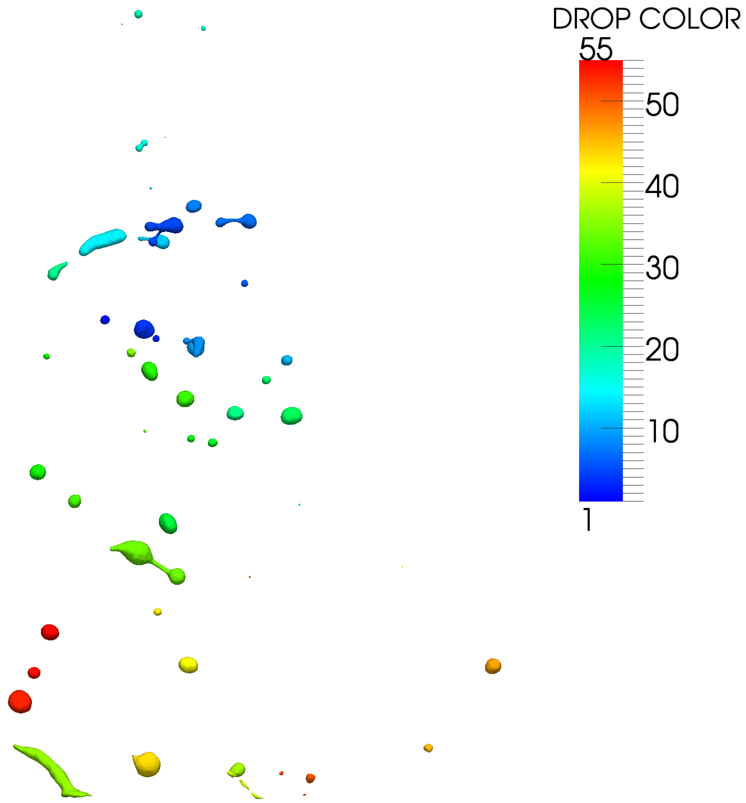


experiment

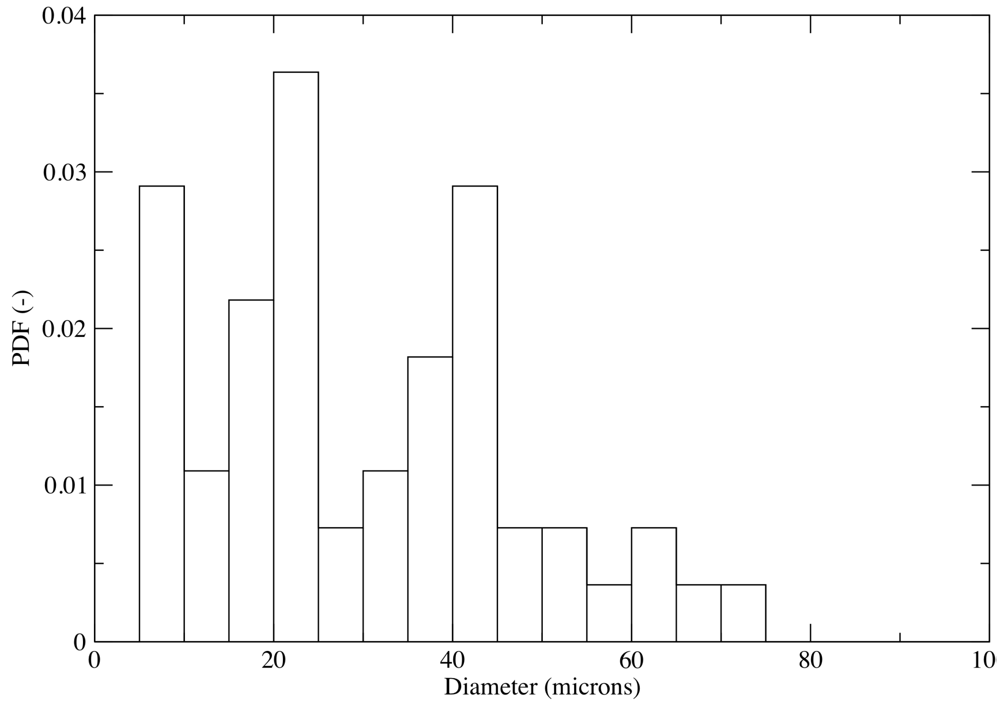


The triple disk injector: analysis

- A droplet identification algorithm has been applied in the triple disk injector on 4096 cores



