HPC for the simulation of turbulent combustion in aeronautical engines

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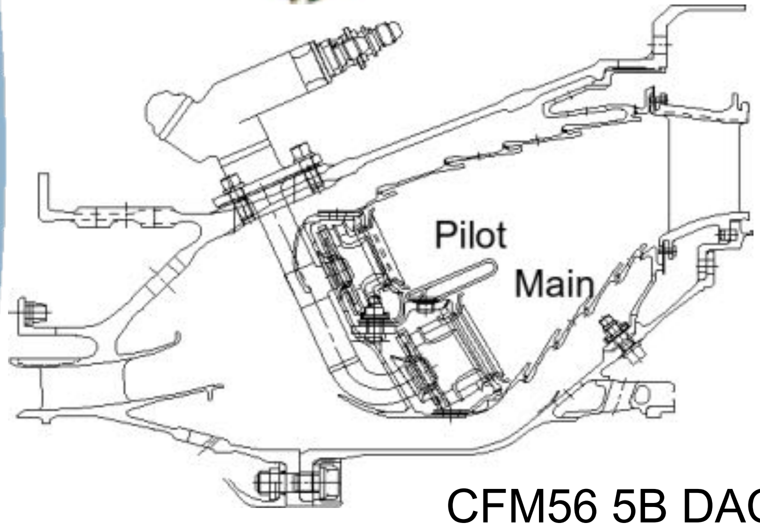
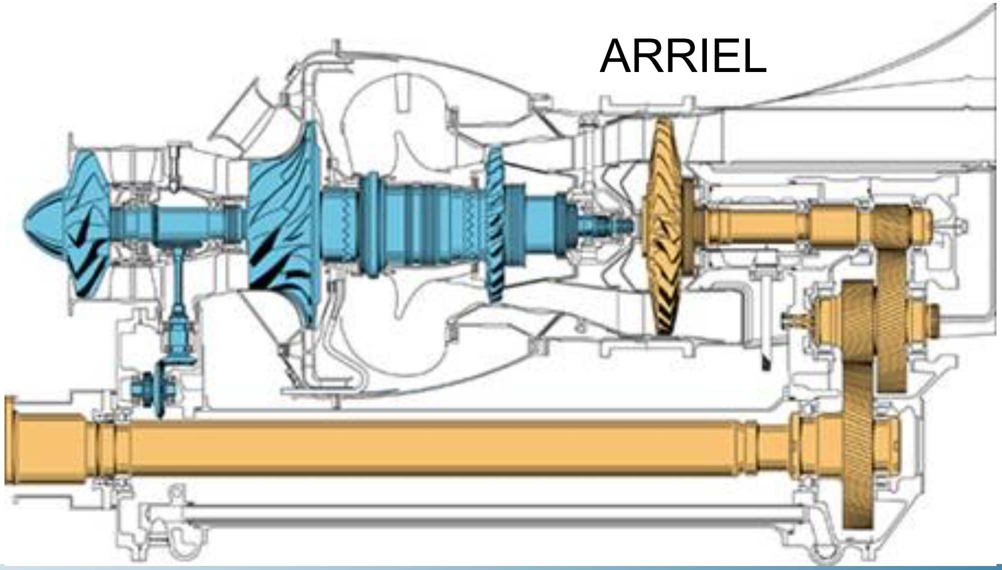
PRACEdays18

29/05/2018 – University of Ljubljana - Slovenia

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 — *Thermal efficiency*

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

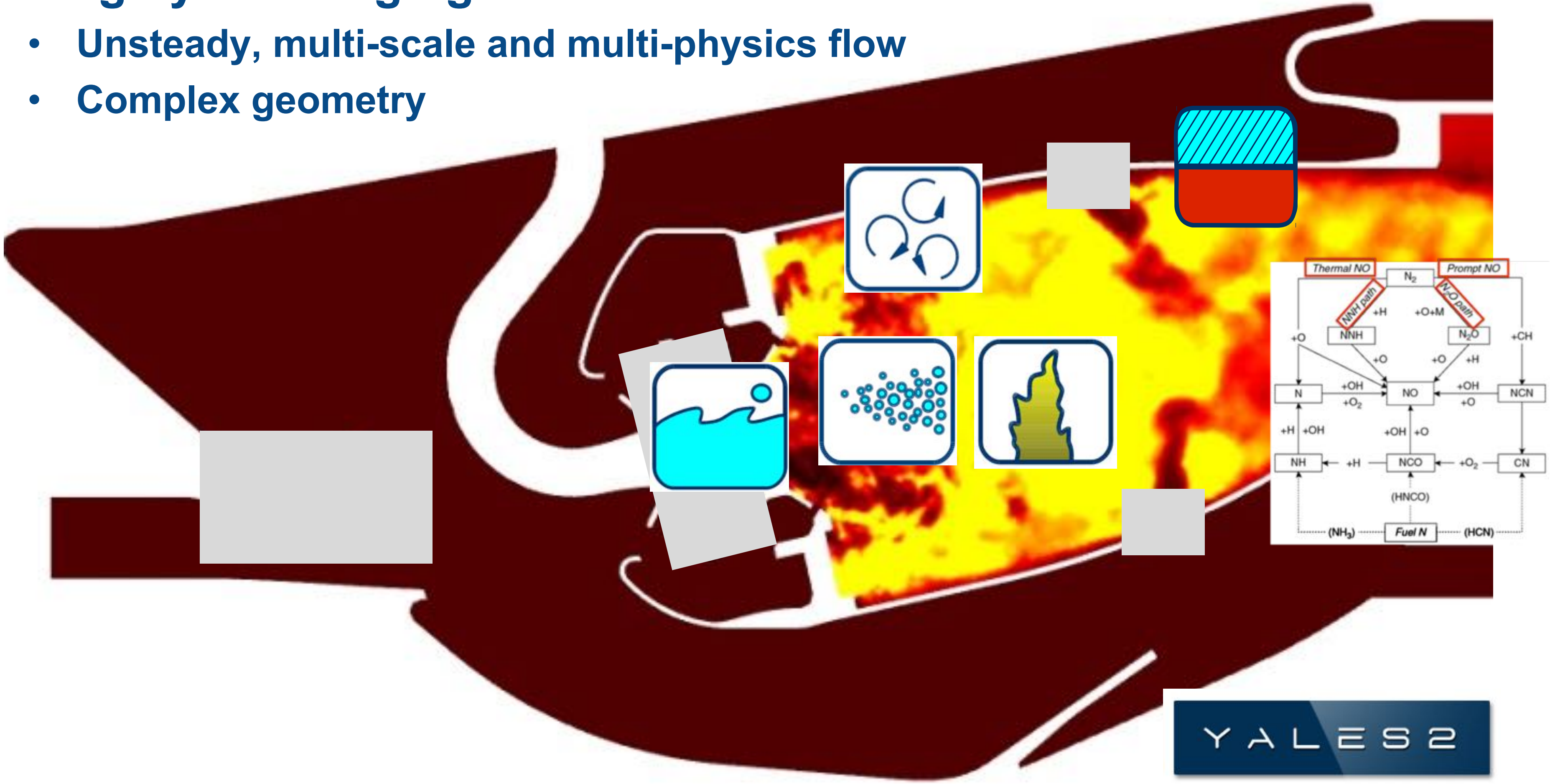
- International regulations
  - ➡ CAEP regulations
- Main pollutants
  - UHC
  - Smoke
  - Carbon Monoxide (CO)
  - Nitrogen Oxides (NOx)

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

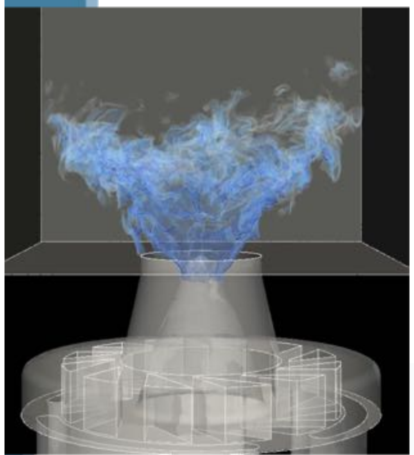


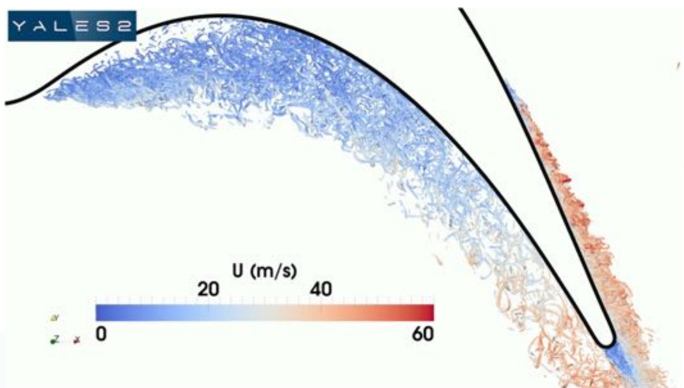
- **Unsteady approaches are mandatory to predict these phenomena**
- **Objective: develop LES models for pollutant predictions**

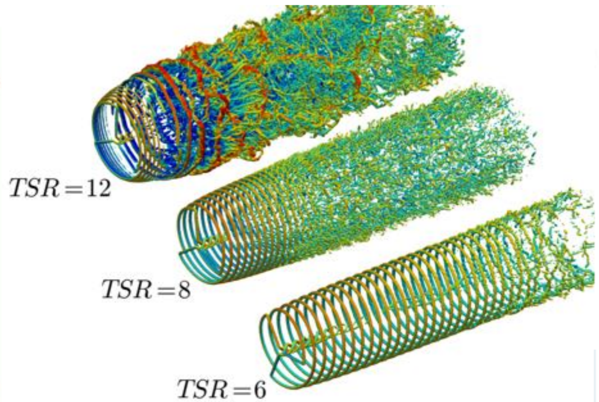
Flow solver

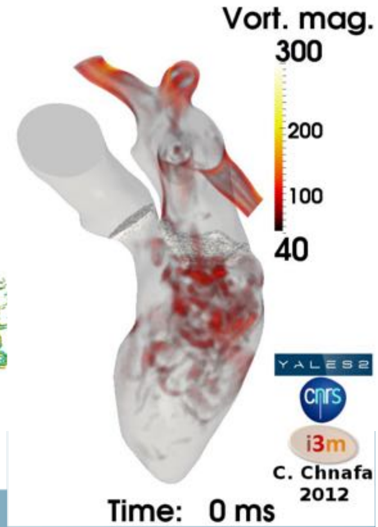
[1] YALES2 web site, http://www.coria-cfd.fr
[2] SUCCESS web site, http://success.coria-cfd.fr

- 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 and 4th-order time integration
- 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)



