HPC and combustion

G. Staffelbach

A. Dauptain, E. Riber, O. Vermorel, L. Gicquel, B. Cuenot, F. Duchaine, J. Dombard

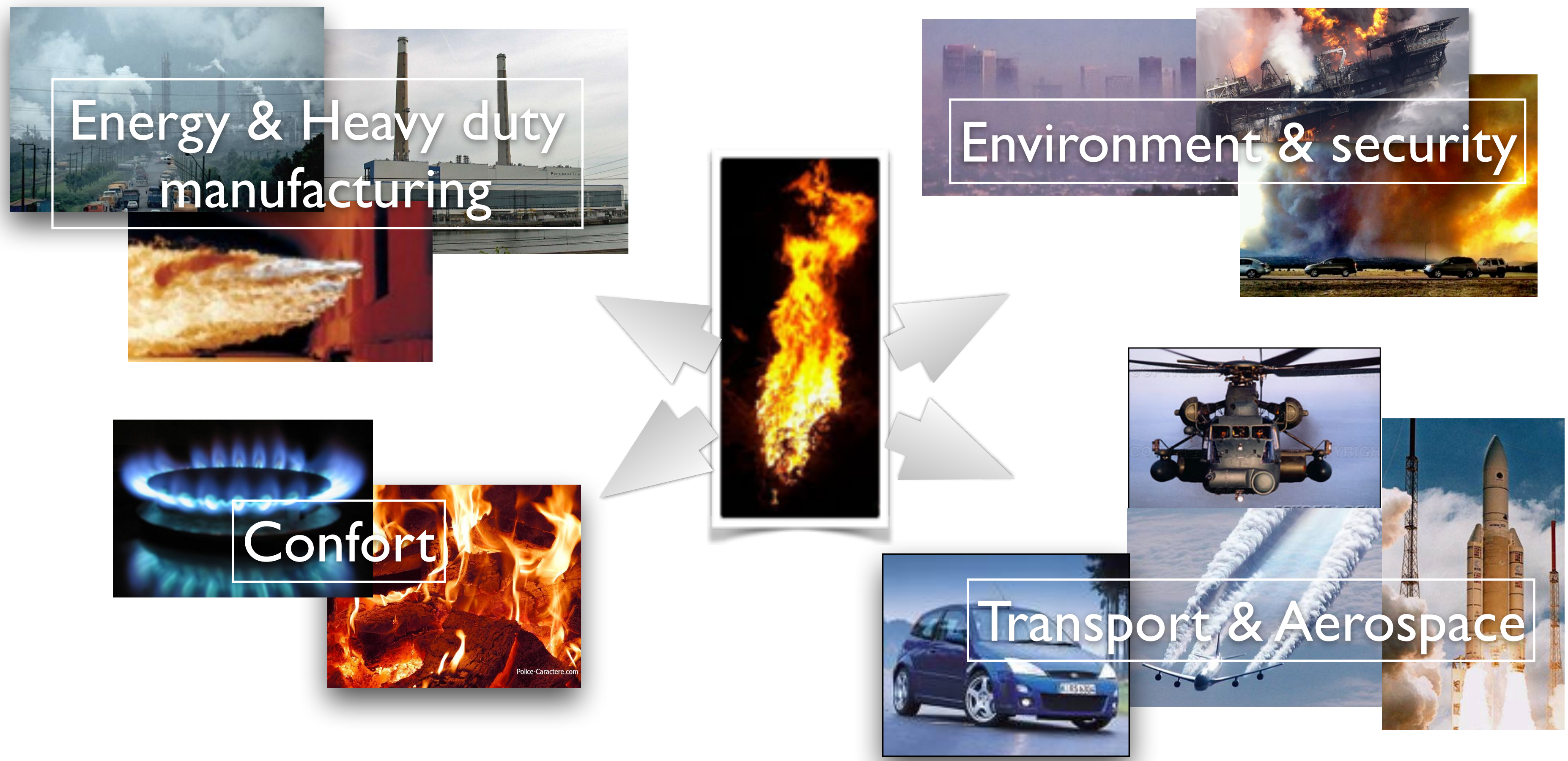
and lots of Phds…

CERFACS

- ➡ non-profit research center in Toulouse France
- ➡ 150 people :
  - Climate change
  - Sparse matrix algorithms
  - Atmospheric pollution
  - Computational Fluid Dynamics
    - Aerodynamics
    - Turbomachinery
    - Combustion

Context

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



Context

➡ Pollution and climate change definitely will …

Context

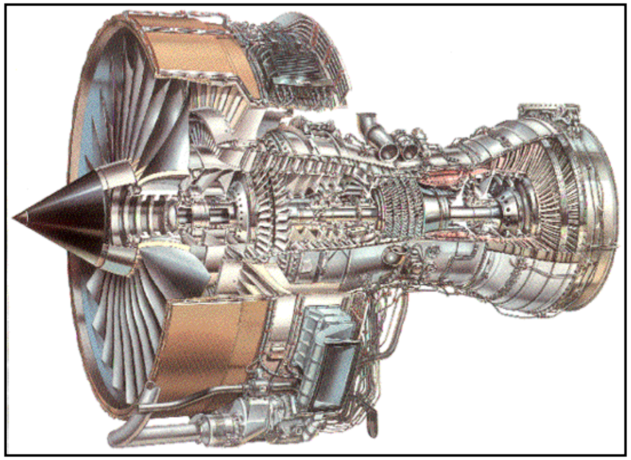
- Definite need to optimise combustion processes

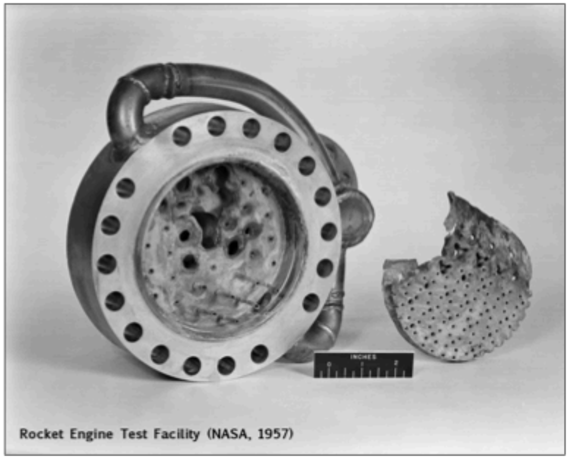
- Via new technologies:
  - New fuels ?
  - New materials ?
  - New operating conditions ?

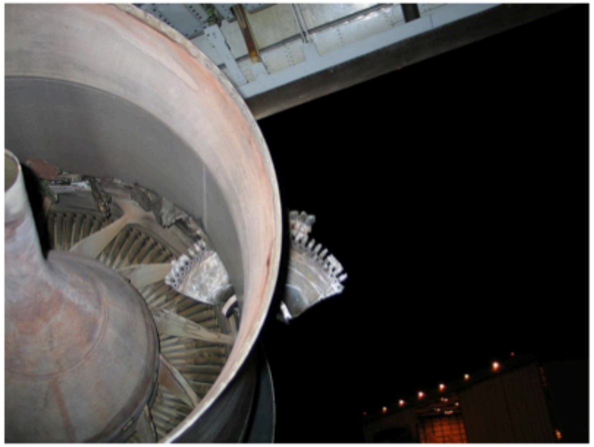
- Optimizing combustion is a priority but ..

Context

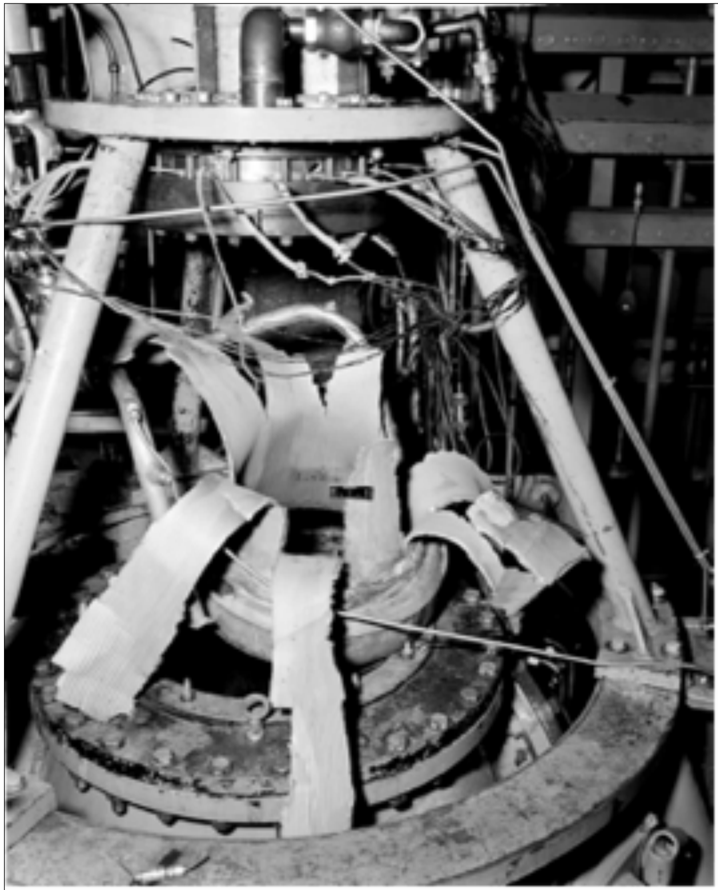
- ➡ New conditions can lead to new problems …
- One of the usual problems encountered during optimization of combustion systems is combustion ***instabilities*** (« thermoacoustics » in combustion)



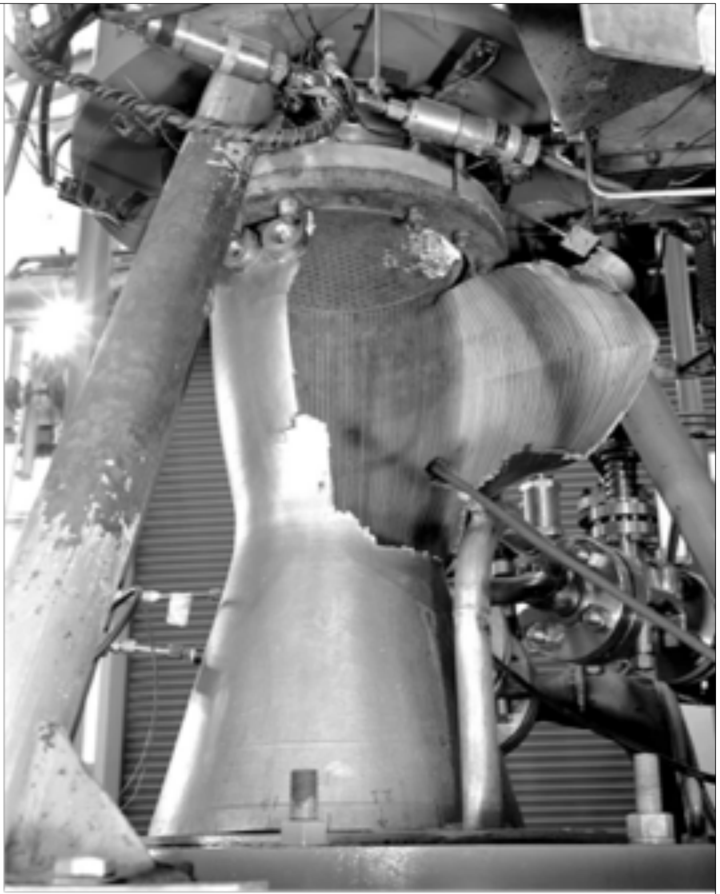




Context



Liquid rocket engine (NASA 1957)



Liquid rocket engine (NASA 1963)

What is a combustion instability ?

- Very simple experiment (40$)

+

What is a combustion instability ?

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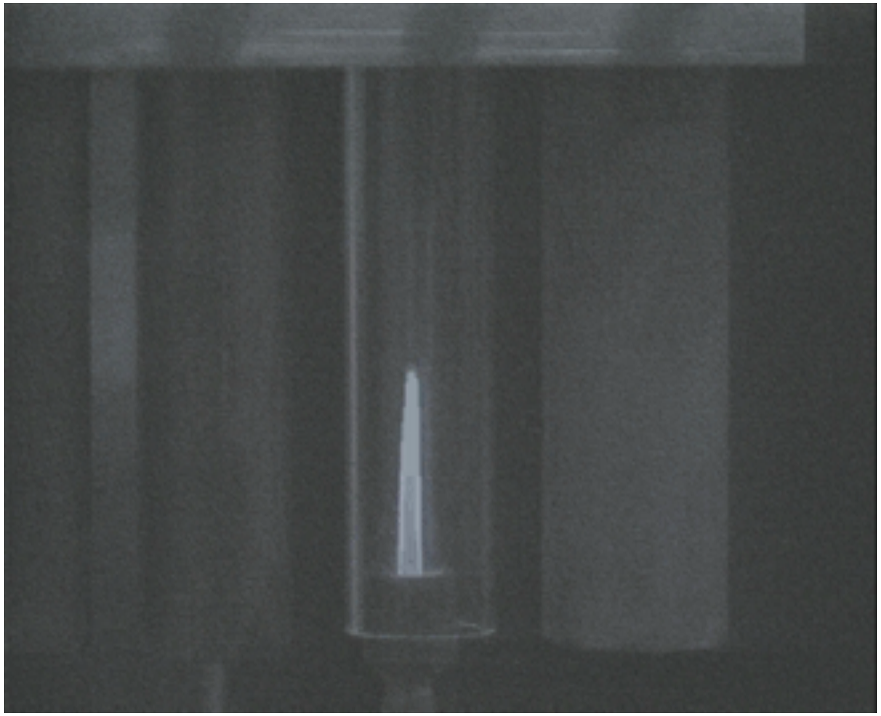
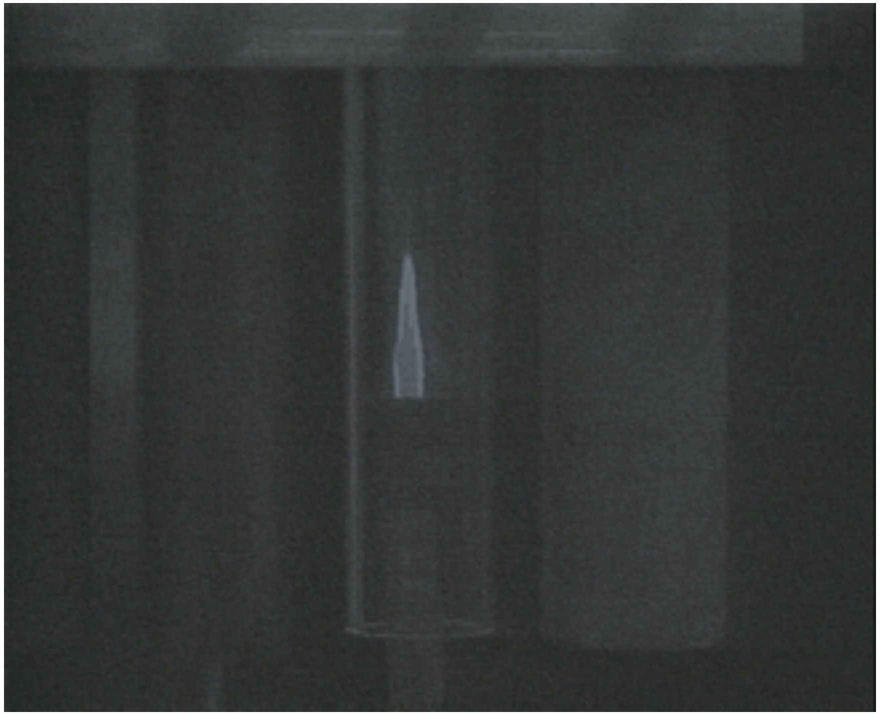
What is a combustion instability ?

- Same experiment with glass walls (Dr Durox, EM2C Paris): 2000 $ experiment (quartz)



STABLE



UNSTABLE

What is a combustion instability ?

