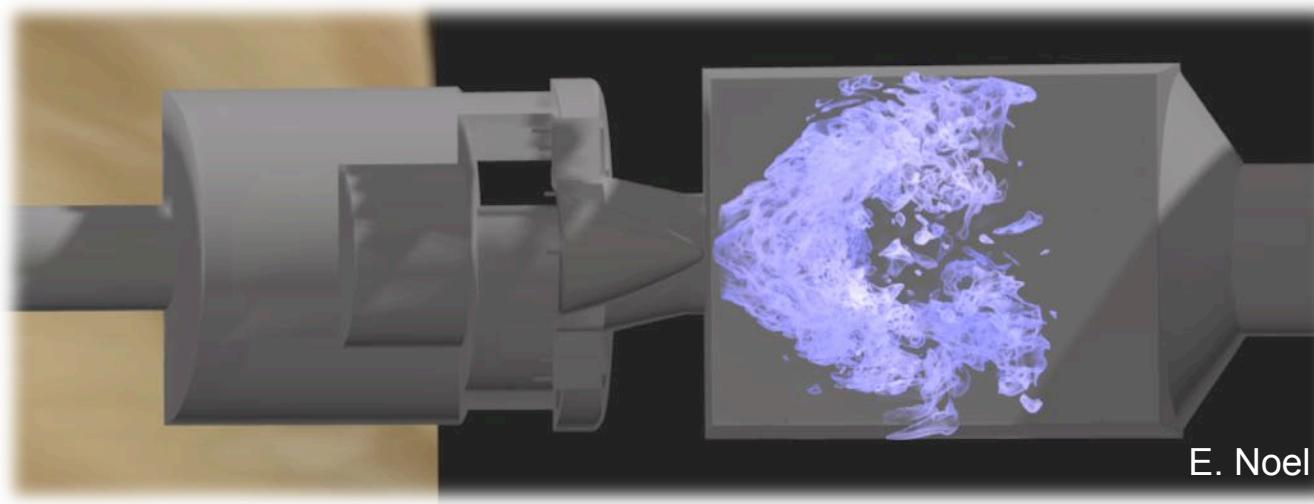


High-performance computing for turbulent combustion modeling

Strategies and challenges



V. Moureau, G. Lartigue

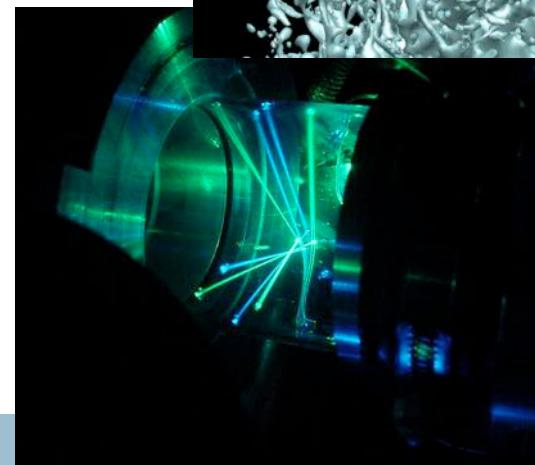
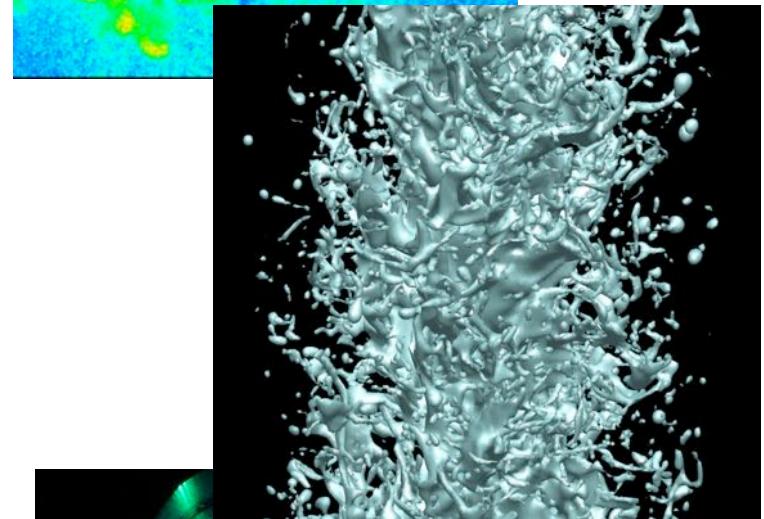
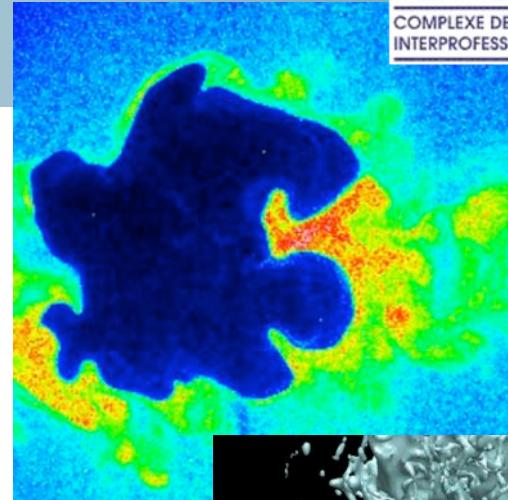
CORIA, CNRS UMR 6614, University and INSA of Rouen, France

<http://www.coria-cfd.fr>

ETSN, 19 – 23 janvier 2015, Puy Saint-Vincent

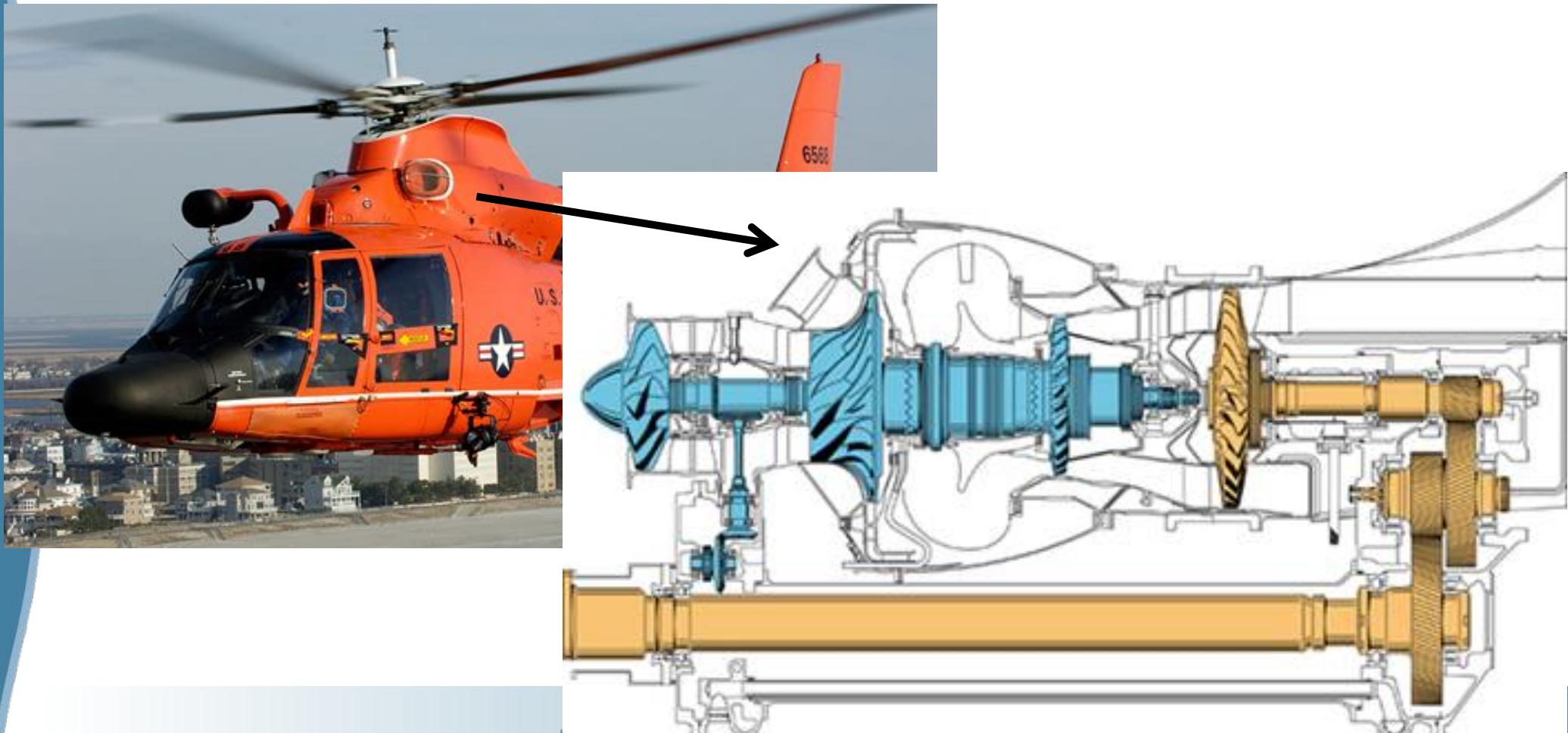
The CORIA lab

- ▶ Joint lab from CNRS, INSA and University of Rouen
- ▶ Located in Rouen (1h from Paris)
- ▶ Key figures
 - 180 employees, 56 senior researchers
- ▶ 3 departments
 - Reactive flows
 - Turbulence, atomization and sprays
 - Optics and lasers
- ▶ Combustion modeling team
 - In the reactive flows department
 - 7 researchers
 - Prof Luc Vervisch, Dr Pascale Domingo, Dr Vincent Moureau, Dr Guillaume Ribert, Dr Ghislain Lartigue, Dr Guido Lodato, Prof Yves D'Angelo,
 - 12 PhDs



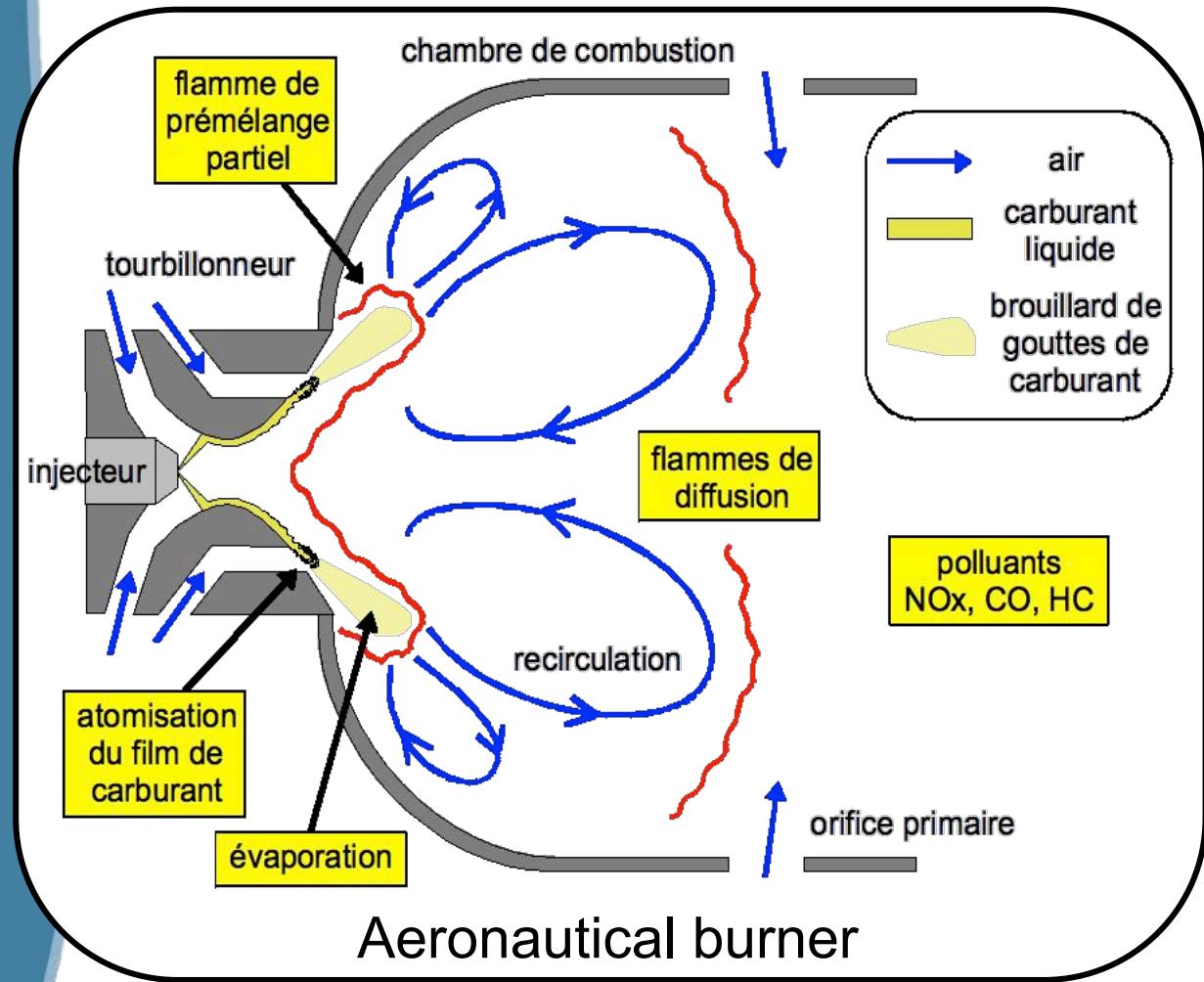
■ Why trying to model turbulent combustion ?

- ▶ 86% of the usable energy on earth is obtained through combustion
- ▶ Combustion occurs in many applications
 - Aeronautical engines, automotive industry, furnaces, ...



The challenge

Many phenomena at very different scales

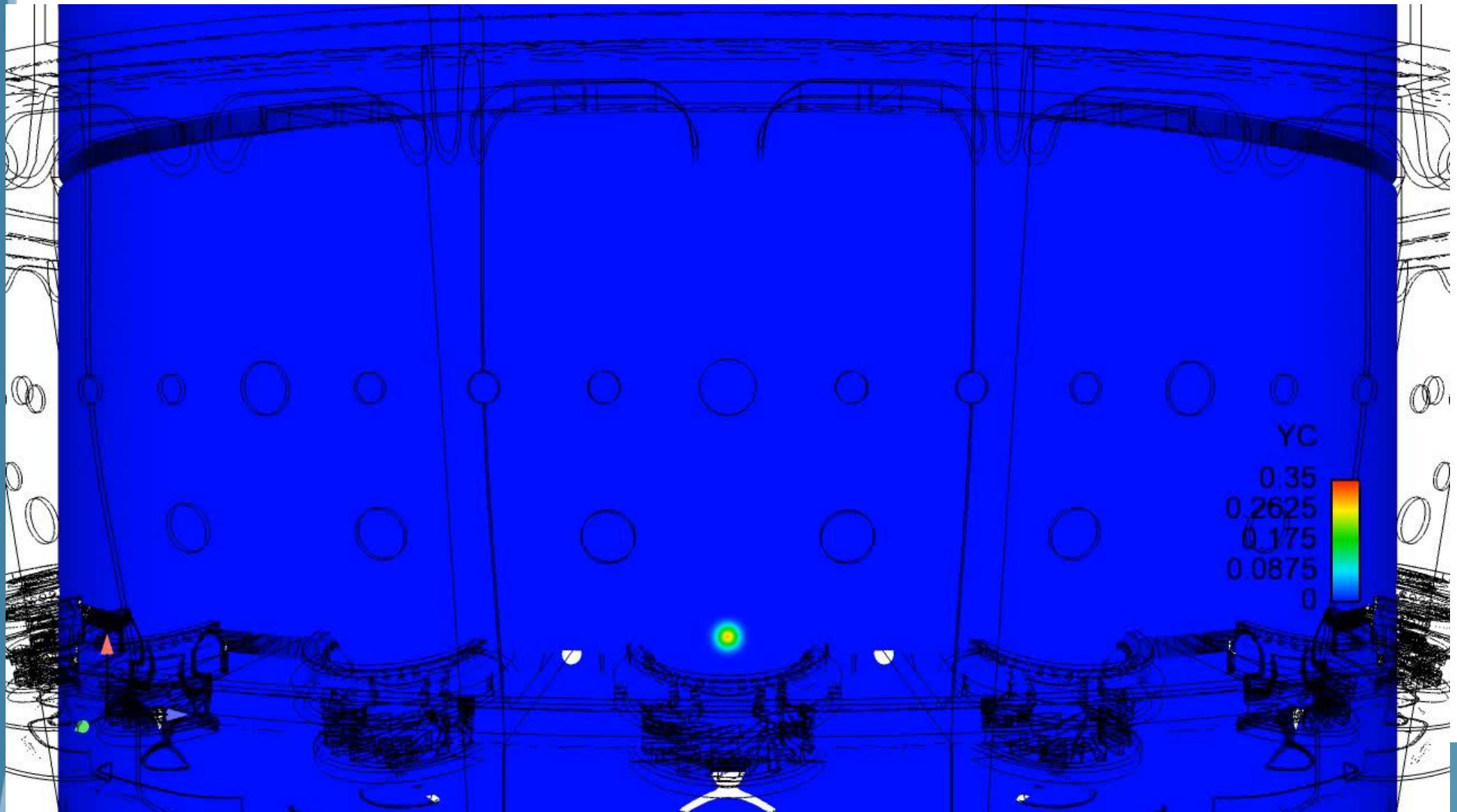


Turbulence	10 mm 0.01mm
Atomization	0.1 mm
Spray transport	10 μm
Evaporation	10 μm
Combustion	0.1 mm

3 to 4 orders of magnitude

■ 2012 extreme calculation: LES of an ignition sequence in a 360° SNECMA combustor

- ▶ 160M tets, 20h on 2048 cores of Airain (J. Leparoux and G. Godel)

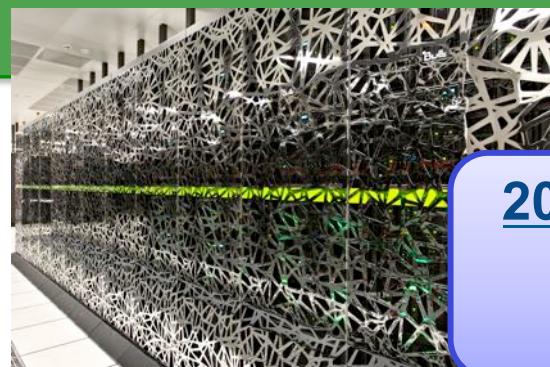


Estimate of resources required for future large-scale computations

- ▶ Simulation time for an aeronautical combustor with a mesh of 10 billion tets (2020 target)



PC : 530 years
with 6 cores



Server
6 years with
256 cores

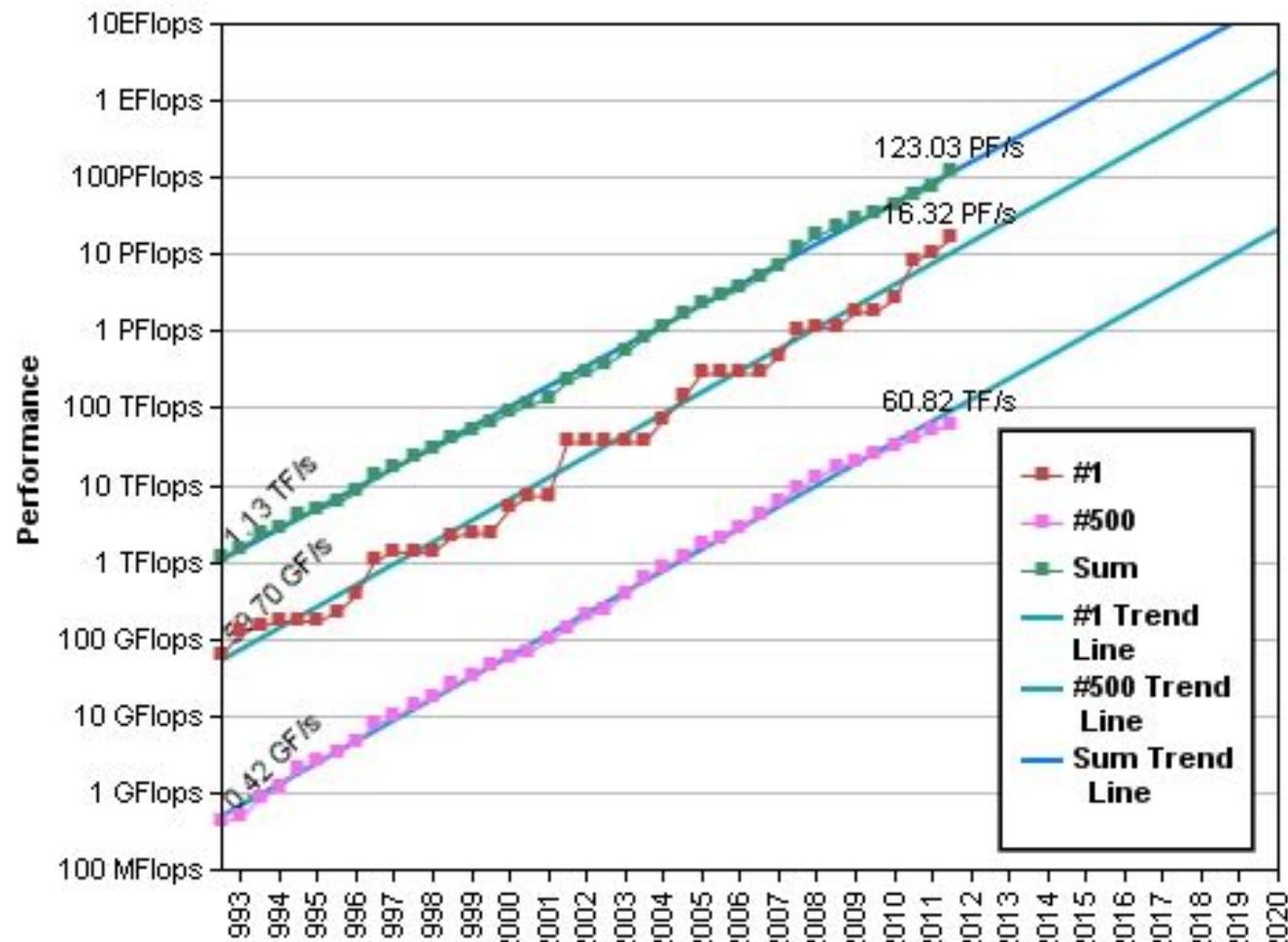
2020 exascale system
1 day with XX million cores

power

- ▶ Many issues have to be addressed
 - Mesh management, solving of large linear systems, load balancing of chemistry integration, data-mining, ...

The CFD driving mechanism

► Moore's law: the power of super-computers doubles every 18 months

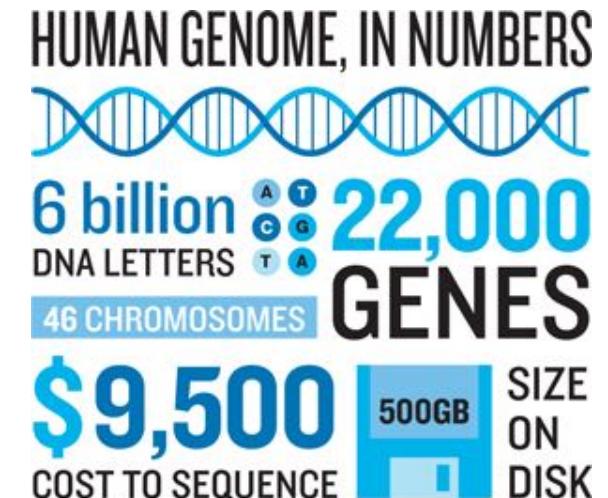


<http://www.top500.org/>

The « big data » challenge

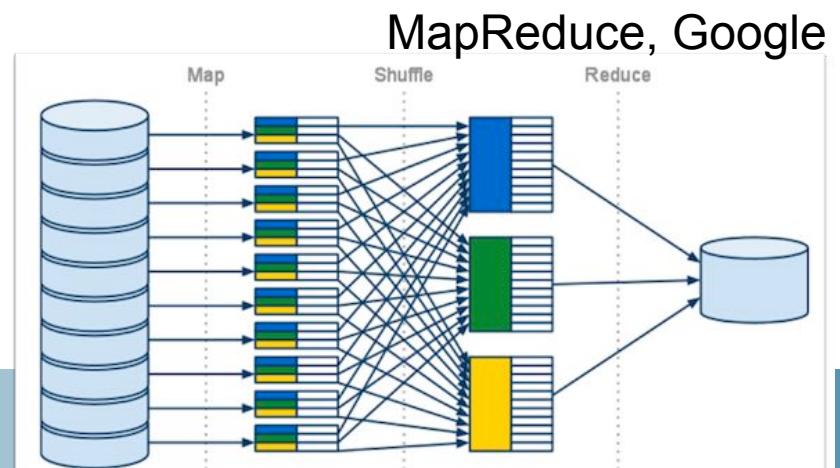
► Large data sets are encountered in many fields

- Internet
- Finance
- Weather forecast
- Genomics
- Computational Fluid Dynamics (CFD)
- ...



► « Big data » denotes a set of techniques used for processing these large amounts of data

- Data partitioning
- Data ordering
- Filtering
- Parallel processing
- ...



■ Outline

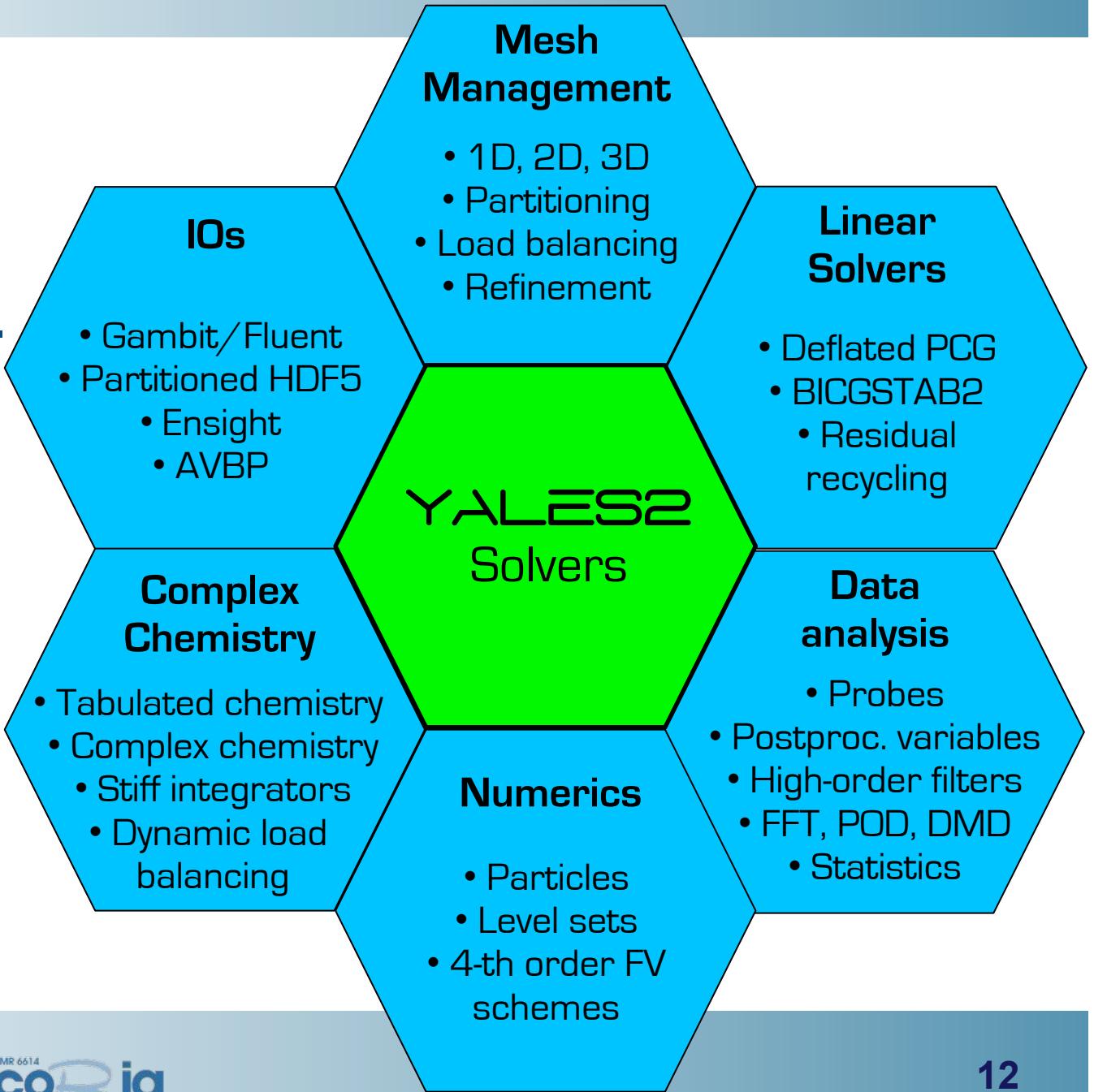
- ▶ **Context**
- ▶ **The YALES2 code**
 - Presentation
 - Specific features of the code
 - Feedback on the development of HPC codes
- ▶ **Case studies**
 - Identification of coherent structures in semi-industrial swirl burners and their interactions with the spray
 - Modeling of heat transfer on a low-Mach number turbine blade
 - Prediction of pollutant emissions in a meso-scale combustion device
 - Large-Eddy Simulation of innovative offshore wind turbines
 - Parallel mesh adaptation and load balancing
- ▶ **Conclusions & Perspectives**

The YALES2 code

- ▶ **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 on massively parallel machines
- ▶ It is used by more than 160 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, ...
 - Collaboration with INTEL/CEA/GENCI/UVSQ Exascale Lab
 - Industry: SAFRAN, RHODIA (SOLVAY), AREVA, ...
- ▶ **Awards**
 - 2011 IBM faculty award
 - 3rd of the Bull-Joseph Fourier prize in 2009
 - Principal investigator of 2 PRACE proposals

The YALES2 library (version 0.5.0)

- ▶ 2 main maintainers
 - V. Moureau
 - G. Lartigue
- ▶ 300 000 lines of object-oriented f90 and f2003
- ▶ Git version management
- ▶ www.coria-cfd.fr
- ▶ Portable on all the major platforms (even ARM or Xeon Phi proc.)



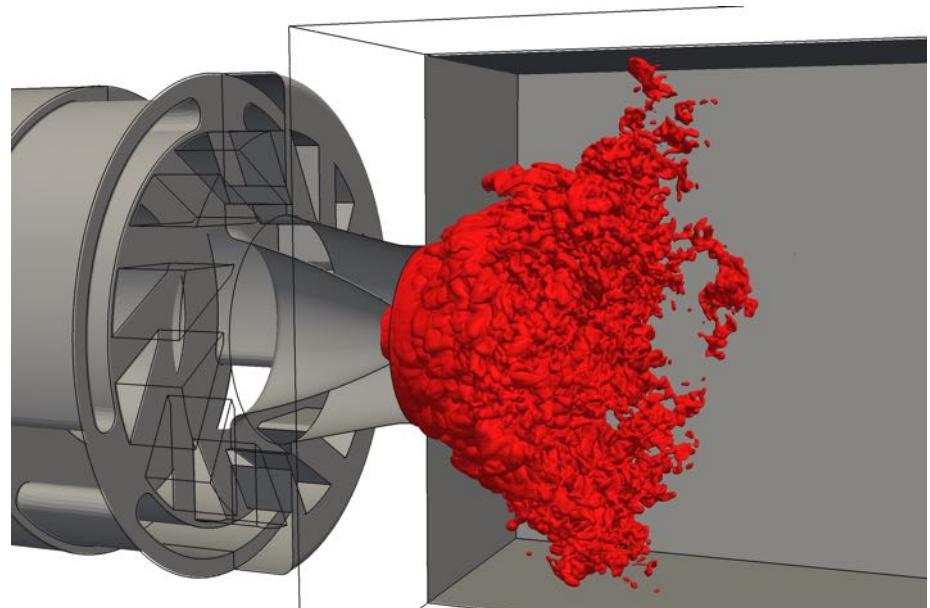
The YALES2 solvers

► Mature solvers

- Scalar solver (SCS)
- Level set solver (LSS)
- Lagrangian solver (LGS)
- Incompressible solver (ICS)
- Variable density solver (VDS)
- Spray solver (SPS)
- Magneto-Hydrodynamic solver (MHD)
- Heat transfer solver (HTS)
- Linear acoustics solver (ACS)
- Chemical reactor solver (CRS)

► Work in progress

- Mesh movement solver (MMS)
- ALE solver (ALE)
- Radiative HT solver (RDS)
- Explicit compressible solver (ECS)
- Immersed boundary solver (IBS)
- Darcy solver (DCY)



PRECCINSTA Burner

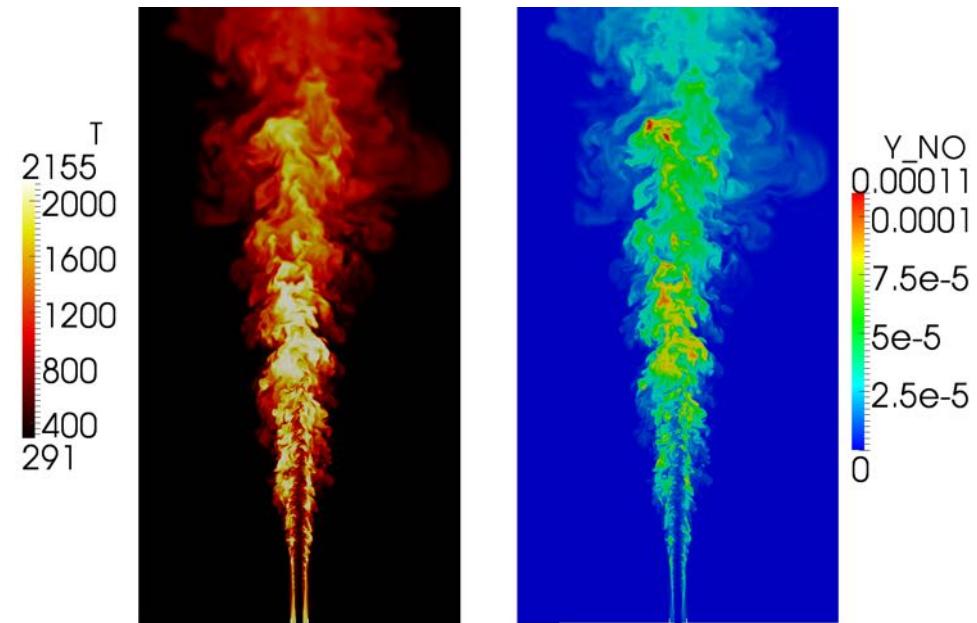
2.6 billion cells, 16384 cores of BG/P

More details:

- www.coria-cfd.fr
- www.youtube.com/user/CoriaCFD

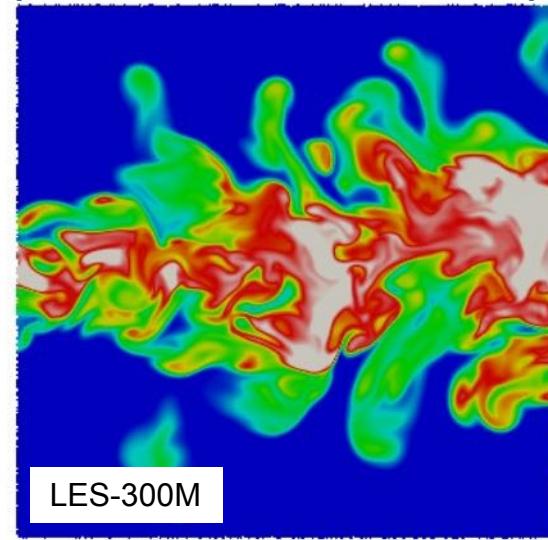
■ Some studies with YALES2

NOx prediction in jet flames (F. Pecquery, C&F 2014)



Flame kernel expansion in stratified mixture

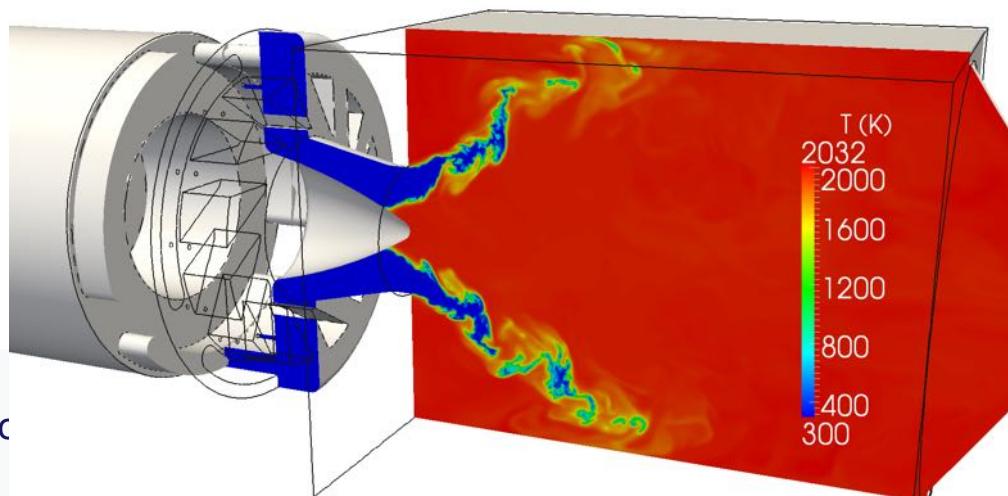
(C. Gruselle, C&F, sub.)



