Parallel and dynamic mesh adaptation of tetrahedral-based meshes for propagating fronts and interfaces: application to premixed combustion and primary atomization.

Vincent Moureau, Pierre Bénard, Ghislain Lartigue
CORIA, CNRS, University of Rouen, France

Renaud Mercier – SAFRAN TECH, France

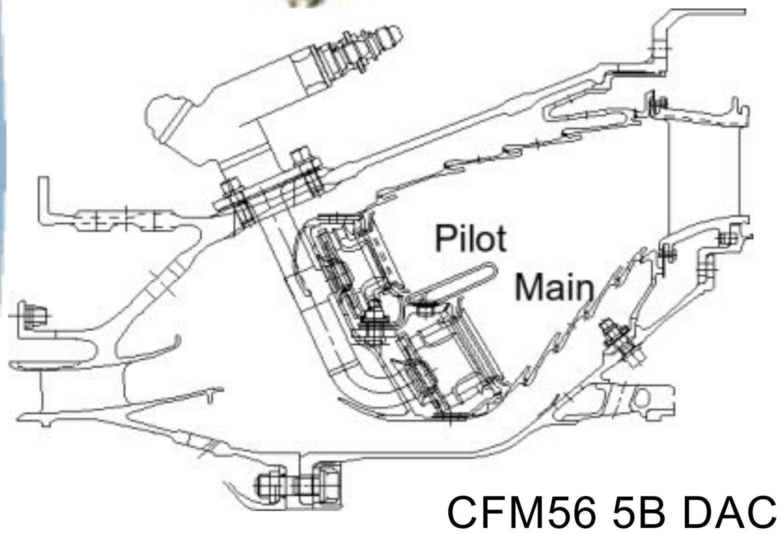
Algiane Froehly – LMB/INRIA Bordeaux

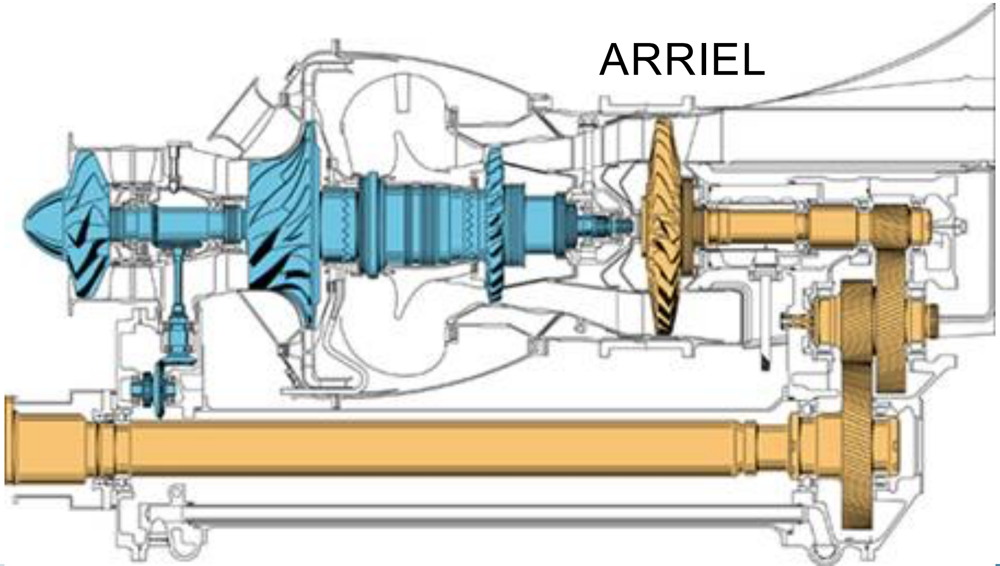
In memoriam C. Dobrzynski – LMB/INRIA Bordeaux

Séminaire INRIA

05/06/2018 – Saclay

Aeronautical engines





Engine design is driven by two major constraints

Fuel efficiency

- Economic constraints
  - ➡ reduced fuel consumption
  - ➡ reduced CO_2 emissions
- Global efficiency of the engine

Turbofan = **Ducted fan** + **Gas turbine (core engine)**

$$\eta_{glob} = \eta_{prop} \times \eta_{th}$$

Propulsive efficiency ← η_{prop} | **Thermal efficiency** ← η_{th}

High bypass ratio architecture

Ultra-high pressure ratio core engine

$$\eta_{th} = 1 - \left(\frac{P_1}{P_2}\right)^{\frac{\gamma - 1}{\gamma}}$$

Pollutant emissions

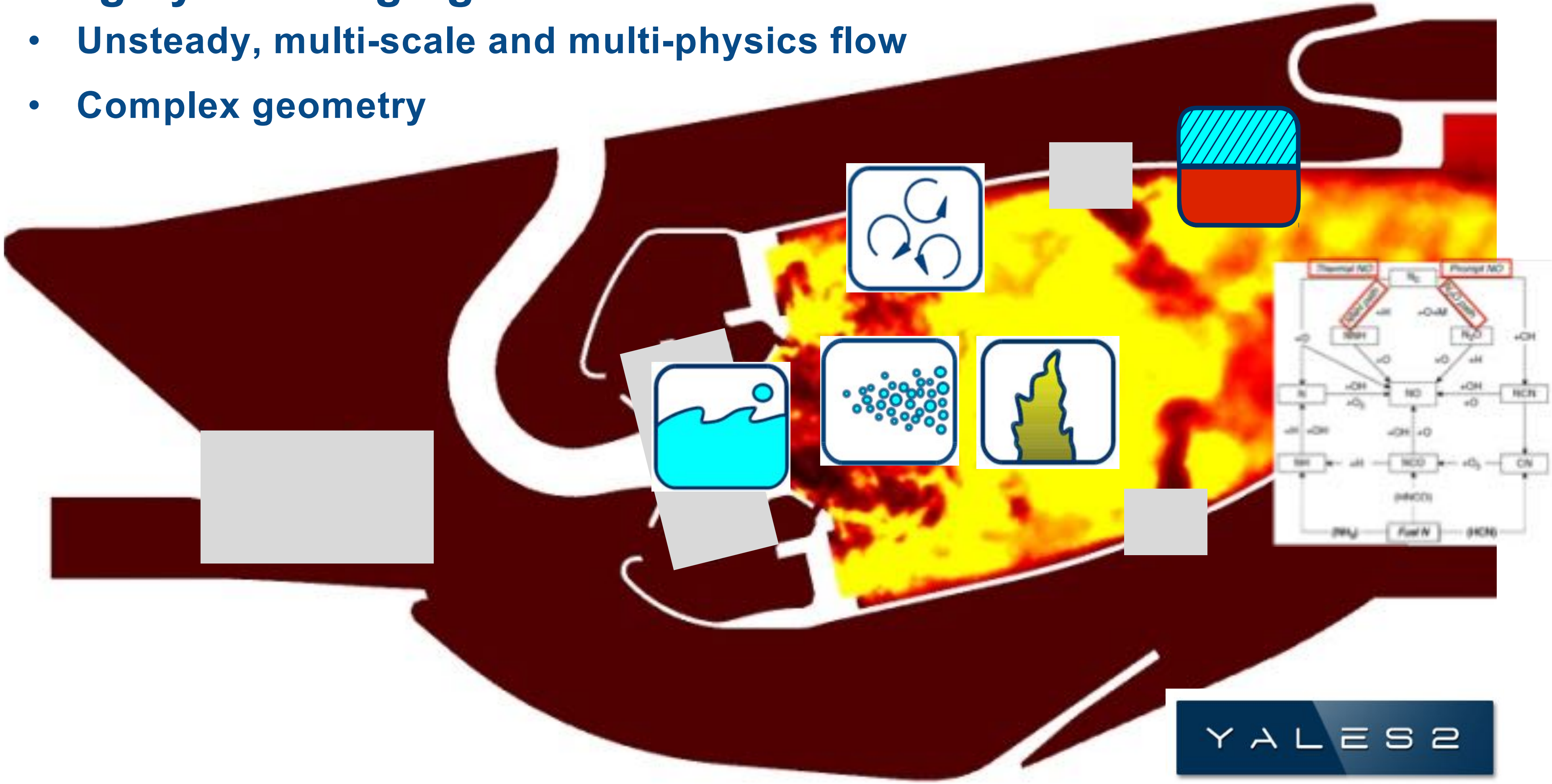
- International regulations
  - ➡ CAEP regulations
- Main pollutants
  - UHC
  - Smoke
  - Carbon Monoxide (CO)
  - Nitrogen Oxides (NOx)

Smoke in the trail of a B-52

Ultra low-NOx combustion chamber

Prediction of performances and pollutant emissions in aeronautical engines

- **A highly challenging task**
  - Unsteady, multi-scale and multi-physics flow
  - Complex geometry



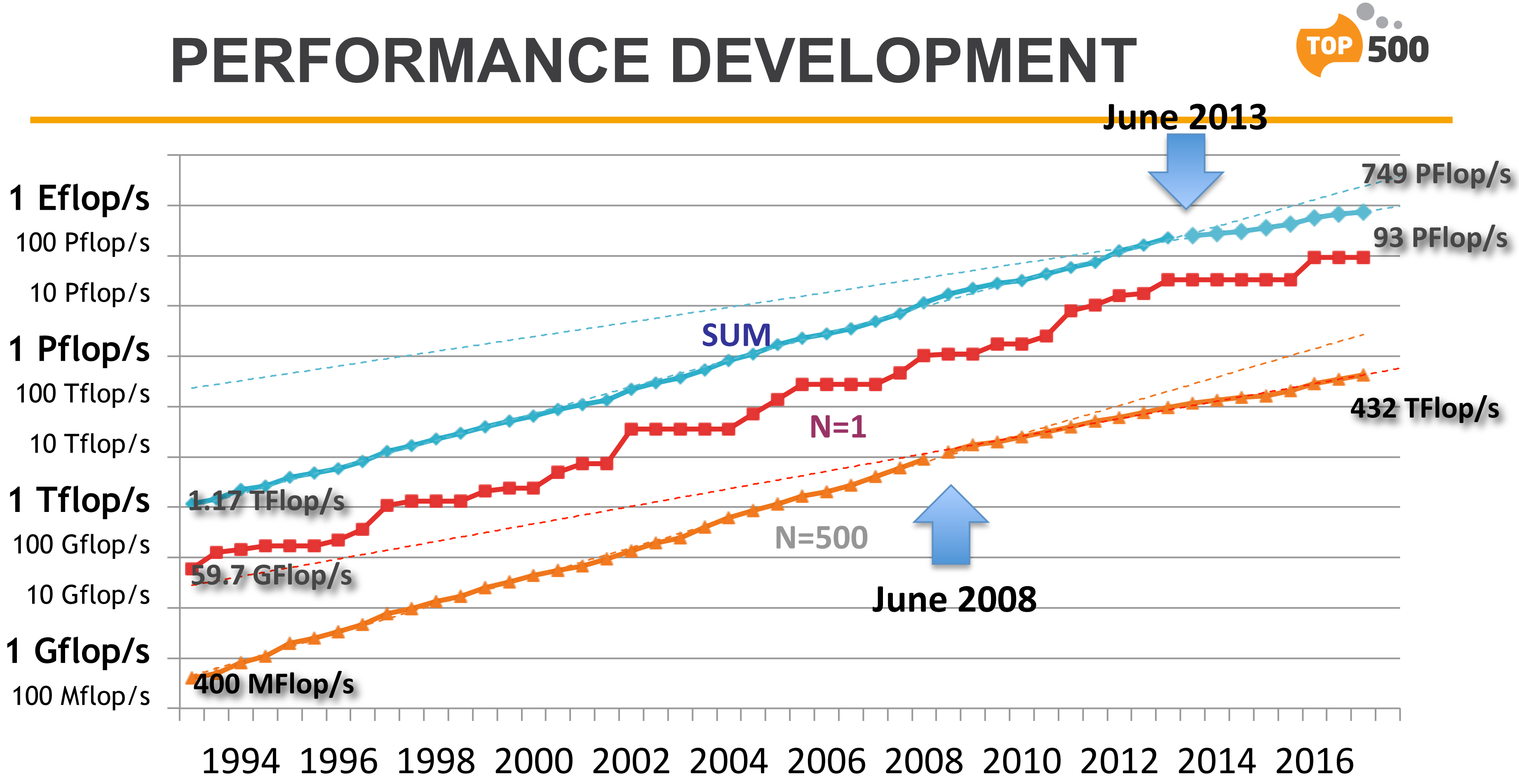
- **Unsteady approaches are mandatory to predict these phenomena**
- **Objective: develop LES models for pollutant predictions**

Driving mechanism: Moore's law

- **The power of super-computers almost doubles every 18 months**

Driving mechanism: Moore's law (revisited)

- **Erich Strohmaier, ISC 2017, Frankfurt**



- **The end of Moore's law has a strong impact on the new architectures**

Top 500, june 2017

- 6 different CPU/GPU types in the top 10…

#	Site	Manufacturer	Computer	Country	Cores	Rmax (Pflops)	Power (MW)
1	National Supercomputing Center in Wuxi	NRCPC	Sunway TaihuLight NRCPC Sunway SW26010, 260C 1.45GHz	China	10,649,600	93.0	15.4
2	National University of Defense Technology	NUDT	Tianhe-2 NUDT TH-IVB-FEP, Xeon 12C 2.2GHz, IntelXeon Phi	China	3,120,000	33.9	17.8
3	Swiss National Supercomputing Centre (CSCS)	Cray	Piz Daint Cray XC50, Xeon E5 12C 2.6GHz, Aries, NVIDIA Tesla P100	Switzerland	361,760	19.6	2.27
4	Oak Ridge National Laboratory	Cray	Titan Cray XK7, Opteron 16C 2.2GHz, Gemini, NVIDIA K20x	USA	560,640	17.6	8.21
5	Lawrence Livermore National Laboratory	IBM	Sequoia BlueGene/Q, Power BQC 16C 1.6GHz, Custom	USA	1,572,864	17.2	7.89
6	Lawrence Berkeley National Laboratory	Cray	Cori Cray XC40, Intel Xeons Phi 7250 68C 1.4 GHz, Aries	USA	622,336	14.0	3.94
7	JCAHPC Joint Center for Advanced HPC	Fujitsu	Oakforest-PACS PRIMERGY CX1640 M1, Intel Xeons Phi 7250 68C 1.4 GHz, OmniPath	Japan	556,104	13.6	2.72
8	RIKEN Advanced Institute for Computational Science	Fujitsu	K Computer SPARC64 VIIIfx 2.0GHz, Tofu Interconnect	Japan	795,024	10.5	12.7
9	Argonne National Laboratory	IBM	Mira BlueGene/Q, Power BQC 16C 1.6GHz, Custom	USA	786,432	8.59	3.95
10	Los Alamos NL / Sandia NL	Cray	Trinity Cray XC40, Xeon E5 16C 2.3GHz, Aries	USA	301,0564	8.10	4.23

- And HPLinpack is not a good benchmark for our CFD applications

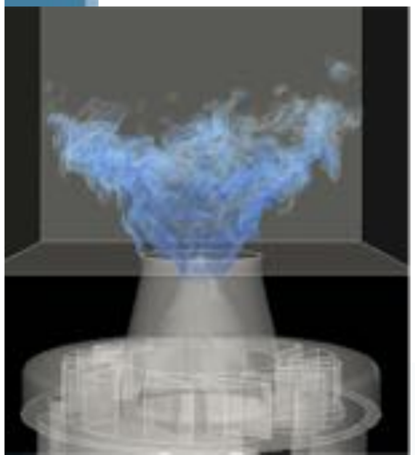
Outline

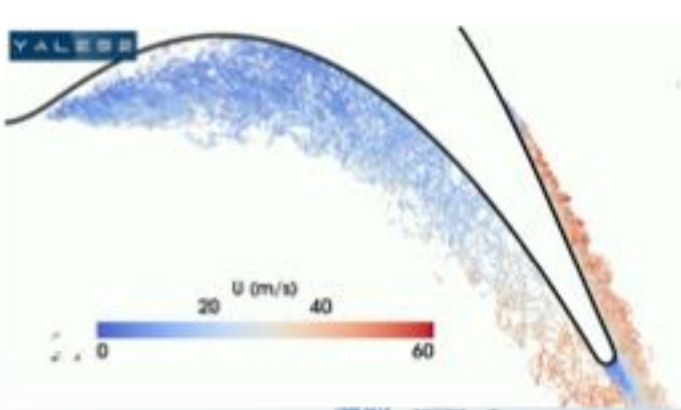
- **Context**
  - LES of aeronautical engines
  - HPC evolution
- **The YALES2 flow solver**
- **LES of the PRECCINSTA burner with finite-rate chemistry**
- **Towards dynamic mesh adaptation of fronts and interfaces**
  - Strategy
  - Application to propagating flames
  - Application to primary atomization
- **Conclusion and prospects**

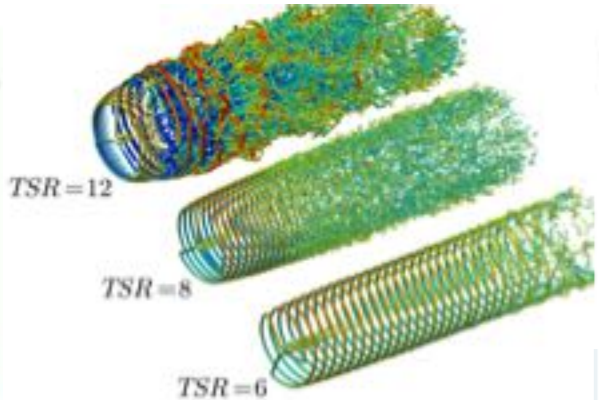
Flow solver

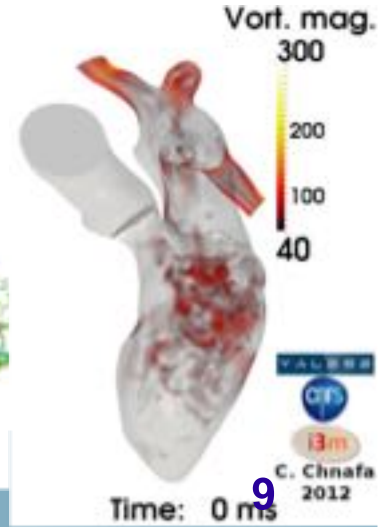
[1] YALES2 web site, http://www.coria-cfd.fr
[2] Chorin, Math. Comp. 22, 1968
[3] Bernard et al., to be submitted, 2018