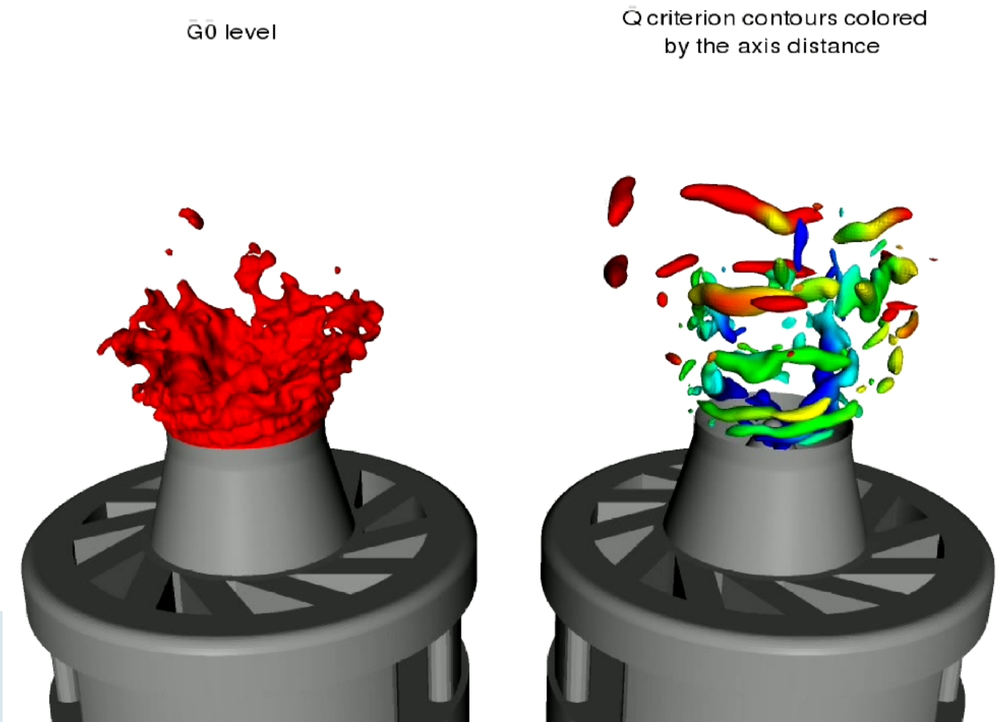
55 droplets identified on the present snapshot



Application to the simulation of swirl burner dynamics

The Precessing Vortex Core

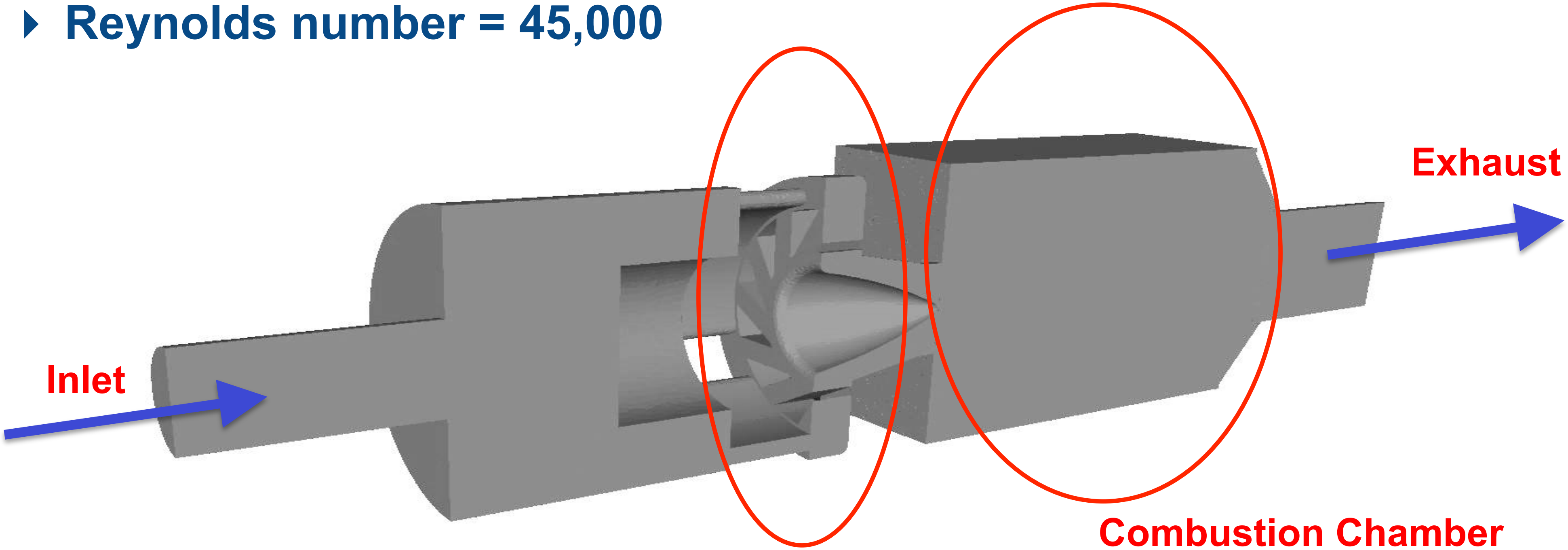
- **The PVC plays an important role in swirl flames (Syred, 2006)**
  - **It is well characterized for isothermal flows but its behavior is more complex for reacting flows**
  - **Its presence strongly depends on the flow topology (Hermeth et al., 2013)**
  - **It may couple non-linearly to thermo-acoustic modes (Durox et al., 2013)**
  - **It may play a role in the spatial distribution of fuel droplets (Linassier 2011, Sierra Sanchez 2012, …)**



