YALES2

A massively parallel solver for multi-physics fluid dynamics

From primary atomization to pollutant prediction in complex geometries

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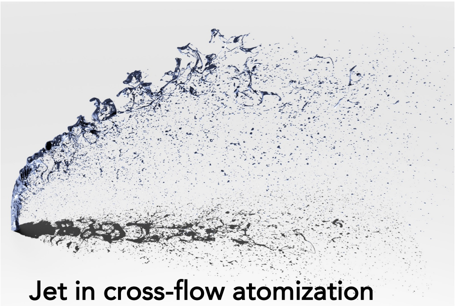
http://www.coria-cfd.fr

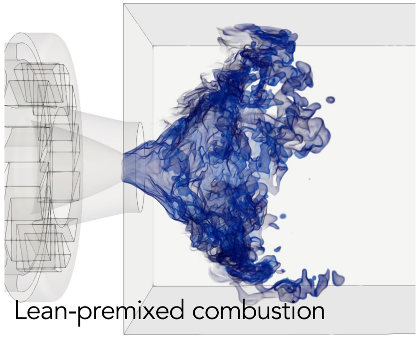
High-fidelity and multi-physics CFD

- A wide range of scientific and application domains

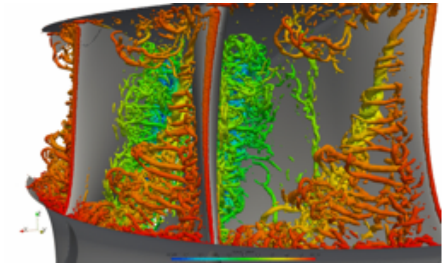
Two-phase flow modeling

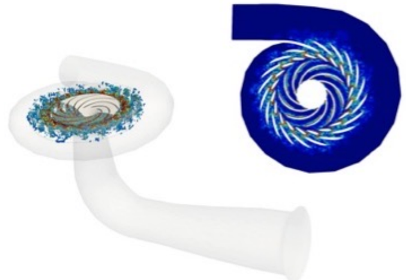


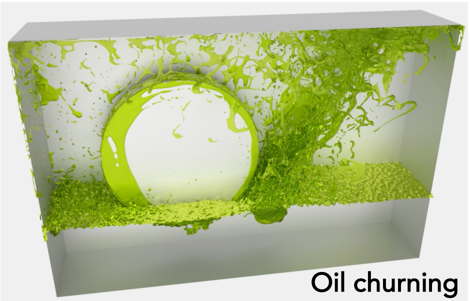
Gaseous combustion

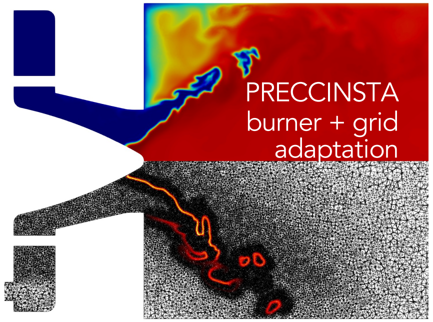


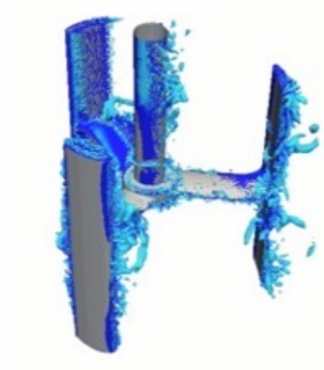
Renewable energies

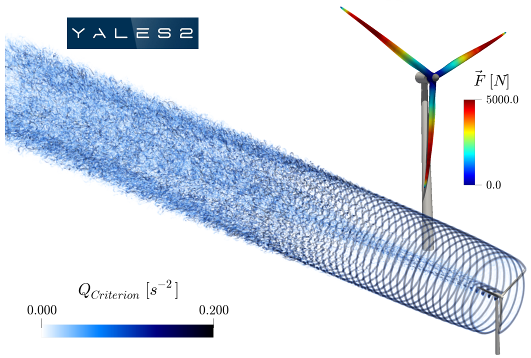