- Low-Mach number Navier-Stokes equations with projection method [1,2]
- Unstructured meshes with adaptive grid refinement
- 400k+ lines of object-oriented fortran2008
- MPI and hybrid OpenMP/MPI
- 4th-order central finite-volume method [3]
- Combustion modeling
  - Tabulated or complex chemistry, NOx prediction model…
- Two-phase flows
  - Spray modeling (Lagrangian particles)
  - Primary atomization (Accurate Conservative Levelset)
- Suited for massively parallel computing (>32 000 procs)









The YALES2 network

- A collaborative network supported by the French combustion community
- More than 200 trained researchers and engineers

Academia

SUCCESS scientific group
(http://success.coria-cfd.fr):
CORIA, CERFACS, IMAG, LEGI
EM2C, IMFT, IFP-EN, LMA

ULB, MONS, UCL, LOMC,
LMB/INRIA, Sherbrooke,
PPRIME

Computing centers

CRIANN, IDRIS, CINES, TGCC
GENCI, PRACE

Industry

SAFRAN
(YALES2-AE)

ARIANE GROUP
SOLVAY
AIR LIQUIDE
ADWEN
…

YALES2

www.coria-cfd.fr

SMEs

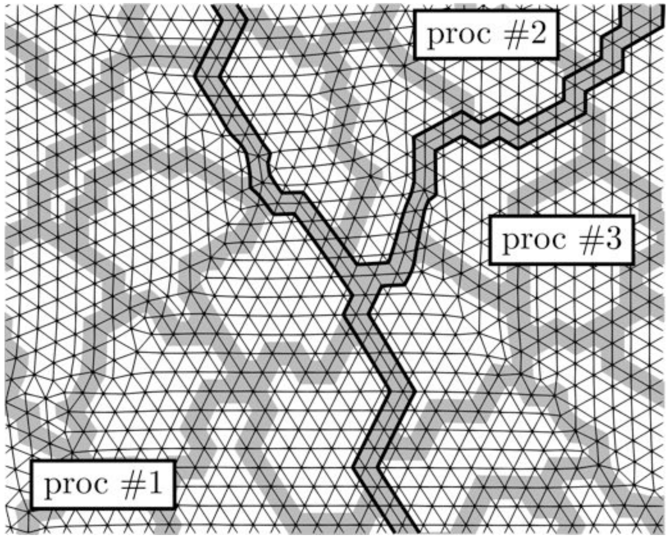
GDTech
Paralgo
Linterweb

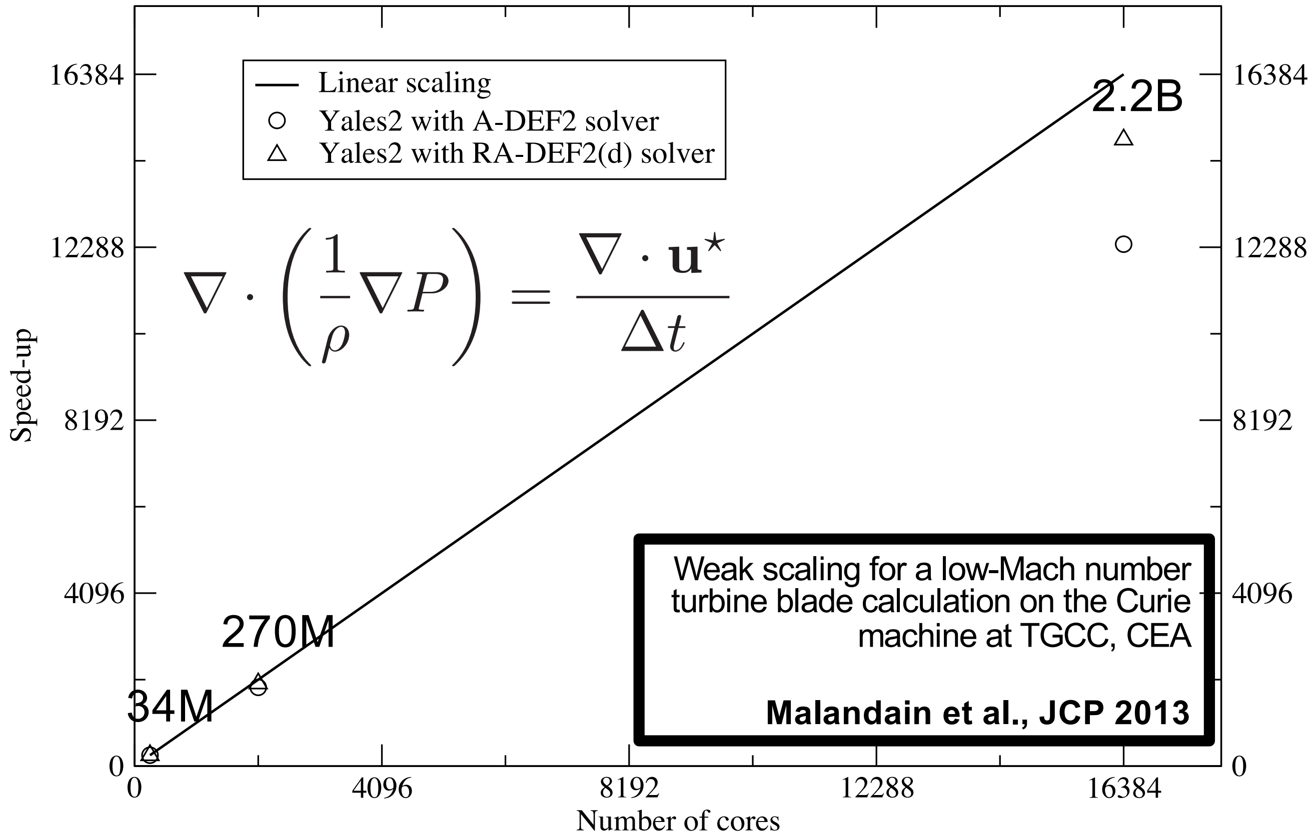
HPC experts

ECR lab
INTEL/CEA/GENCI/UVSQ

In-core and parallel performances

- **Two-level domain decomposition [1]**
  - Mesh is split into cell groups at the core level
  - Enables to fit in L2 cache memory
  - Used for the preconditioning of the linear solvers
- **In-house linear solvers**





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

[1] Moureau et. al., CR Mecanique, 2011

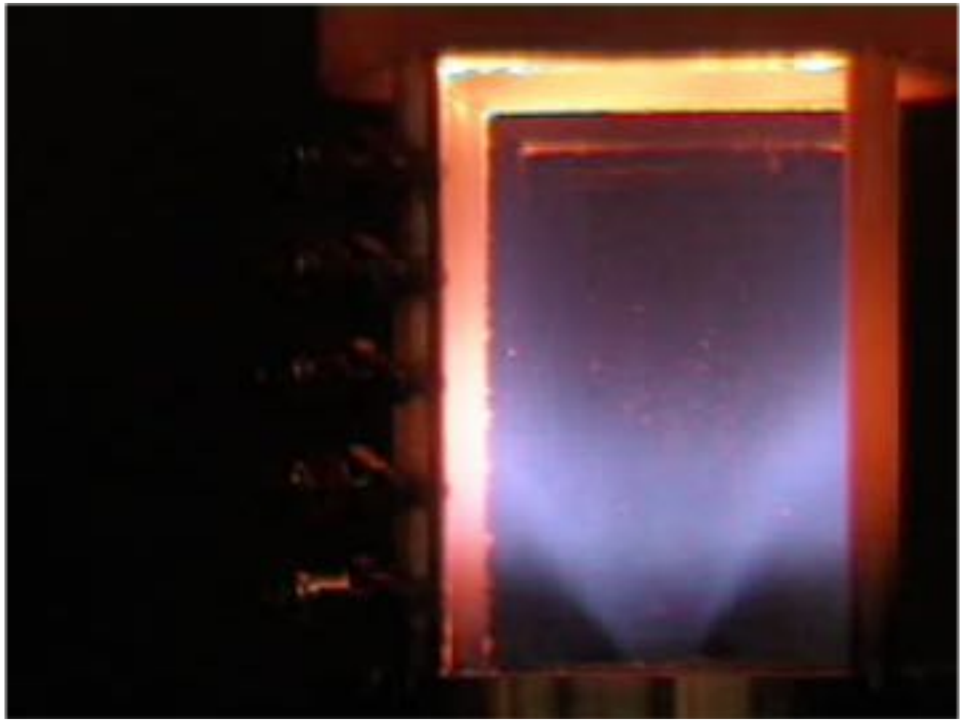
Towards lean-premixed low-NOx burners

LES of the PRECCINSTA burner with finite-rate chemistry

The PRECCINSTA burner (1/2)

- Experimental lean-premixed CH4/air combustor with swirl
- Designed by SAFRAN Helicopter Engines (Turbomeca)
- Built to test LES capability for prediction of combustion instabilities
- Different equivalence ratios corresponding to stable or unstable regimes
- Non-intrusive measurements perfomed at DLR (Germany)

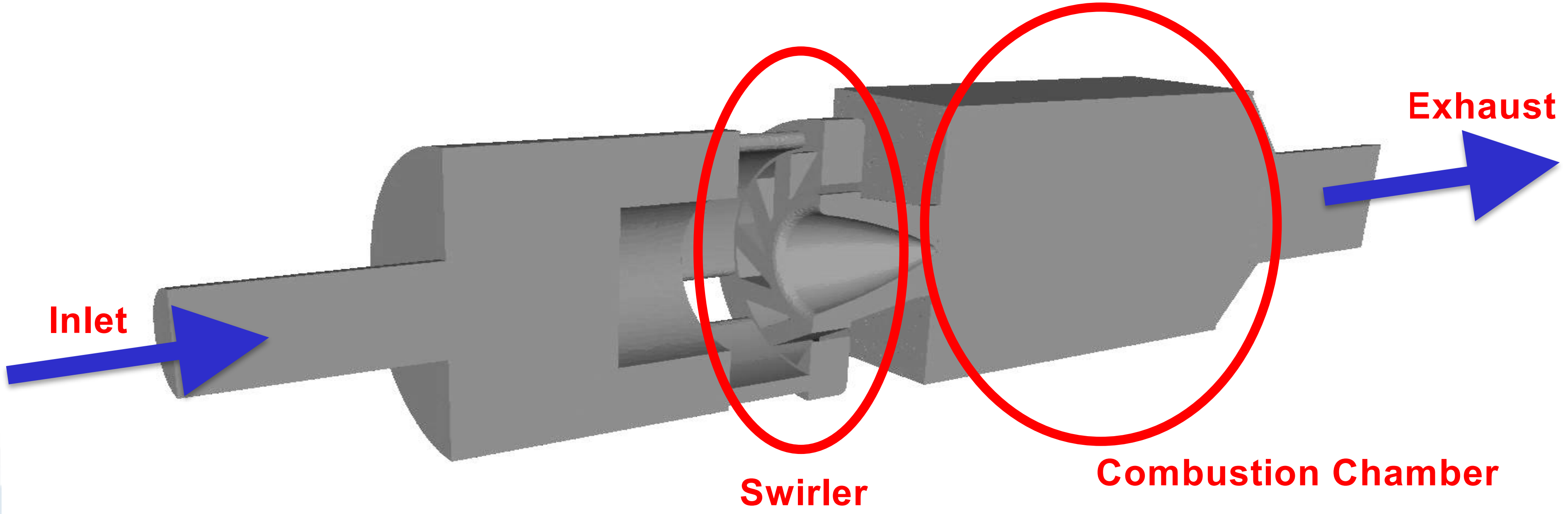
PRECCINSTA experimental burner



Equivalence ratio is decreasing slightly from 0.8 to 0.5

The PRECCINSTA burner (2/2)

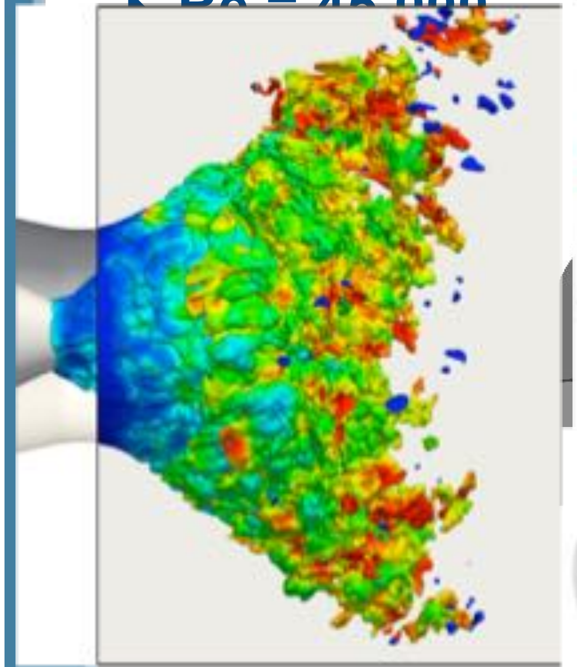
- **Re = 45,000**

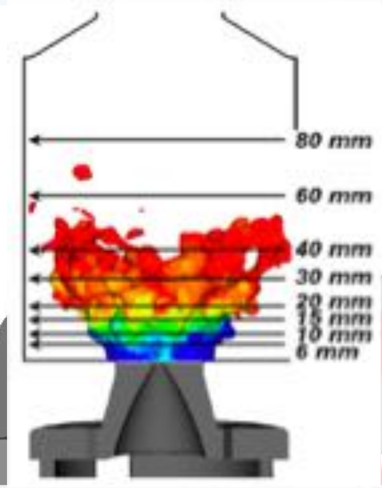


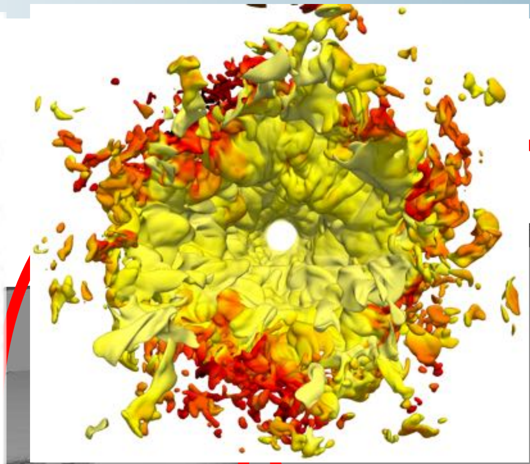
- **Many related studies**
  - Roux et al., Comb. & Flame (2005)
  - Moureau et al., J. Comp. Physics (2007)
  - Galpin et at., Comb. & Flame (2008)
  - Moureau et al., Comb. & Flame (2011)
  - Franzelli et al., Comb. & Flame (2012)
  - Veynante et al., Comb. & Flame (2016)

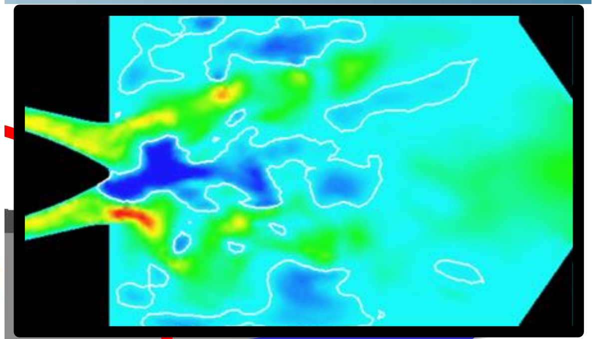
The PRECCINSTA burner (2/2)