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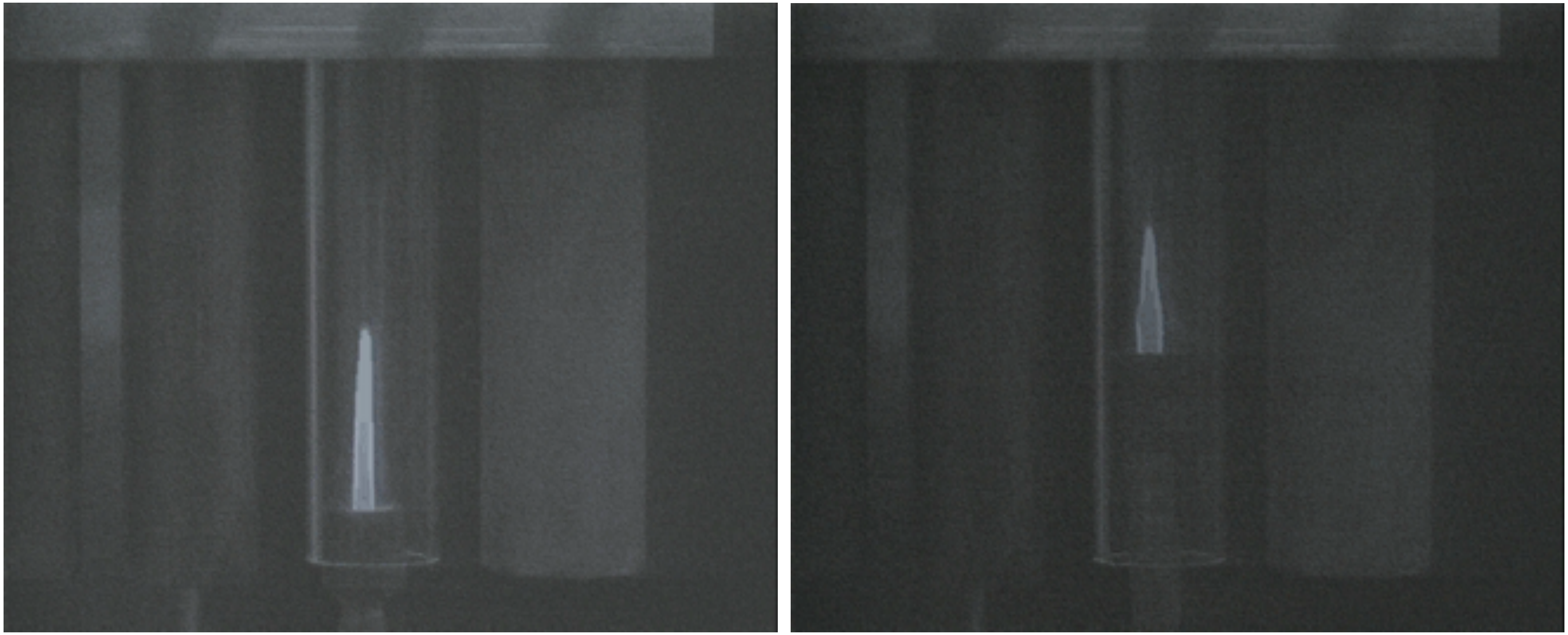

STABLE UNSTABLE

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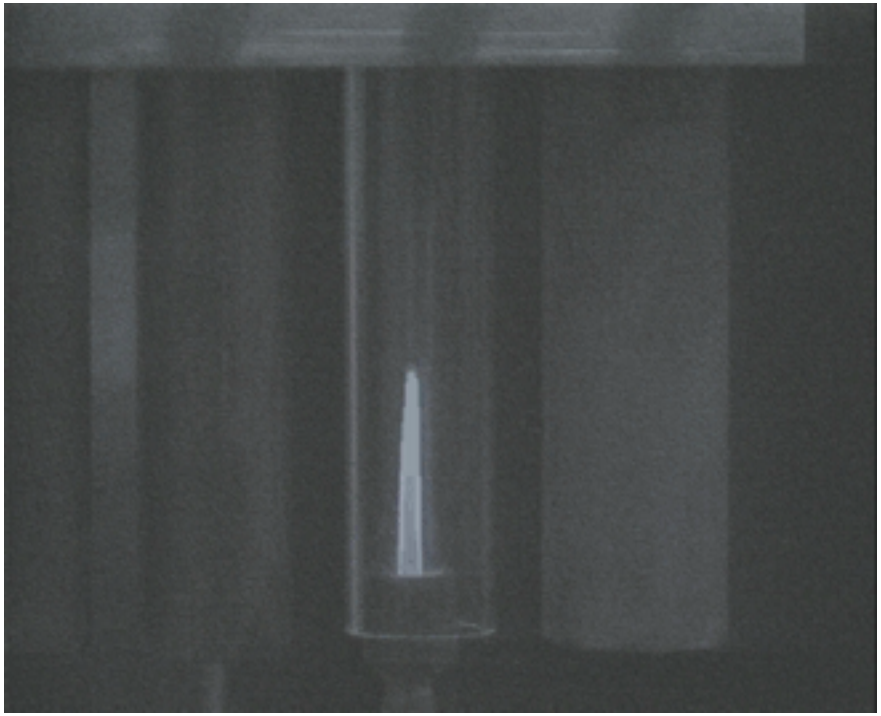
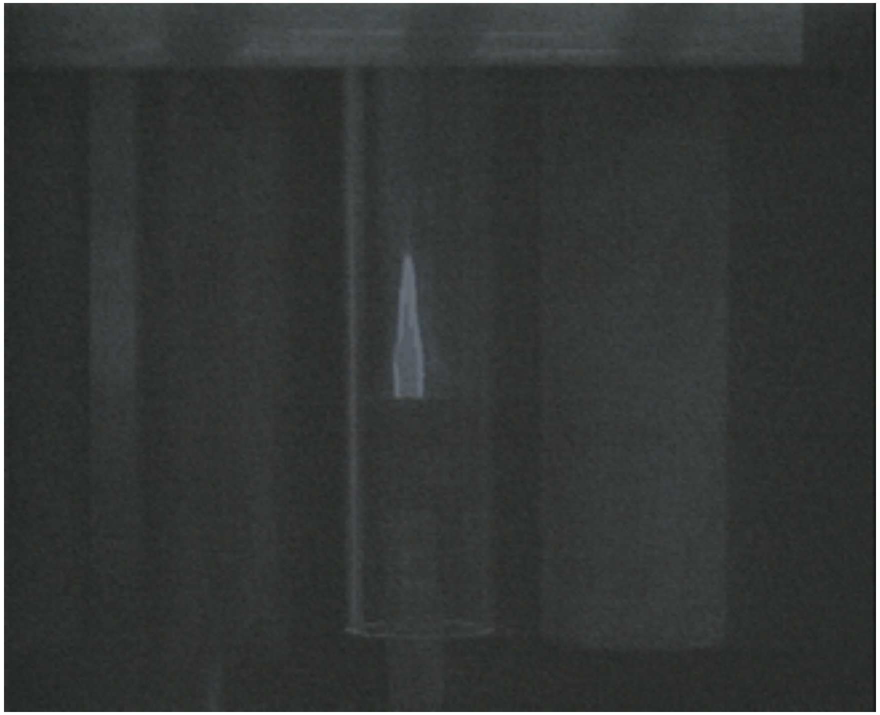
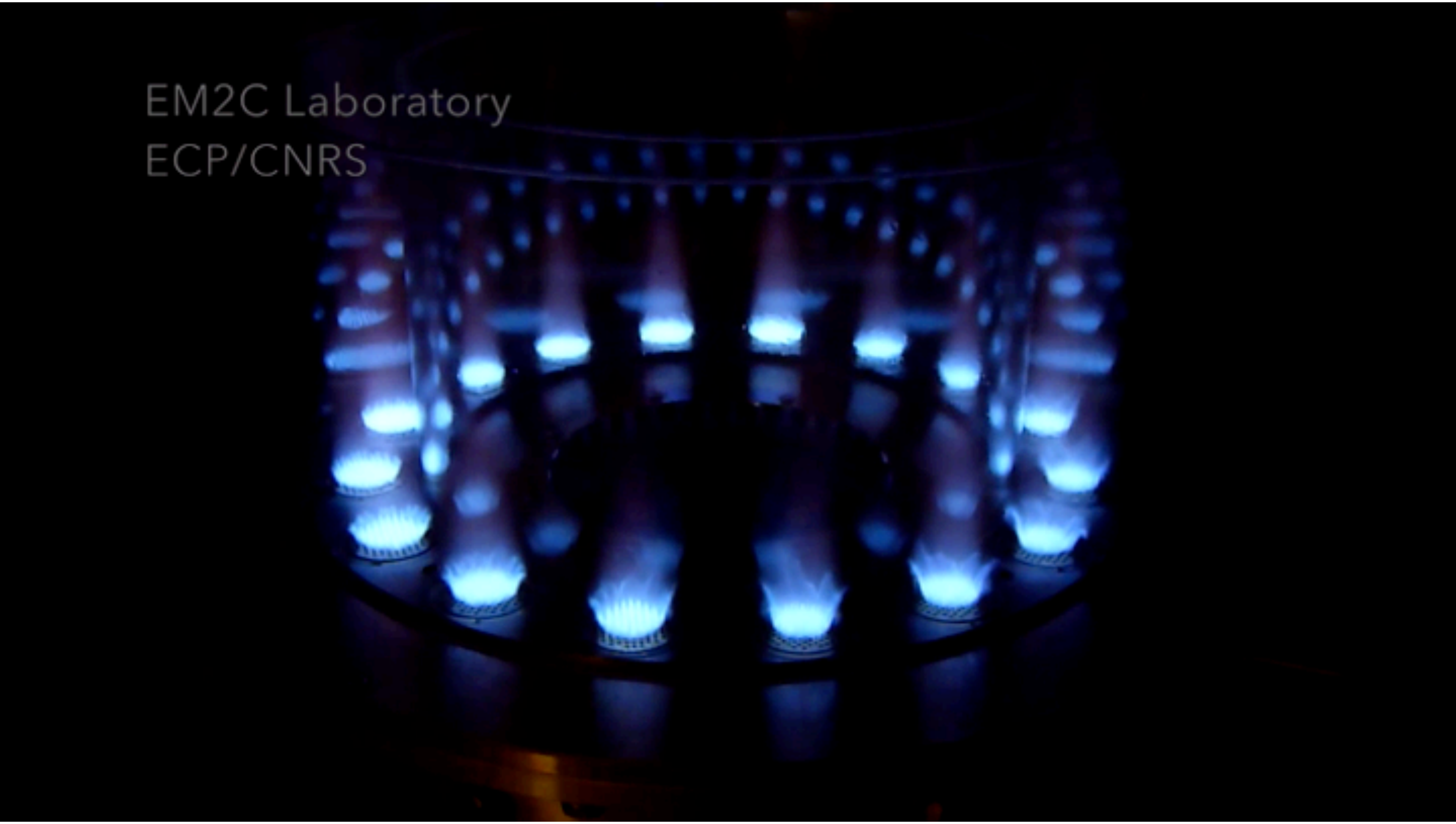


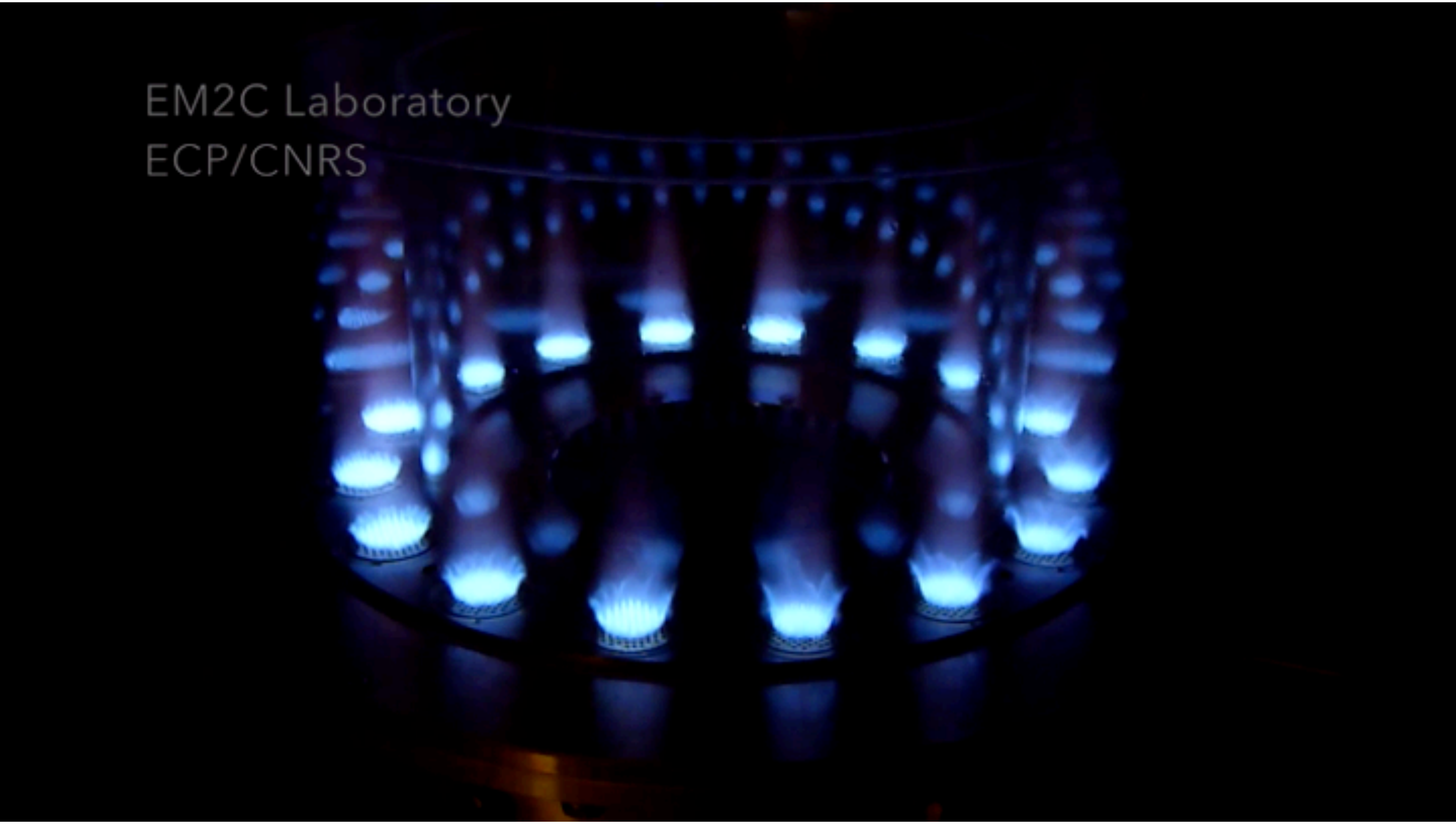


STABLE UNSTABLE

What is a combustion instability ?

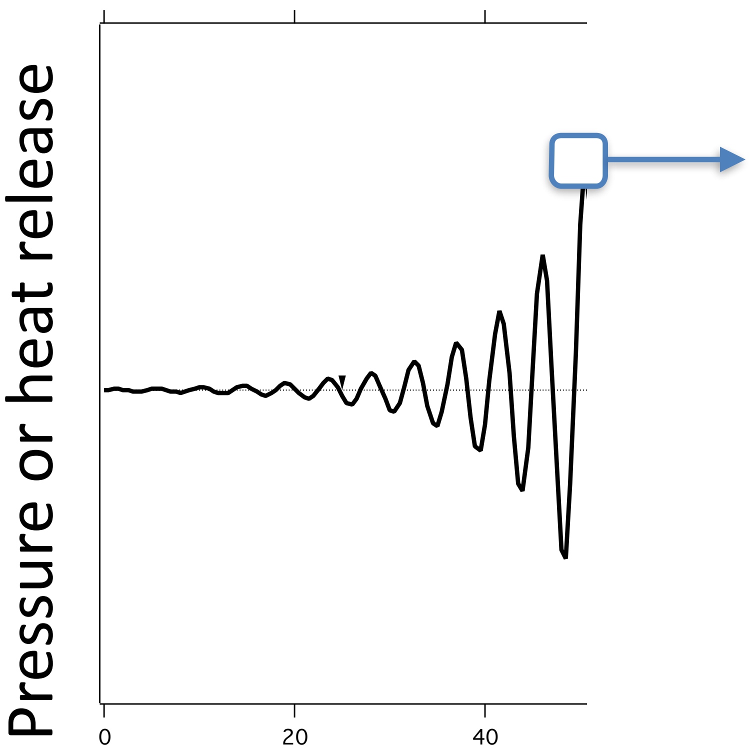


What is a combustion instability ?

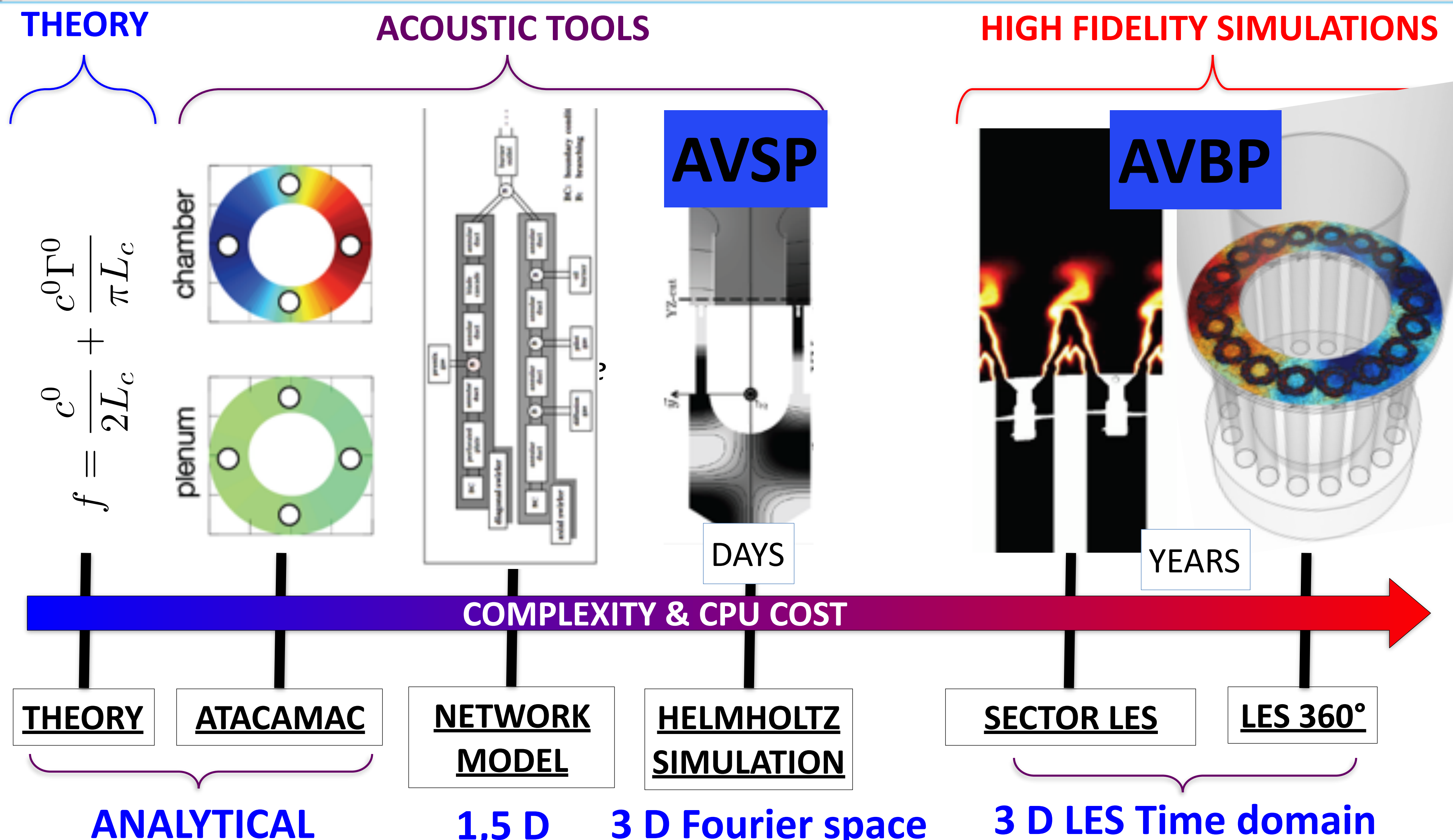


What is a combustion instability ?