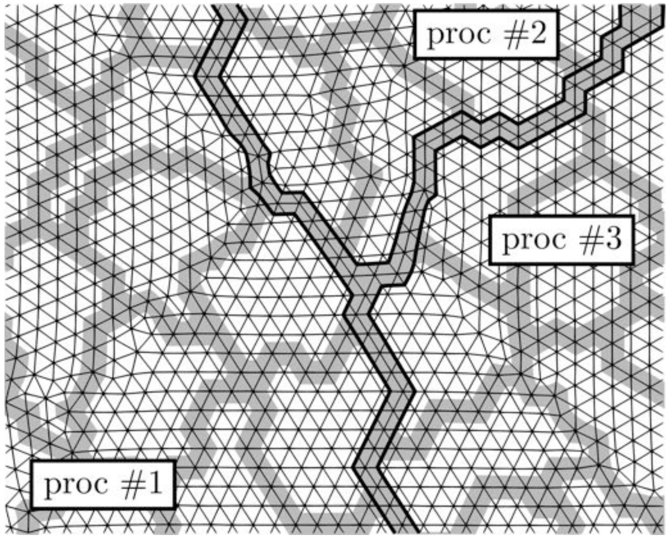




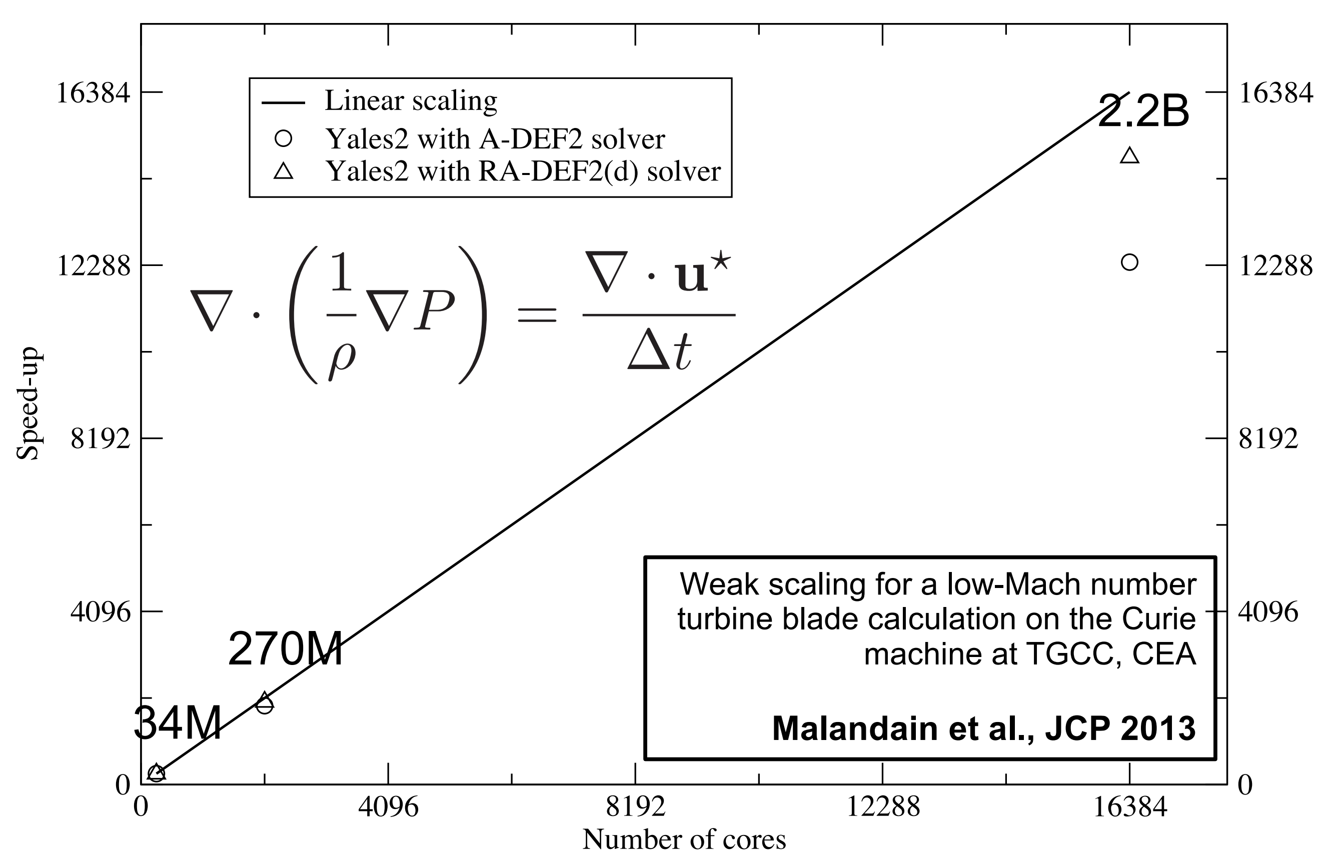


YALES2 in-core and parallel performances

- **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**



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

HPC experts

ECR lab
INTEL/CEA/GENCI/UVSQ

SMEs

GDTech
Paralgo
Linterweb

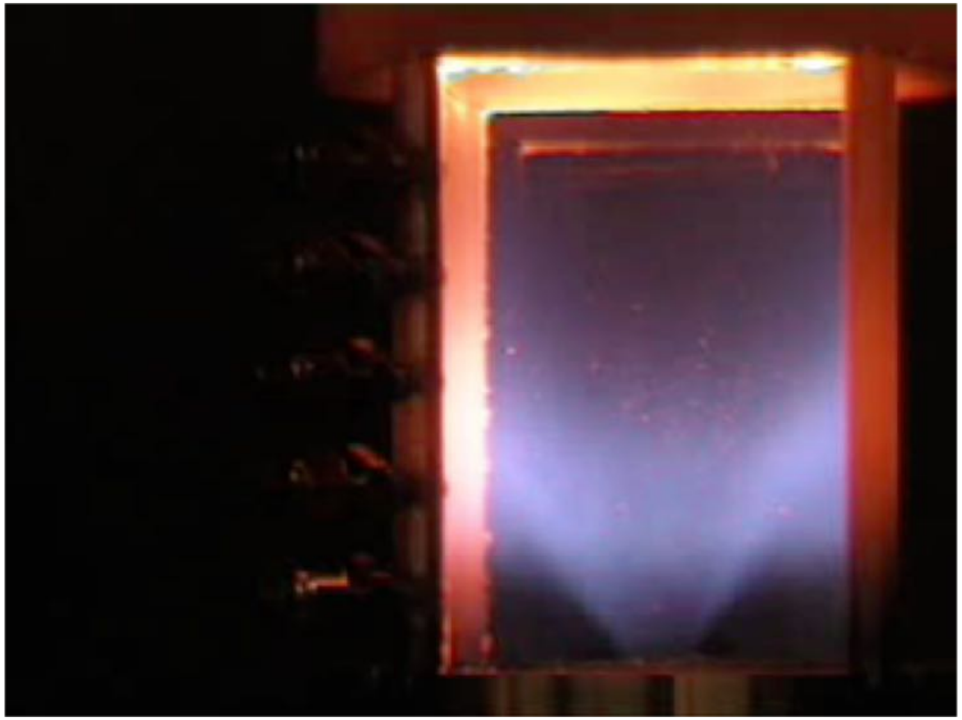
Towards lean-premixed low-NOx burners

LES of the PRECCINSTA burner with finite-rate chemistry

The PRECCINSTA burner (1/2)

- Experimental lean-premixed CH_4/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)

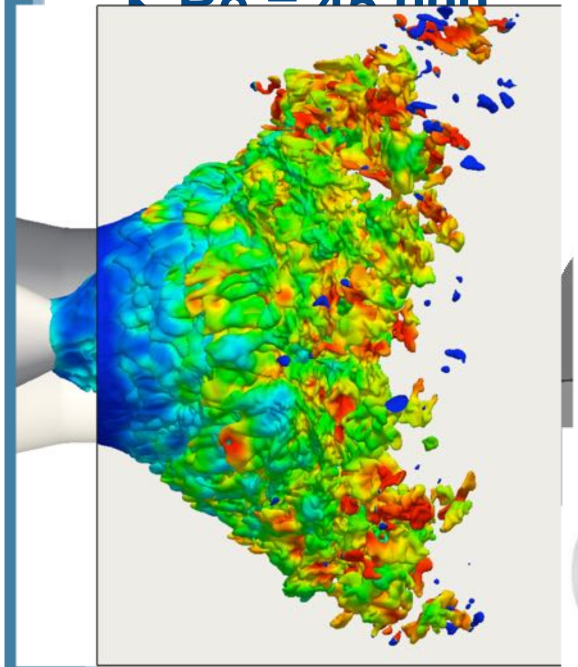
PRECCINSTA experimental burner

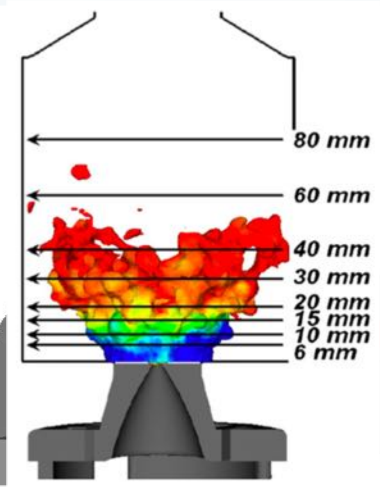


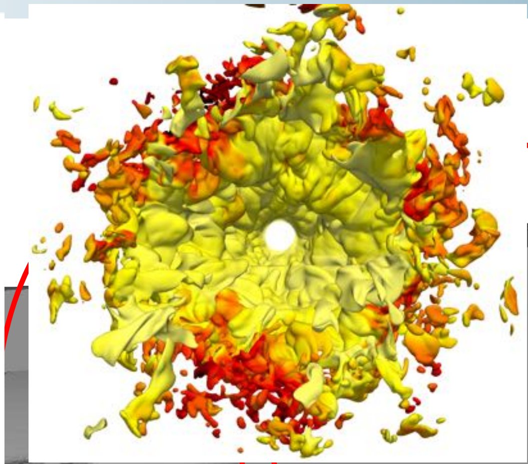
Equivalence ratio is decreasing slightly from 0.8 to 0.5

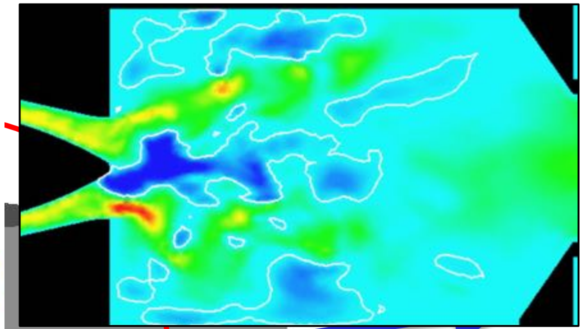
The PRECCINSTA burner (2/2)

