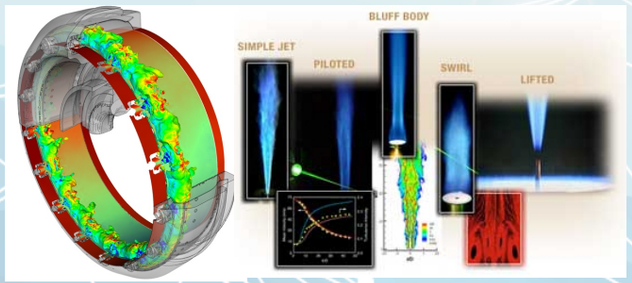
CERFACS

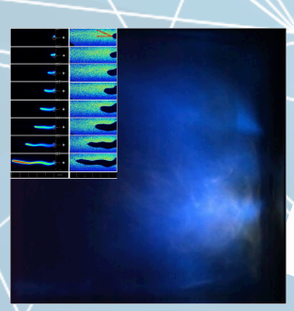
CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

ORAP
PROMOUVOIR LE CALCUL HAUTE PERFORMANCE

Forum ORAP: spécial 20 ans,
Maison de l'UNESCO, Paris,
14-15 octobre 2014

High Performance Computing and Turbulent Reacting Flows: past and potential trends





L.Y.M. Gicquel[1†]
B. Cuenot[1], E. Riber[1], G. Staffelbach[1], A. Dauptain[1],
F. Duchaine[1], O. Vermorel[1], J. Dombard[1]
T. Poinsot[2]

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[2] CNRS - IMFT, Toulouse
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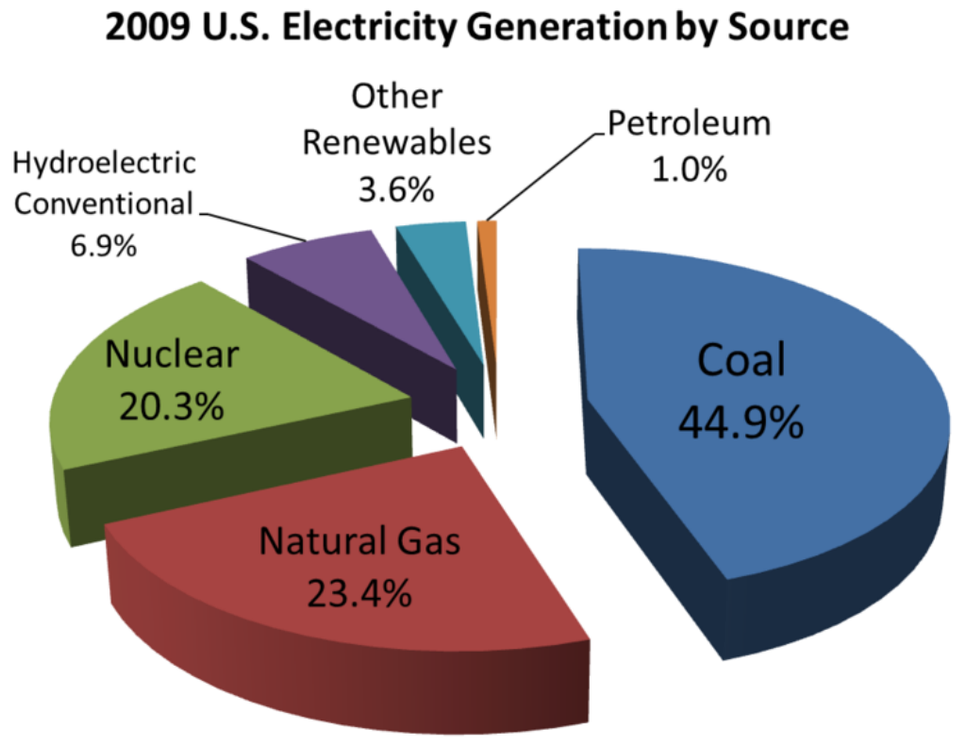
Context and Objectives

Combustion: An engineering science at the cross-road between *chemistry & fluid mechanics* with strong *technological/industrial and societal* implications

Context and Objectives

<u>Recent political and societal awareness</u> impose new guidelines and regulations to energy related industries - ACARE 2020, ICAO ….

- **Combustion** equals 80% of the energy produced worldwide
- Control climate change with increased access to renewable energies while better managing available fossil fuel ressources
- Sustain the global demand for energy (+ 2.6%)
- Improve existing technology efficiencies and emission productions…

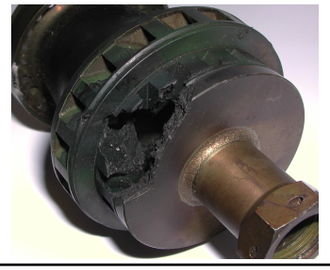


Although **<u>combustion</u>** has been around for quite some time (1st gas turbine & piston engines produced in chain by early 1900's), the research / engineering community is faced with quite a challenge !!

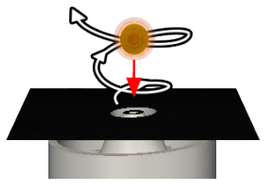
Context and Objectives

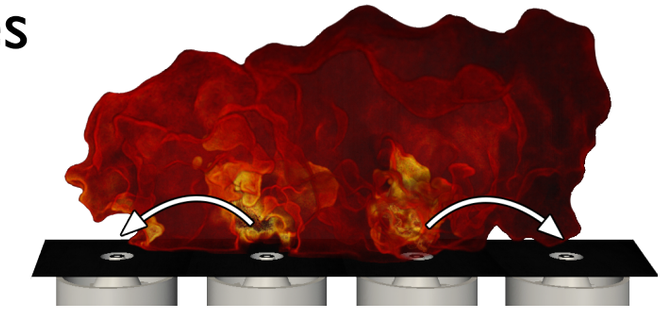
Lean Premixed (LP) combustion is a concept that has been known for quite a while. It never made it in the GT early development phases because it comes with major problems:

- Flashback



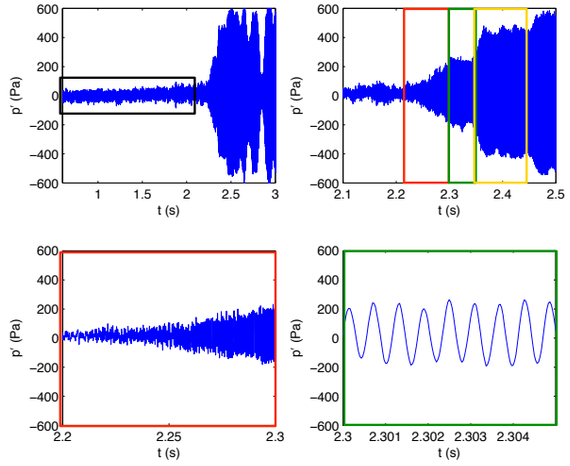
- Ignition issues





- … etc

- Thermo acoustic instabilities



Courtesy of Worth and Dawson (private communication)

What made the difference is an improved understanding of *«combustion dynamics»* through **CFD turbulent reacting flow models** addressing fundamental, *laboratory scale burners as well as real burner complex flows*.

Layout of the talk

I] HPC & turbulent reacting flow CFD

- Modeling: from simplified and steady models to fully unsteady simulations
- Combustion predictions: increase in model fidelity and complexity
- Current capacities & challenges: model development and validation on fully transient problems

II] Potential trends and developments

- Towards improved numerical predictions require improved physics description - multi-physics codes
- Improved engines/applications will require technological breakthrough where more *engine components will need to be addressed in an integrated fashion* because they will interfere

I] HPC & turbulent reacting flow CFD

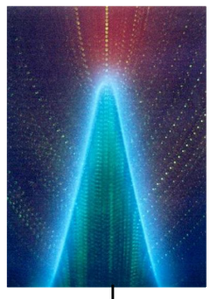
Turbulent reacting flows have been from the beginning studied and theoretically addressed as true/pure multi-scale multi-physics problems:

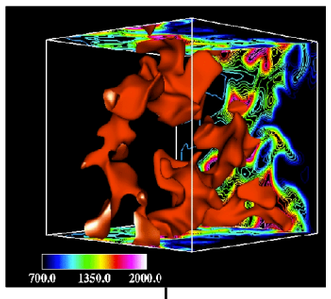
Chemical reactions

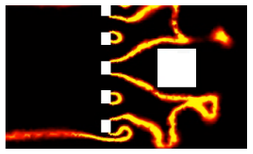
Turbulence

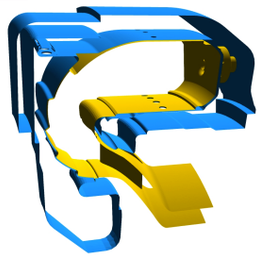
Flame Flow/Obstacle interactions

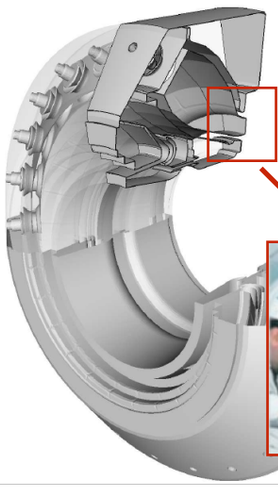
Large scale industrial problems
Geometrical complexities









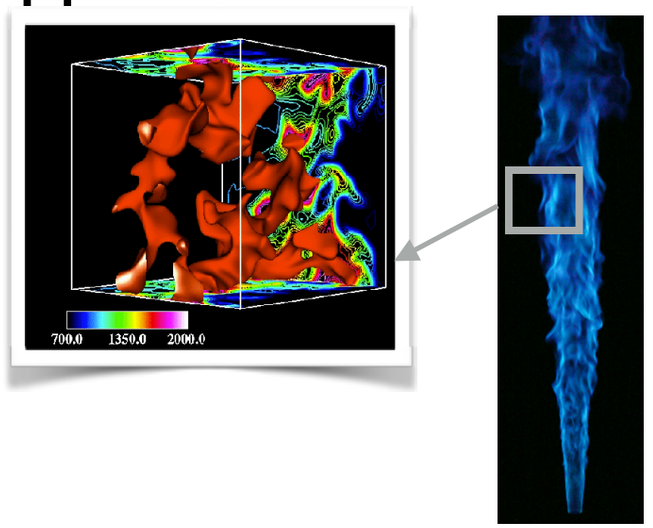


~100 μm ~1 mm ~10 mm ~100 mm ~1 m ~10 m ~100 m ~1 km

~1 ms ~10 ms ~1 s ~10 s ~1 min ~10 min ~1 h ~1 jour

1) Modeling

To go forward (whatever the context) different approaches were naturally proposed in the 1980's, 1990's and on:



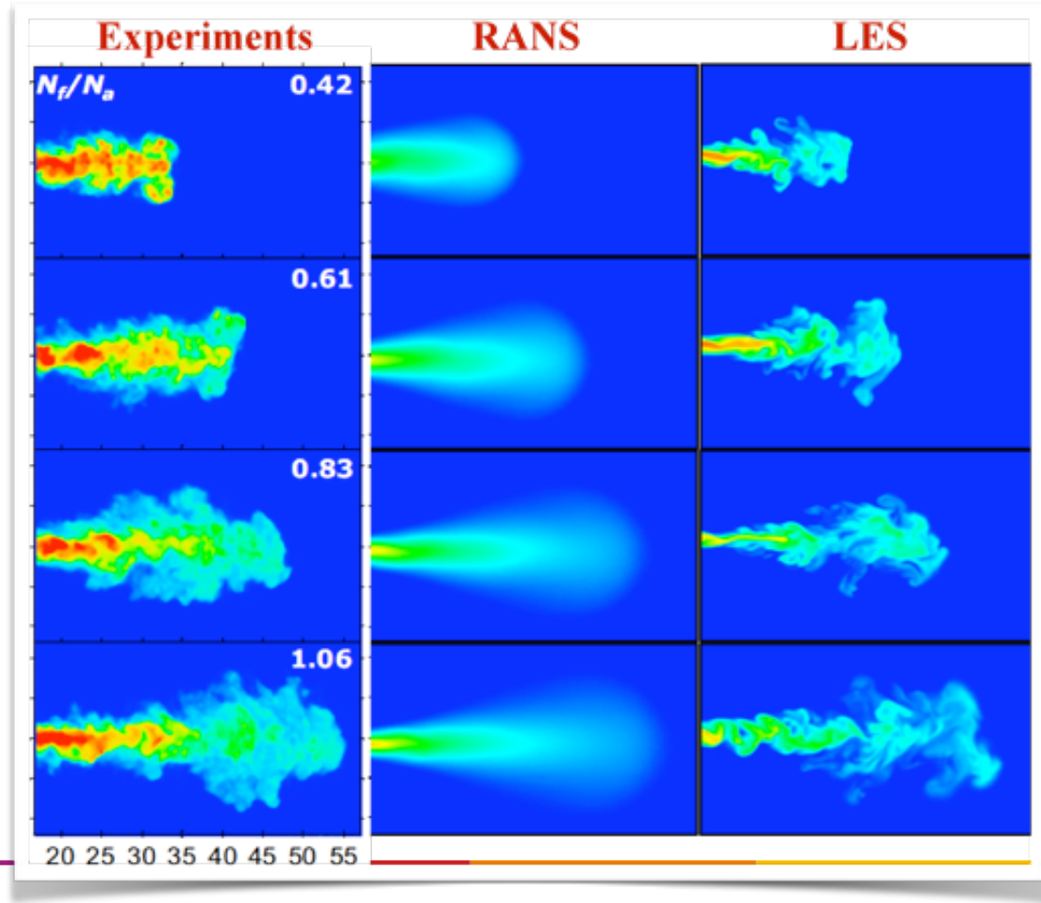
- No trade-of (i.e. solve everything): **DNS**
  However restrained to simple flows

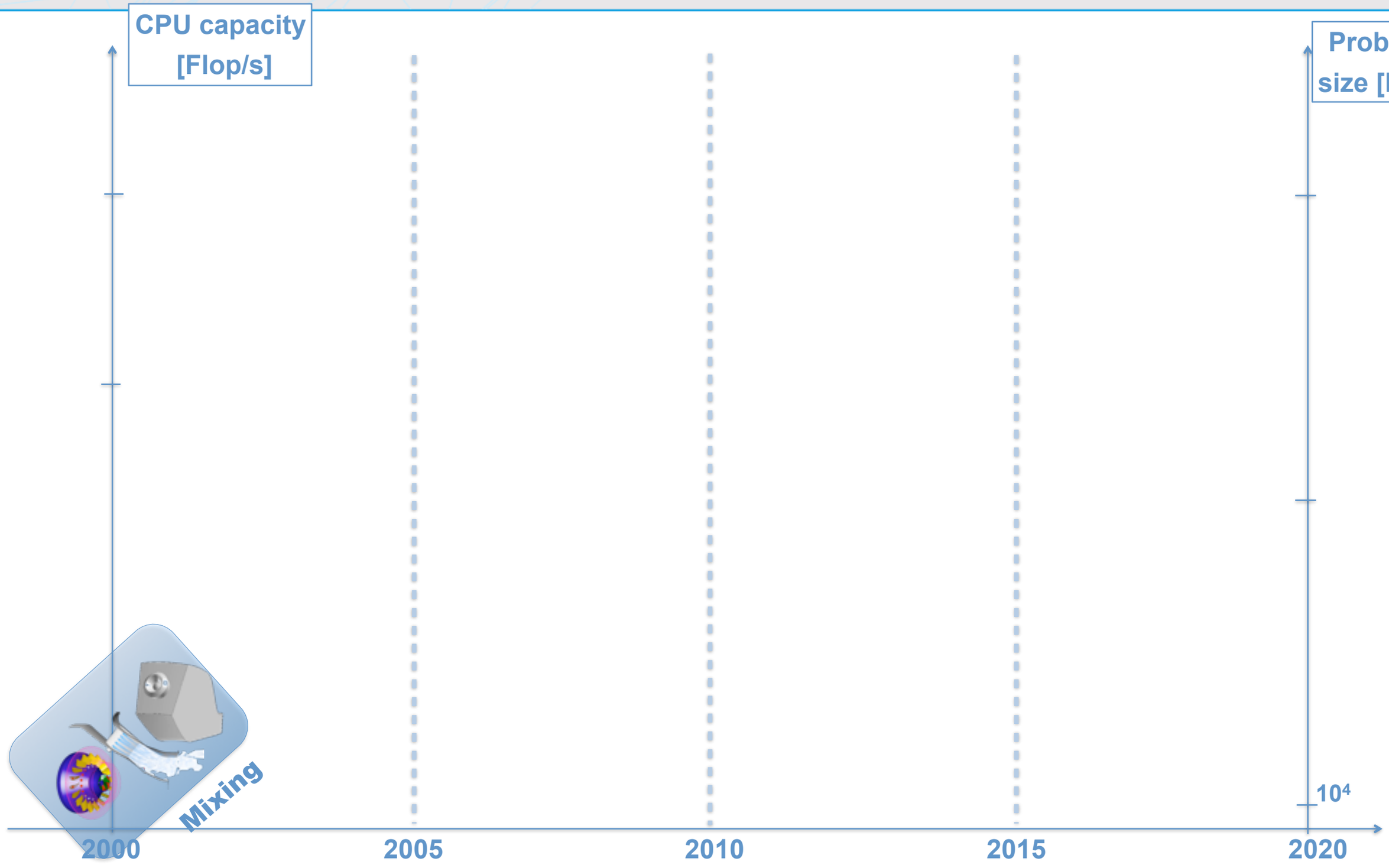
- To address more complex problems ***modeling*** is introduced so to have a tractable CFD solution:

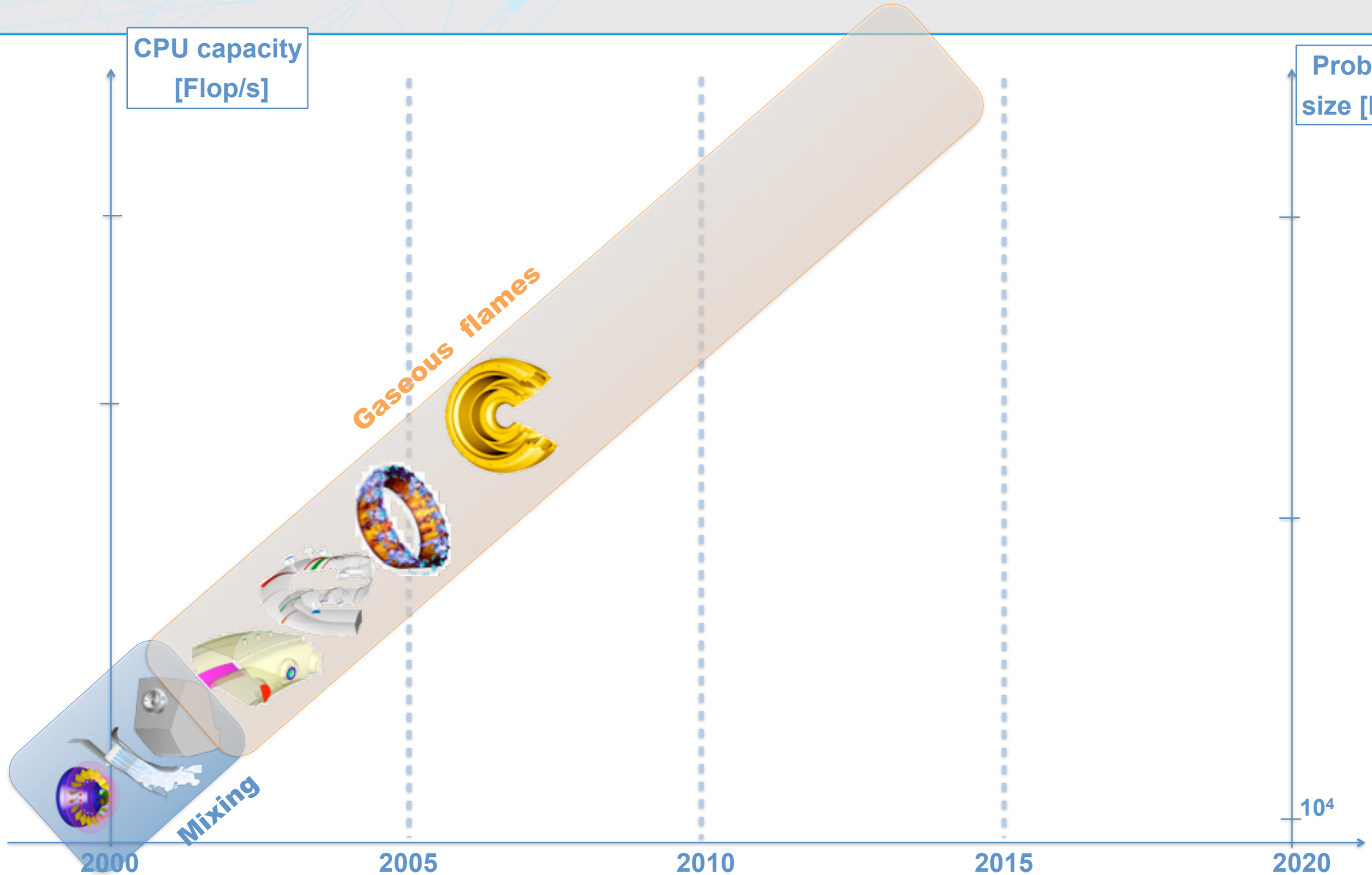
  - **Modeling formalisms**:

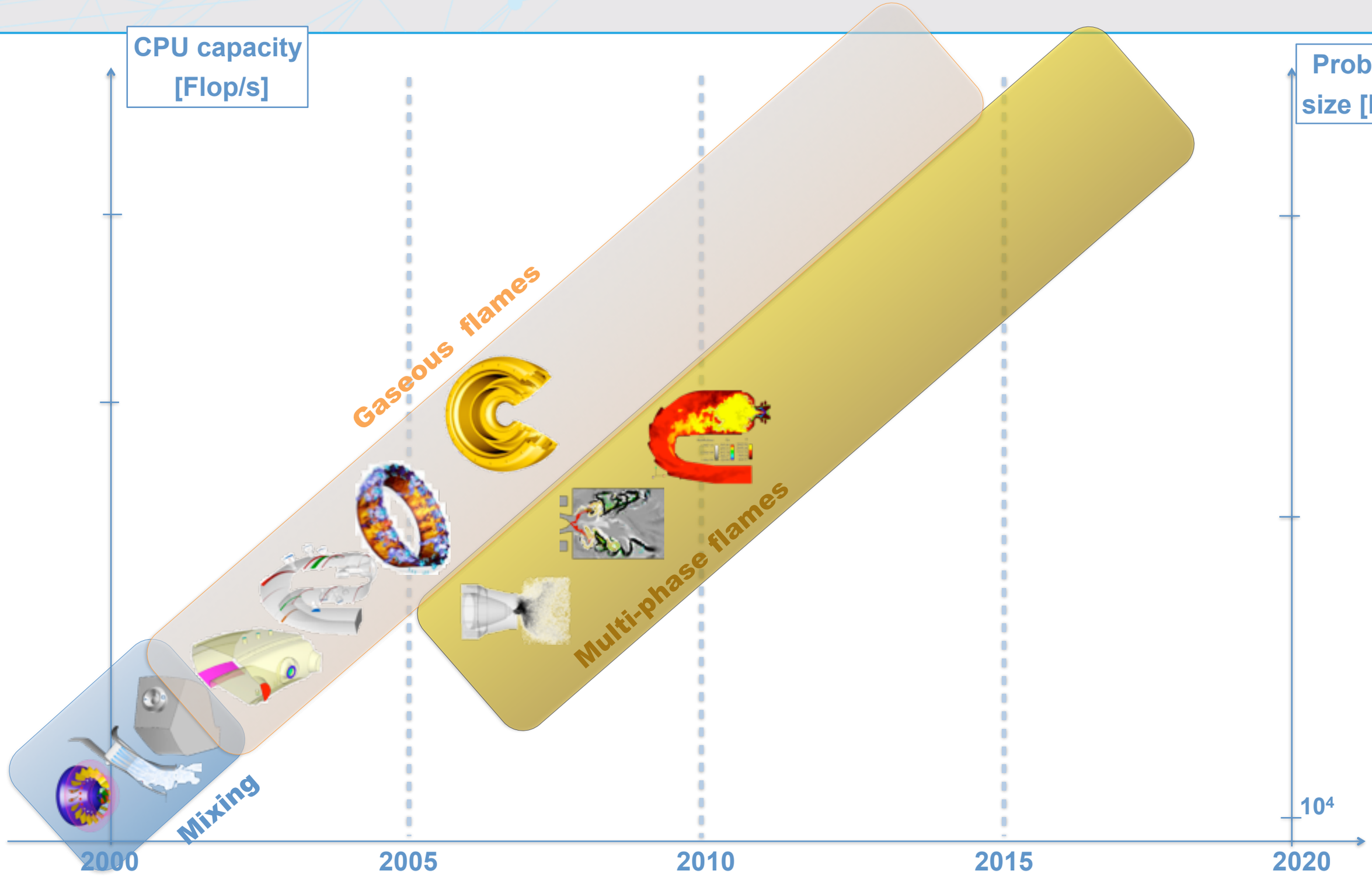
    RANS (steady) or **URANS** (unsteady)
    vs
    LES (filtering)

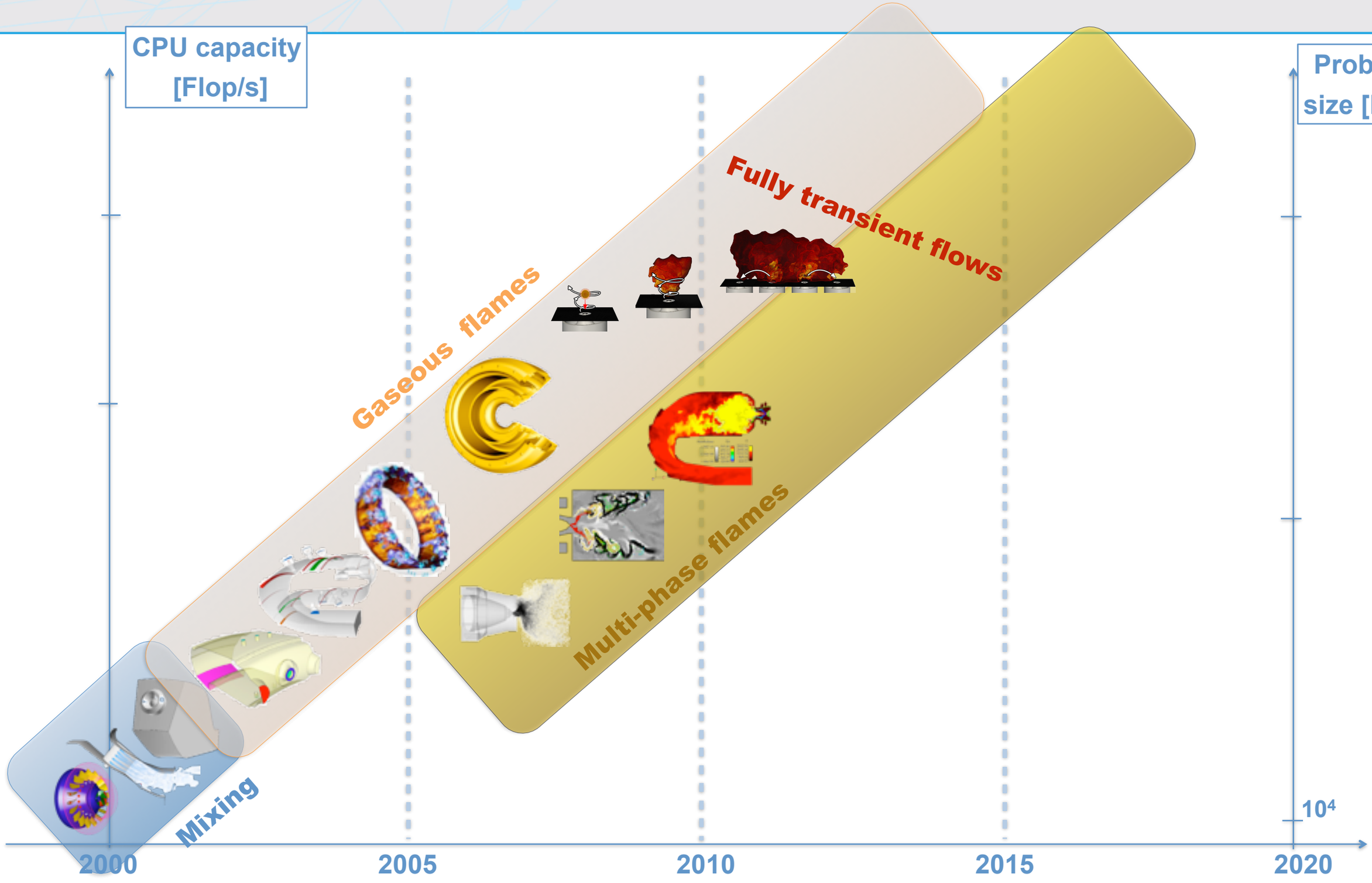
  - Reduced chemistry, turbulence model, turbulence/chemistry models…




CPU capacity [Flop/s]
Problem size [DoF]
Mixing
10^4
2000
2005
2010
2015
2020


CPU capacity [Flop/s]
Problem size [DoF]
Gaseous flames
Mixing
10^4
2000
2005
2010
2015
2020


CPU capacity [Flop/s]
Problem size [DoF]
Gaseous flames
Multi-phase flames
Mixing
2000
2005
2010
2015
2020
10⁴


CPU capacity [Flop/s]
Problem size [DoF]
Gaseous flames
Fully transient flows
Multi-phase flames
Mixing
2000
2005
2010
2015
2020
10⁴

CPU capacity [Flop/s]

Problem size [DoF]

Fully transient flows

Gaseous flames

Multi-phase flames

Mixing

10^4

2000 2005 2010 2015 2020

CPU capacity [Flop/s]

Problem size [DoF]