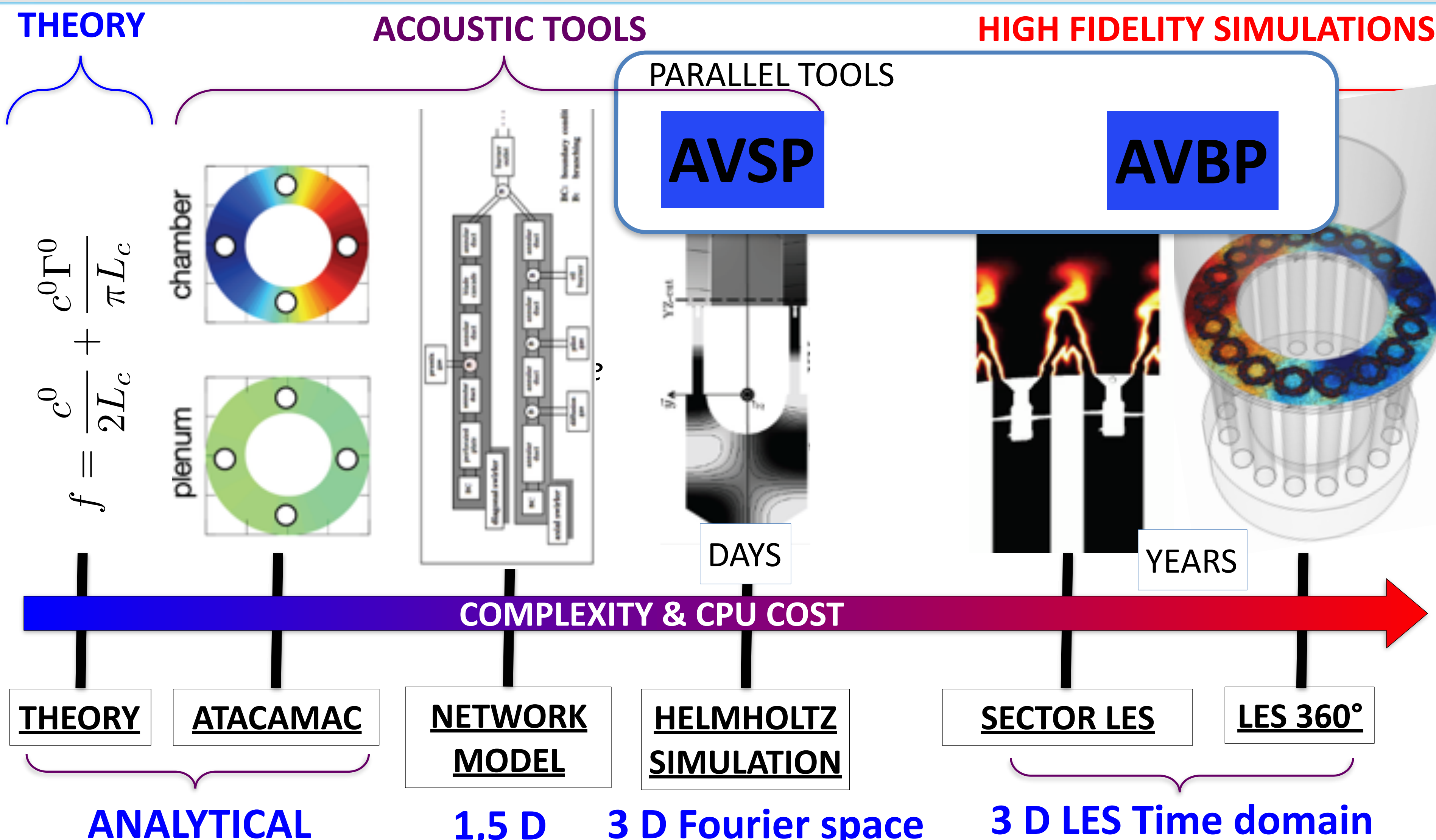
- If oscillation attain a high enough level …



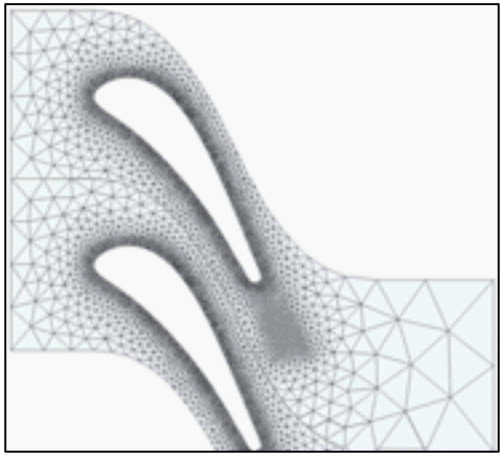
CERFAC Tools



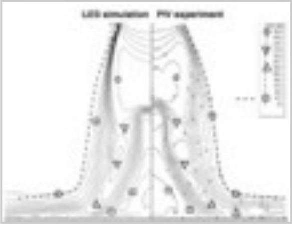
CERFAC Tools

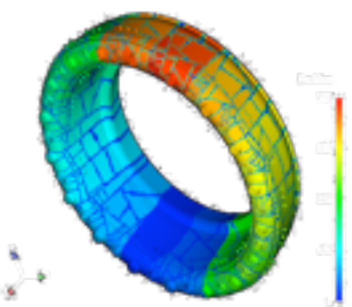


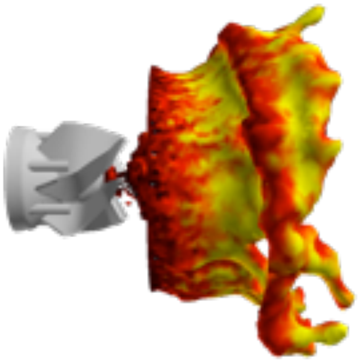
The AVBP code

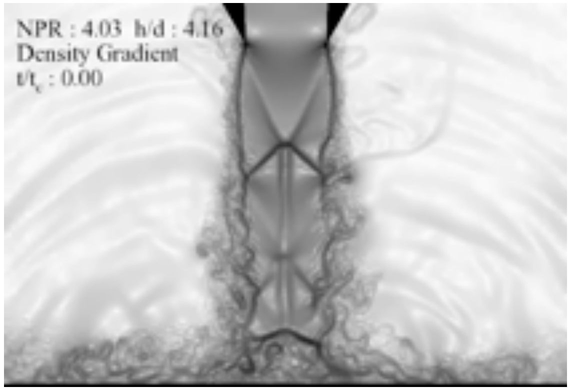


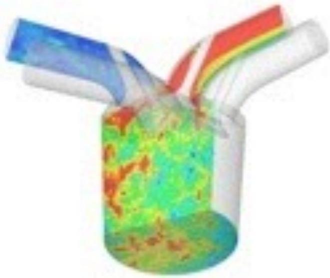
- Developed by CERFACS and IFP-EN,
- External/internal flows,
- Fully compressible turbulent reacting flows (ideal & real gases),
- DNS/LES approaches,
- Unstructured hexahedral, tetrahedral, prisms & hybrid meshes,
- Massively parallel,
- C/Fortran languages,
- SPMD approach.
- Multi-phase solvers (Lagrangian & Eulerian)











2013 PRACE Scientific Annual Report 'success story'

'Most innovative industrial HPC solution in Europe' in ISC'2013

An open science project

RESEARCH ENTITIES

EM2C (Centrale Paris)
IMFT (Toulouse)
CORIA (Rouen)
ONERA
TU Munich
U. Twente
Von Karman institute
U. Sherbrooke
CIEMAT Madrid
ETH Zurich
Gent University

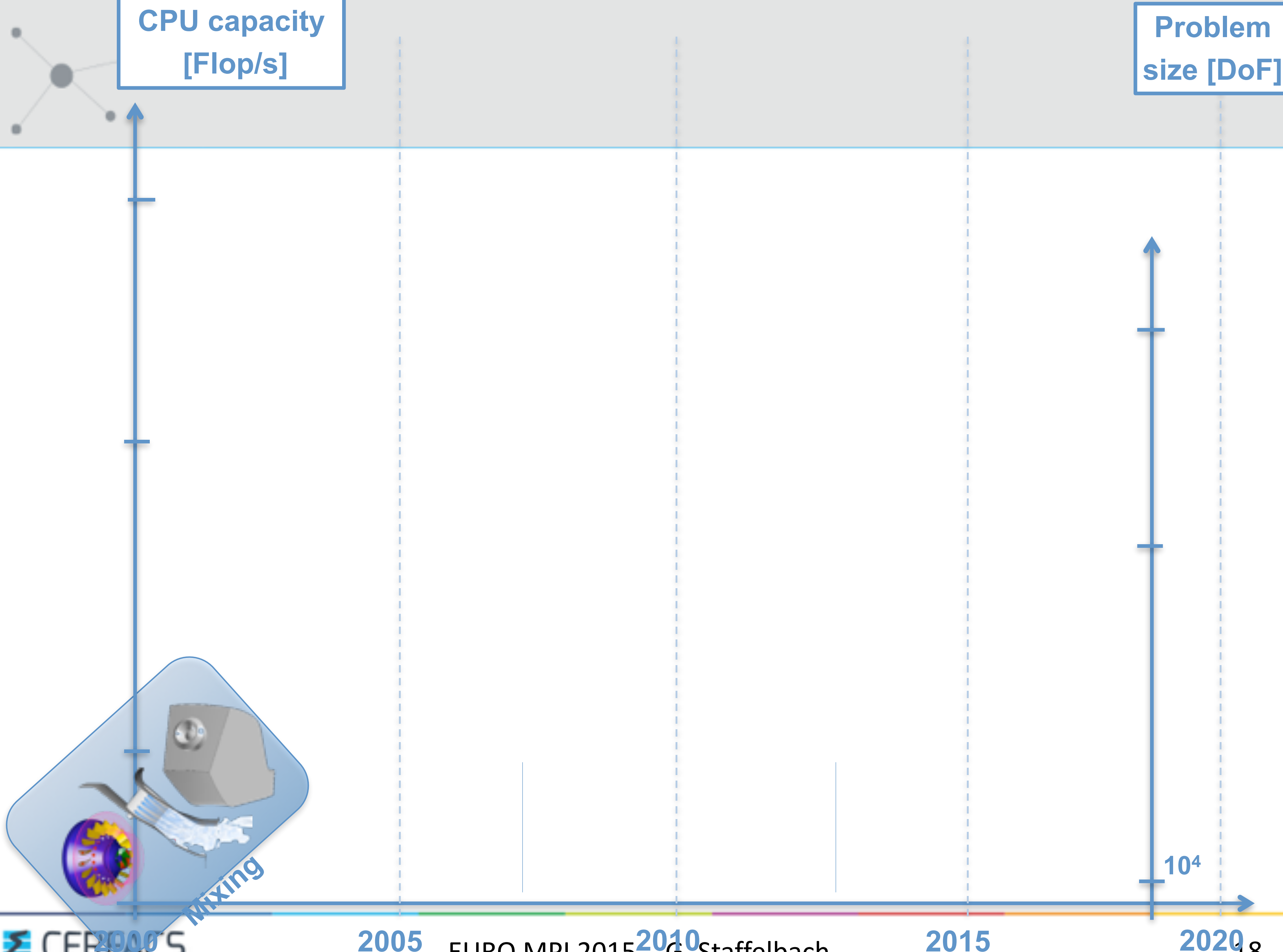
CERFACS

INDUSTRY

SNECMA
TURBOMECA
TOTAL
SNECMA Vernon
RENAULT
PSA
ALSTOM
ANSALDO
HONEYWELL
SIEMENS
AIR LIQUIDE
GDF

HPC centers (IDRIS,CINES,BSC,GENCI, CEA TGCC, ARNL,ORNL,JSC)