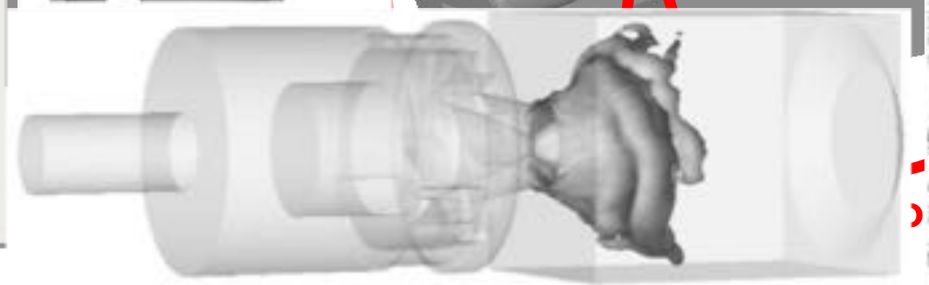
- Re = 45 000

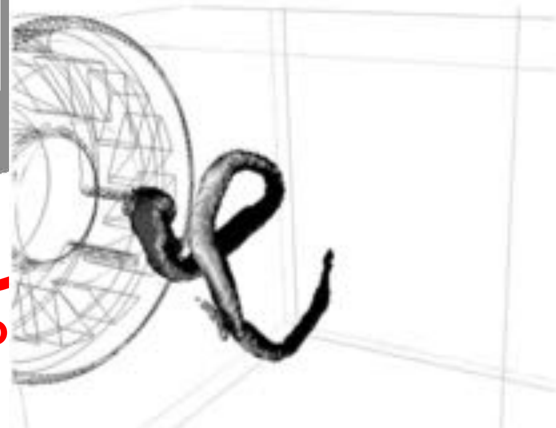




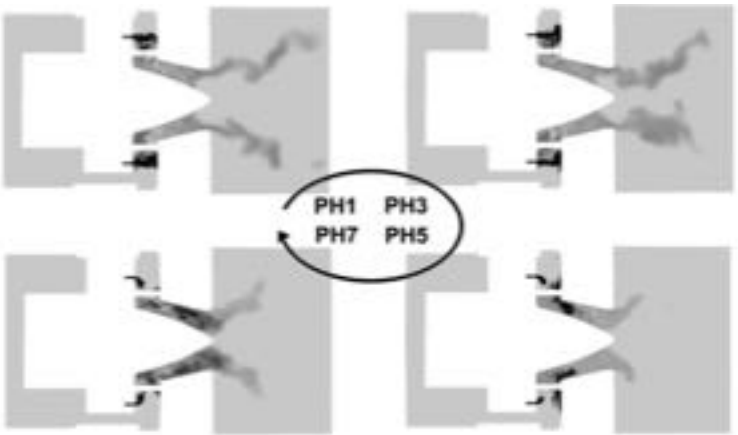


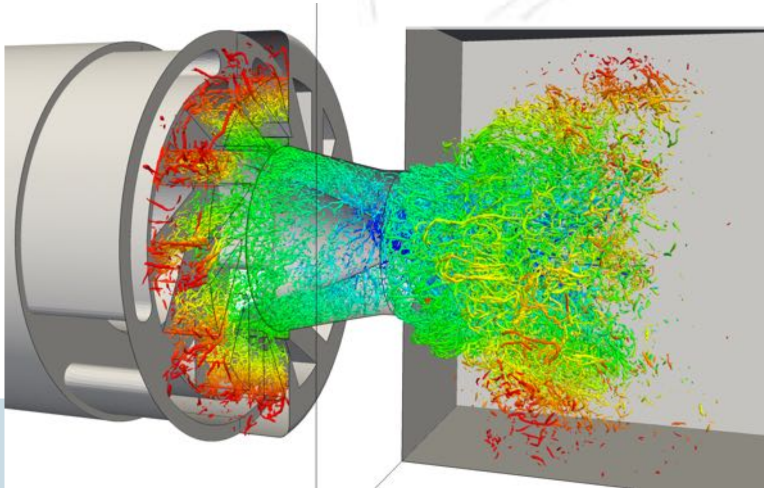






- Ma
  - 2011)
  - ') 2012)
  - 2016)

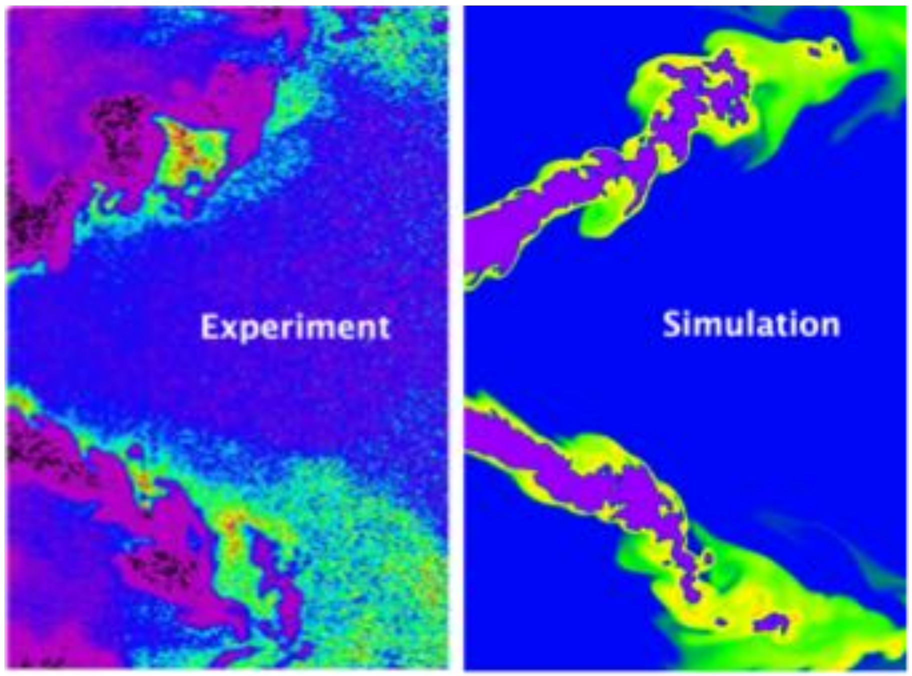




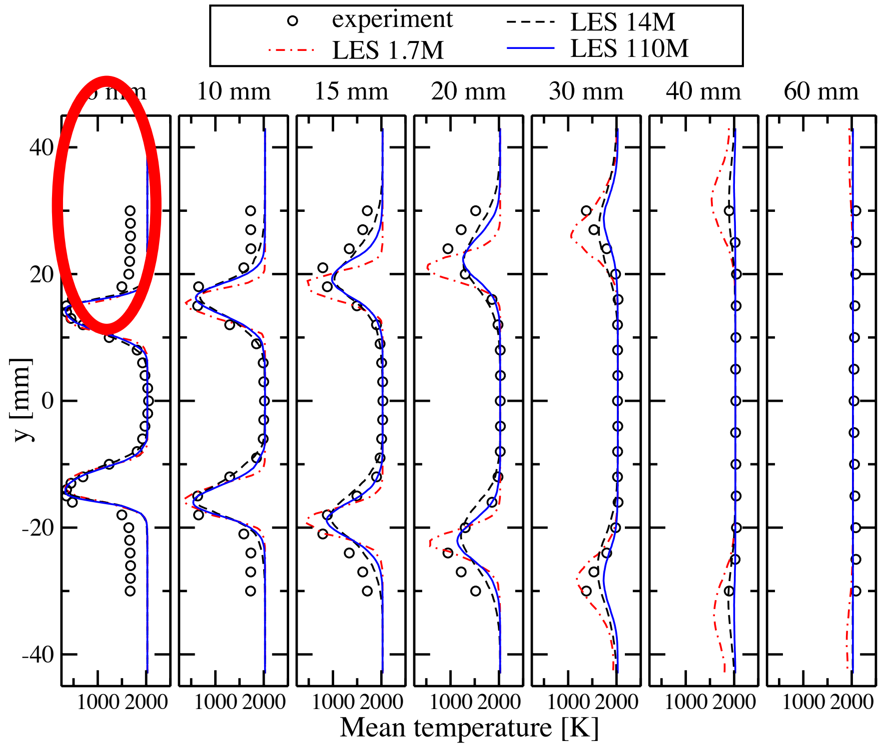
A remaining open question…

- No wall temperature/heat flux are available in the experiment
- Results from adiabatic simulations versus experiment

OH field



Moureau et al., C&F 2011



- V flame (heat loss) versus M flame (adiabatic) ?
- Difficult to model with tabulated chemistry => finite-rate chemistry

HPC for finite-rate chemistry

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot \rho Y_k \mathbf{u} = \nabla \cdot (-\rho \mathbf{V}_k Y_k) + \dot{\omega}_k \qquad 10 \leq k \leq 100$$

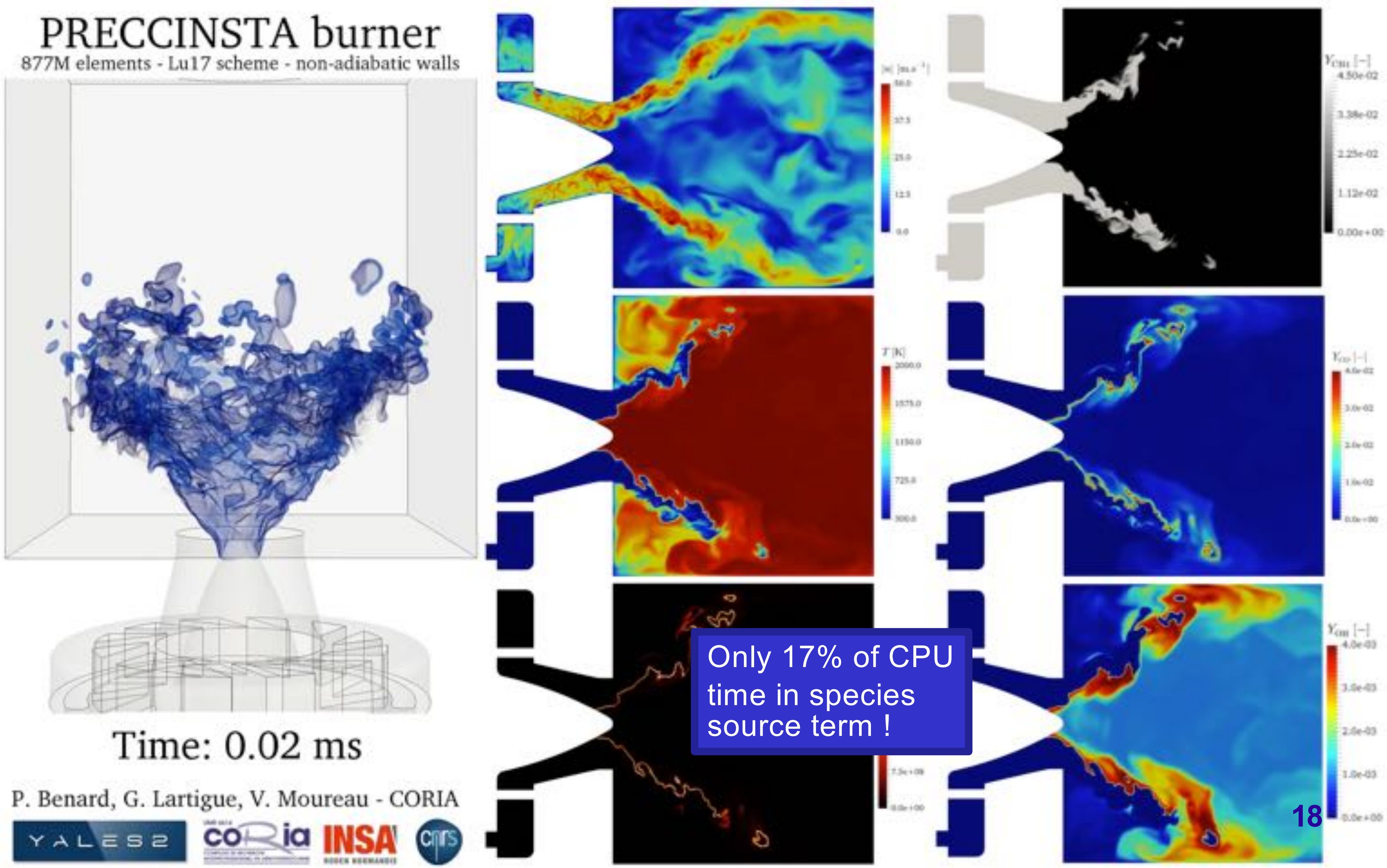
transport $10^{-6} s$ diffusion $10^{-9} s$ reactions $10^{-12} s$

Key ingredients

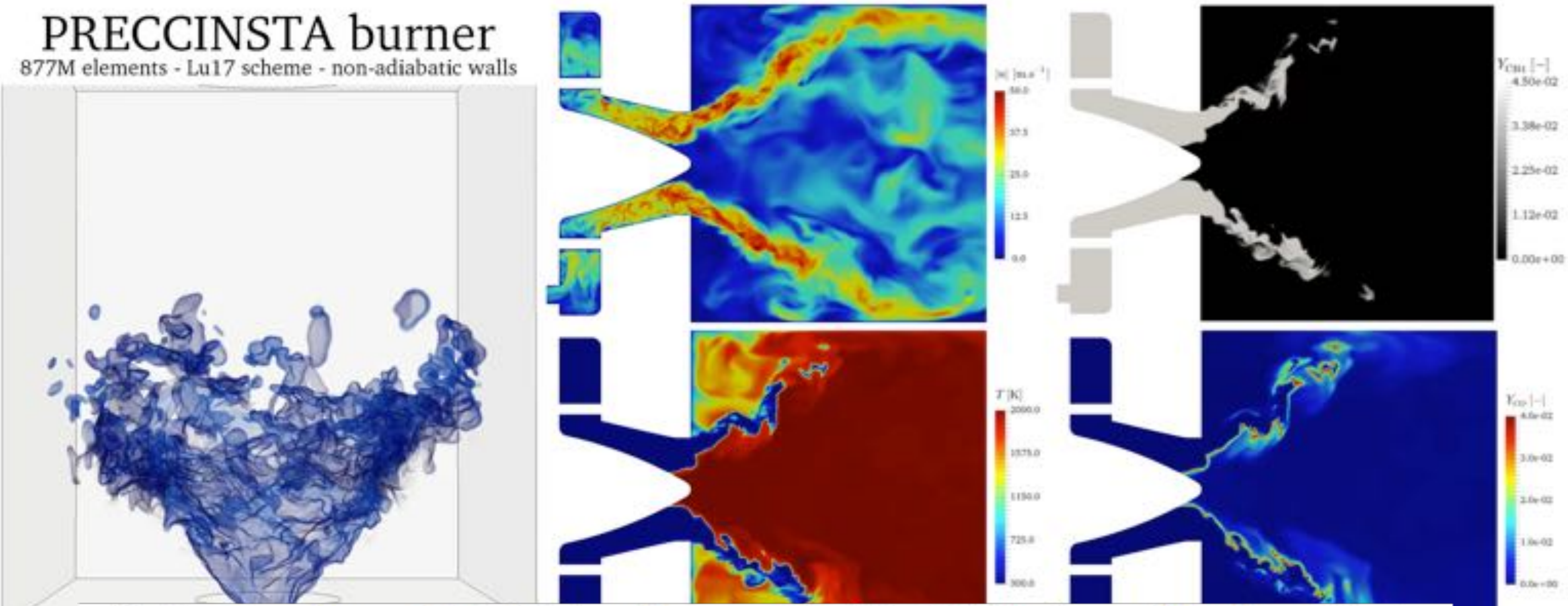
Dynamic TFLES model	• Allows to resolve the flame front on the LES grid (Colin et al. 2000)
Operator splitting	• Each phenomenon is advanced at its own characteristic time
CVODE stiff integrator	• Variable order and variable timestep integration with error control + analytical Jacobian + full vectorization of reaction rates and Jacobian
Dynamic load balancing	• 2-level task sharing algorithm based on MPI (Fontenaille et al., submitted to EUROPAR 2018)

- Validated with up to 91 species and 700 reactions (kerosene/air combustion)
- Good performances up to 32'000 cores

Mesochallenge Myria 2017 @ CRIANN
FIRELES PRACE project, 16384 cores on Curie



Mesochallenge Myria 2017 @ CRIANN
FIRELES PRACE project, 16384 cores on Curie



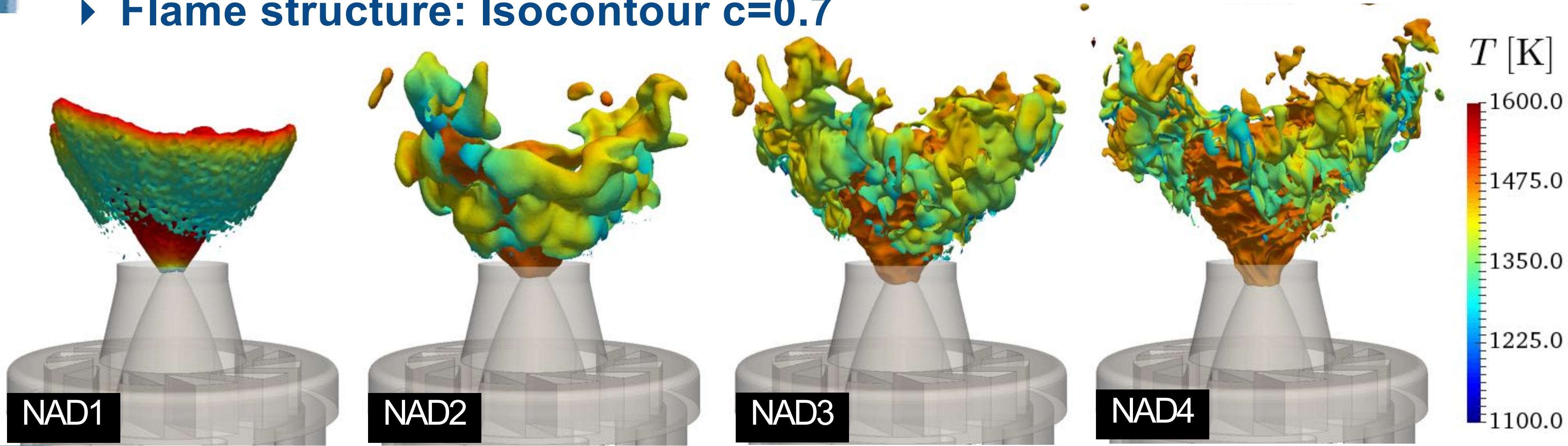
Portion du solveur	Part de la boucle temporelle [%]	RCT [μs/noeud/iteration $* N_{proc}$]
Advection	0.78	6.5
Implicit diffusion	3.41	28.7
Pressure correction	8.48	71.2
Scalar advection	9.26	77.8
Scalar diffusivity	10.29	86.4
Scalar source term	16.62	139.6
Scalar diffusion	47.09	395.7
GLOBAL	100.0	840.2

Only 17% of CPU time in species source term !