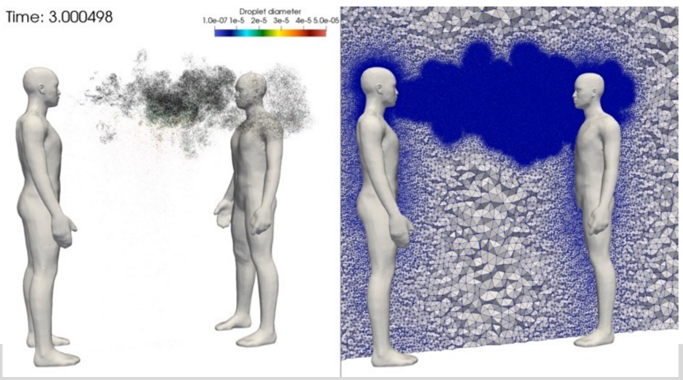




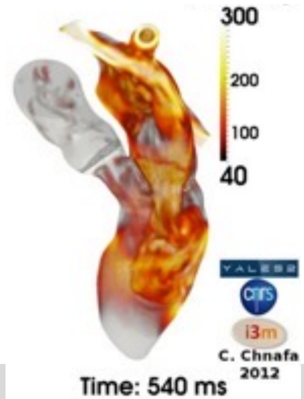




Aerosol dispersion

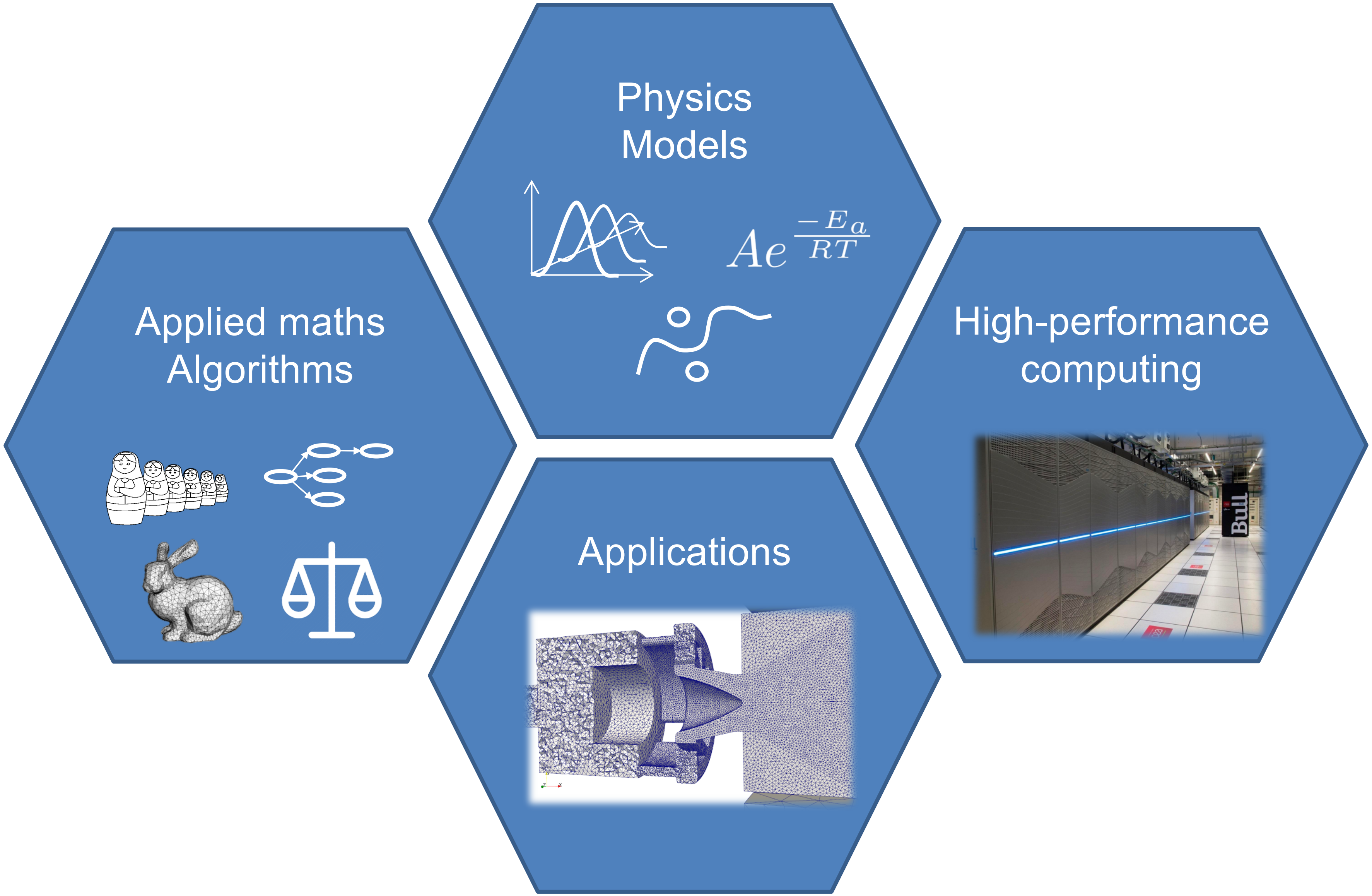


Bio-mechanics



The challenge

- High-fidelity and multi-physics CFD is a multi-disciplinary science



The YALES2 network

- Developed by CORIA, the French Combustion Community and others
  - 350+ researchers/engineers trained at CORIA since 2009
  - 150+ articles (Google Scholar)
- A unique network to ease collaboration and disseminate numerics, algorithms and models to the community

Academic partners

SUCCESS scientific group [1]
CORIA, IMAG, LEGI, EM2C
IMFT, CERFACS, IFP-EN, LMA

ULB, UMONS, UCL, LOMC,
PPRIME, LMB/INRIA,
CORNELL U., SHERBROOK U.
VERMONT U.