INTEL IPCC DEEP FP7 EU project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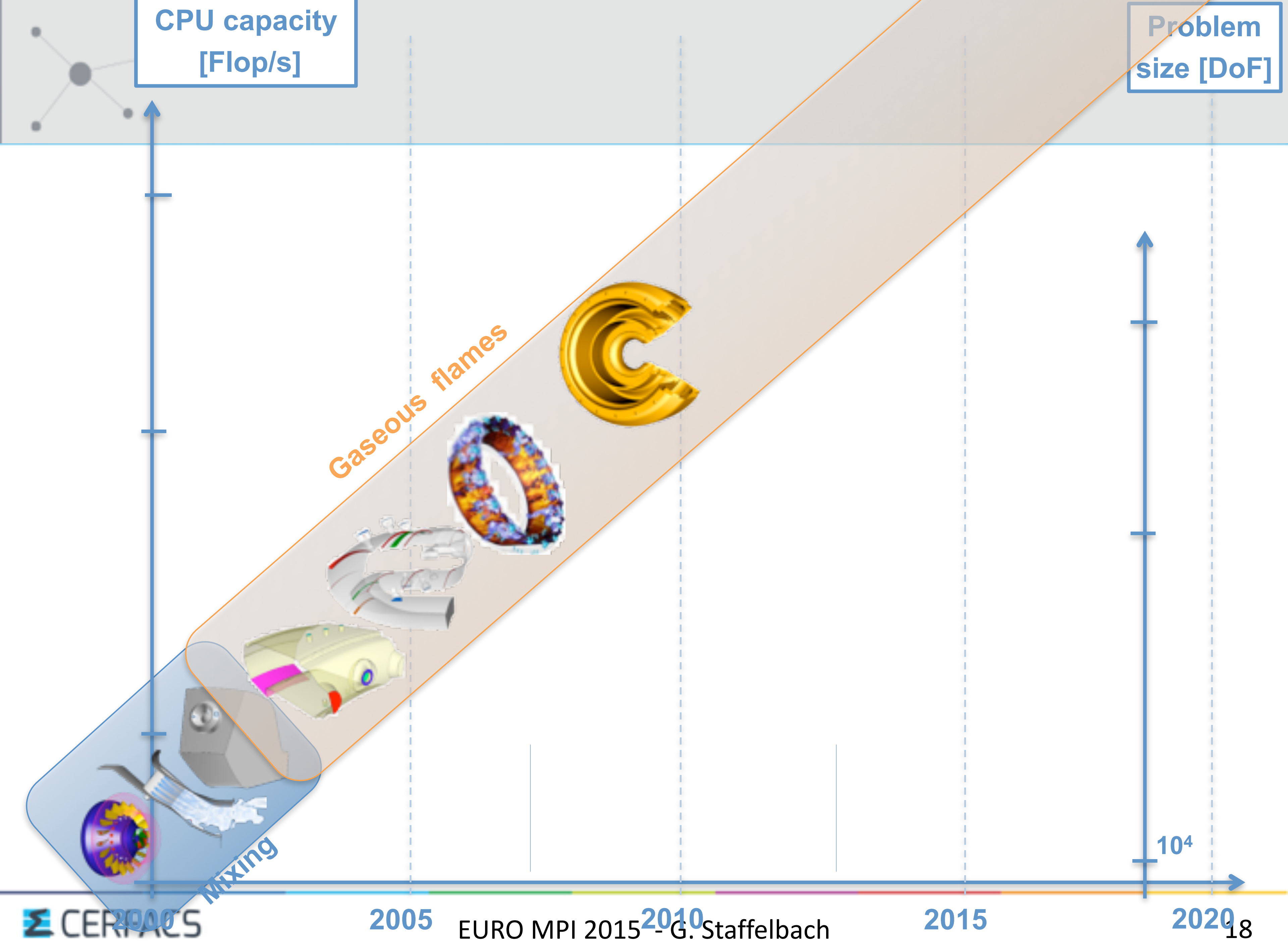
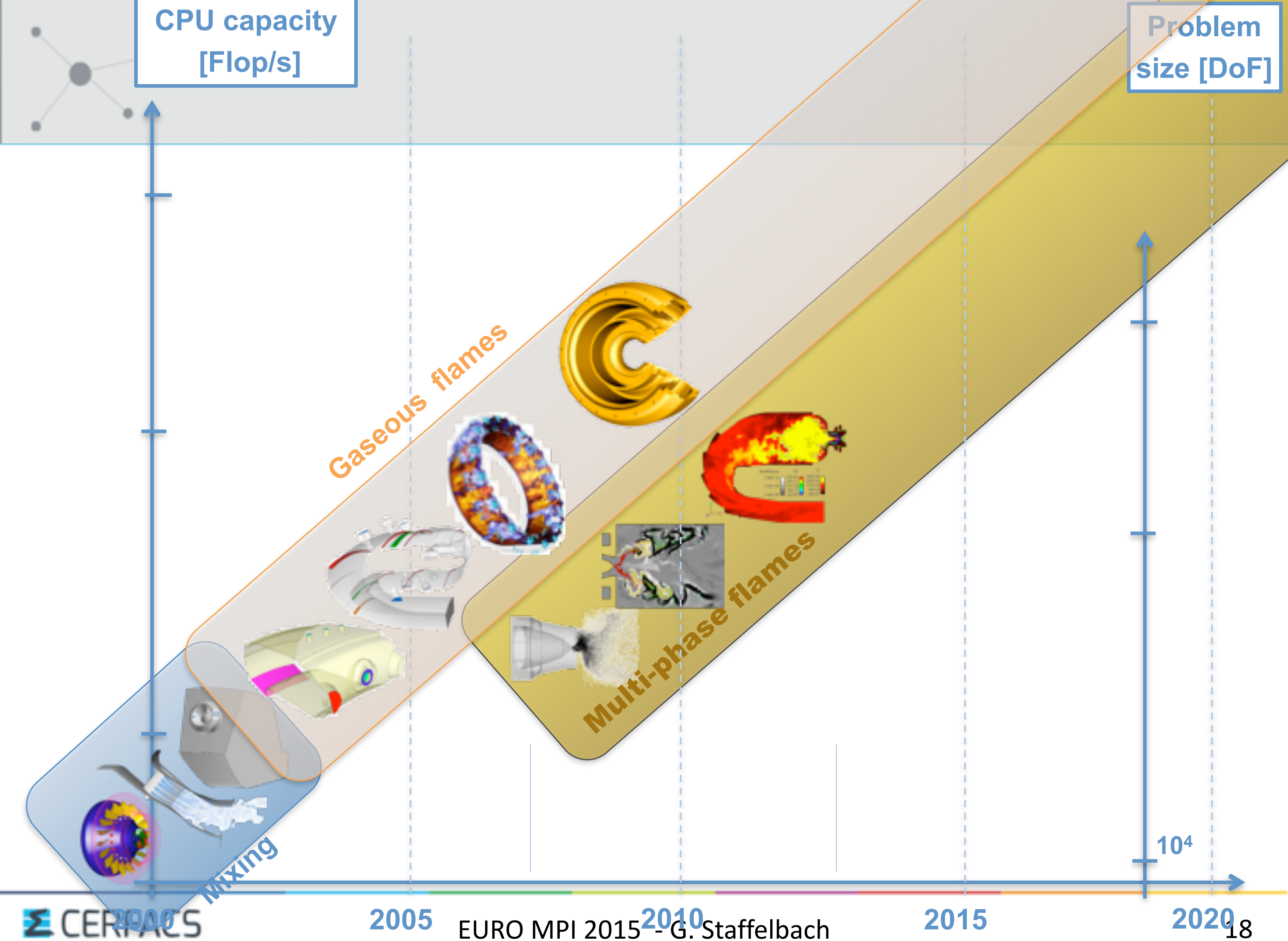
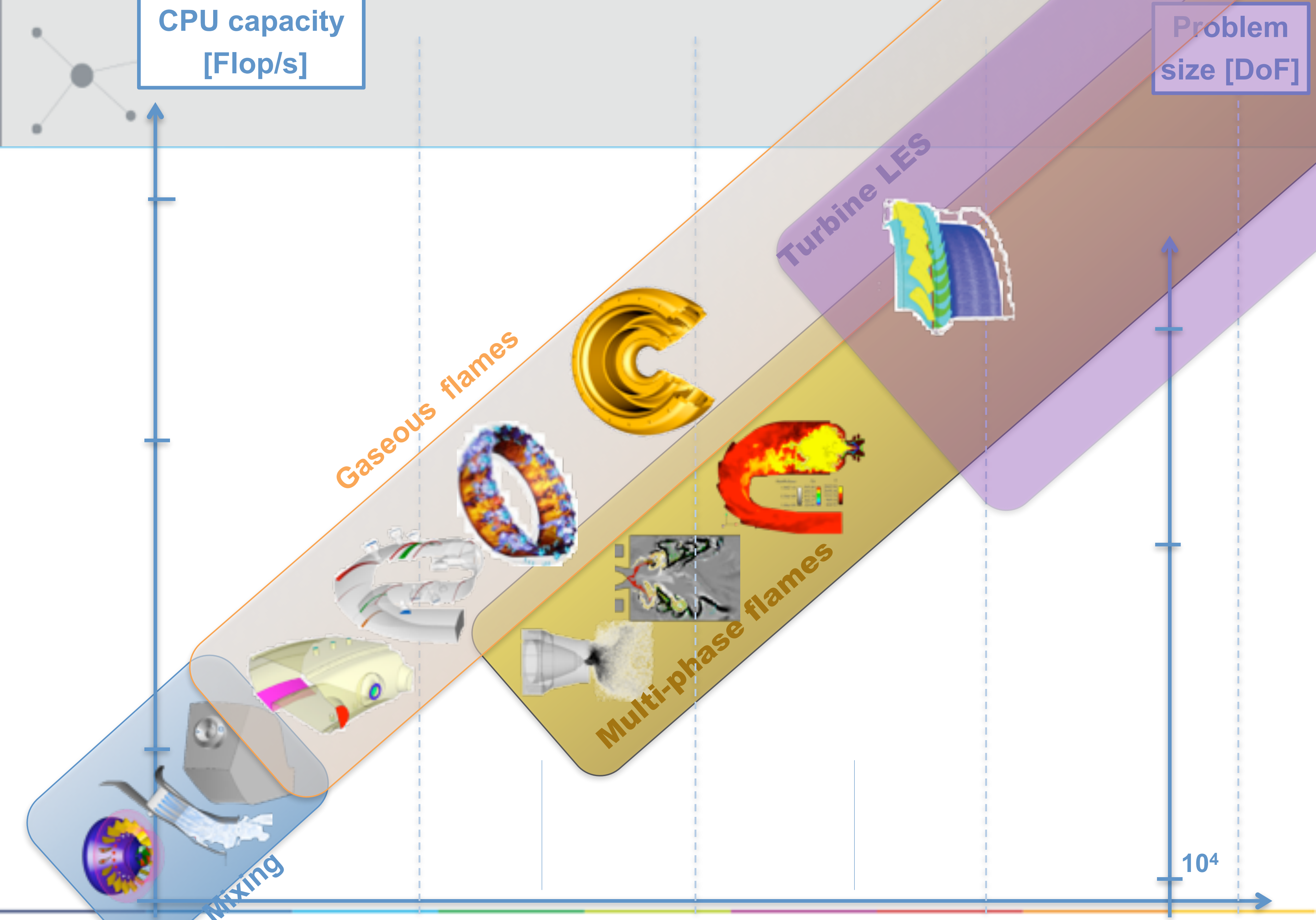
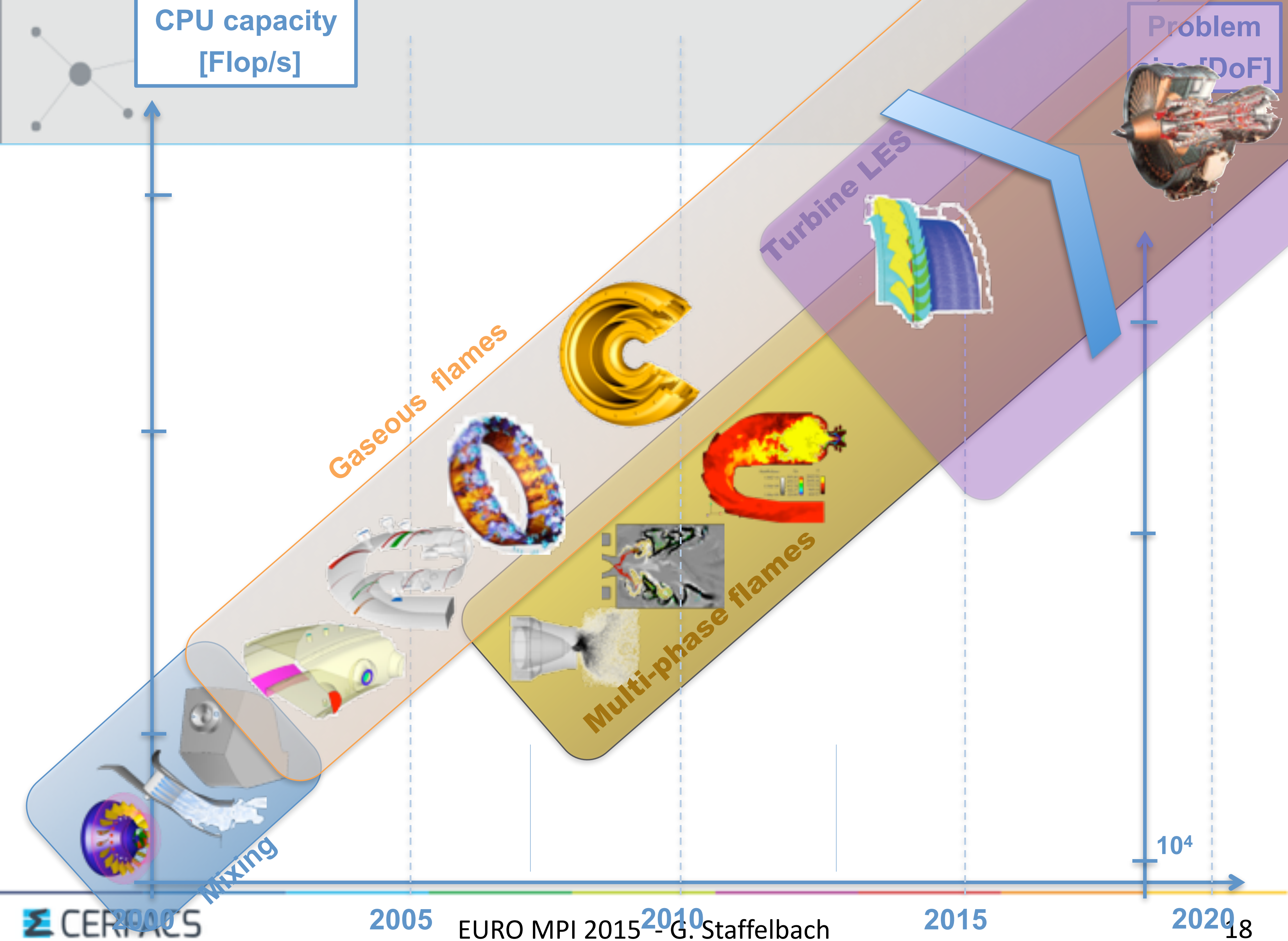
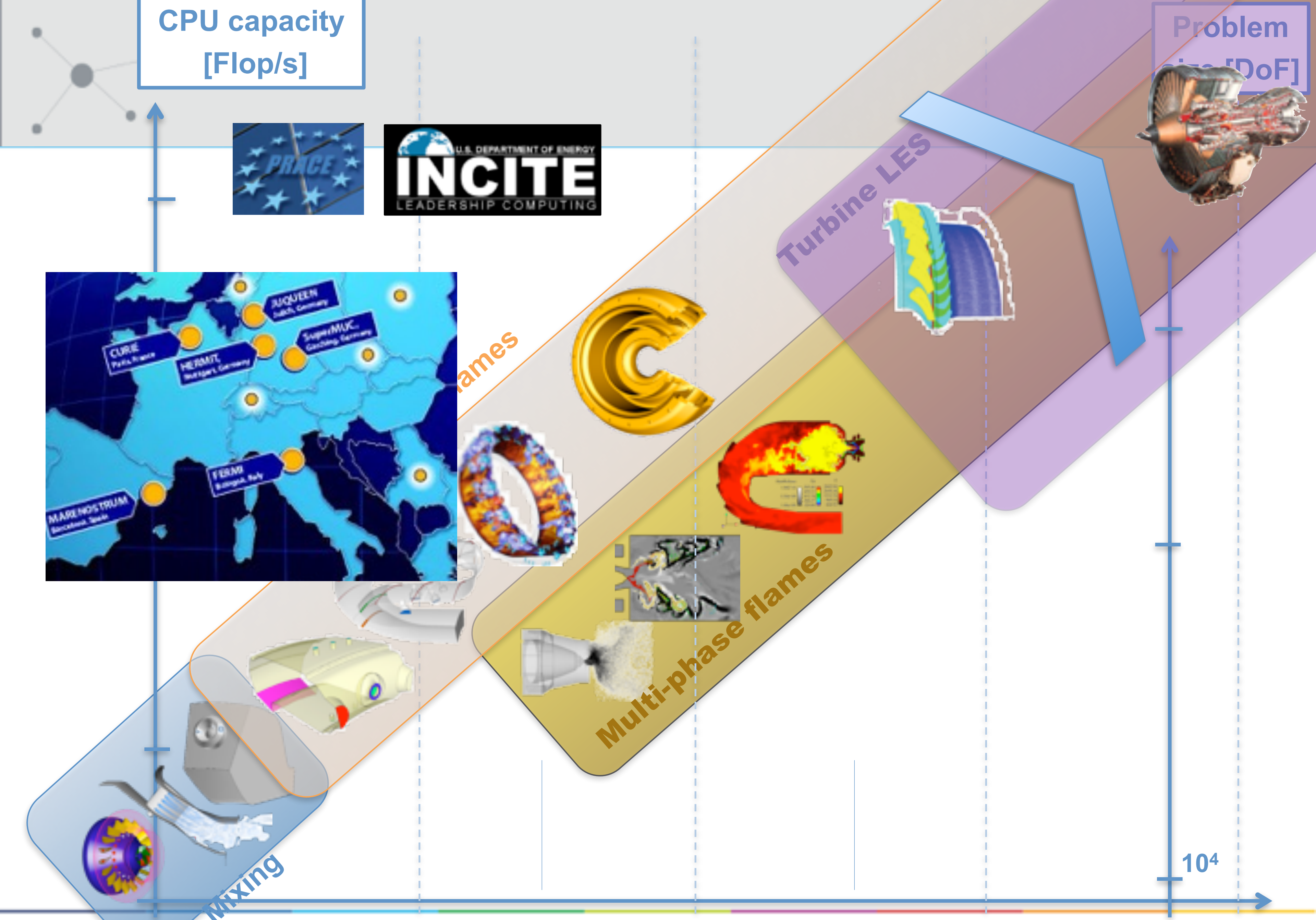
Problem size [DoF]
10^4
Mixing
2000
2005
2010
2015
2020

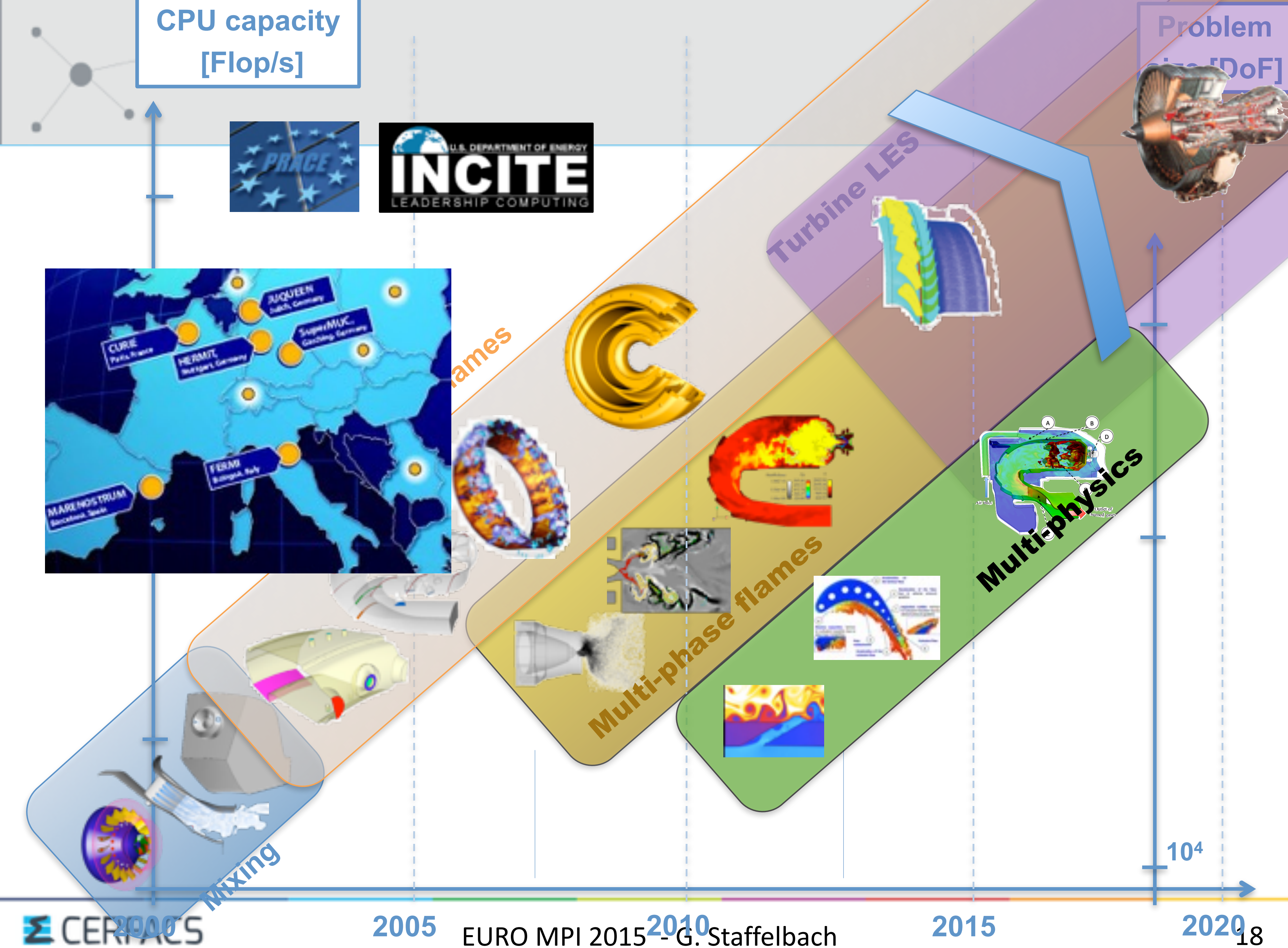

CPU capacity [Flop/s]
Problem size [DoF]
Gaseous flames
Mixing
10^4
2000
2005
2010
2015
2020


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


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


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


CPU capacity [Flop/s]
Problem size [DoF]
PRACE
U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING
JUQUEEN
CURIE
HERMIT
SuperMUC
FERMI
MARENOSTRUM
Turbine LES
Multi-phase flames
Mixing
10^4
2000
2005
2010
2015
2020