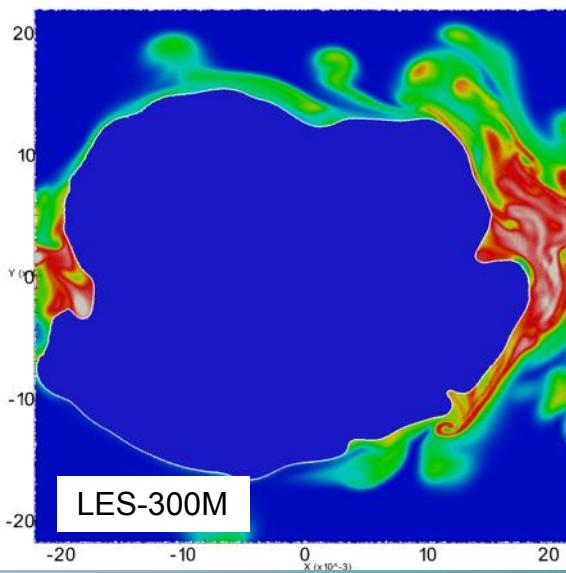
Mixture fraction

Investigation of partial premixing in a swirl burner

12B tets, 16384 cores of Curie, MS-COMB PRACE project

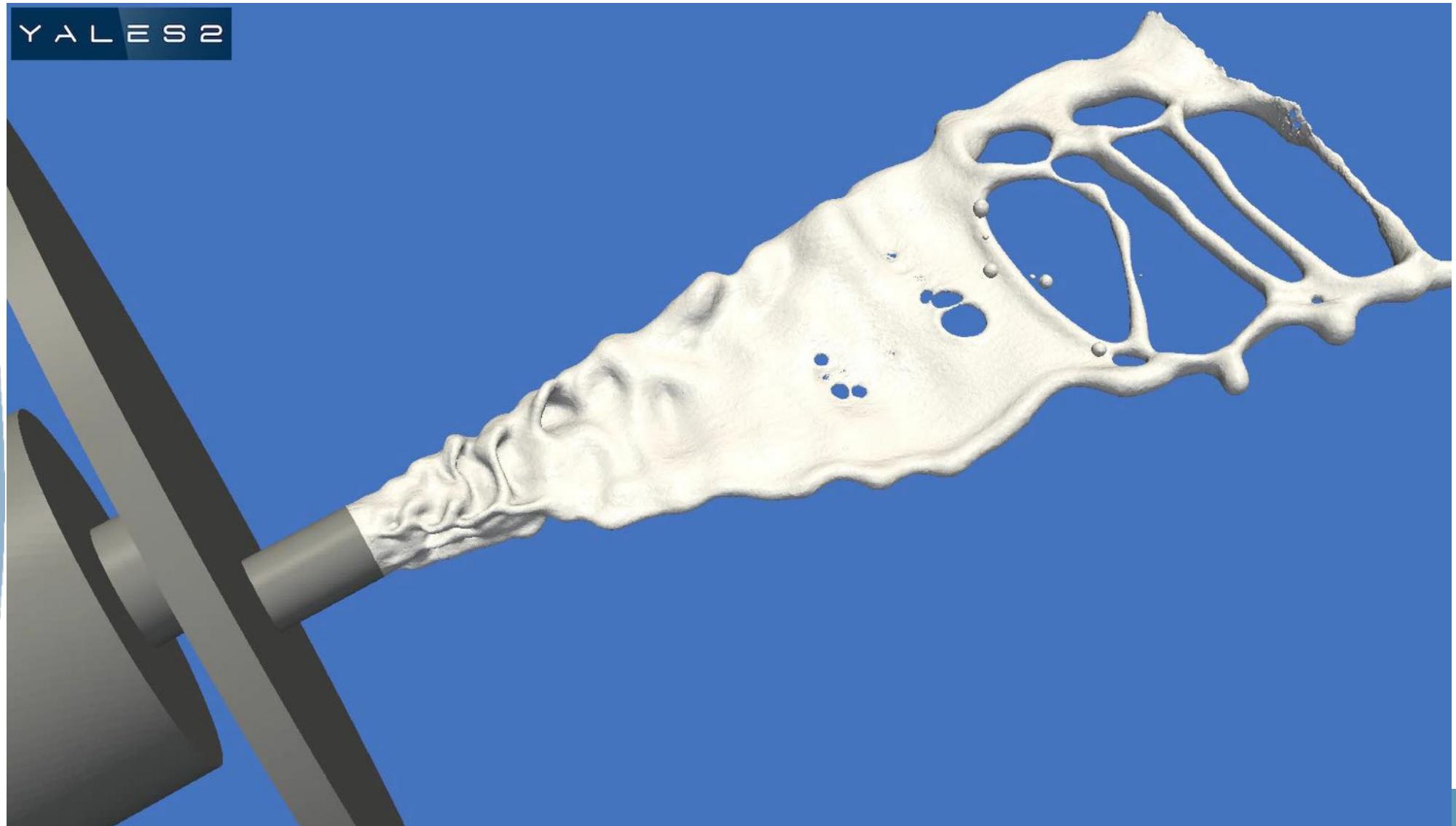


et INSA de Rouen



Some studies with YALES2 Primary atomization

- ▶ 1.6 billion cells, Curie machine, TGCC, CEA



V. Moureau, CORIA

■ Some studies with



- ▶ Project led by S. Mendez and F. Nicoud @ I3M, Montpellier

Vort. mag.



C. Chnafa
2012



CNRS – UNIVERSITE et INSA de Rouen



A few lesson learned during the development of HPC codes

- ▶ Software engineering is very important when the number of lines and users increases
- ▶ Some key ingredients
 - Versioning system: **git + SourceTree + gitorious.coria-cfd.fr**
 - Inline documentation: **doxygen**
 - Automated building of the code on various architectures: **Jenkins**
 - Automatic verification and validation tests
 - Centralized documentation and bug tracking: **yales2.coria-cfd.fr**
- ▶ When working with industrials, new constraints emerge
 - Specific software environment (Windows...)
 - Graphical User Interface !!! : OpenTea/C3SM GUI generation by CERFACS

SourceTree

The screenshot shows the SourceTree application interface for a Git repository named 'yales2-trunk'. The main window displays a timeline of commits, a detailed commit view, and a diff viewer.

File Status: Working Copy

Branches:

- CORIA**:
 - closed_volume
 - adaptation
 - AV_scalars
 - Ben
 - c3sm
 - cav
 - compressible
 - compressible2
 - deflation
 - deflation2
 - dev_curie_last
 - dynamic
 - element_weighting
 - high_order_filters
 - improved_implicit_diffusion
 - lastTFLES_merge_dynScheduler...
 - ms_openmp
 - pointcloud
 - starfish4
 - yales2_lite
- EM2C**:
 - ftacles
 - ftacles2
 - ftacles3
 - palm
- EXASCALE**:
 - master
 - optim
 - optim_allocatable
- I3M**:
 - tracers
- IMFT**:
 - two_phase_euler
- master**: (selected)
- SAFRANTECH**:
 - dynamic_adaptation
- ULB**:
 - Bernard_RT
 - update_solver_mhd
- old_svn_versions**

Timeline (All Branches):

Description	Commit	Author	Date
Added a temperat...	9231b6b	Vincent MOUREAU <vincent....	Jan 20, 2015, 0:35
* Refactoring lagra...	ce12f40	Benjamin Farcy <benjamin.far...	Jan 19, 2015, 16:58
* Clean-up	e204093	Vincent Moureau <vincent.mo...	Jan 17, 2015, 21:56
* NOT WORKING. Refactoring lagrangian. backup of a devel version.	bf4f316	Benjamin Farcy <benjamin.far...	Jan 16, 2015, 16:31
Added source term mask for reactive scalars	fd5ff4c	Lola Guedot <lola.guedot@co...	Jan 16, 2015, 15:56
Merge branch 'CORIA/mask_source_terms' of shannon.insa-rouen.fr:ho...	76e112e	Vincent MOUREAU <vincent....	Jan 16, 2015, 15:38
* bug correction	2d6c182	Vincent MOUREAU <vincent....	Jan 16, 2015, 11:23
* Added the Safran Tech platform	6591fa4	Vincent MOUREAU <vincent....	Jan 16, 2015, 11:23
* Bug correction	6e98ada	Vincent MOUREAU <vincent....	Jan 16, 2015, 11:04
Merge branch 'master' into SAFRANTECH/merging	7263ec1	Vincent MOUREAU <vincent....	Jan 16, 2015, 10:58
Dynamic mesh adaptation	e161f0e	Vincent MOUREAU <vincent....	Jan 16, 2015, 10:45
* Added T = INITIAL_FIELD for multispecies VDS calculations	a0b3d13	Vincent MOUREAU <vincent....	Jan 16, 2015, 10:44
* Change to the occigen platform	99802a0	Vincent MOUREAU <vincent....	Jan 15, 2015, 18:02
Refactoring lagragian. oneway/toway ok	9b20d6d	Vincent MOUREAU <vincent....	Jan 15, 2015, 16:25
Refactoring lagrangian ...	0027624	Vincent MOUREAU <vincent....	Jan 14, 2015, 22:33
Refactoring lagrangian ...	e823507	Benjamin Farcy <benjamin.far...	Jan 14, 2015, 16:51
Refactoring lagrangian ...	e402a58	Benjamin Farcy <benjamin.far...	Jan 13, 2015, 19:58
Some tests with the cavitation solver	a7fd63a	Vincent MOUREAU <vincent....	Jan 13, 2015, 18:32
Update of the occigen platform	4f3c0a7	moureauv <moureauv@occige...	Jan 13, 2015, 18:29
Refactoring lagrangian in progress	7f60164	Benjamin Farcy <benjamin.far...	Jan 13, 2015, 17:52
Merge commit '40d2c6be288b30eb07e829167bdb6a47930b...' into 'master'	a770a2b	Locci Carlo <carlo.locci@hot...	Jan 13, 2015, 9:57

Commit View (e161f0e5ab1cec2929edcb478860b1a41):

Commit: e161f0e5ab1cec2929edcb478860b1a41
Parents: 99802a030b, 06445b7305
Author: Vincent MOUREAU <vincent.moureau@coria.fr>
Date: January 16, 2015 at 10:45:44
GMT+1
Labels: yales2private.coria-cfd.fr/master
yales2devel.coria-cfd.fr/master
yales2_safrantech.coria-cfd.fr/master
yales2_pierre/master
yales2_milou/master yales2.coria-cfd.fr/master master

Diff Viewer (src/main/grid_adaptation_m.f90):

Hunk 1 : Lines 1-31

```
1 1 !*****
2 2 !***** COPYRIGHT (C) 2006-2014, CORIA - CNRS, ALL RIGHTS RESERVED. *****
3 3 !*****
4 4 !-----#
5 5 #! <MODULE NAME=grid_adaptation_m>
6 6 #! <DESCRIPTION>
7 7 !#   routines to adapt a grid in parallel
8 8 #! </DESCRIPTION>
9 9 !-----
10 10 module grid_adaptation_m
11 11
12 12 - use defs_m,          only: WP, LEN_MAX, alargeint, ahuge, small
13 13 + use defs_m,          only: WP, LEN_MAX, alargeint, ahuge, small, one_third
14 14 use mpi_m,
15 15 - use misc_m,          only: are_bbox_intersecting, bbox_distance
16 16 + use misc_m,          only: use_r1_buffer, use_i1_buffer, free_r1_buffer, free_i1_buffer
17 17 + use buffers_defs_m,   only: use_r1_buffer, use_i1_buffer, free_r1_buffer, free_i1_buffer
18 18 + use conn_defs_m,      only: elem_face2node, NFACE_OF_ELEMENT
19 19 + use buffers_defs_m,   only: use_r1_buffer, use_r2_buffer, use_i1_buffer, use_i2_buffer, &
```

■ gitorious.coria-cfd.fr

The screenshot shows the Gitorious web interface for the 'yales2' repository. The top navigation bar includes links for Dashboard, Administration, user ~moureauv, 11 notifications, and Logout. The main header features the GITORIOUS logo and navigation tabs for Activities, Projects, and Teams.

Repository Overview: The central area displays basic repository information: Project: yales2, Owner: +yales2admin (through -lartigue), and Created: 23 Jan 13:17. It also shows clone options via SSH and Git URLs, and a search bar.

Activities: A sidebar lists recent activities:

- Tuesday November 12 2013
 - COMMIT 23:34: moureauv deleted branch beta/yales2_0.4.3_beta on yales2/yales2
 - COMMIT 23:34: moureauv created branch releases/yales2_0.4.3 on yales2/yales2
- Sunday November 10 2013
 - PUSH 14:25: moureauv pushed 3 commits to yales2/yales2:beta/yales2_0.4.3_beta. View diff
beta/yales2_0.4.3_beta changed from ada81ed to 01c2549
 - PUSH 14:25: moureauv pushed 3 commits to yales2/yales2:master. View diff
master changed from ada81ed to 01c2549
- Monday November 04 2013
 - PUSH 18:13: moureauv pushed 1 commit to yales2/yales2:master. View diff
master changed from a152609 to ada81ed
 - PUSH 18:13: moureauv pushed 1 commit to yales2/yales2:beta/yales2_0.4.3_beta. View diff
beta/yales2_0.4.3_beta changed from a152609 to ada81ed
 - PUSH 15:57: moureauv pushed 26 commits to yales2/yales2:master. View diff
master changed from 041f819 to a152609
 - PUSH 15:57: moureauv pushed 26 commits to yales2/yales2:beta/yales2_0.4.3_beta. View diff

Right Sidebar: Includes sections for Clone repository, Manage collaborators, Manage read access, Edit repository, Committers (listing Linterweb, Ghislain Lartigue, moureauv, Emmanuel Oseret, Andres Charif-Rubial, Jean-Baptiste Besnard, +yales2admin, +yales2_committer, +yales2), Repository clones (Team clones: yales2-devel, yales2admin), and Personal clones (yangs-yales2, Chen Yang).



CORIA-CFD

Home page
Users
Publications
Conferences

YALES2
Public page
Gallery
Private wiki (login req'd)

SITCom-B
Public page
Gallery
Private wiki (login req'd)

Navigation
Community portal
Recent changes
Help

Toolbox
What links here
Related changes
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Permanent link
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CORIA-CFD

Welcome on the CORIA-CFD wiki!

This wiki is dedicated to the users of CFD codes developed at [CORIA](#), a French combustion laboratory located in Rouen.

The CORIA-CFD platform consists of public and private wikis and svn/trac systems to help in the development of these codes. The codes using this platform are:

- YALES2
- SITCom-B
- H-Allegro

Coming conferences

All the coming conferences and meetings may be found on the [conferences](#) page.

Some useful links to start with

- [YALES2](#)
 - [YALES2 public page](#)
 - [YALES2 Gallery](#)
 - [YALES2 private wiki \(login required\)](#)
- [SITCom-B](#)
 - [SITCom-B public page](#)
 - [SITCom-B Gallery](#)
 - [SITCom-B private wiki \(login required\)](#)
- [Users and Publications](#)
 - Industrial partners, associated lab and people working on the projects
 - Publications of the combustion modeling group at CORIA

Registration

If you want to be given access to the private wikis, please send a mail to the webmaster [✉](mailto:webmaster@coria-cfd.fr)

Logos

The official logos of YALES2 and SITCom-B can be downloaded here (jpg, 160x160):



For higher resolutions and different file formats, the following tar.gz file is available: [File:Logos.tar.gz](#).

This project is supported by



90.23.213.174 Talk for this IP address Log in

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[Special page](#)

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Discussion board

[Overview](#) > [YALES2 users' forum](#) > [General usage](#)

[New topic](#)

General usage

	Replies	Views	Latest reply
Stop run properly & Dumping all data	1	10	08:46, 6 December 2011 by Moureauv
Posted at 15:39, 5 December 2011 by Ourlac			
Initialization with INTERPOLATION	3	19	08:41, 6 December 2011 by Moureauv
Posted at 15:53, 24 November 2011 by Ourlac			
Restart with NDUMP=24	2	24	21:11, 8 November 2011 by Granet
Posted at 21:14, 7 November 2011 by Granet			
Friction factor in pipes	5	33	10:37, 4 November 2011 by Granet
Posted at 14:37, 18 October 2011 by Granet			
Issues with periodicity	6	30	15:55, 24 October 2011 by Granet
Posted at 16:18, 20 October 2011 by Granet			
Restart after a change of platform	2	17	18:09, 10 October 2011 by Moureauv
Posted at 17:57, 10 October 2011 by Mercier			
Problem with 'svn checkout' : error message "Mot de passe du porte-clé GNOME '(null)' "	1	21	12:40, 20 July 2011 by Mendez
Posted at 12:35, 20 July 2011 by Lartigue			
Memory issue with an heavy mesh (.cas)	3	48	09:23, 18 July 2011 by Moureauv
Posted at 21:49, 7 July 2011 by Mercier			
Dumping of the cells on a boundary condition	0	22	
Posted at 08:41, 12 July 2011 by Moureauv			
Mesh manipulation (transformation, gluing)	1	27	11:28, 11 July 2011 by Moureauv
Posted at 09:54, 11 July 2011 by Duchaine			
Cartesian Mesh Stretching	1	51	17:03, 31 May 2011 by Gruselle
Posted at 16:27, 31 May 2011 by Gruselle			

Project page Discussion Read Edit View history Go Search

Moureau My talk My preferences My watchlist My contributions Log out

YALES2 Doxygen

YALES2 Search

logged in as moureau Logout Preferences Help/Guide About Trac

WIKI Timeline Roadmap Browse Source View Tickets New Ticket Search Admin Available Reports Custom Query

{6} All Tickets By Milestone (Including closed) (11 matches)

A more complex example to show how to make advanced reports.

Edit report Copy report Delete report

Ticket	Summary	Component	Status	Resolution	Version	Type	Priority	Owner	Modified
#10	Shift from ICS TO VDS - Density issue	yales2	new		trunk	defect	major	moureauv	07/15/11
#11	r560 : negative time step at initialization	yales2	new		trunk	defect	major	moureauv	11/17/11
#1	Create an object to perform Lagrange interpolation	yales2	accepted			task	minor	lartigue	02/02/11
#4	add system dependent routines in include.f90	yales2	new			enhancement	minor	lartigue	02/02/11
#9	Probe dumping : RMS not updated	yales2	closed	fixed	trunk	defect	minor	somebody	10/28/11
#8	TIME_MAX usage	yales2	closed	fixed	0.3.0	defect	minor	somebody	10/28/11
#2	Store the absolute simulation time in solution	yales2	closed	fixed		enhancement	minor	vahé	06/18/11
#7	Compute and dump Vorticity	yales2	closed	fixed	0.3.0	enhancement	minor	lartigue	02/17/11
#3	Pb with slip wall velocity after a restart	yales2	closed	fixed		defect	major	taieb	02/14/11
#6	toto	yales2	closed	invalid		defect	major	moureauv	02/07/11
#5	test	yales2	closed	invalid		defect	major	lartigue	02/07/11

Note: See [TracReports](#) for help on using and creating reports.

Download in other formats:

RSS Feed | Comma-delimited Text | Tab-delimited Text | SQL Query

Jenkins: automation of tasks based on scripts

V. 2

Jenkins

search ? Vincent Moureau | log out

ENABLE AUTO REFRESH

New Item People Build History Manage Jenkins Credentials My Views

Build Queue

No builds in the queue.

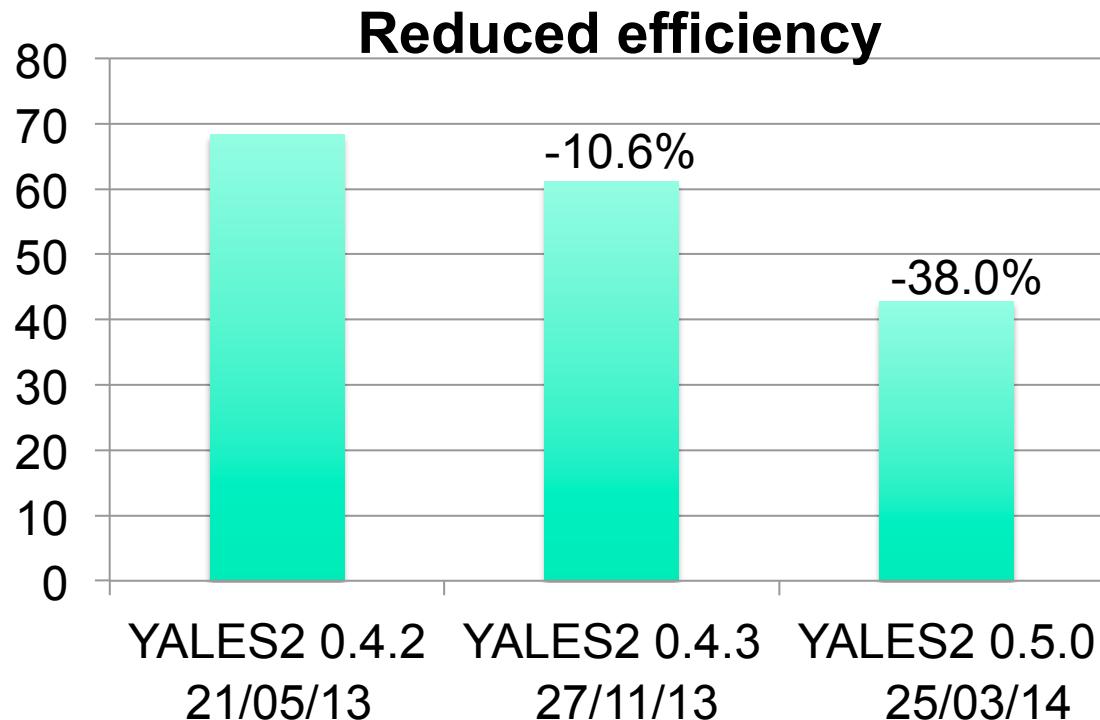
Build Executor Status

1 Idle
2 Idle
3 Idle
4 Idle
5 Idle

All	Bench	Build	Make	Run	+	Last Success	Last Failure	Last Duration
get_cpu_hours	1 mo 26 days - #3	N/A	1 min 15 sec					
myruns	3 mo 13 days - #3	N/A	26 sec					
yales2_bench_all	8 mo 6 days - #1	N/A	17 ms					
yales2_bench_on_antares	3 mo 17 days - #6	N/A	22 sec					
yales2_bench_on_curie	3 mo 17 days - #4	N/A	27 sec					
yales2_bench_on_milou	3 mo 24 days - #4	N/A	2 min 2 sec					
yales2_bench_on_turing	3 mo 17 days - #4	N/A	1 min 38 sec					
yales2_bench_result_all	8 mo 5 days - #1	N/A	15 ms					
yales2_bench_result_on_antares	3 mo 17 days - #6	N/A	1.9 sec					
yales2_bench_result_on_curie	3 mo 17 days - #8	N/A	17 sec					
yales2_bench_result_on_milou	8 mo 5 days - #2	N/A	1.6 sec					
yales2_bench_result_on_turing	3 mo 17 days - #7	N/A	3.7 sec					
yales2_build_all	1 mo 17 days - #28	N/A	90 ms					
yales2_build_on_antares	1 mo 17 days - #78	N/A	1 hr 8 min					
yales2_build_on_antares_master_module	2 mo 16 days - #5	N/A	4 min 55 sec					
yales2_build_on_curie	6 days 7 hr - #94	1 yr 1 mo - #12	2 min 8 sec					
yales2_build_on_milou	1 mo 17 days - #112	11 mo - #41	3 min 54 sec					
yales2_build_on_turing	1 mo 17 days - #87	N/A	1 hr 8 min					
yales2_make_agat_on_milou	3 mo 17 days - #24	N/A	1 min 12 sec					
yales2_make_avvt_on_milou	3 mo 17 days - #24	N/A	1 min 52 sec					
yales2_run_agat_on_milou	3 mo 17 days - #21	N/A	13 min					

A few lesson learned during the development of HPC codes

- ▶ A network of CFD, applied math, and HPC experts is required
- ▶ 2 examples
 - Optimization of the YALES2 code with the Exascale Lab, INTEL/CEA/GENCI/UVSQ



- Optimization of a dynamic load balancing algorithm on the Curie machine with the « Application support team » from TGCC

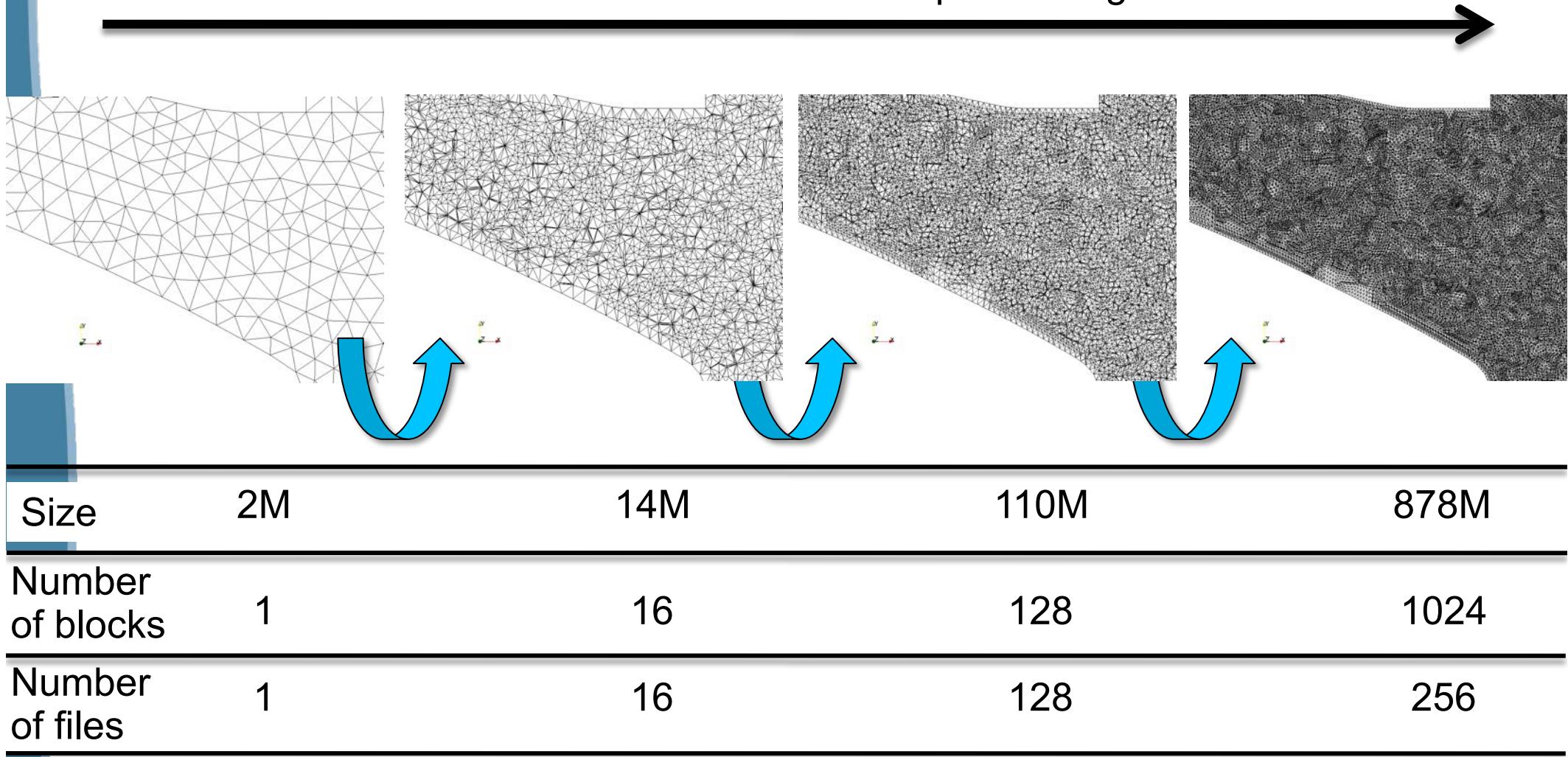
Specific features of the code

Mesh management

- MOUREAU, V., DOMINGO, P. & VERVISCH, L. (2011) Design of a massively parallel CFDcode for complex geometries. *Comptes Rendus Mécanique* 339 (2-3), 141–148.

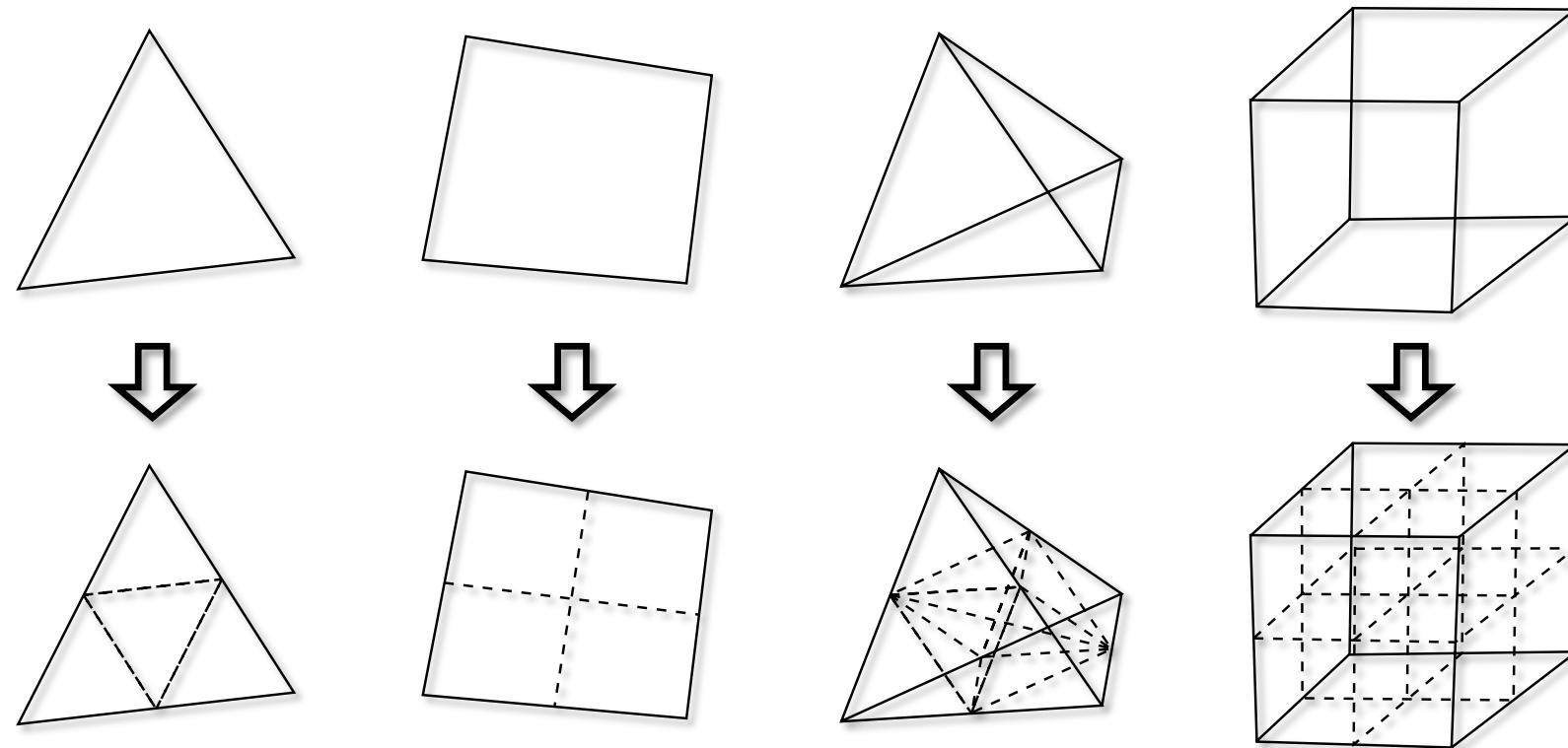
■ Strategy: refinement and partitioning

Automatic mesh refinement + partitioning



■ Mesh generation

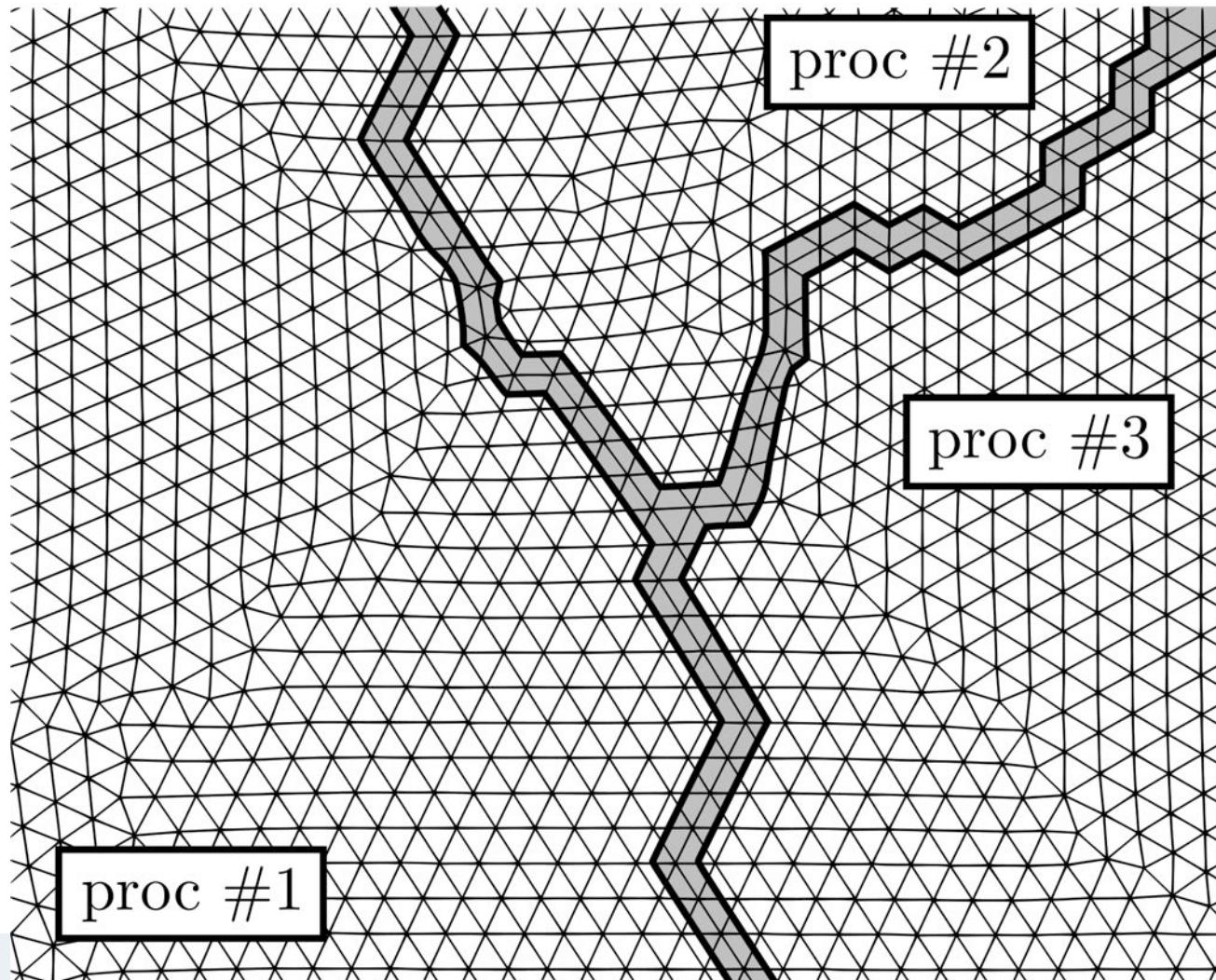
- ▶ Homogeneous mesh refinement allows to reach massive mesh sizes. The only constraint is that the geometry has to be well described by the first mesh.



- ▶ For tets, mesh refinement is not obvious (Rivara 1984)

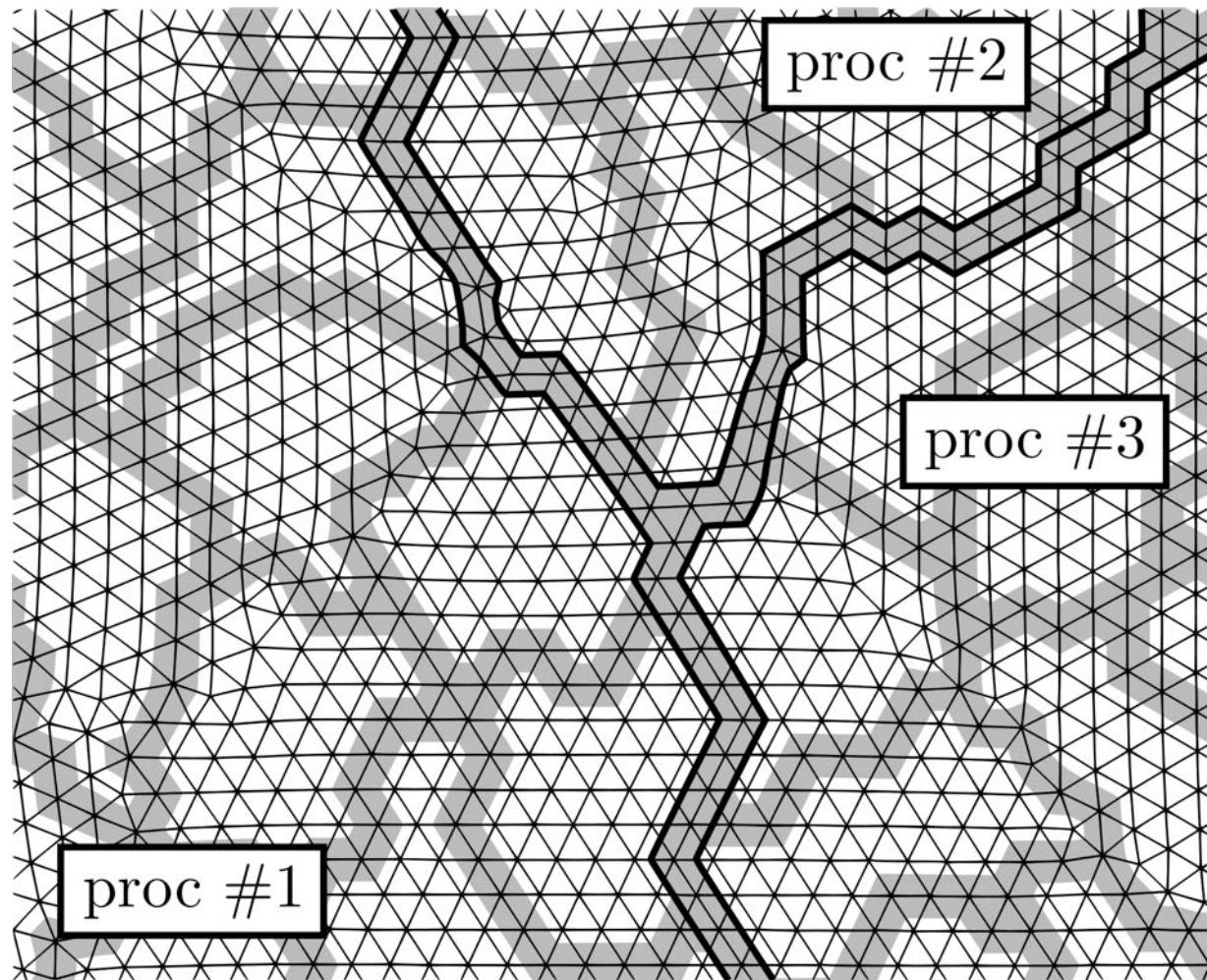
■ Mesh management on the processors

- ▶ **1st solution: single-level domain decomposition**
- ▶ **Several available libraries: Metis, Scotch, ...**



■ Mesh management on the processors

- ▶ 2nd solution: two-level domain decomposition (Moureau et al 2011) which is cache aware



Specific features of the code

High-performance linear solvers

- MALANDAIN, M., MAHEU, N. & MOUREAU, V. (2013) Optimization of the deflated conjugate gradient algorithm for the solving of elliptic equations on massively parallel machines. *Journal of Computational Physics*, 238, 32-47

■ Governing equations

- ▶ For DNS of iso-thermal flows at low-Mach number
- ▶ Velocity equation

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

- ▶ Divergence-free constraint

$$\nabla \cdot \mathbf{u} = 0$$

- ▶ Often solved with projection methods (Chorin 1968)

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

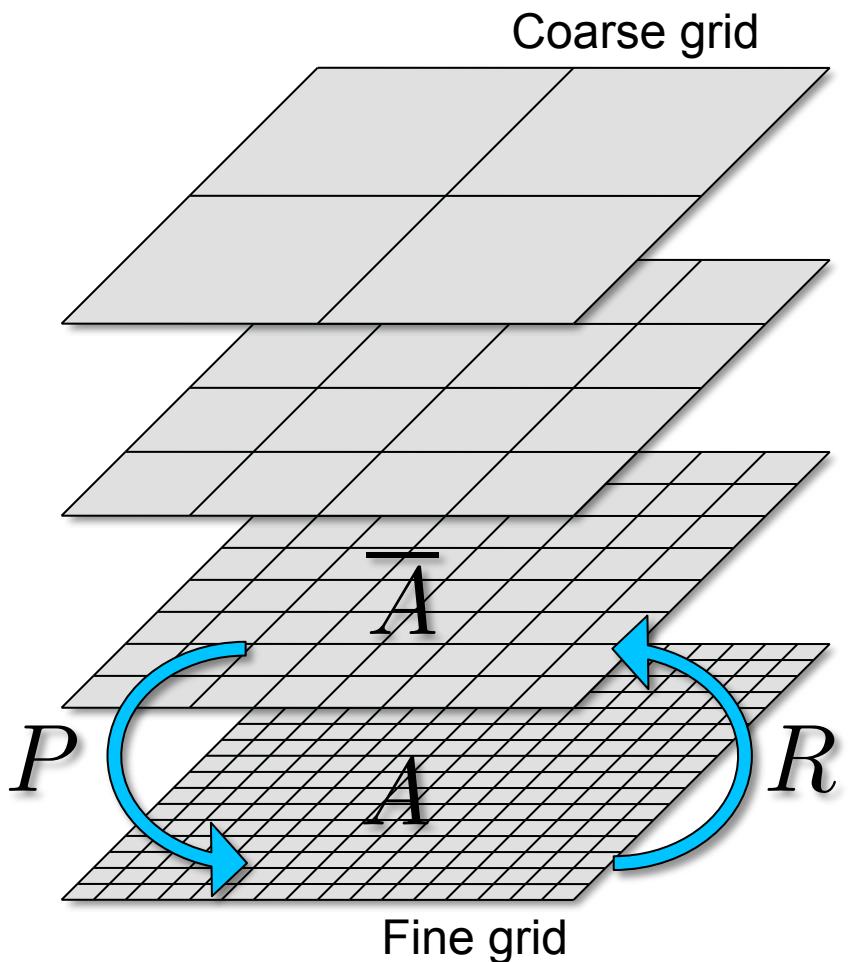
■ Multigrid methods for the Poisson equation solving