HPC experts

ECR lab
INTEL/CEA/GENCI/UVSQ
IBM/ROMEO

HPC centers

CRIANN, IDRIS, CINES, TGCC
GENCI, PRACE

YALES2

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Industrial partners

SAFRAN
ARIANE GROUP
SOLVAY
SIEMENS/GAMESA
AIR LIQUIDE
…

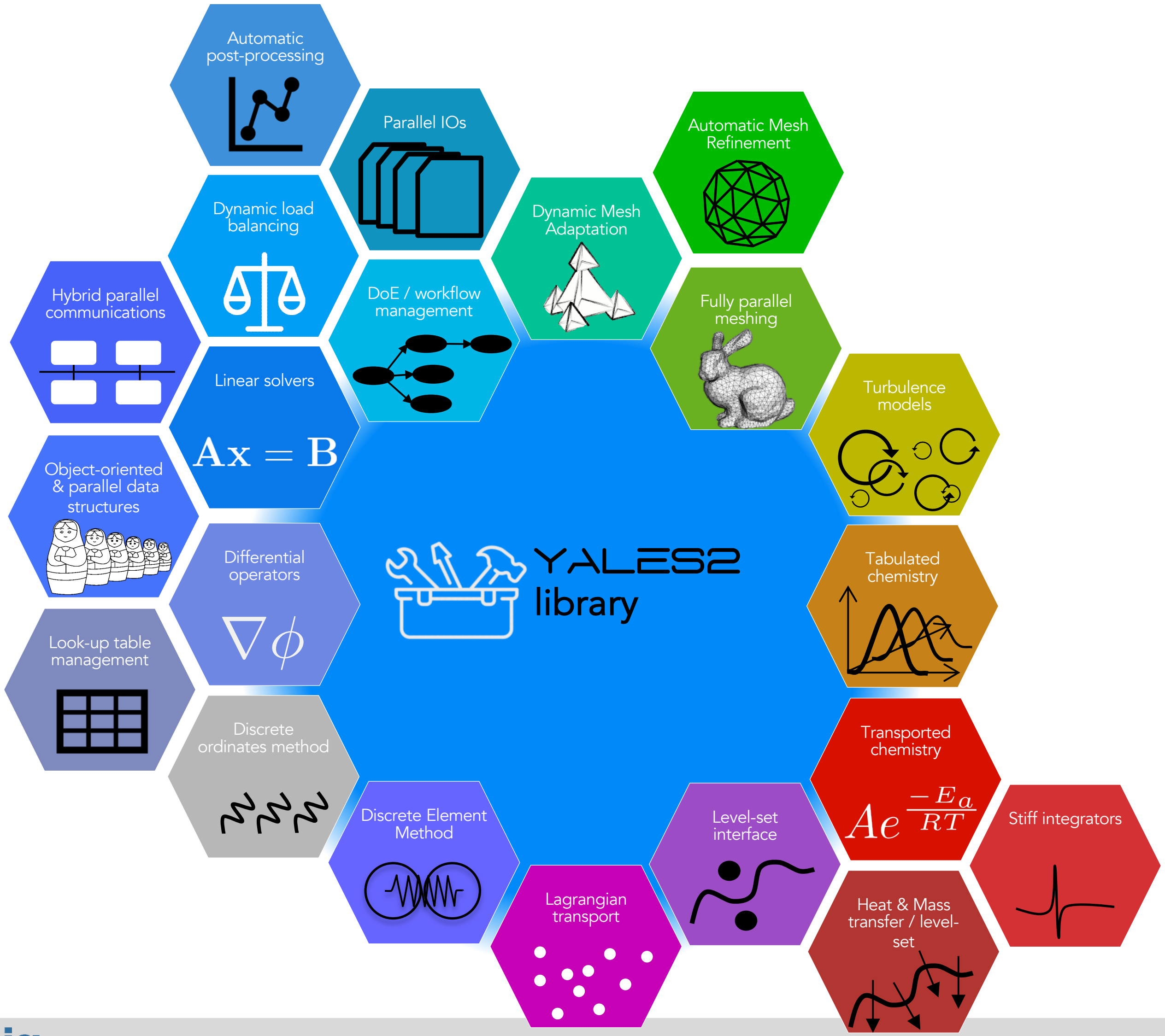
SMEs

GDTech

[1] http://success.coria-cfd.fr

The CFD platform: YALES2

- The numerical library YALES2LIB consists of all the numerical methods required to develop solvers



YALES2 solvers

ICS Incompressible at constant density

VDS Incompressible at variable density

SPS Spray with level-set and ghost-fluid method

ALE Arbitrary Lagrangian Eulerian

GFS Granular flow with Discrete Element Method

HTS Heat transfer

MHD Magneto-hydro-dyn

SMS+FSI Structural mech.

ACS Acoustics

BOI Boiling

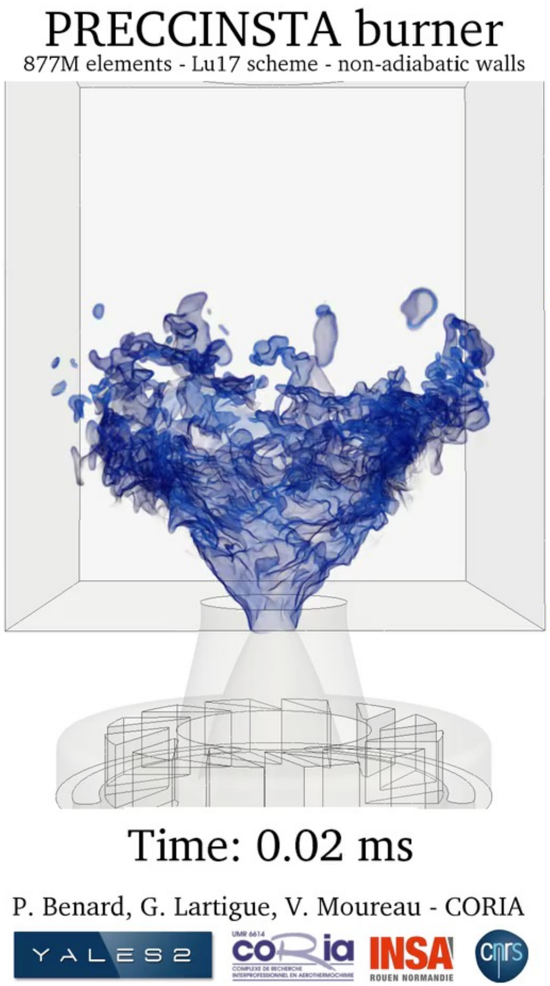
CPS Compressible flow ($Ma>1$)