CPU capacity [Flop/s]
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LEADERSHIP COMPUTING
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CURIE
Paris, France
HERMIT
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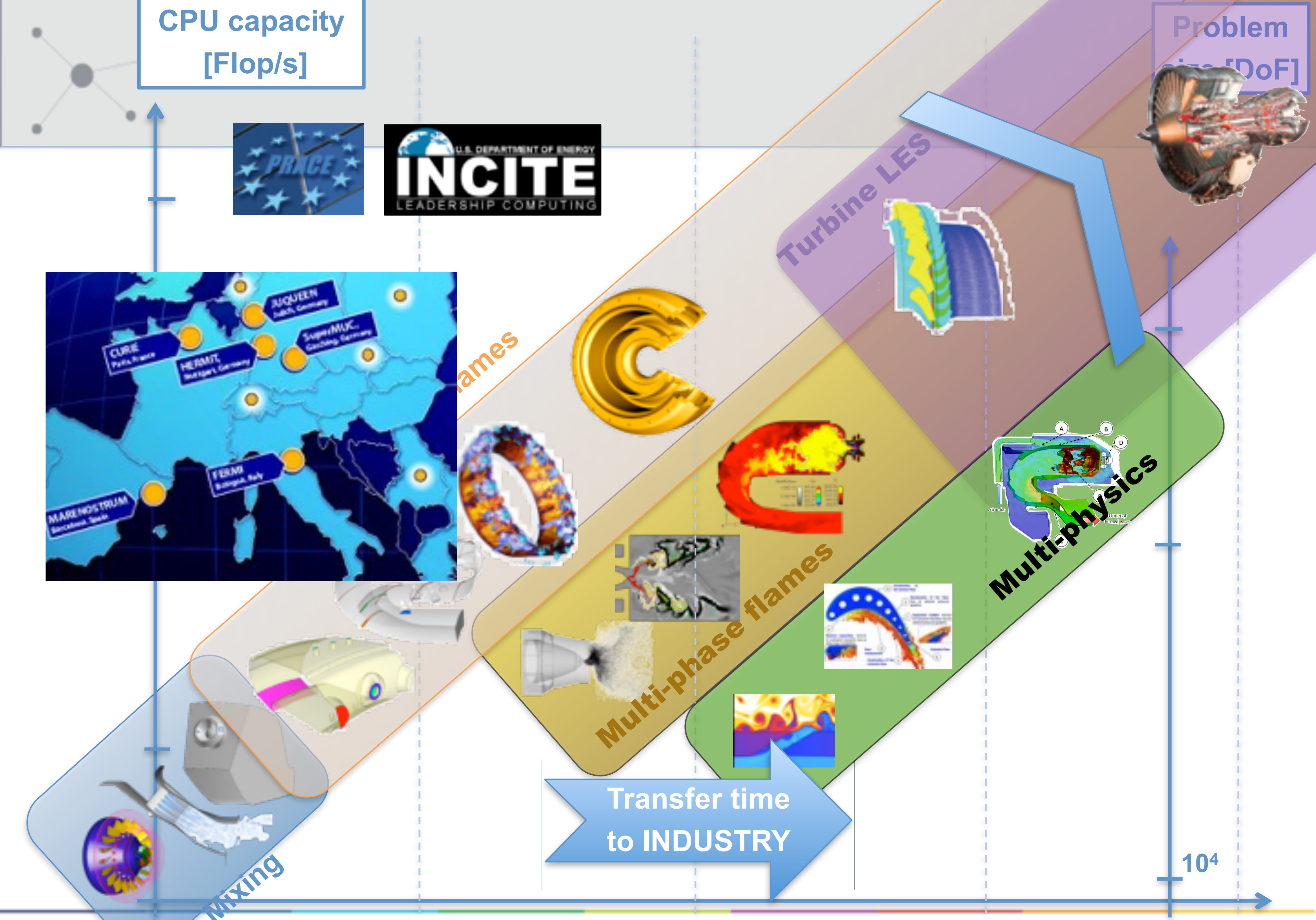
FERMI
MARENOSTRUM
Mixing
ames
Multi-phase flames
Turbine LES
Multi-physics
10^4
2000
2005
2010
2015
2020


CPU capacity
[Flop/s]
Problem
size [DoF]
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CURIE
HERMIT
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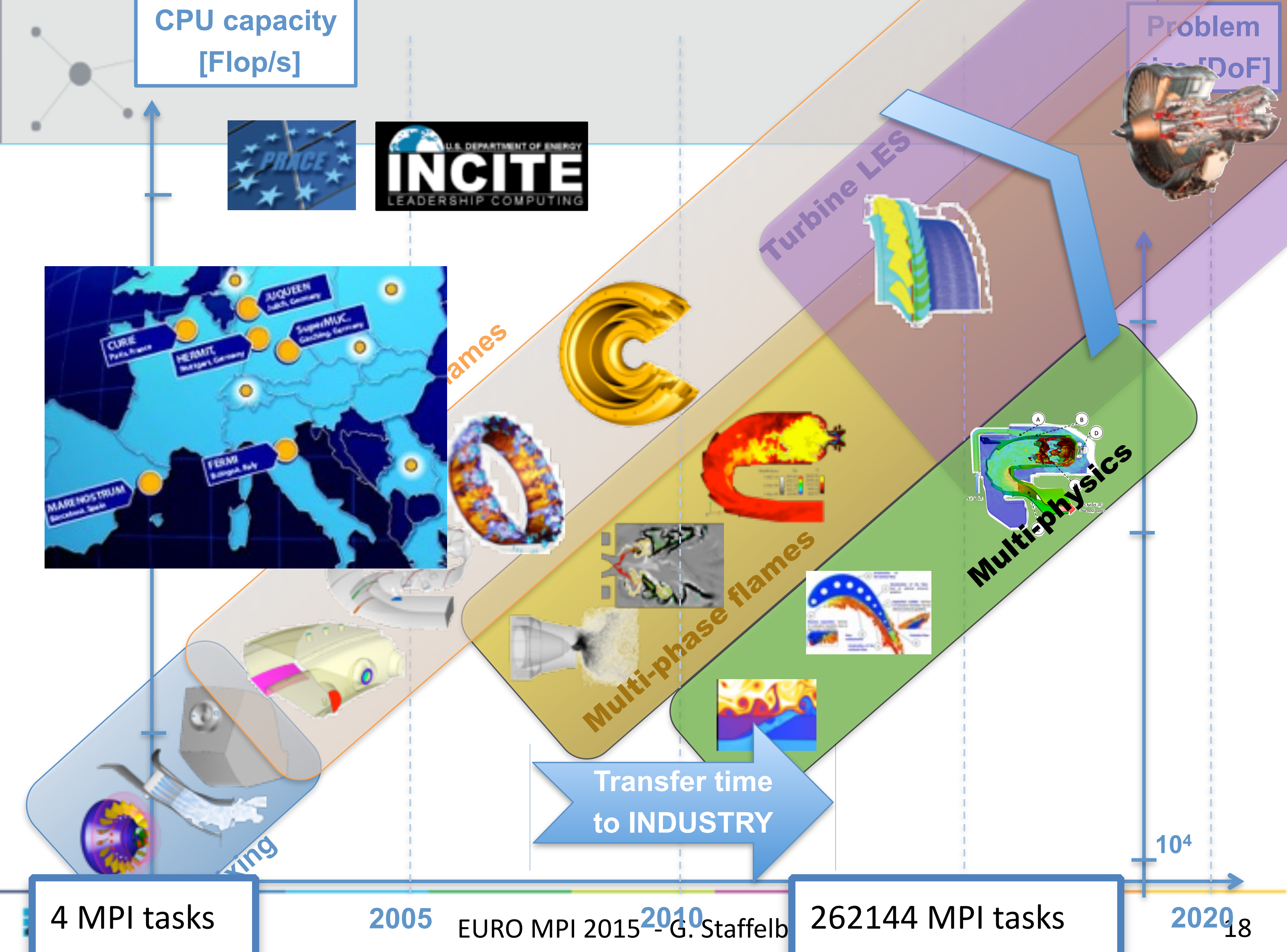
MARENOSTRUM
Turbine LES
ames
Multi-phase flames
Multi-physics
Mixing
Transfer time
to INDUSTRY
10^4
2000
2005
2010
2015
2020


CPU capacity [Flop/s]
Problem size [DoF]
PRACE
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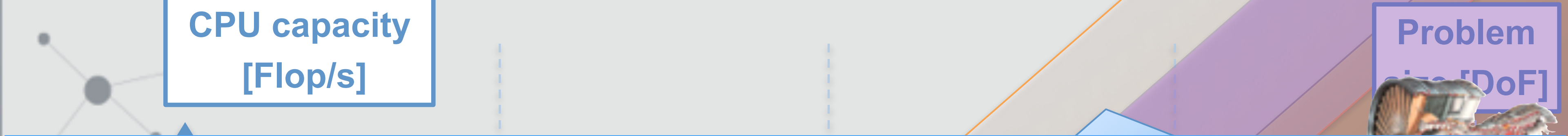
LEADERSHIP COMPUTING
JUQUEEN
CURIE
HERMIT
SuperMUC
FERMI
MARENOSTRUM
Turbine LES
Multi-phase flames
Multi-physics
Transfer time to INDUSTRY
10^4
4 MPI tasks
262144 MPI tasks
2005
2010
2020



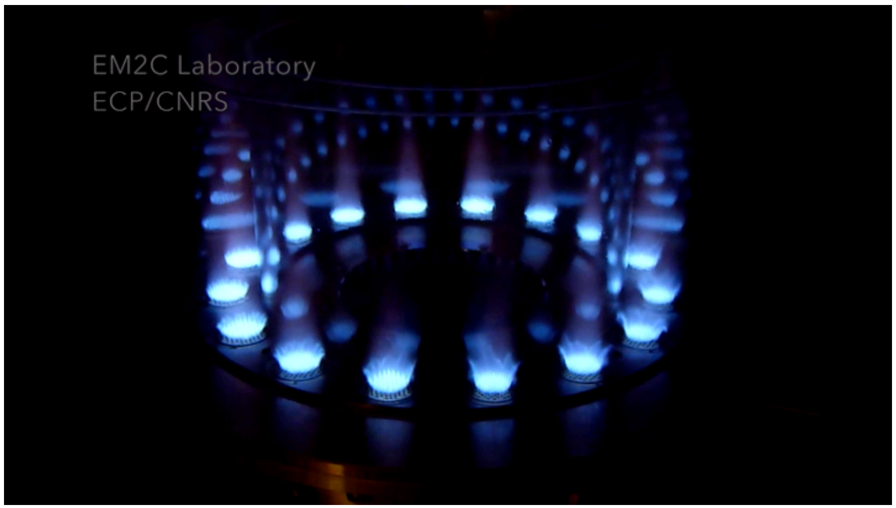
"We acknowledge Intel for its support through the Intel Parallel Computing Center program"

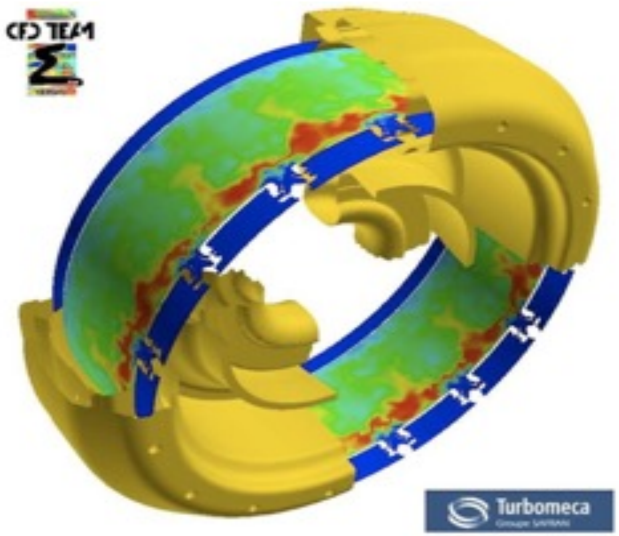
This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

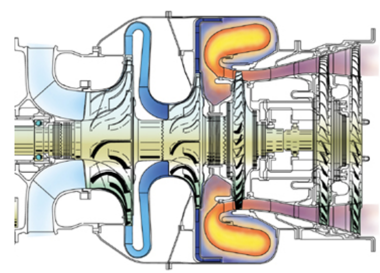
"We acknowledge PRACE for awarding us access to resource CURIE based in France at *Très Grand Centre de calcul du CEA* **(TGCC)."**
"We acknowledge PRACE for awarding us access to resource JUQUEEN based in Germany at *Jülich Supercomputing Centre* **(JSC)."**
"We acknowledge PRACE for awarding us access to resource HERMIT based in Germany at *High Performance Computing Center Stuttgart* **(HLRS)."**
"We acknowledge PRACE for awarding us access to resource FERMI based in Italy at ***CINECA*****."**

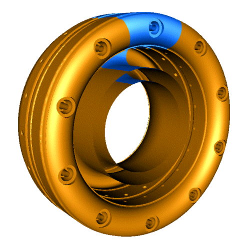
Combustion instabilities in Gas turbines

- From experiment to real turbines
- Use LES to ‘predict’ instabilities









Wolf et al Comb. Flame, 159: 3398-3413, 2012
Gicquel et al Progress in Energy and Combustion Science. 38, 782-817. 2012.
Parmentier et al Combustion and Flame 159, 7, July 2012, 2374-2387.

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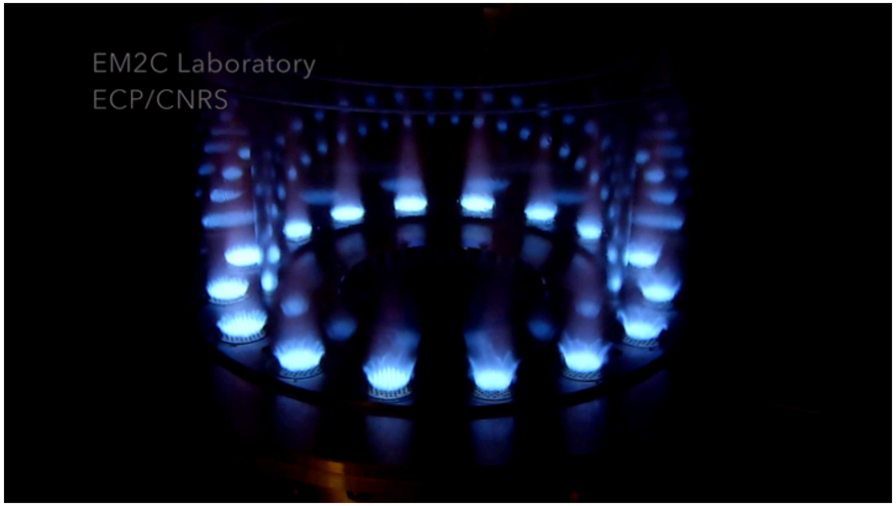
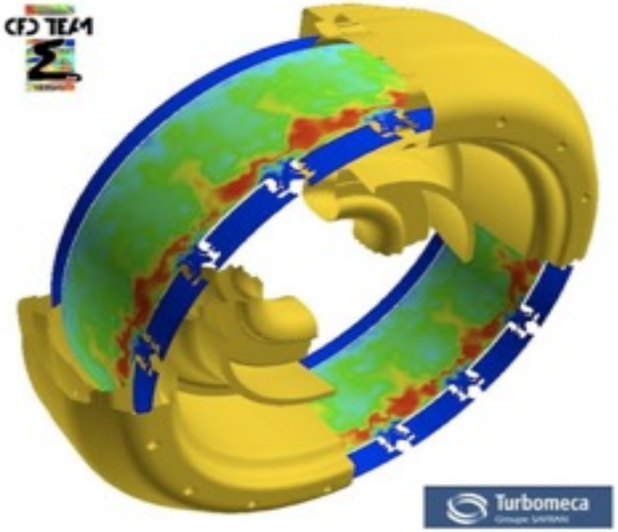
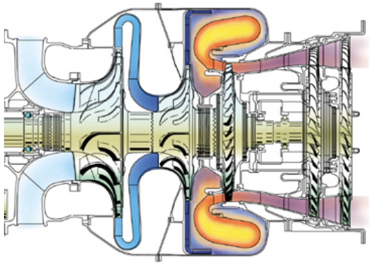
CFD TEAM







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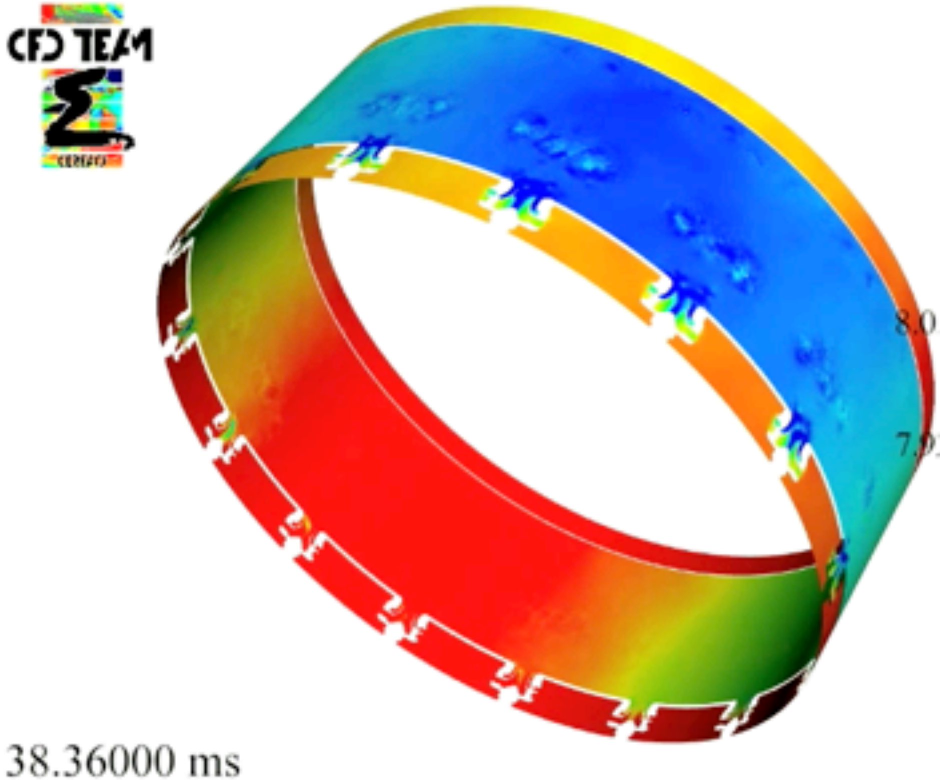
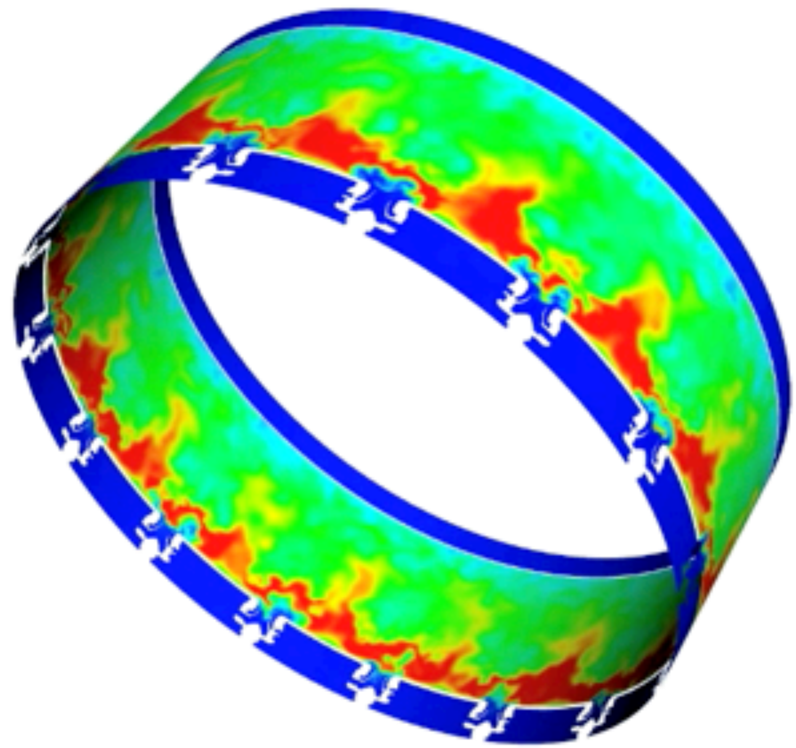
LES of full 360 Gas Turbine