Gaseous flames

Fully transient flows

Multi-phase flames

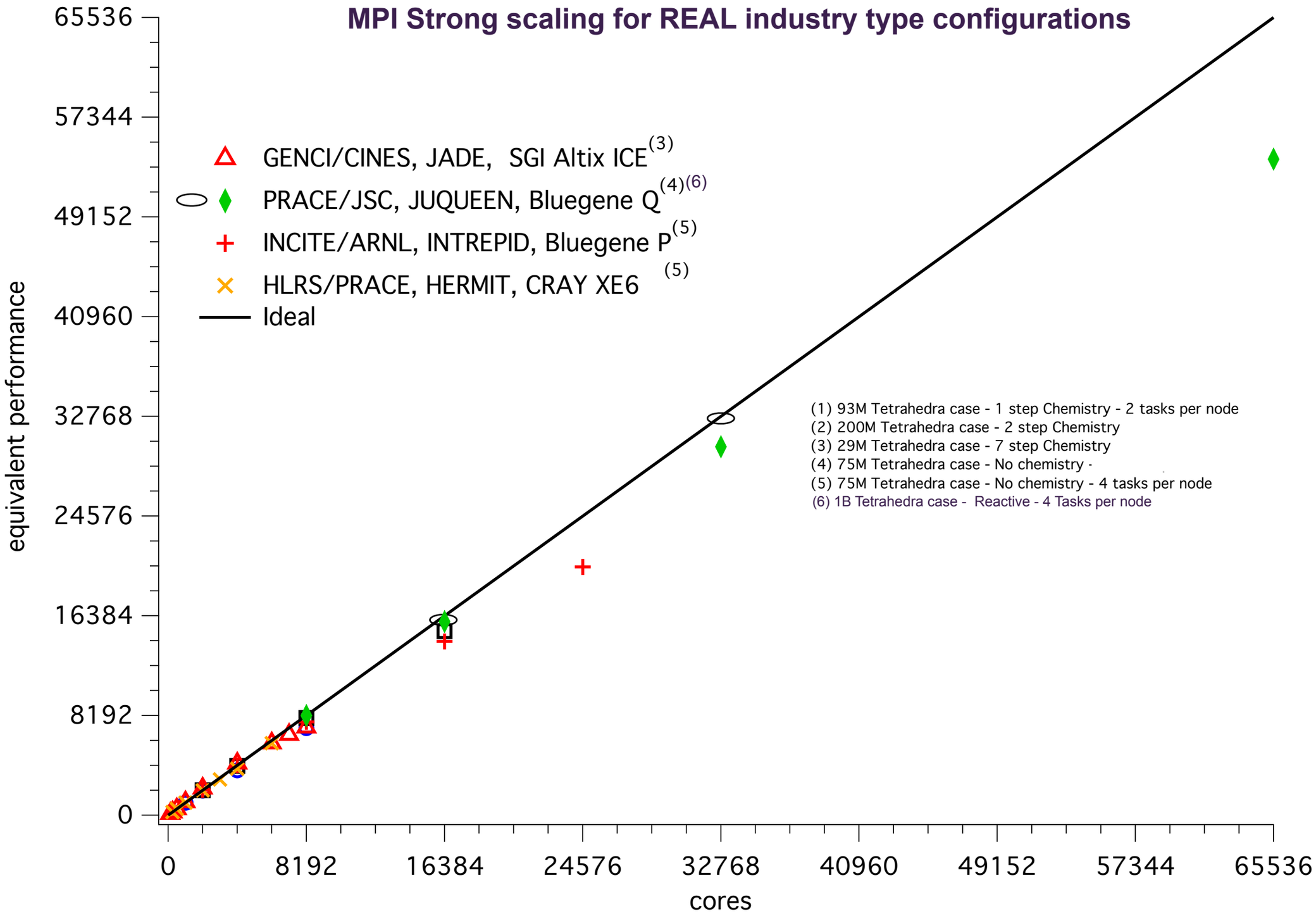
Mixing

Transfer time to INDUSTRY

10^4

2000 2005 2010 2015 2020

MPI Strong scaling for REAL industry type configurations



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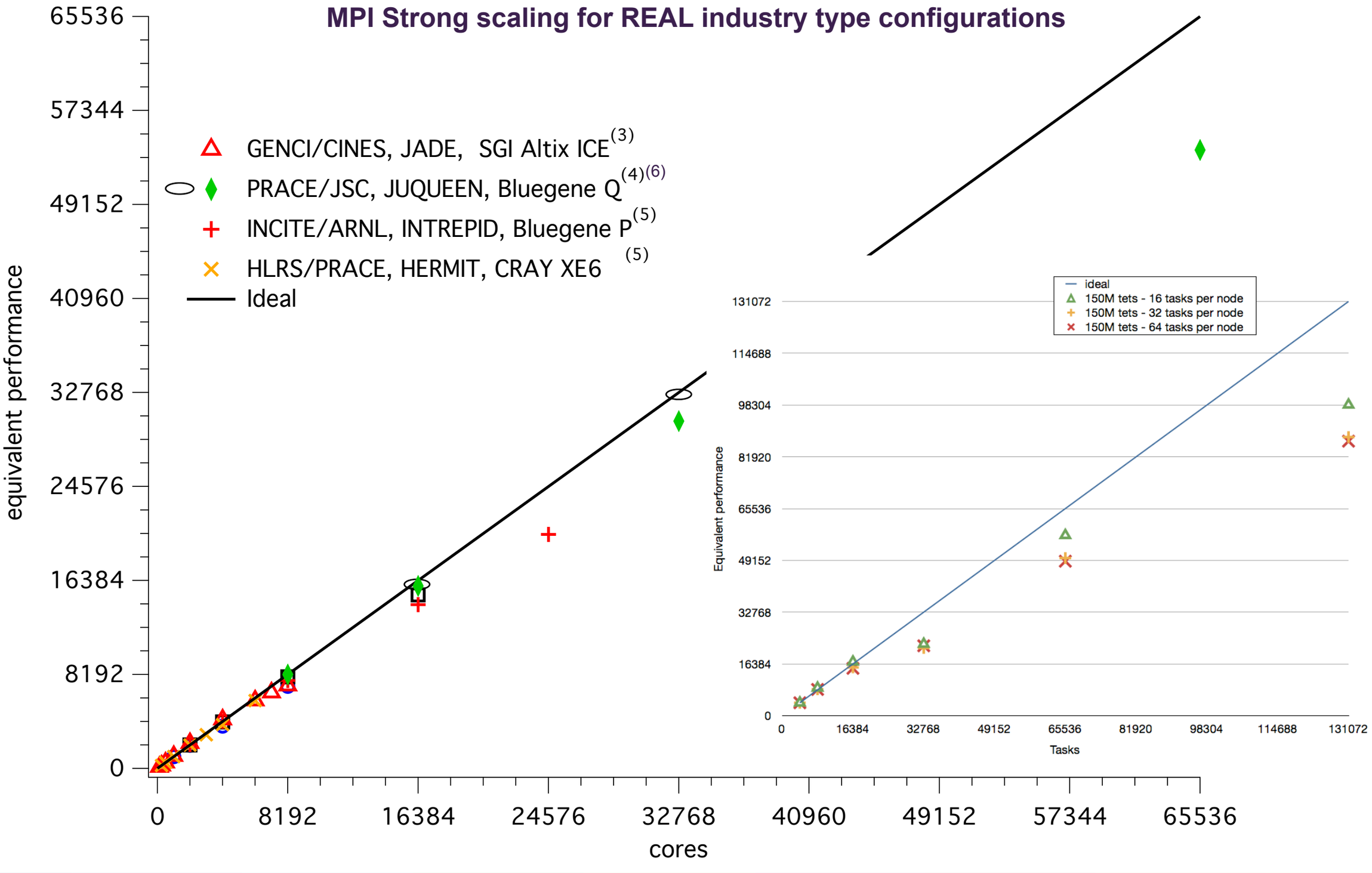
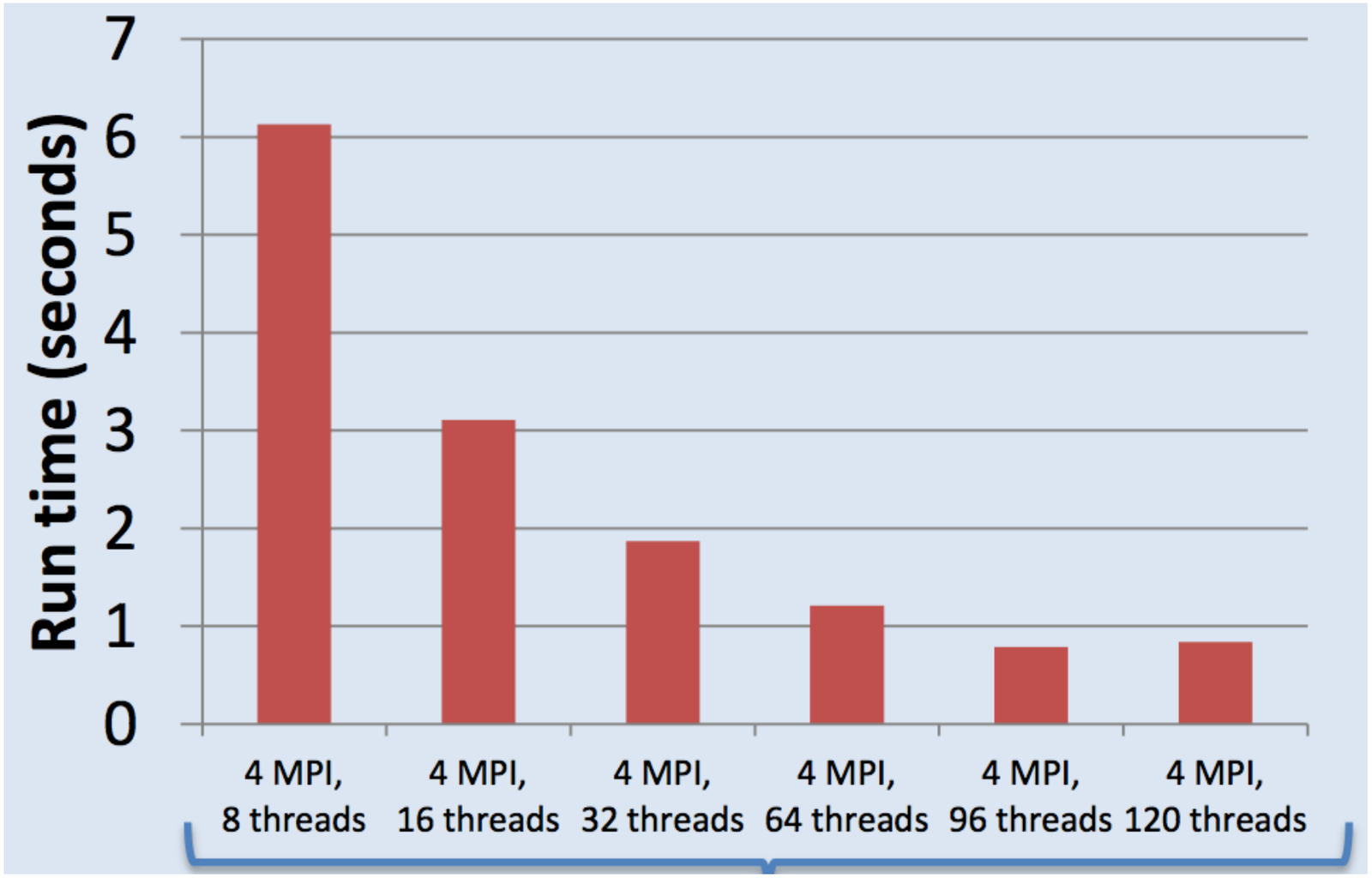
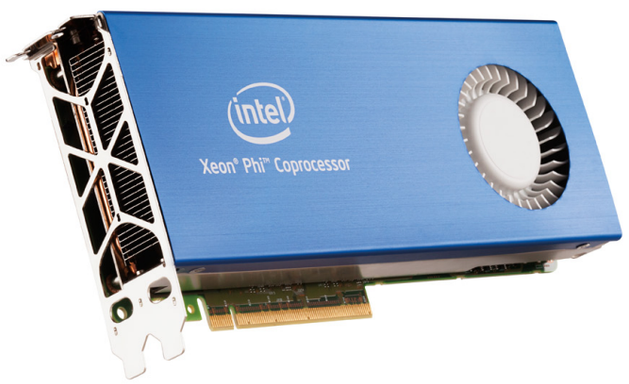


MPI + OmpSS Strong scaling on Xeon Phi



Using 2 Xeon Phi

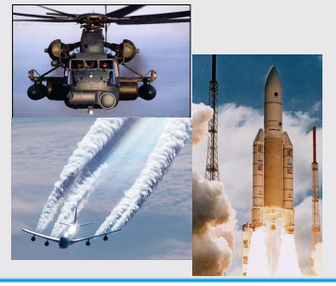
Dynamical exascale entry platform



Introduction of Coarse grain parallelism on a legacy code

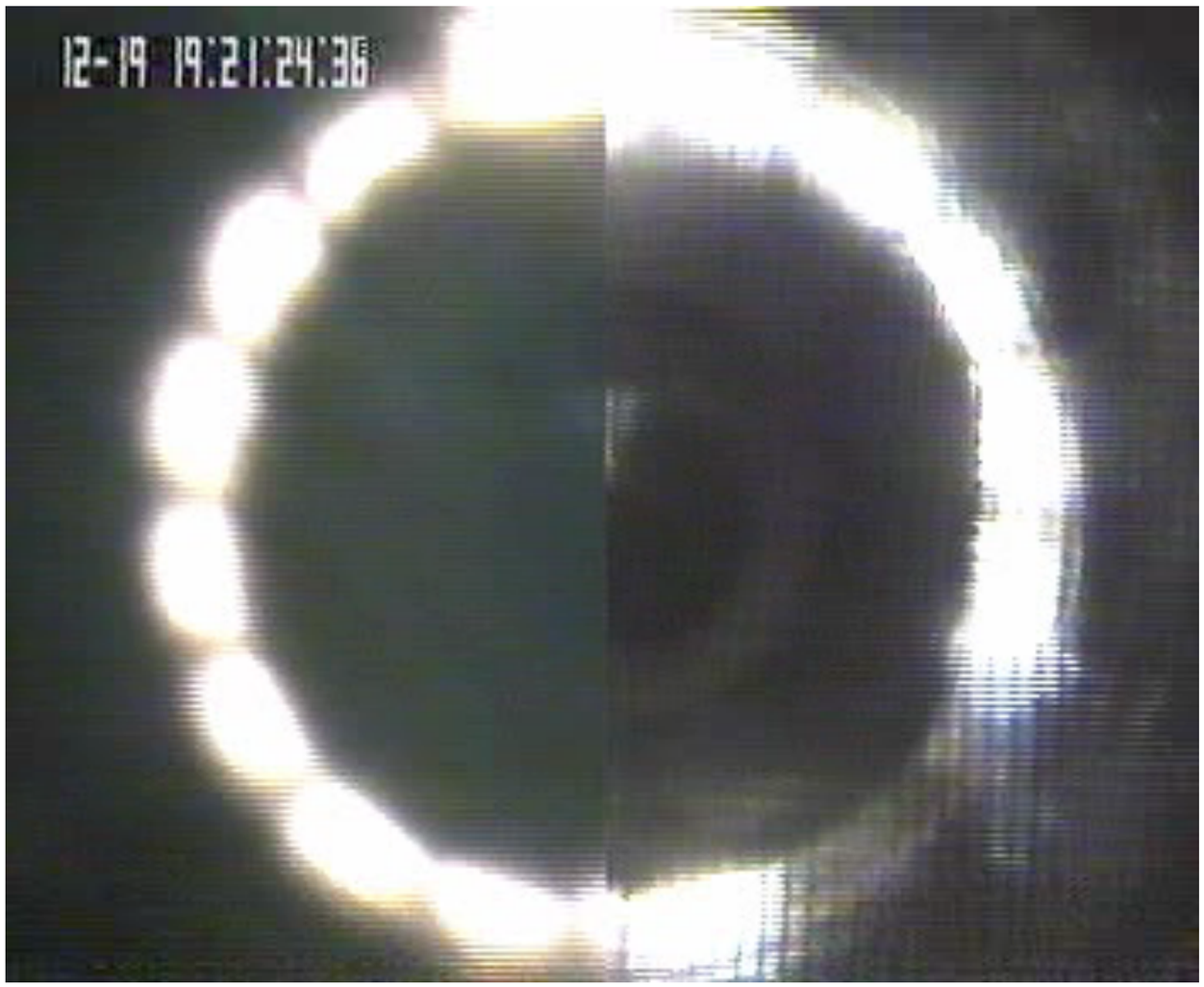
Test limited by available access … TACC granted access to Stampede 10days ago

3) Current capacities and challenges



In the aeronautical context: ignition is of paramount importance (where everything starts…)

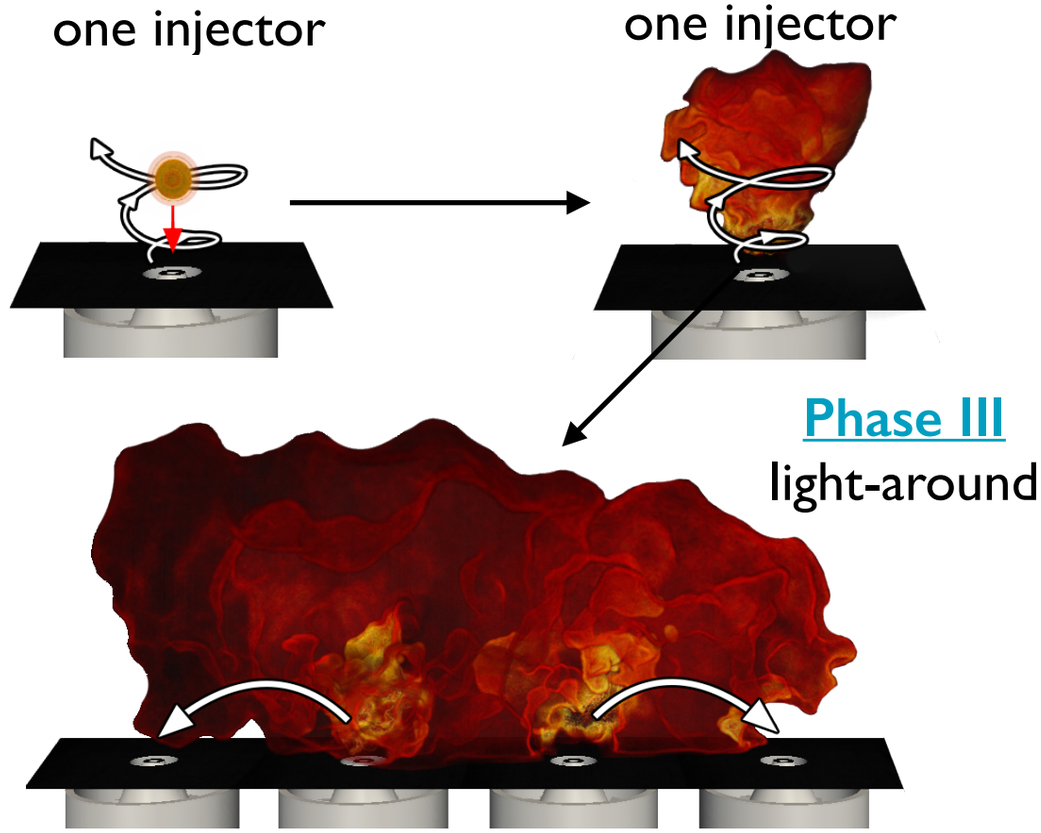
- Number of fuel injection systems which calibrate the effective cost and power of the engine
- Operability as well as security issue of the engine



Phase I
deposit near one injector

Phase II
flame on one injector

Phase III
light-around



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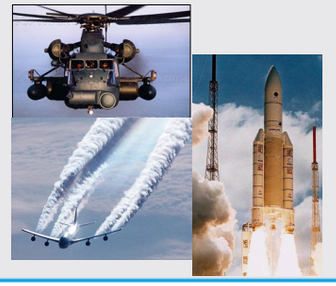

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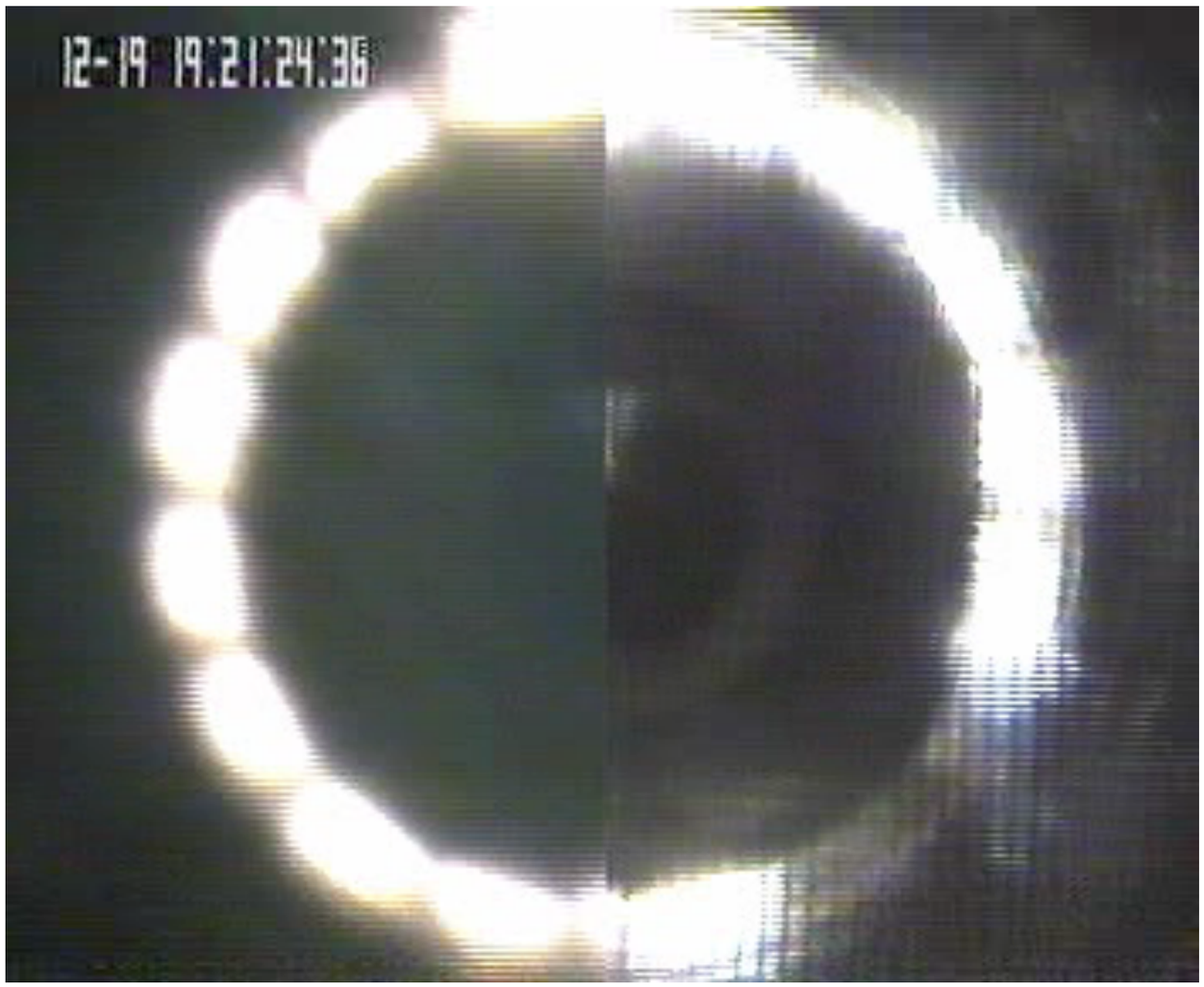