► Formally, on a coarse grid

$$\bar{A} = RAP$$

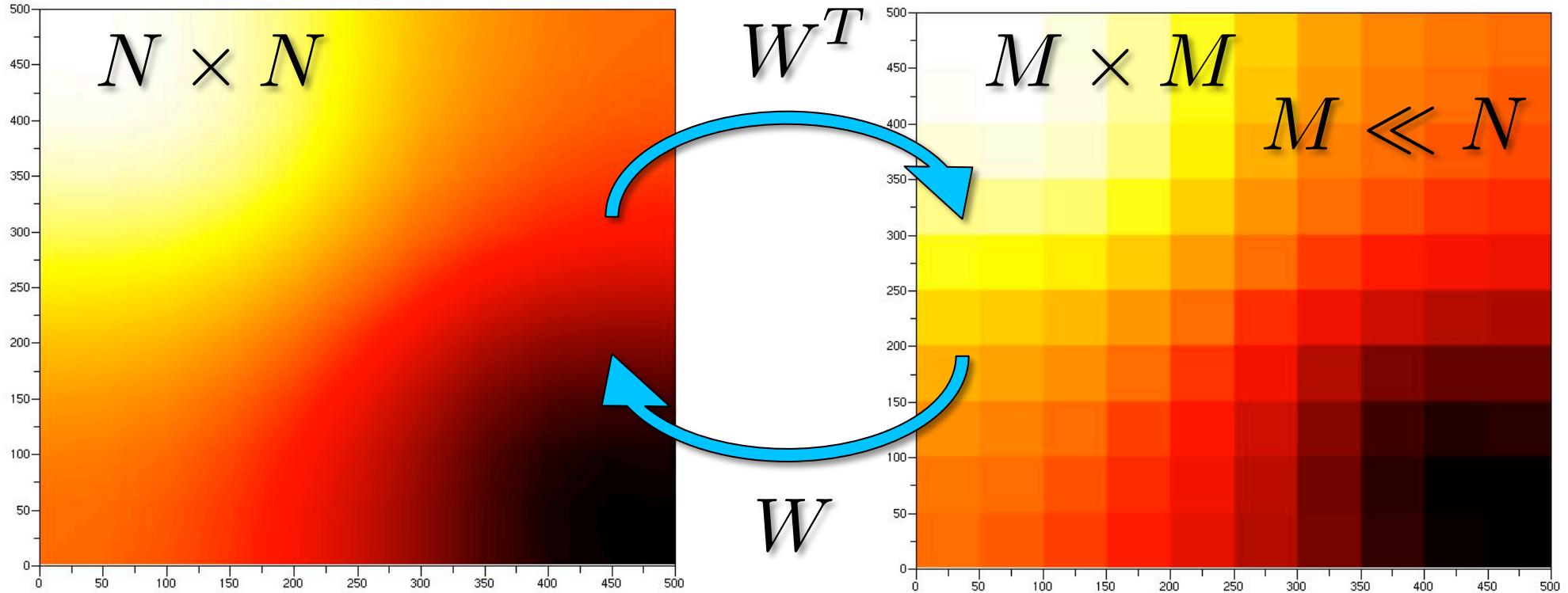
► Some issues encountered with geometric and algebraic multigrids

- The coarse meshes must be compatible with the processor count
- On the coarse meshes : few work for many communications
- Unstructured meshes are still difficult to handle with algebraic multigrids
- Variable coefficients in the Laplacian operator may force to rebuild the grid hierarchy



The Deflated Preconditioned Conjugate Gradient (Nicolaides 1987)

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

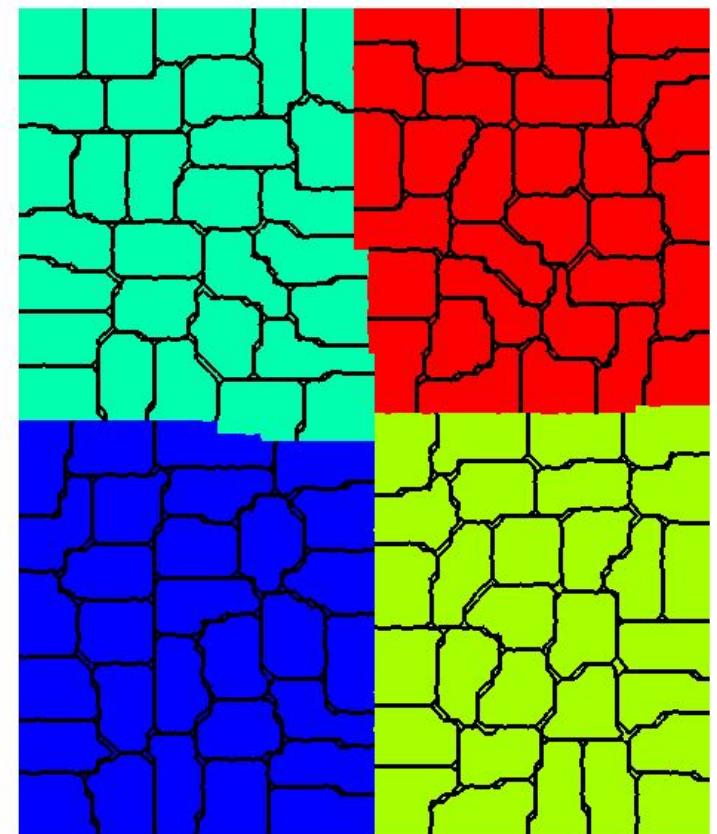
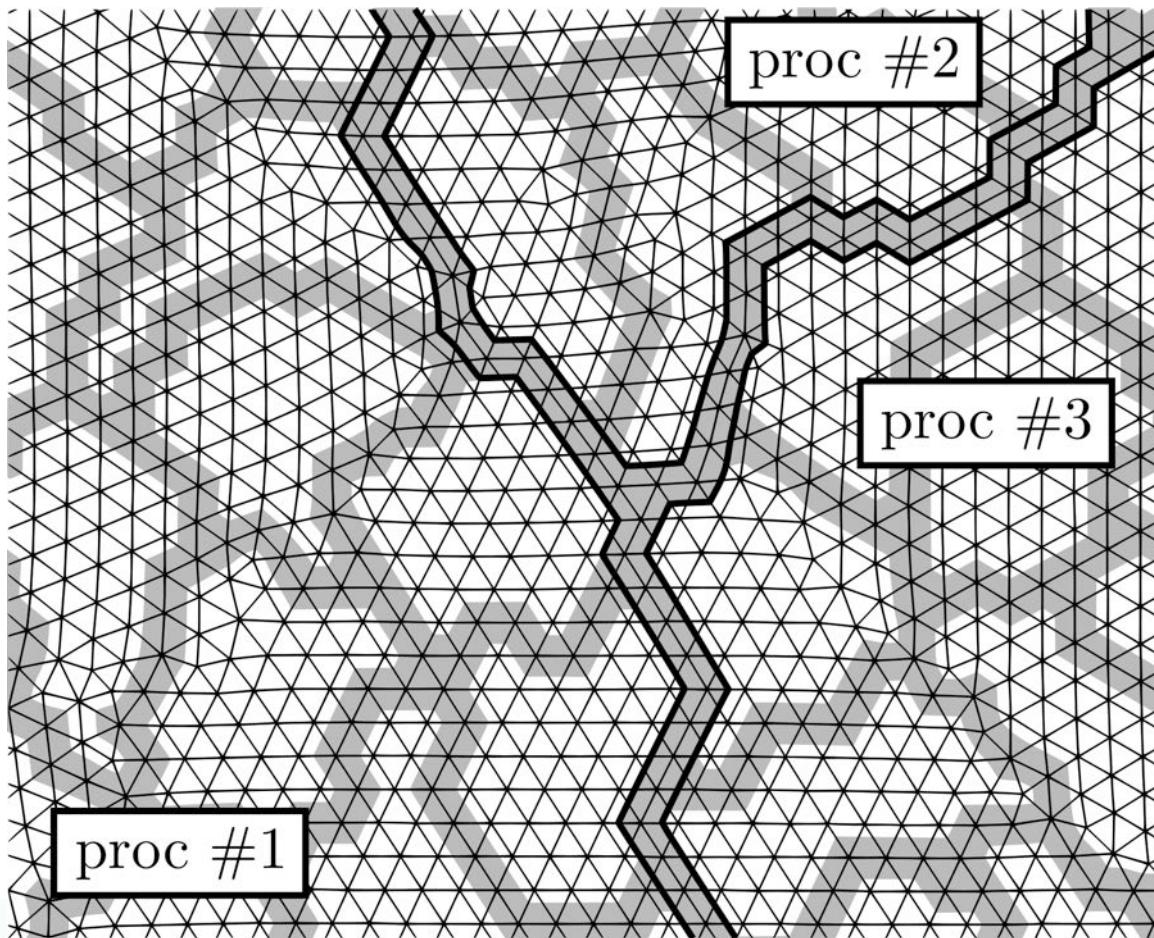


- ▶ The PCG preconditioning is based on a projection operator

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

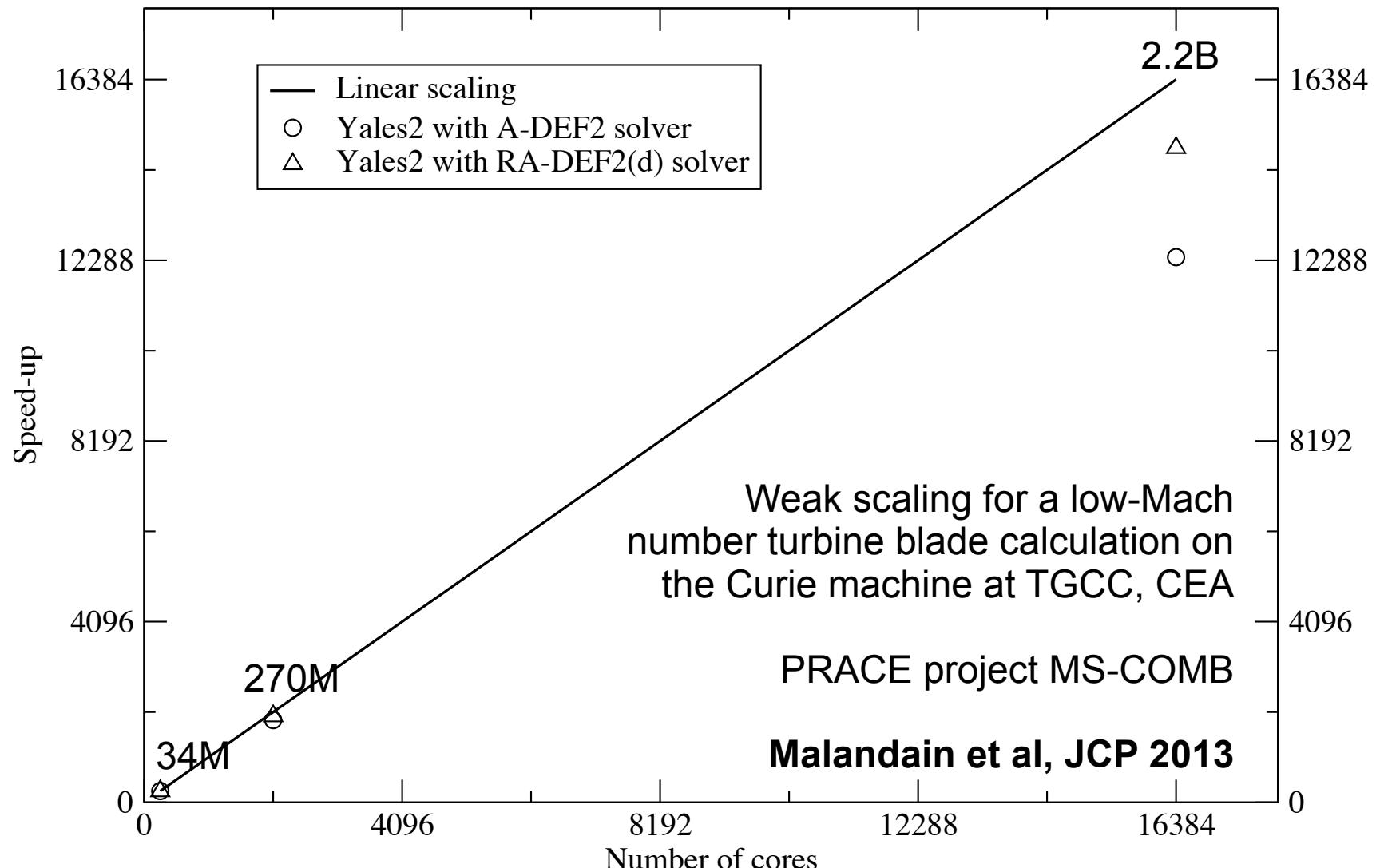
■ Implementation in YALES2

- ▶ Deflation is quite easy to implement if a coarse mesh is available.
Restriction and prolongation operators are well defined.
- ▶ In YALES2, the DPCG uses the two-level domain decomposition.



Optimized deflated PCG

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

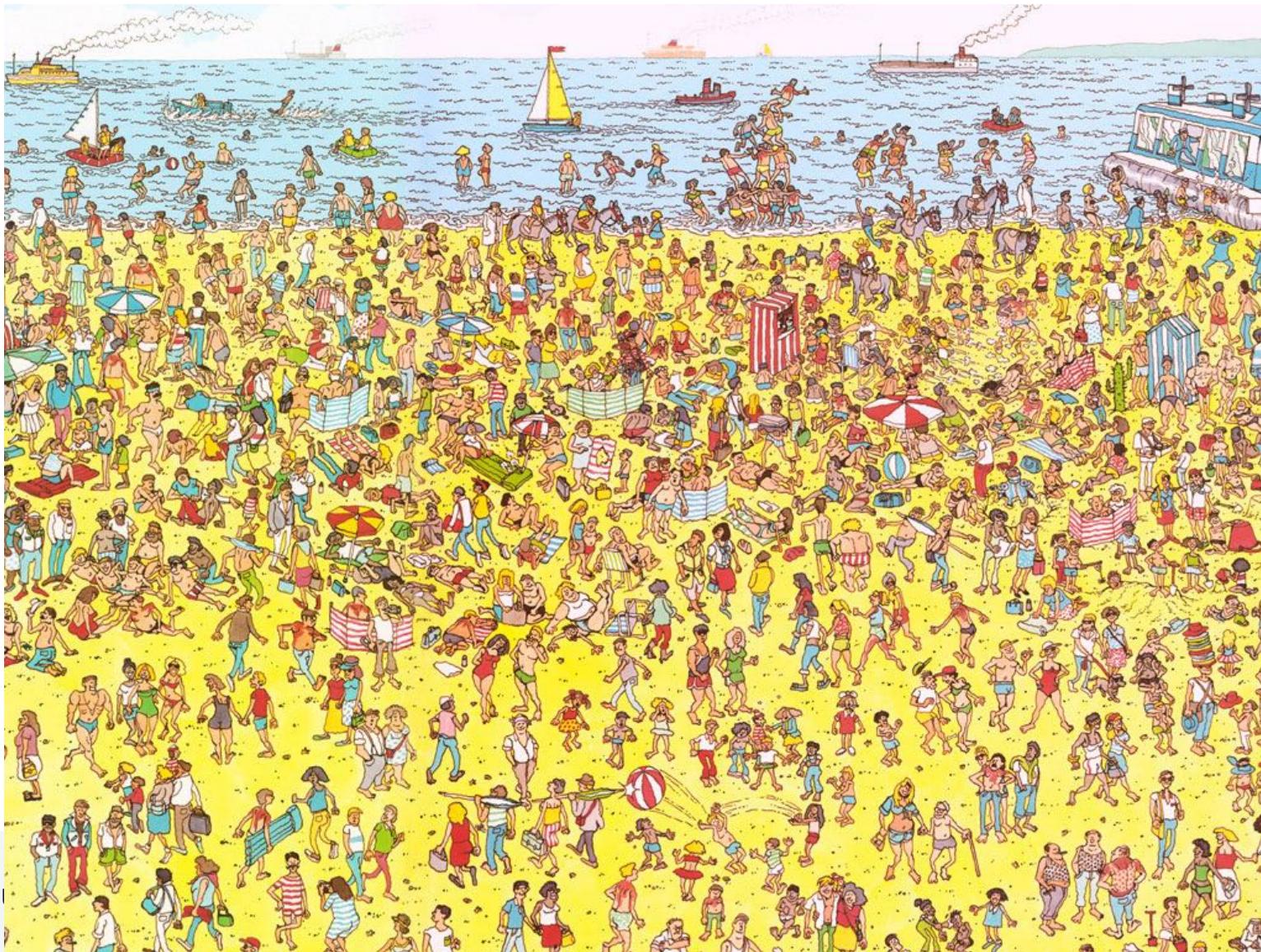


Specific features of the code

Selective sampling

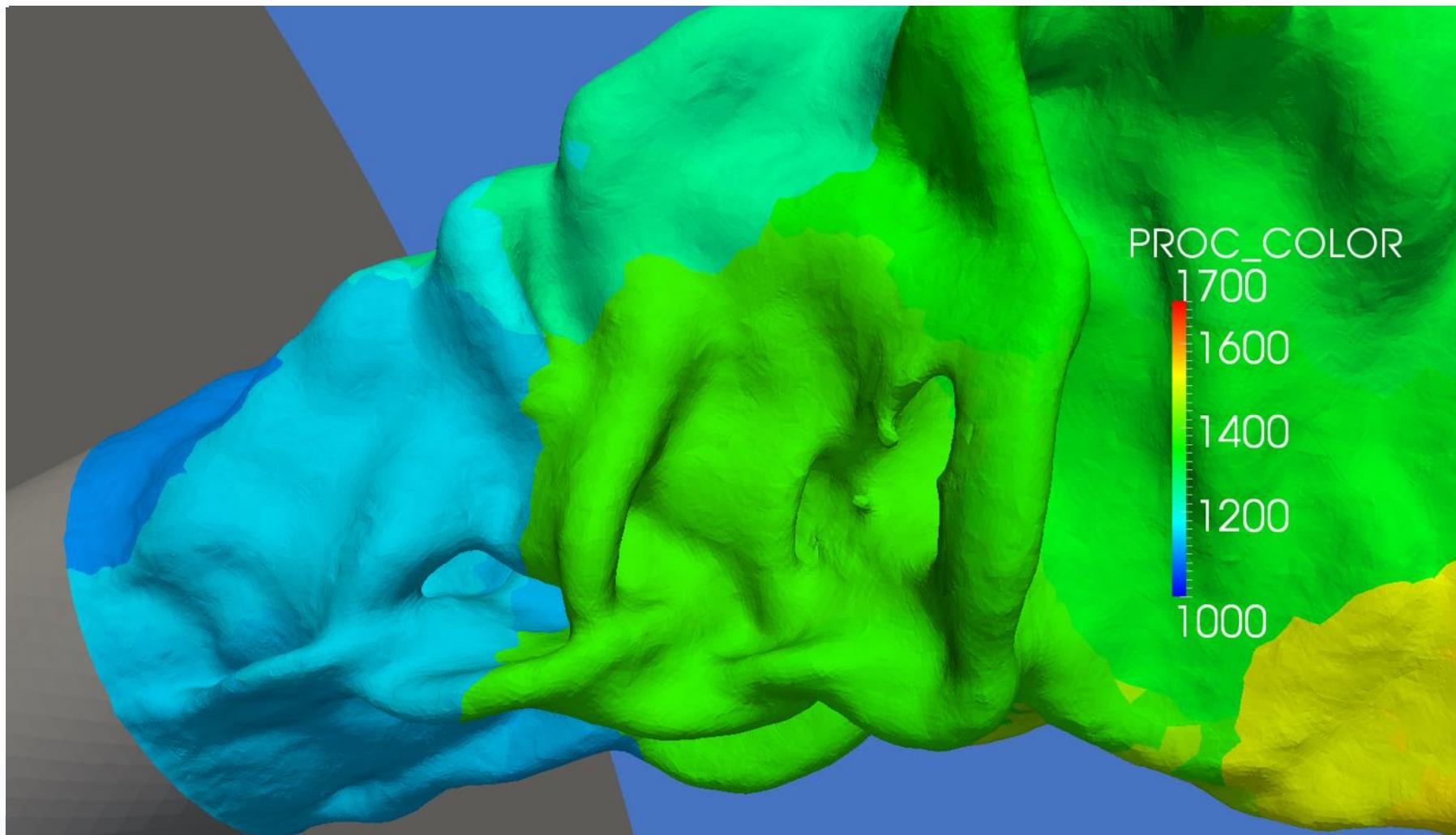
■ Principle

- ▶ Selective sampling consists in identifying the important data
- ▶ Often similar to the “where’s Waldo” game...



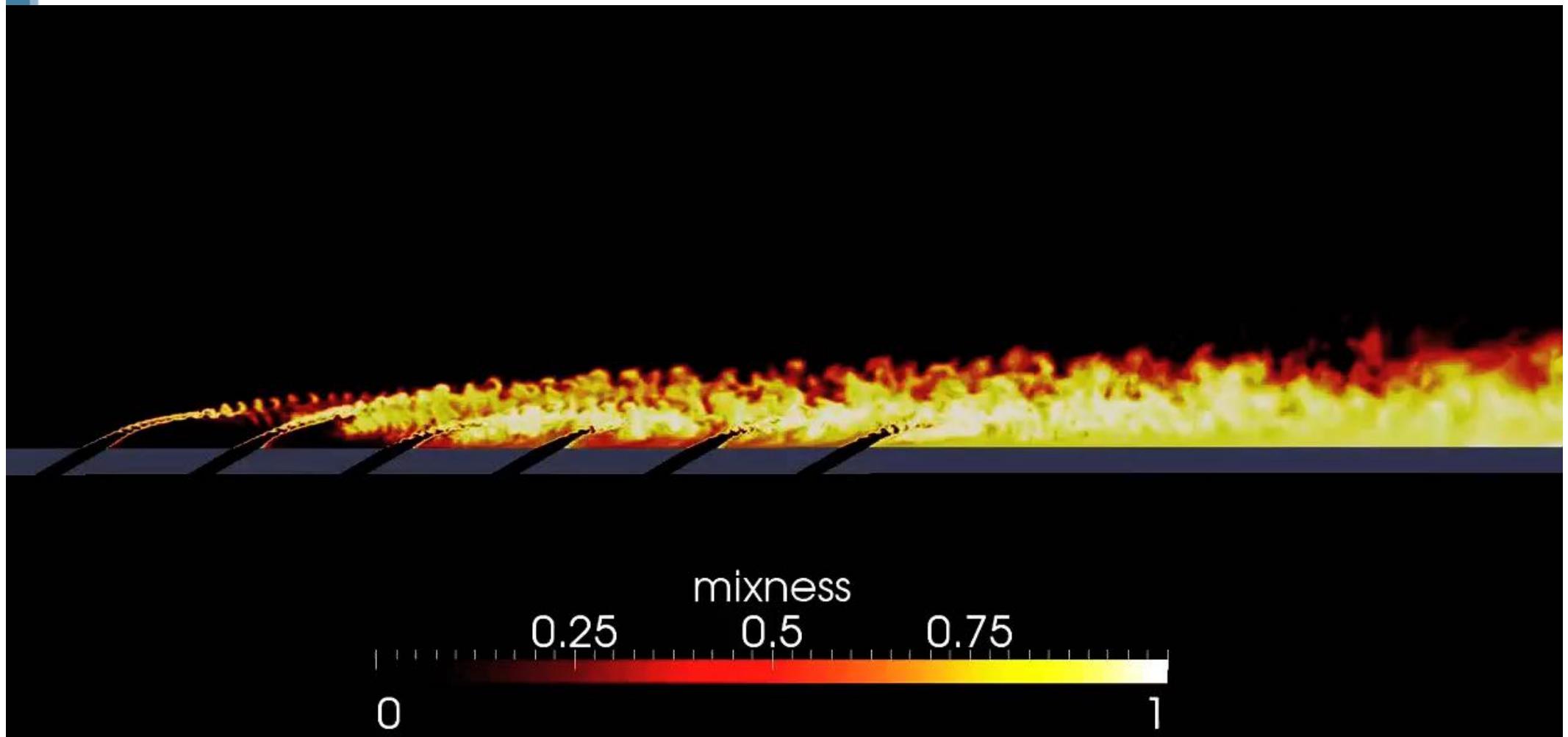
■ Selective sampling of iso-contours

- ▶ In the code or in the post-processing tools, only the cells crossing a certain iso-surface may be of interest
- ▶ Sampling of these few cells still allows to rebuild the full iso-surface



■ Selective sampling of planes

- ▶ Example with a mesh of 110 million tets on 1024 cores of Curie, CEA
- ▶ Extraction of 300 planes at the center of the domain



Case studies

Identification of large-scale coherent structures in semi-industrial swirl burners and analysis of their interactions with the spray

L. Guédot, G. Lartigue, V. Moureau, CORIA

Vortex identification

▶ Some references

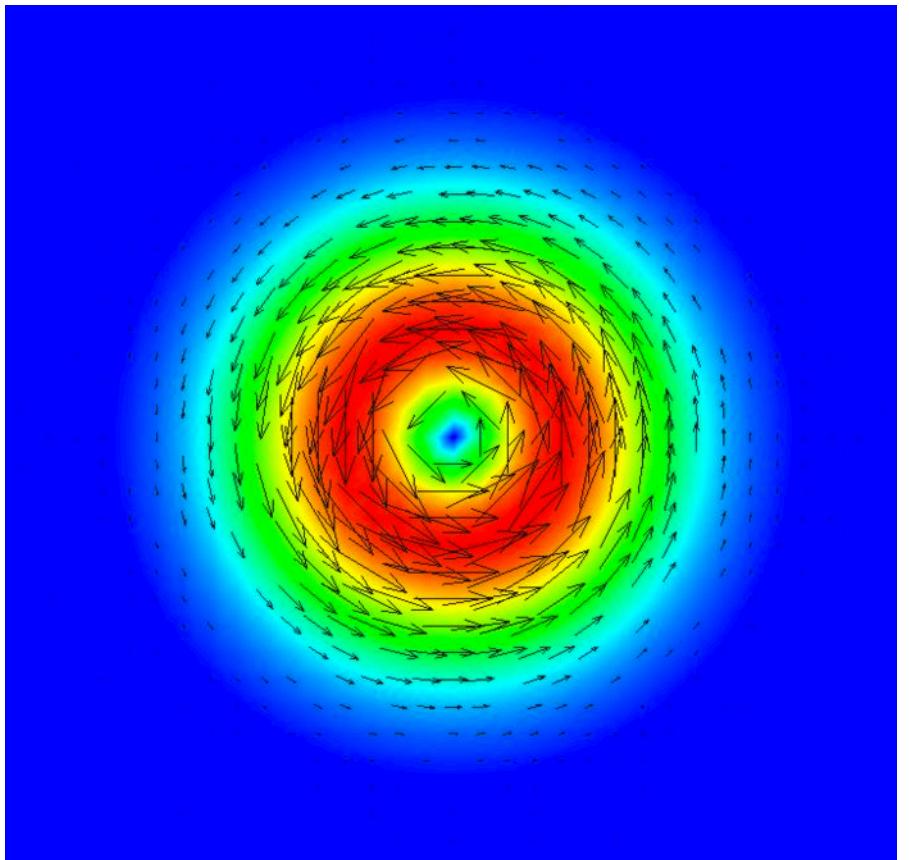
- Jeong J. and Hussain F., JFM 1995
- Dubief Y. and Delcayre F., JoT 2000

▶ Starting from the Gauss vortex

$$\Psi(x, y) = \exp\left(-\frac{x^2 + y^2}{\tau^2}\right)$$

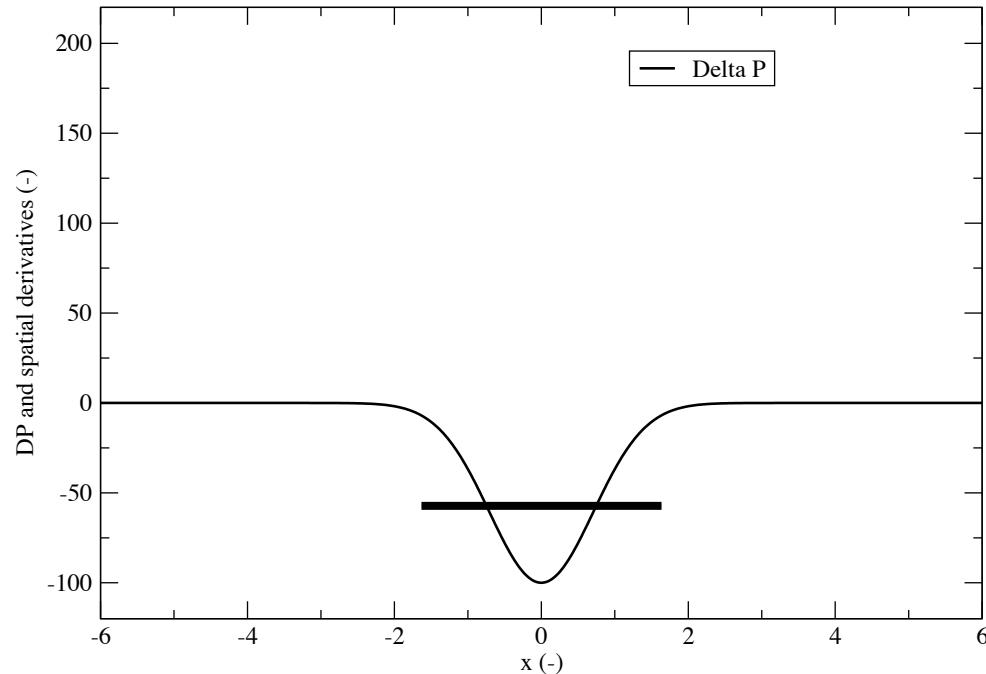
$$\mathbf{u}(x, y) = 2U_0 \frac{\Psi(x, y)}{\tau} \begin{pmatrix} -y \\ x \end{pmatrix}$$

$$P(x, y) = P_0 - \rho_0 U_0^2 \Psi^2(x, y)$$

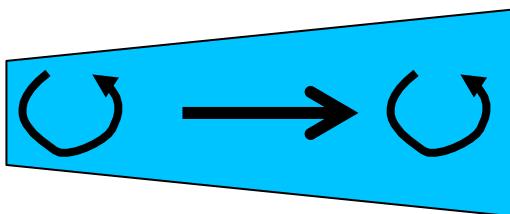


Vortex identification

► First idea: pressure iso-surface

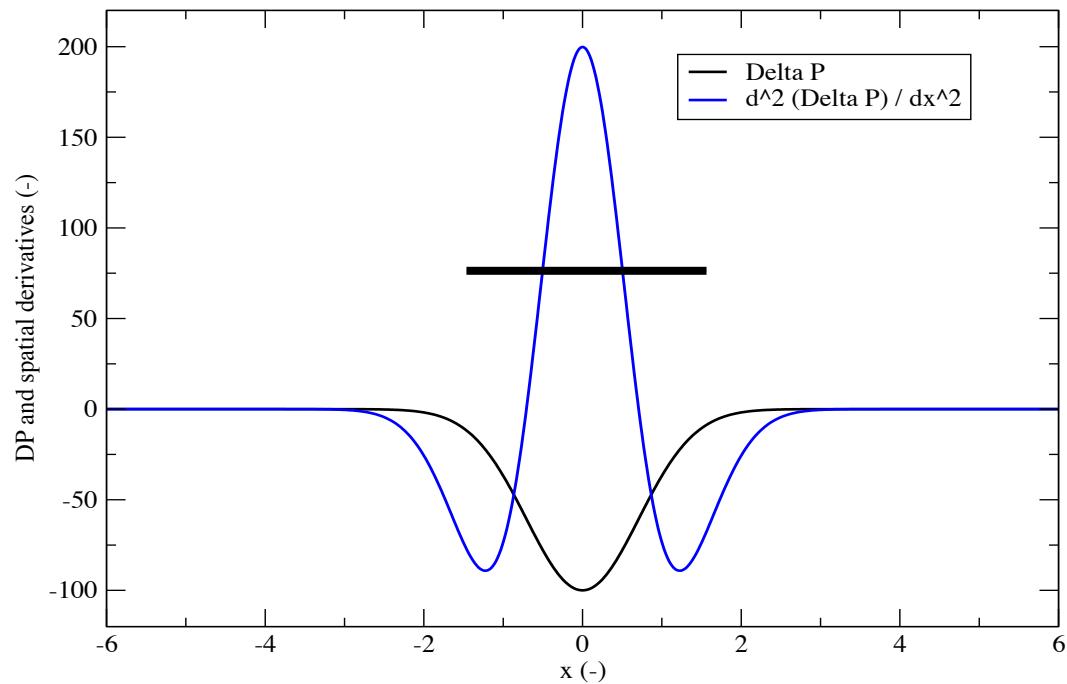


► Not perfect because pressure varies for many reasons (Bernoulli, ...)



Vortex identification

- ▶ Second idea: iso-surface of the second derivative of the pressure



- ▶ In incompressible flows, the pressure Laplacian is the Q-criterion (Hunt et al., CTR 1988)

$$Q = \frac{1}{2\rho} \Delta P$$

$$Q = \frac{1}{2} (\Omega_{ij} \Omega_{ij} - S_{ij} S_{ij})$$
$$S_{ij} = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \quad \Omega_{ij} = \frac{1}{2} (\nabla \mathbf{u} - \nabla \mathbf{u}^T)$$

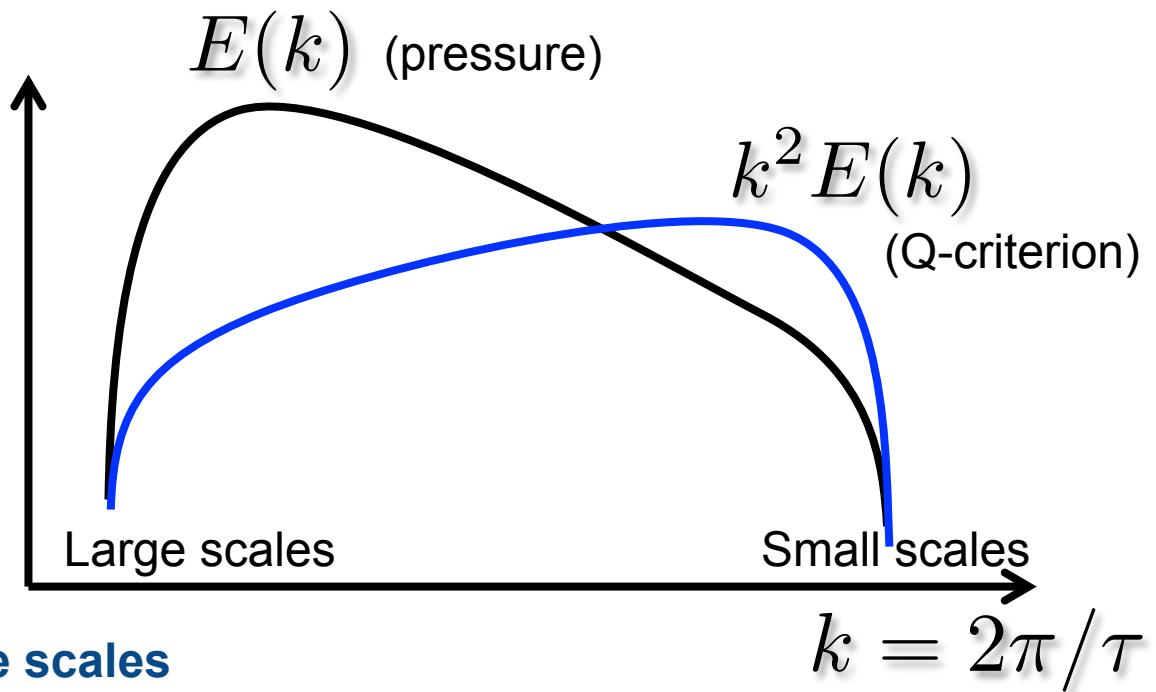
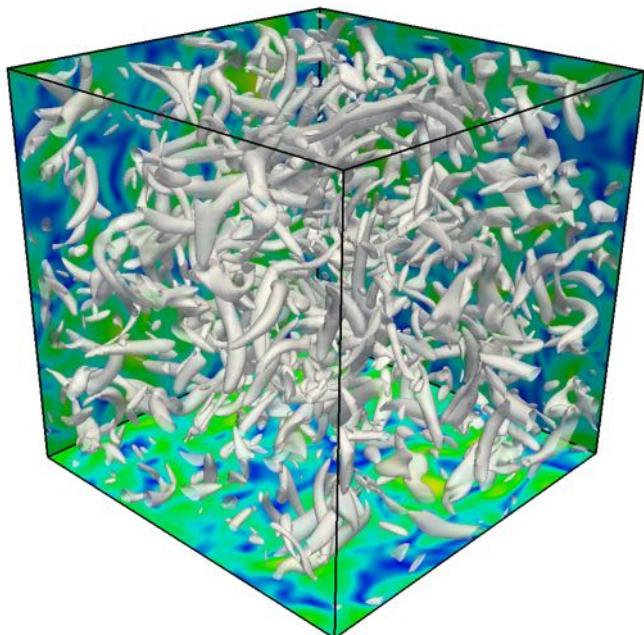
Vortex identification in turbulent flows

▶ Scaling of the two different methods

- Pressure iso-surface : ρU_0^2

Q-criterion : $\rho U_0^2 / \tau^2$

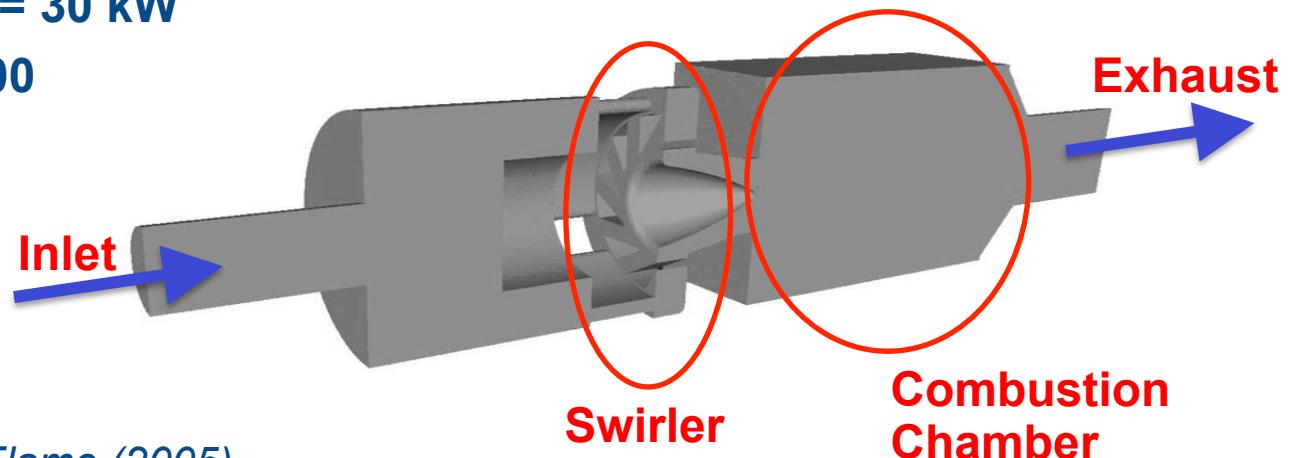
▶ Application to turbulent flows



- Pressure iso-surfaces => large scales
- Q-criterion => small scales

■ Application: the PRECCINSTA burner

- ▶ Industrial lean air/methane burner investigated at DLR (*Meier et al. 2007*)
- ▶ Aim: to help validating LES models for turbulent premixed flames
- ▶ Operating conditions
 - Partially premixed (often considered fully premixed)
 - $\Phi = 0.75$ to 0.83 , power = 30 kW
 - Reynolds number = $45,000$
 - Atmospheric



▶ Related publications

- *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)*
- *Mercier et al., Int. Symp. Comb. (2014)*
- ...