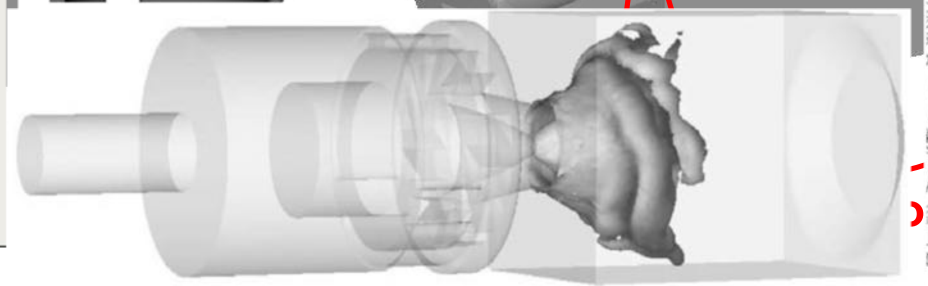
- Re = 45 000

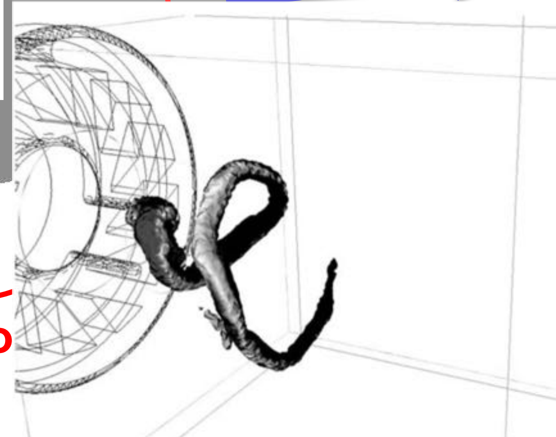




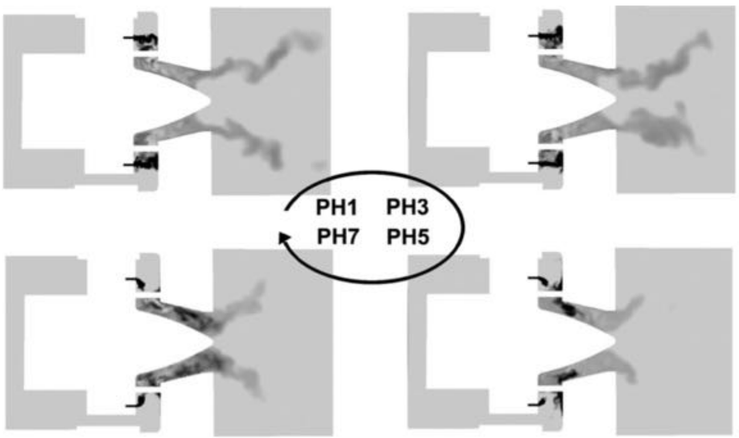


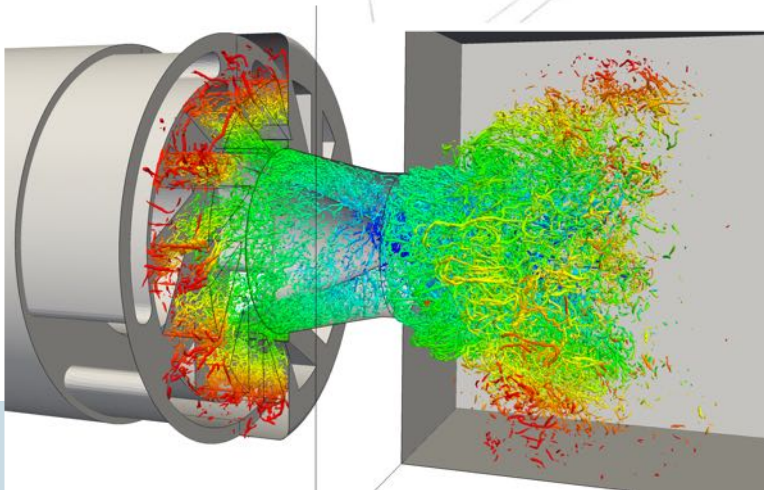






- Ma[illegible]
  - [illegible] 2011)
  - [illegible] 012)
  - [illegible] 2016)

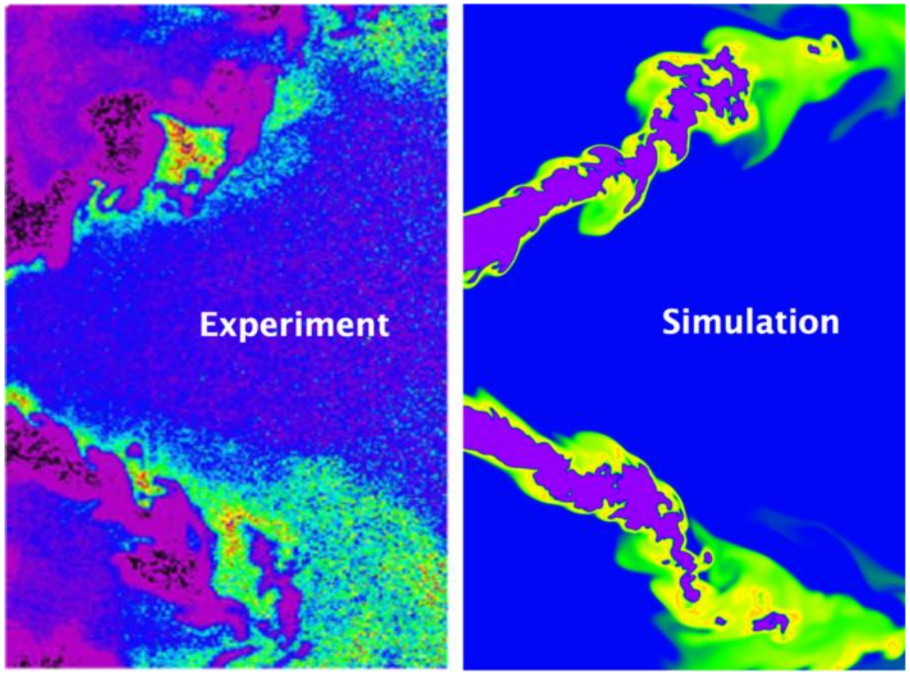




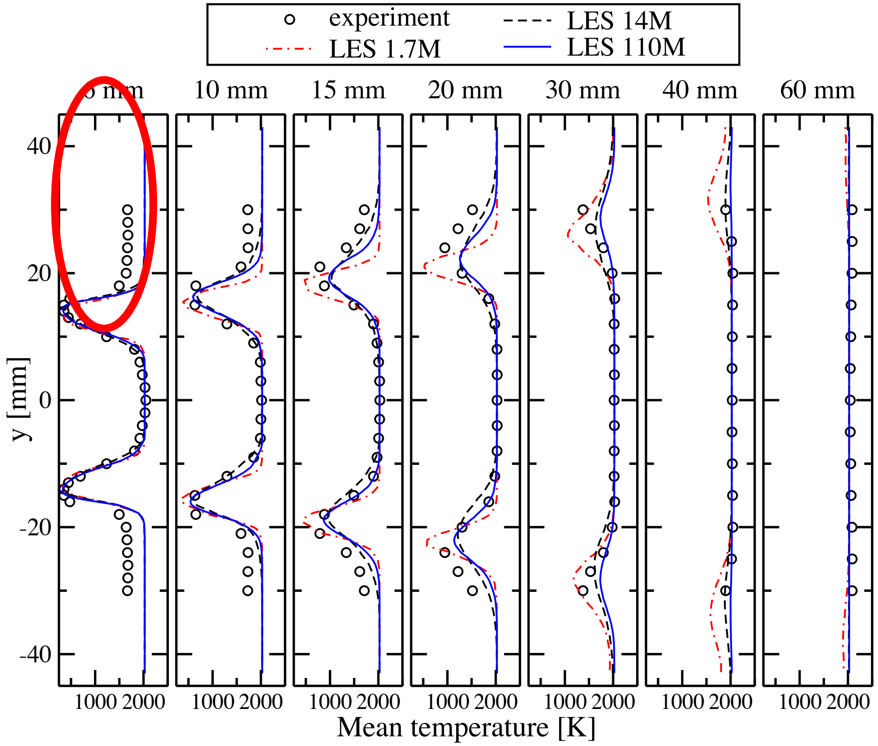
A remaining open question…

- 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

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

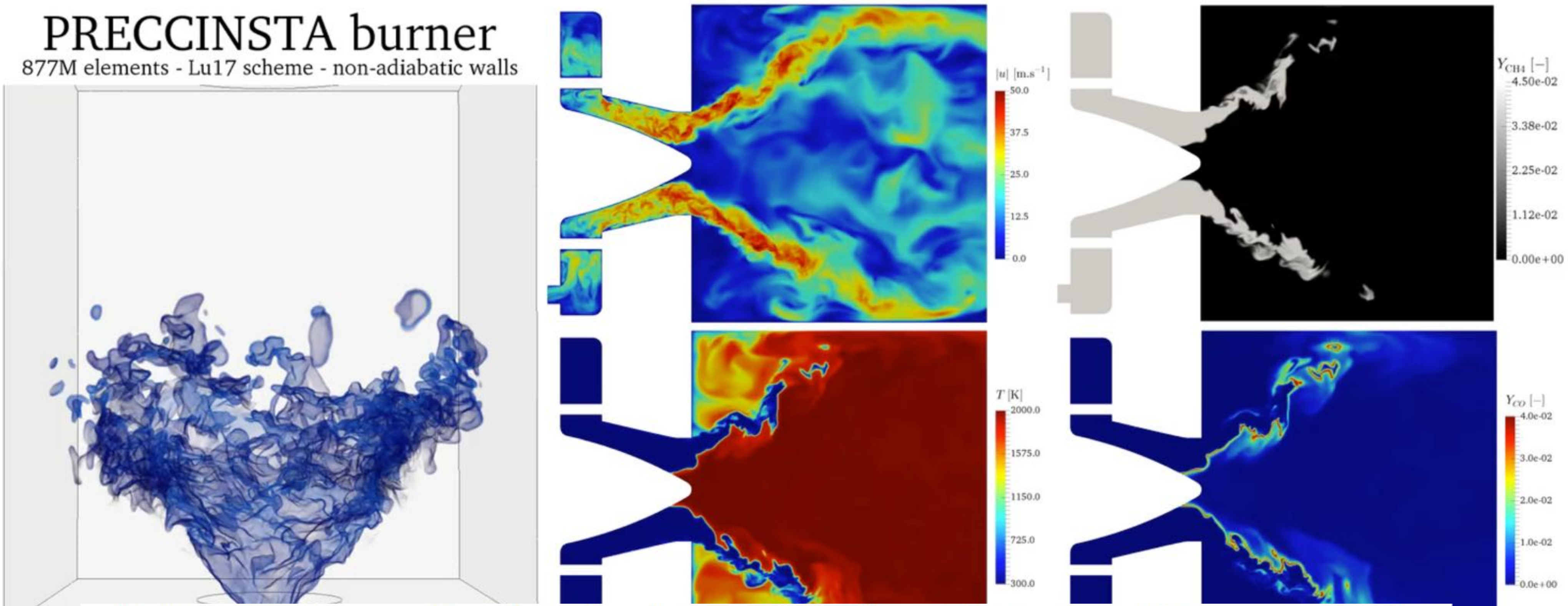
transport $10^{-6} s$ — diffusion $10^{-9} s$ — reactions $10^{-12} s$