Non-adiabatic cases

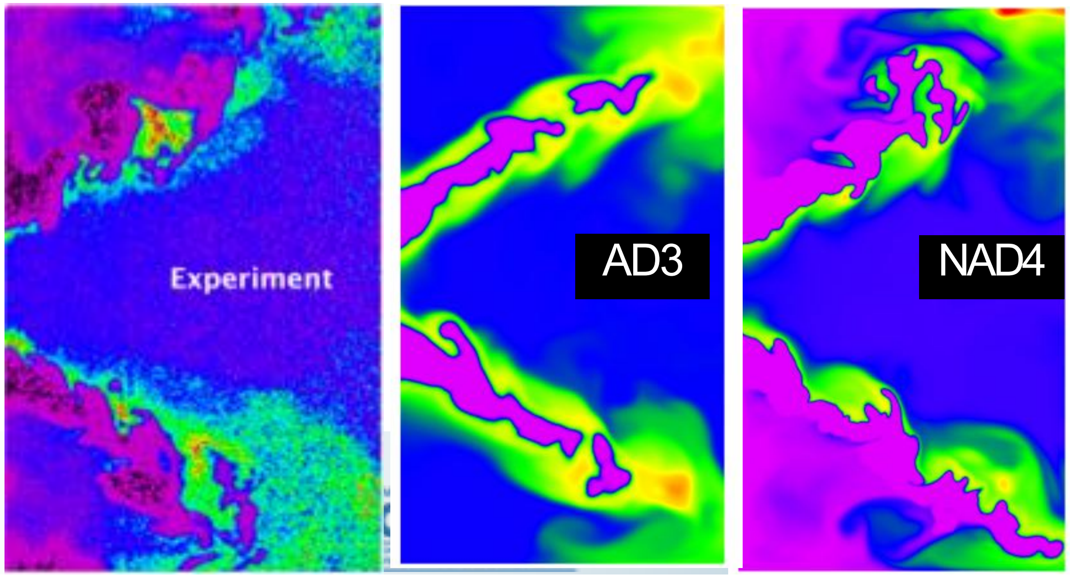
Mesh name	1	2	3	4
#cells [million]	1.7	14	110	877
Cell size [mm]	1.2	0.6	0.3	0.15
Heat loss/Total HR [%]	3.4	6.1	6.5	6.0

- **Flame structure: Isocontour c=0.7**



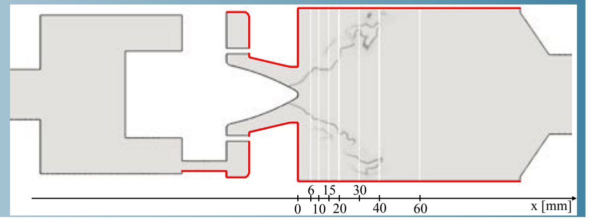
Complete extinction of external flame => V-shape flame

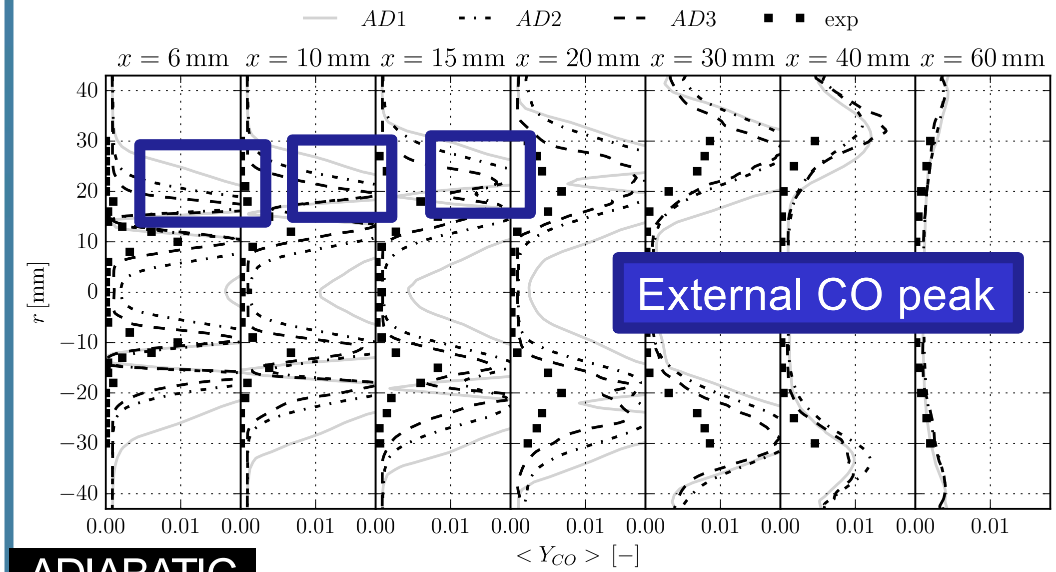
OH field

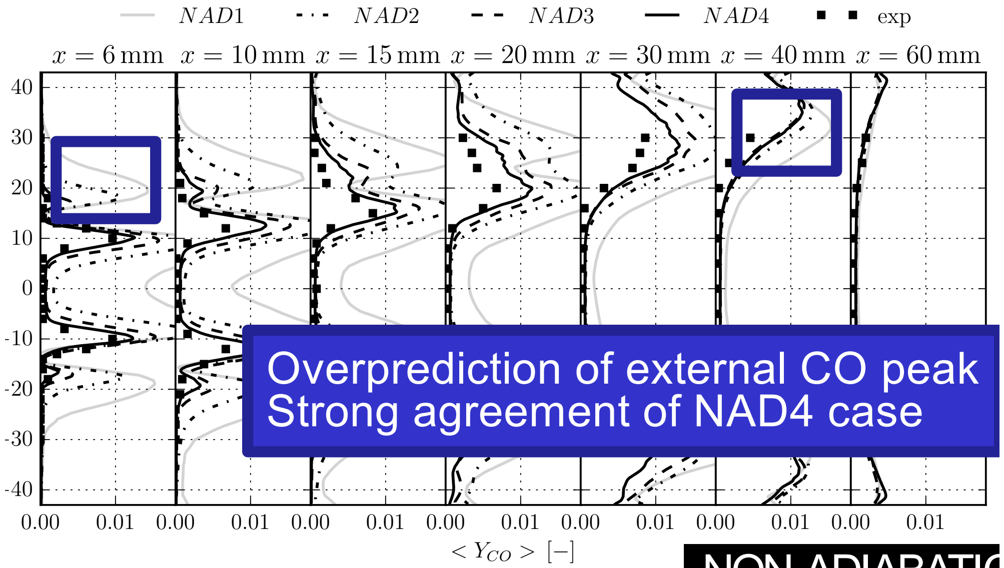


P. Bénard et al.,
accepted to the 2018 Int. Comb. Symp., Dublin

Mean and RMS CO mass fraction

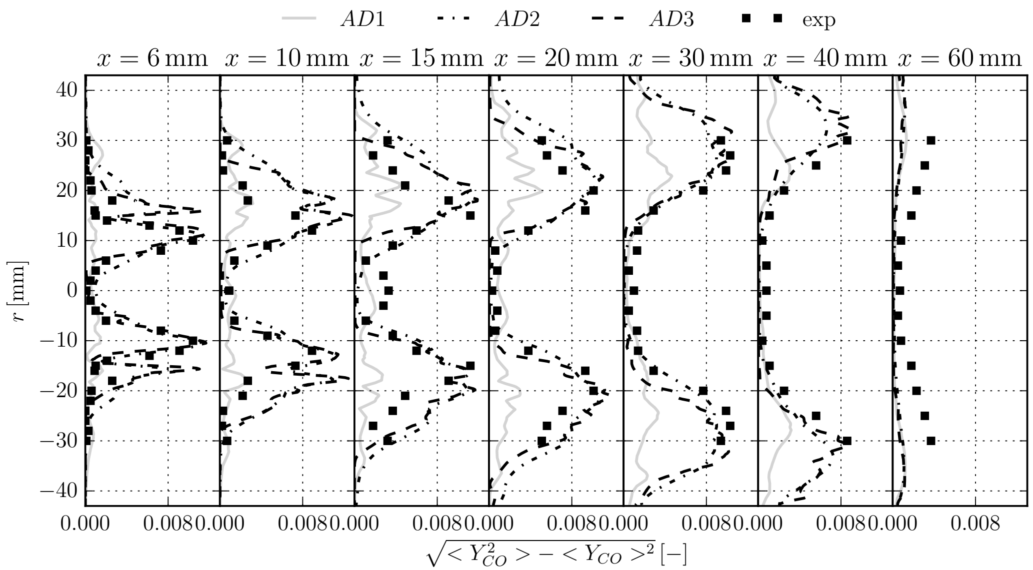


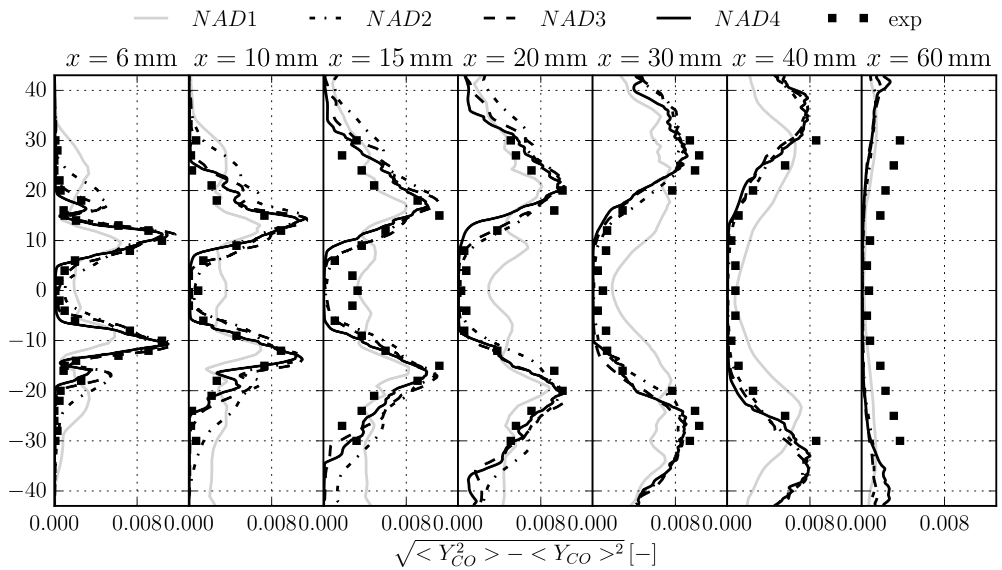




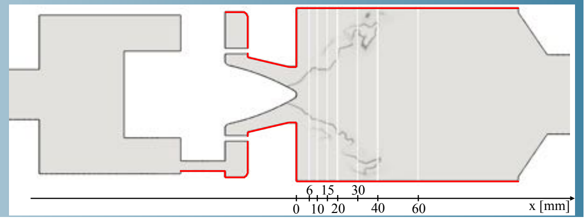
ADIABATIC

NON-ADIABATIC

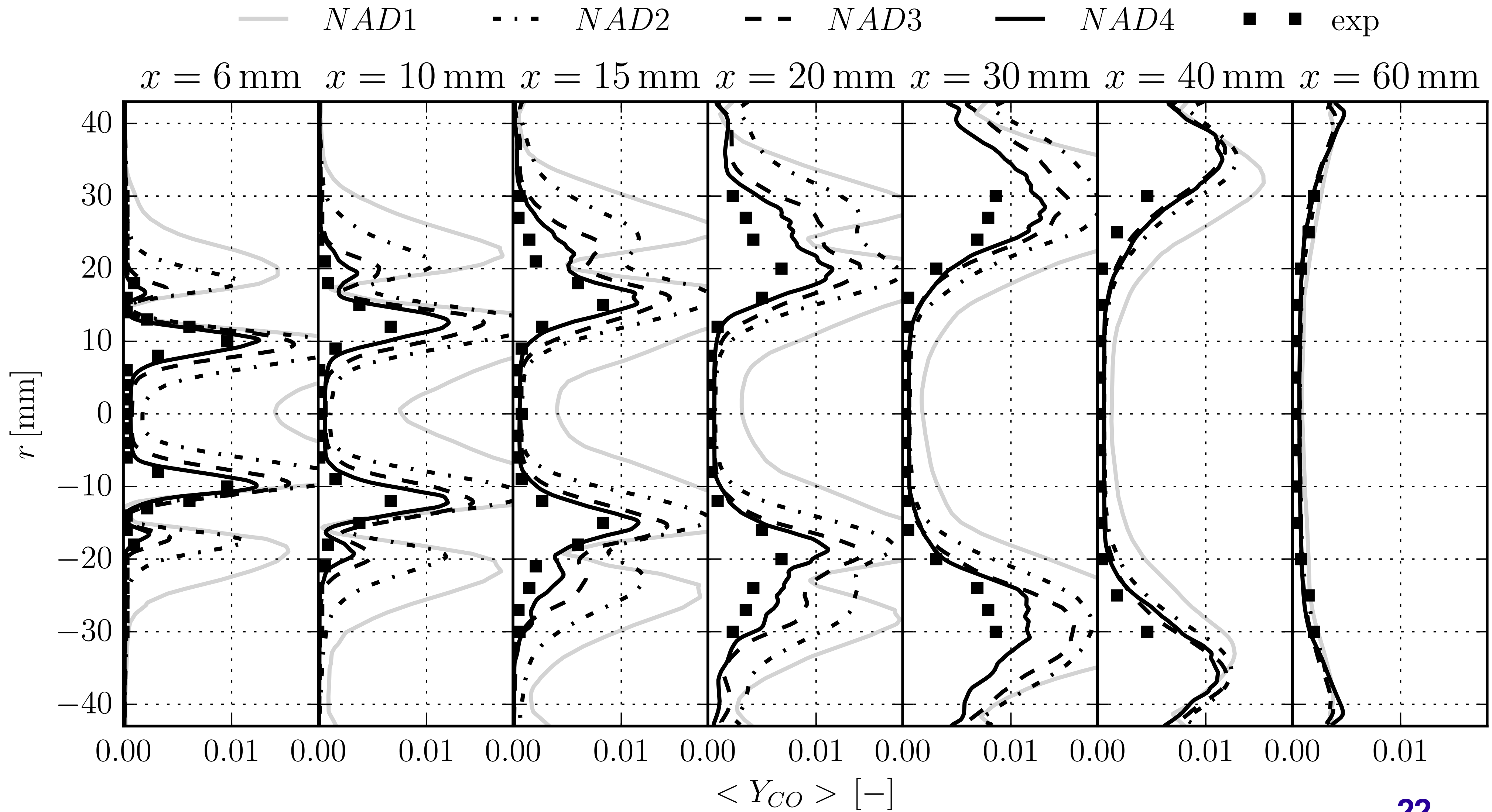




Mean and RMS CO mass fraction



- Some error on CO remain due to TFLES combustion model



When can we expect a DNS of PRECCINSTA? (or of lab-scale burners)

???

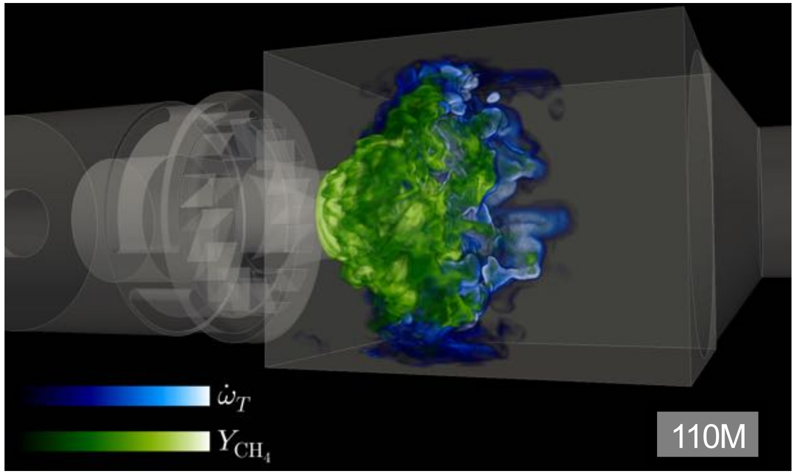
Exaflops

Petaflops

- DNS (species profile resolving)
  - 10 microns
  - 89’000B tets
  - ???

- DNS (flame/turbulence interactions resolving)
  - 50 microns
  - 143B tets, 442M CPUh
  - 200’000 cores, 13 weeks

- LES of PRECCINSTA burner
  - 17 species, 72 reactions
  - 150 microns
  - 877M tets, 4M CPUh
  - 8000 cores, 2 weeks



- Alternative to reach DNS faster ?