■ PRECCINSTA: numerical set up

► Meshes

Cells in Million	1.7	14	110	329	2634
Δ [mm]	1.2	0.6	0.3	0.2	0.1
ℓ_T/Δ	5.8	11.7	23.3	35.0	70.0
Δ/η	41.4	20.7	10.3	6.9	3.4
δ_L/Δ	0.35	0.71	1.41	2.12	4.24
S_c	0.8	0.7	0.25	0.15	0.0

► Machine

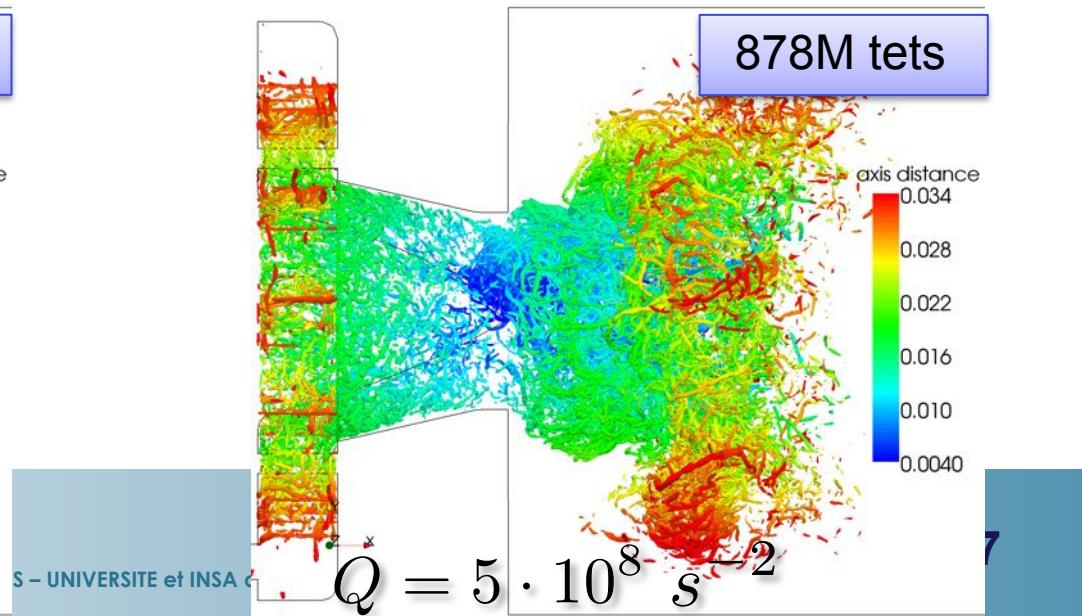
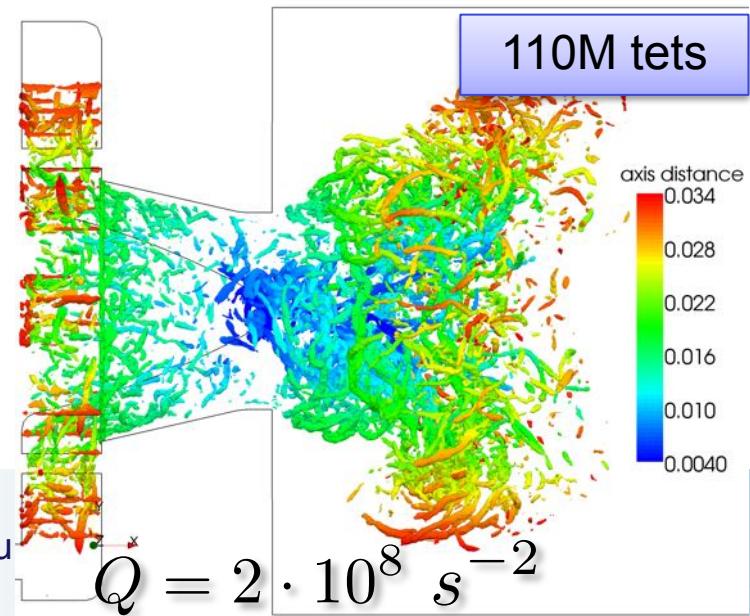
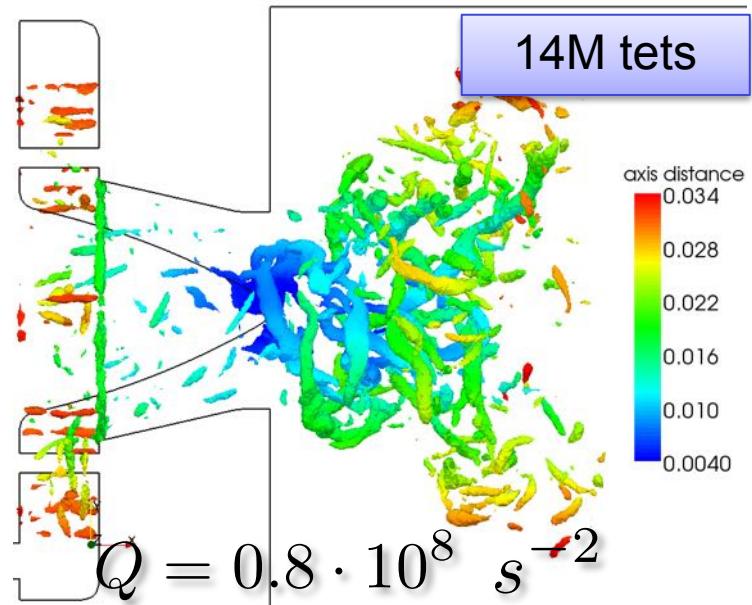
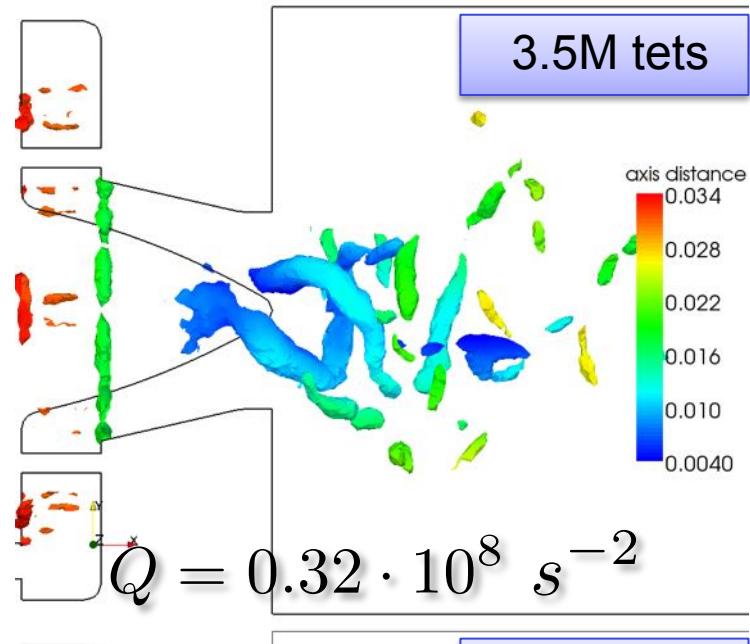
- **Babel, IDRIS, IBM Blue Gene/P**
- **Up to 16384 cores**

► Models

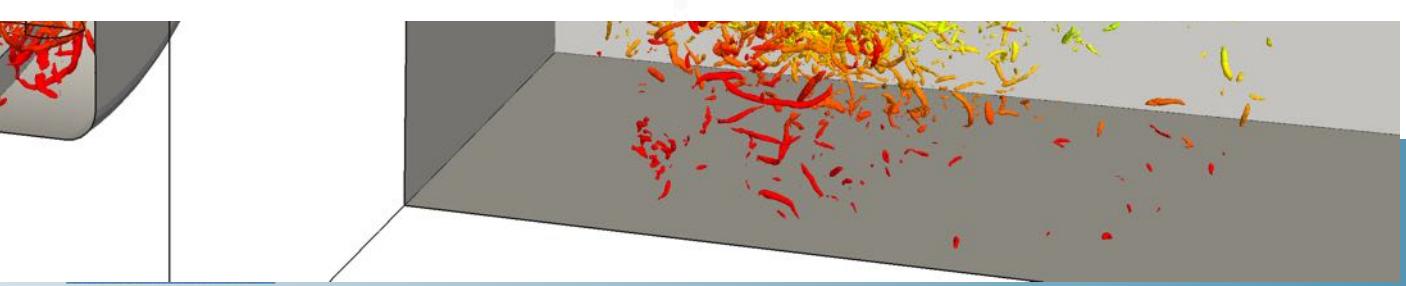
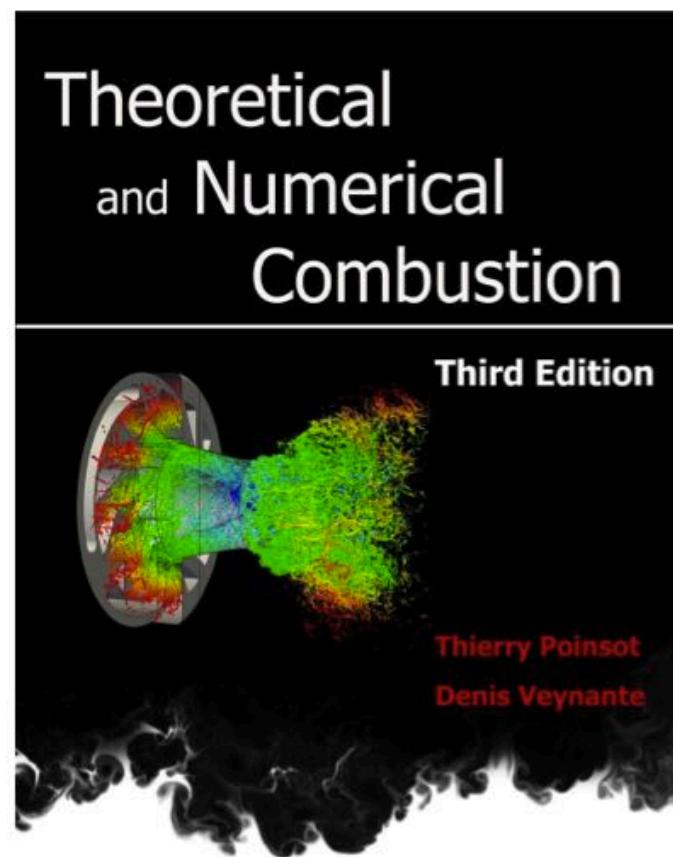
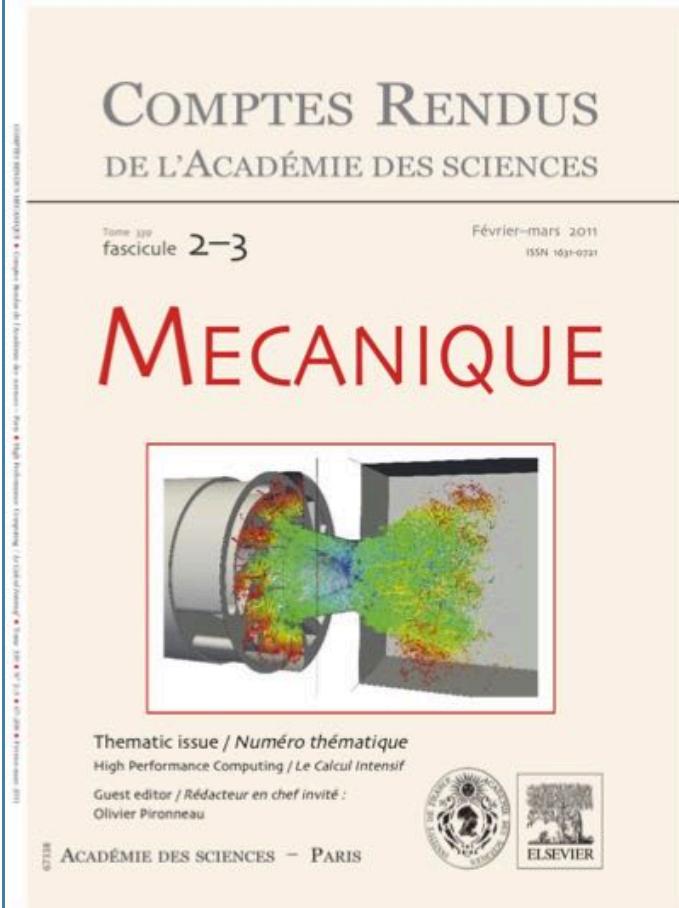
- **Turbulence: localized dynamic Smagorinsky model**
- **Walls: no slip boundary condition**

■ PRECCINSTA: coherent structures (1/2)

► Q-criterion iso-surfaces

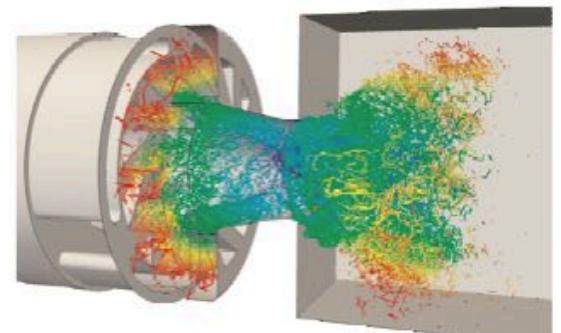


■ PRECCINSTA: coherent structures (2/2)



Studying Turbulence Using
Numerical Simulation
Databases - XIII

Proceedings of the 2010 Summer Program

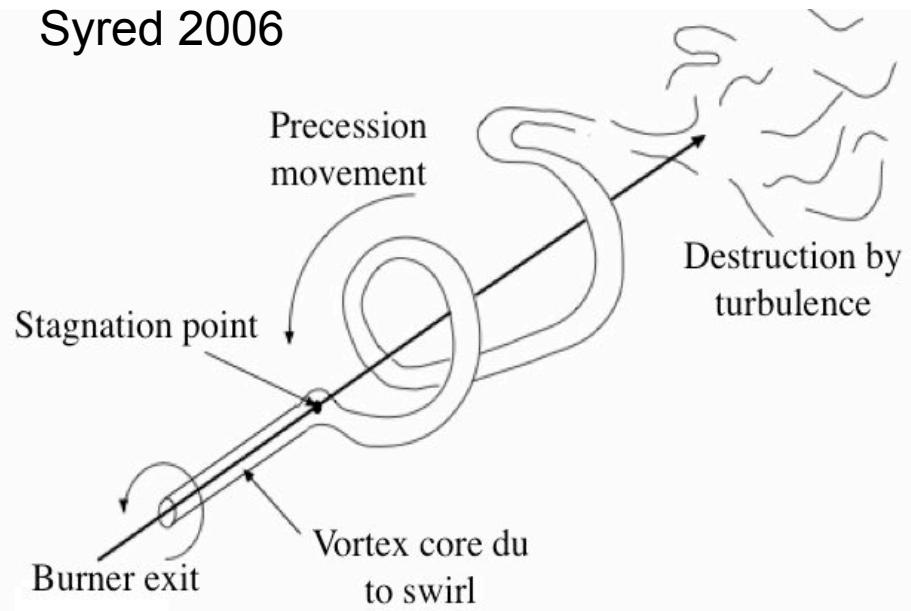


The Precessing Vortex Core

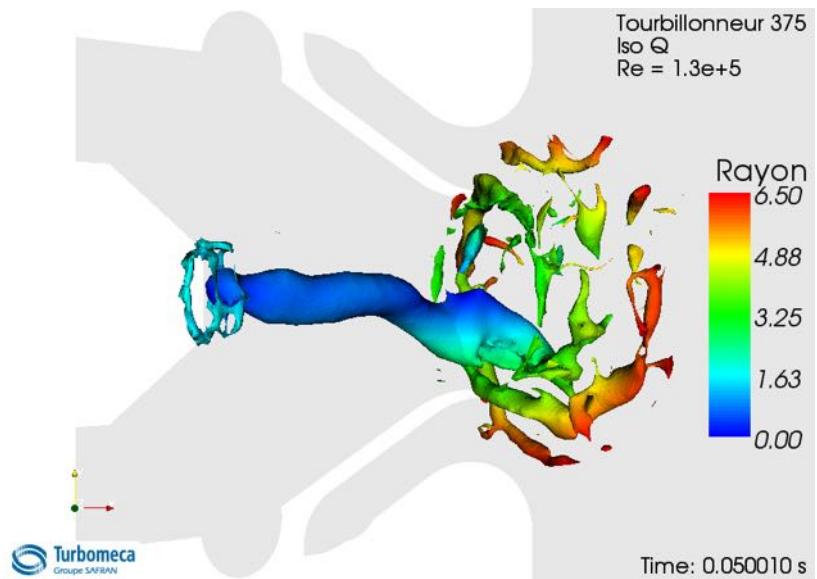
- Occurs if swirl number > 0.6

$$S = \frac{\int_0^R u_\theta u_z r^2 dr}{R \int_0^R u_z^2 r dr}$$

Syred 2006



Pedot et al., courtesy TURBOMECA

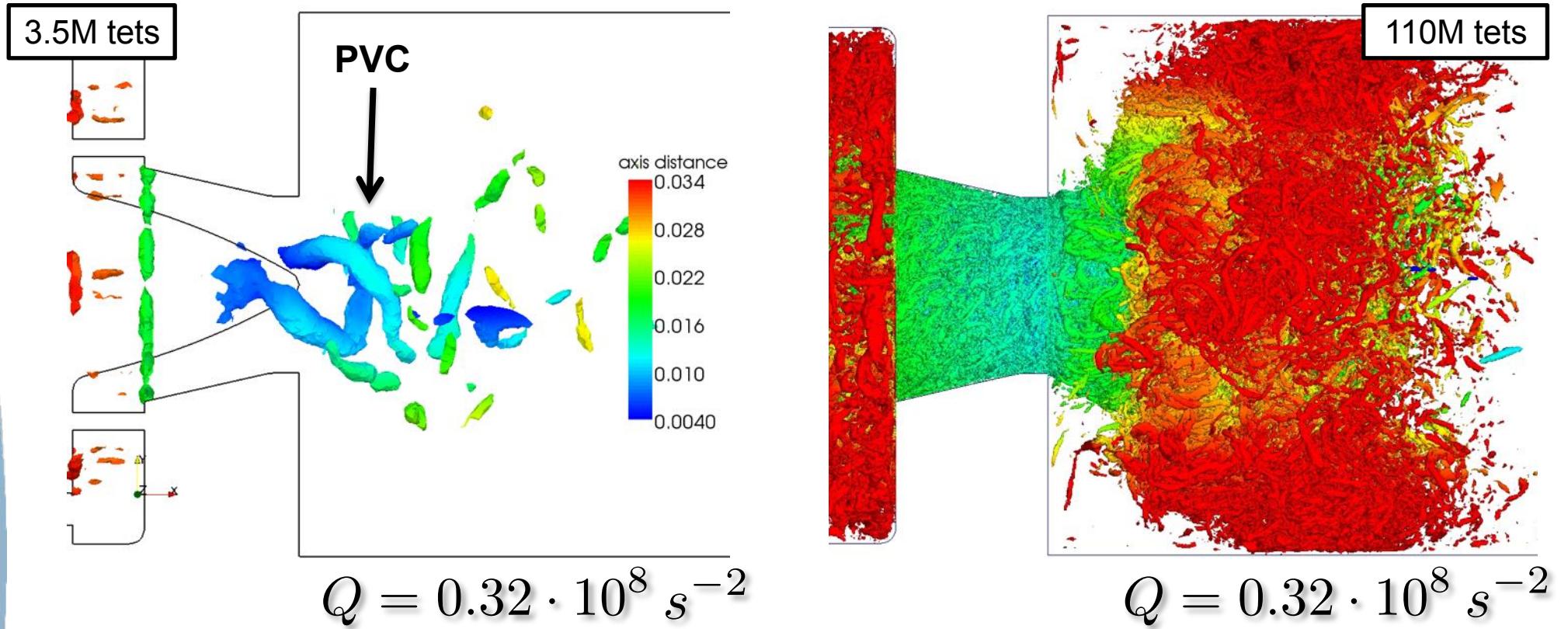


- Interactions with spray [Sanjose 2009]
- Interactions with combustion [Syred 2006]

M. Sanjose (2009), PhD thesis.

N. Syred (2006), A review of oscillation mechanisms and the role of the precessing vortex core (PVC) in swirl combustion systems, Prog. Energy Combust. Sci., 32 93-161.

■ Extraction of the PVC in PRECCINSTA



- As expected, the PVC is completely masked by the small vortices on fine meshes. One solution = filtering !

■ High-order filters for large-scale extraction

- ▶ High-order implicit filters (Raymond et al., Guédot et al.)
- ▶ Designed for the filtering of weather data

$$\bar{\phi} + \beta^p D^p \bar{\phi} = \phi$$

$$\beta = \frac{\Delta x^2}{-4 \sin^2(k_c \Delta x / 2)}$$

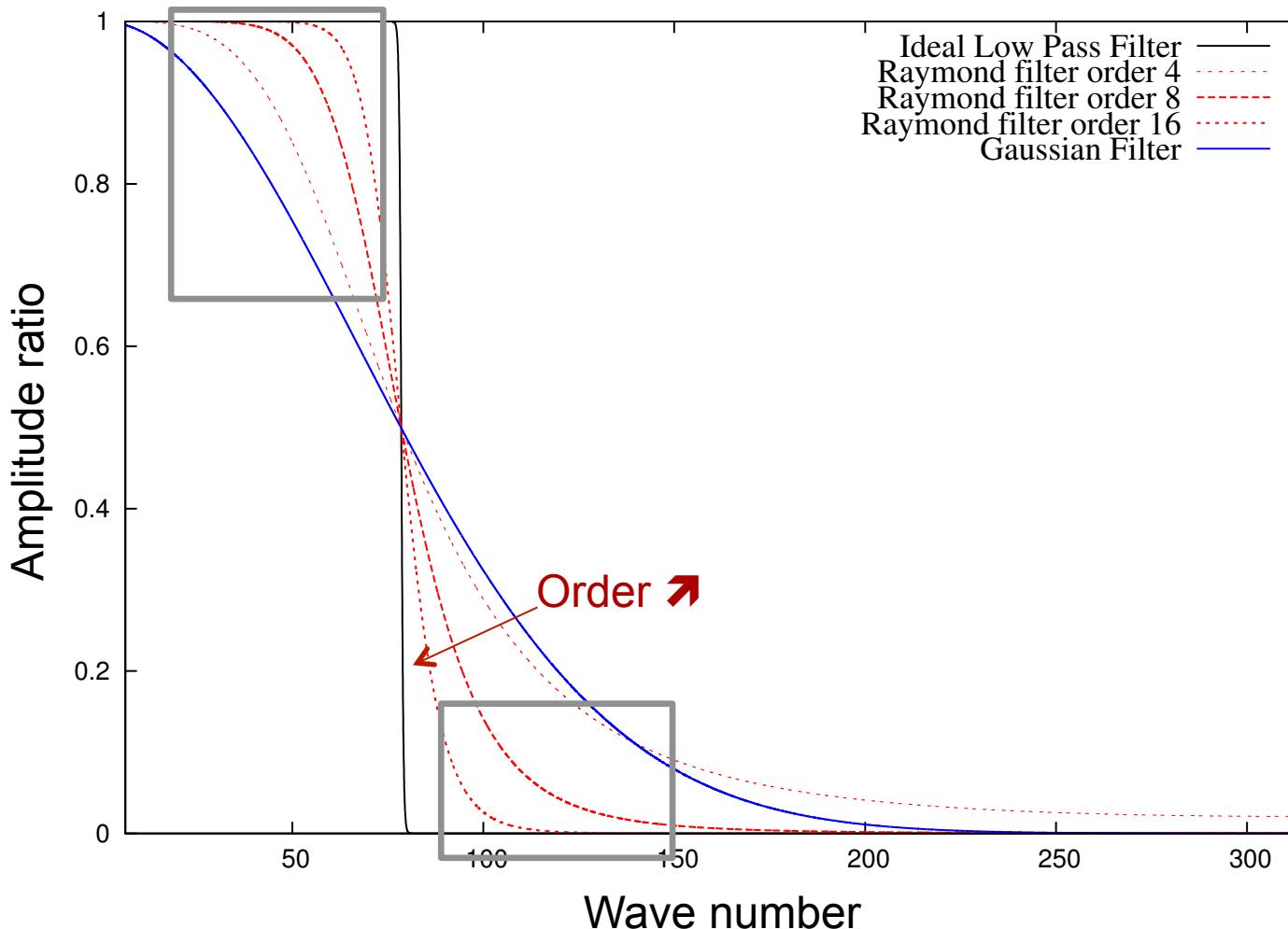
$$D\phi \simeq \frac{\partial^2 \phi}{\partial x^2}$$

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

■ High-order filters for large-scale extraction

► Selectivity increases with the order

- Large structures are less dissipated and small structures more dissipated



■ High-order filters for large-scale extraction

- ▶ Generalization to complex geometries / unstructured grids

(Guedot et al., submitted)

- ▶ Definition of a modified Lapacian operator

- Coefficient β in the Laplacian operator
 - Symmetric tridiagonal operator

$$\bar{\phi} + \beta^p D^p \bar{\phi} = \phi \quad \longrightarrow \quad \bar{\phi} + (\nabla \cdot \beta \nabla)^p \bar{\phi} = \phi$$

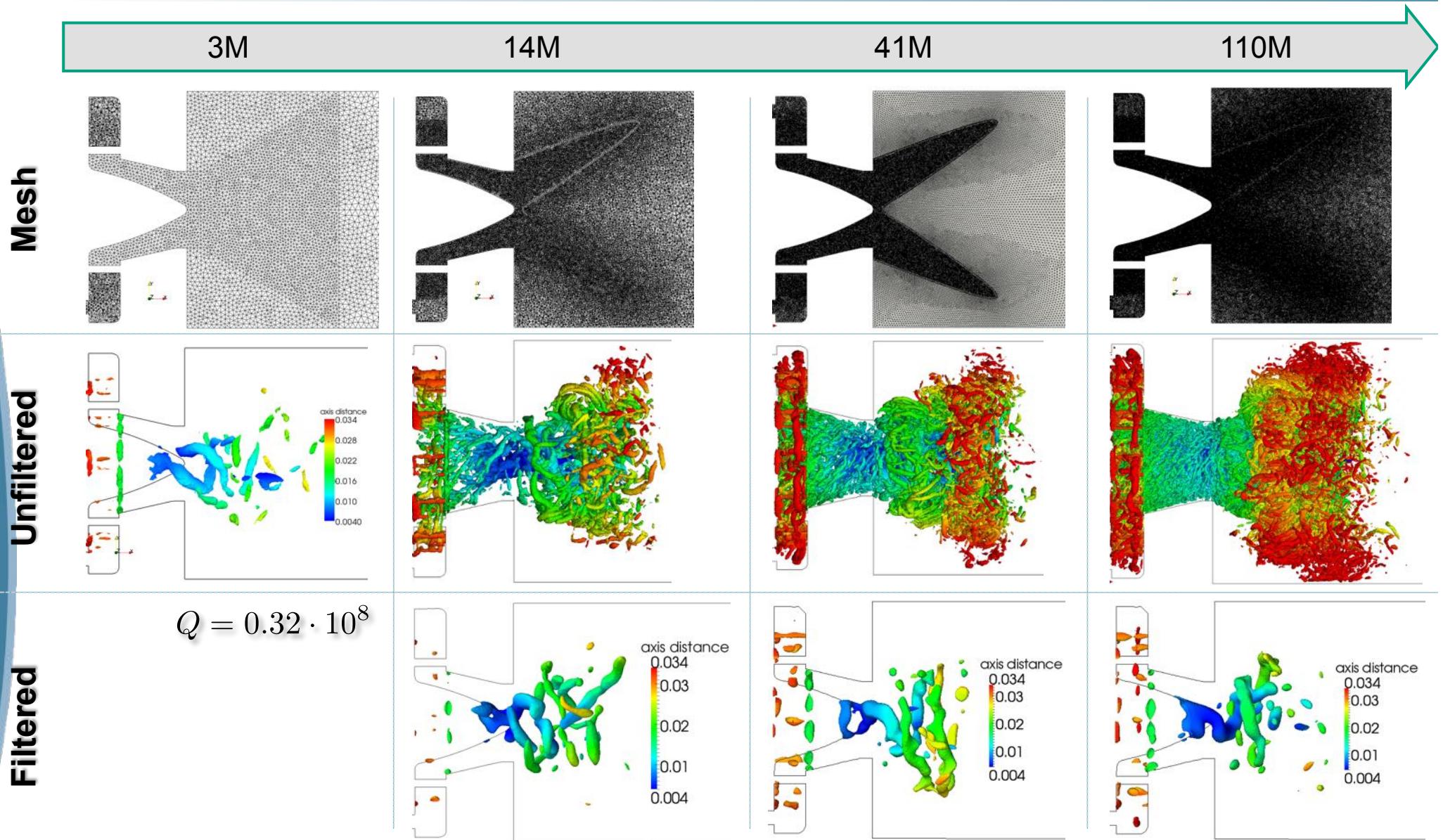
- ▶ Linear system

$$(I + \Delta'^p) \bar{\phi} = \phi$$

- ▶ Algorithms used to invert the system

- Factorization in first or second order matrix polynomials
 - Real or complex preconditioned conjugate gradient

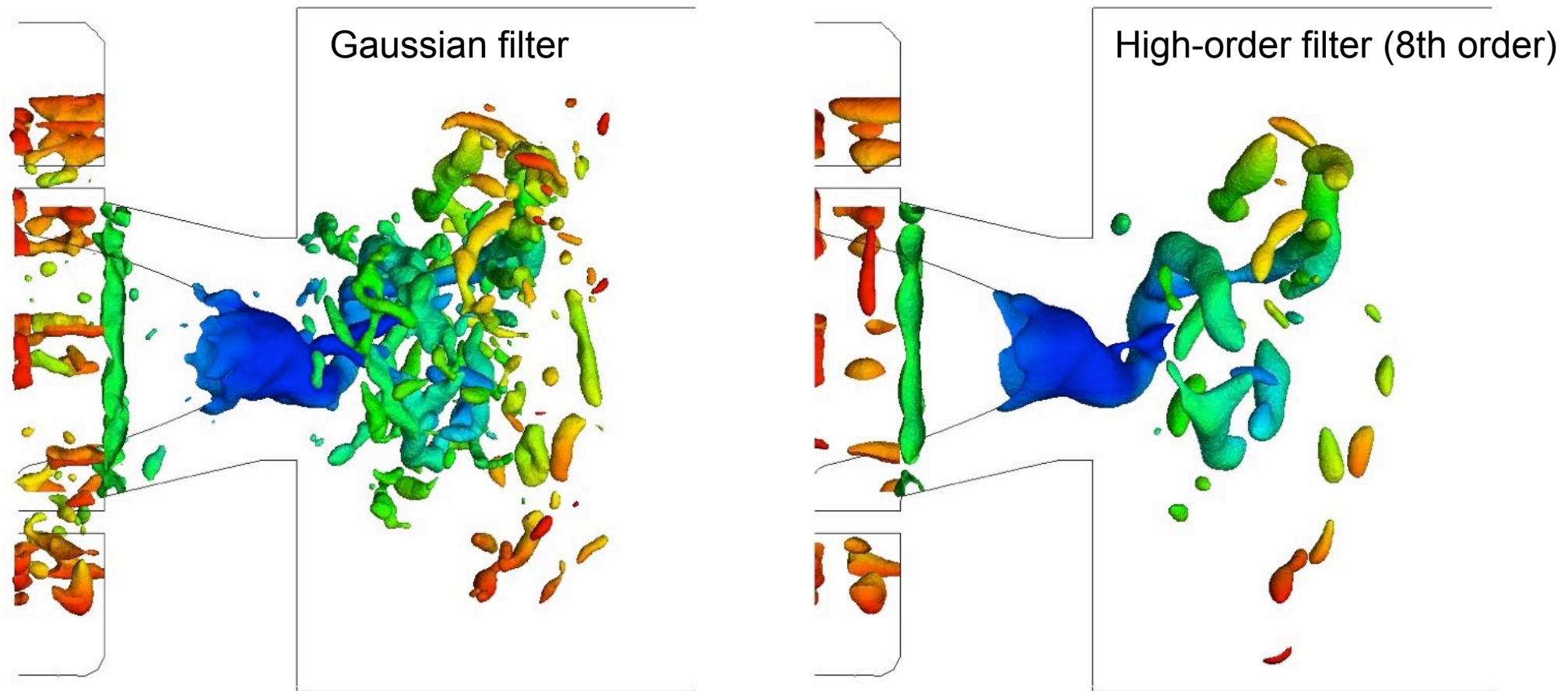
Large-scale feature extraction in the PRECCINSTA burner



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

Large-scale feature extraction in the PRECCINSTA burner

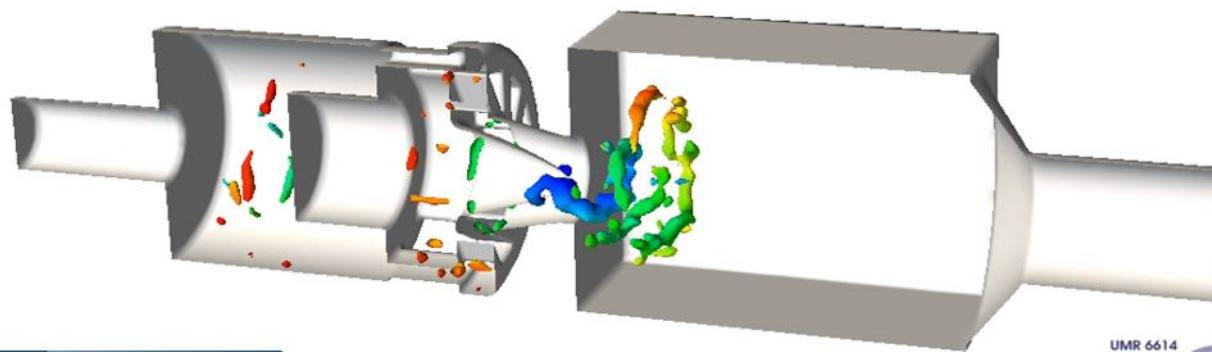
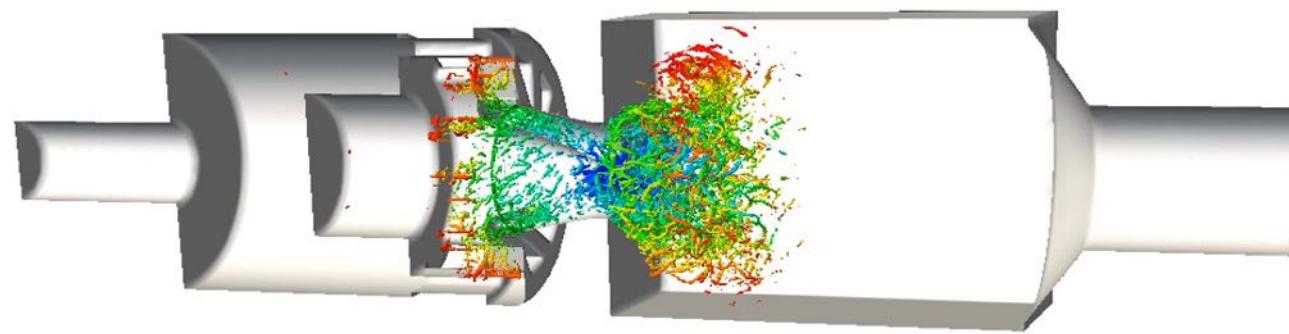
- ▶ Only high-order filters are able to extract large scale features on highly resolved meshes with a large range of scales
- ▶ The CPU cost of post-processing increases dramatically



■ Large-scale feature extraction

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

Time : 0.00 ms

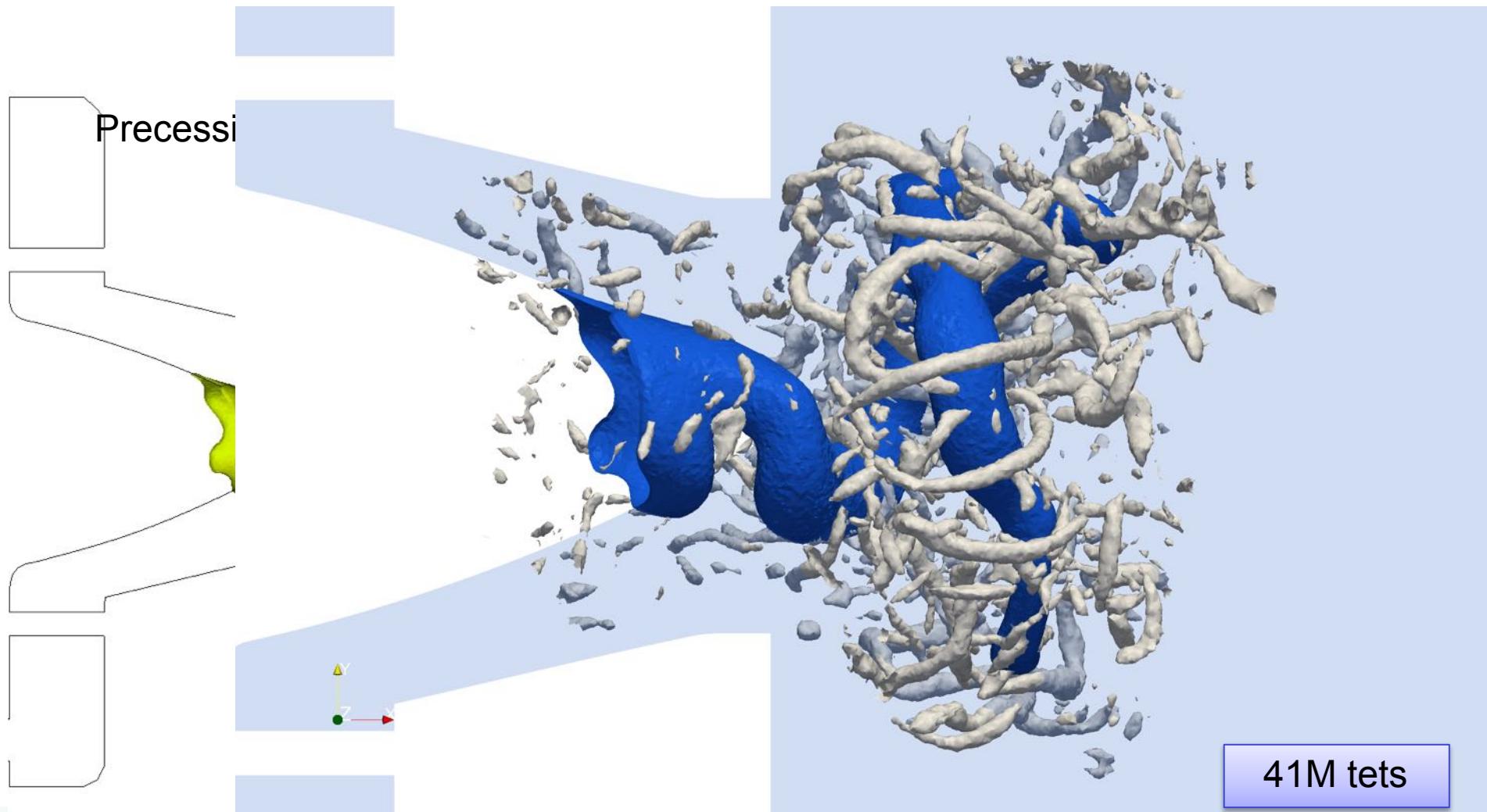


YALES2

UMR 6614
coria
COMPLEXE DE RECHERCHE
INTERPROFESSIONNEL EN AEROTHERMOCHEMIE

■ Large-scale feature extraction

- ▶ Combining high-order filters with level set and segmentation algorithms allows a better extraction of the PVC