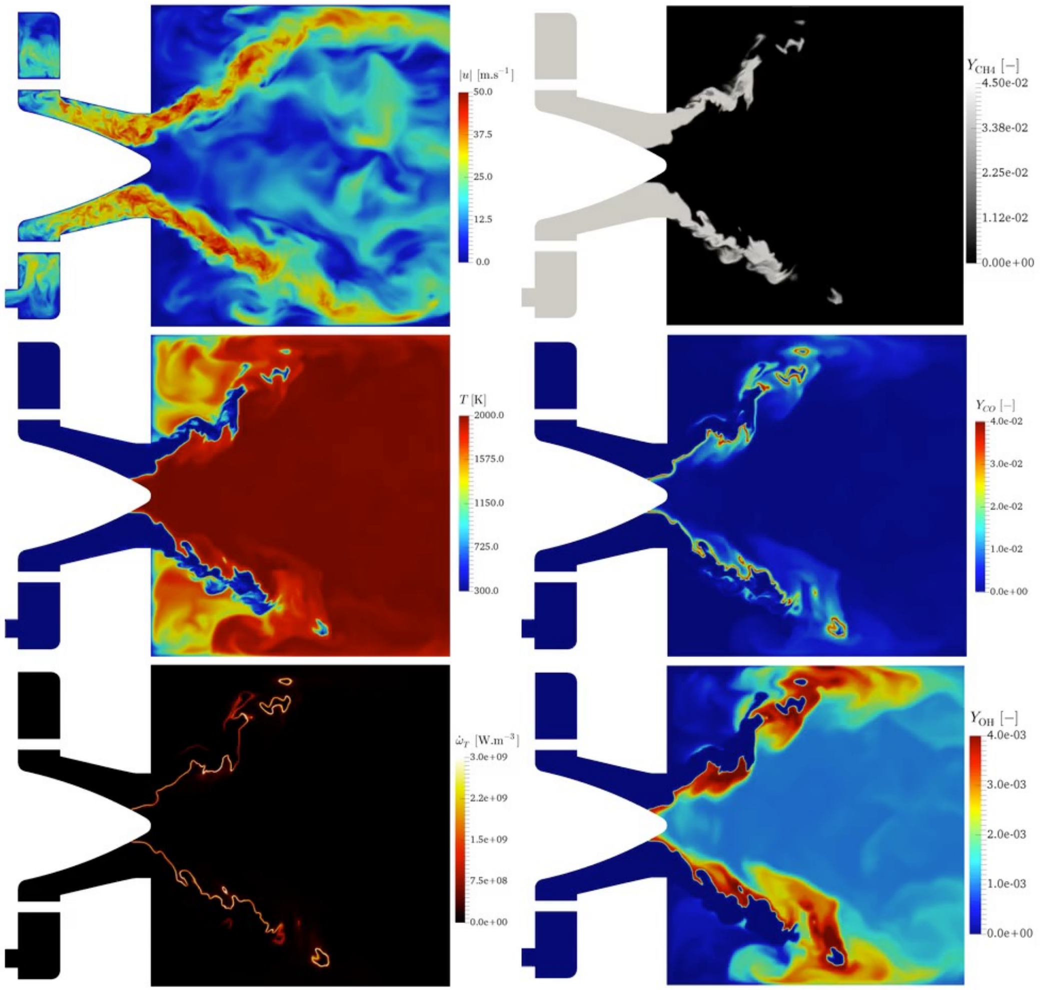
YALES2 features

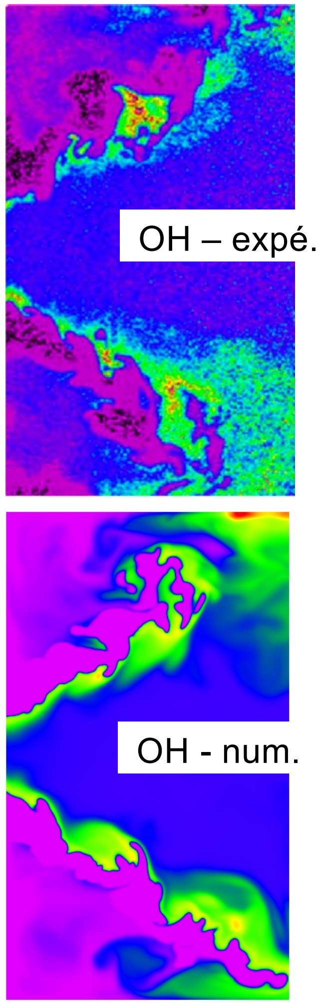
- High fidelity
- Multiphysics
- High performance