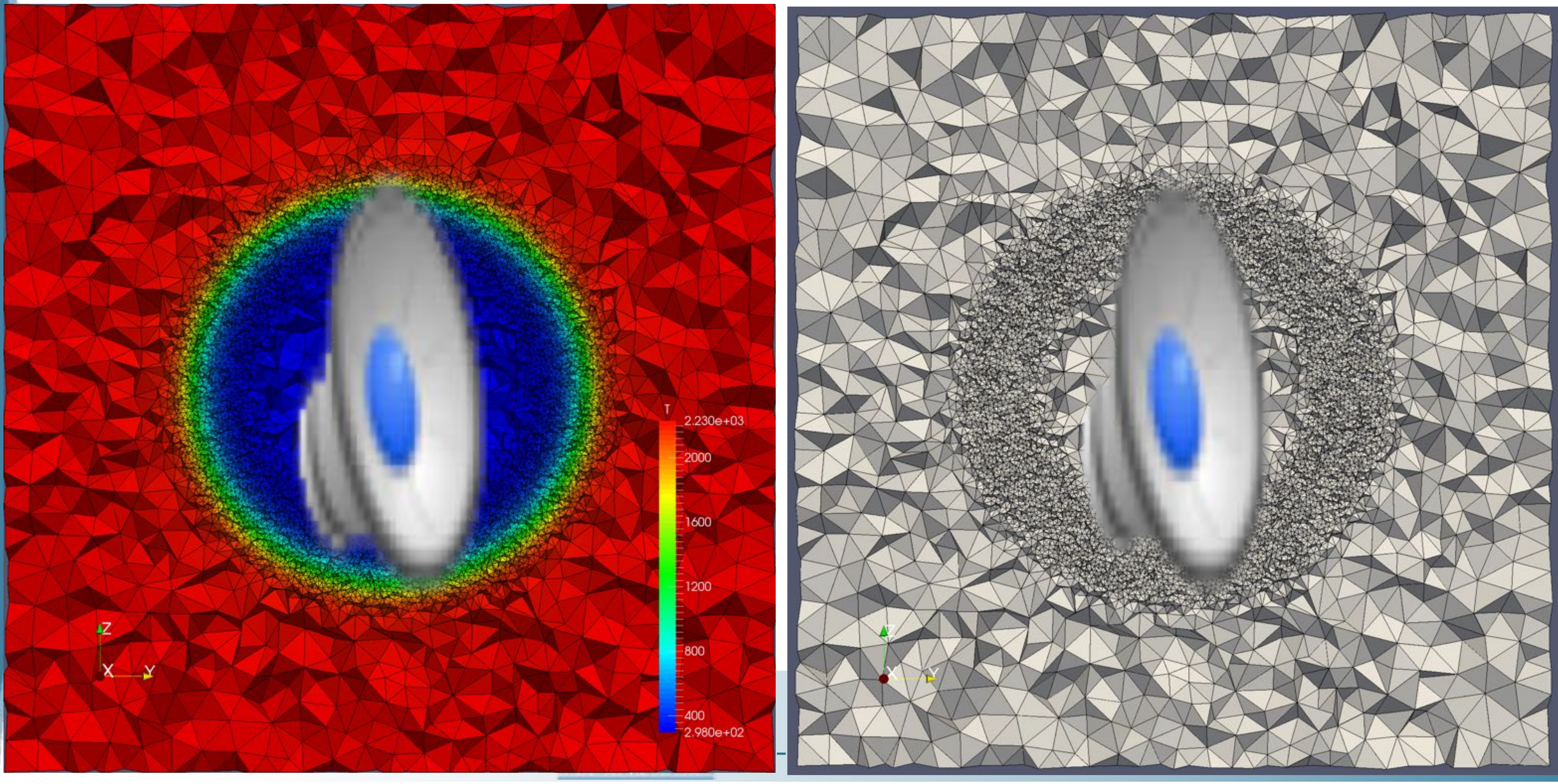
Dynamic h-adaptation of a premixed flame

- **F-TACLES combustion model [1], refinement ratio = 6**
- **H-adaptation performed with the MMG library from INRIA**

upgrade your meshes

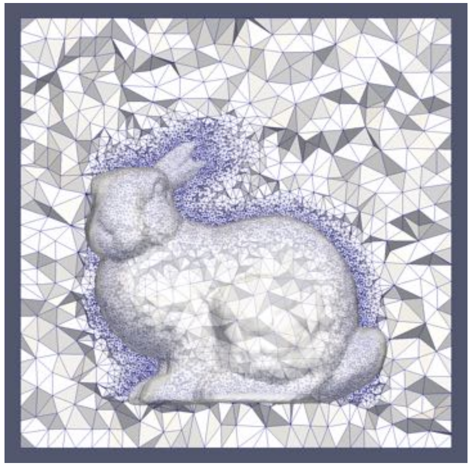
www.mmgtools.org

[1] Fiorina et al., C&F, 2009



H-adaptation of tetrahedral-based meshes

- **Consists in topology changes to refine or unrefine the mesh locally**
  - **Node insertion in Delaunay triangulations**
  - **Edge or face swapping**
  - **Element collapsing**
  - **…**



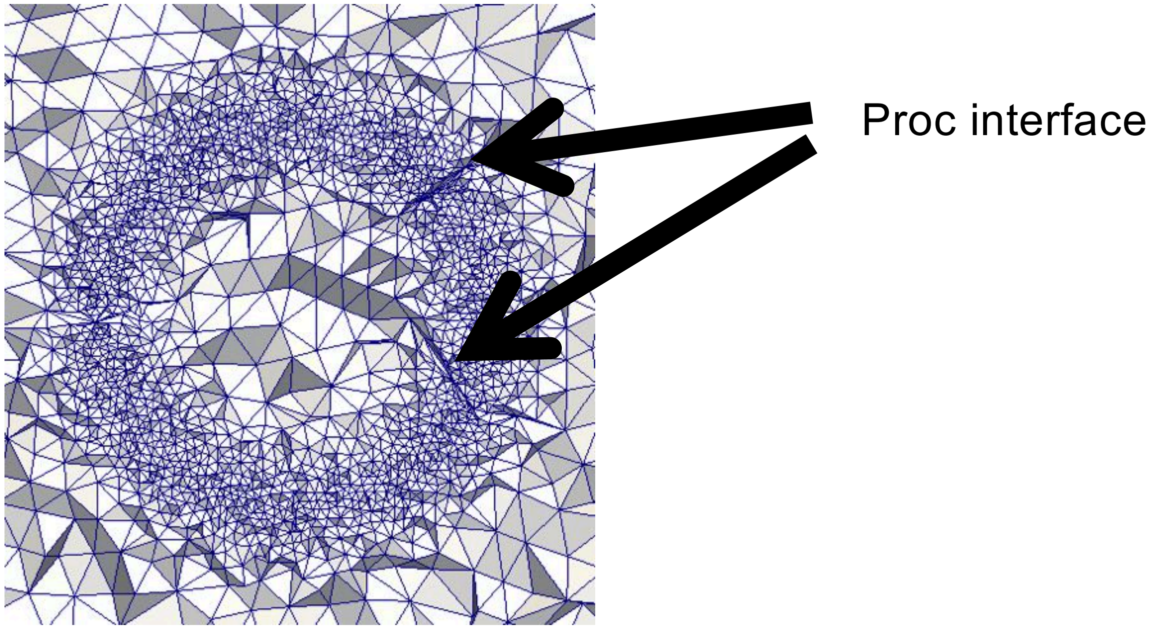
- **Several open-source libraries exist**
  - **MMG3D,** http://www.mmgtools.org
  - **MADLIB,** http://sites.uclouvain.be/madlib/
  - **NETGEN,** http://www.hpfem.jku.at/netgen/
  - **TETGEN,** http://wias-berlin.de/software/tetgen/
  - **CGAL,** http://www.cgal.org/
  - **MeshAdapt,** http://www.scorec.rpi.edu/~xli/MeshAdapt.html

- **Very few libraries are (massively) parallel**
- **Other constraint: need to have a fine control on the mesh quality to continue using finite-volume schemes**

Parallel h-adaptation strategy

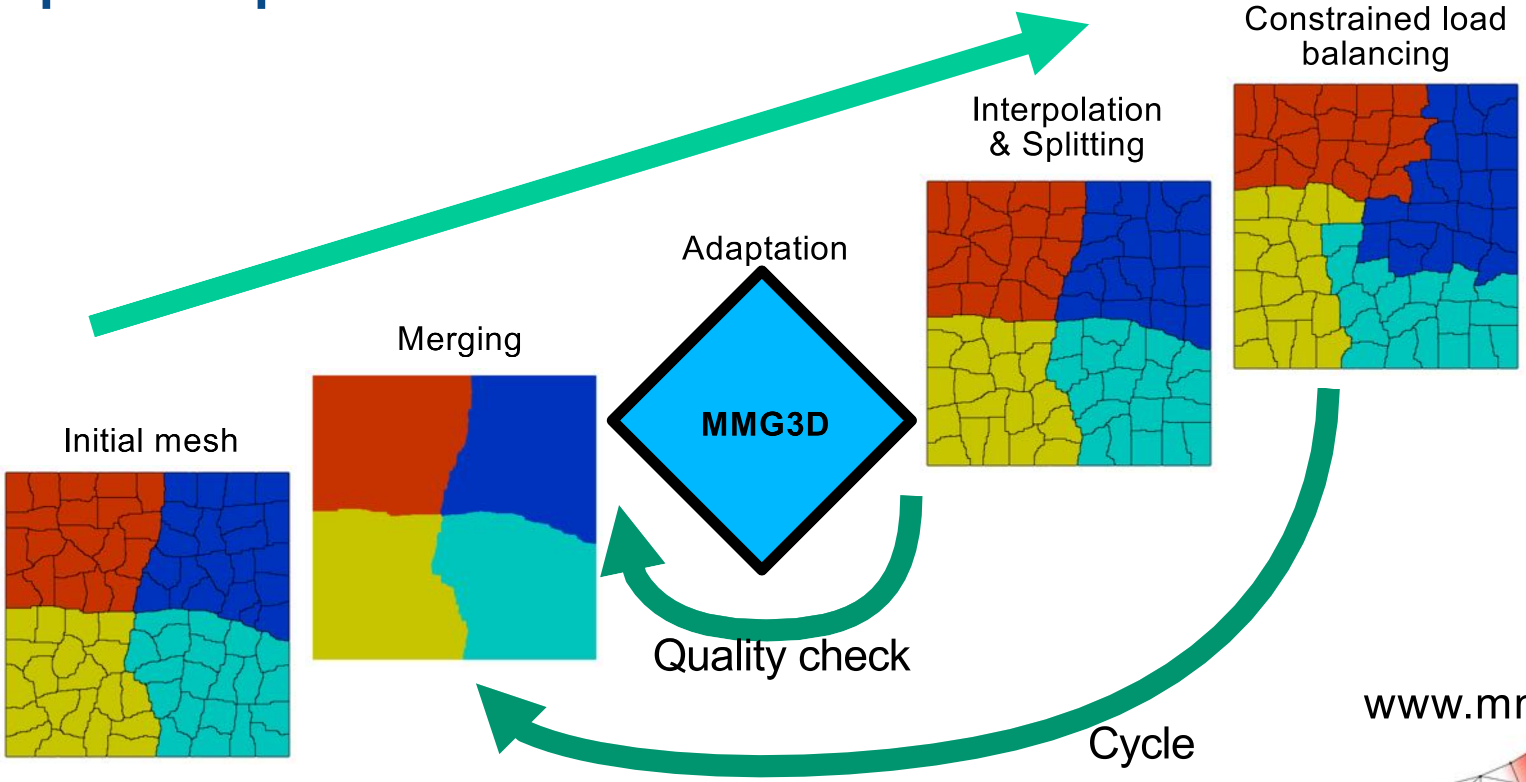
- **Can we imagine a parallel algorithm based on sequential adaptation libraries such as MMG3D?**

- **If mesh adaptation is performed on each processor, problems will arise at the proc interface. The choice made in YALES2 is to leave the processor interface untouched**



Parallel h-adaptation strategy

- Designed for massively distributed meshes [Bénard et al., IJNMF, 2015]
- Skewness is a key parameter for 4th-order central schemes
- Example for 4 processors



www.mmgtools.org

Upgrade your meshes

- MMG input: isotropic metric (or the desired local cell size)

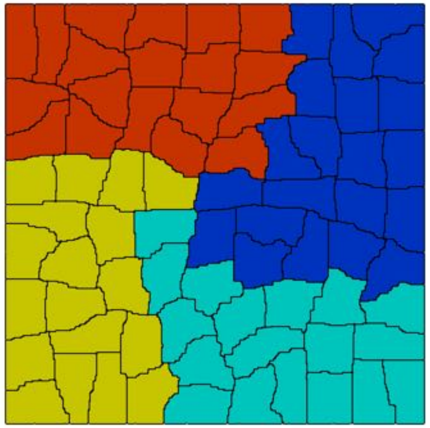
Load balancing strategies

1. **Parallel load balancing with PARMETIS4 [1]**
   - The cell group graph is built and repartitioned in parallel
   - Edge weights multiplied by 100 at the interface
   - Uncontiguous partition and may lead to empty processors

2. **Sequential load balancing with METIS5 [2]**
   - The cell group graph is built on master and partitioned
   - Partition is then modified to minimize data movement
   - Contiguous partition if input graph is contiguous

3. **Selective load balancing based on skewness**
   - Only the cell groups with a bad skewness on the interface are moved

Constrained load balancing

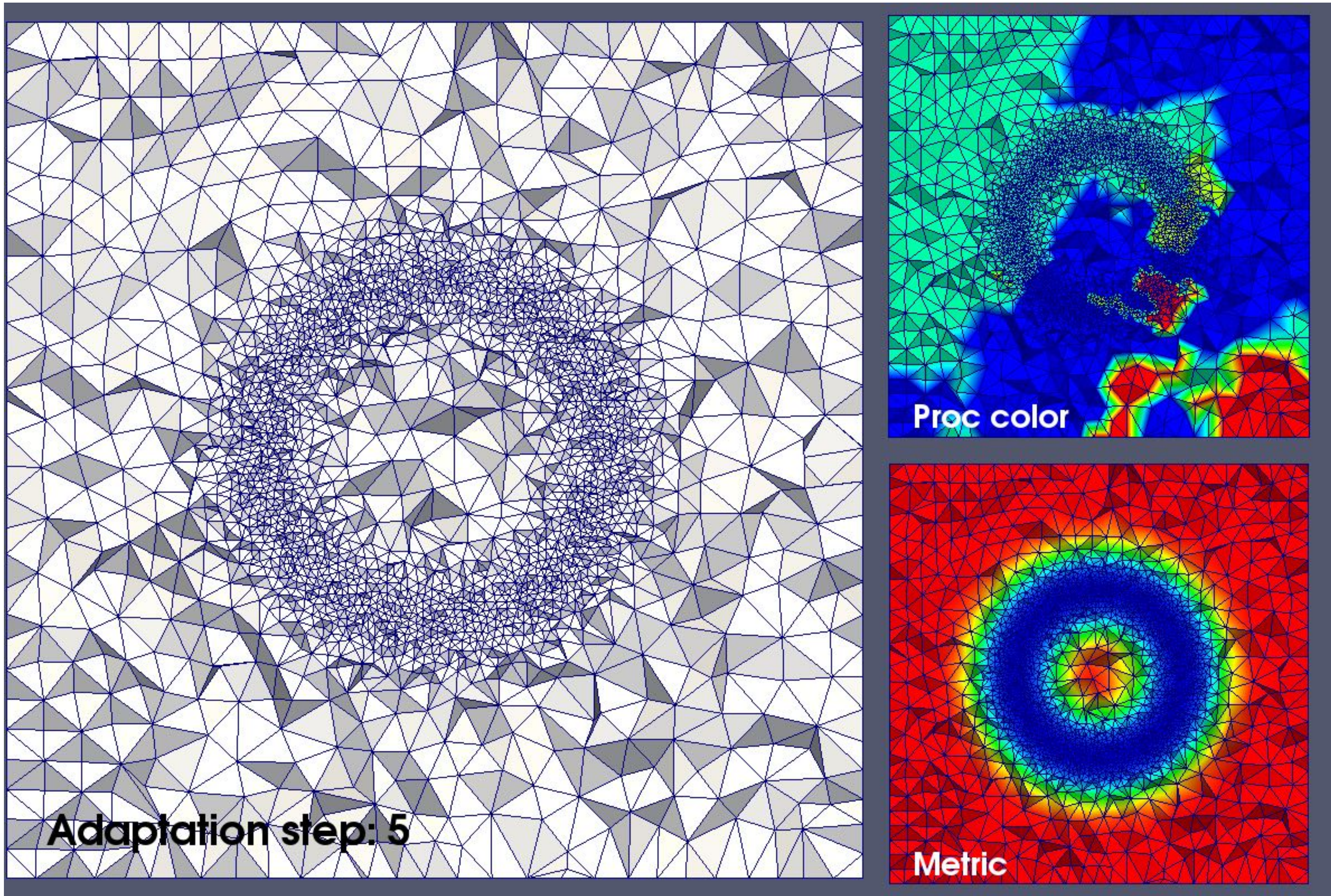


- **In following examples, #3 is used during the inner steps and #2 is performed at the end.**

[1] Karypis et al., JPDC, 1998
[2] Karypis et al., SIAM JSC, 1999

Refinement example 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

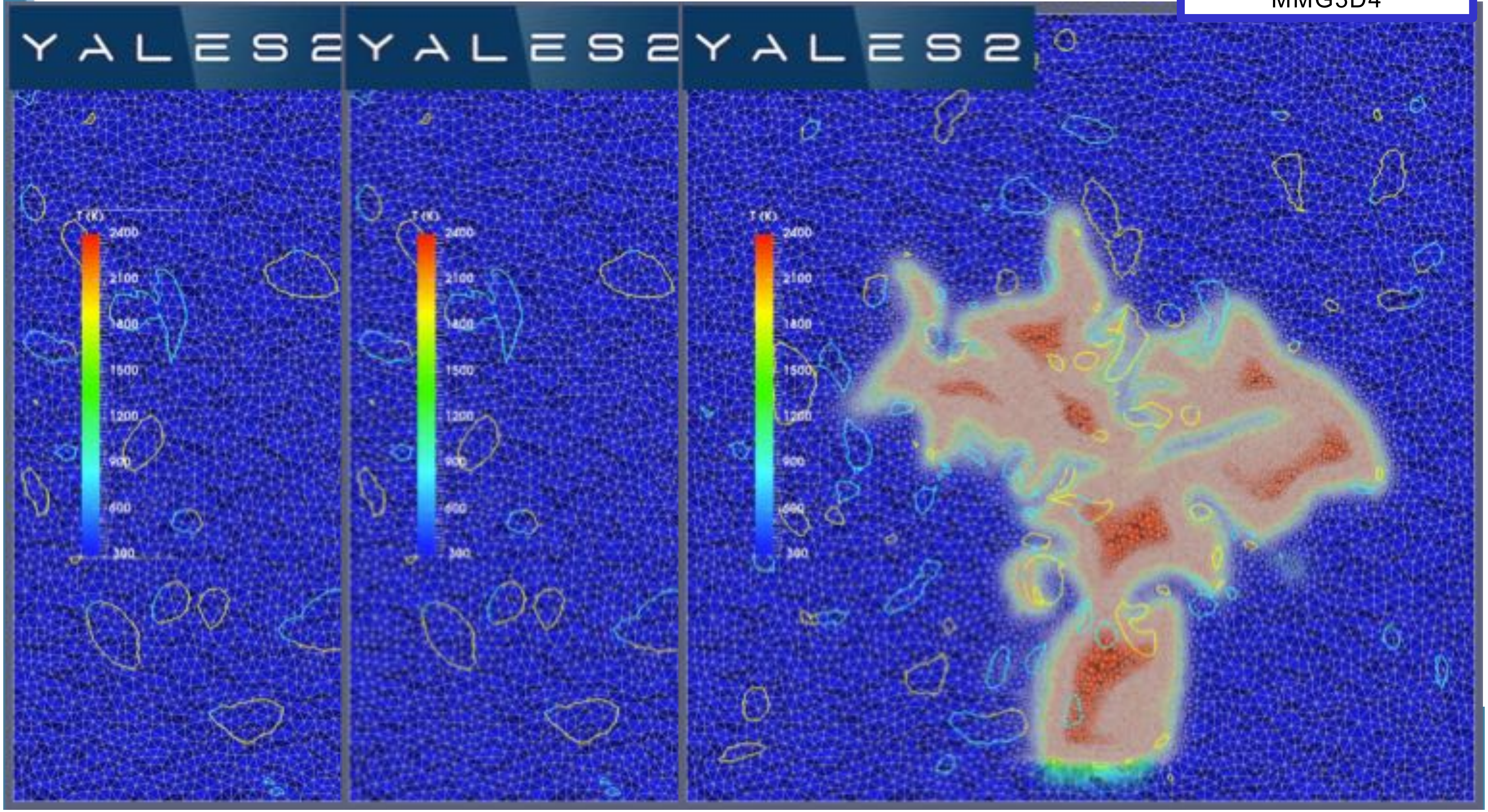


Application of dynamic mesh adaptation to propagating flames

Application: Turbulent flame kernel propagation

- CH4/air BFER scheme, DTFLES model, phi = 1.0, u'/S_L = 22.5
- Refinement ratios = 1, 3, 6