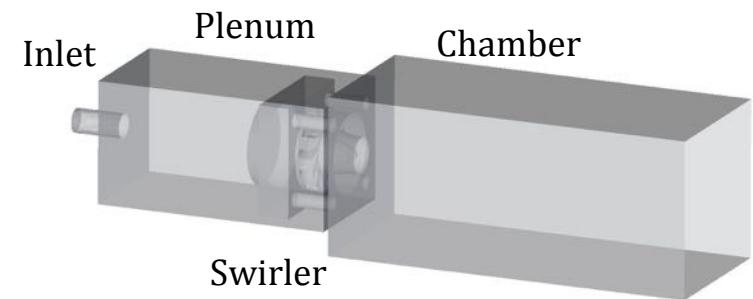


Spray/PVC interactions in the MERCATO burner

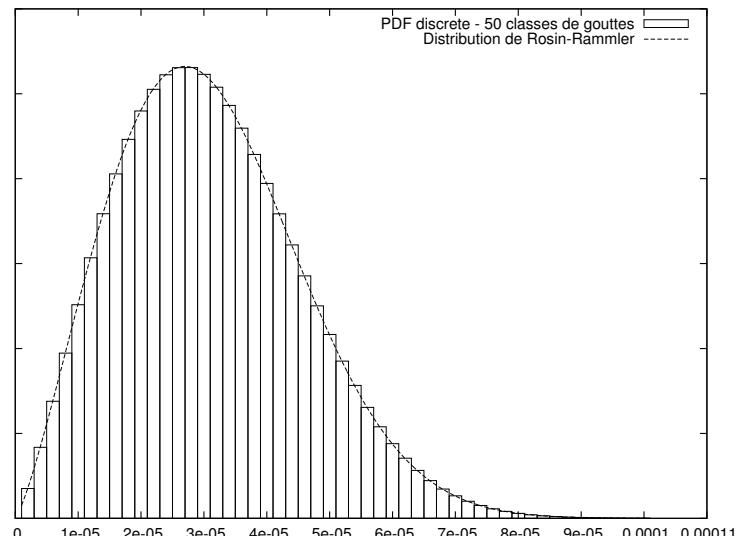
- Operating conditions

[Sanjose 2009]

	Non reactive operating point
Air mass flow rate	15 g/s
Air temperature	463 K
Fuel mass flow rate	2 g/s



- Numerical setup [Hannebique 2013]

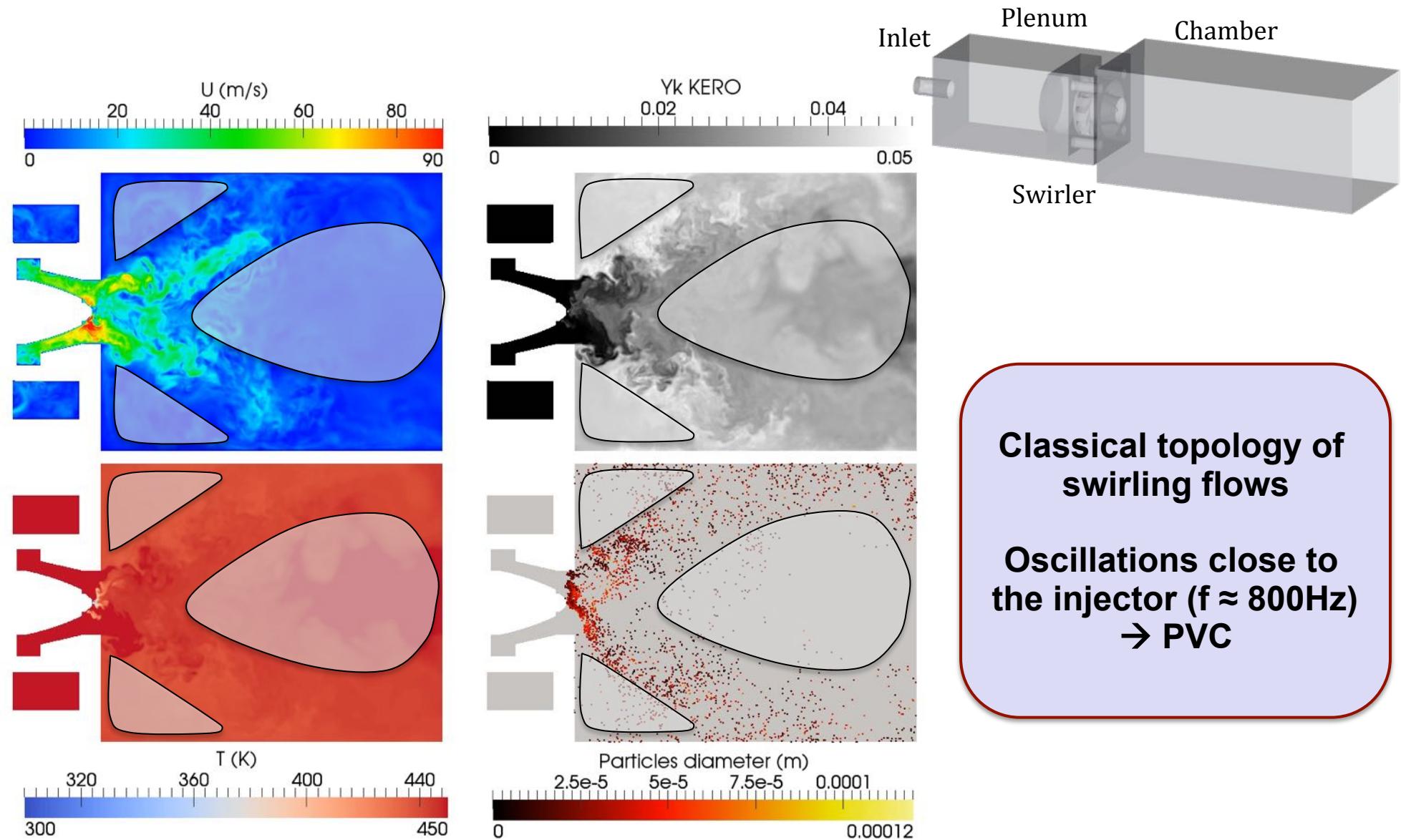


M. Sanjose (2009), PhD thesis.

G. Hannebique (2013), PhD thesis.

	Numerical parameters
CFD code	YALES2
Mesh	40M tetras
Subgrid-scale model	Dynamic Smagorinsky
Method for dispersed phase	Euler - Lagrange
Particles diameter distribution	Rosin-Rammler
Particles size	4 – 100 µm

Spray/PVC interactions in the MERCATO burner

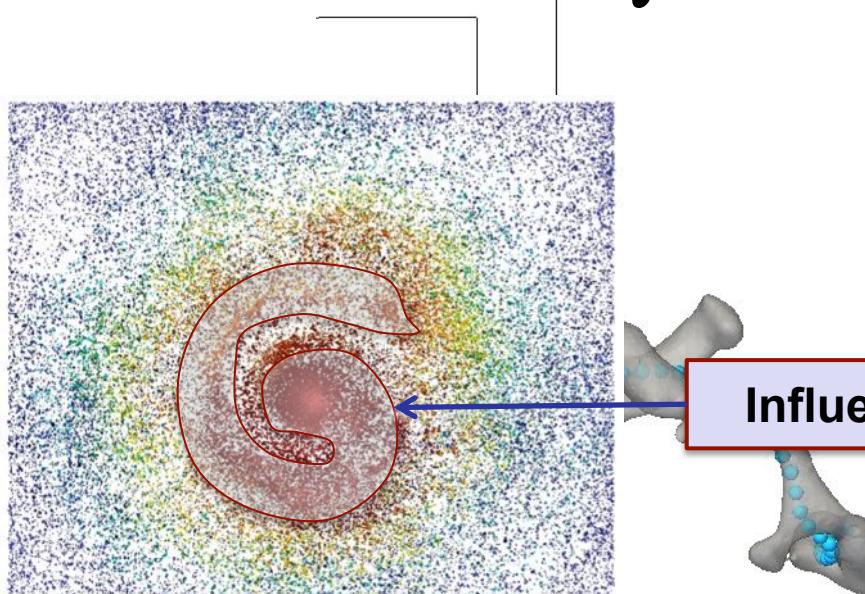
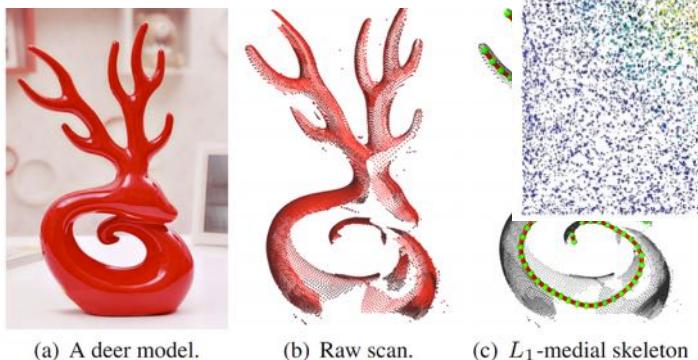


Spray/PVC interactions in the MERCATO burner

PVC identification

- 1) Filtering of Q-criterion with a filter size $\Delta=8\text{mm}$ of order 12
- 2) Isolation of the PVC
- 3) Downsampling of the PVC
- 4) Extraction of the PVC (performed with the open source software PointCloud Pro [Huang 2013])

$$\overline{Q} = 3 \cdot 10^7$$



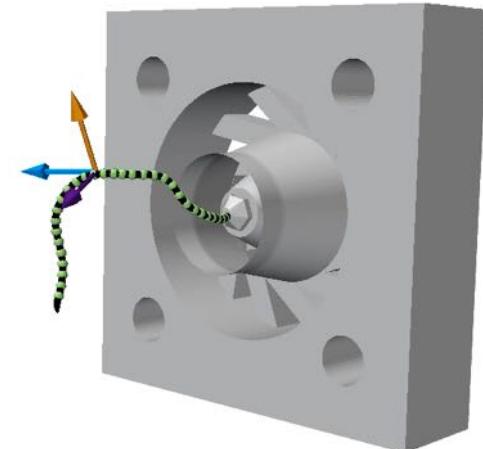
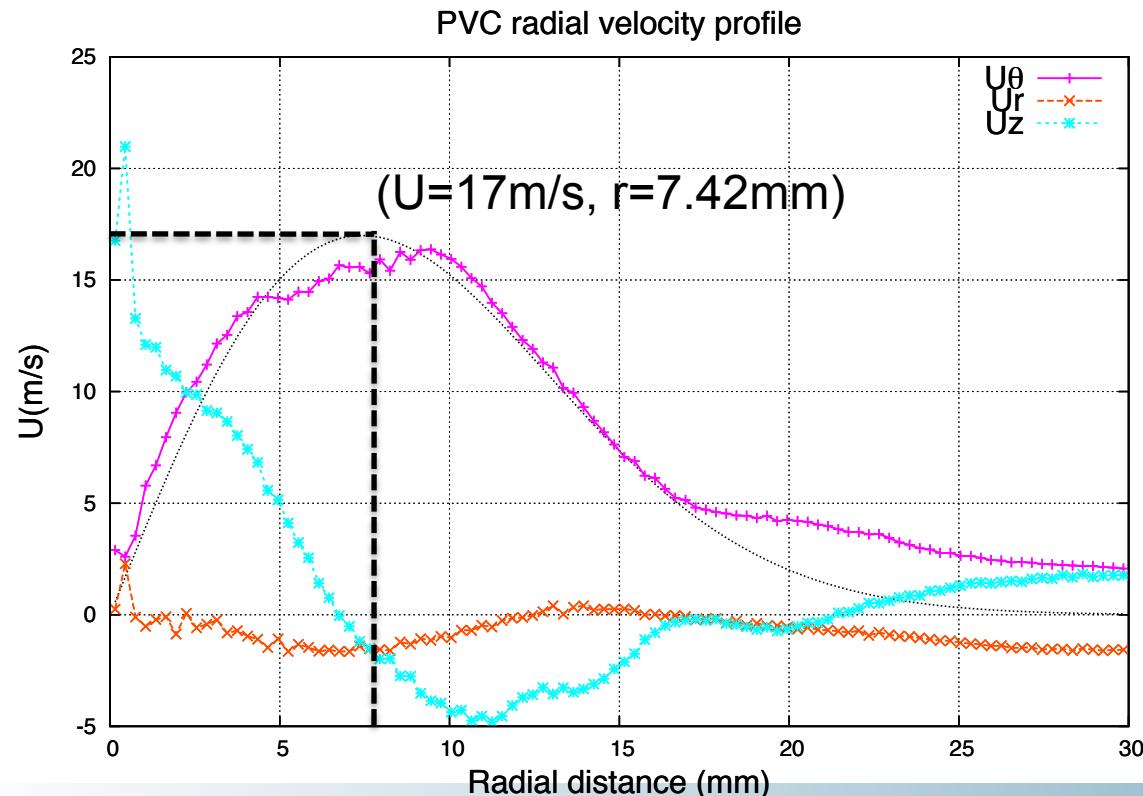
H. Huang, S. Wu, D. Cohen-Or, M Gong, H Zhang, G Li, and Chen B. L1 medial skeleton of point cloud. ACM Transactions on Graphics, 32 :65 :1–65 :8, 2013.

Spray/PVC interactions in the MERCATO burner

Reconstruction of the PVC velocity profile :

- 1) Projection of u_{PVC} on PVC coordinate system
- 2) Averaging over all PVC length
- 3) Fitting with analytical Gaussian vortex velocity profile

$$u_{PVC} = \begin{pmatrix} u_z \\ u_r \\ u_\theta \end{pmatrix}$$



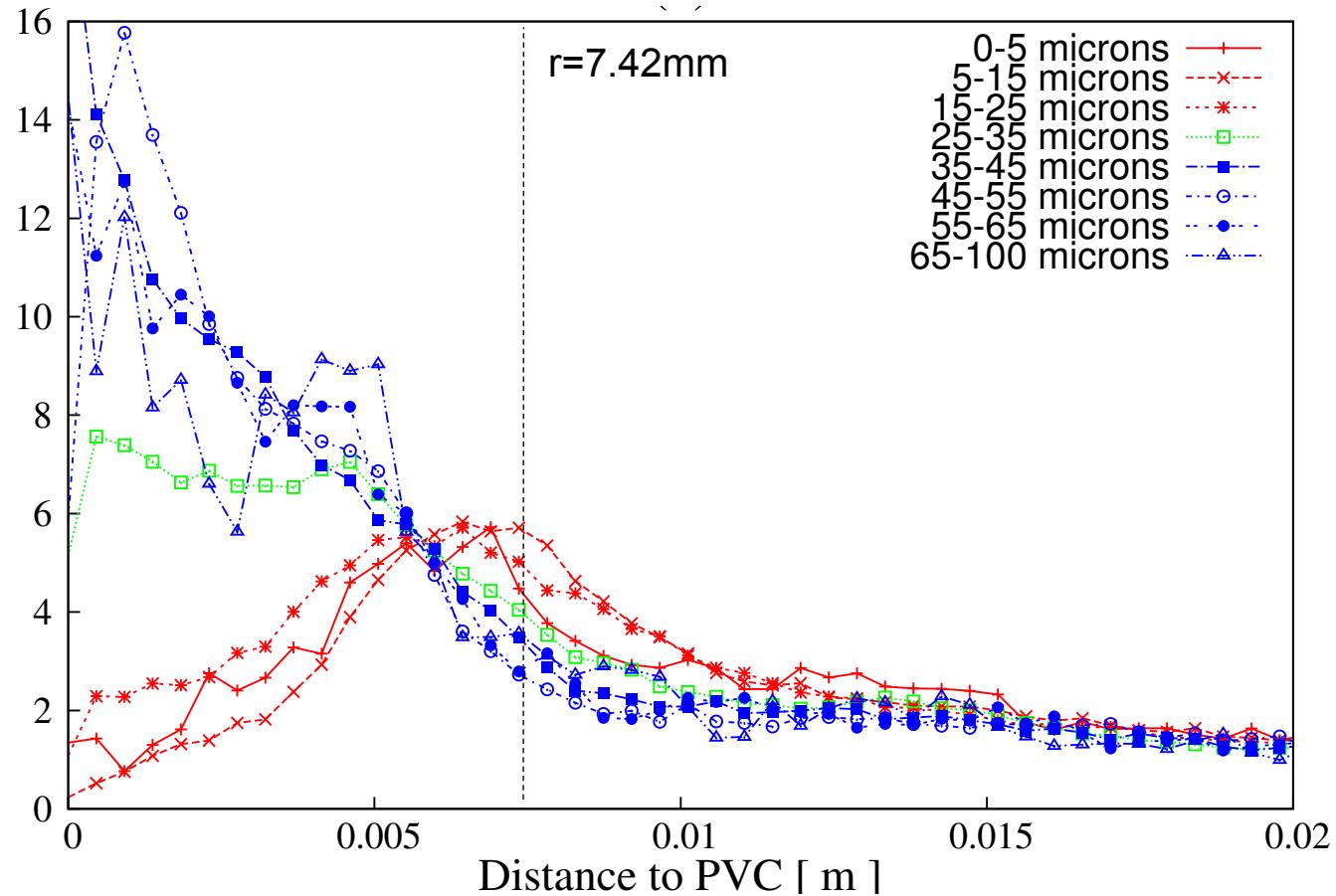
PVC characteristic time scale:

$$\tau_{PVC} = \frac{2\pi r}{u_{max}} = 2.74\text{ms}$$

Spray/PVC interactions in the MERCATO burner

Interaction with fuel droplets

PDF of the distance to the PVC for each diameter class

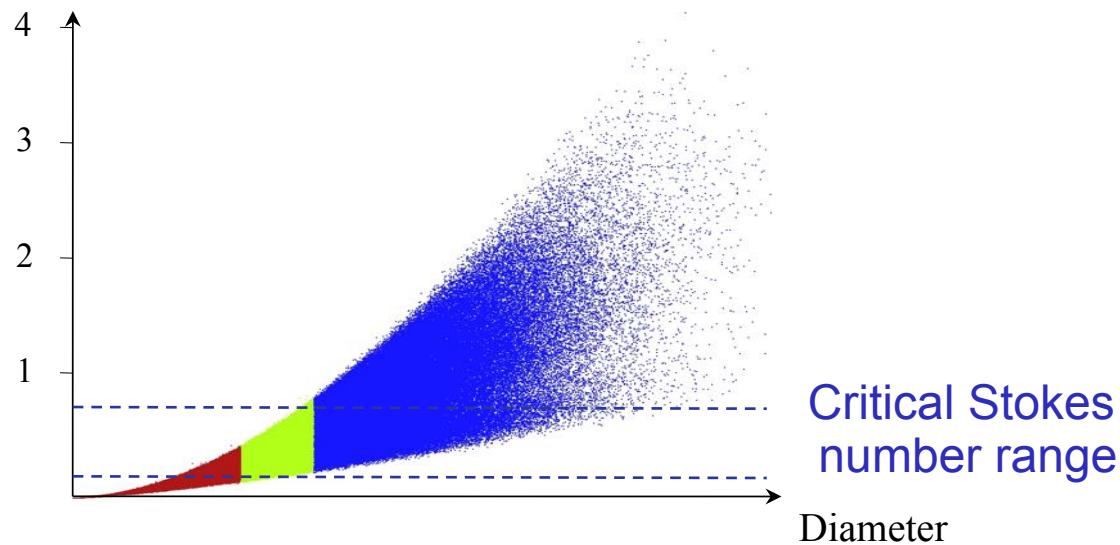


Important segregation effect of the PVC

Spray/PVC interactions in the MERCATO burner

► Stokes number based on PVC time scale

Stokes number



Inertial particles ($St > St_c$) are present
in the PVC inner core
Small particles ($St \ll St_c$) tend to
accumulate at the periphery of the PVC

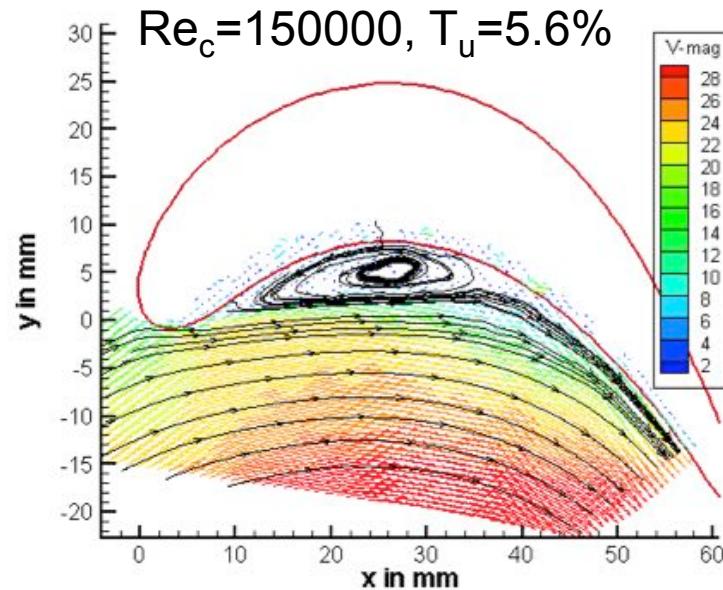
Modeling of heat transfer on a low-Mach number turbine blade

**N. Maheu, V. Moureau, P. Domingo, CORIA
G. Balarac, LEGI
F. Duchaine, CERFACS**

- MAHEU, N., MOUREAU, V., DOMINGO, P., DUCHAINE, F. & BALARAC, G. (2012) 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.
- MAHEU, N., MOUREAU, V. & DOMINGO, P. (2012) High fidelity simulation of heat transfer between a turbulent flow and a wall. *ERCOFTAC ETMM9*. Thessaloniki, Greece.

■ Study of heat exchanges on a turbine blade

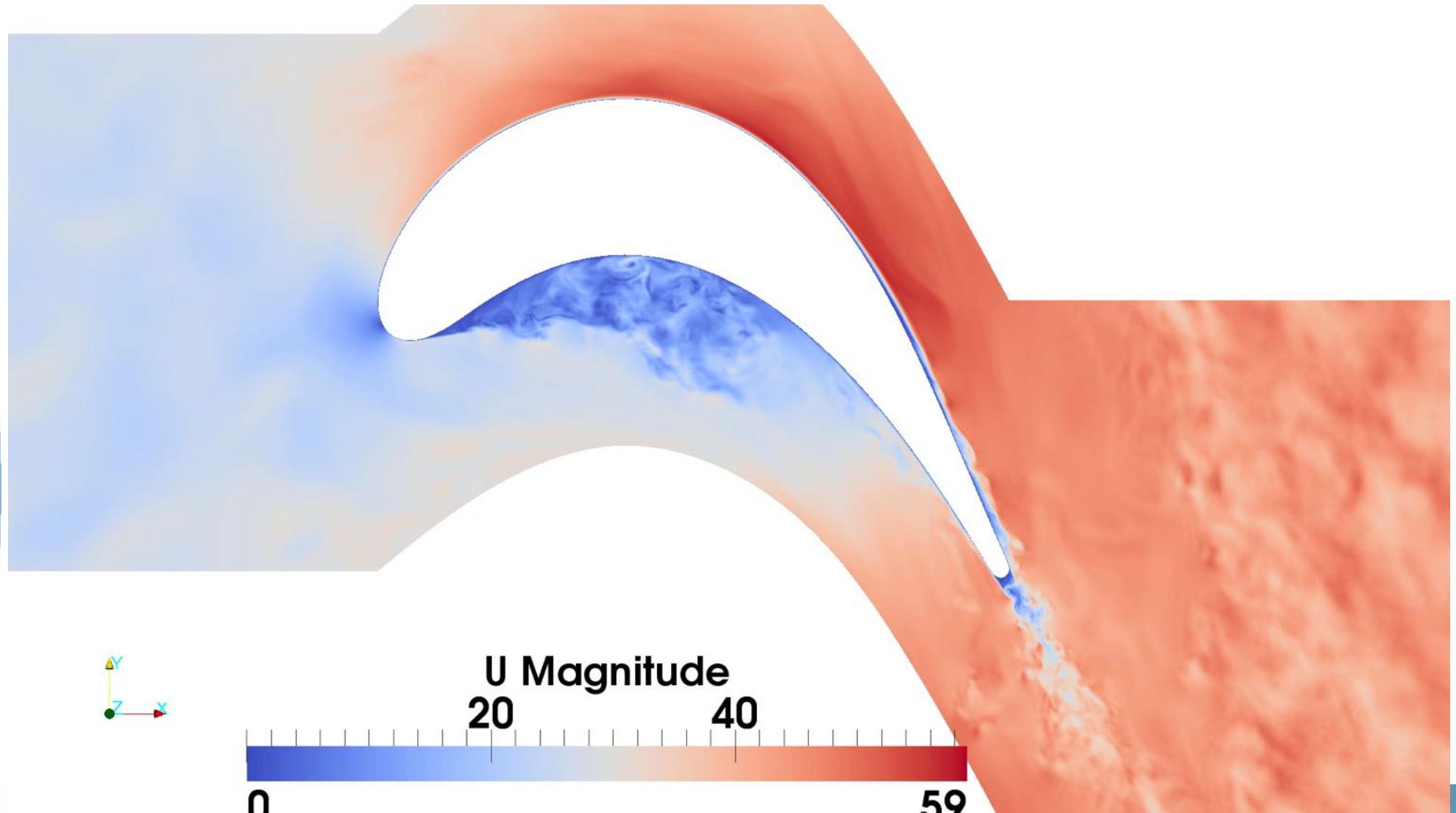
- ▶ T7.2 blade from AlTEB2 project
- ▶ Low-Mach number blade
- ▶ Experiments from Karlsruhe University
- ▶ Aim: to build a reference LES database for the derivation of heat transfer models



Mesh	Cell count	Node count	Min. cell size	Max $\Delta y^+, \Delta x^+, \Delta z^+$	Blade Flow-Through time
M0	1.2M	220K	90 μm	93.3	32.0
M1	35M	5.8M	30 μm	30.4	33.9
M2	280M	47M	15 μm	15.2	11.1
M3	2.2B	367M	7.5 μm	7.6	4.5
M4	17.9B	3.0B	3.75 μm	3.8	0.9
M5	143B	23.8B	1.9 μm	(2.0)	(40 Δt)

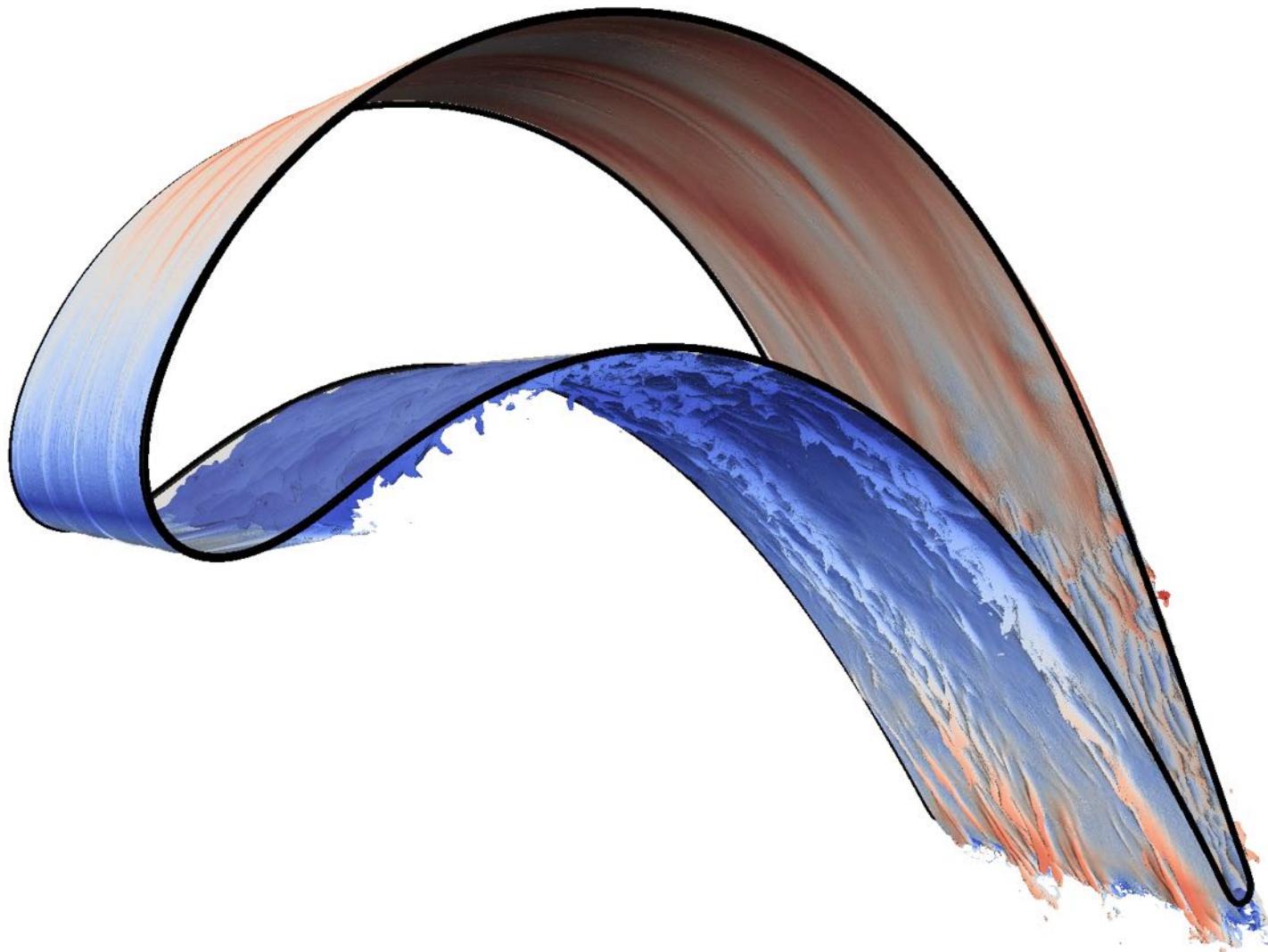
■ Flow topology – M2 (280M tets)

► Velocity magnitude in the midplane



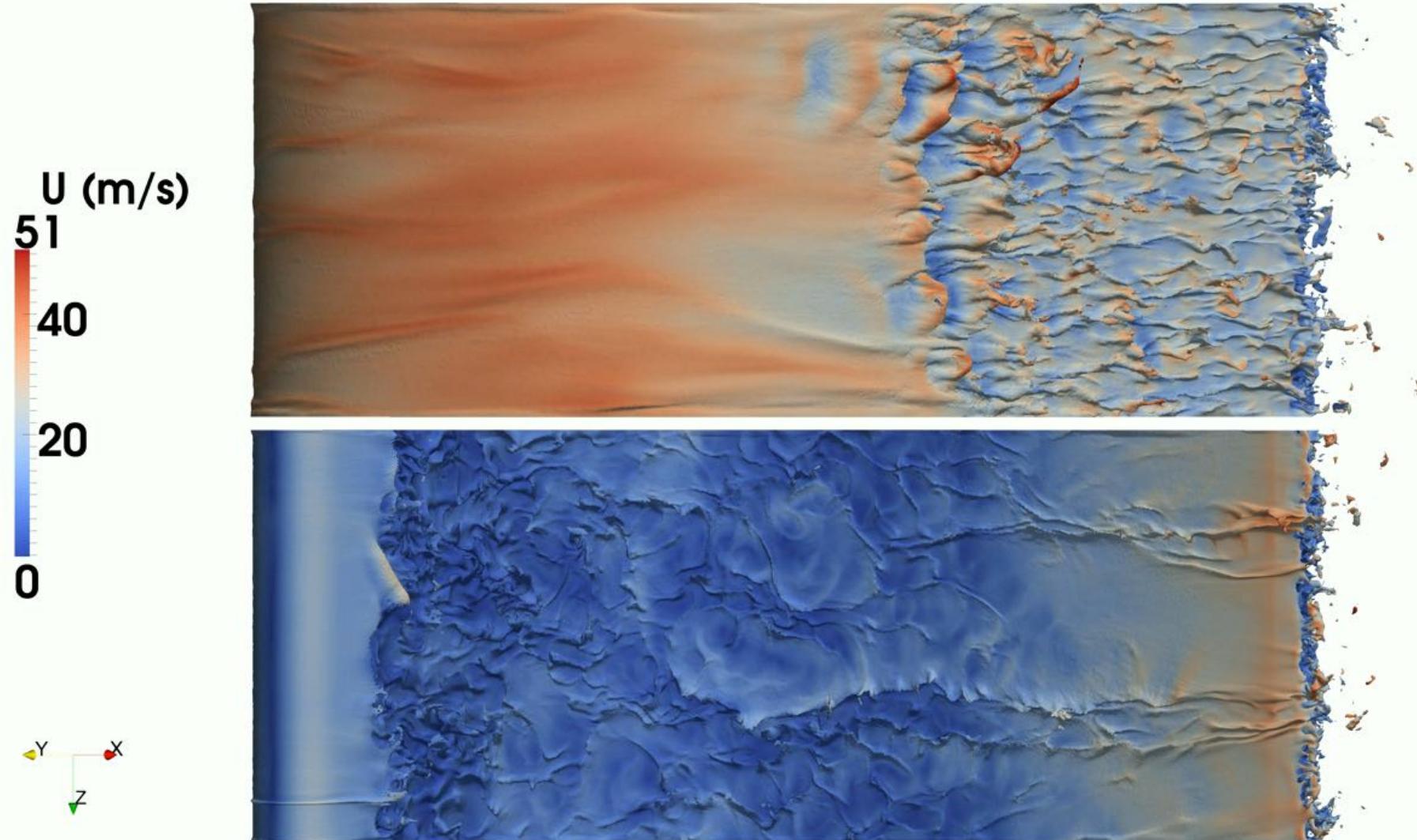
■ Flow topology – M2 (280M tets)

- ▶ Temperature iso-surface colored by the velocity magnitude



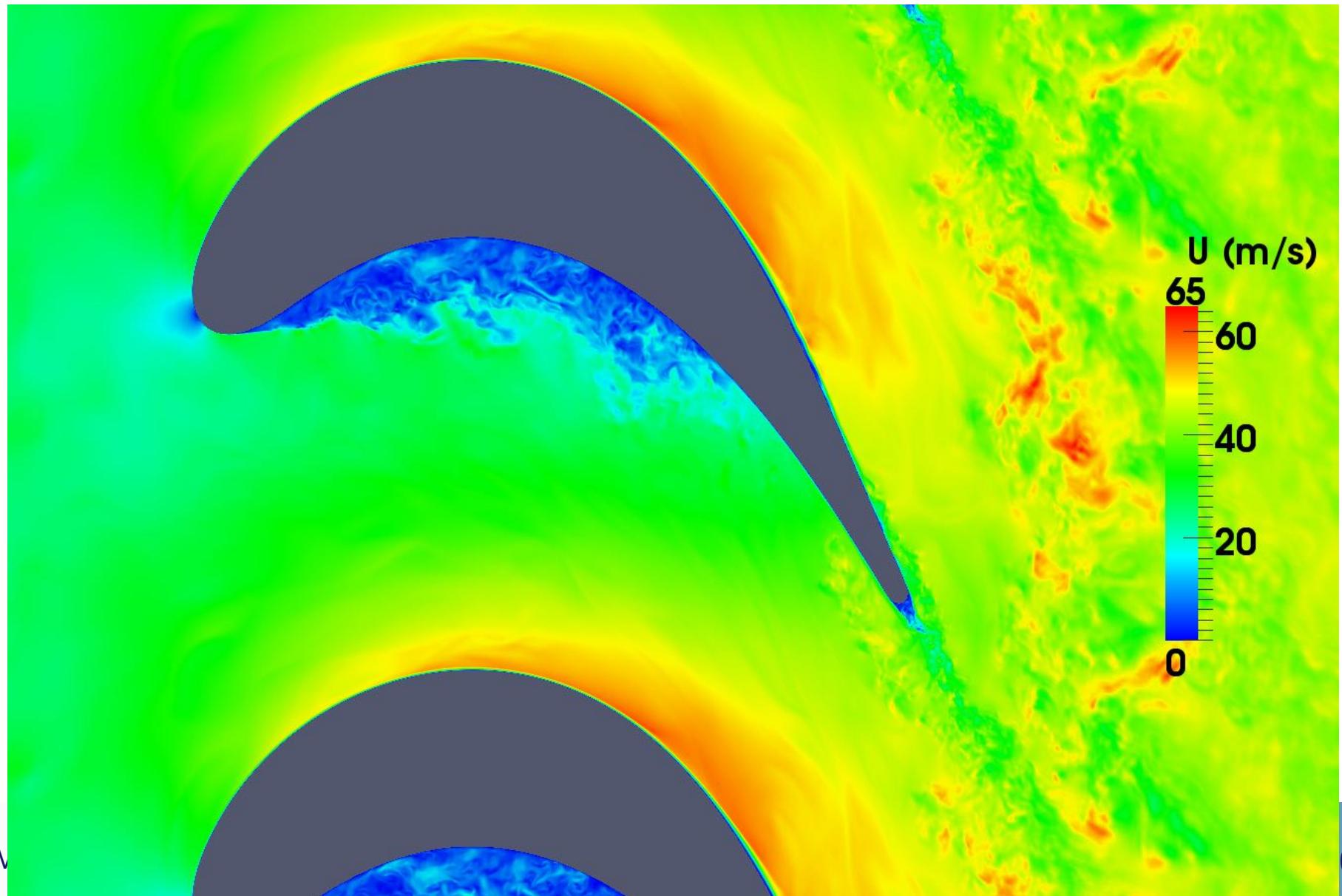
■ Flow topology – M2 (280M tets)