Frontier finite-rate chemistry LES of PRECCINSTA burner

- LES with Sankaran scheme (17 species, 73 reactions) and heat loss [1]
- 878 millions cells, 150 microns in the flame region
- CPU hours from CRIANN and FIRELES PRACE project, 16384 cores on Curie, CEA



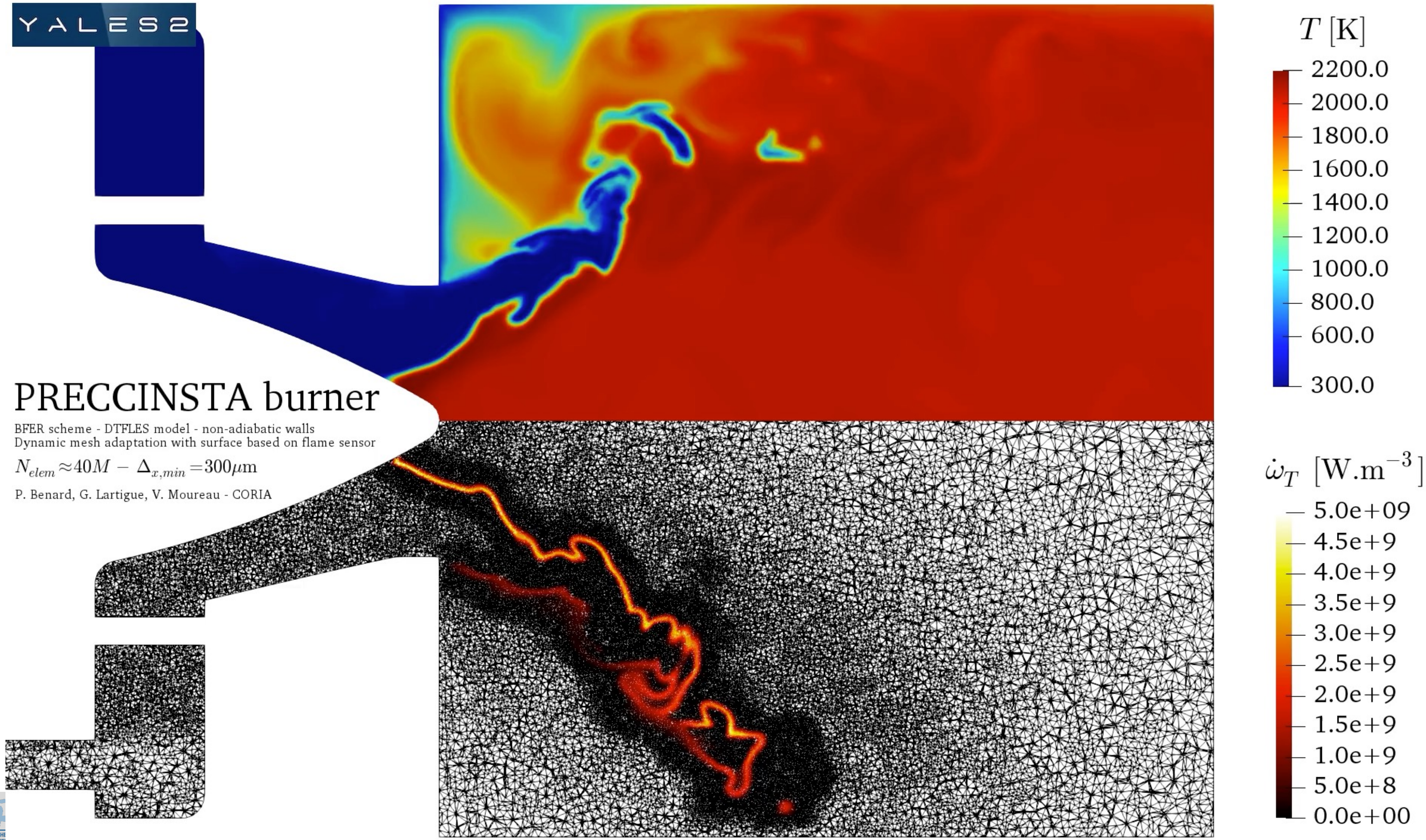




[1] P. Bénard et al. (2018) Int. Comb. Symp., Dublin

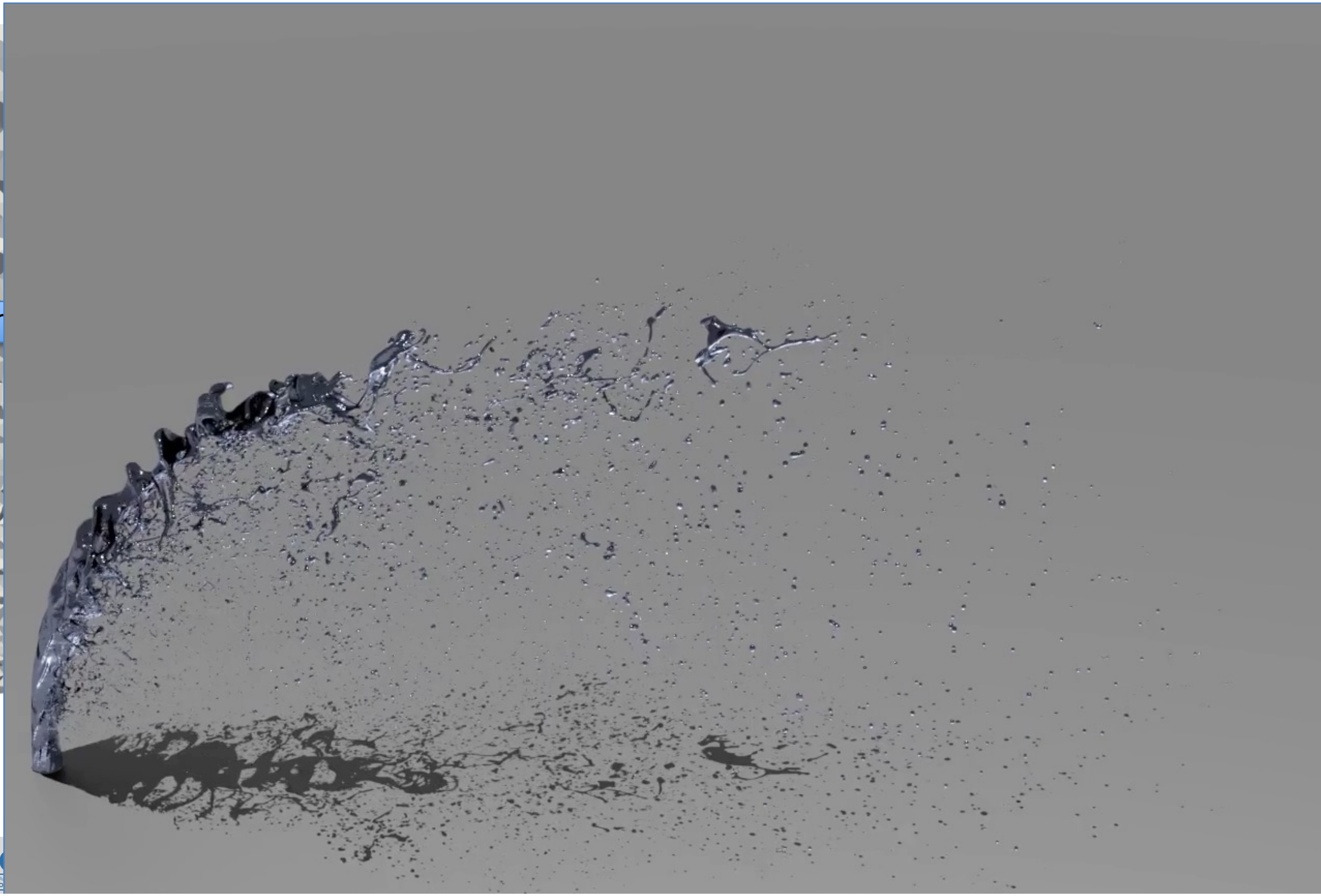
Application to the PRECCINSTA burner

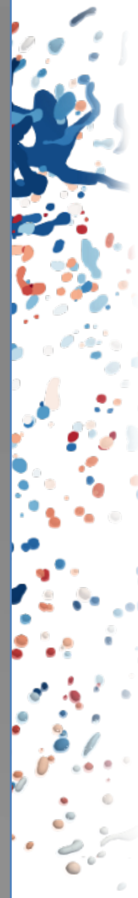