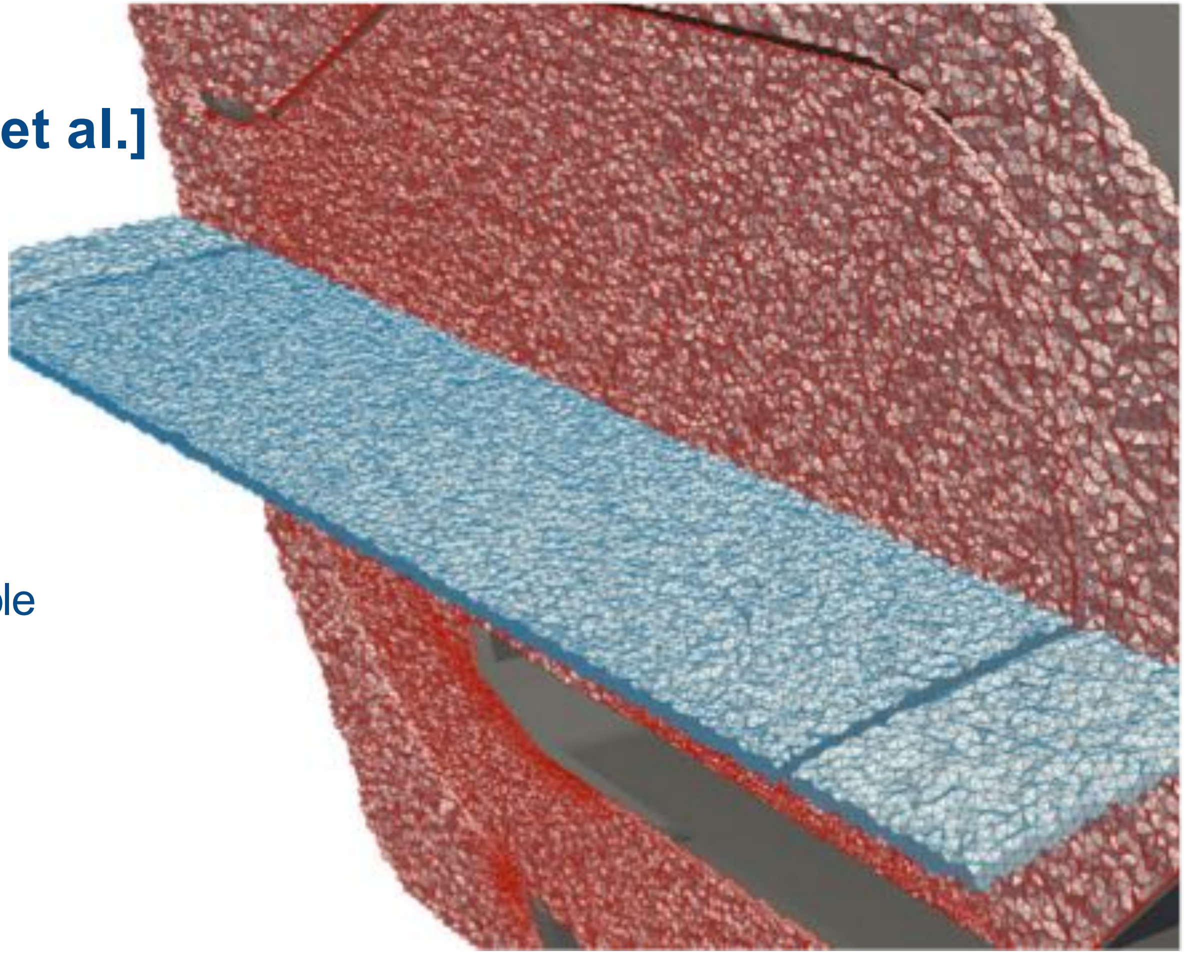
Finite-rate chemistry
MMG3D4



Application: Ignition in a SAFRAN HE combustor

- **SAFRAN Tech simulation**
- **F-TACLES model [Fiorina et al.]**
- **Iso-temperature at 1300K colored by vorticity**
- **Parameters**
  - Based on gradient of progress variable
  - Refinement ratio = 5
  - **41M to 75M tets**
  - Physical duration = 0.3 ms
  - **5h on 512 Cobalt cores**
  - 1 adaptation every 15 iter.
  - 1 adaptation = 4 minutes
  - Adaptation cost = 50%

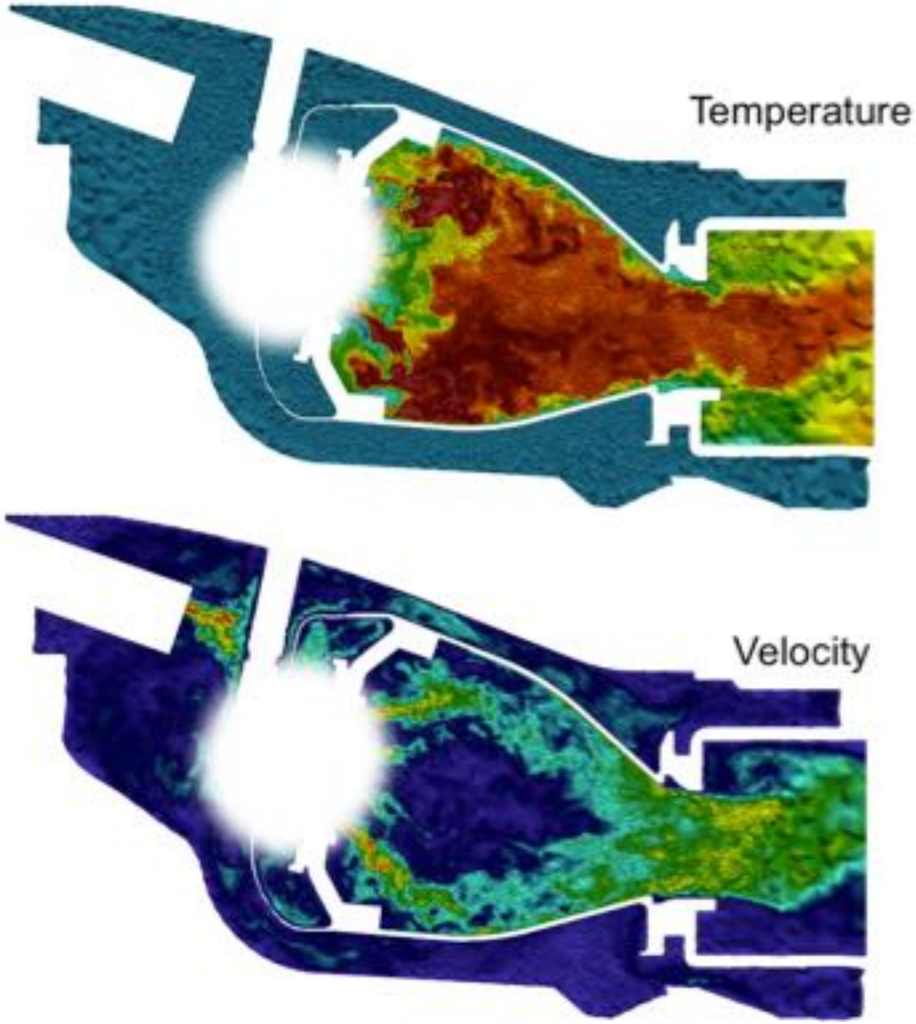
Courtesy R. Mercier



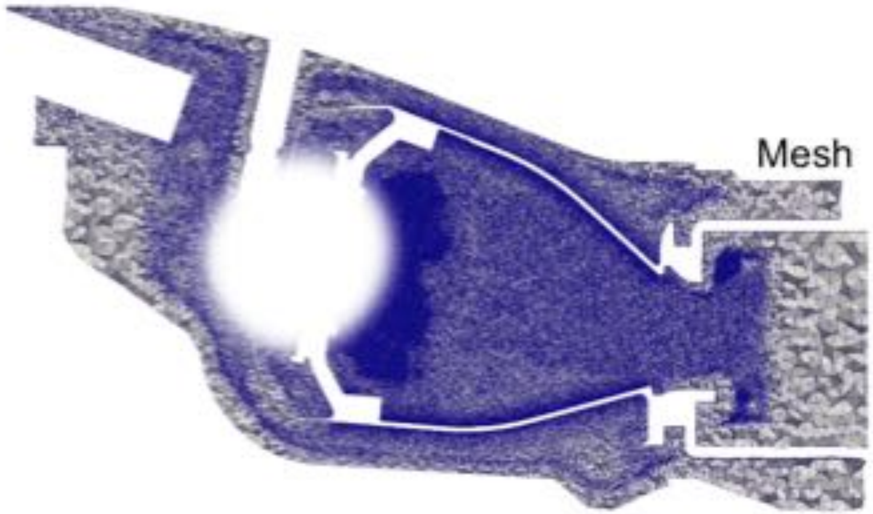
On-going simulations with periodic dynamic remeshing by G. Vaudor

Towards optimal and user-independent LES of aeronautical burners

- **With R. Mercier, SAFRAN TECH and C. Dobrzynski, IMB/INRIA**
- **Finalist at the 2018 TERATEC simulation awards**



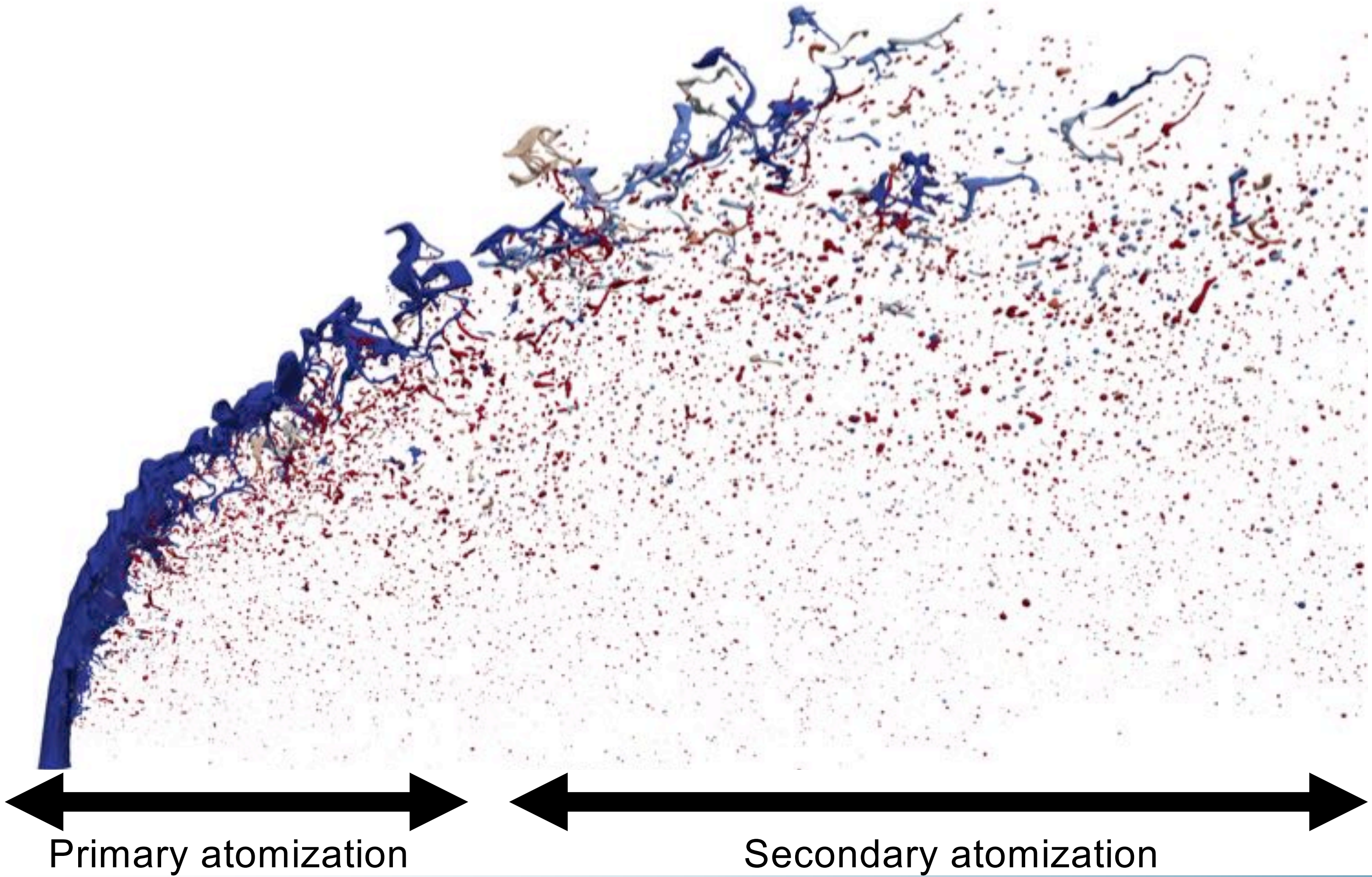
- **Proof of Concept**
  Safran combustion chamber
  - **Return time : 3 days (versus 15 days)**
  - **"All in one run"** : Embedded run scenario (initialization, fuel injection, ignition, stabilization,…)
  - **Automatic mesh convergence** included
  - User-specified CPU budget



Application of dynamic mesh adaptation to primary atomization

Typical flow topology

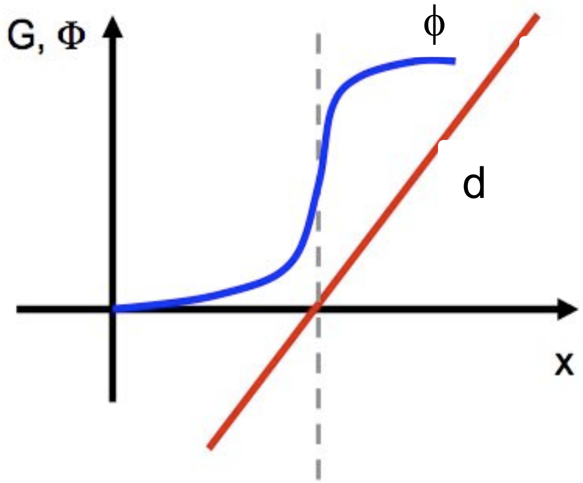
- **Jet in cross-flow configuration**



Level set tracking: the ACLS method
(Desjardins et al., JCP 2009)

- **Hyperbolic tangent**

$$\phi(\mathbf{x},t) = \frac{1}{2}\left(\tanh\left(\frac{\mathrm{d}(\mathbf{x},\mathrm{t})}{2\epsilon}\right)+1\right)$$



- **In YALES2, the hyperbolic tangent is used so that transport and reinitialization are conservative (Olsson and Kreiss, JCP, 2005)**

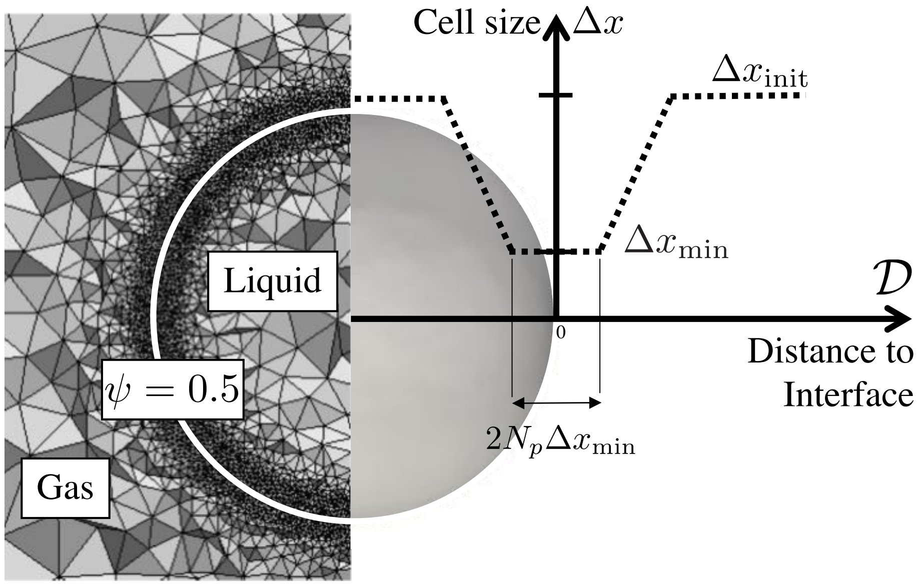
$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = 0$$

$$\frac{\partial \phi}{\partial \tau} + \nabla \cdot (\phi(1-\phi)\mathbf{n}) = \nabla \cdot (\epsilon(\nabla\phi \cdot \mathbf{n})\mathbf{n})$$

- **The ACLS is coupled to the Ghost-Fluid Method (Fedkiw et al., 2000) for the pressure jump**