- ▶ Temperature iso-surface colored by the velocity magnitude



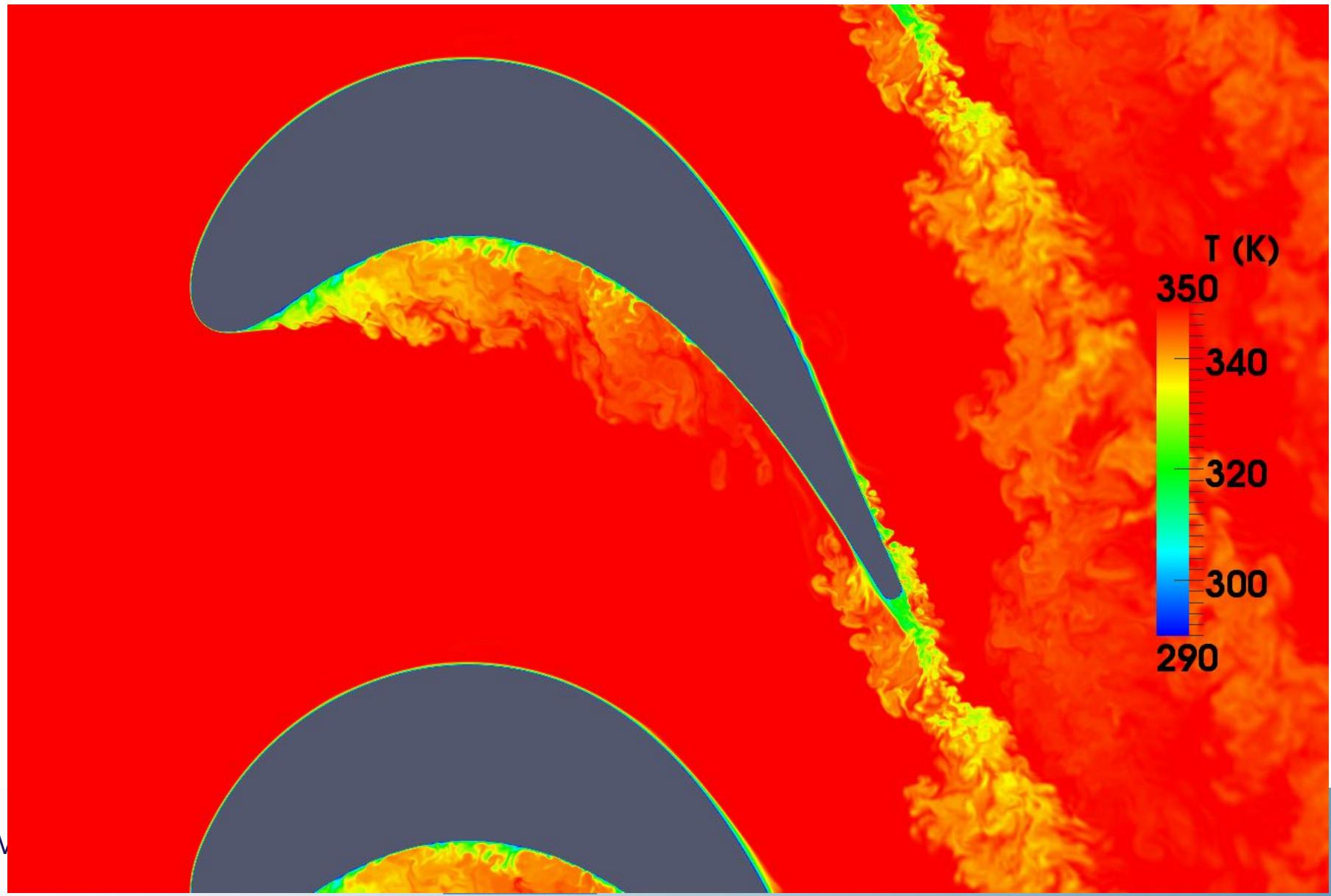
■ Flow topology – M4 (18B tets)

► Velocity magnitude



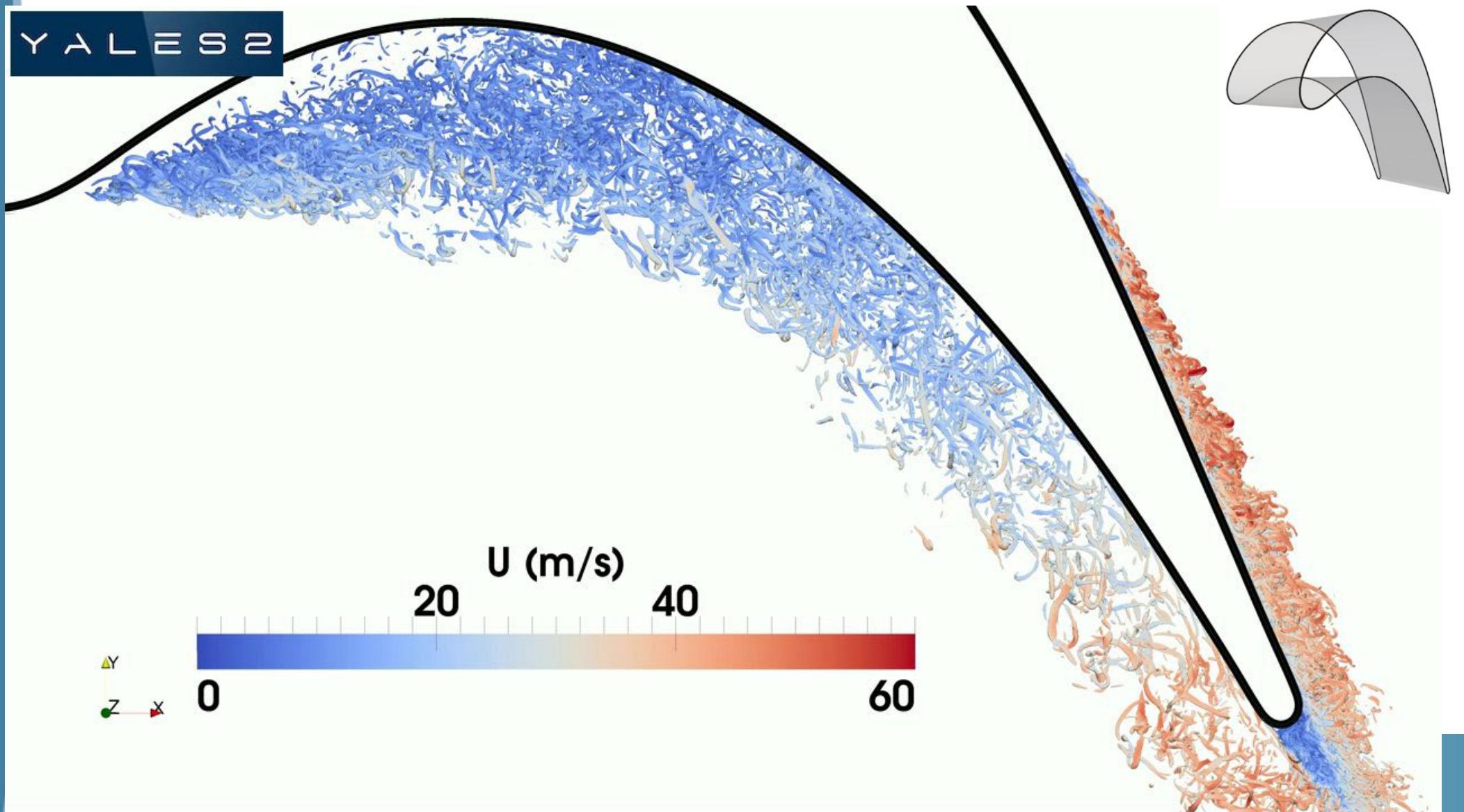
■ Flow topology – M4 (18B tets)

► Temperature

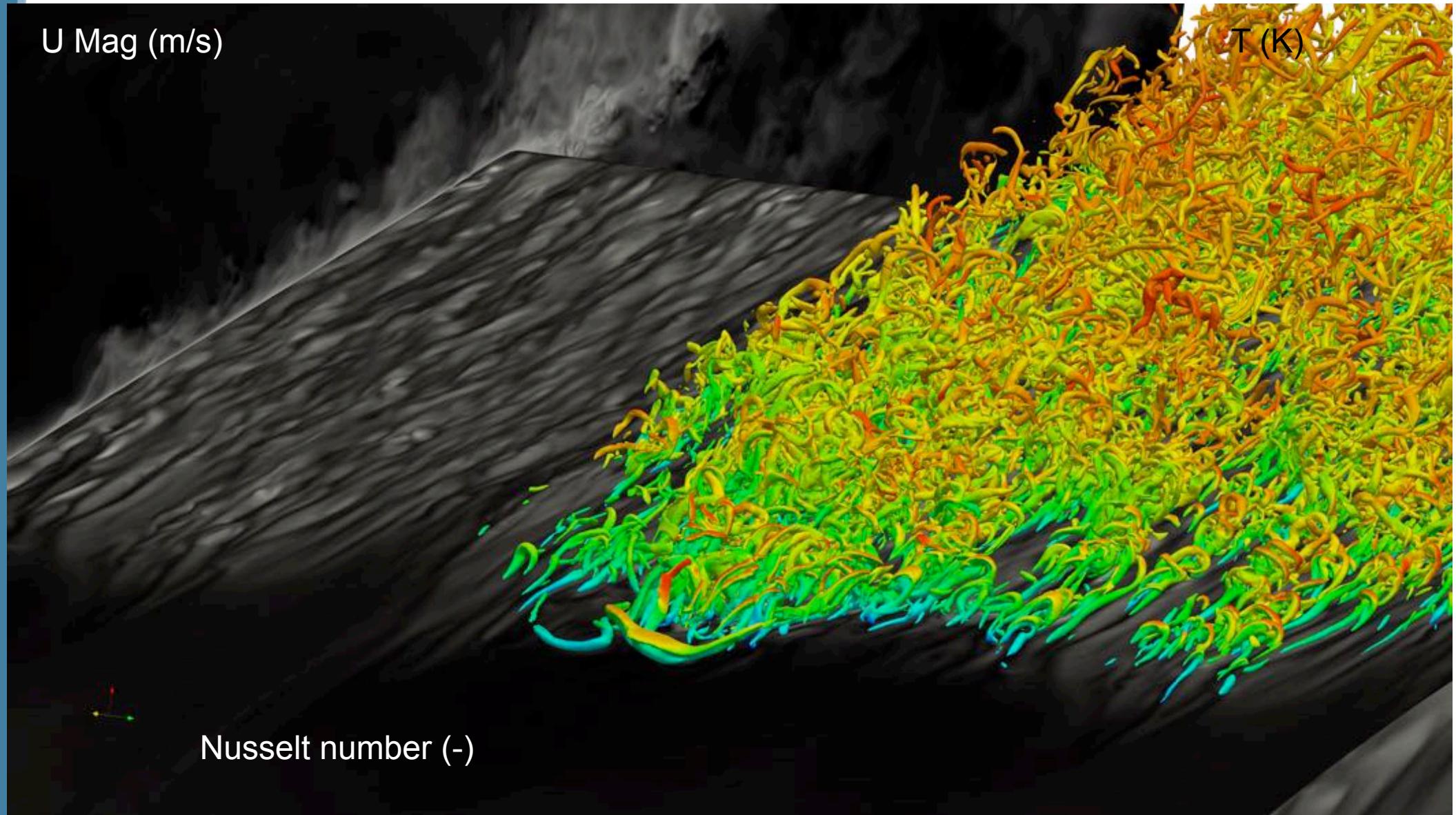


■ Smallest resolved vortices – M4 (18B tets)

- ▶ Selective sampling of Q-criterion iso-surfaces

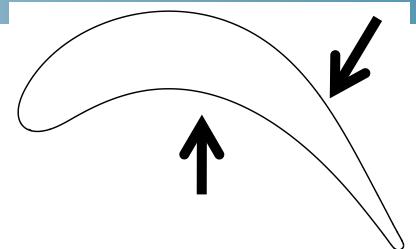


■ Transition on the suction side – M4 (18B tets)



■ Effect of turbulent eddies on heat transfer

- ▶ Study of local heat transfer – M4 (18B tets)
- ▶ Selective sampling of temperature iso-surfaces

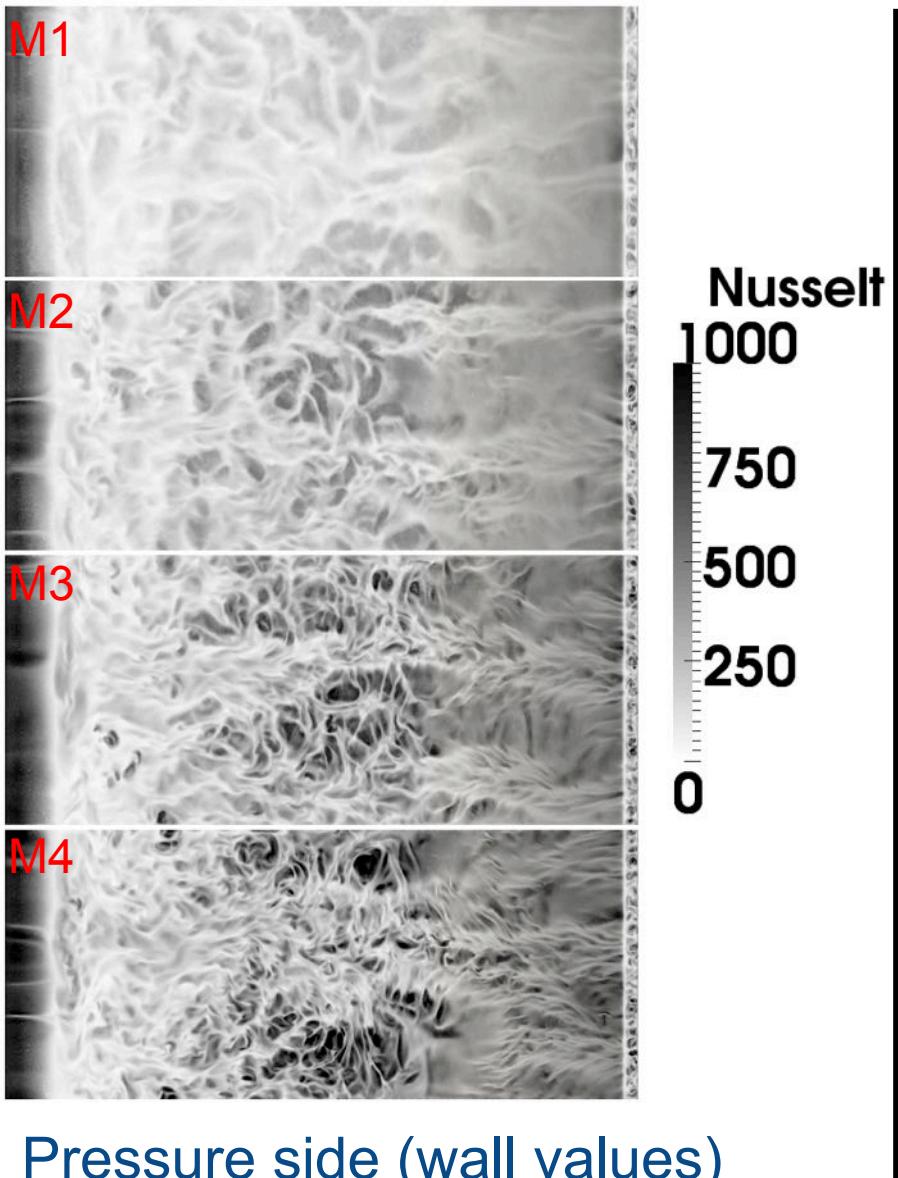


U (m/s)
10 20

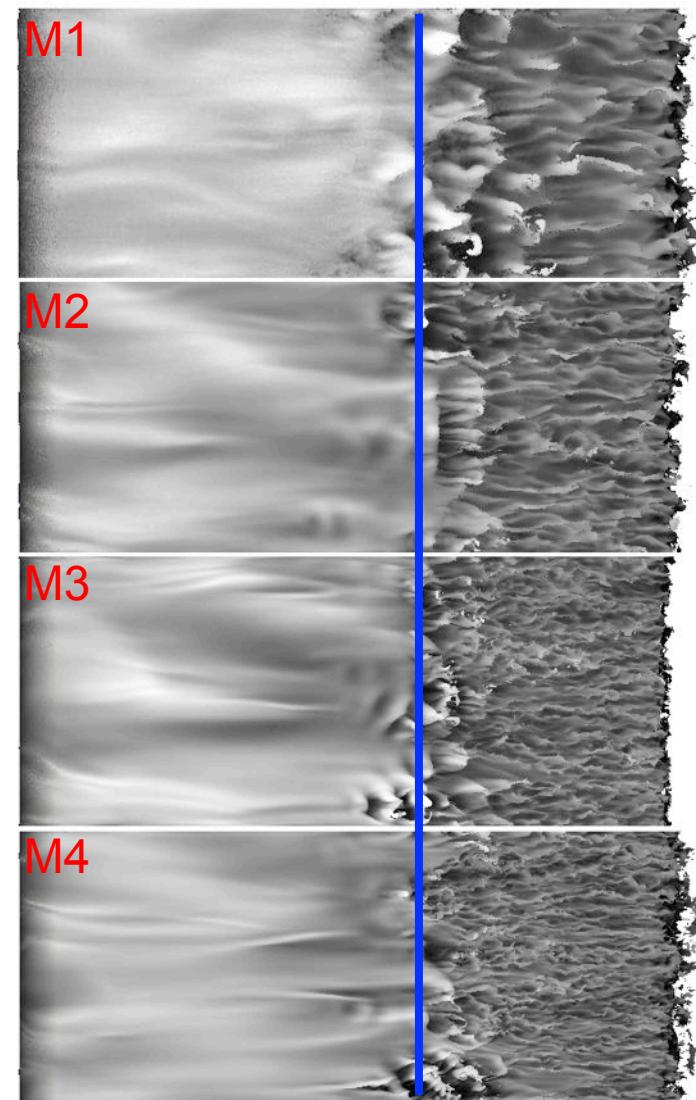
0

25

Effect of turbulent eddies on heat transfer Mesh resolution effect

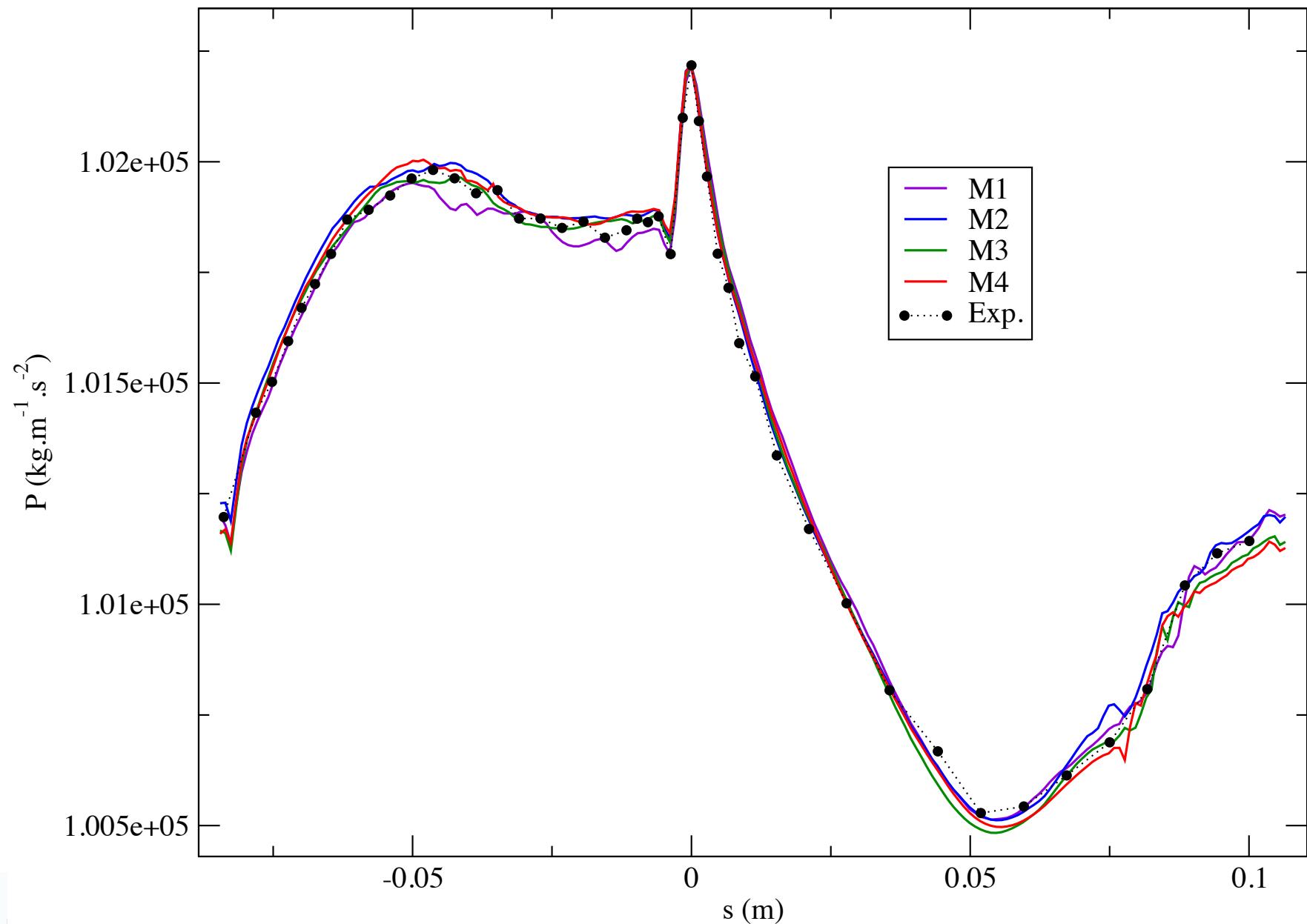


► Pressure side (wall values)

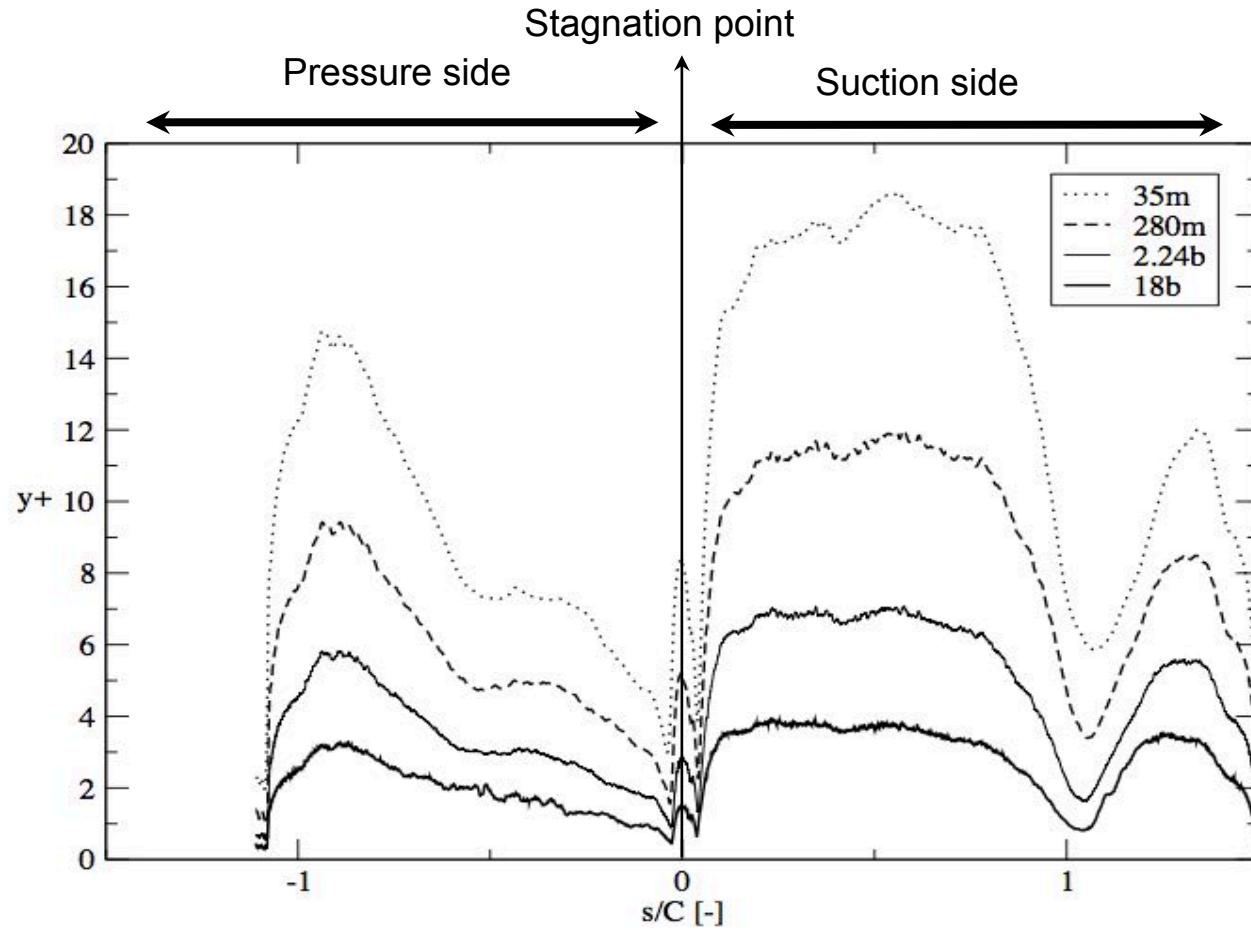


► Suction side ($\text{isoZ} = 0.5$
colored by velocity)

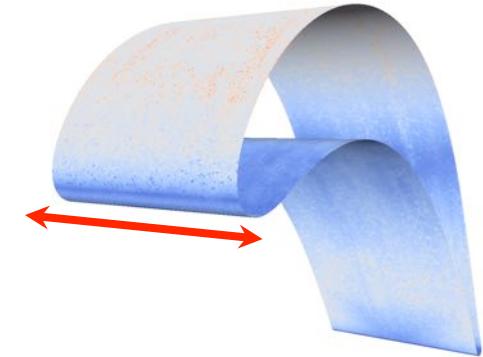
■ Pressure distribution on the blade



■ Assessment of mesh resolution at the wall



Resolution at the surface of the blade

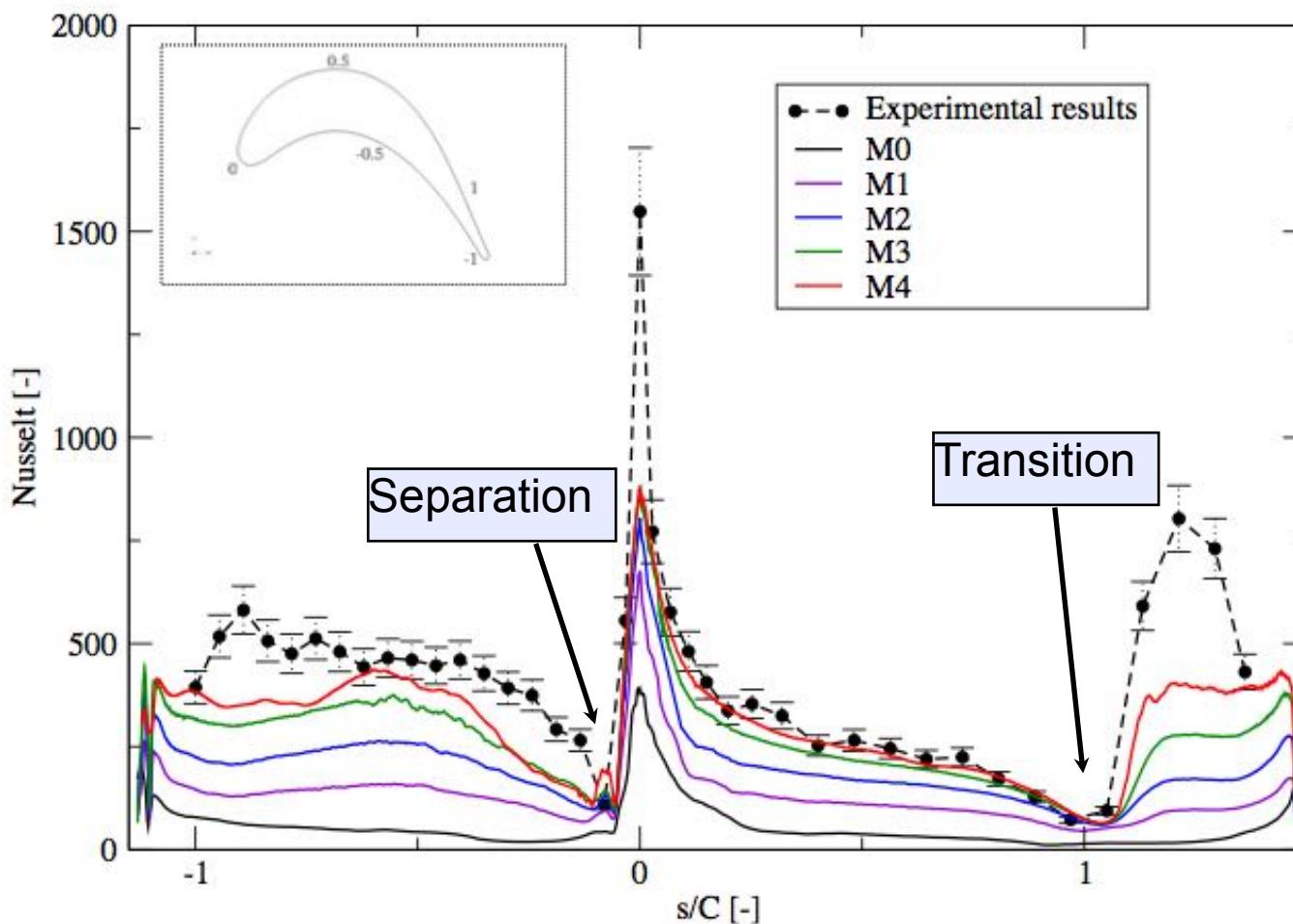


Span (z-direction) of the computational domain:

$$\frac{1}{3}C$$

■ Heat transfer on the blade

- Resolved Nusselt number at the blade surface on each mesh, used as a heat transfer resolution indicator



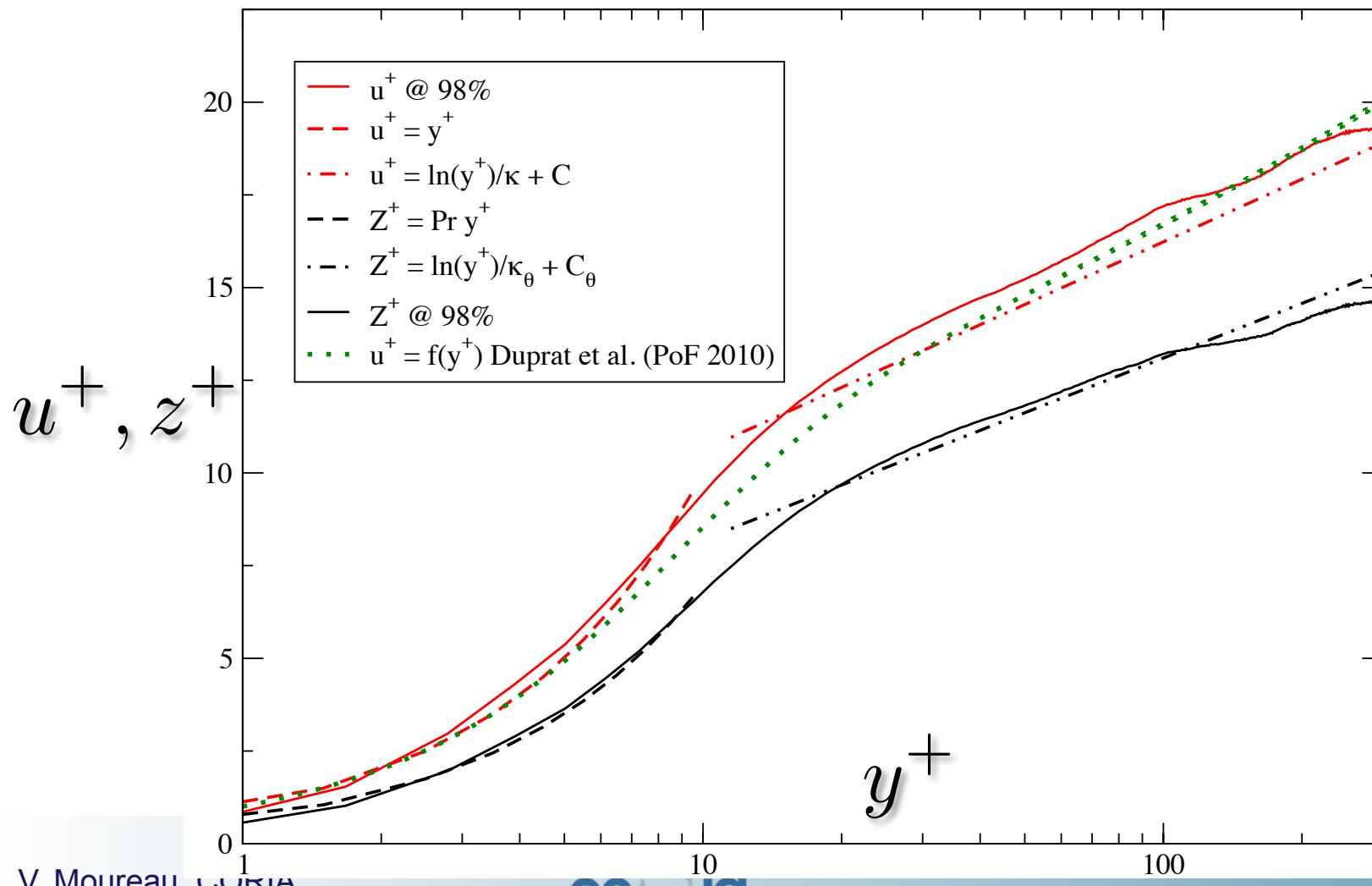
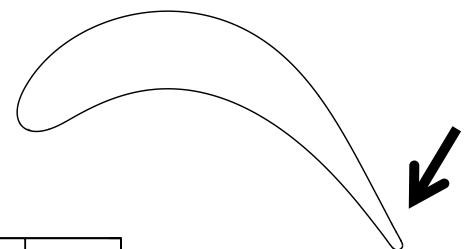
Nusselt number:

$$Nu = \frac{\tilde{q}C}{(T_\infty - T_w) \alpha}$$

with $\tilde{q} = \alpha \nabla \tilde{T}$

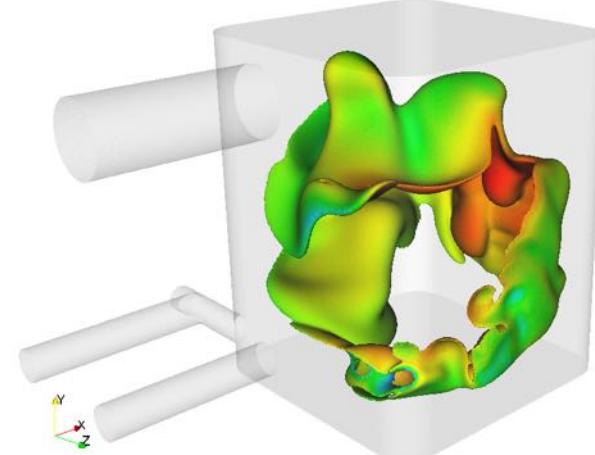
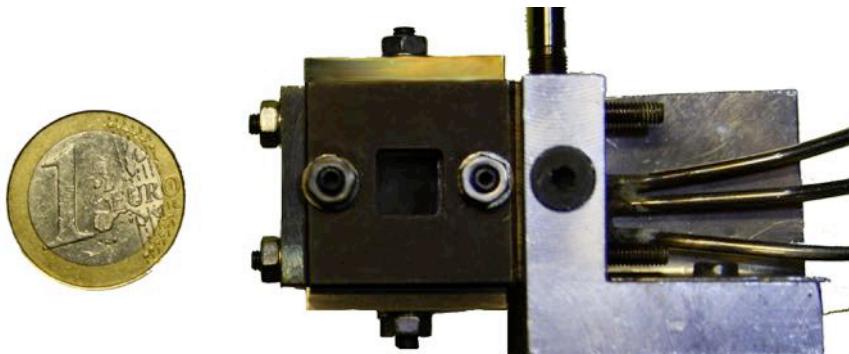
Velocity and scalar profiles at the trailing edge

- Thanks to the level set function, the streamwise velocity and the temperature in wall units may be plotted as functions of the wall distance



A finite-rate chemistry approach for Large Eddy Simulation of pollutant emissions in a meso-scale combustion device

Pierre Bénard, Vincent Moureau, Ghislain Lartigue,
Yves D'Angelo



■ Context

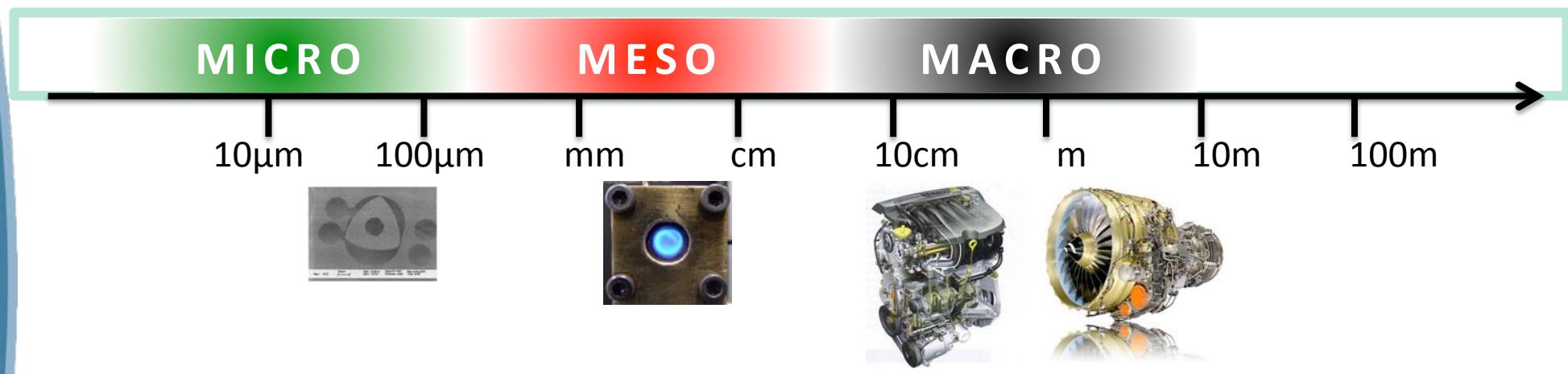
► New applications

- Need of power supply (from 1 to 100 W)



► Interest for the centimeter scale combustion

- Fuel energy density benefits [1]



Lightweight, robust, compact and instantly rechargeable

[1] Maruta, Micro and mesoscale combustion, PCI, 2010

■ Context

► Small scale combustion issues [2]

- High heat losses
- Low Reynolds number => poor mixing
- Short residence time



Complex combustion regime, incomplete combustion

► Goals of the study

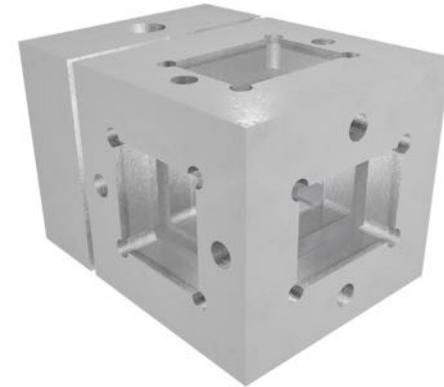
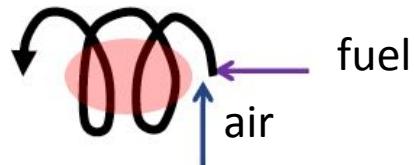
- Predictive simulations of the reactive flow
 - LES 3D with reduced chemistry approach
 - Turbulence and heat losses consideration
- H₂ enrichment influence

[2] Fernandez-Pello, Micropower generation using combustion: Issues and approaches, PCI, 2002

■ Set-up

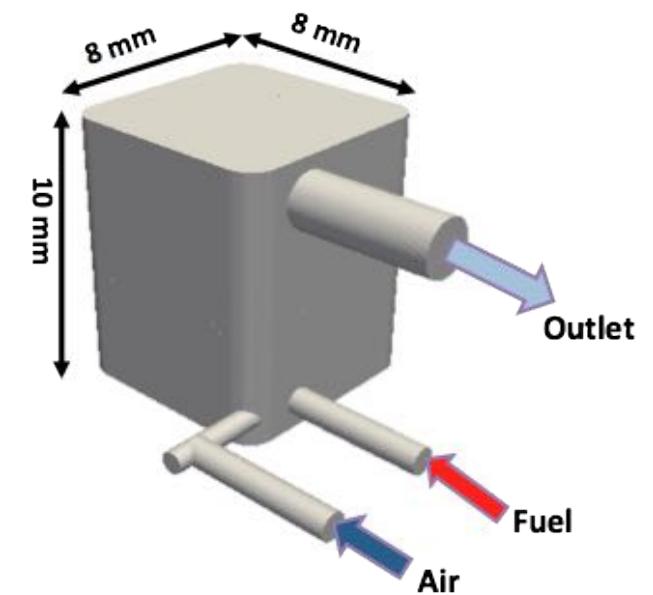
► Meso-combustor experiment [3]

- $8 \times 8 \times 10 \text{ mm} = 0.640 \text{ cm}^3$
- 2 inlets & 1 outlet
- whirl flow topology



► Numerical methods

- Low-Mach number YALES2 solver [4]
- Finite-rate chemistry
- CH₄/air Coffee chemical scheme
 - 14 species, 38 reactions
- 34M elements mesh
 - average cell size = 50 microns



[3] S. Liu, B. Renou, Y. D'Angelo, 15th Int. Symp. on Applications of Laser Techniques to Fluid Mechanics, 2010

[4] www.coria-cfd.fr

► Equations resolved with finite rate chemistry in

- Low Mach number approach, Hirschfelder-Curtiss approximation, ...