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)

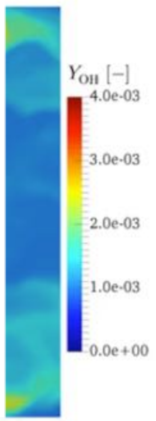
- Validated with up to 91 species and 700 reactions (kerosene/air combustion)
- Good performances up to 32’000 cores

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



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

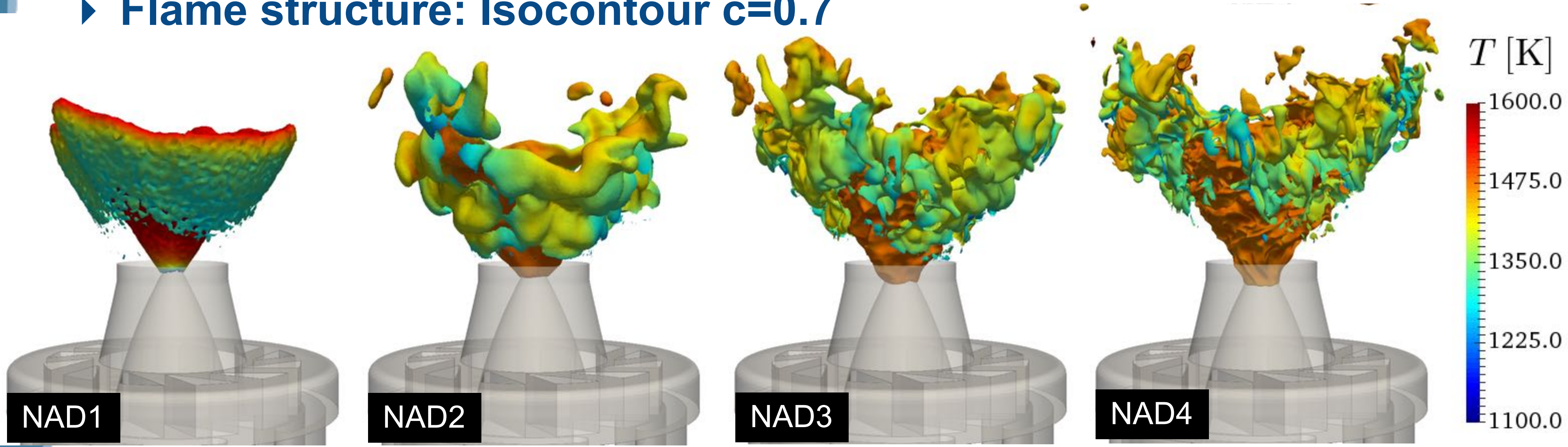
Only 17% of CPU time in species source term !



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

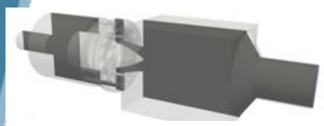
Non-adiabatic cases

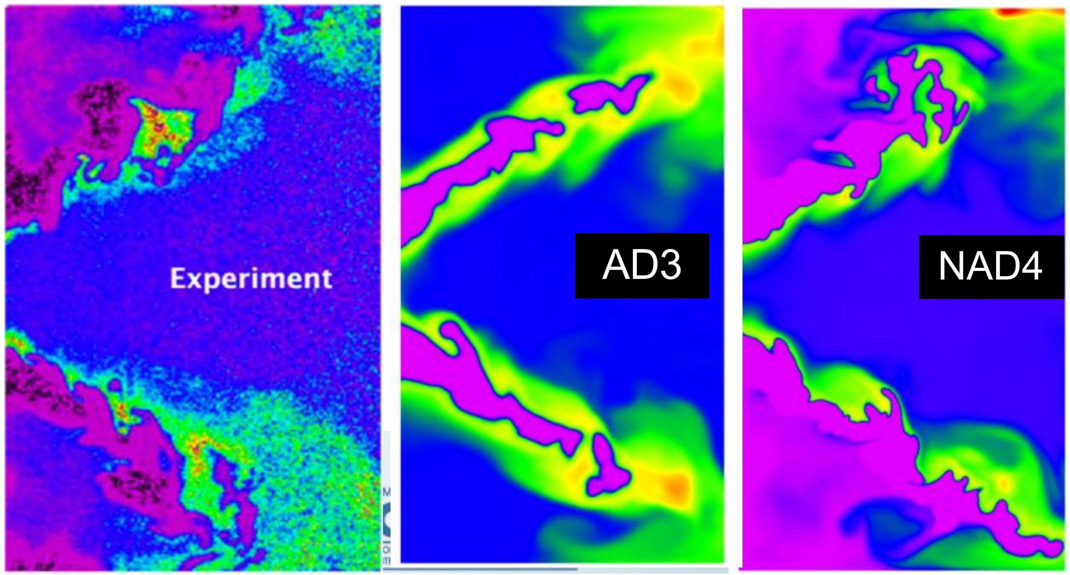
- **Flame structure: Isocontour c=0.7**



Complete extinction of external flame => V-shape flame

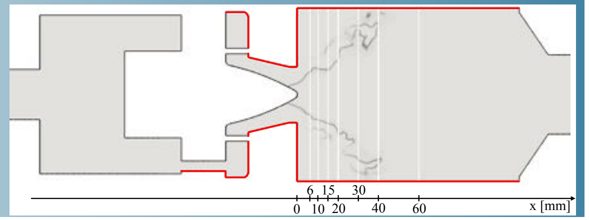
OH field

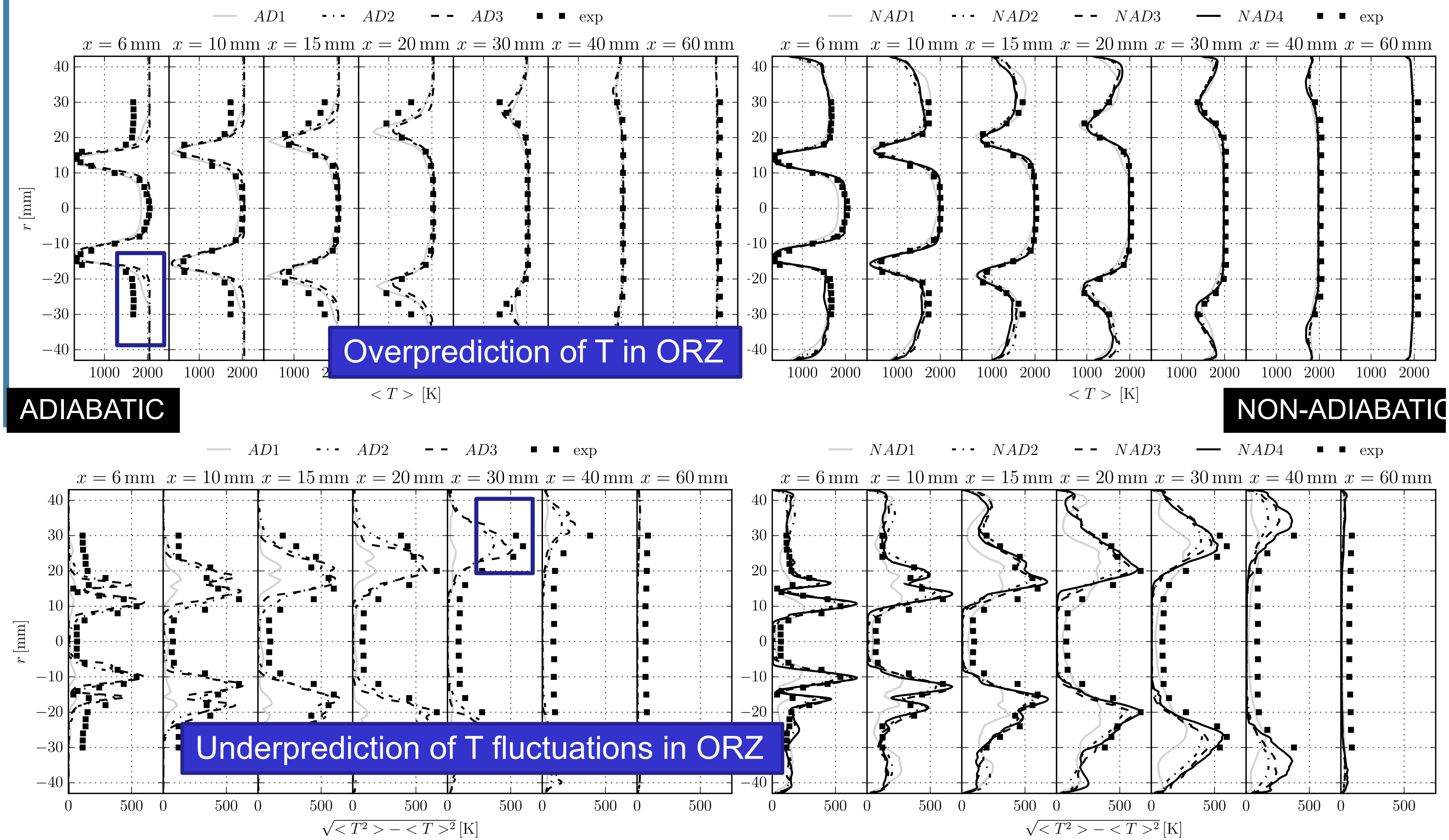




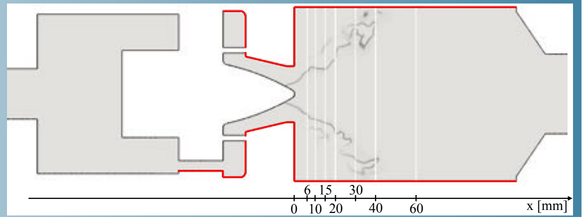
P. Bénard et al., accepted to the 2018 Int. Comb. Symp., Dublin