Moureau et al., JCP 2007

PRECCINSTA burner

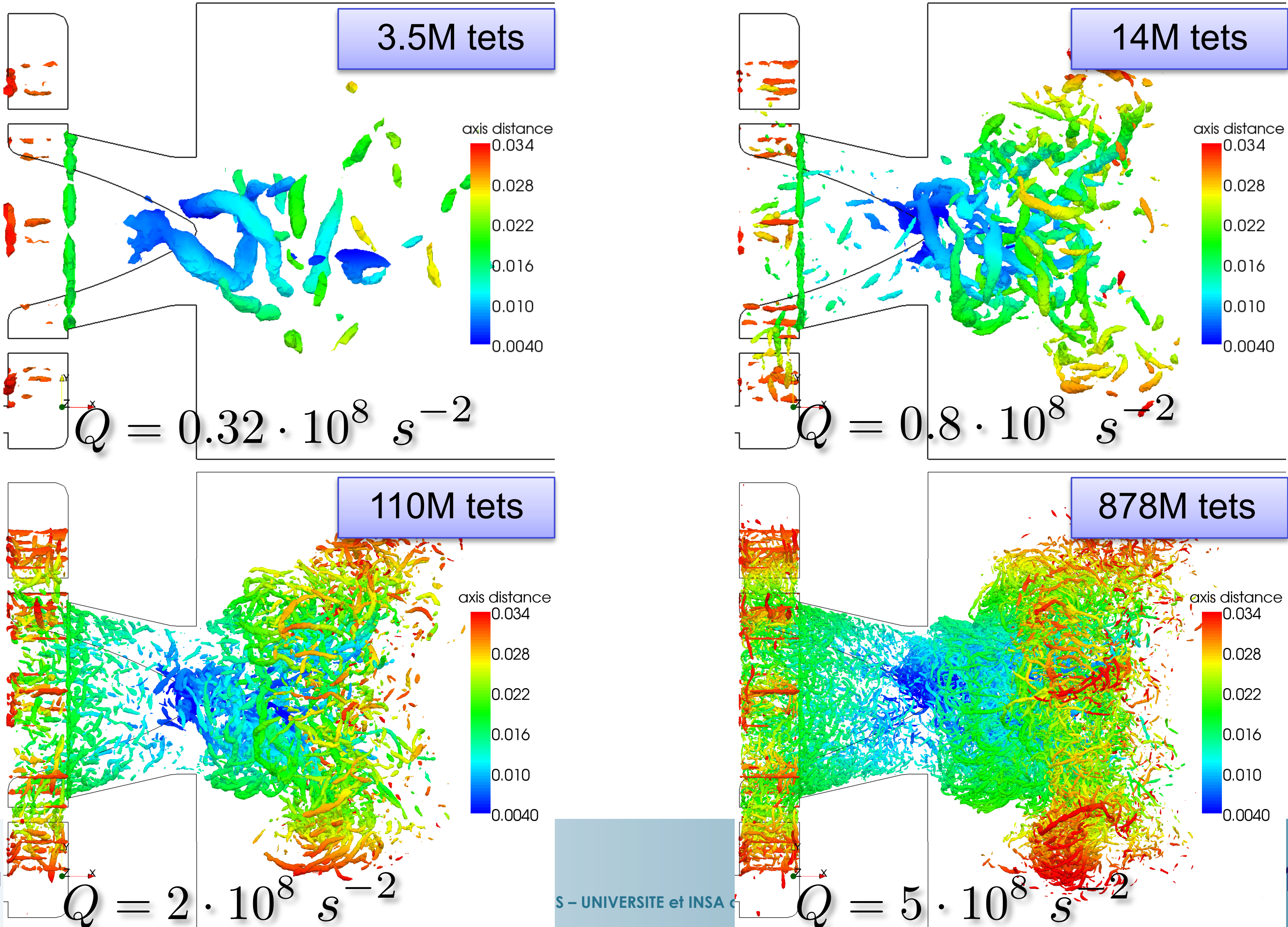
- Industrial lean air/methane burner designed by Turbomeca (SAFRAN)
- Reynolds number = 45,000