➡ LES of a gas turbine is able to predict the azimuthal combustion instability

10 million CPU hours Bluegene P
32768 MPI tasks



Pressure



Temperature

G. Staffelbach, L. Gicquel, G. Boudier, and T. Poinsot. Large Eddy Simulation of self excited azimuthal modes in annular combustors. Proc. of the Combustion Institute, 32:2909-2916, 2009.
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LES of full 360 Gas Turbine

- LES of a gas turbine is able to predict the azimuthal combustion instability

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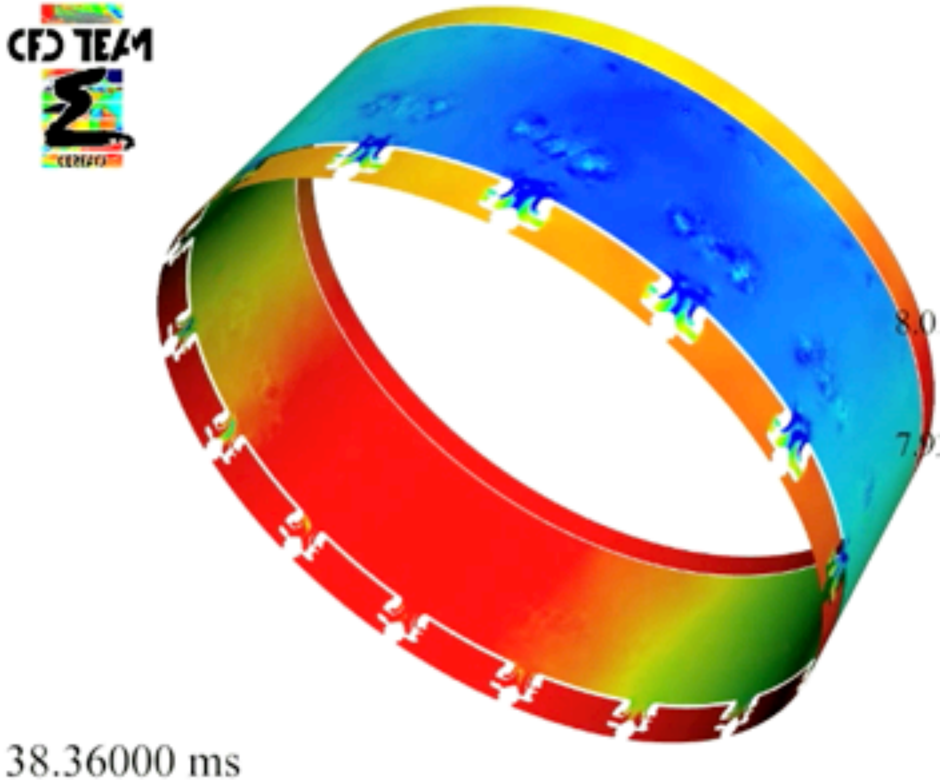
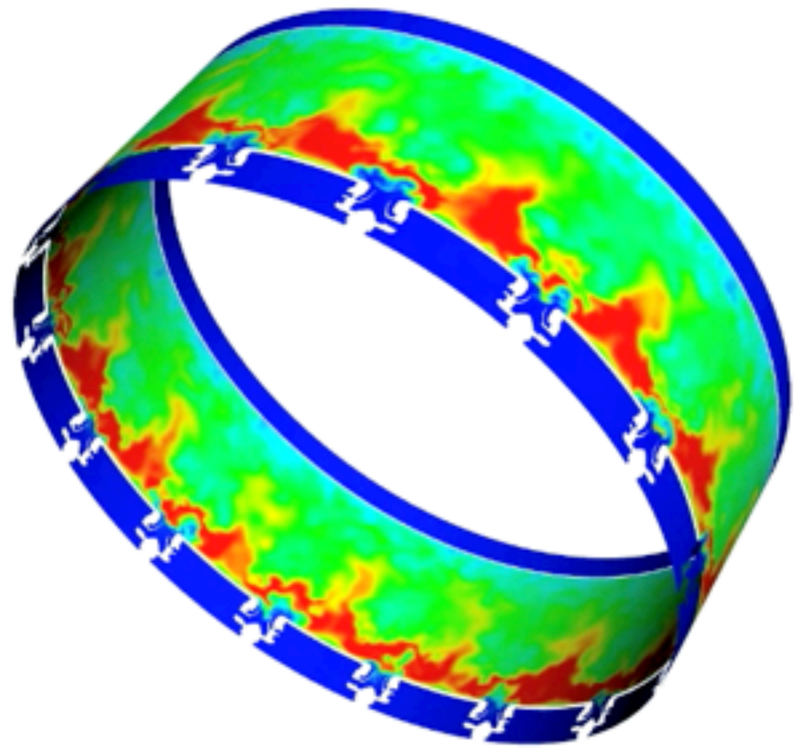


Pressure



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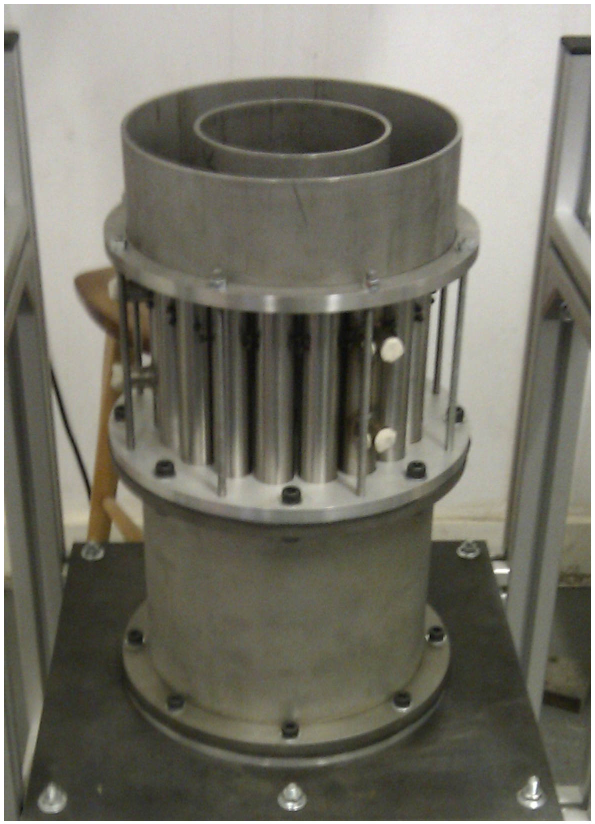
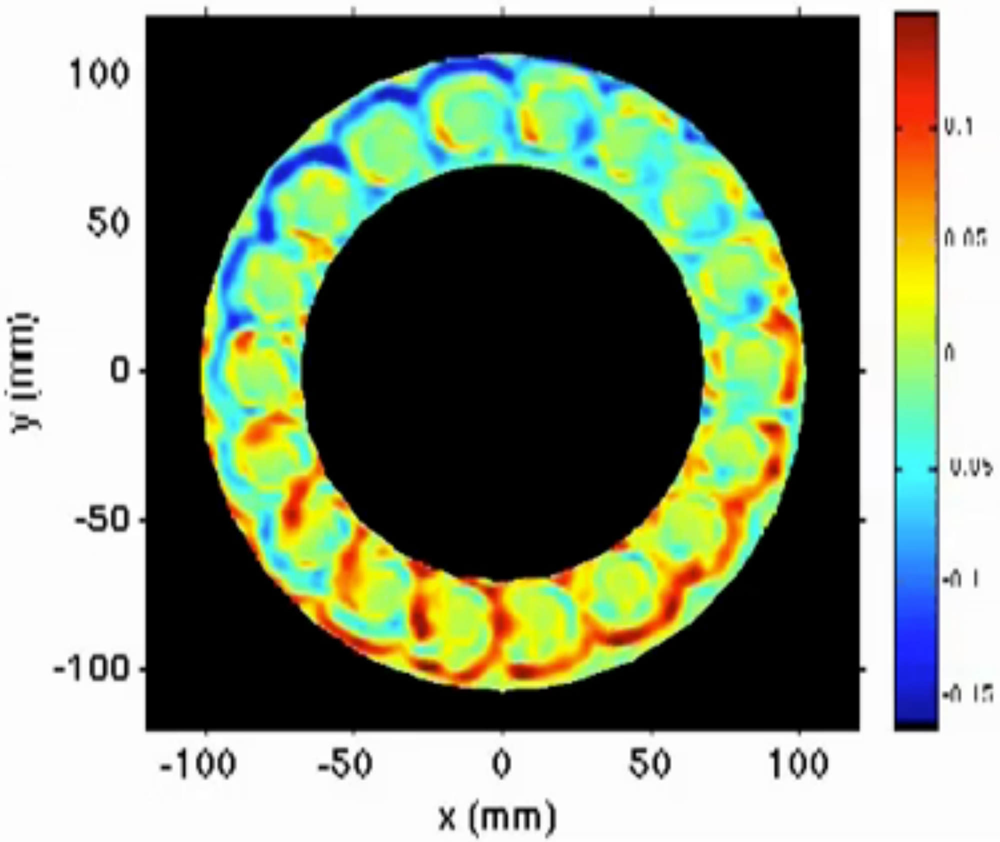
- DAWSON Experiment (Cambridge 2011)



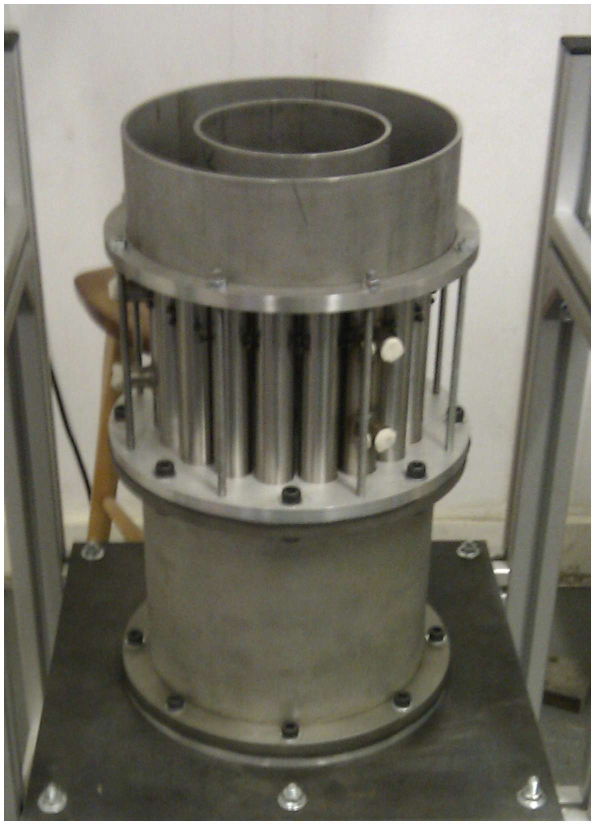
Fluctuating Heat Release

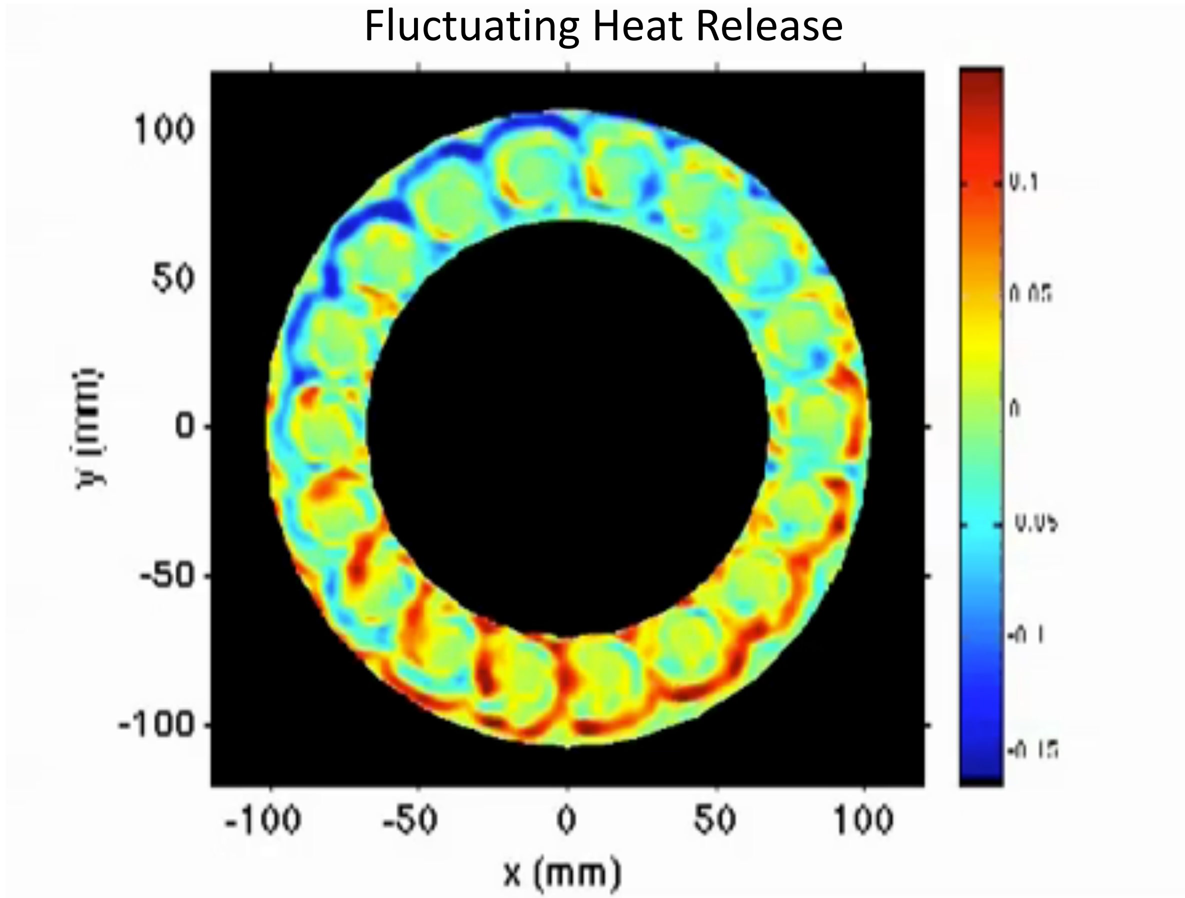


N.A. Worth, J.R. Dawson, Proc. Combust. Inst. (2012), http:// dx.doi.org/10.1016/j.proci.2012.05.061

Illustration in the lab

- ➡ DAWSON Experiment (Cambridge 2011)





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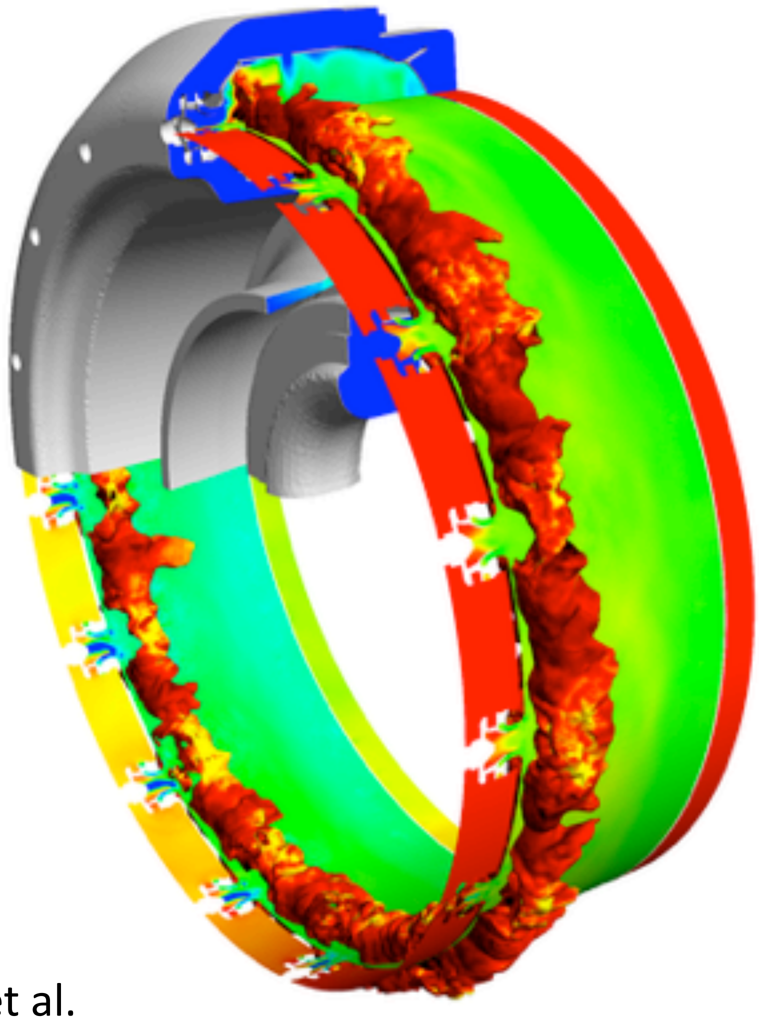
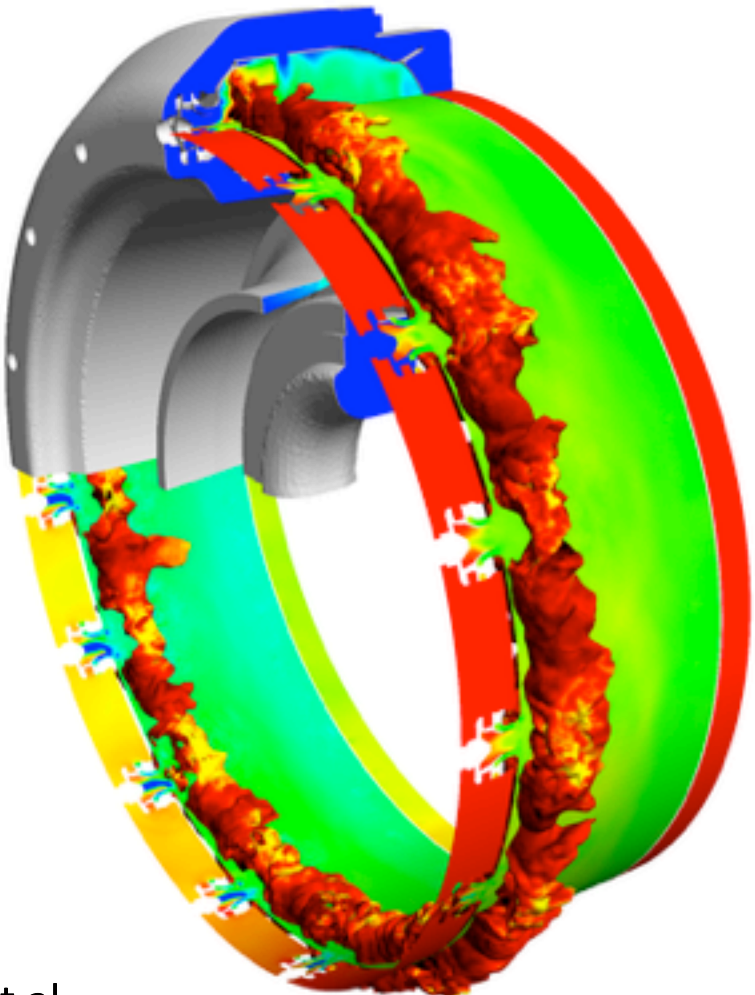
Stability prediction



wolf et al.