Coupling of ACLS with dynamic mesh adaptation

- **Interface driven adaptation with imposed maximum metric gradient**



- **Metric definition**

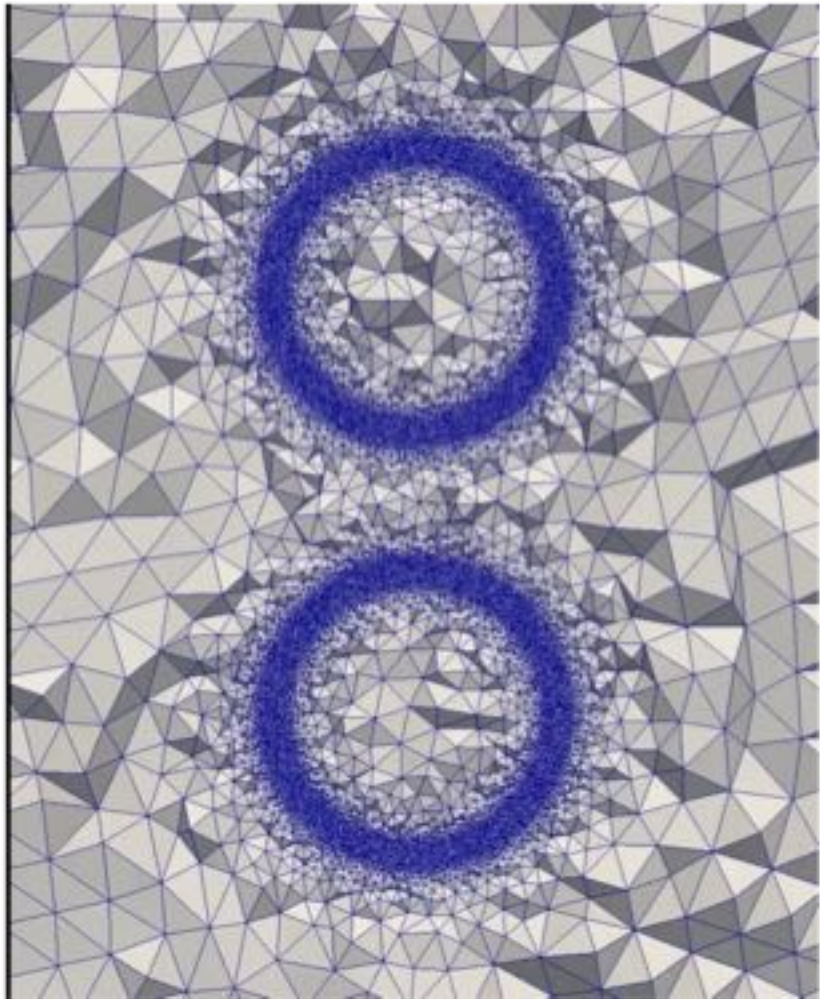
$$M(\mathcal{D}) = \min\left(\Delta x_{\mathrm{init}}, \max\left(\Delta x_{\mathrm{min}}, (|\mathcal{D}| - N_p\Delta x_{\mathrm{min}}) * |\nabla M|_0\right)\right)$$

- **Control of adaptation events**

$$N_{\mathrm{iter}}^{\mathrm{adapt}} = \frac{N_p}{\mathrm{CFL}} \frac{\Delta t^{\mathrm{CFL}}}{\Delta t}$$

Validation for droplet collision

- $N_p = 7$



Ashgriz et al., JFM 1990

Water/air

We = 23

Oh = 0.0047

d_{drop} = 400 µm

Δx_{min} = 4 µm

Δx_{max} = 80 µm

6M cells

Validation for droplet collision

Ashgriz et al., JFM 1990

Water/air

We = 23

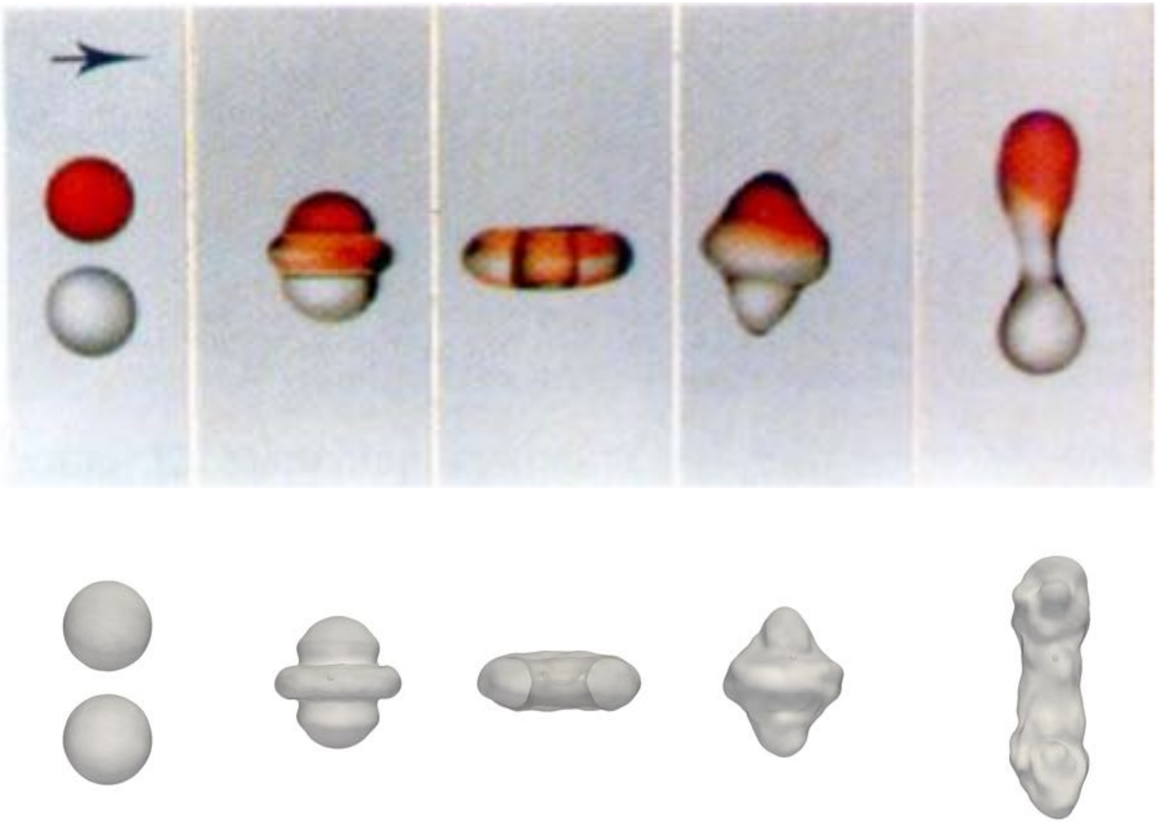
Oh = 0.0047

d_{drop} = 400 µm

Δx_{min} = 4 µm

Δx_{max} = 80 µm

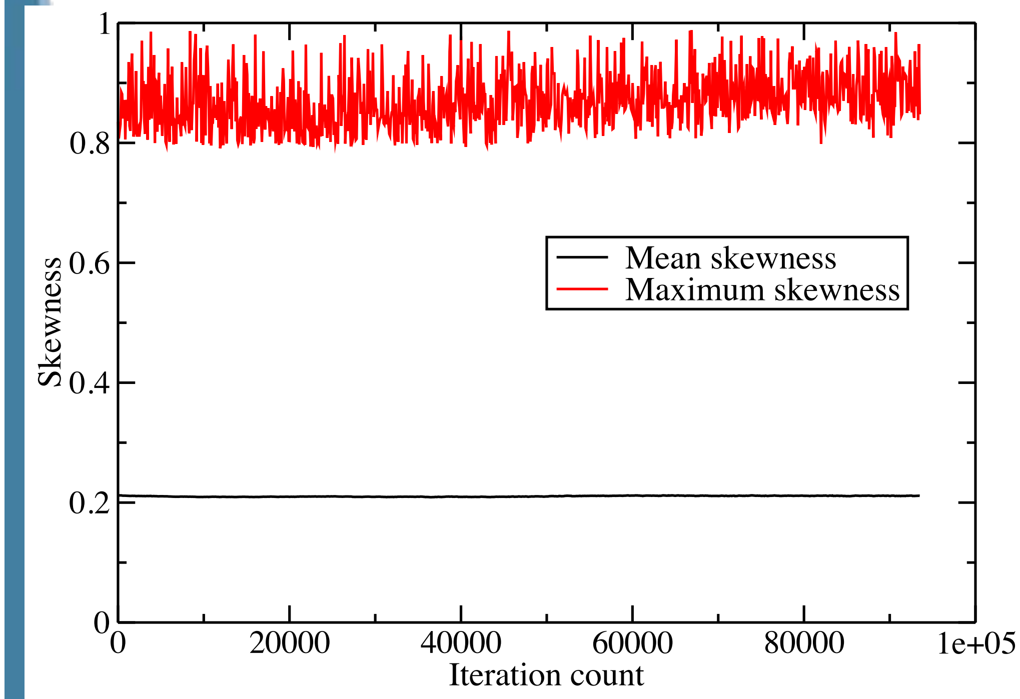
6M cells



Interface dynamics correctly reproduced at an affordable cost

Validation for droplet collision: performances

Mesh skewness evolution



MMG_v5 skewness filters are mandatory to keep a reasonable skewness

CPU cost

112 cores, Intel Xeon Broadwell, Myria super-computer @ CRIANN

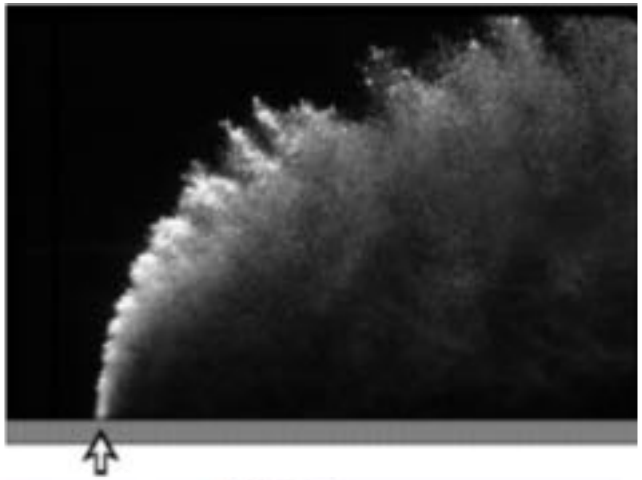
	Relative cost	RCT (ms.proc/ite/node)
Adaptation	23.1%	19.3
Interface tracking	26.8%	22.4
Advection	13.9%	11.6
Poisson equation	34.2%	28.5

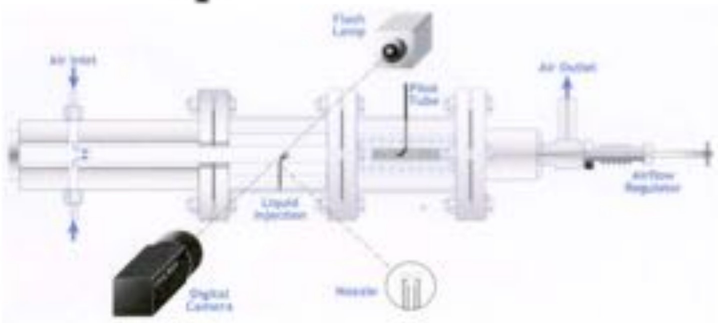
Mean iteration count between remeshing events is 94. Adaptation loop lasts 20s on average.

This affordable adaptation cost has been obtained after numerous optimizations

Application to a jet in cross flow
with R. Mercier, J. Leparoux, H. Musaefendic, SAFRAN

- High-pressure kerosene jet in cross-flow
- Relevant for multi-point injection systems
- Ragucci et al., Atomization & Sprays, 2007



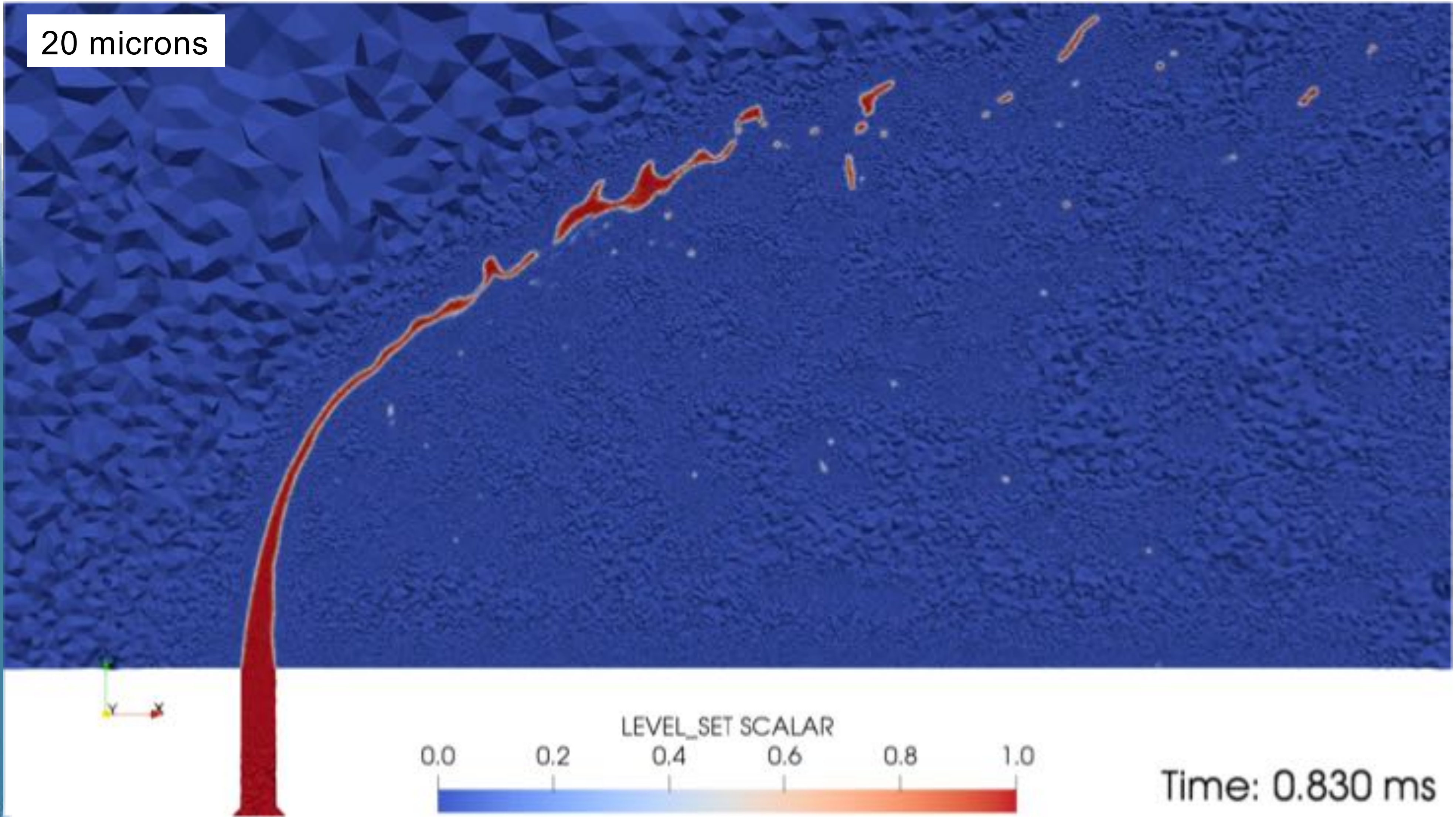


- Reference operating conditions
  - Injector diameter: D=0.5 mm
  - Flow section: 25 mm x 25 mm
  - Pressure: 10 bars
  - V_{air}= 37 m/s and $V_{kerosene}$= 17 m/s
  - Re_{air}= 590 287 and $Re_{kerosene}$= 4477
  - $We_{aero} = \rho_{air} V^2_{k\acute{e}ro} D/\sigma = 63.5$
  - Momentum ratio $q = \rho_{kero} V^2_{kero} / \rho_{air} V^2_{air} = 14.2$

- Numerics
  - Ghost-Fluid Method [Fedkiw et al., 2000]
  - Accurate Conservative Levelset [Desjardins et al., 2009]