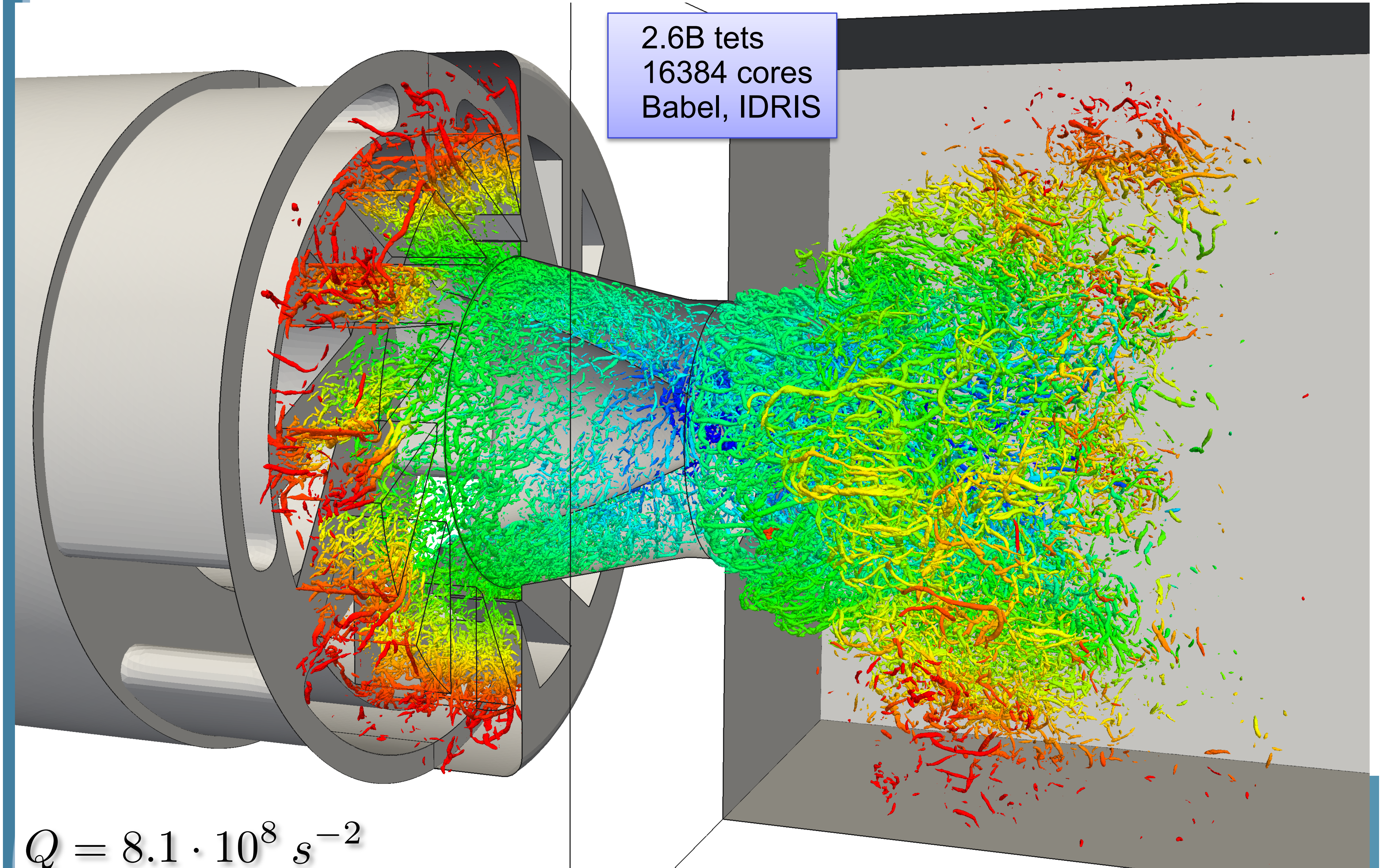
- Roux et al., Combustion and Flame (2005)
- Moureau et al., Journal of Computational Physics (2007a,2007b)
- Galpin et al., Combustion and Flame (2008)
- Moureau et al., Combustion and Flame (2011)
- Franzelli et al., Combustion and Flame (2012)
- …

Mesh refinement study of the smallest resolved scales

- **For HIT, the Q-criterion at the cut-off freq. scales as** $Q \simeq \epsilon^{2/3} \Delta^{-4/3}$