- Increasing the fuel consumption rate reduces the delay and stabilised the system

Stability prediction



wolf et al.

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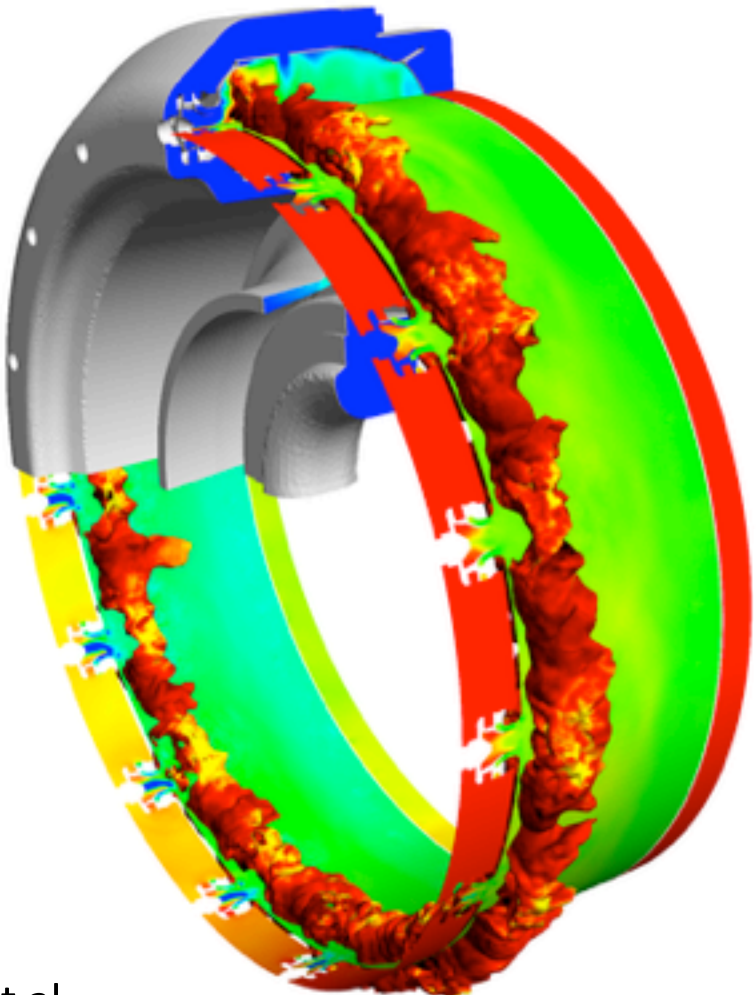
Stability prediction



wolf et al.

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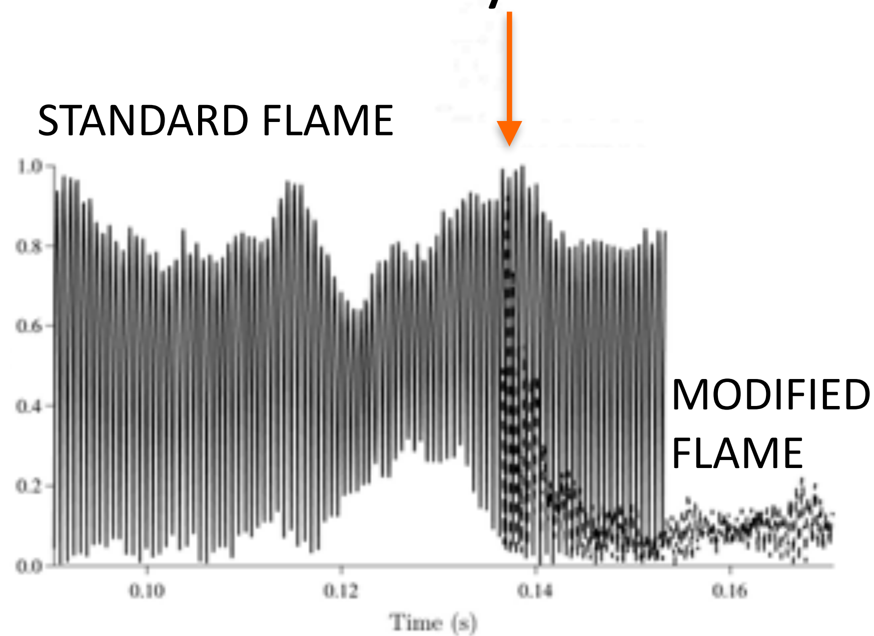
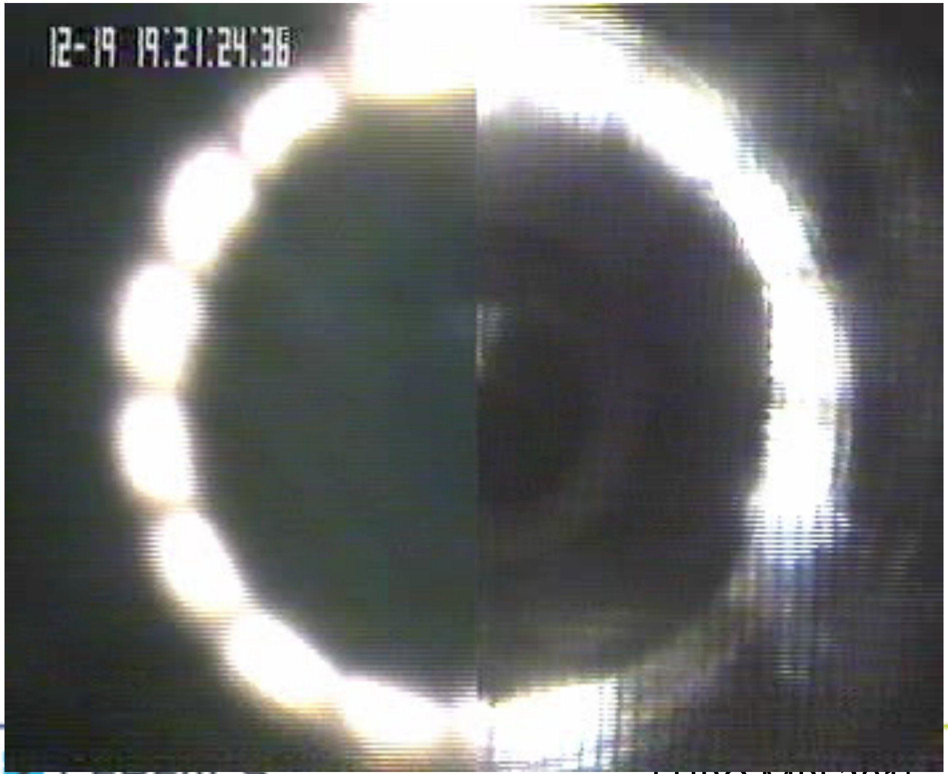


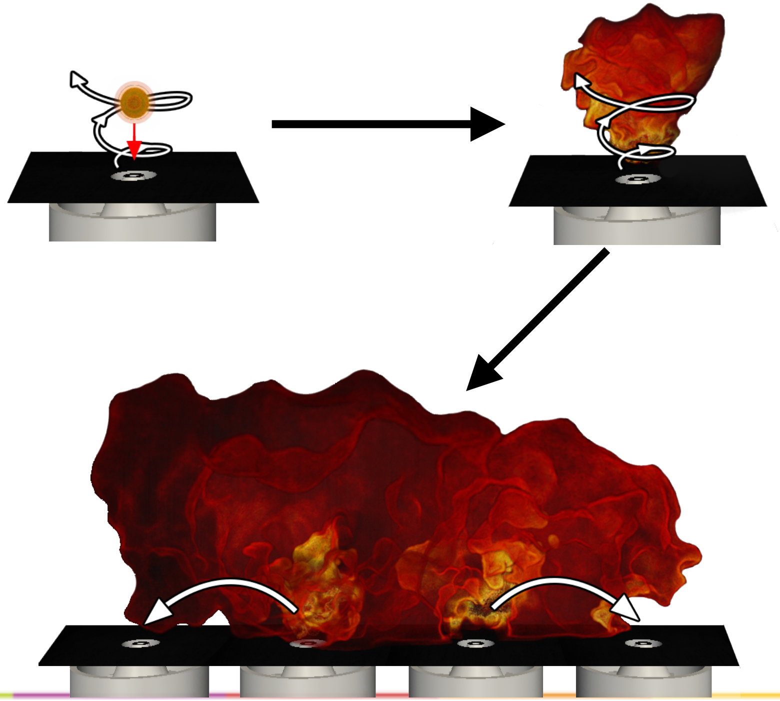
Using simulation to assist combustor design : Ignition

Efficient ignition is paramount for safety and economic reasons

Where to add the energy to start the flame?

How to ensure burner to burner flame propagation ?





Using simulation to assist combustor design : Ignition

Efficient ignition is paramount for safety and economic reasons

Where to add the energy to start the flame?

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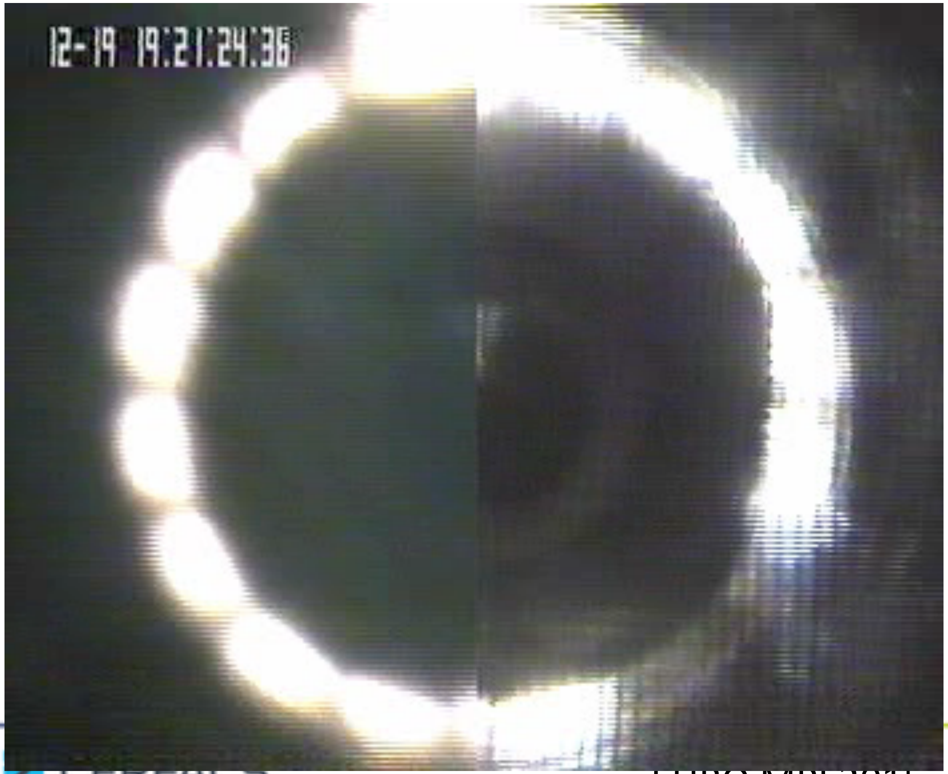
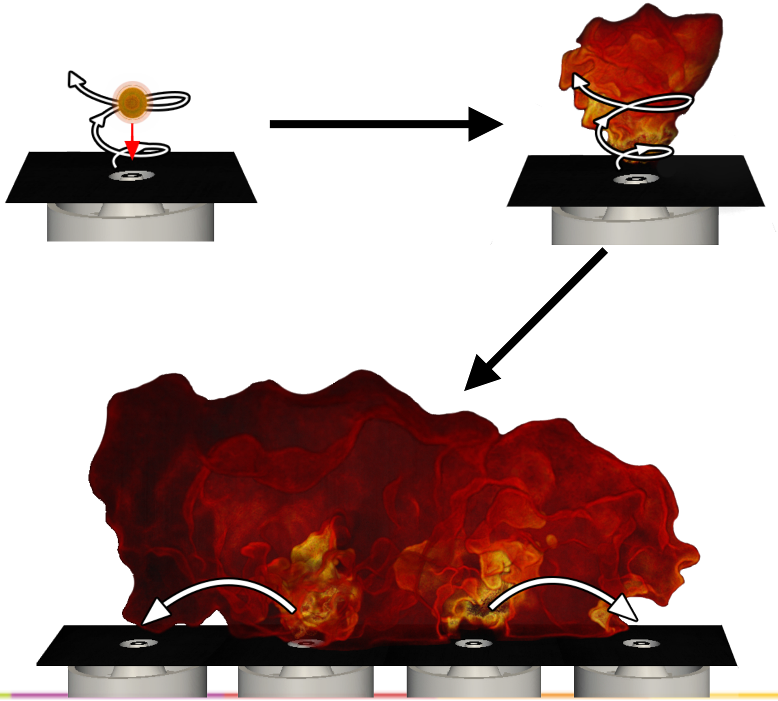
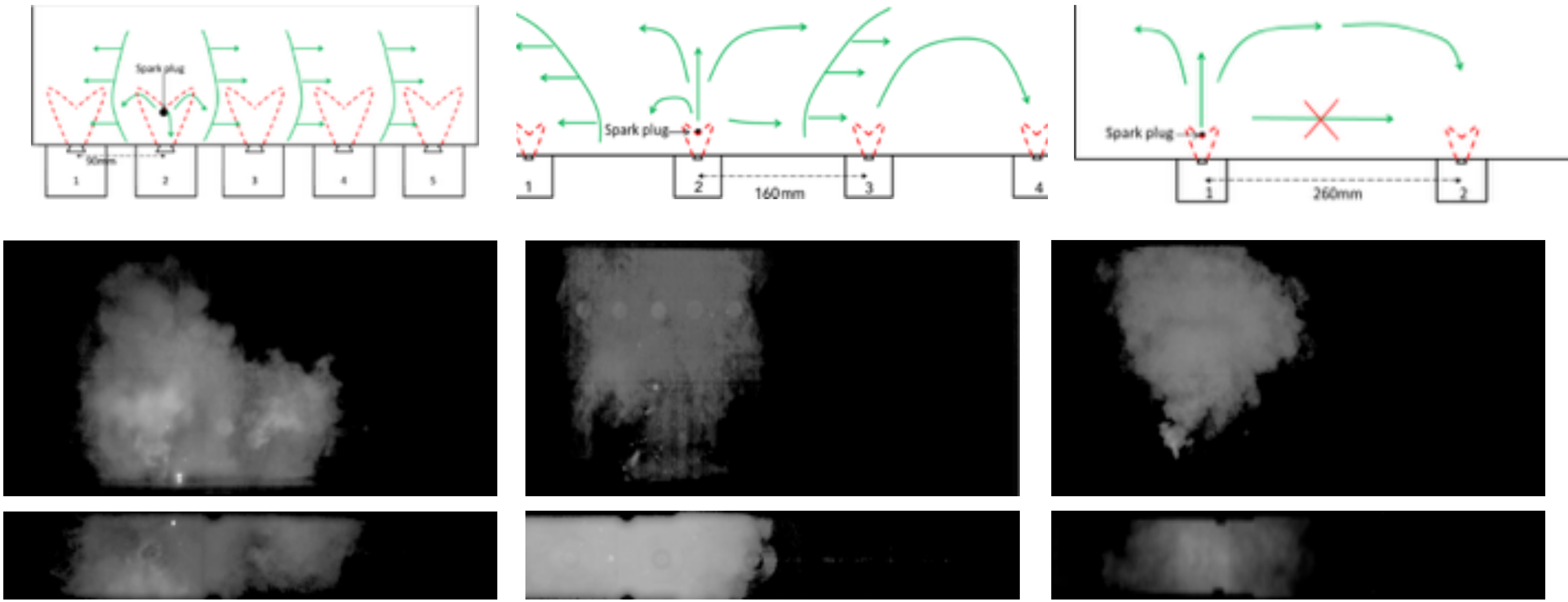




Using simulation to assist combustor design : Ignition

How many burner ? Ignition spark position ?