- **Volume/surface adaptation with MMG5.3 and YALES2 2018.11**
- Metric definition based on a calculated progress variable gradient
- Same resolution as 110M (300 microns) but with 38M cells: **global x3 speed-up**



Application to gas/liquid interfaces

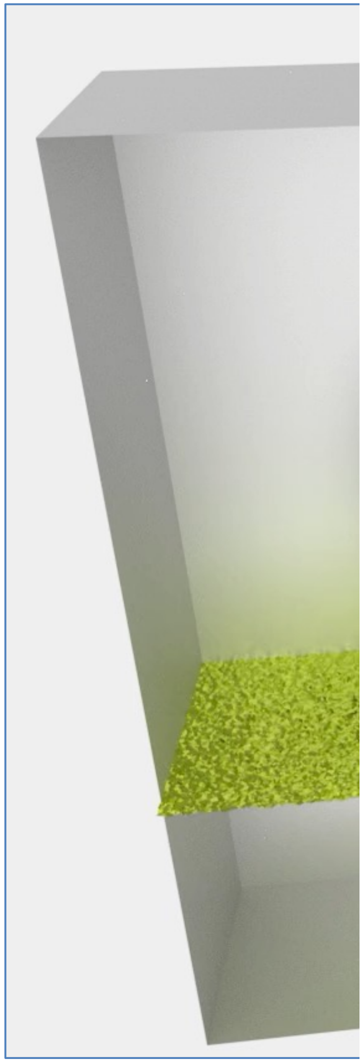
- Kerosene jet-in-cross flow at 10 bar, We_{aero} = 60 to 400 [1]
- Accurate Conservative Levelset [2], up to 1.6 billion tets on 8192 cores [3]