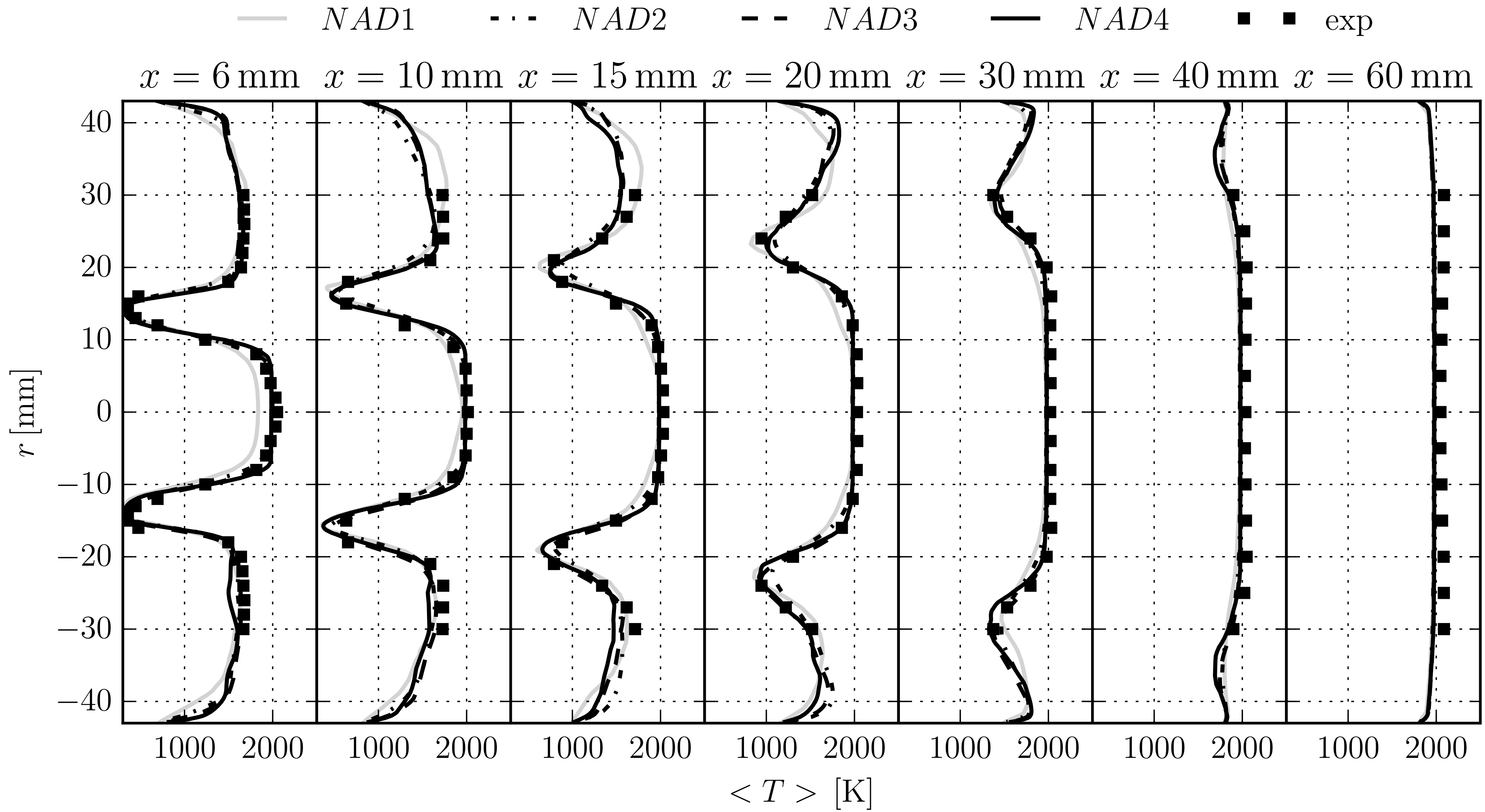
Mean and RMS temperature



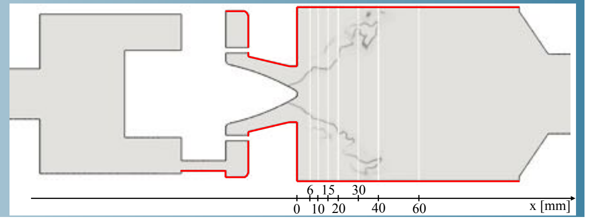


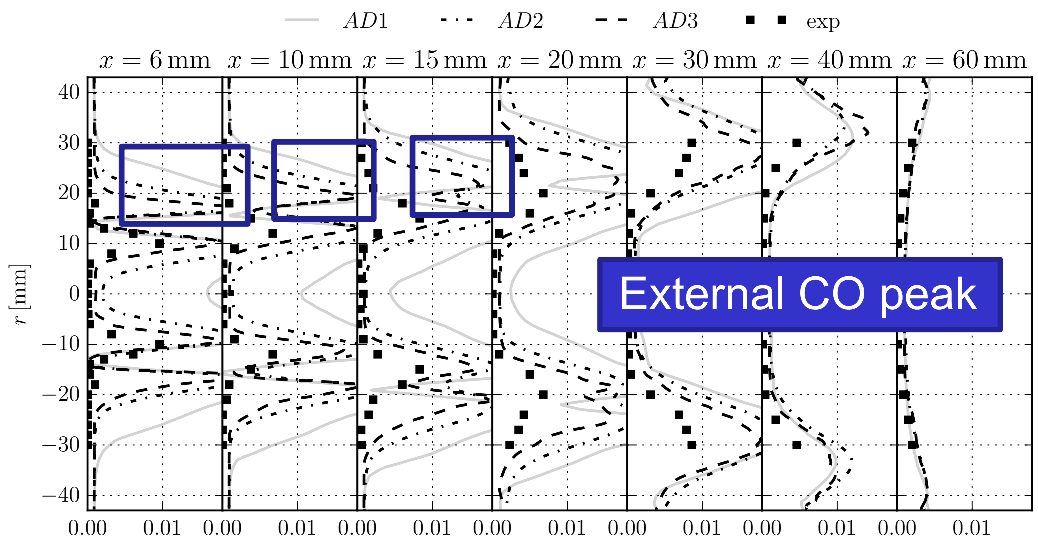
Mean and RMS temperature

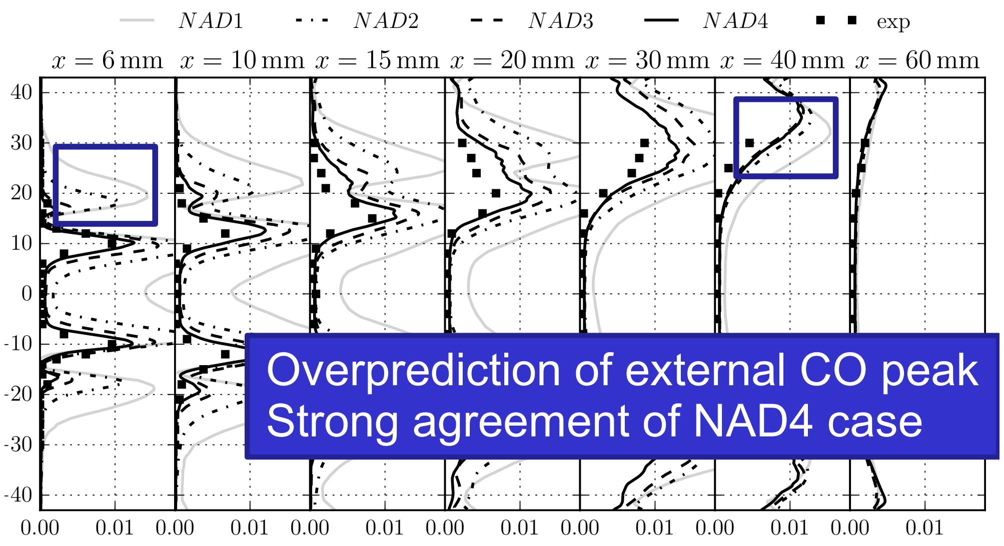




Mean and RMS CO mass fraction

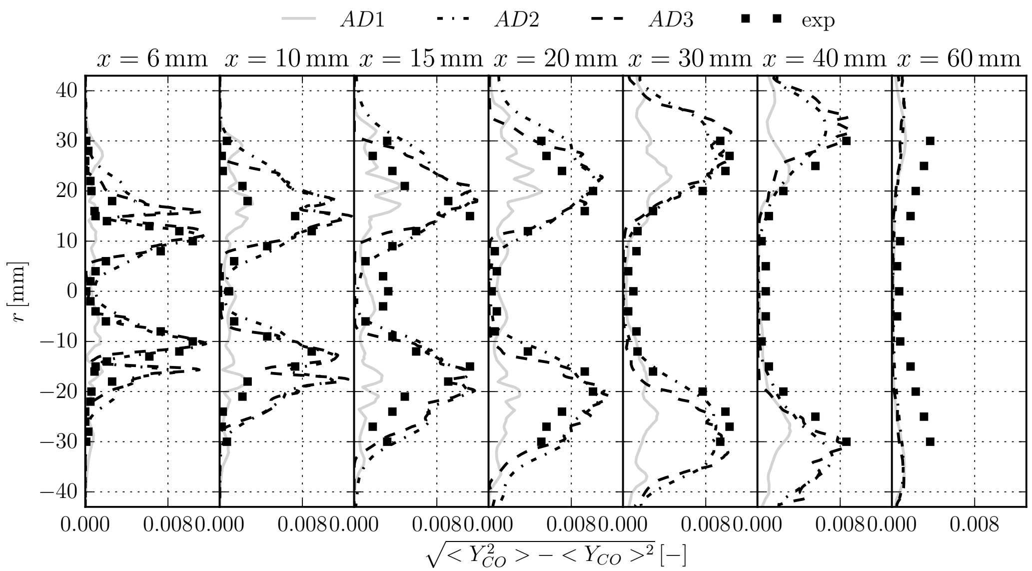


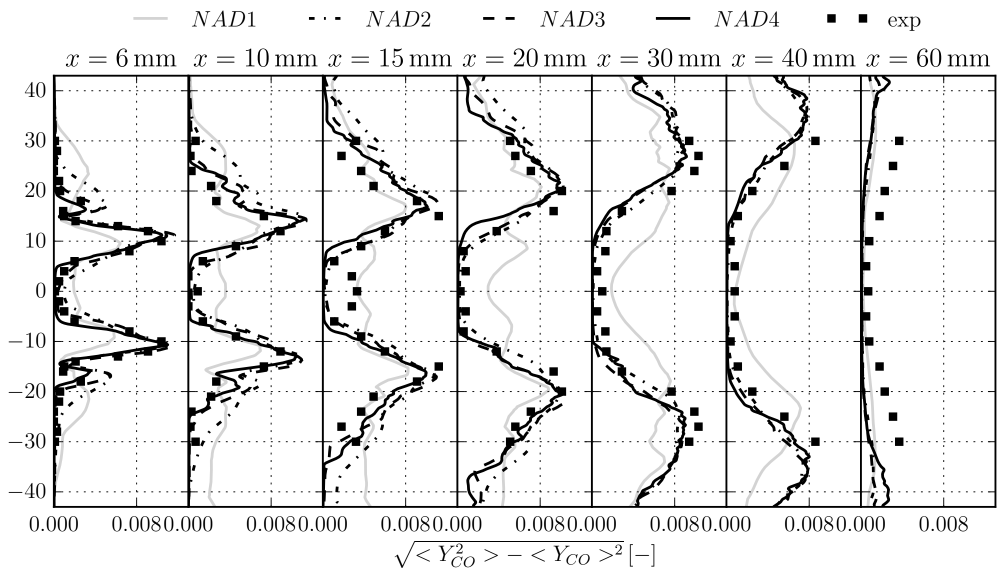