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

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

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot \rho Y_k \mathbf{u} = \nabla \cdot (-\rho \mathbf{V}_k Y_k) + \dot{\omega}_k$$

$$\frac{\partial \rho h_s}{\partial t} + \nabla \cdot \rho h_s \mathbf{u} = \frac{\partial P_0}{\partial t} + \nabla \cdot (-\rho \mathbf{V}_h h_s)) + \dot{\omega}_T$$

► Numerical methods

- Operator splitting approach
- Stiff integration with analytical Jacobian of the source terms with CVODE
- Dynamic load balancing of the species source term computation

■ Modeling

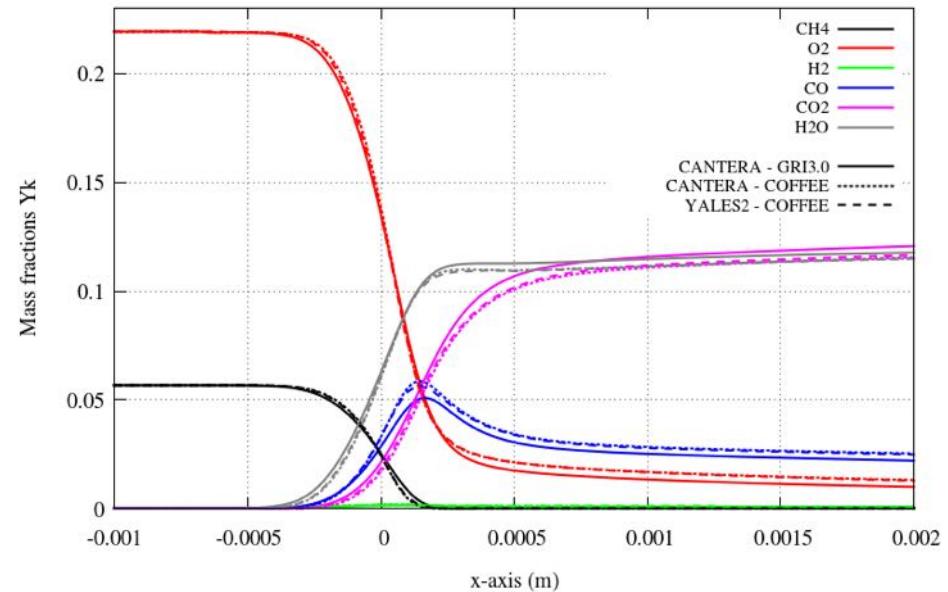
- ▶ **CH₄/air reduced chemistry**
 - **Coffee [5] : 14 species, 38 reactions**

- ▶ **Mesh**
 - **34M of elements**
 - **Uniform cell size of 50 µm**
 - enables to get the correct flame speed and mass fraction profiles

- ▶ **Turbulence model**
 - **Dynamic Smagorinsky [6]**
 - **Acts only in the air jet and at the wall impact**
 - **$\mu_T/\mu_{\text{max}} = 5$**

[5] T. P. Coffee, 1984

[6] Lilly, 1992



Operating conditions

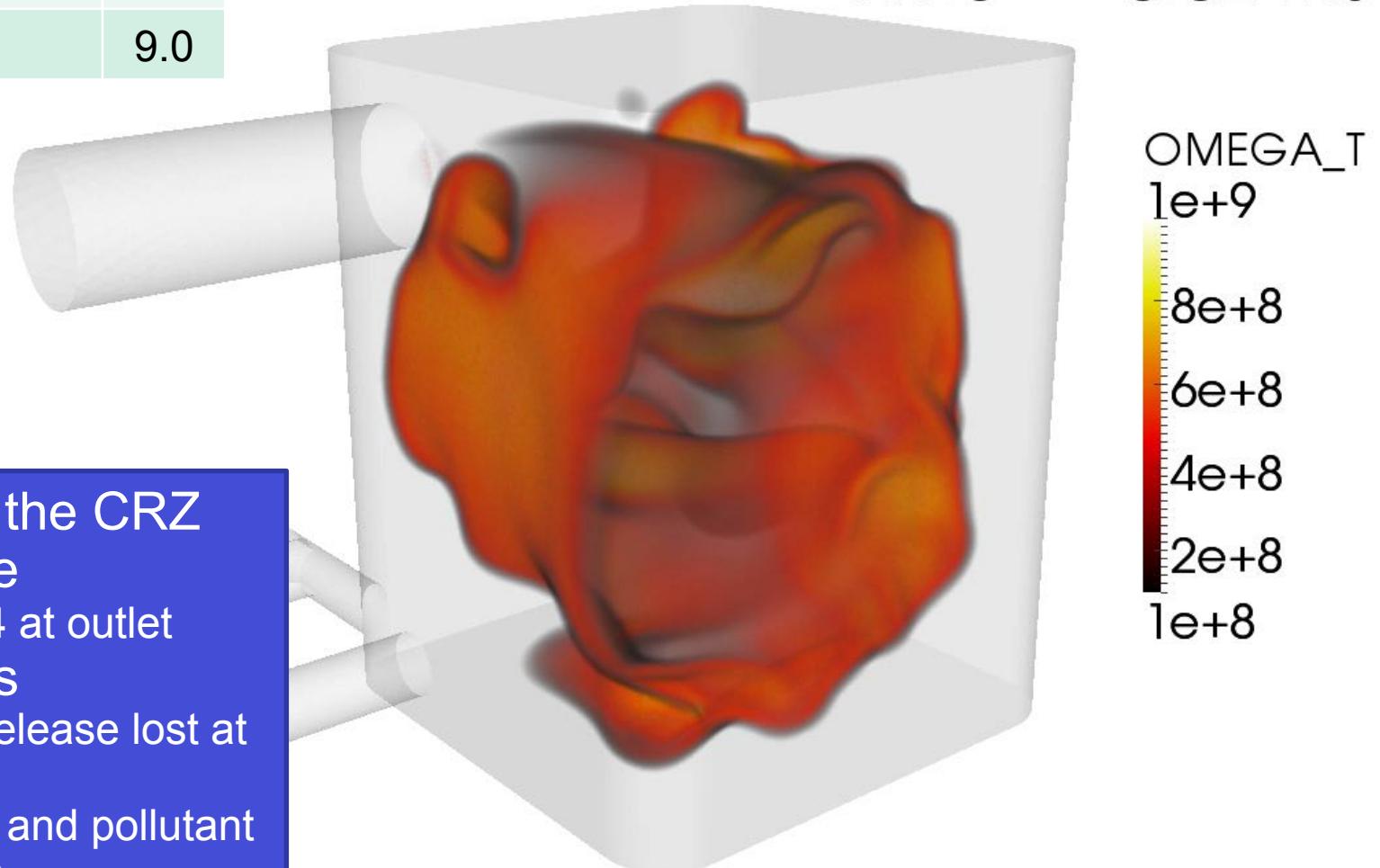
CH ₄ mass flow rate [x10 ⁻⁶ kg/s]	1.74
Air mass flow rate [x10 ⁻⁶ kg/s]	29.0
Equivalence ratio	1.03
Injected power [W]	87.0
Wall temperature[K]	417

Pure CH₄/air reactive flow

Operating conditions

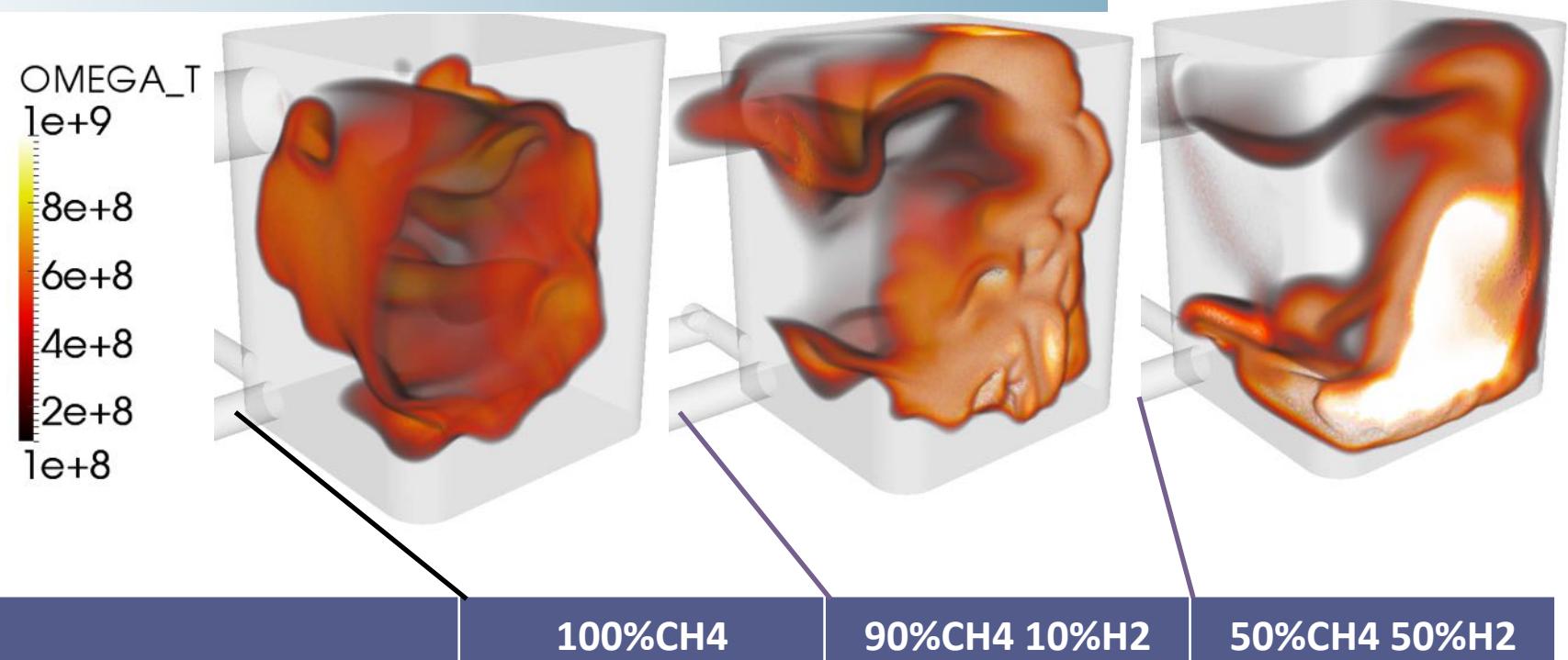
Equivalence ratio	1.03
Wall temperature [K]	417
Flow through time [ms]	9.0

Time = 0.02 ms



- Flame confined to the CRZ
- Globally lean flame
 - ✓ 25% unburnt CH₄ at outlet
- Poor performances
 - ✓ 60% of the heat release lost at the walls
 - ✓ Flame quenching and pollutant emissions (CO...)

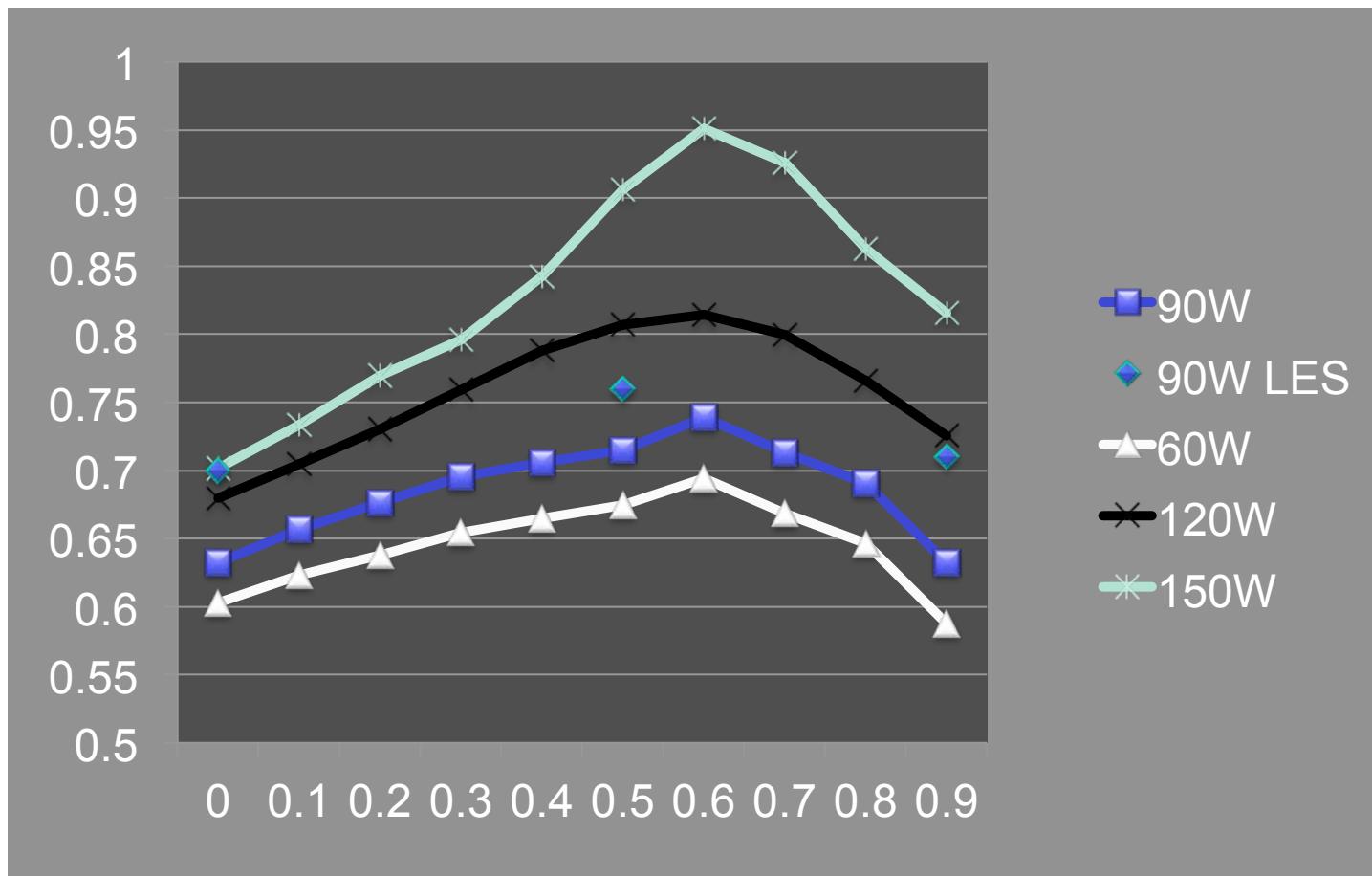
■ Hydrogen enrichment



- Strong influence of H₂ enrichment
 - Small amount of H₂ **improves** performances while keeping the flame topology
 - Large amount of H₂ changes front topology

■ Hydrogen enrichment

- ▶ Comparison of the conversion efficiency with experimental data



- ▶ LES enables predicting the conversion efficiency

The load balancing issue in the stiff integration of source terms

- ▶ Operator splitting and stiff integration of the source terms
- ▶ Chemical source terms are considered constant during the time step

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot \rho Y_k u = \nabla \cdot (-\rho V_k Y_k) + \dot{W}_k$$

$$\frac{\partial \rho h_s}{\partial t} + \nabla \cdot \rho h_s u = \frac{\partial P_0}{\partial t} + \nabla \cdot (-\rho V_h h_s) + \dot{W}_T$$

- ▶ The constant source terms are computed as

$$W_k = \int_{t^n}^{t^{n+1}} \dot{\omega}_k dt$$

$$W_T = \int_{t^n}^{t^{n+1}} \dot{\omega}_T dt$$

- ▶ from the solving of a homogeneous reactor

$$\frac{d\rho Y_k}{dt} = \dot{\omega}_k$$

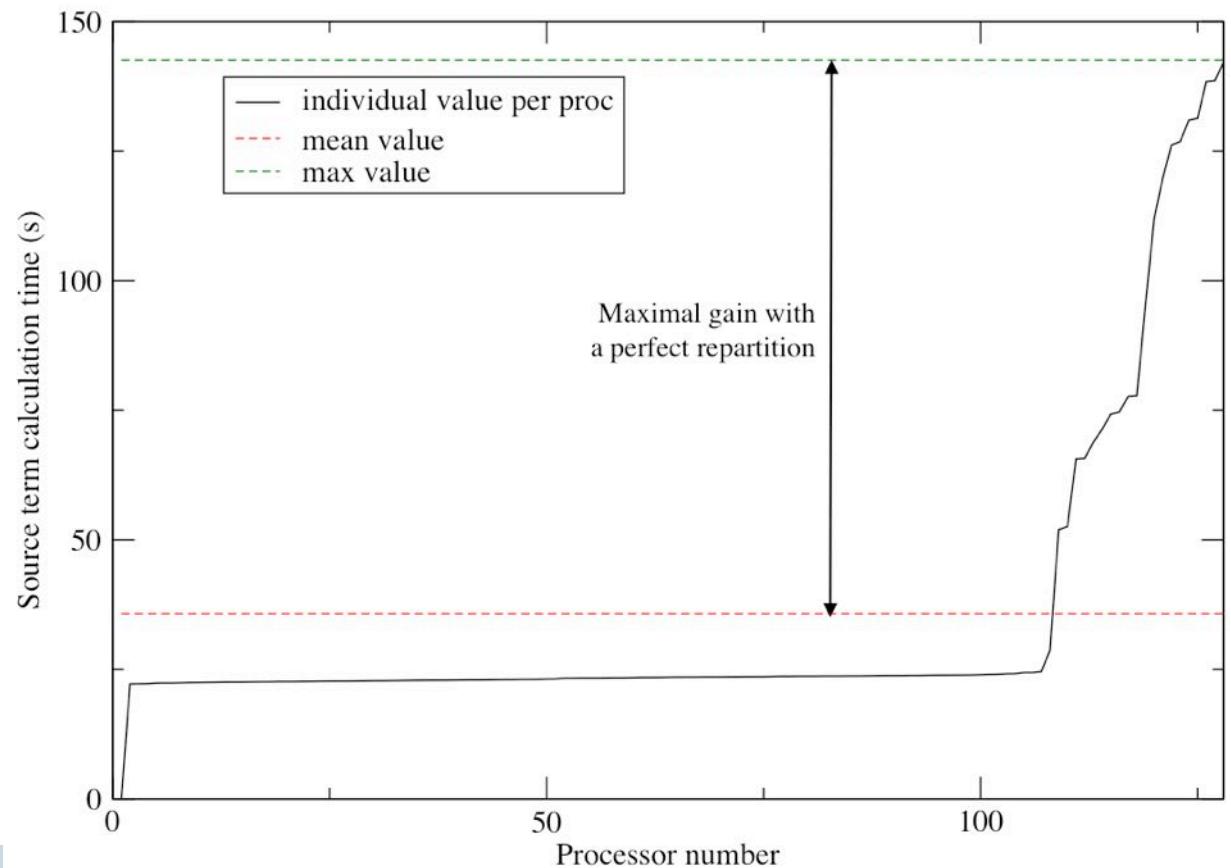
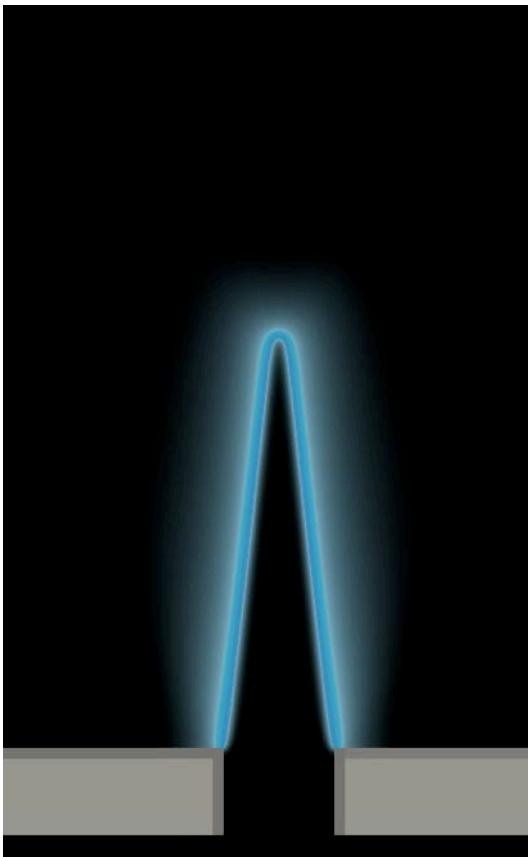
$$\frac{d\rho h_s}{dt} = \dot{\omega}_T$$

$$P = \text{const}$$

The load balancing issue in the stiff integration of source terms

▶ Calculation of a 2D bunsen burner

- Methane/air premixed burner
- 14 species, 38 reactions (T.P. Coffee, 1983) integrated with CVODE
- Even for small mechanisms, a huge gain could be obtained with ideal load balancing



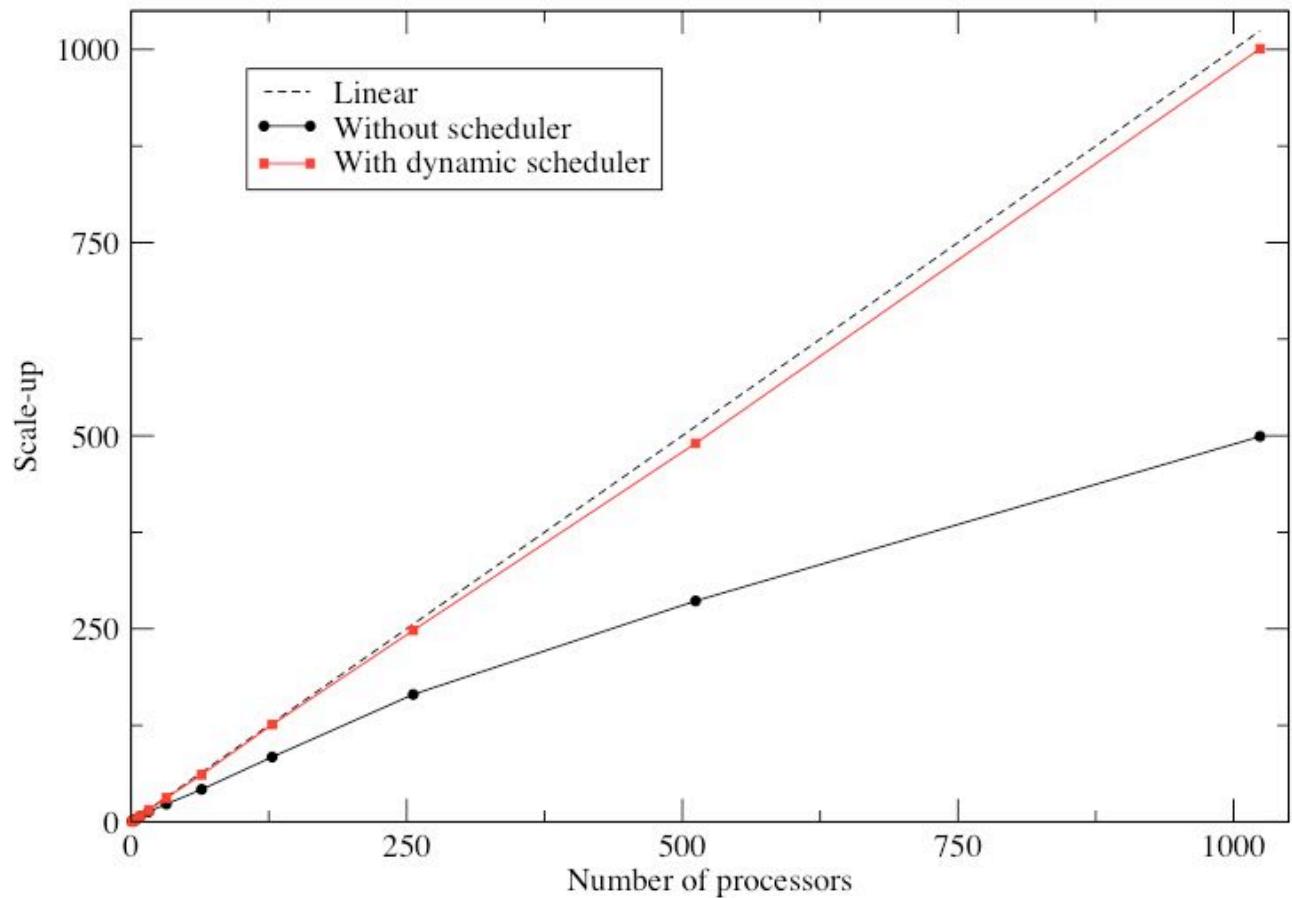
A load balancing algorithm for the source term stiff integration

- ▶ An MPI dynamic scheduler has been implemented in YALES2

- ▶ Principle

- A master is designated
- The master gives chunks of source term calculations to a number of slaves
- Available slaves designate a new master
- Repeat

- ▶ Linear scaling is recovered up to 32k cores on Turing

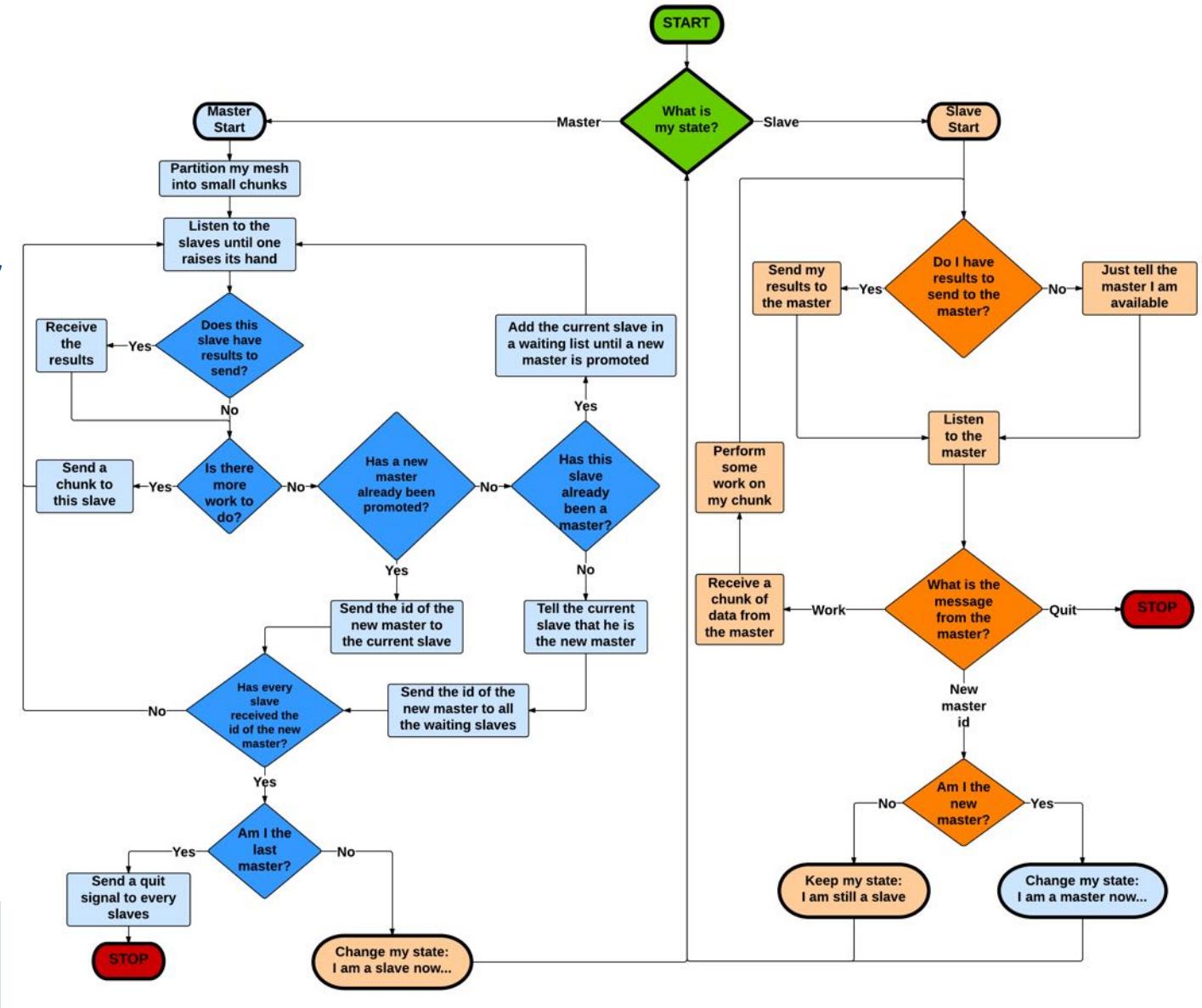


Solution: dynamic scheduler

► An MPI dynamic scheduler has been implemented in YALES2

► Principle

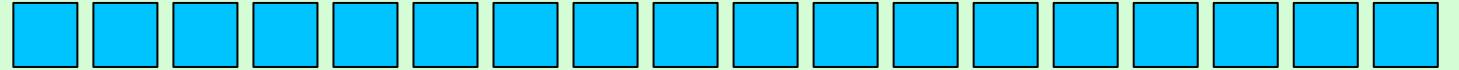
- A master is designated
- The master gives chunks of source term calculations to a number of slaves
- Once finished, the master tells the other slaves it is done
- Available slaves designate a new master
- Repeat



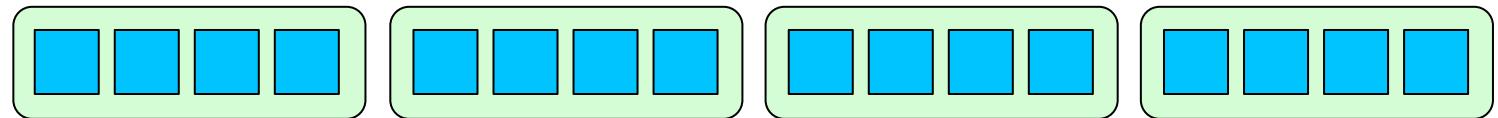
■ Performances

- ▶ The cost of the MPI communications scales as N_{cores}^2
- ▶ Beyond 1000 cores, MPI sub-communicators must be introduced to reduce the MPI overhead

One MPI comm.



Multiple MPI comm.



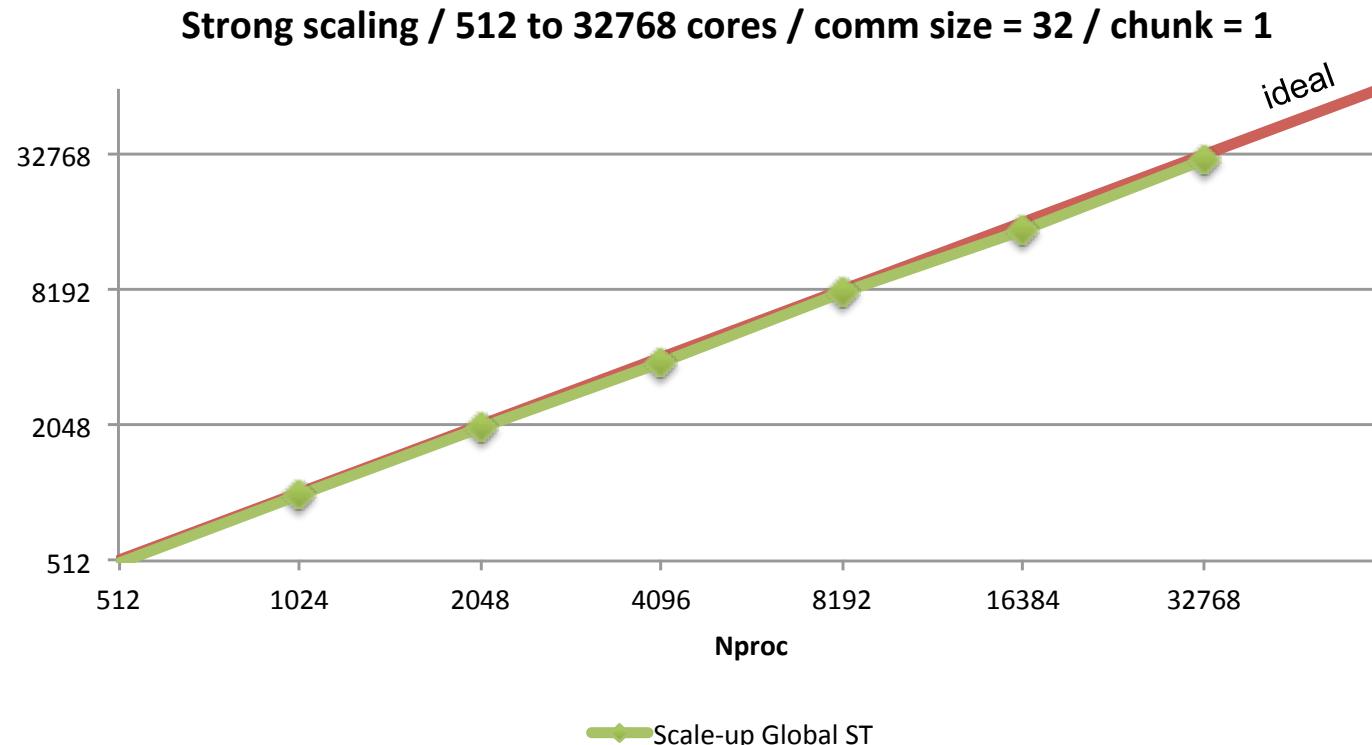
▶ Steps

- Analysis of the cost of the chemistry source term on each core (it is assumed that the cost is the same from one fluid iteration to another)
- Sorting and grouping of the cores to create well balanced MPI sub-communicators
- Dynamic scheduling on each MPI sub-communicator

- ▶ Linear speed-up recovered up to 65,000 cores on a Blue Gene/Q machine and up to 8192 cores on the Curie machine (CEA, TGCC)

■ Performances

- ▶ **Strong scaling on a IBM Blue Gene/Q machine at IDRIS**
 - Scales up to 32k processors for the meso-scale burner
 - Spends only 40% of the temporal loop time in source term integration



Large-Eddy Simulation of innovative offshore wind turbines

V. Moureau, G. Lartigue, F. Barnaud, P. Deglaire



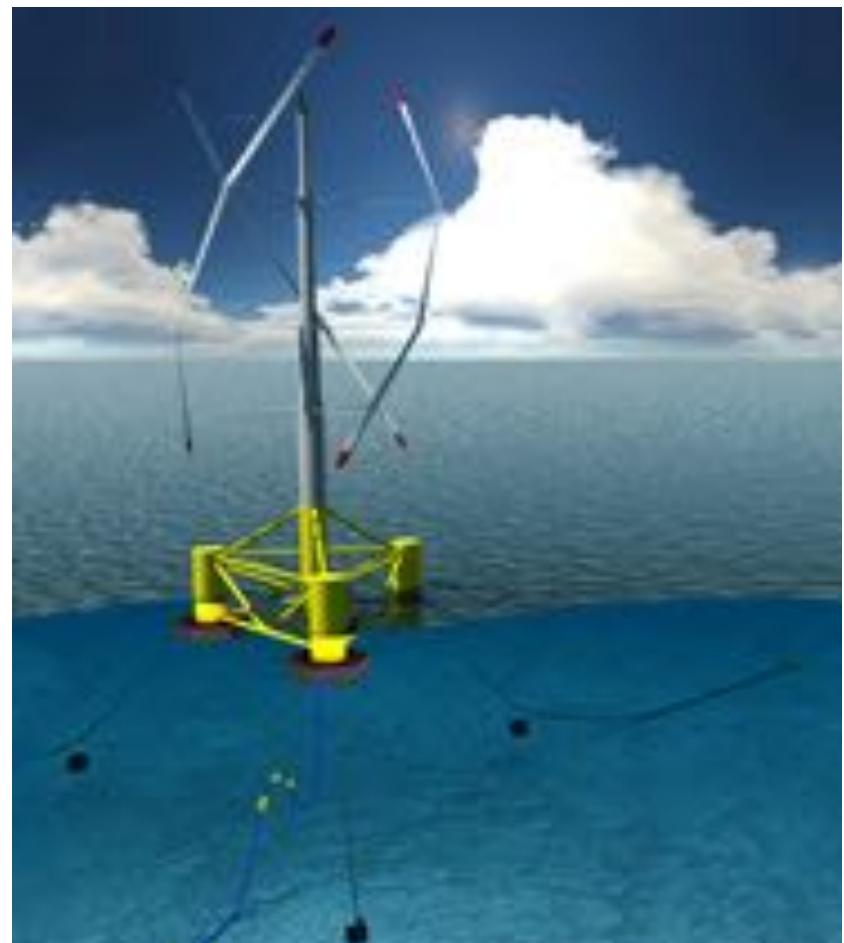
■ LES for wind turbines

- ▶ Large-Eddy Simulation is a promising tool for the prediction of wind turbine performances as it gives access to unsteady flow features
- ▶ Some challenges
 - High Reynolds number flows with very thin boundary layers
 - Low-Mach number
 - Rotation of the blades (moving geometry)



■ The Nenuphar concept

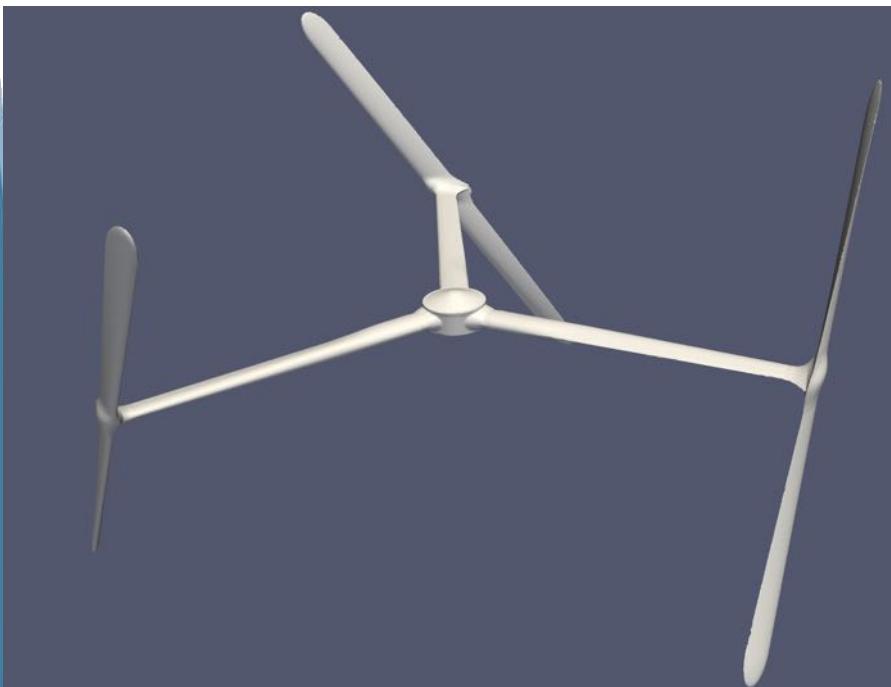
- ▶ The Nenuphar concept relies on a floating vertical axis wind turbine
- ▶ Advantages
 - Simple and robust
 - Limited environment impact
 - Ease of maintenance
- ▶ Challenges for LES
 - Novel concept: lack of experience
 - Angle of attack of the blades changes continuously leading to dynamic stall
 - Floating of the wind turbine induces a sensitivity to waves