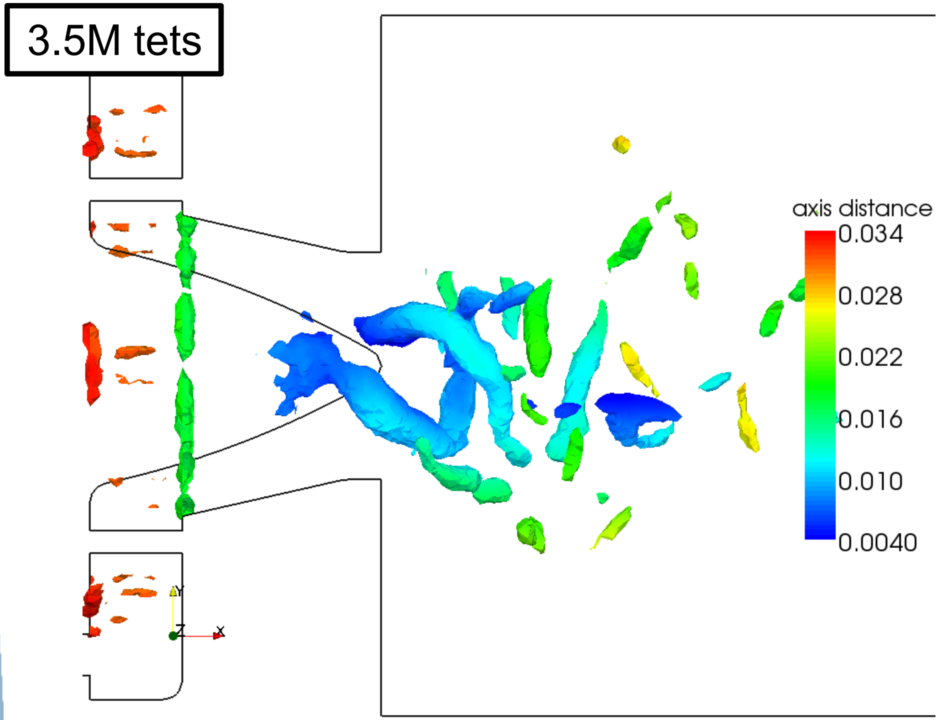


PRECCINSTA: coherent structures (2/2)

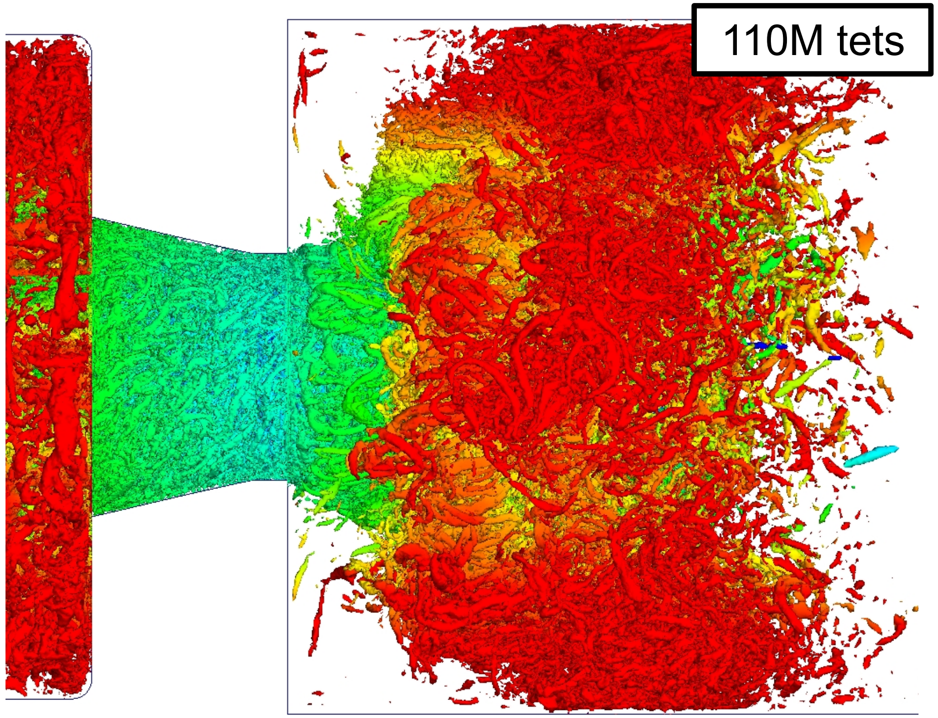


$Q = 8.1 \cdot 10^8\ s^{-2}$

A data-mining challenge: large-scale feature extraction



$$Q = 0.32 \cdot 10^8 \ s^{-2}$$



$$Q = 0.32 \cdot 10^8 \ s^{-2}$$

- **Issue with the Q-criterion (based on L2 norm of velocity gradients)**
  - **High values => smaller strutures resolved on the mesh**
  - **Low values => large structures + smaller ones**
- **Solution: filtering of the solution**

A data-mining challenge: large-scale feature extraction

High-order implicit filter (L. Guédot et al.)