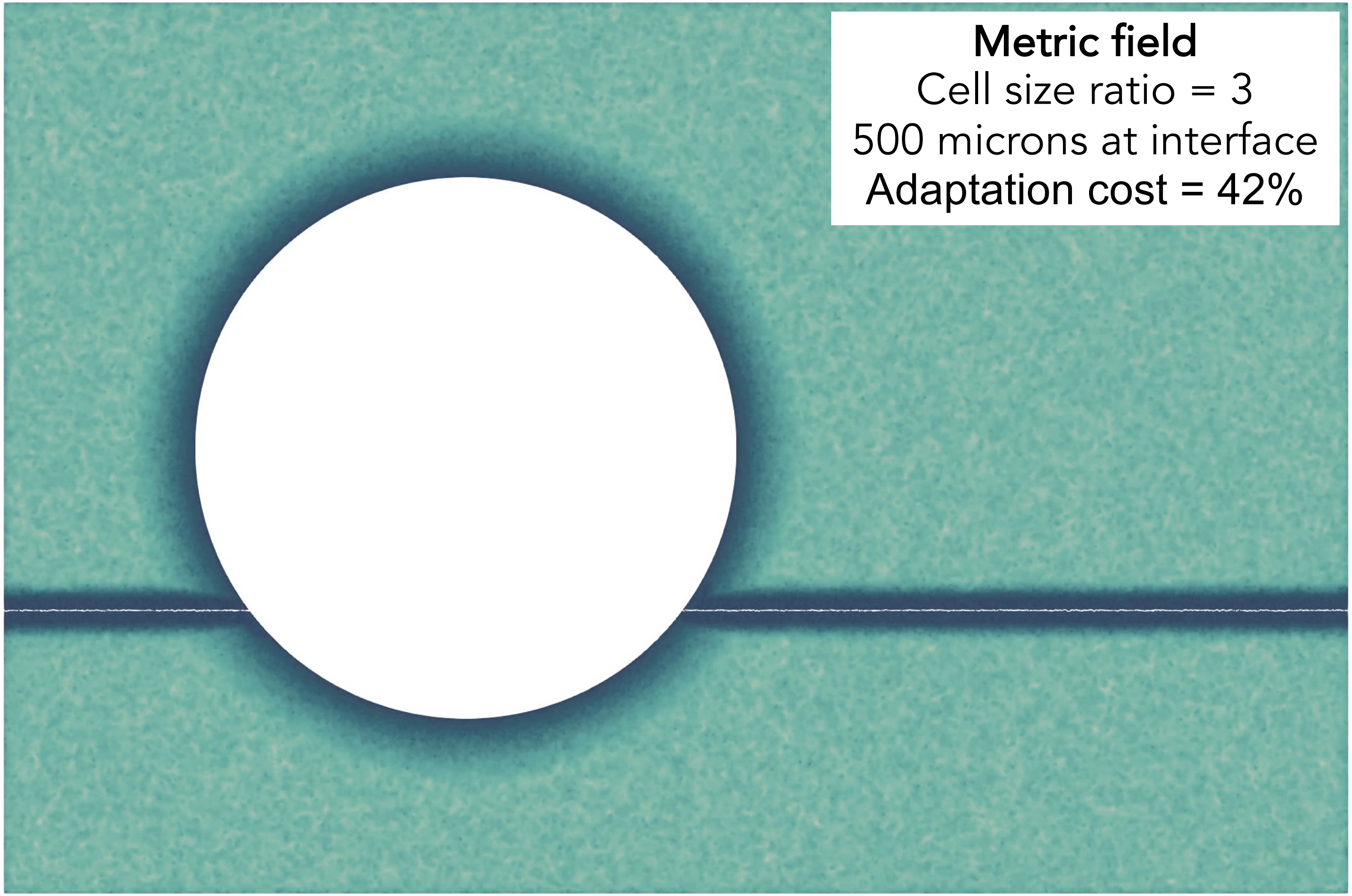




Application to gas/liquid interfaces

- Simulation of oil churning by M. Cailler, SAFRAN TECH [1,2]
- Real fluid properties, 206 million tets on 1250 cores (Cobalt, CEA)





[1] Cailler et al., ICMF, 2019
[2] Leprince et al., Advances in Tribology, 2012

Some studies with YALES2
Wind turbines

- Impact of yaw on wake develpoment behind offshore wind turbines
- Collaboration with SIEMENS/GAMESA Renewable Energies