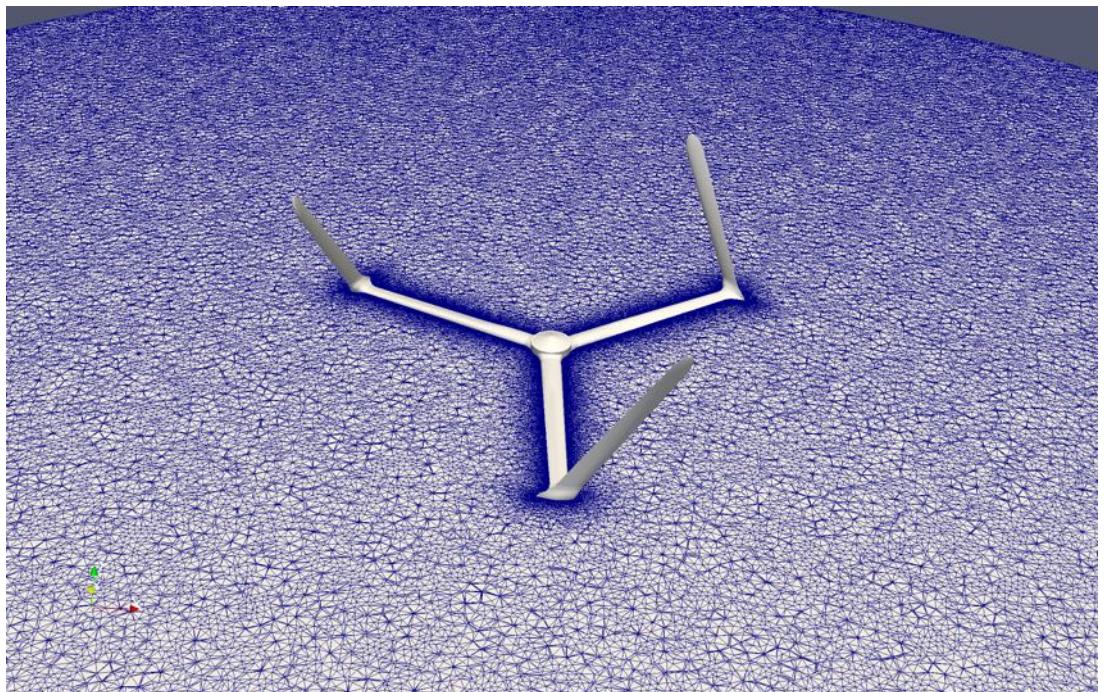
■ The Nenuphar concept

► First LES attempt with YALES2

Triblade geometry

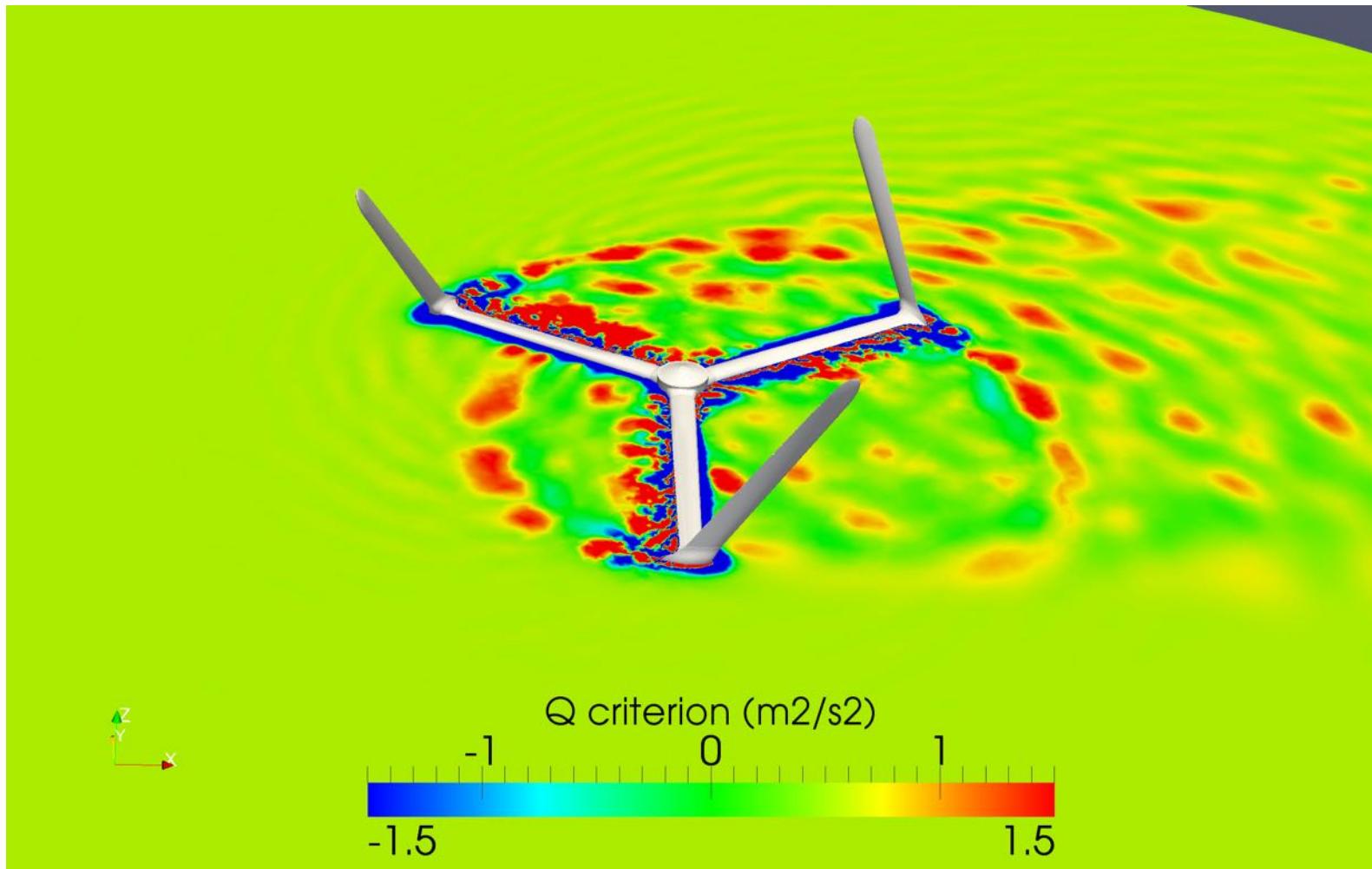


Unstructured 3D mesh with 41 or 325 million cells



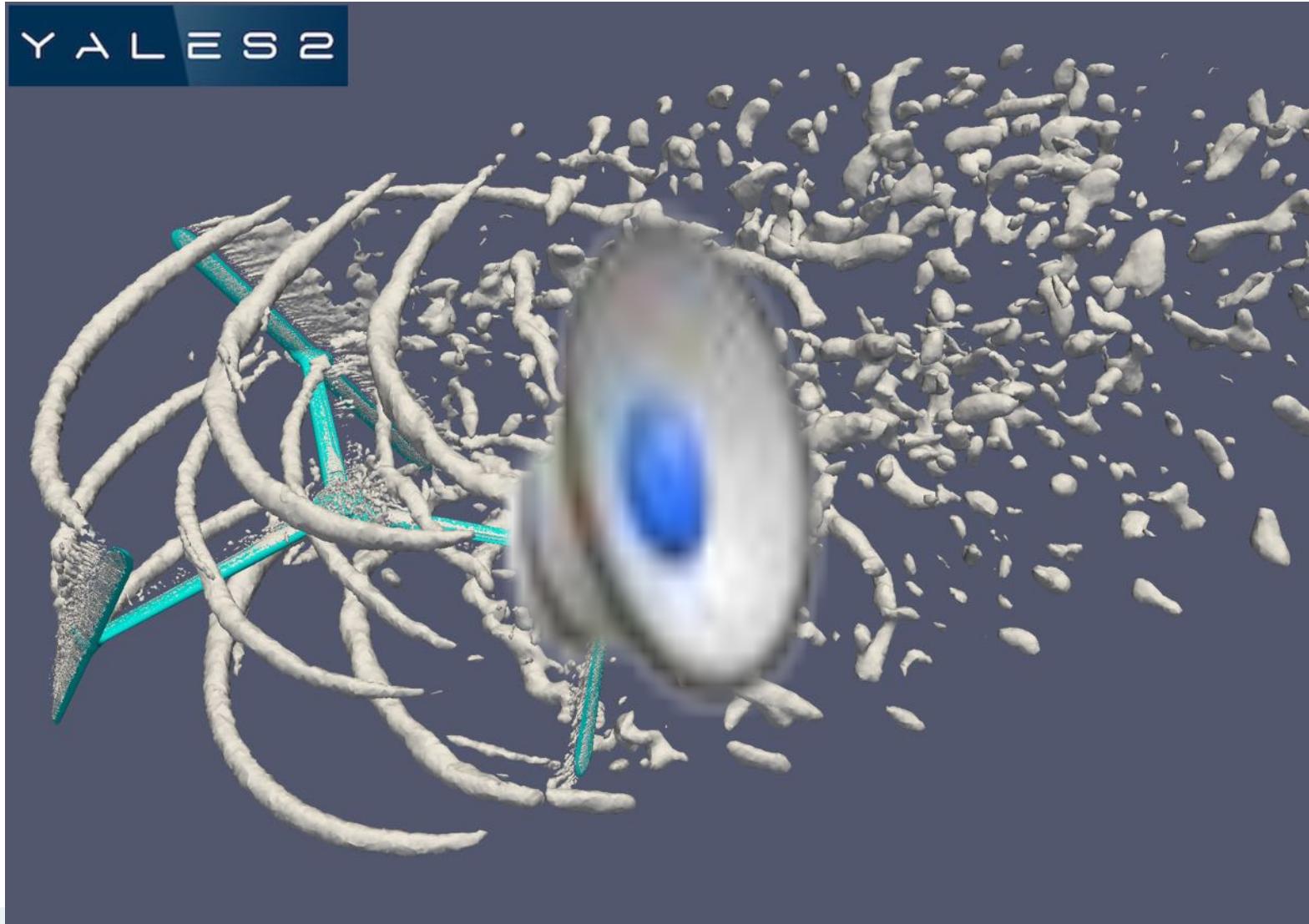
The Nenuphar concept

- Q-criterion at Tip-Speed Ratio 3.5 after 4 full rotations (41M mesh)



The Nenuphar concept: Grand Challenge on the OCCIGEN machine at CNES

- Q-criterion at Tip-Speed Ratio 3.5 on the M2 mesh (300 million tets)



Parallel mesh adaptation and load balancing with YALES2

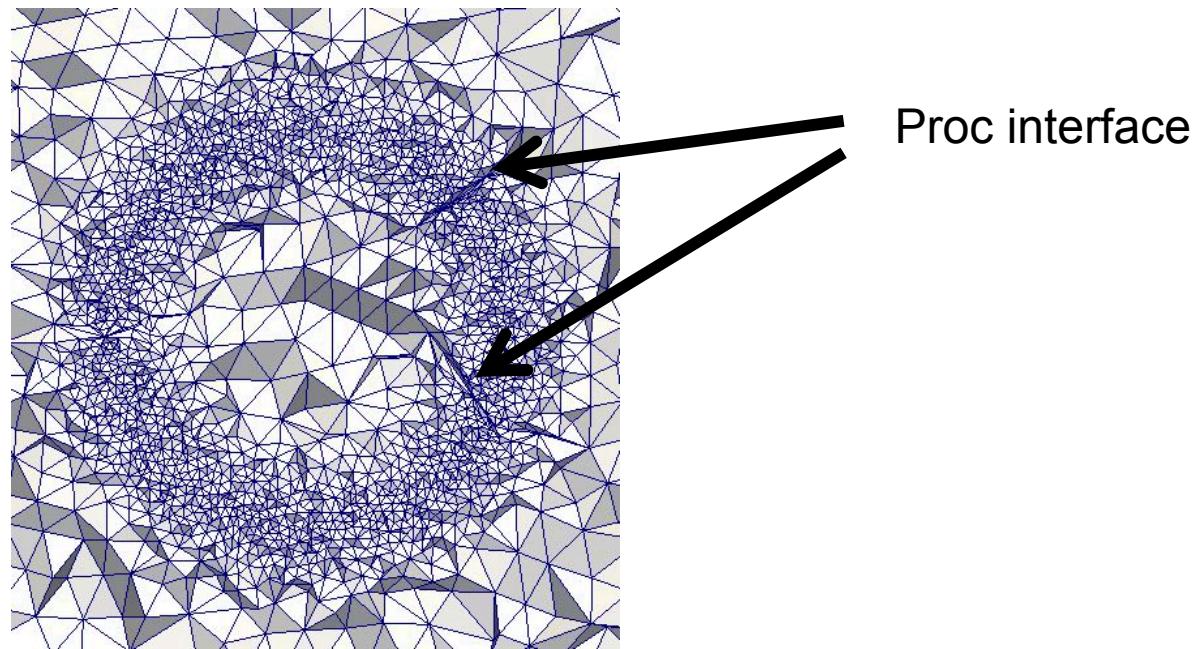
**V. Moureau, G. Lartigue, P. Bénard
C. Dobrzynski, G. Balarac**

■ Mesh adaptation

- ▶ **Mesh adaptation consists in the use of numerical techniques to refine or unrefine the mesh locally**
 - Node insertion in Delaunay triangulations
 - Edge or face swapping
 - Element collapsing
- ▶ **Several sequential libraries exist**
 - **MMG3D, C. Dobrzynski**, <http://www.math.u-bordeaux1.fr/~dobrzyns/logiciels/mmg3d.php>
 - **MADLIB**, <http://sites.uclouvain.be/madlib/>
 - **NETGEN**, <http://www.hpfem.jku.at/netgen/>
 - **TETGEN**, <http://wias-berlin.de/software/tetgen/>
 - **CGAL**, <http://www.cgal.org/>
 - **MeshAdapt**, <http://www.scorec.rpi.edu/~xli/MeshAdapt.html>
- ▶ **Very few libraries are (massively) parallel**

■ Strategy

- ▶ Can we imagine a parallel algorithm based on sequential adaptation libraries like MMG3D (our preferred choice) ?
- ▶ If mesh adaptation is performed on each processor, problems will arise at the proc interface. The choice made in YALES2 is to leave the proc interface and the boundaries untouched



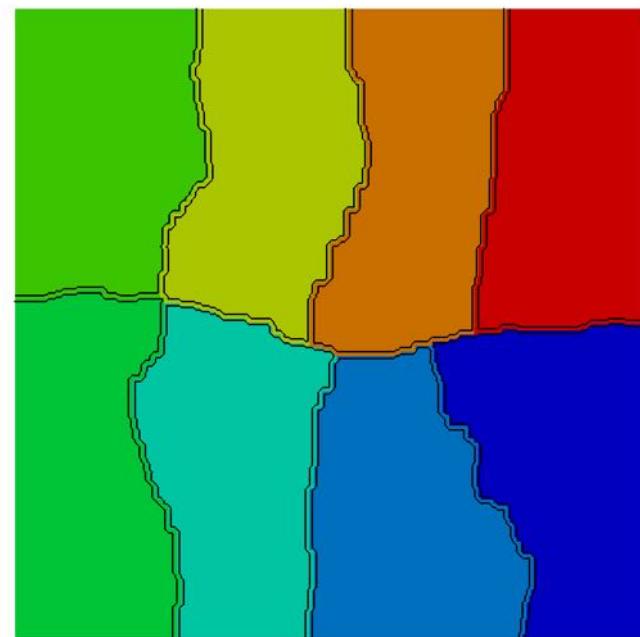
■ Strategy

- ▶ Then, mesh adaptation will be performed several times with a moving proc interface
 - Requires parallel load balancing...
- ▶ Parallel algorithm given the YALES2 double domain decomposition
 - Merge the cell groups
 - Adapt the mesh on each processor leaving the boundaries untouched
 - Split the mesh into cell groups
 - Balance the mesh with ParMETIS taking into account the non-adapted interface
 - Start again
- ▶ Key ingredients
 - Parallel load balancing
 - Merging/splitting of the mesh into cell groups on each processor
 - Fast connectivity reconstruction

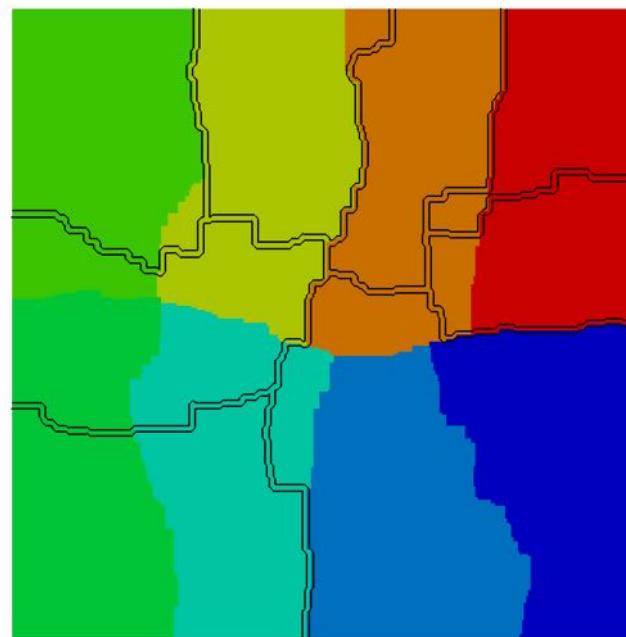
■ Parallel load balancing example

- ▶ YALES2 is coupled to ParMetis 4.x and enables to load balance a calculation on-the-fly
- ▶ 2D example

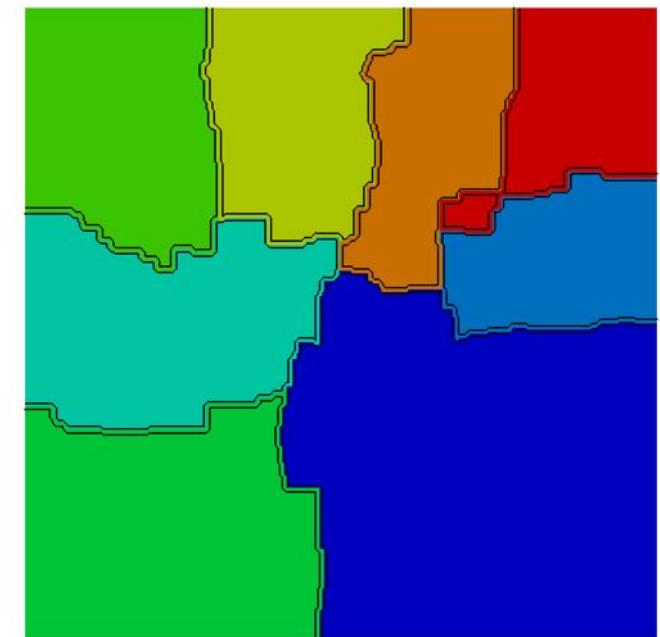
Parallel partition with weights equal to the proc color



Cell-group graph adaptation with ParMetis 4.x

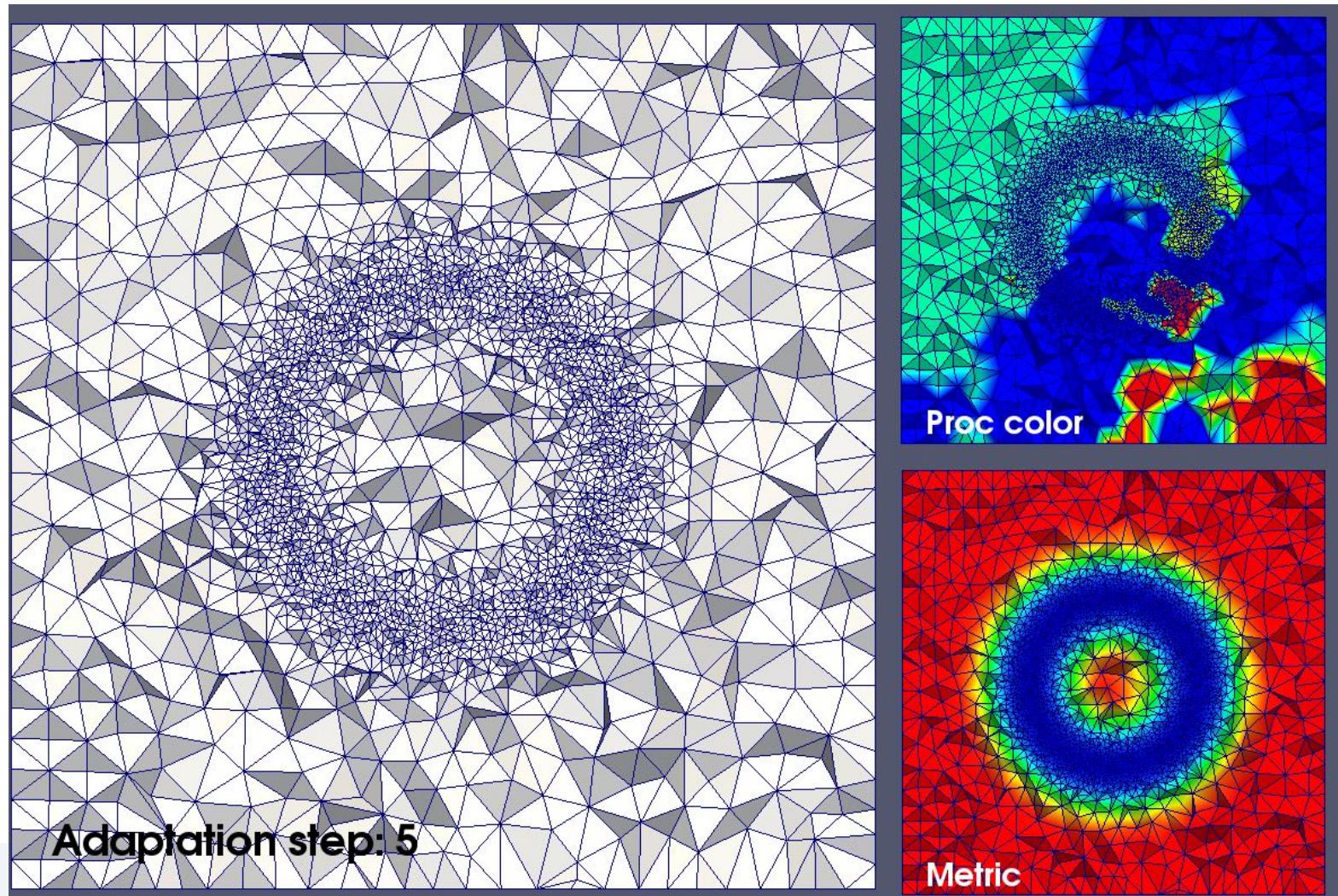


Migration of the cell groups to the other procs



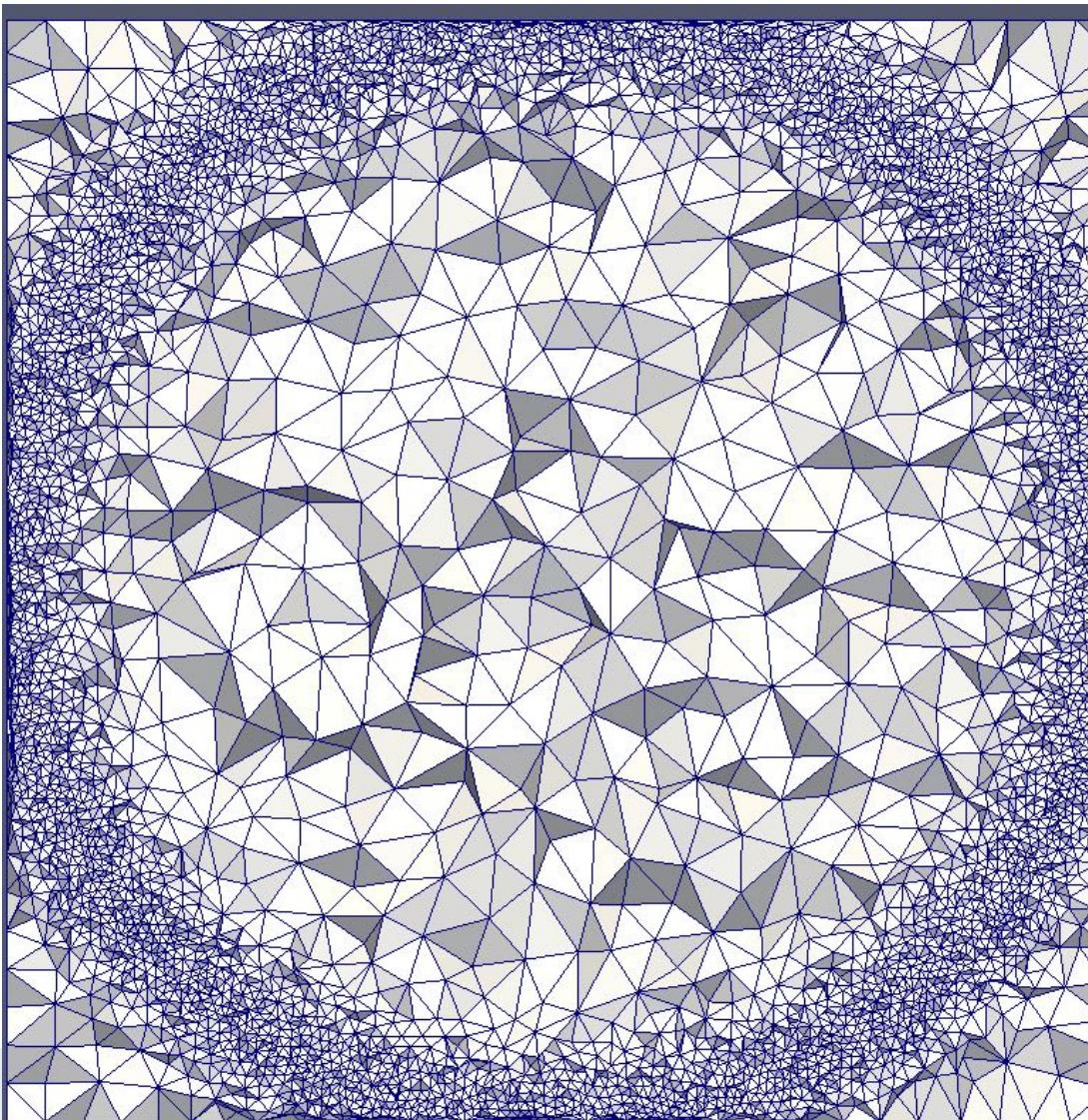
■ 3D example: refinement of a sphere on 4 procs

- ▶ Step 1 to 4: same procedure based on MMG3D + load balancing
- ▶ Step 5: optimization of the mesh for LES + better load balancing



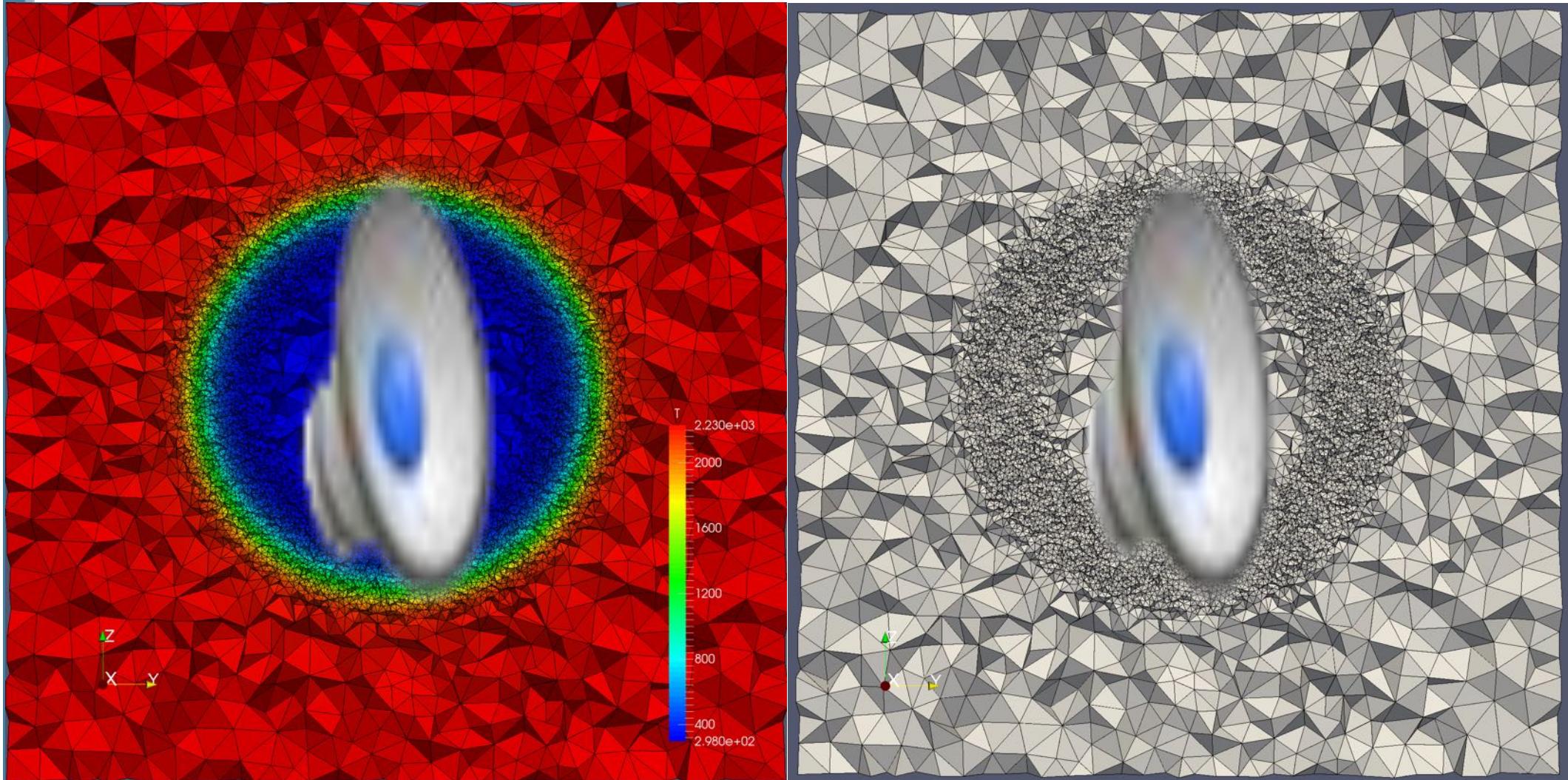
■ 3D example: dynamic mesh on 4 procs

- ▶ 5 steps per adaptation



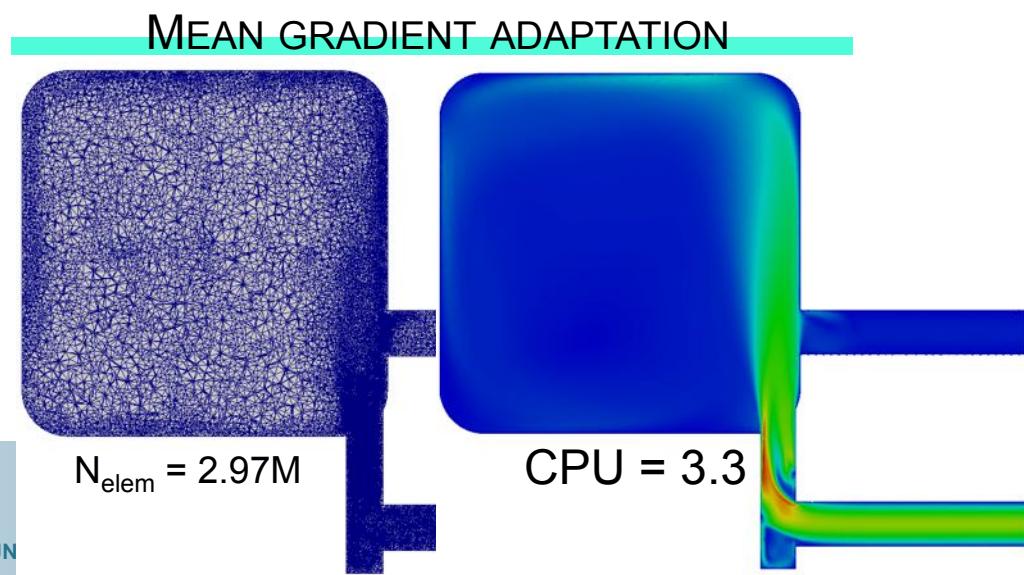
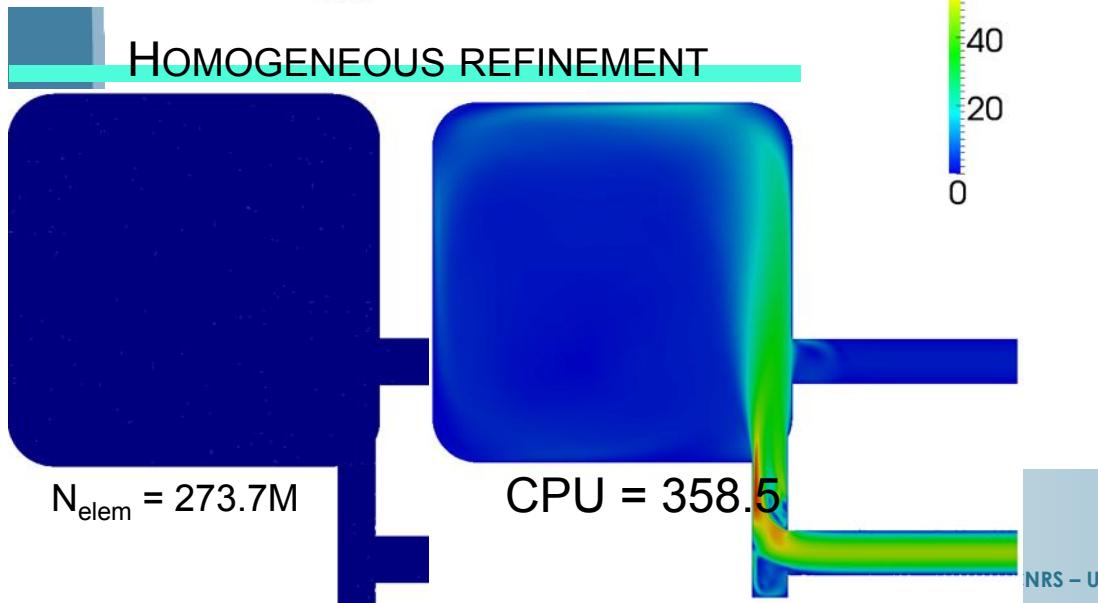
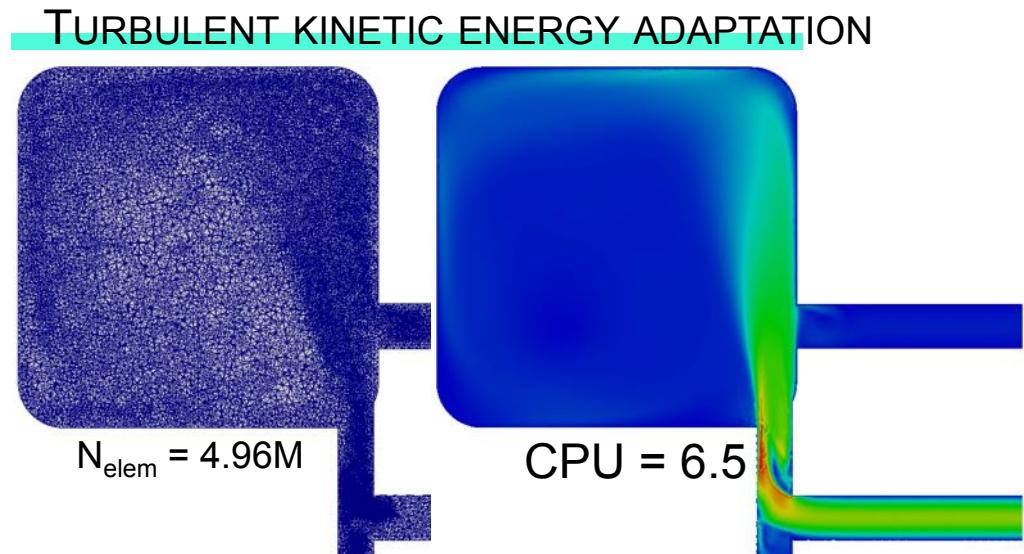
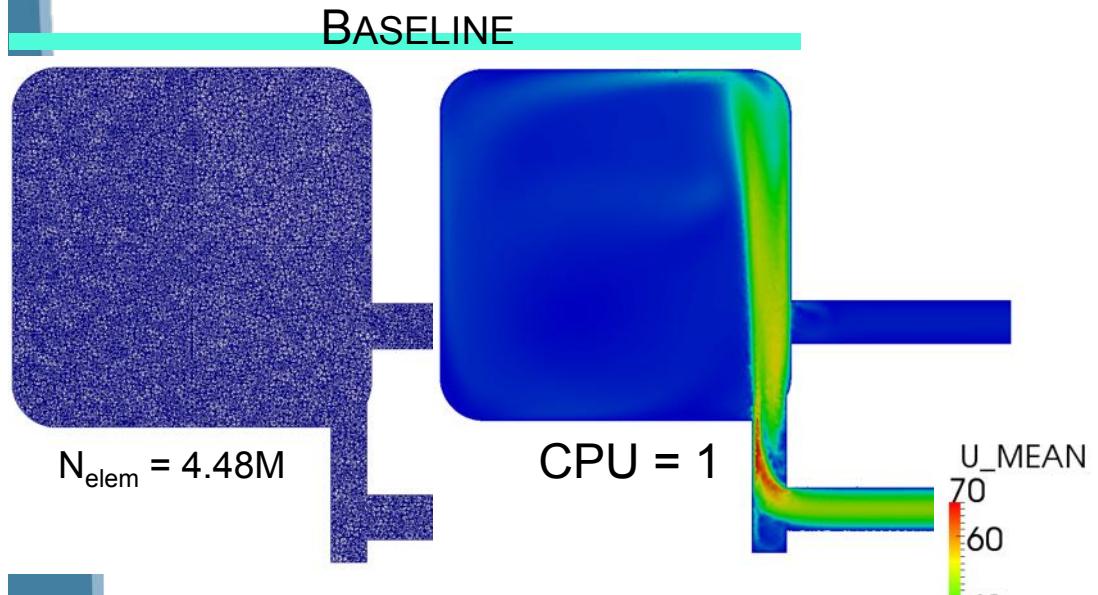
A real application: collapse of a flame ball with dynamic mesh adaptation

- ▶ F-TACLES combustion model, refinement ratio = 6, 20 cores



■ Combination with mesh adaptation criteria

- ▶ Isothermal flow adaptation on 8 cores of the meso-scale burner



Conclusions & perspectives

■ Conclusions & Perspectives

- ▶ With exascale computing, the size of the simulations will still increase and the post-processing cost will also increase...
- ▶ Sequential and parallel performances will continue to be critical
 - Memory contiguity, vectorization
 - Work/communication overlapping
 - Asynchronous communications
- ▶ The pre- and post-processing of large-scale simulations are very challenging
 - Handling of large amount of data
 - Data-mining for large-scale feature extraction
 - Need to combine many techniques using massively parallel machines
- ▶ New solutions will need to be found
 - Multi-grid techniques for solution visualization
 - Highly selective filters to extract the features of interest
 - Combination of all these techniques plus POD, DMD, Wavelets, ...

■ References & Acknowledgements

► Additionnal references

- Moureau, V. et al., Analysis of large amounts of numerical data, 2013 VKI training course
- 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
- 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

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- INTEL/GENCI/CEA/UVSQ Exascale Lab
- Computing centers: TGCC, IDRIS, CINES, CRIHAN, JULICH

■ Thank you !