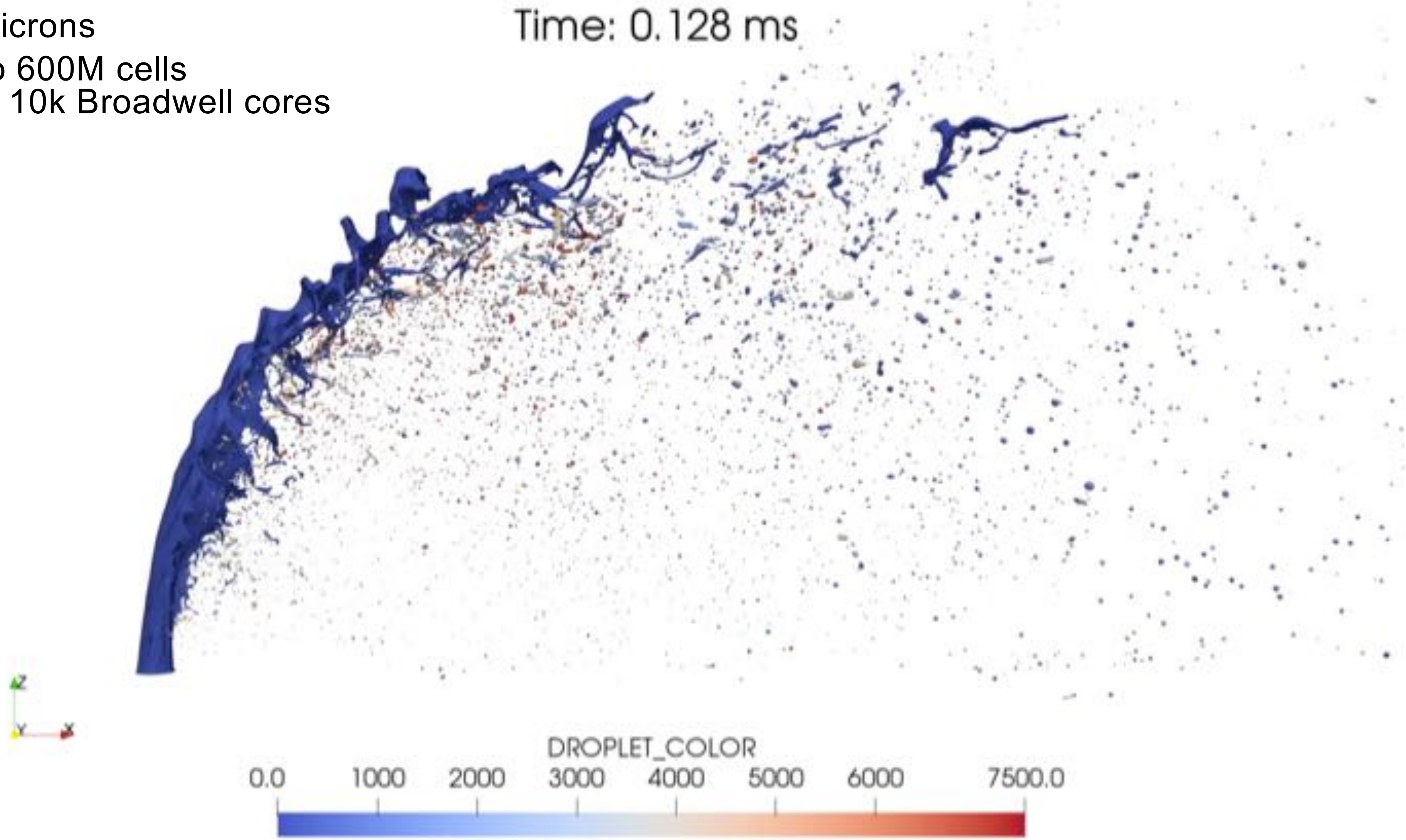
- Paper accepted to ICLASS 2018, Chicago

Application to a jet in cross flow
with R. Mercier, J. Leparoux, H. Musaefendic, SAFRAN



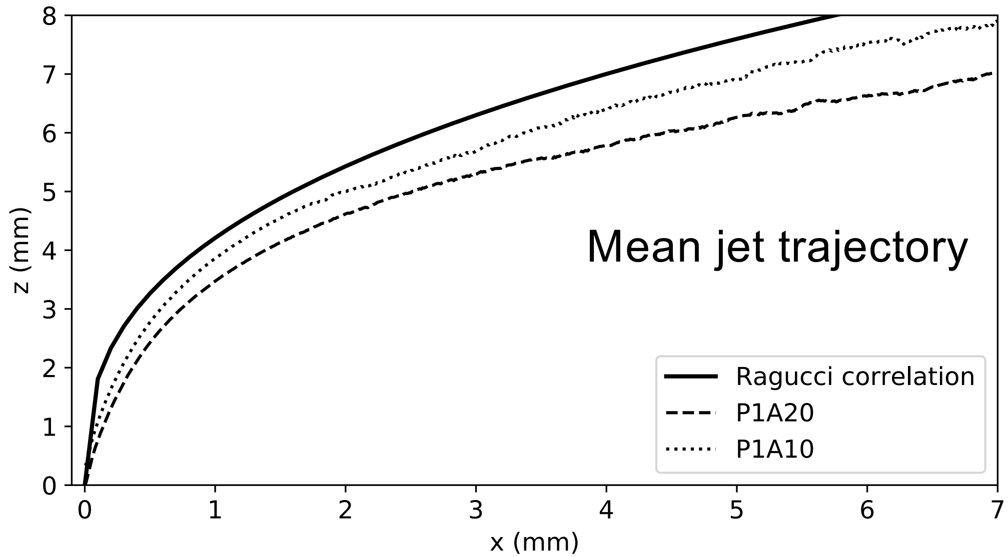
Application to a jet in cross flow
with R. Mercier, J. Leparoux, H. Musaefendic, SAFRAN

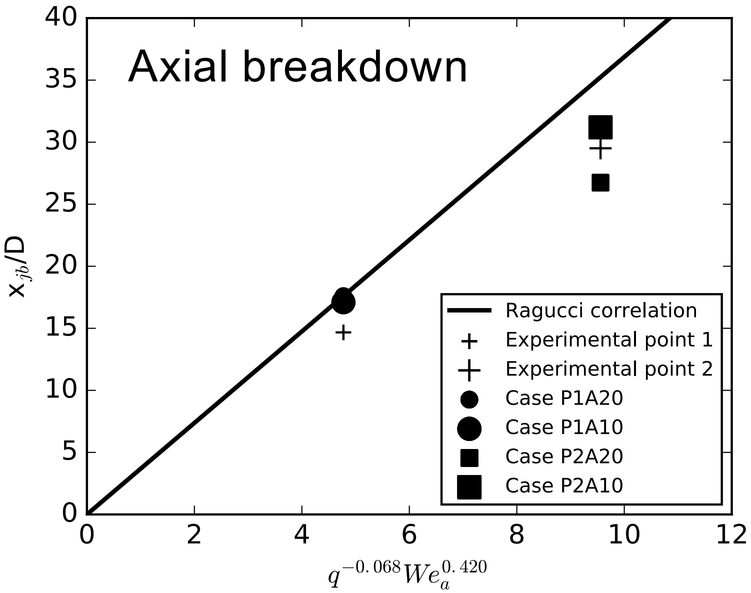
10 microns
Up to 600M cells
6k to 10k Broadwell cores

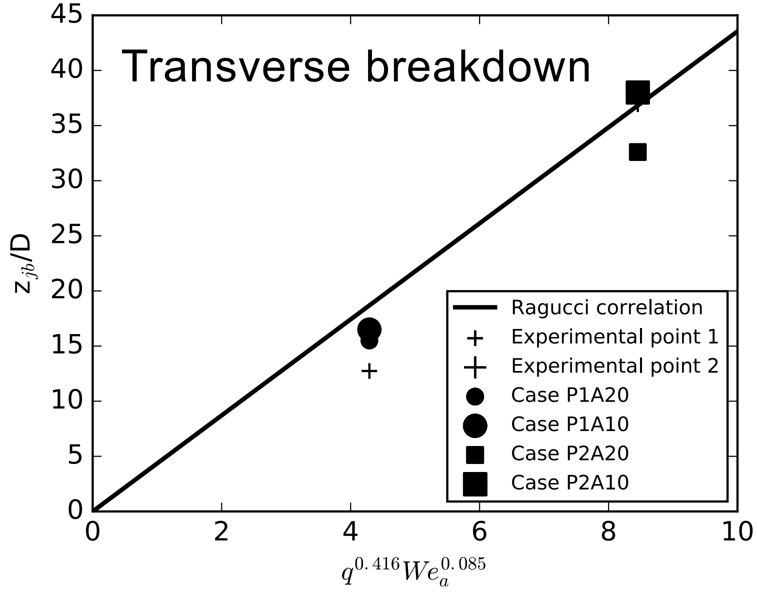


Application to a jet in cross flow
with R. Mercier, J. Leparoux, H. Musaefendic, SAFRAN

- Quantitative comparisons







Application to a SAFRAN Aircraft Engines injector

- Pressure-swirl atomizer
- Simulation includes the full injector geometry

Parameters

Kerosene/Air @ P_0

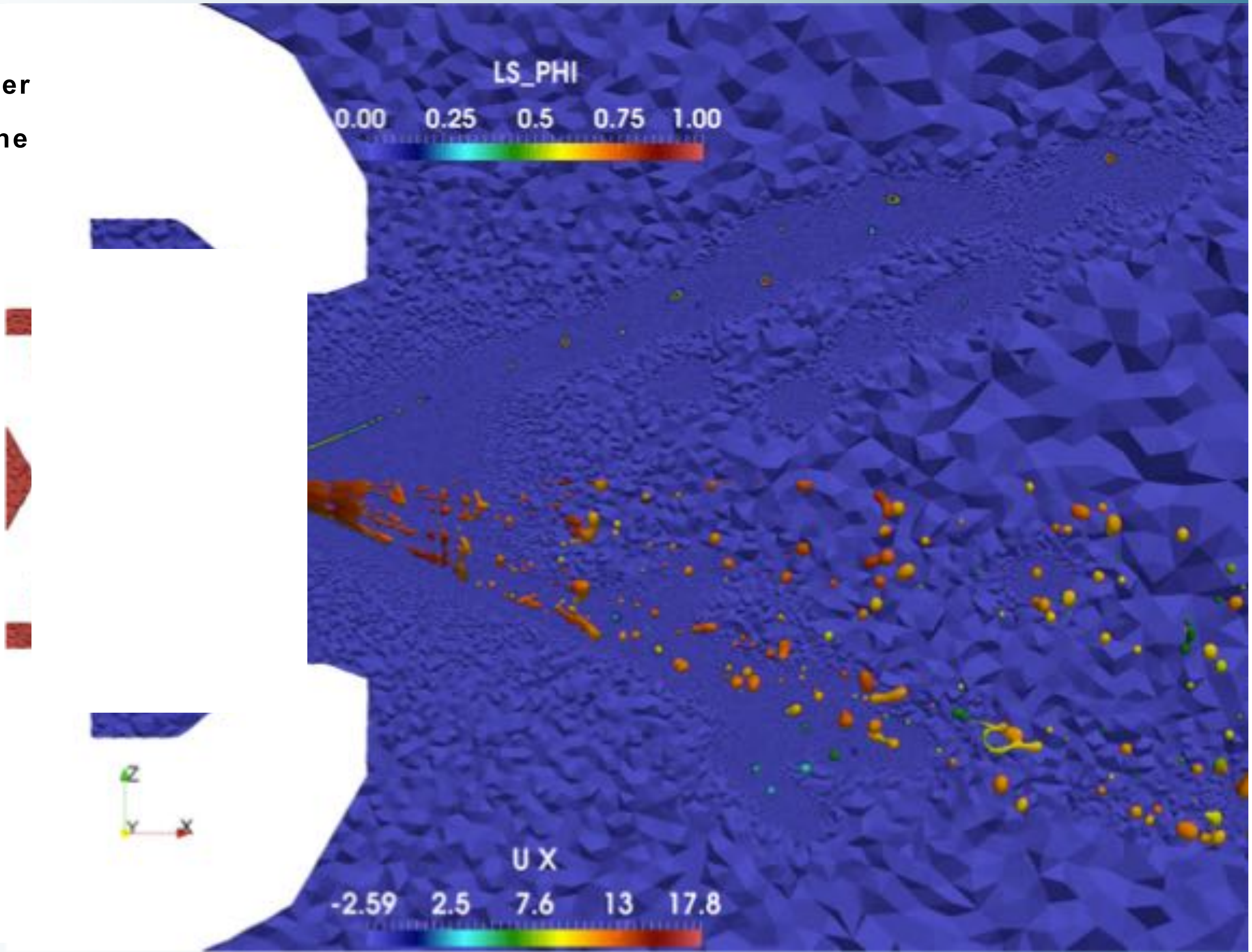
33 to 390 Mcells

Δx_{min} = 4.4 to 15 µm

180h on 1120 cores

Cobalt @ TGCC

Adaptation cost: 50%

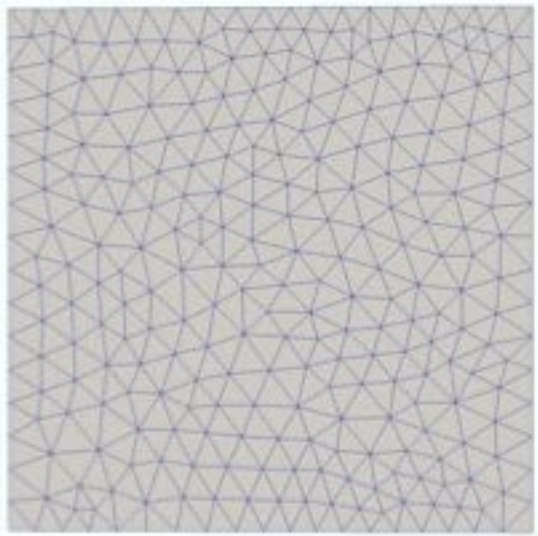


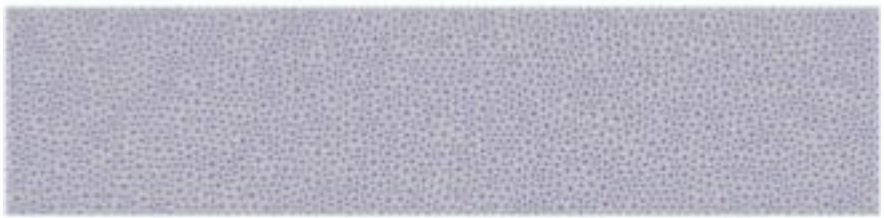
Conclusions

- **LES of complex burners with finite-rate chemistry becomes feasible**
  - On-going PRACE simulations with GRI3 mechanism (52 species, 300+ reactions)

- **Dynamic mesh adaptation is a solution to achieve more accuracy for a given cell count**

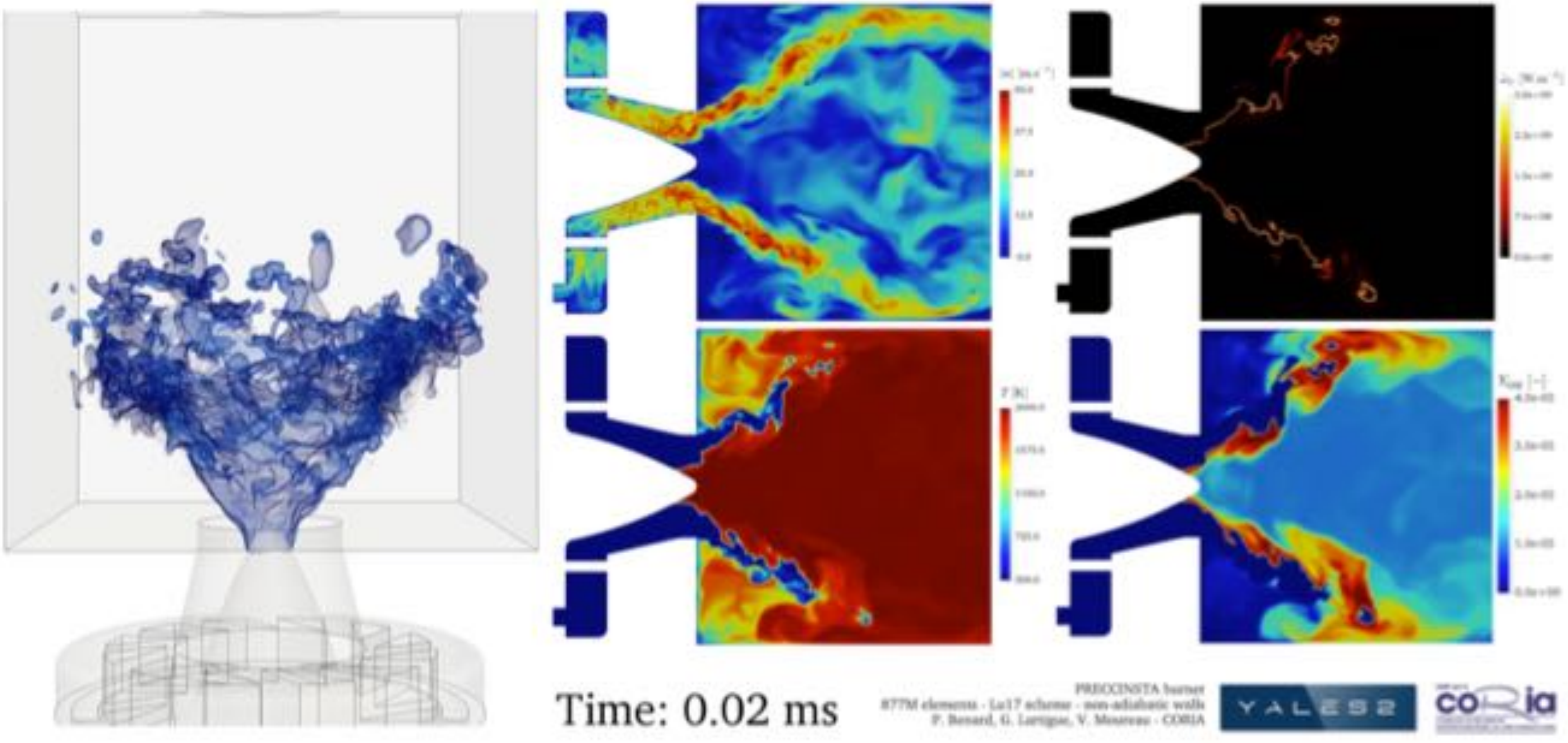
- **Many theoretical and numerical developments are still required**
  - Modeling of space/time commutation errors in LES
  - Performance model for better time control of adaptation
  - Automatic hgrad control from user metric
  - Surface remeshing





Acknowledgments

- PhDs and postdocs of the YALES2 team
- R. Mercier - SAFRAN Tech, France
- C. Dobrzynski, A. Froehly – IMB/INRIA Bordeaux, France
- A. Pushkarev, G. Balarac – LEGI, Grenoble, France
- L. Bricteux and his team, UMONS, Belgium
- CPU hours from PRACE, GENCI and CRIANN



References

- High performance linear solvers
  - 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
- Numerics
  - Vantieghem, S., "Numerical simulations of quasi-static magnetohydrodynamics using an unstructured finite volume solver: development and applications", 2011, PhD Thesis.
  - Kraushaar, M., « Application of the compressible and low-Mach number approaches to Large-Eddy Simulation of turbulent flows in aero-engines », 2011, PhD Thesis
- References on the code
  - 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
- Other references
  - http://www.coria-cfd.fr/index.php/User:Moureauv