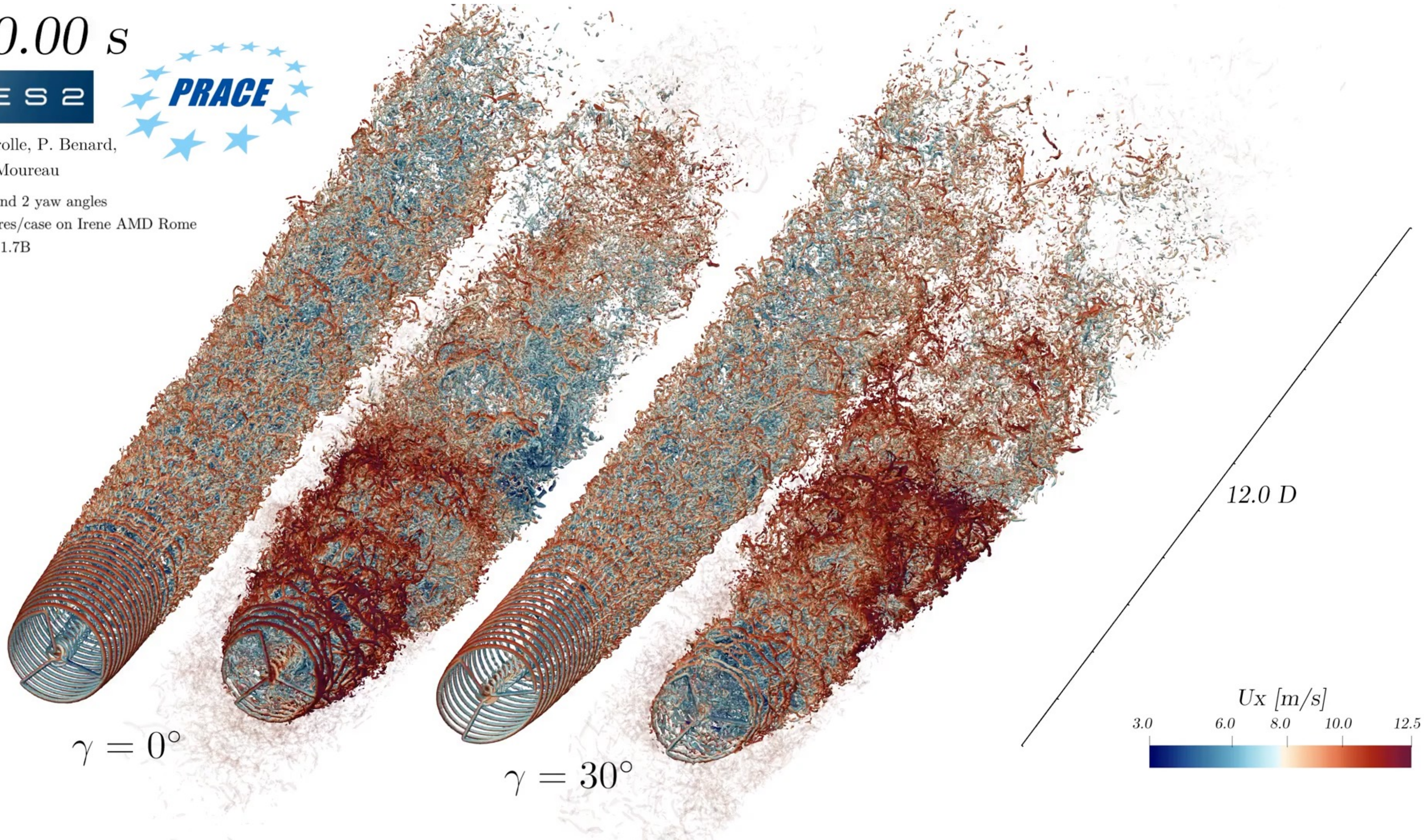
$t = 0.00\ s$

YALES2

PRACE

F. Houtin Mongrolle, P. Benard, G. Lartigue, V. Moureau

4 cases: 2 inflows and 2 yaw angles
Resources: 8448 cores/case on Irene AMD Rome
Mesh sizes: 1.5B – 1.7B



The parallelism paradigm

- Many solvers ➔ many different ways to deal with parallelism
  - Euler description for the fluid phase
  - Lagrangian description for particles
  - Parallelism on spectral band and directions for radiation
  - Dynamic load balancing for chemistry
- Full MPI since 2009
- Working on hybrid OpenMP / MPI (coarse grain) since 2017
- Attempts to use GASPI
- Attempts to port a Mini-App on GPU with HPE and IDRIS

- Domain decomposition: the domain is partitioned (METIS/Scotch) and distributed among processors
- Two main parallel tasks:
  - Exchange data between neighbouring subdomains (P2P)
  - Perform dot products (reduce / allreduce)

The key numerical ingredients

- For classical use 80% of CPU spent in solving Poisson equation for pressure (elliptic problem) by Conjugate Gradient algorithm
- Preconditioning does the performance…

- For combustion applications the load balancing does the performance…
  - In-house MPI dynamic scheduler for work-sharing
  - TITUS_DLB library with E. Petit for work-stealing
  - Both use small world approach
  - Highly scalable up to 100'000 cores

- Dynamic mesh adaptation: interpolation and P2P communications do the performance

CPU or Memory bound?

- YALES2 uses unstructured meshes
  - Only non-sequential access…
  - Poor vectorization
  - Low arithmetic intensity
  - Low reusability (depend on connectivity)
  - Sparse Matrix-Vector product + dot products

- Double domain decompostion
  - We partition the mesh a second time on each core to have « groups » of cells
  - These are small enough to fit in L2
  - Cache blocking
  - Also used for our in-house « multigrid » approach to solve the Poisson equation that arises in Low-Mach number Navier-Stokes

Conclusion

- Already a lot of work on code optimization at all levels:
  - Vectorization
  - Alignement
  - Loop improvement for better memory access
  - Algorithm (mesh adaptation is kind of auto-tuning…)
  - Parallelism

- We expect a lot from new hardware:
  - DDR5, HBM, …
  - ARM, RISC V, …

- And from software / environment:
  - Auto-tuning
  - Mixed precision for preconditioning
  - Loop specialization (ndim=1, 2 or 3),