- **1D description of the filter (Raymond et al.)**

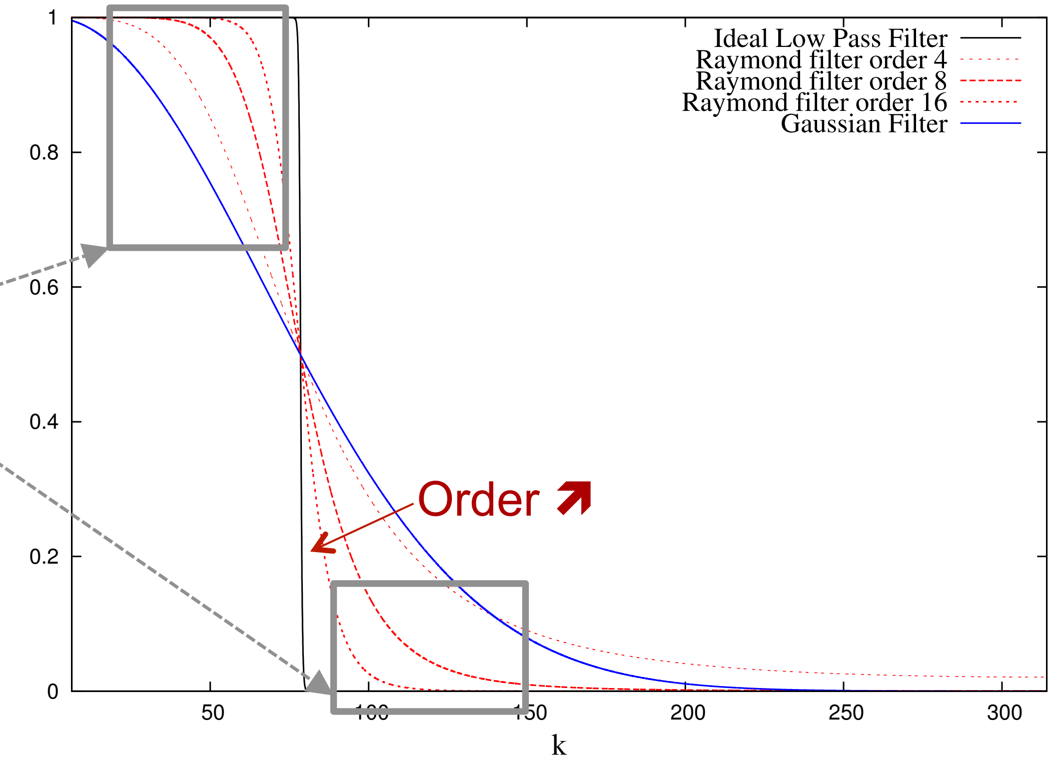
$$\bar{\phi} + \beta^p D^p \bar{\phi} = \phi \text{ with } \beta = \frac{\Delta x^2}{-4\sin^2(k_c \Delta x/2)}$$

D = second order derivative operator
Δx = homogeneous grid spacing
$2p$ = filter order
$k_c = \frac{2\pi}{\Delta}$ (cut-off wave number)
Δ = filter width

- **Damping function**

$$\frac{\bar{A}}{A} = \left(1 + \frac{\sin^{2p}(k\Delta x/2)}{\sin^{2p}(k_c\Delta x/2)}\right)^{-1}$$