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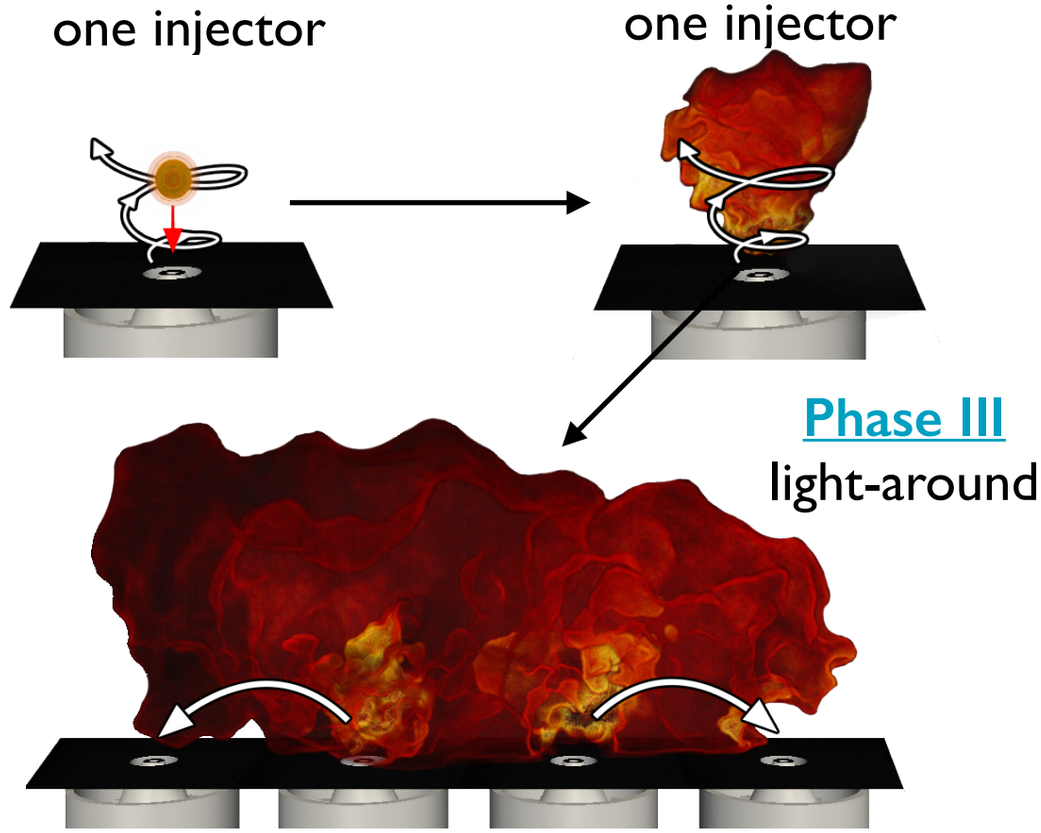
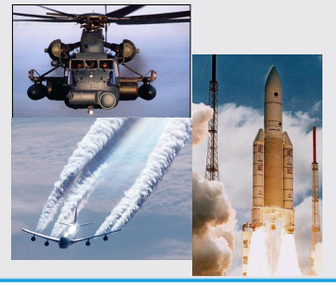
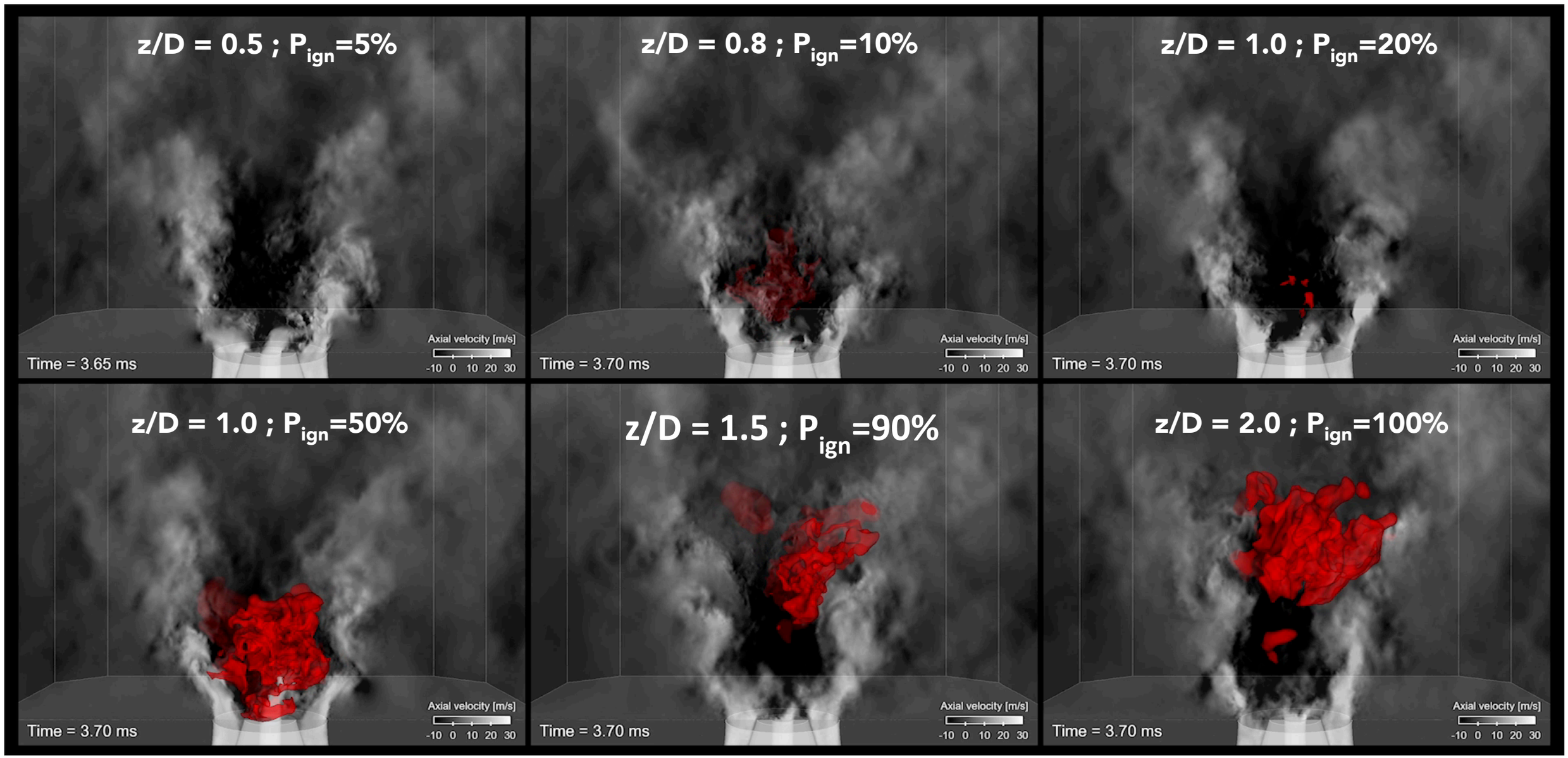




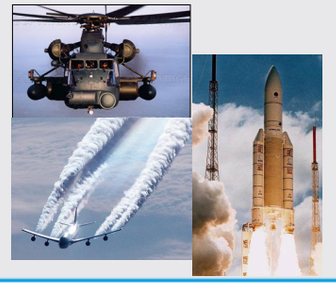
Phase II

Where and how much energy to deposit for a successful ignition of the first burner ?

PhD's of D. barré & L. Esclapez, (SAFRAN Cifre)



Parametric analysis of the numerical models as wells to determine the best practices



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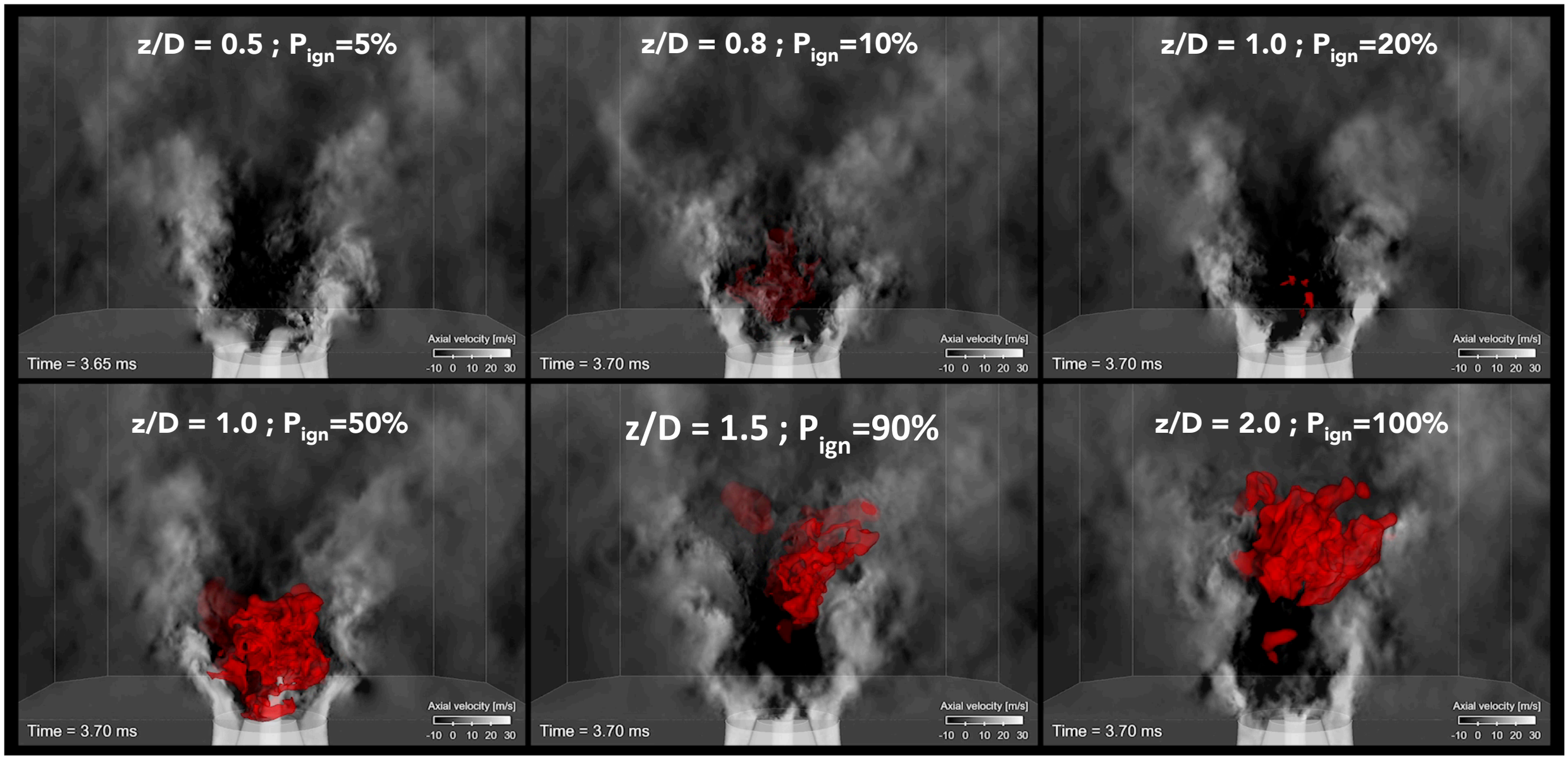

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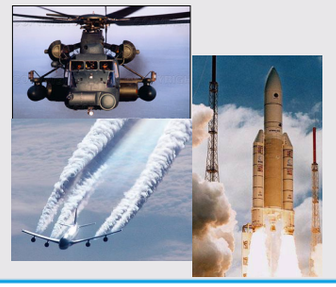


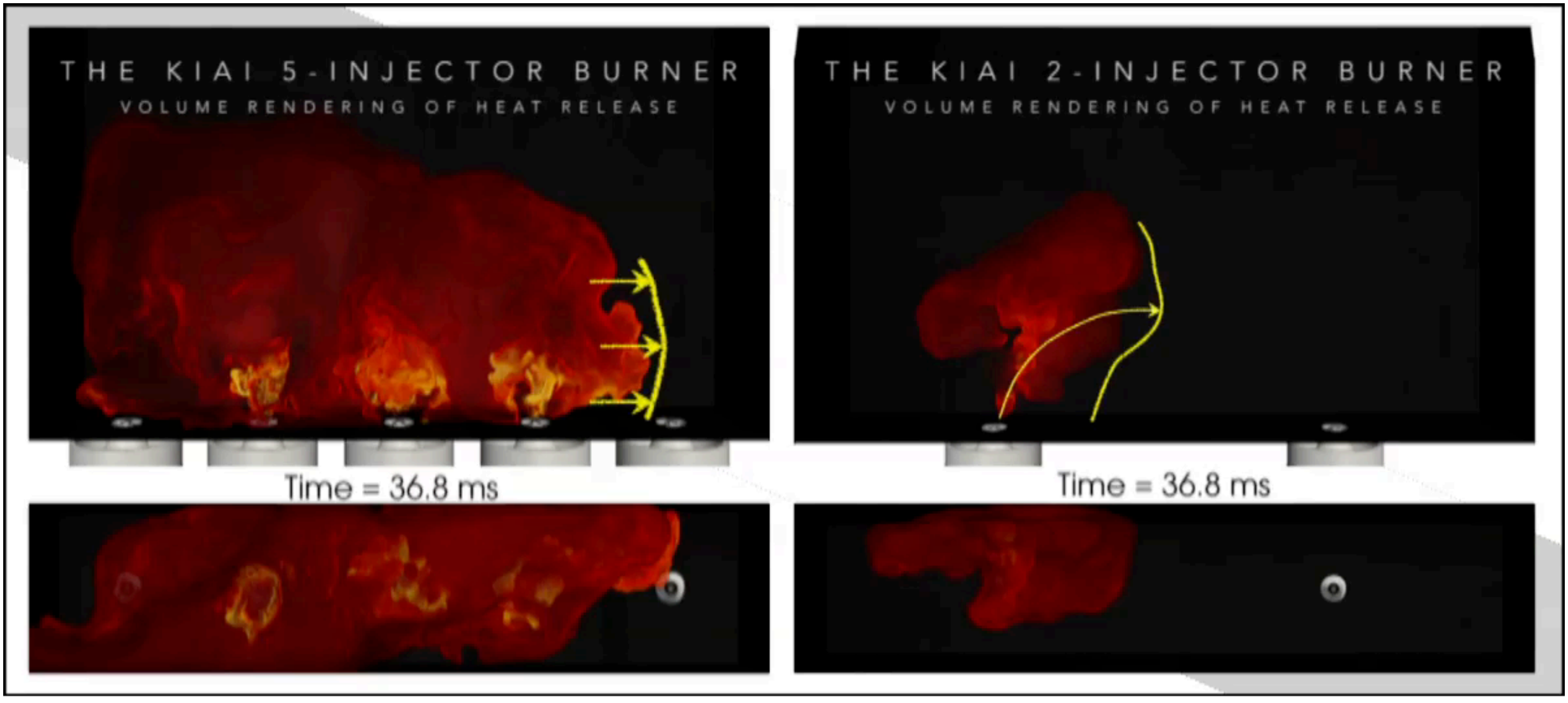
Phase III

Light-around: timing and transient process for potential optimisation

PhD's of D. barré & L. Esclapez, (SAFRAN Cifre)

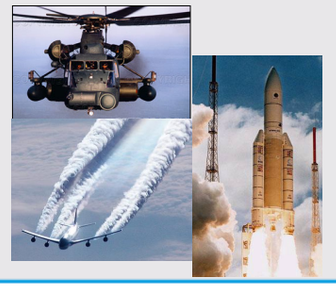
SP9: L = 90mm

SP26: L = 260mm



Radial flame propagation

Axial flame propagation



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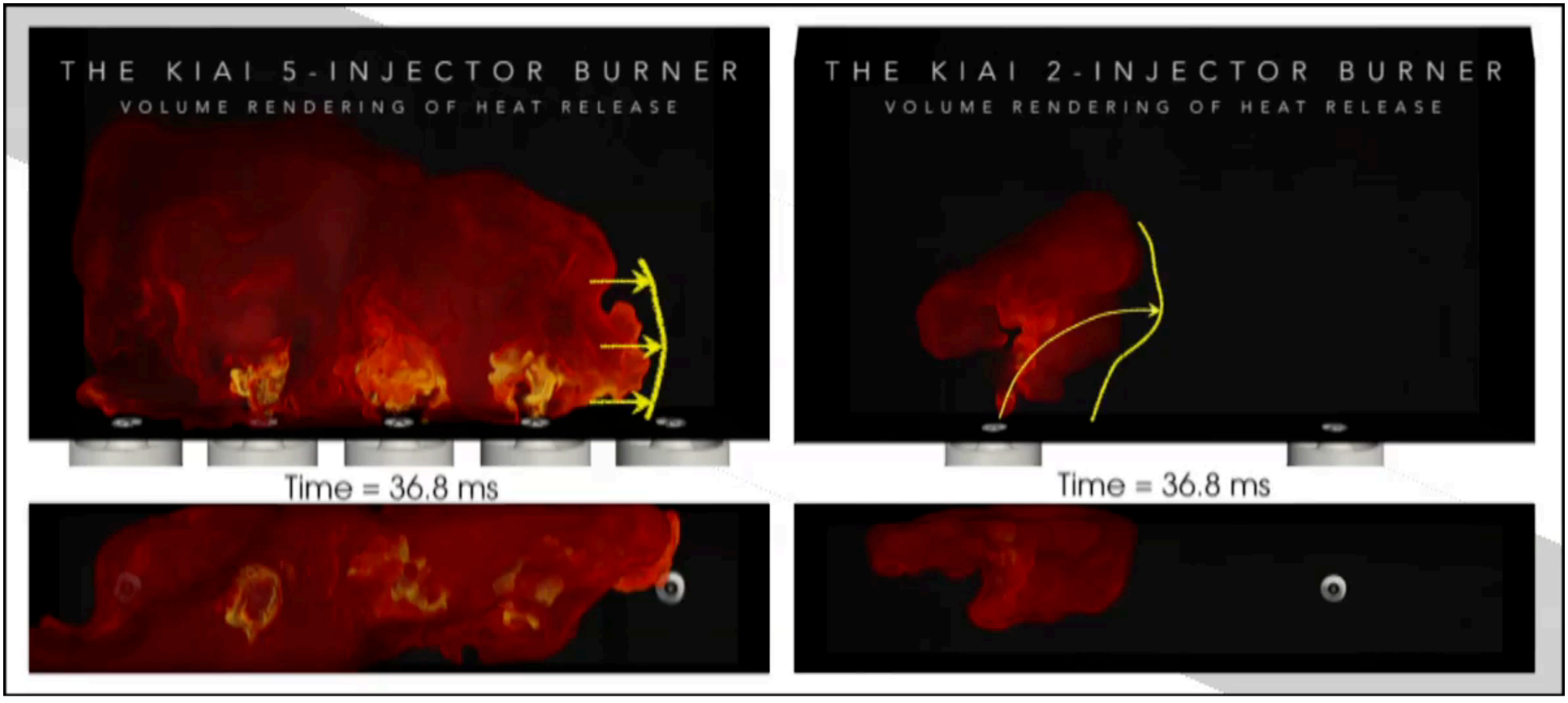