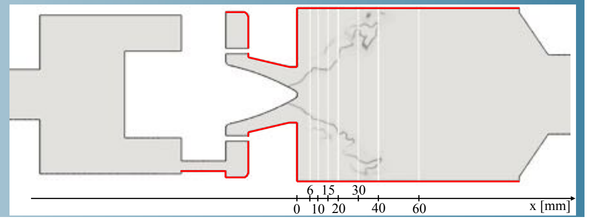
ADIABATIC

NON-ADIABATIC

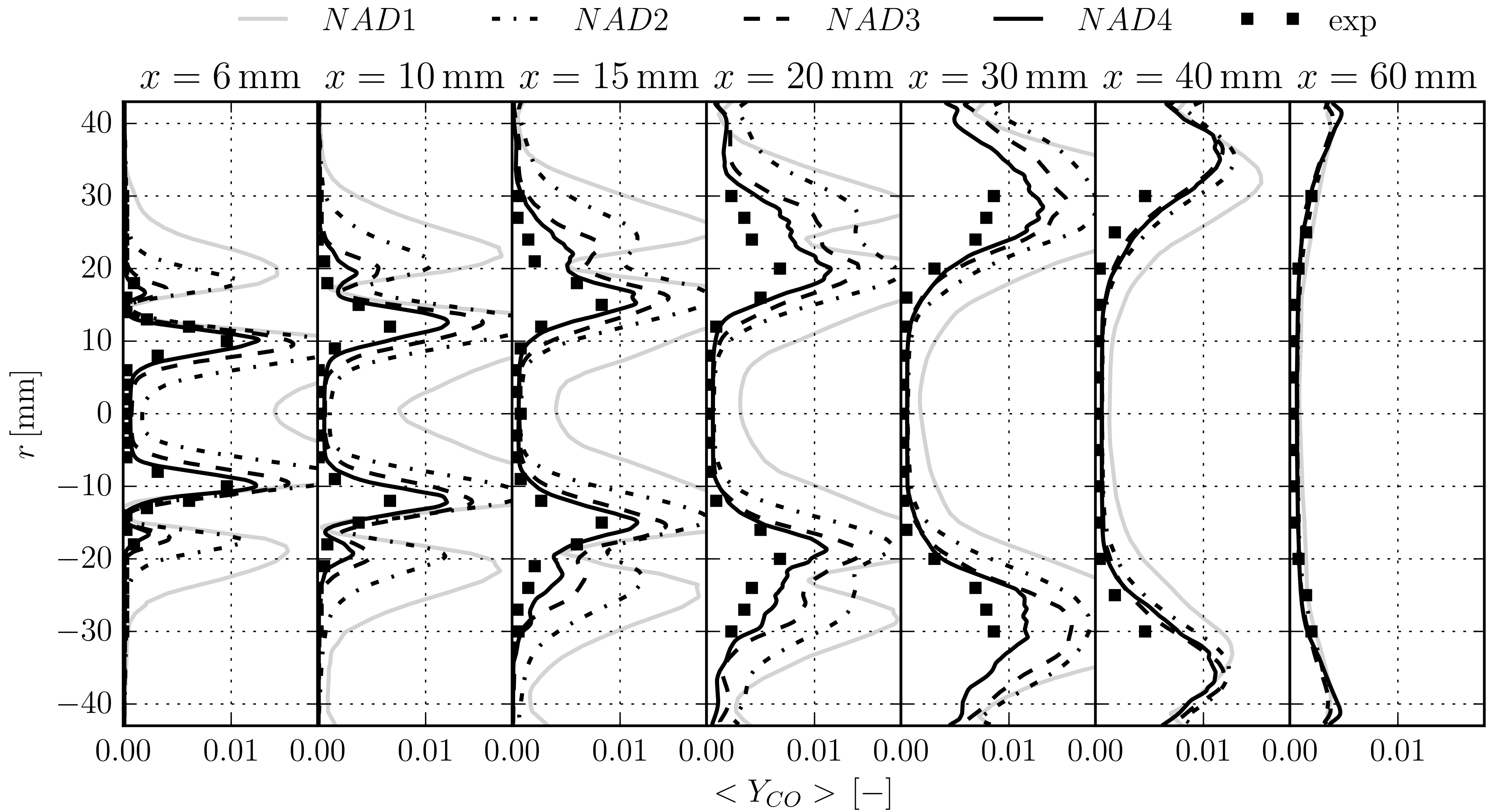




Mean and RMS CO mass fraction



- Some error on CO remain due to TFLES combustion model



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

???

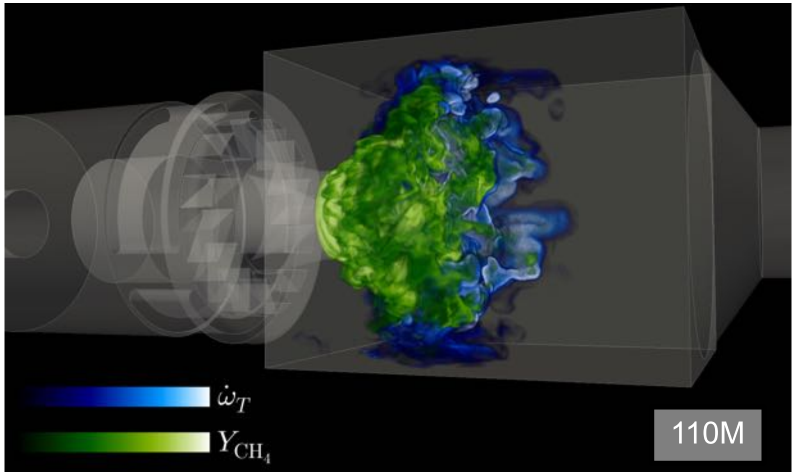
- DNS (species profile resolving)
  - 10 microns
  - 89’000B tets
  - ???