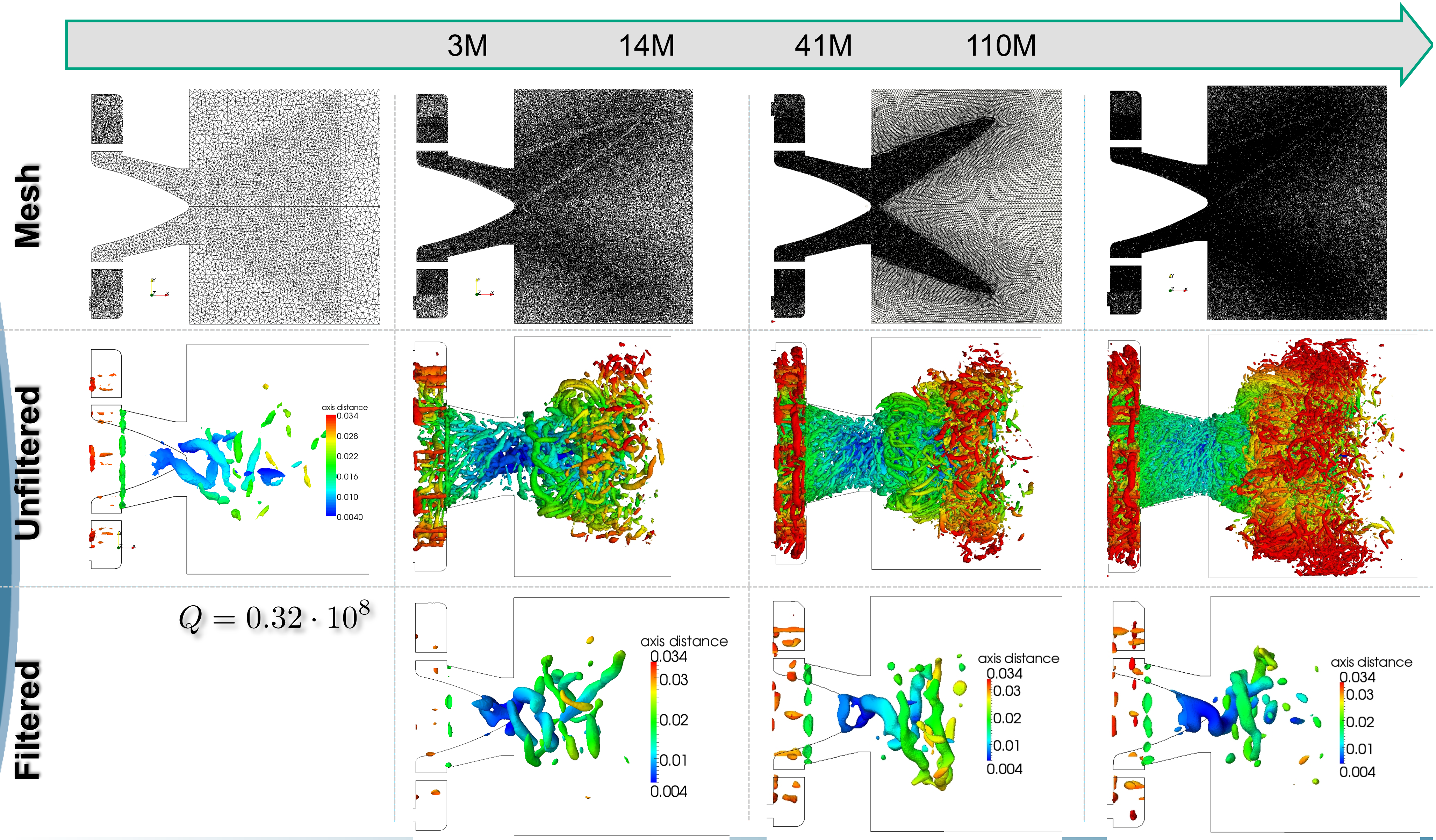
  - Large structures less dissipated
  - Small structures more dissipated



- **Numerics :**
  - Factorization
  - Solving of multiple Conjugate Gradient in the Complex domain

L. Guédot, G. Lartigue, V. Moureau, Design of high-order implicit filters on unstructured grids for the identification of large scale features in large-eddy simulations, DLES9, 2013
W.H. Raymond, A review of recursive and implicit filters. Monthly Weather Review, 1991