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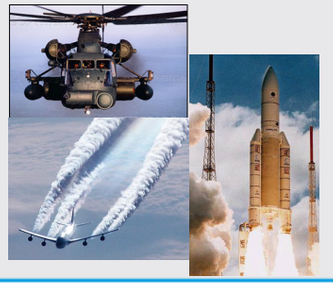
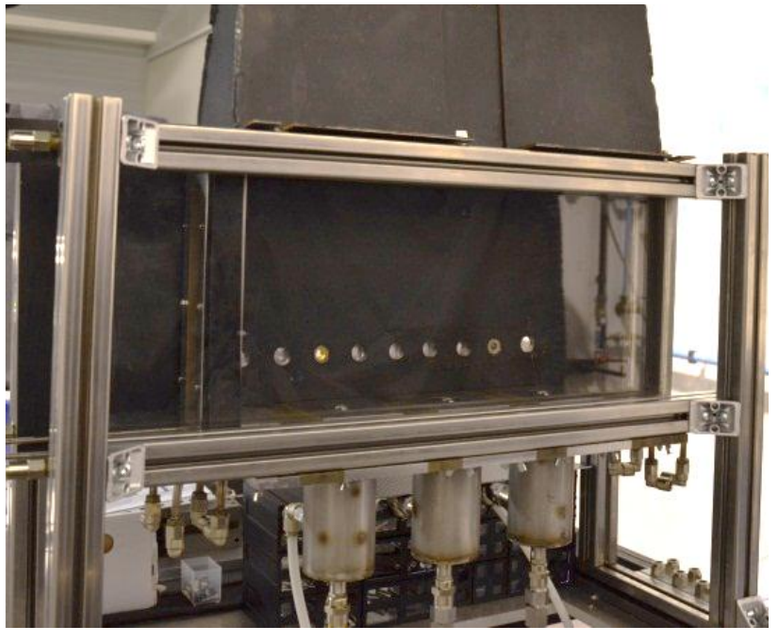


EU project KIAI

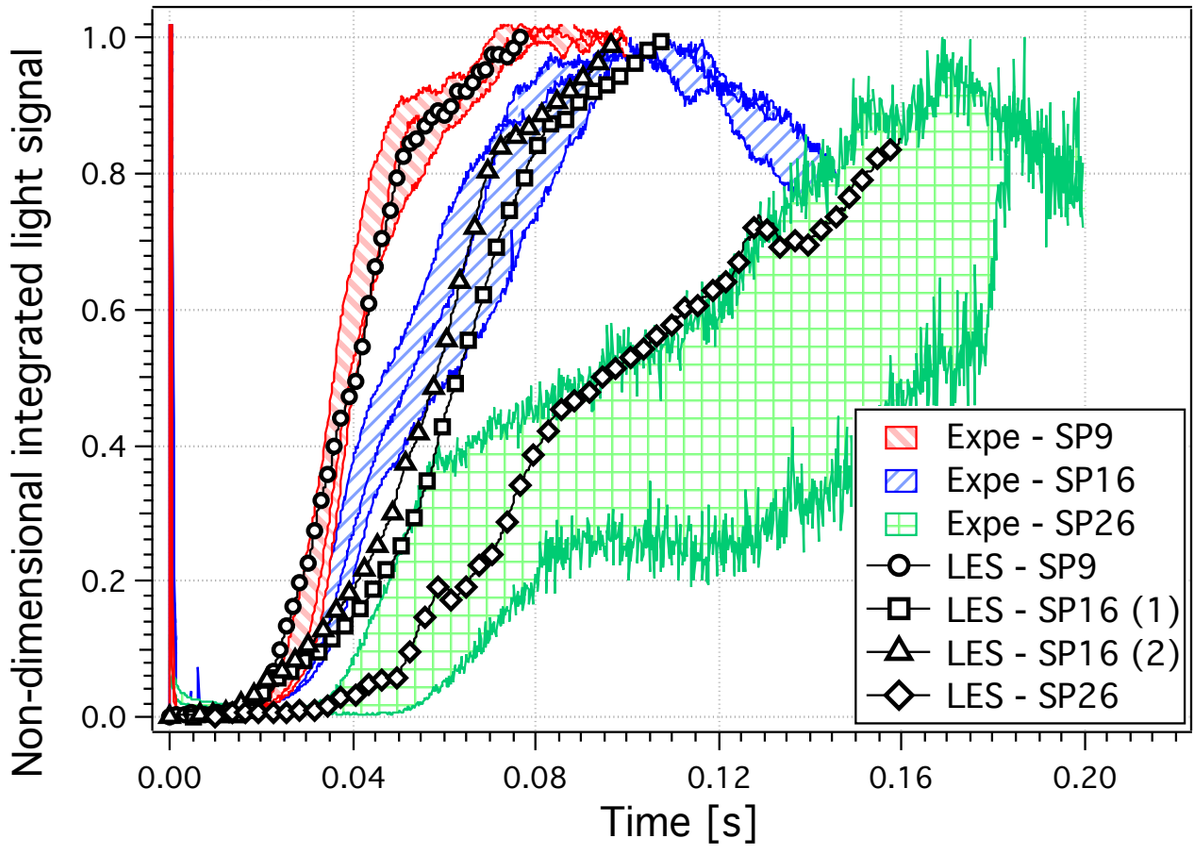


SAFRAN Snecma

UMR 6614 CORIA COMPLEXE DE RECHERCHE INTERPROFESSIONNEL EN AEROTHERMOCHIMIE

KIAI

Evolution of the luminous signal (CH emissions vs. Heat release images):

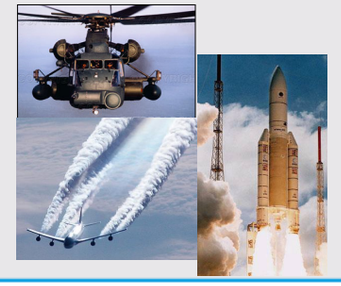


Flame propagation in aeronautical swirled multi-burners: experimental and numerical investigation.

D. Barré, L. Esclapez, M. Cordier, E. Riber, B. Cuenot, G. Staffelbach, B. Renou, A. Vandel, L.Y.M. Gicquel, G. Cabot

Symposium on Combustion

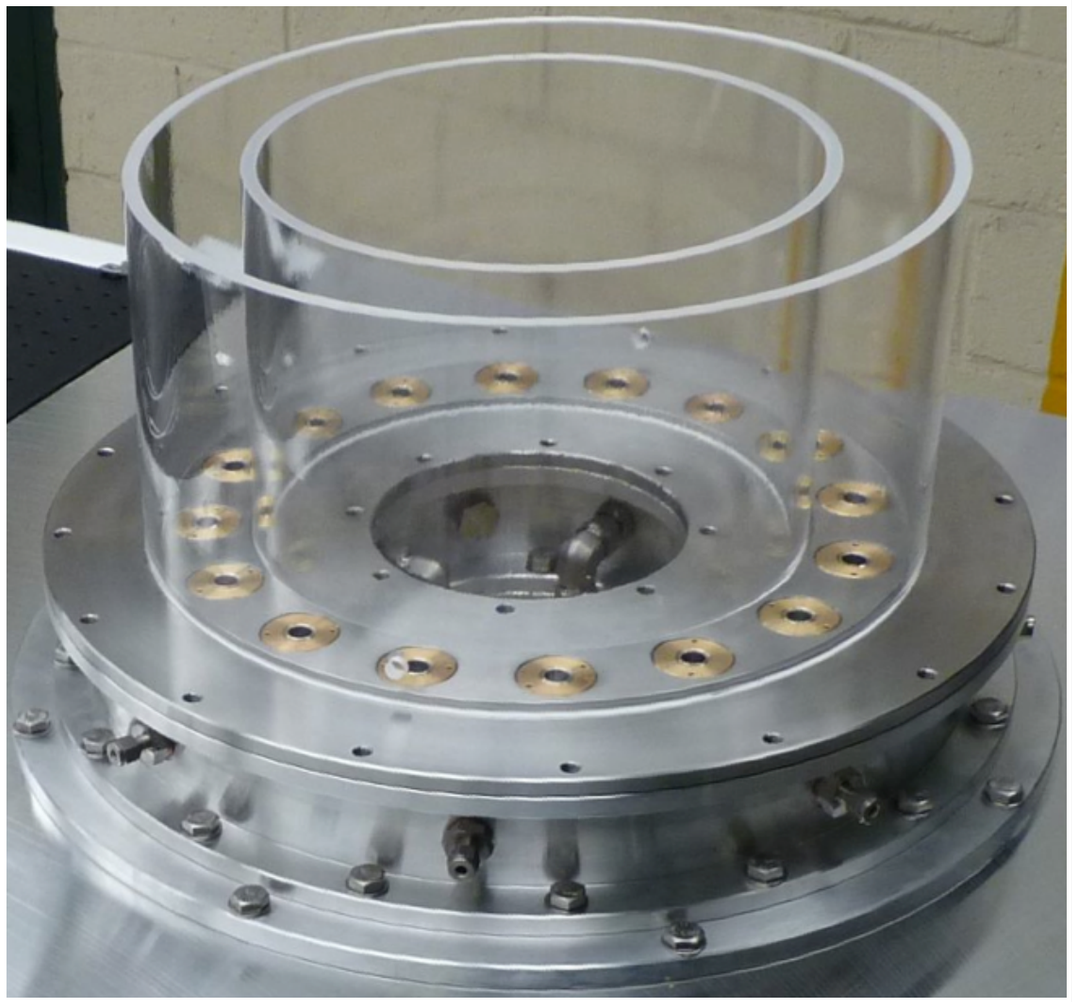
CURIE
6144 cores / run
15M CPU.h

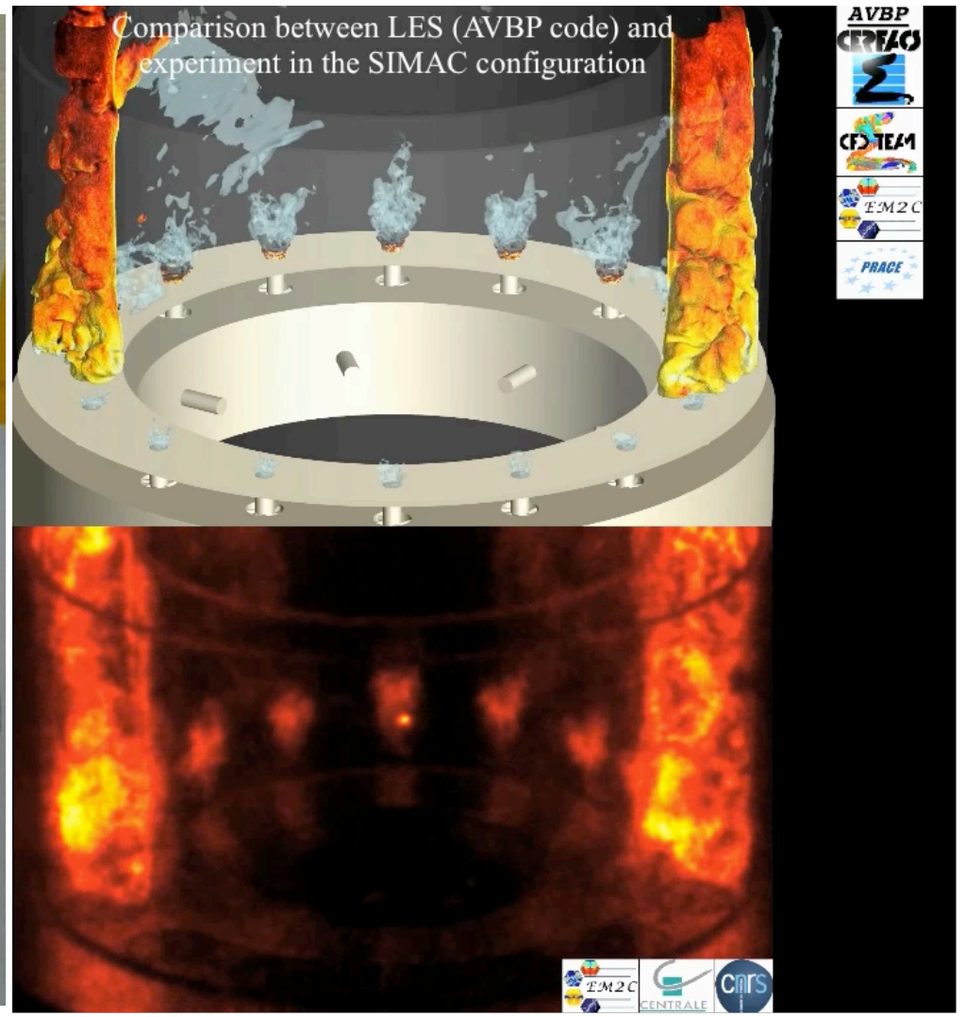


E. Riber, B. Cuenot, F. Duchaine (CERFACS),

R. Vicquelin, M. Boileau, M. Philip , T. Schmitt, S. Candel (EM2C)

Simulation of Ignition in a Multiple Annular Combustor injector and comparison with experiments