Exaflops

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

Petaflops

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

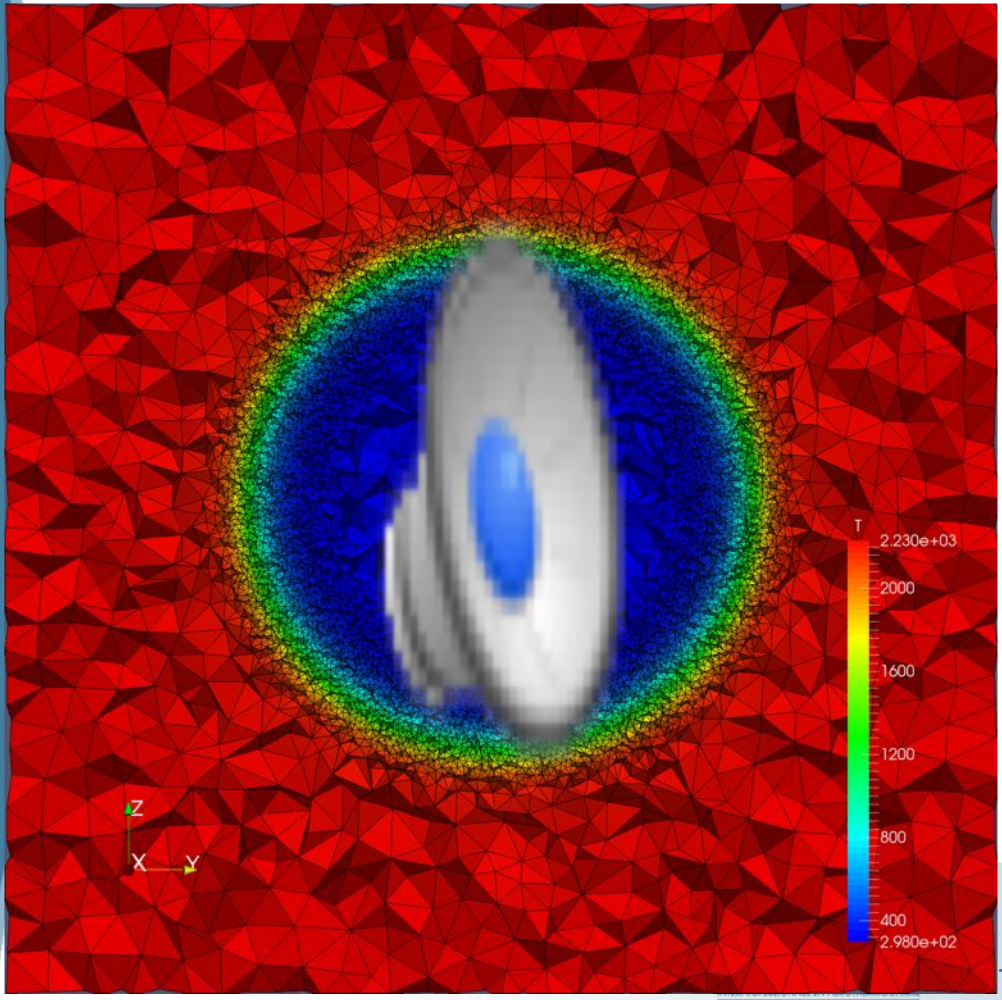


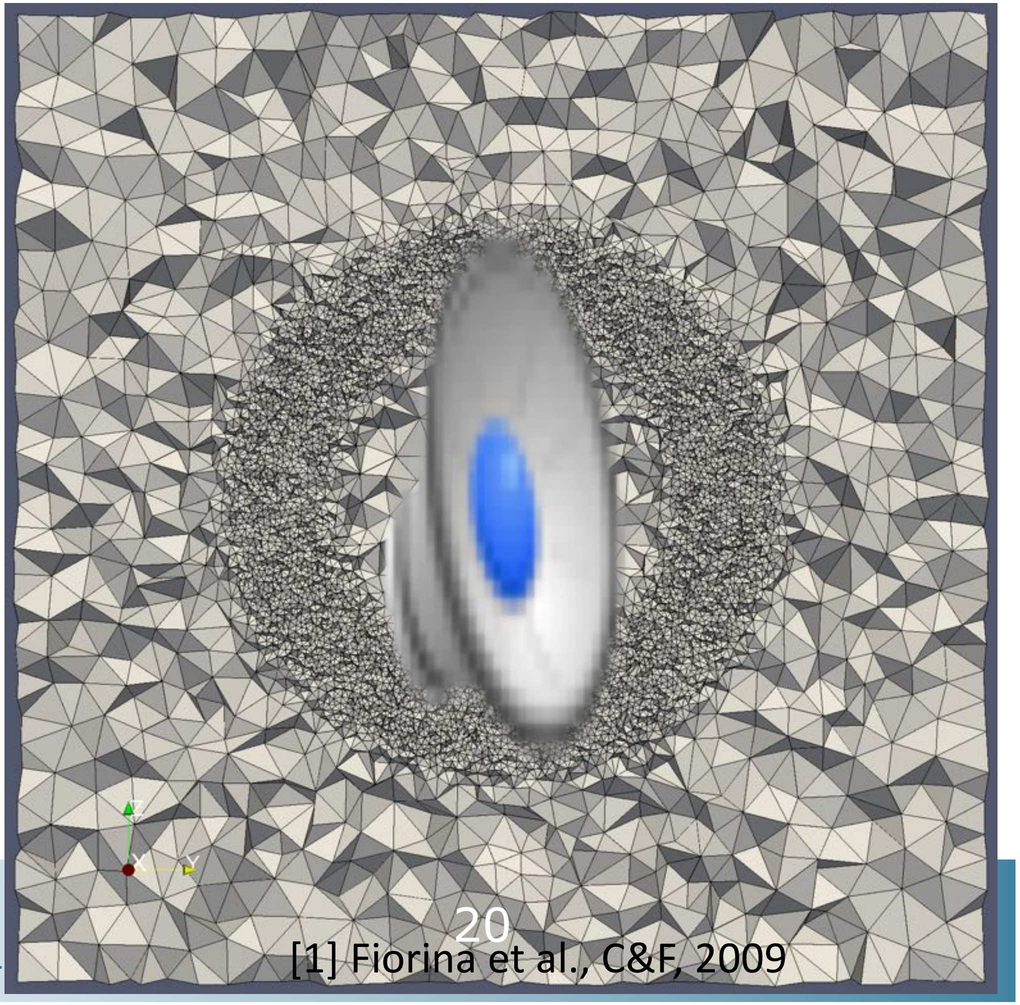
- Alternative to reach DNS faster ?

Dynamic h-adaptation of a premixed flame

- F-TACLES combustion model [1], refinement ratio = 6
- H-adaptation performed with the MMG library from INRIA
- More details in Bénard et al., IJNMF, 2015

upgrade your meshes
www.mmgtools.org

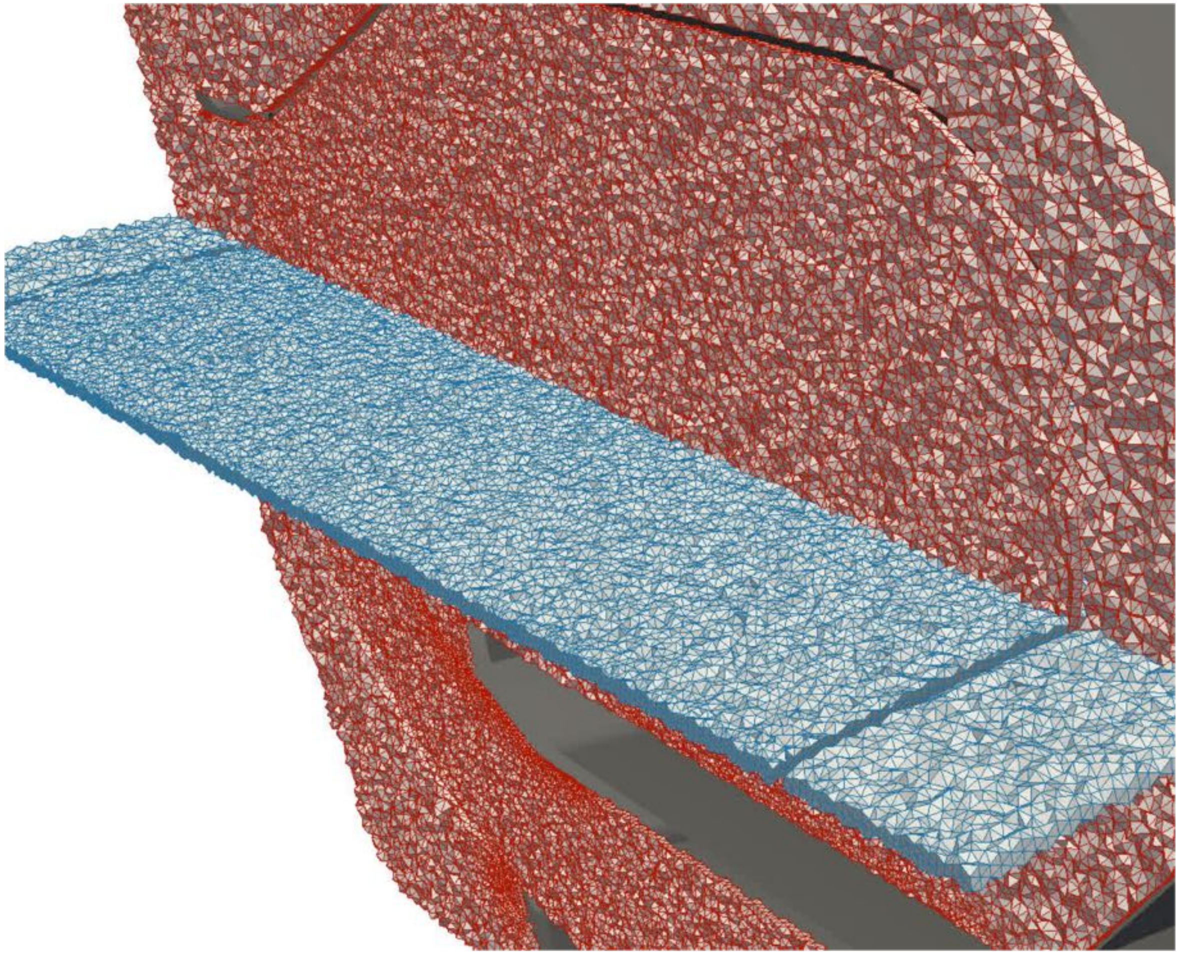




[1] Fiorina et al., C&F, 2009

Application: Ignition in a SAFRAN HE combustor

- **SAFRAN Tech simulation (R. Mercier)**
- **F-TACLES model with variable filter width**
- **Iso-temperature at 1300K colored by vorticity**
- **Parameters**
  - 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%

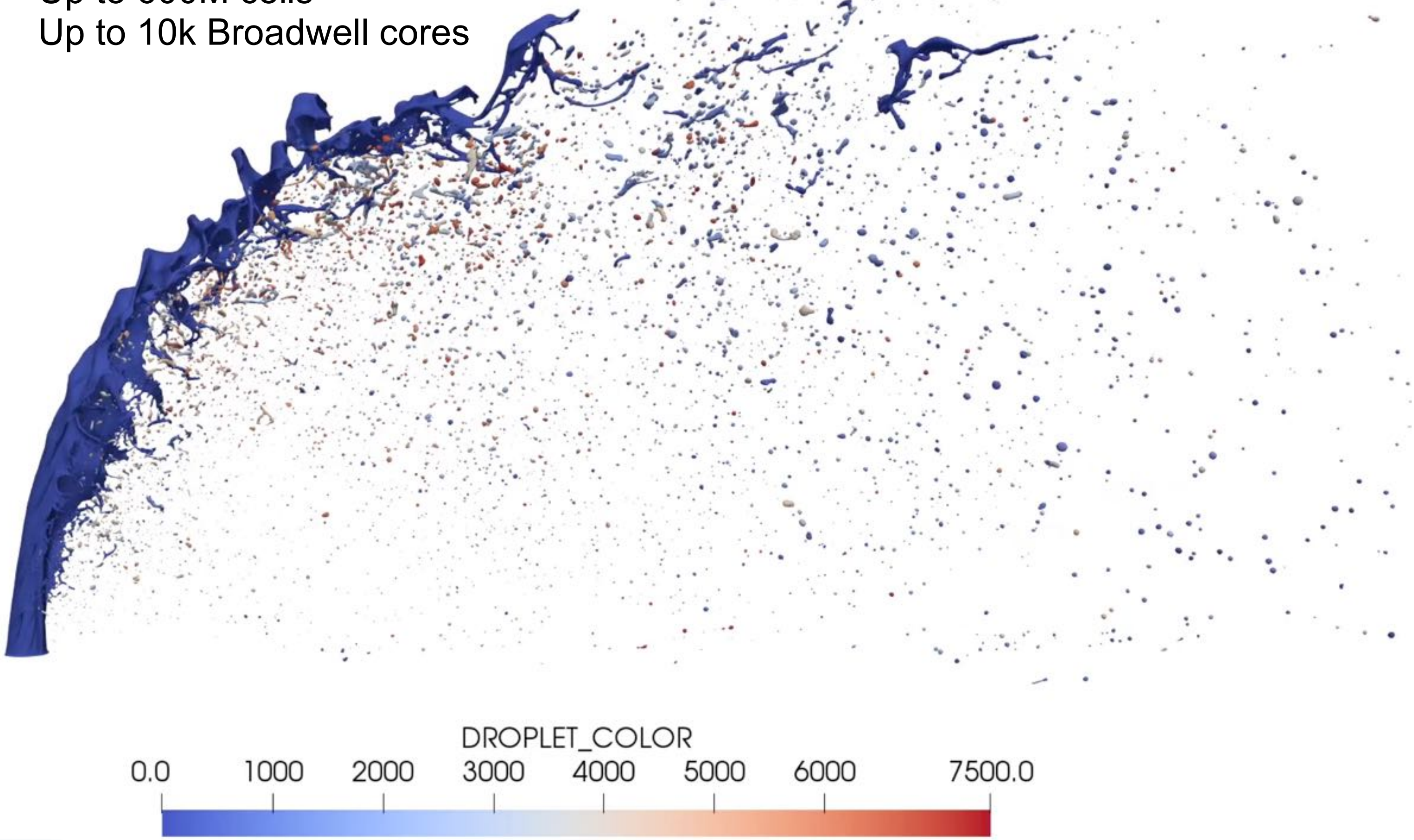


On-going simulations with periodic dynamic remeshing by G. Vaudor

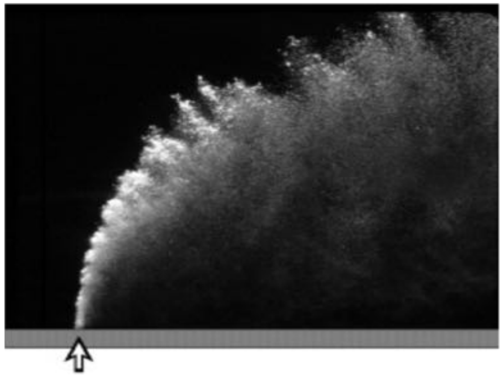
Primary atomization of a jet-in-cross-flow