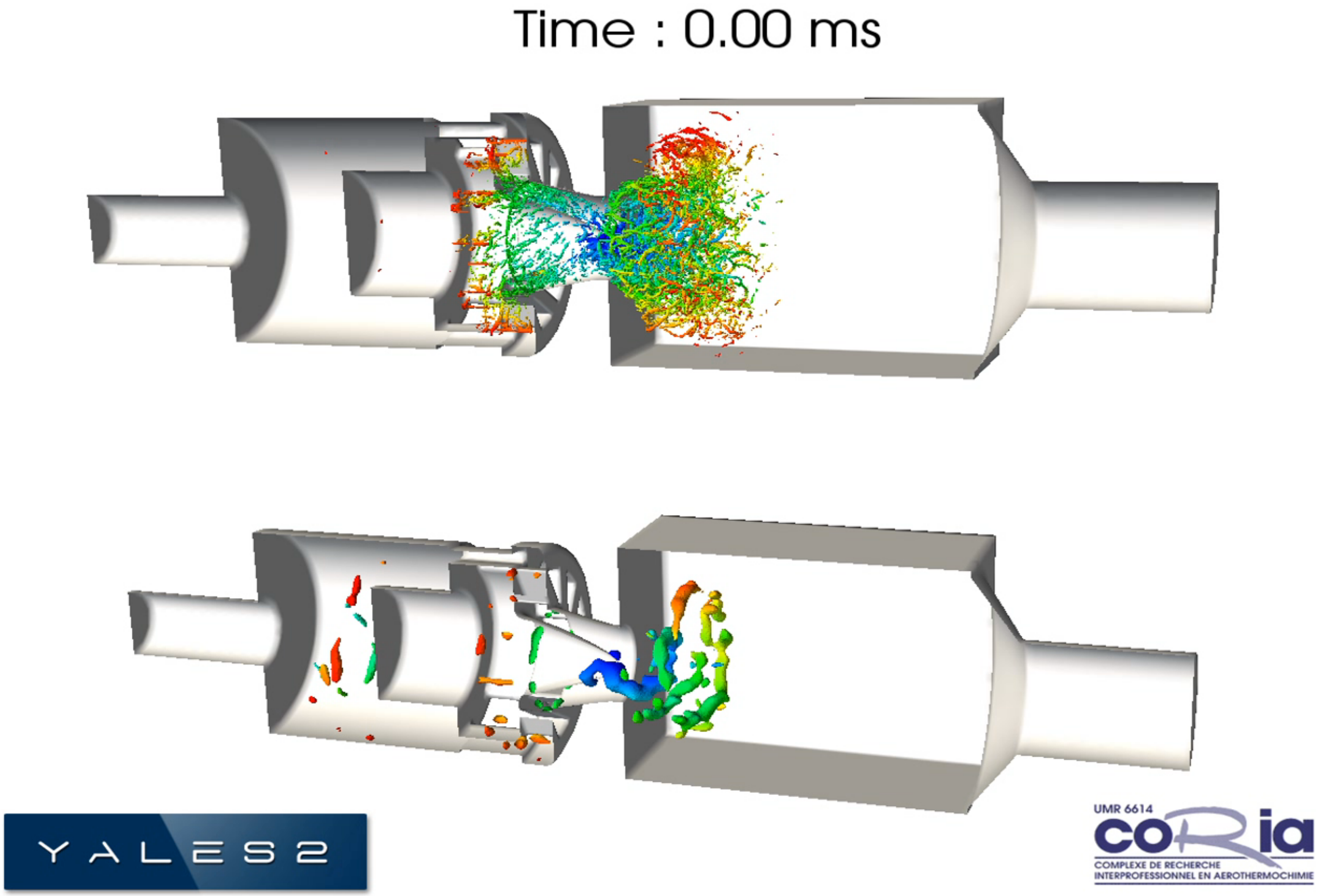
A data-mining challenge: large-scale feature extraction



The high-order filters successfully extract large-scale features on massive unstructured grids

A data-mining challenge: large-scale feature extraction

- With optimized filters, making a video of the PVC is feasible



110M tets

Conclusions & perspectives

Conclusions & Perspectives

- **HPC is a strong driving mechanism in the modeling of aeronautical combustors**

- **Many ingredients are required to build a scalable 3D unsteady combustion solver**
  - **Multi-level mesh partitioning**
  - **Highly efficient linear solvers**
  - **Suitable combustion models and algorithms**

- **The pre- and post-processing of billion cell simulation are still difficult**

- **Some remaining challenges**
  - **Data-mining for large-scale feature extraction**
  - **Efficiency of low-Mach number algorithms (linear solvers) on 1 million cores**

References & Acknowledgements

References

- Malandain, M., Maheu, N., and Moureau, V., “Optimization of the deflated Conjugate Gradient algorithm for the solving of elliptic equations on massively parallel machines“, J. Comp. Physics, 2013, 238, 32-47
- Maheu, N., Moureau, V., Domingo, P., Duchaine, F. & Balarac, G., « Large-eddy simulations of flow and heat transfer around a low-mach turbine blade ». CTR Summer Program. Center for Turbulence Research, NASA Ames/Stanford Univ, 2012.
- Moureau, V., Domingo, P., and Vervisch, L., "From Large-Eddy Simulation to Direct Numerical Simulation of a lean premixed swirl flame: Filtered Laminar Flame-PDF modelling", Comb. and Flame, 2011, 158, 1340–1357
- Moureau, V., Domingo, P., and Vervisch, L., "Design of a massively parallel CFD code for complex geometries", Comptes Rendus Mécanique, 2011, 339 (2-3), 141-148

Acknowledgements

- G. Lartigue, E. Noel, P. Domingo, L. Vervisch, Y. D’Angelo
- O. Desjardins, P. Pepiot, …
- PhD and internship students: P. Benard, C. Gruselle, L. Guédot, N. Maheu, M. Malandain, F. Pecquery, T. Roger, …
- Computing centers: IDRIS, TGCC, CINES, CRIHAN, JULICH