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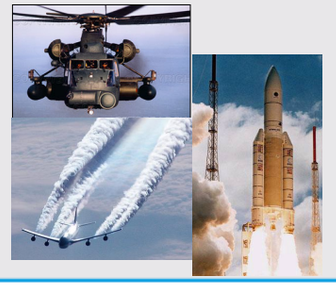
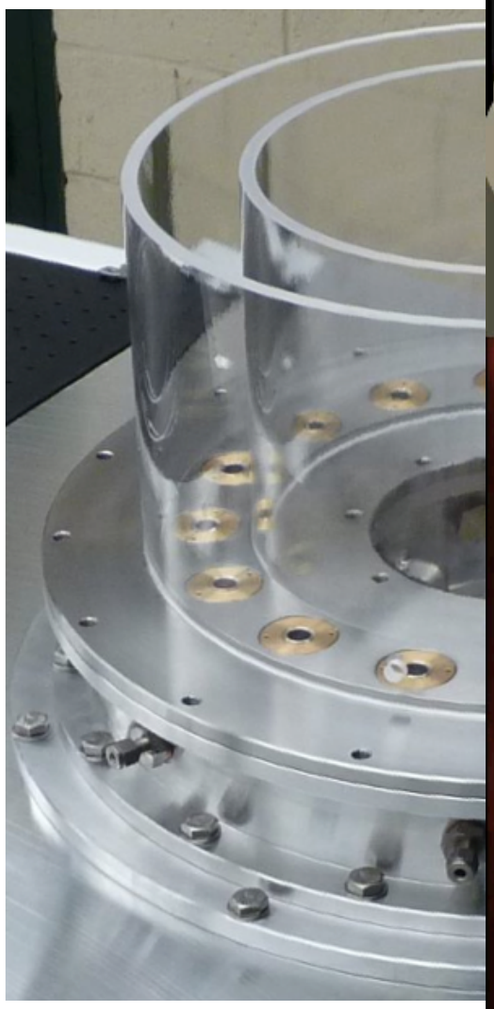
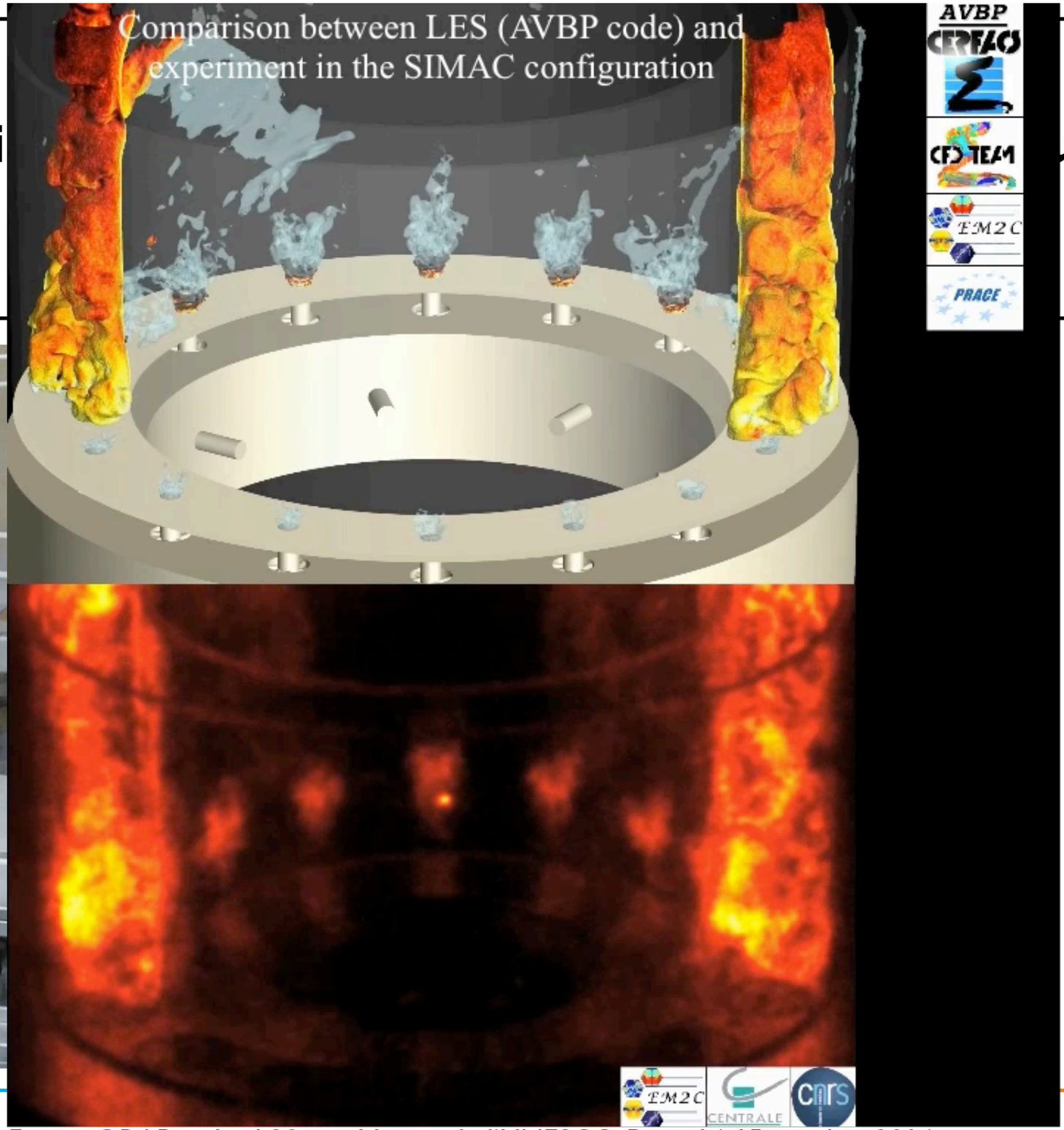
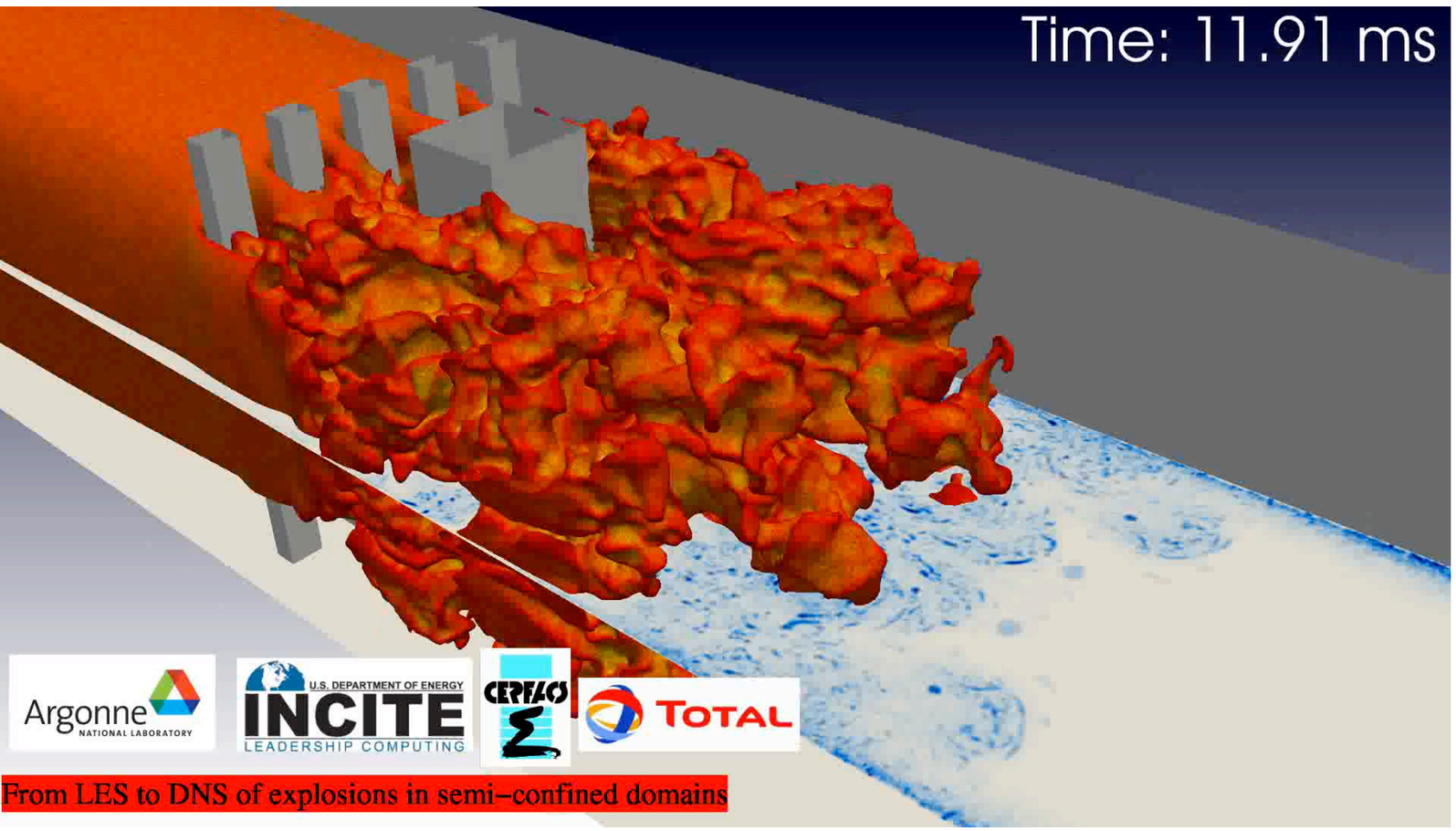


Si ular





Security and risks: « **From LES to DNS of explosions in semi-confined domains** » **-** Understand the physical phenomena involved in confined space explosions and validate the methodology for multiple scales



Sydney experiment, Masri et al

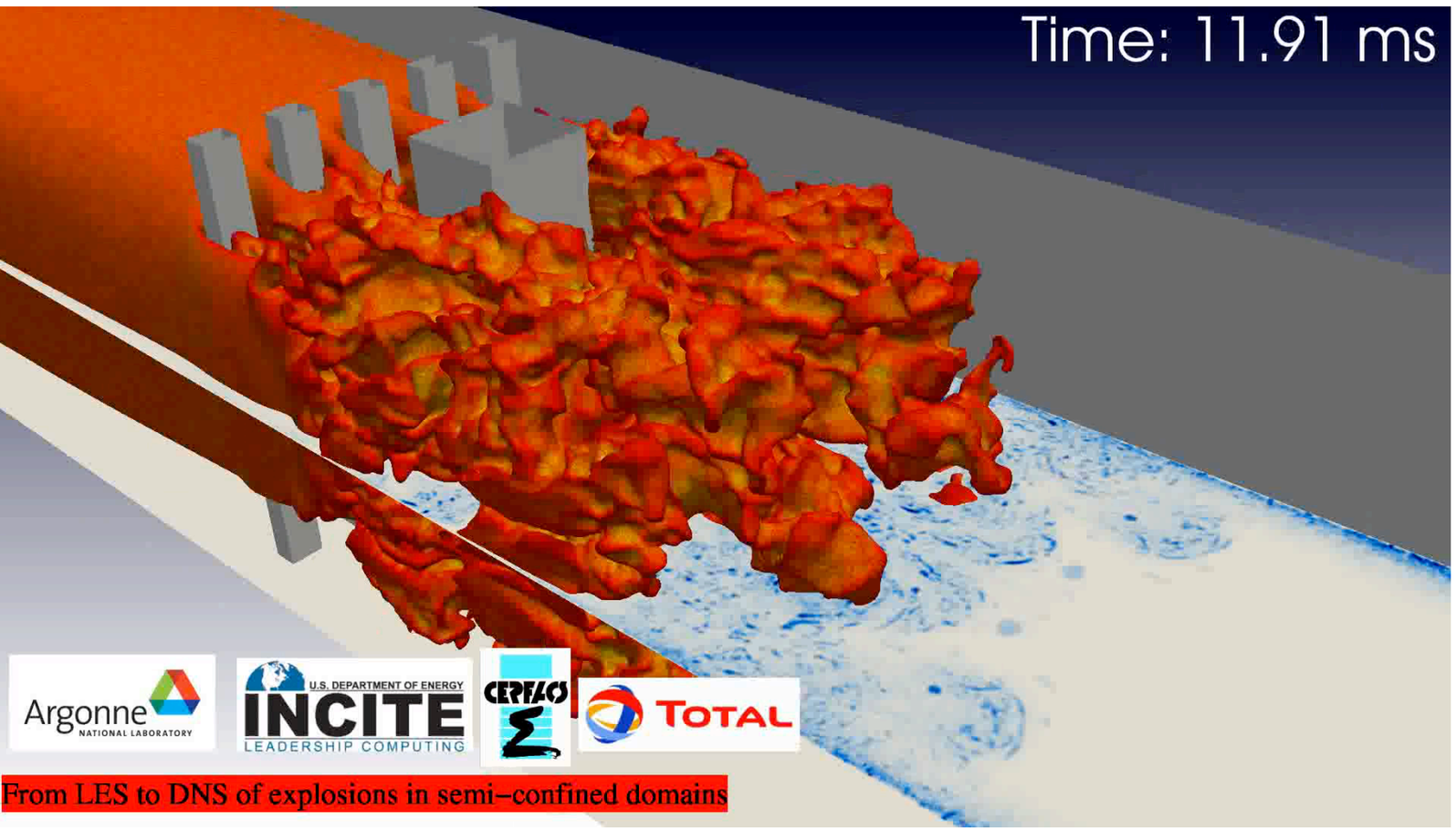
25cm length
LES and DNS (1B elements)

PhD of P. Quillatre (TOTAL Cifre)

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

2013 - 20M BG P
2014 - 86M BG Q

Security and risks: « **From LES to DNS of explosions in semi-confined domains** » **-** Understand the physical phenomena involved in confined space explosions and validate the methodology for multiple scales



Sydney experiment, Masri et al

25cm length
LES and DNS (1B elements)

PhD of P. Quillatre (TOTAL Cifre)

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

2013 - 20M BG P
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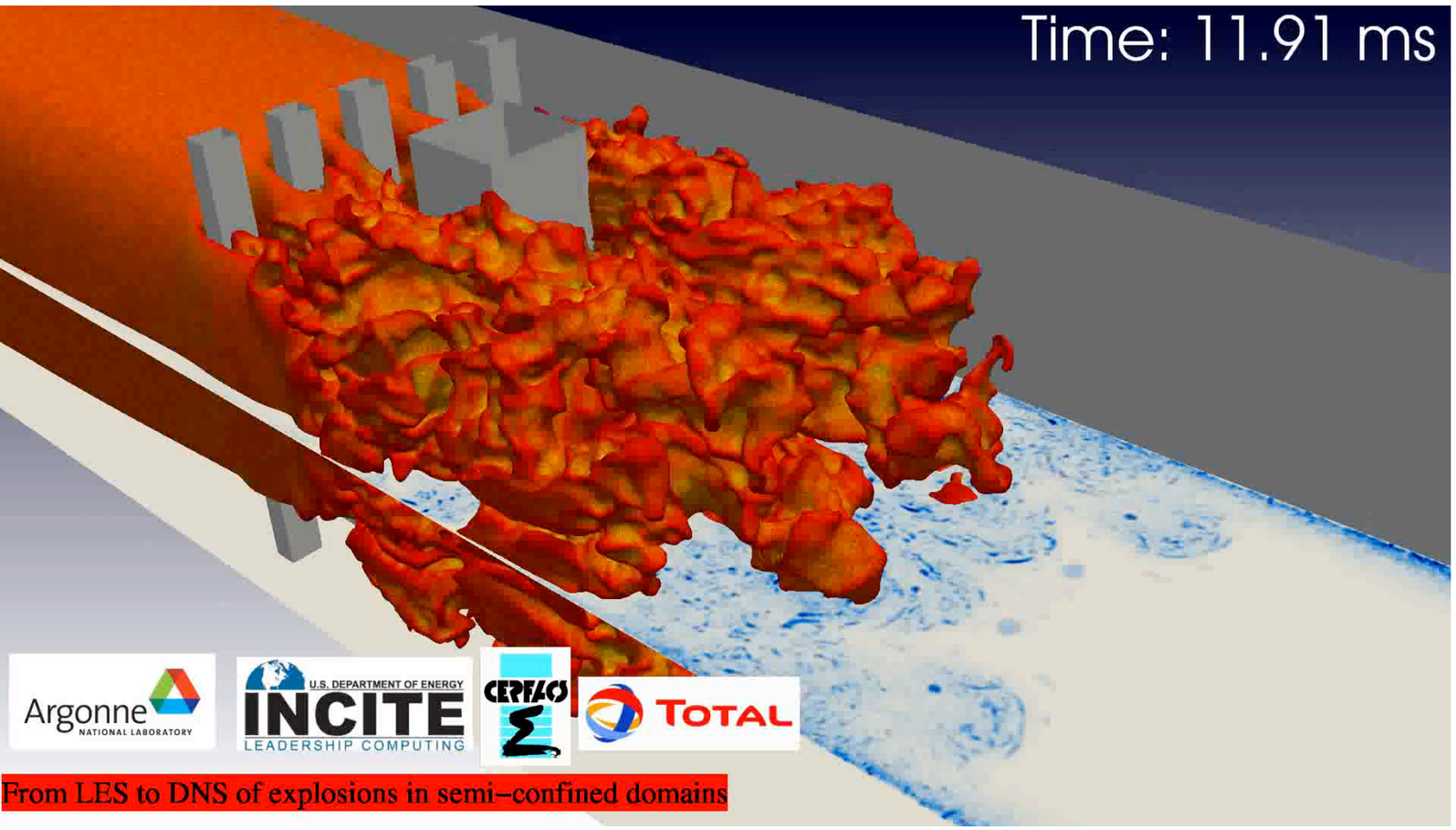

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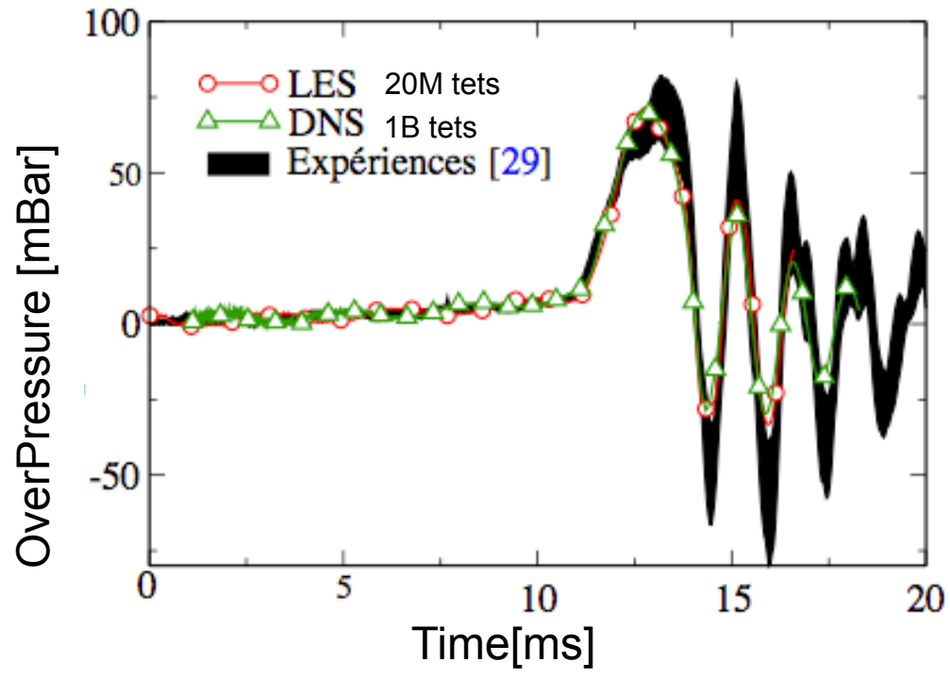