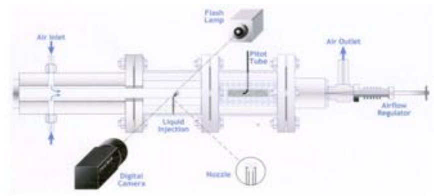
10 microns at the interface
Up to 600M cells
Up to 10k Broadwell cores

Kerosene jet in air at 10 bar



Ragucci et al. 2007
Atomization & Sprays





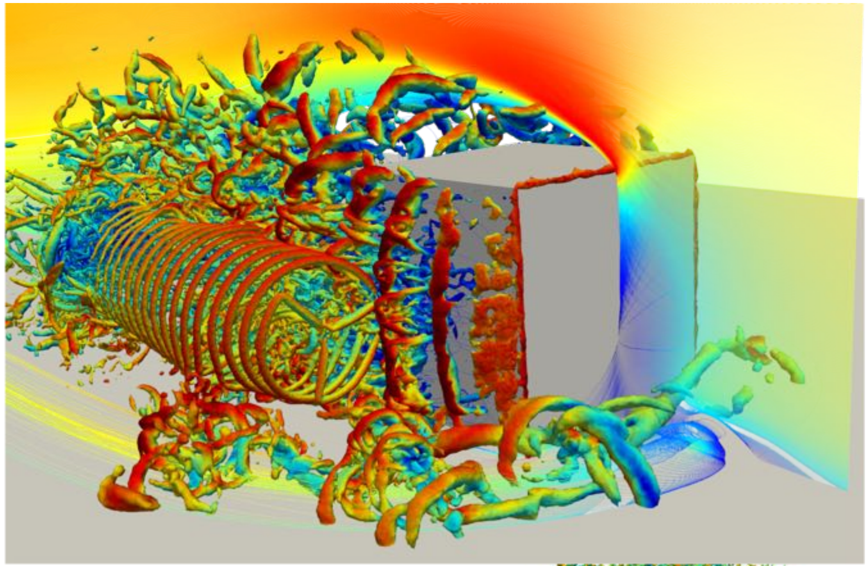
- Injector diameter: D=0.5 mm
- Flow section: 25 mm x 25 mm
- Pressure: 10 bars
- V_{air}= 37 m/s and $V_{kerosene}$= 17 m/s
- Re_{air}= 590 287 and Re_{kero}= 4477
- $We_{aero} = \rho_{air} V^2_{kéro} D/\sigma = 63.5$
- $q = \rho_{kero} V^2_{kero} / \rho_{air} V^2_{air} = 14.2$

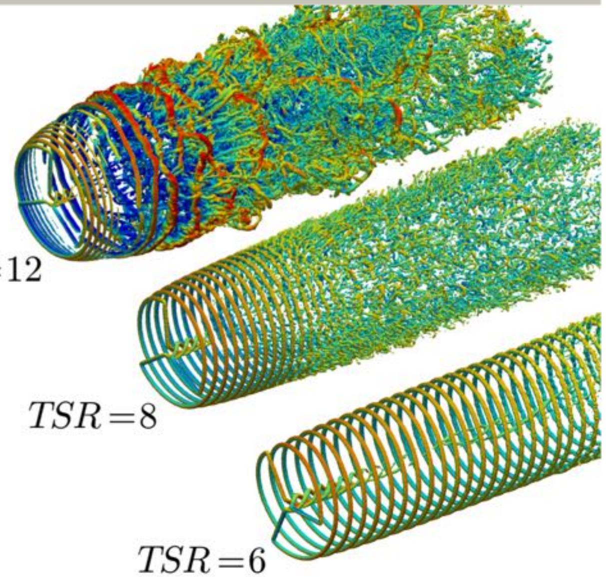
Dynamic mesh adaptation of a kerosene jet in cross flow. J. Leparoux, H. Musaefendic, R. Mercier, V. Moureau, accepted to ICLASS 2018, Chicago.

Application to wind turbines

- **Modeling of wind turbine wakes is important to evaluate wind farm effects on the rotor loading**
  - **Becomes critical when reaching 10MW and 200m diameter rotors**

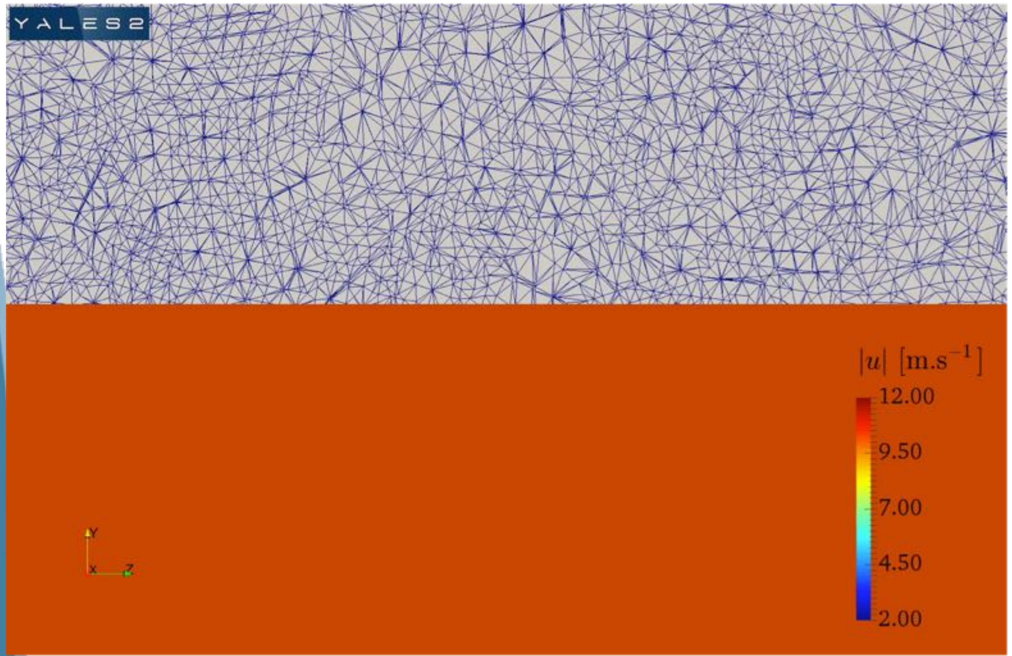
- **LES-actuator line framework**
  - **Based on unstructured grids**
  - **Takes into account any geometric detail**
  - **Bénard et al., Comp. Fluids, 2018**

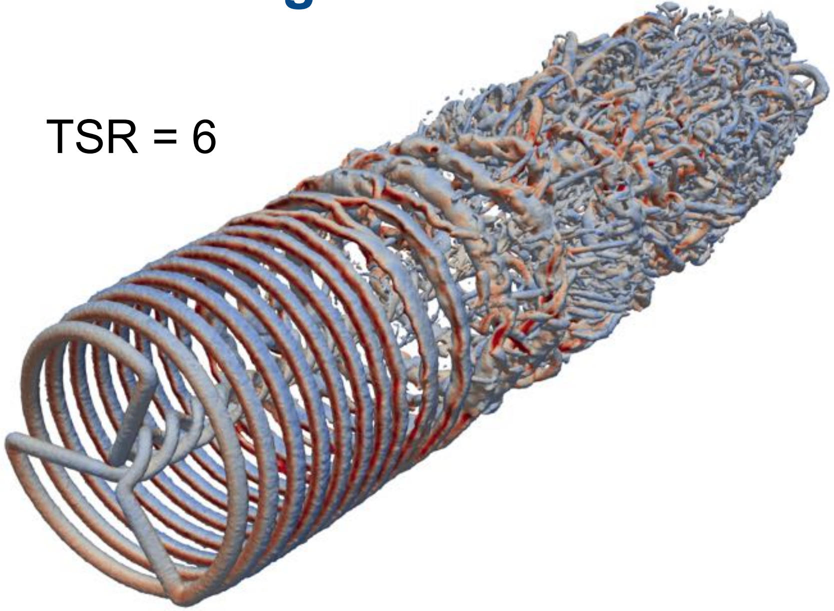




Application to wind turbines

- H-adaptation refinement criterion based on local vorticity
- Enables to reach unprecedented precision for a given cell count

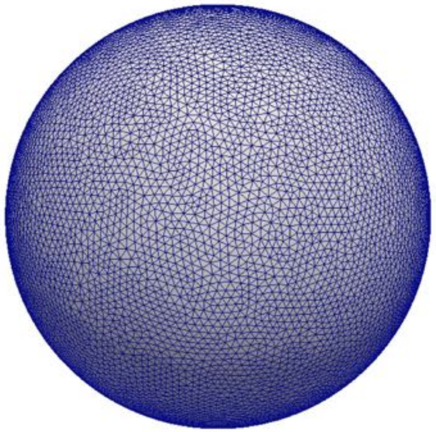


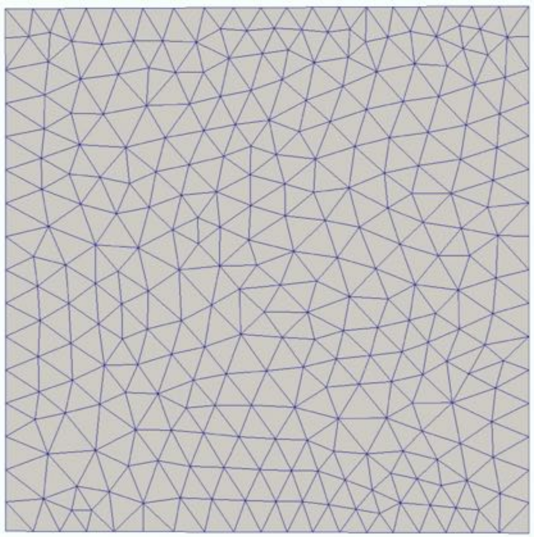


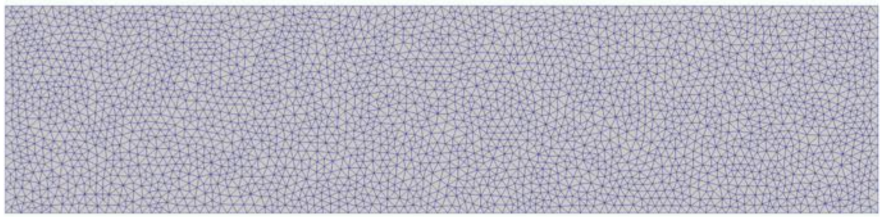
Ultimately: application to wind turbine interactions

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 developments are still required to be widely applied**
  - 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