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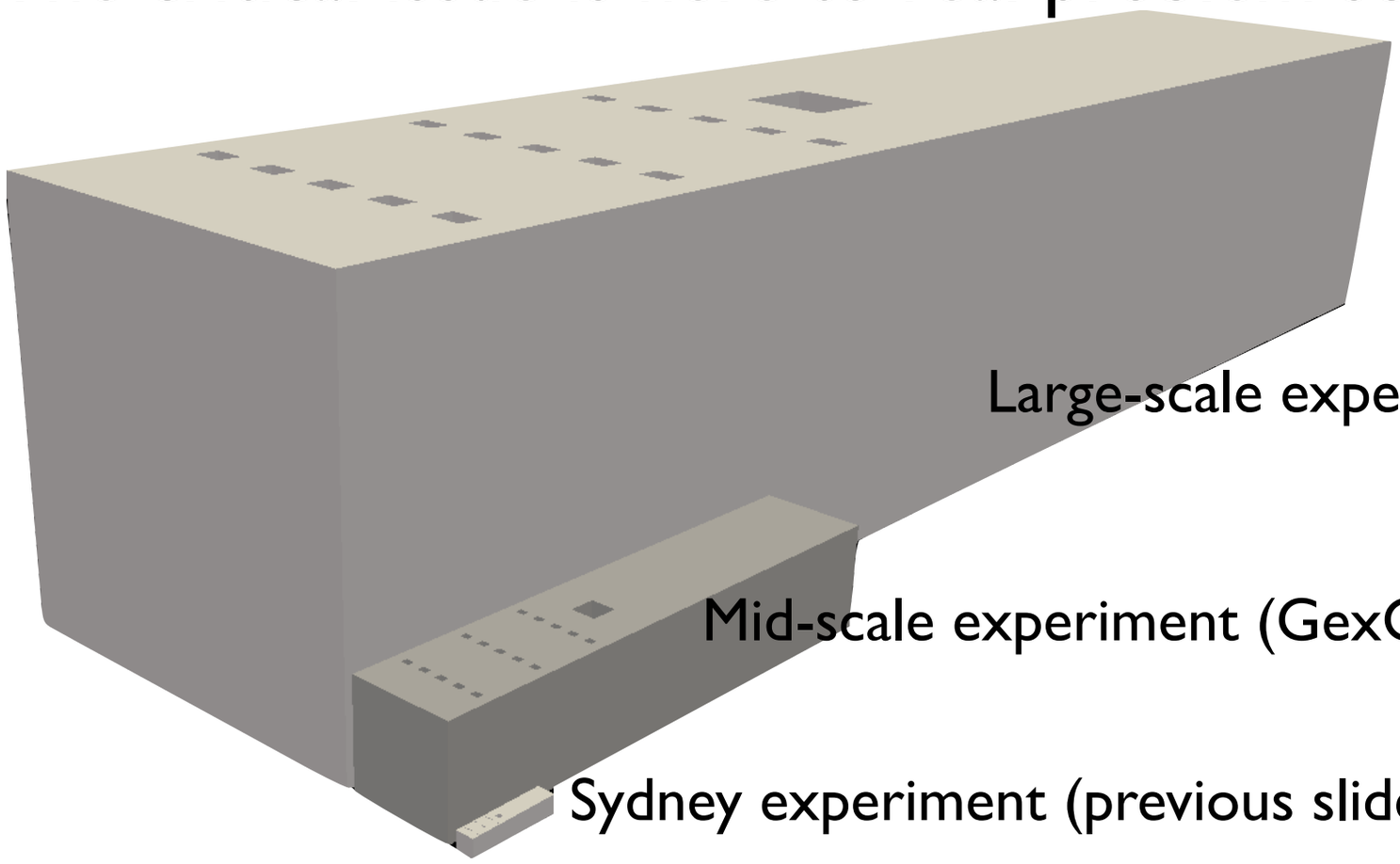
The critical issue is here to real problem scales…



Large-scale experiment (GexCon) - 6 m

Mid-scale experiment (GexCon) - 1.5 m

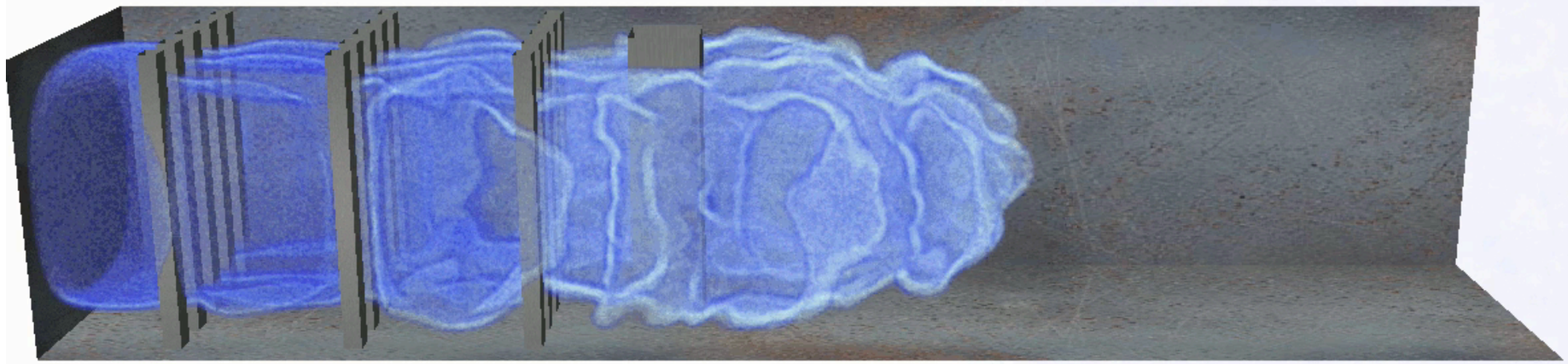
Sydney experiment (previous slide) - 25 cm

Note: 1 B elements simulations

- 1 file = 30 Gb (over 2000 snapshots needed for a temporal view of the evolution)
- One shot simulation on 32 k cores: 20 M CPUh at ALCF BG\ P
- 1 B elements scales up to 131 072 cores

Large Eddy Simulation of the 1.5 m configuration versus experiment

Experiment performed by Gexcon



Large Eddy Simulation

Time: 58.0

Large Eddy Simulation of the 1.5 m configuration versus experiment

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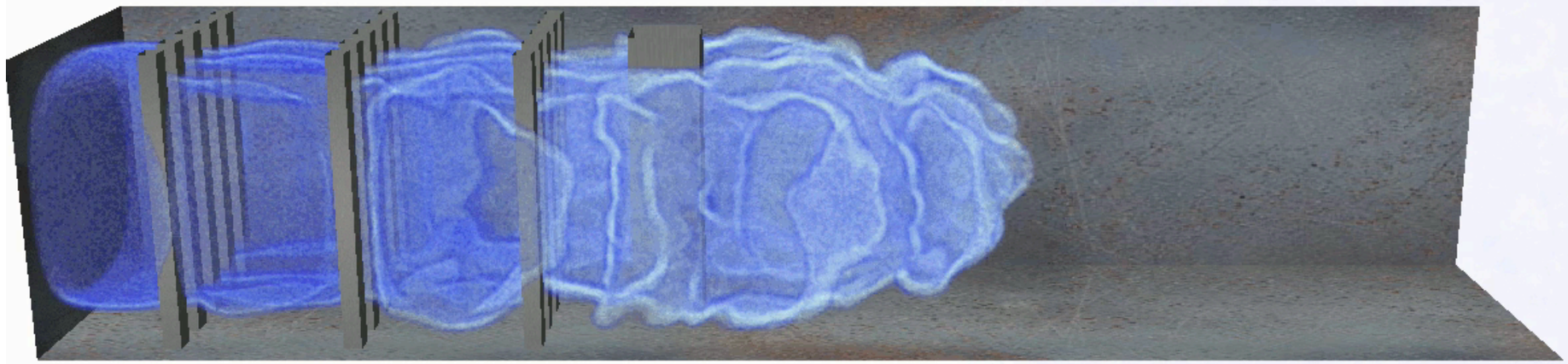


Large Eddy Simulation

Time: 58.0

Layout of the talk

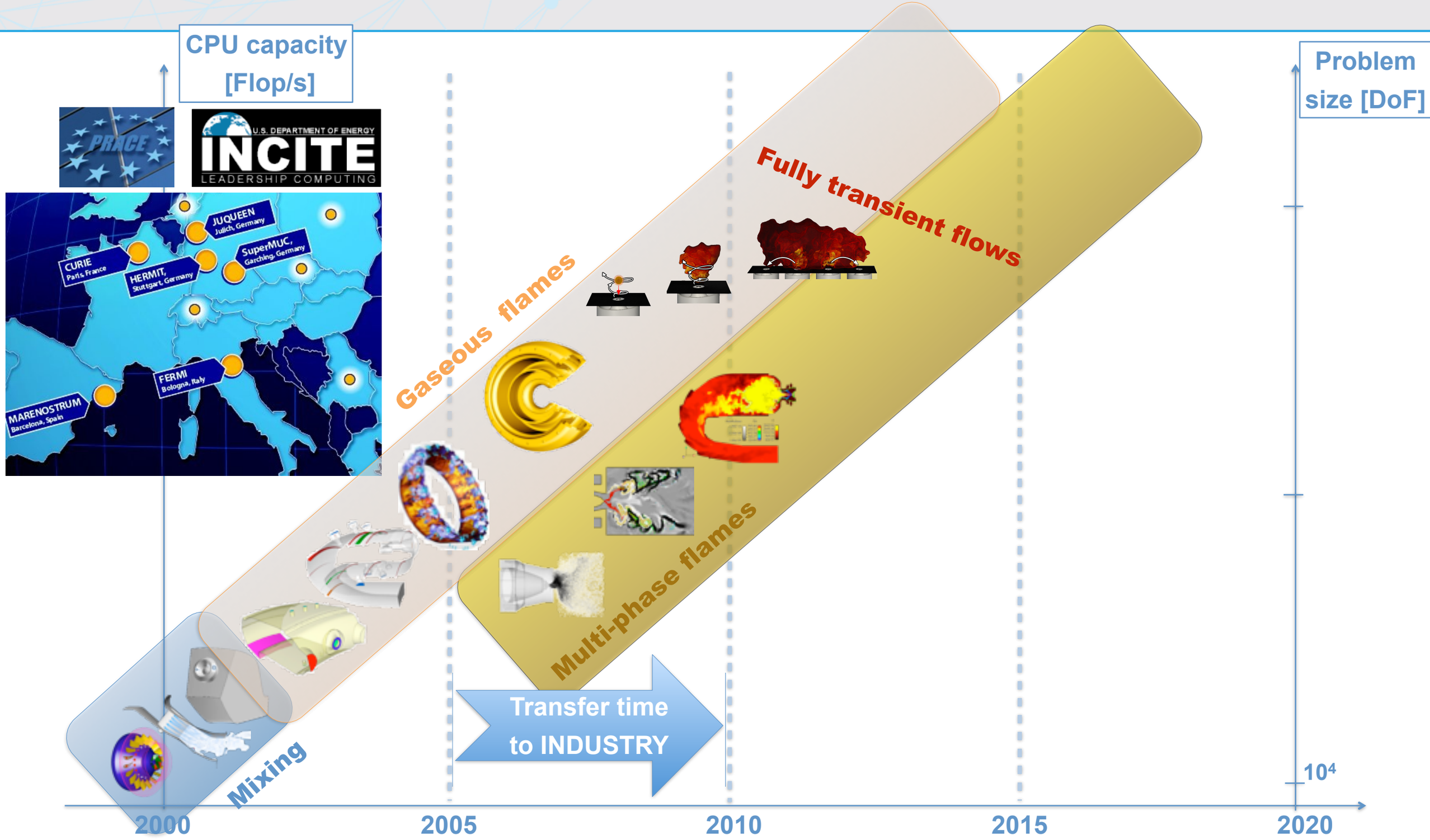
I] HPC & turbulent reacting flow CFD

- Modeling: from simplified and steady models to fully unsteady simulations
- Combustion predictions: increase in model fidelity and complexity
- Current capacities & challenges: model development and validation on fully transient problems

II] Potential trends and developments

- Towards improved numerical predictions require improved physics description - multi-physics codes
- Improved engines/applications will require technological breakthrough where more *engine components will need to be addressed in an integrated fashion* because they will interfere

II] Potential trends and developments



II] Potential trends and developments

CPU capacity [Flop/s]

Problem size [DoF]

PRACE

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

Gaseous flames

Fully transient flows

Multi-phase flames

Multi-physics

Mixing

Transfer time to INDUSTRY

Palm & CWIPI

Open Source LGPL

O-Palm*

* http://www.cerfacs.fr/globc/PALM_WEB/

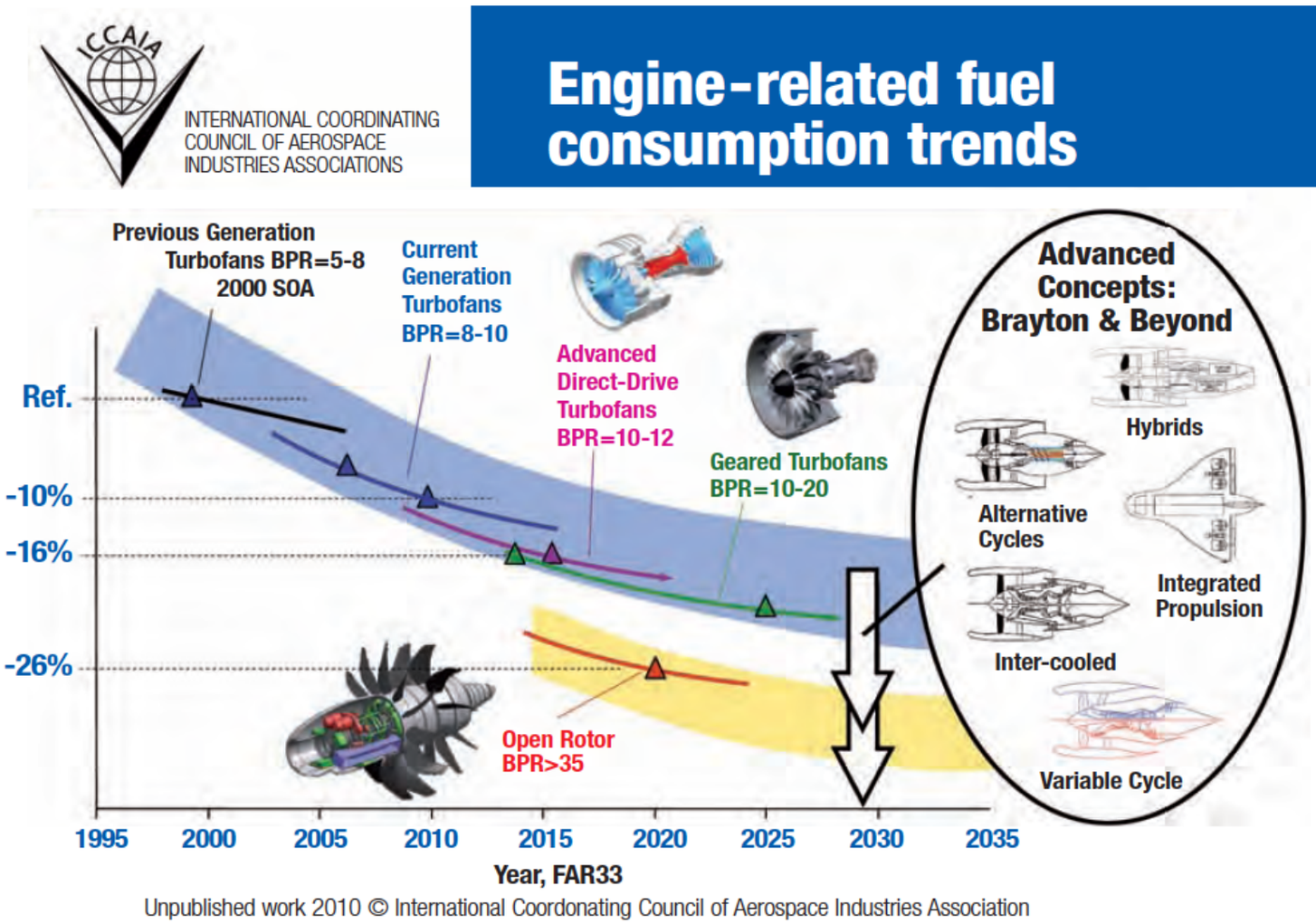
2000 2005 2010 2015 2020

10^4

Industrial needs point to the look for technological breakthroughs: i.e. new thermodynamic cycles, downsizing, integrated systems…

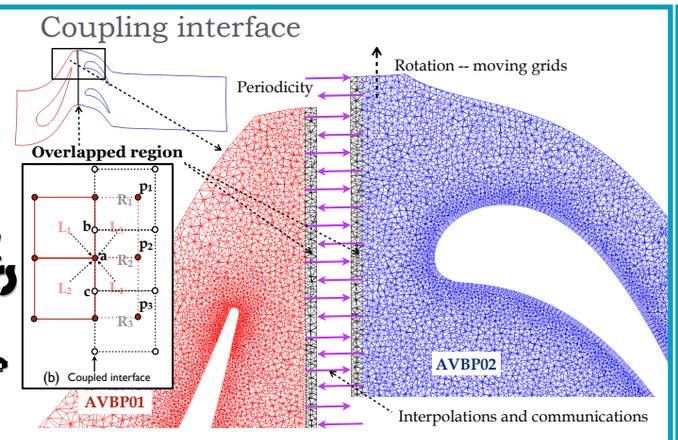
Again CFD is a potential tool to invest in this uncharted territory. The « only investment » and « risk » to manage are the **ability of codes and models to address properly the problems**…

… *as well as the CPU that will go with it* …



Multi-scale/Multi-instance CFD solution to address geometrically or temporally imbalanced systems [1,2]…

Moving parts



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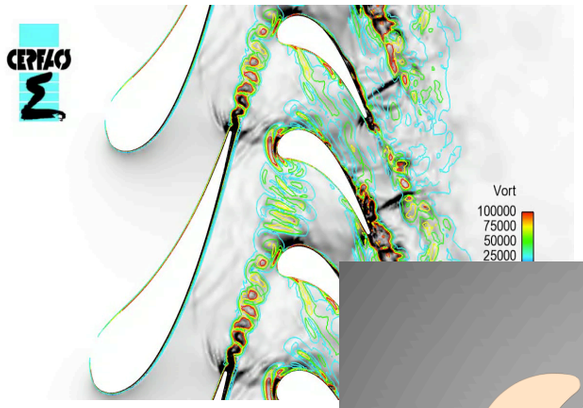
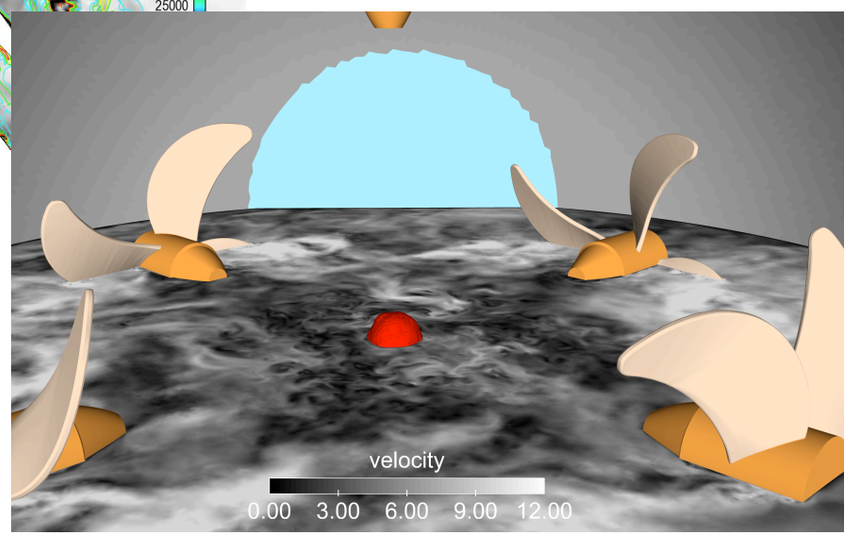
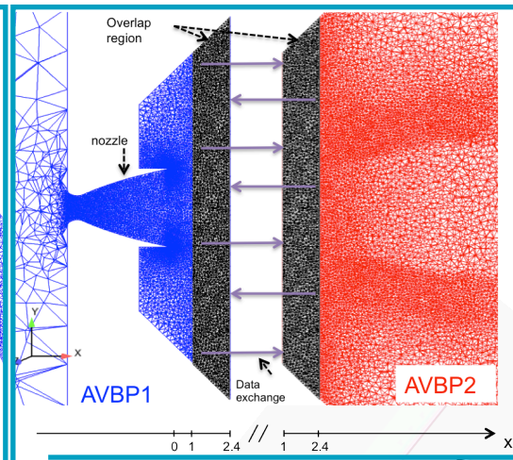




STAE TOULOUSE

SAFRAN AEROSPACE · DEFENCE · SECURITY

Wide range of time scales



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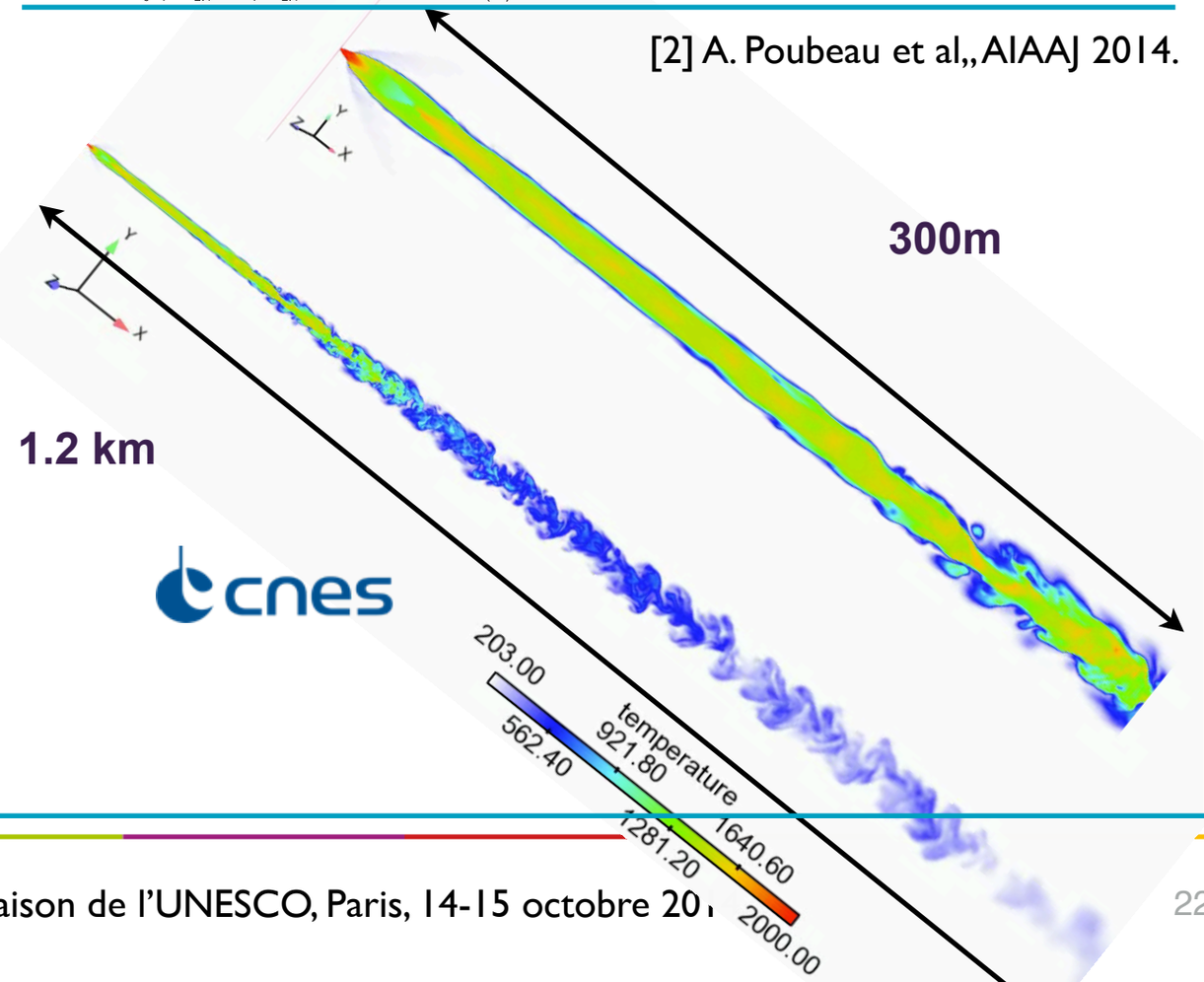

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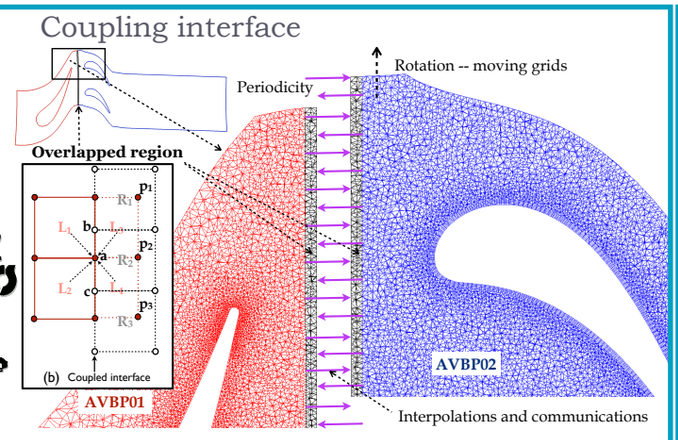

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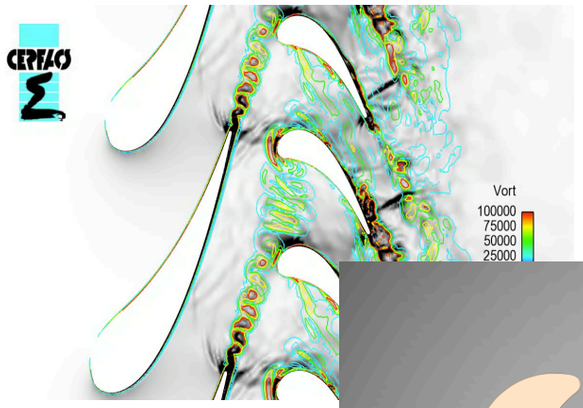

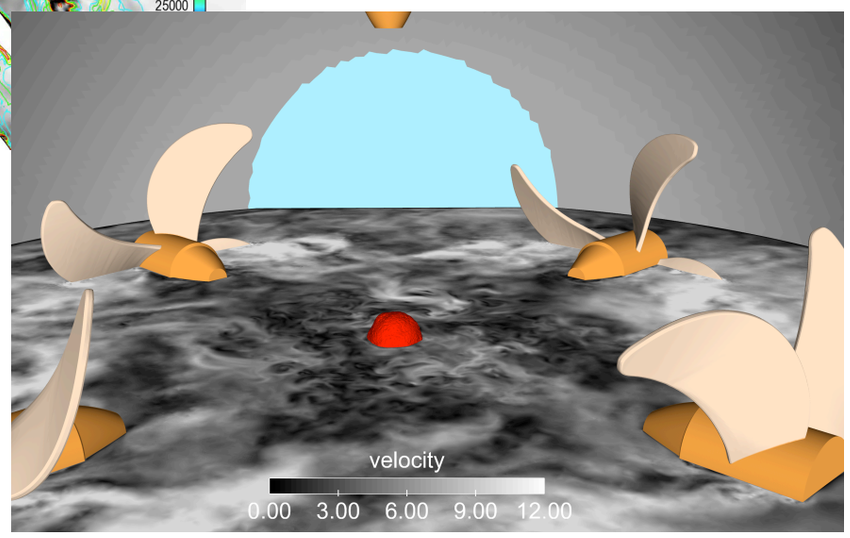

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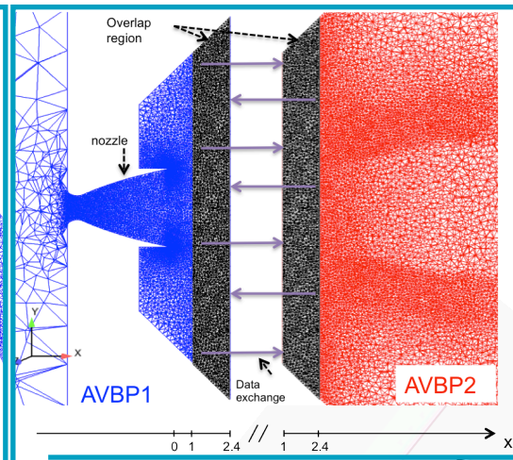

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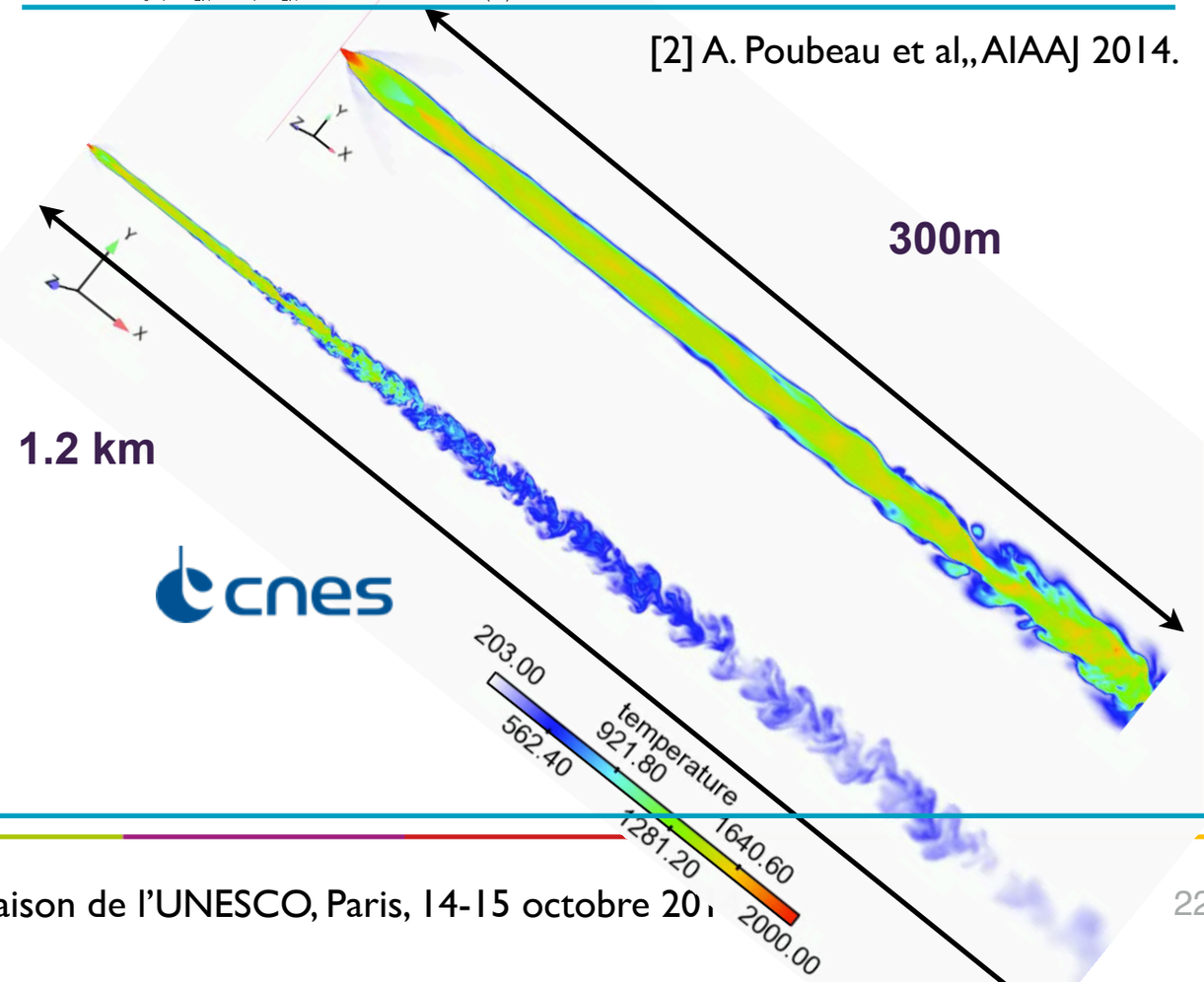

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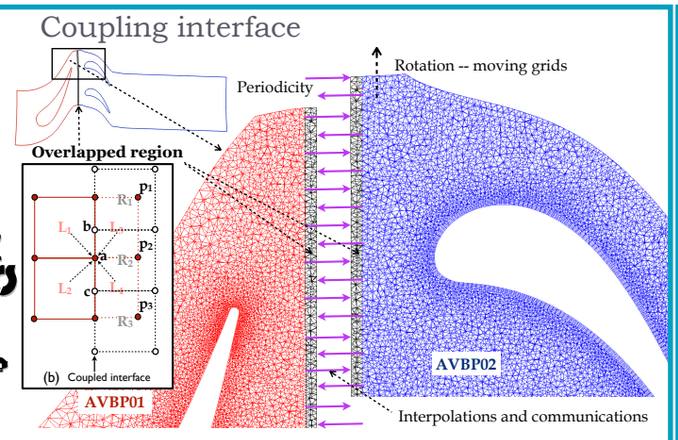

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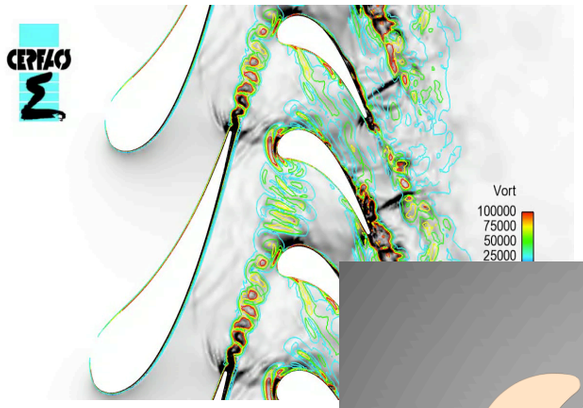

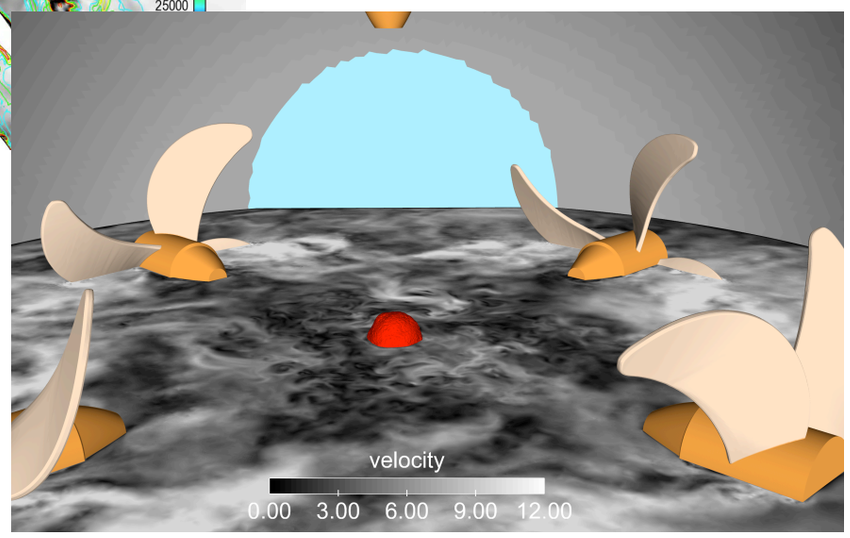

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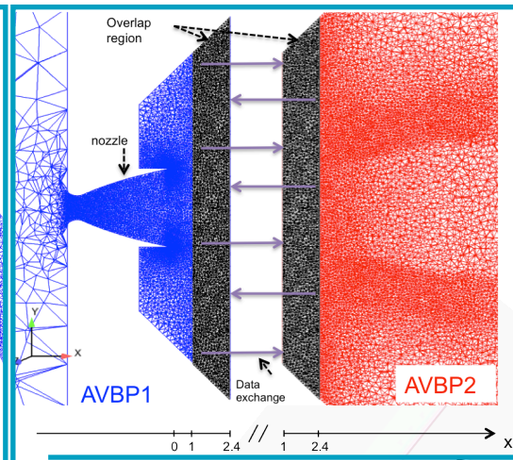

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