SP9: L = 90mm

SP16: L = 160mm

SP26: L = 260mm

EXPERIMENTS ! B. Renoud et al CORIA

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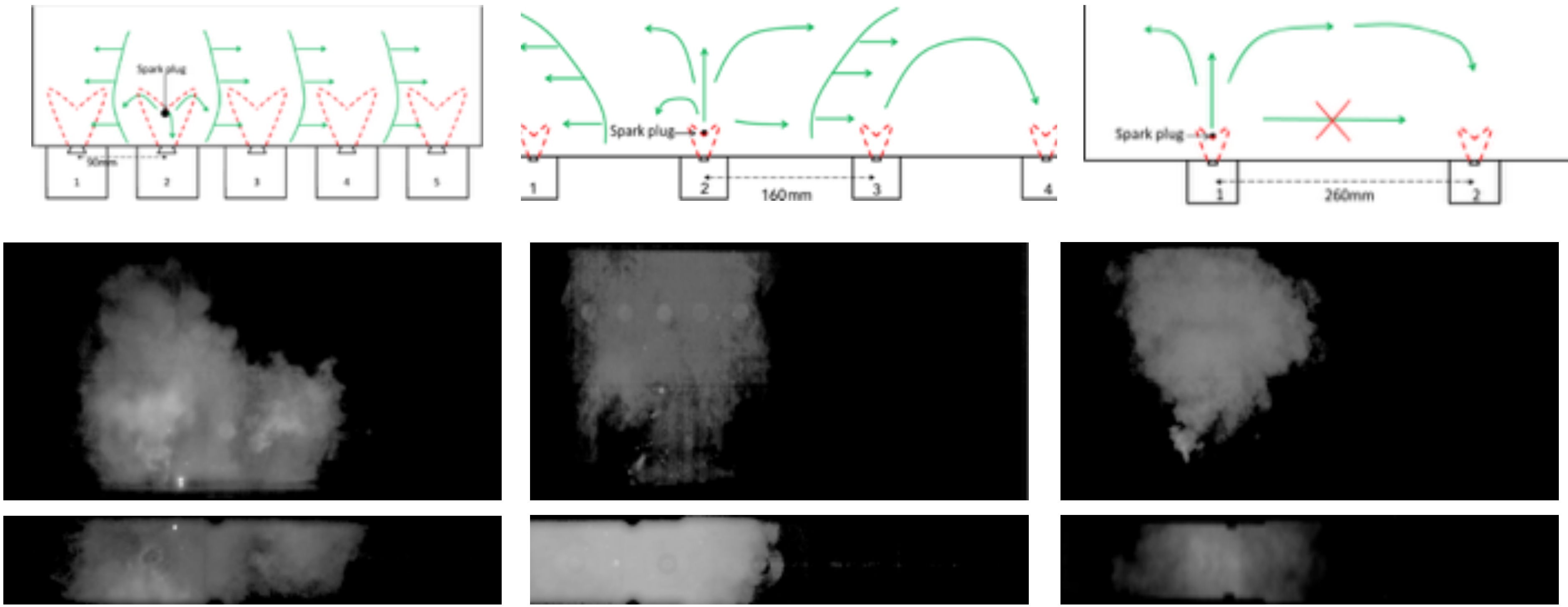

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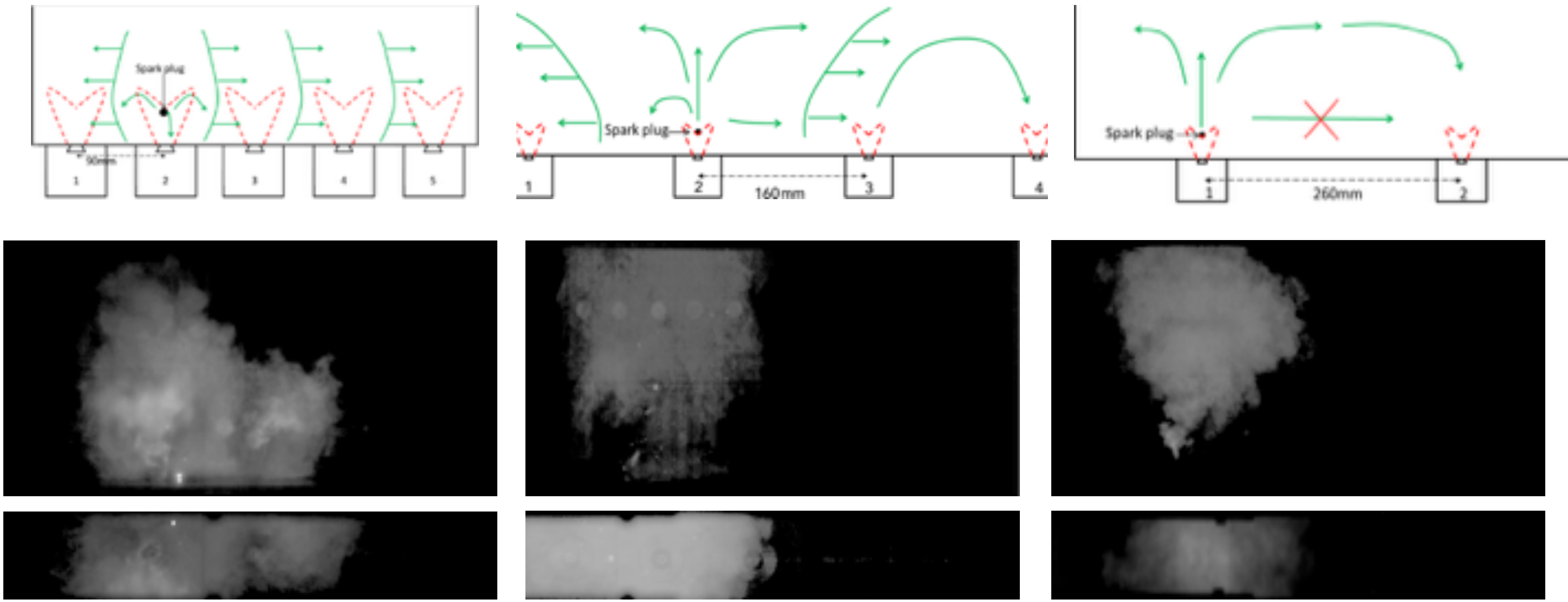

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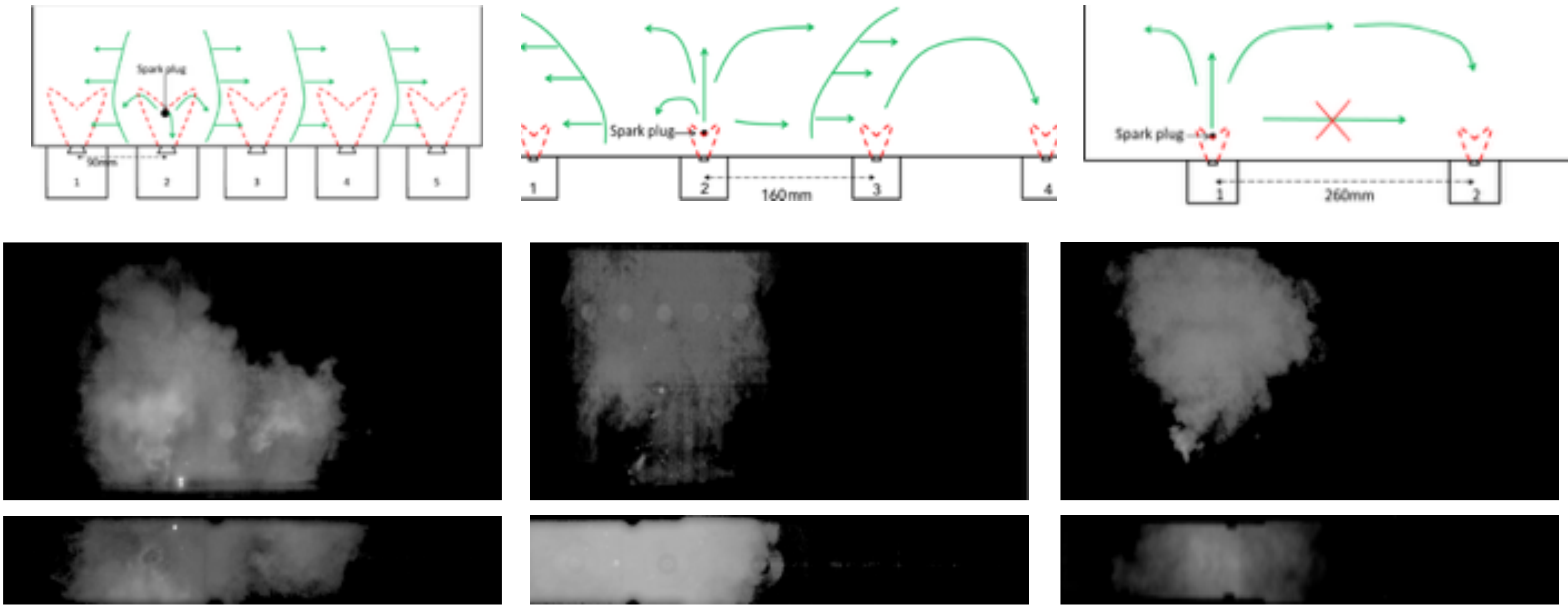

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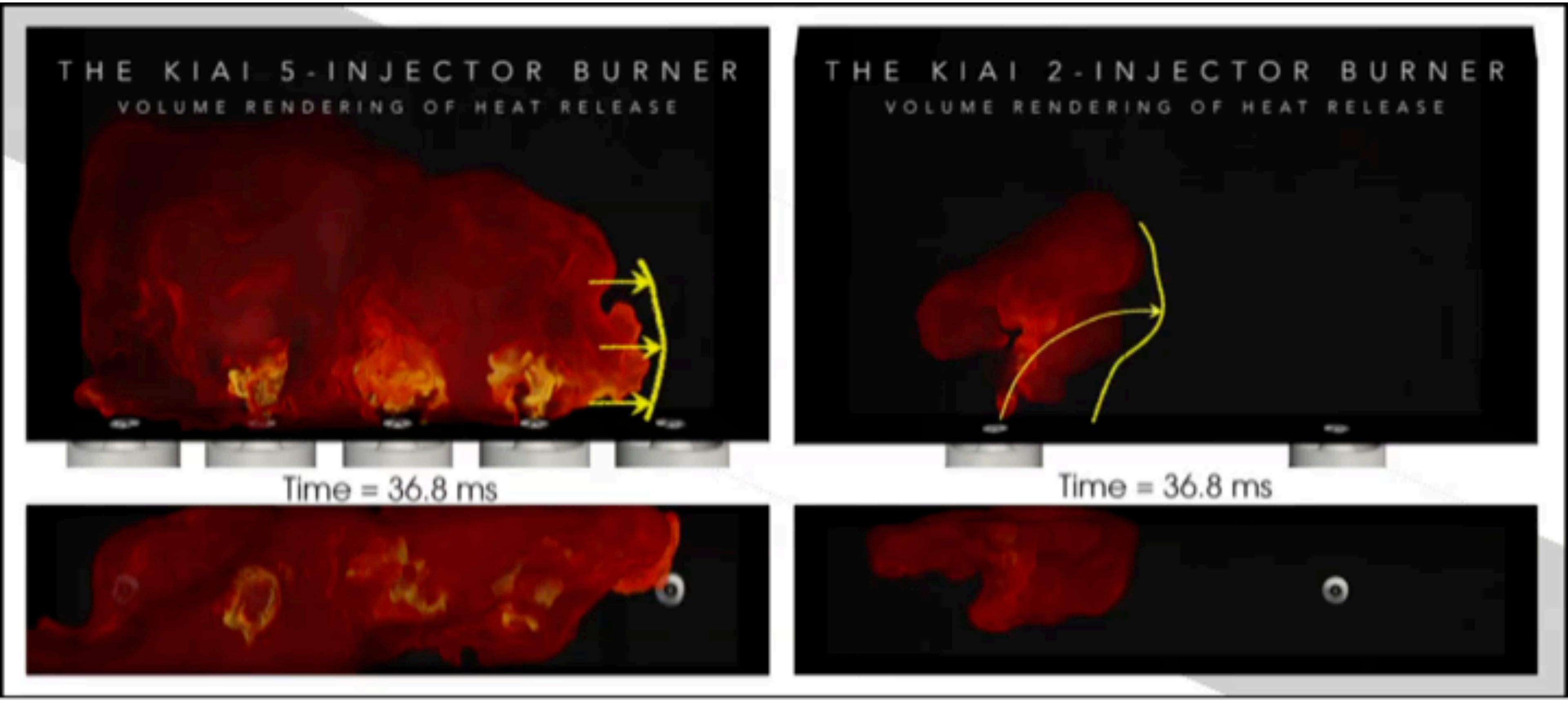

Radial flame propagation

Axial flame propagation

D. barre L. Esclapez

8192 MPI tasks BG Q IDRIS - 10M cpu hours

Using simulation to assist combustor design : Ignition

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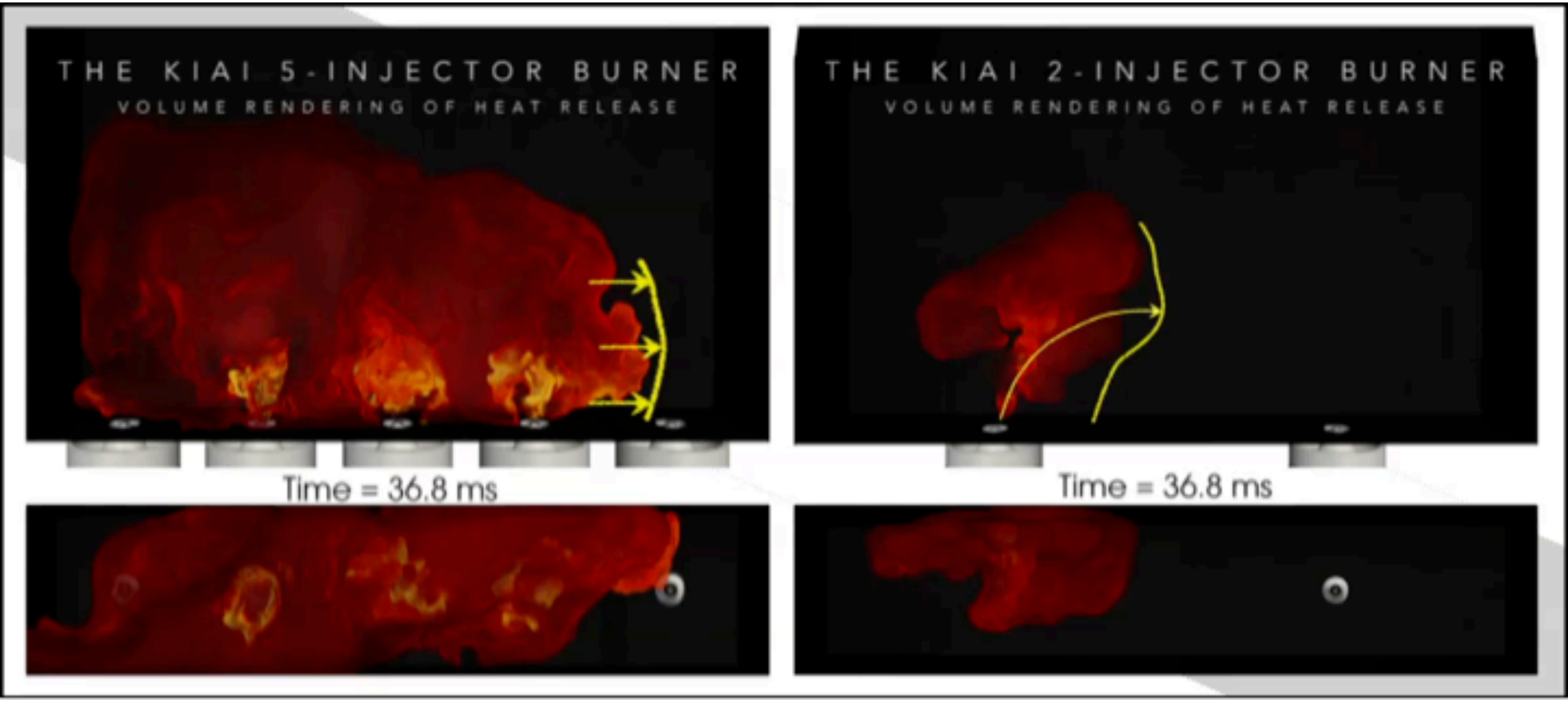
SP26: L = 260mm



Radial flame propagation

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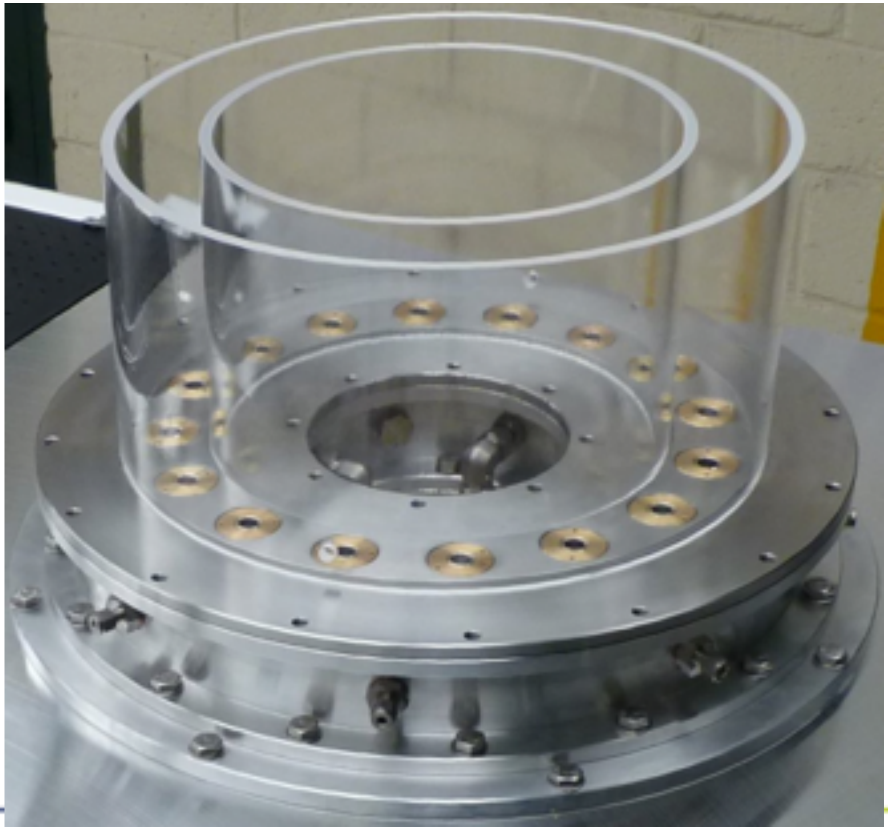
8192 MPI tasks BG Q IDRIS - 10M cpu hours

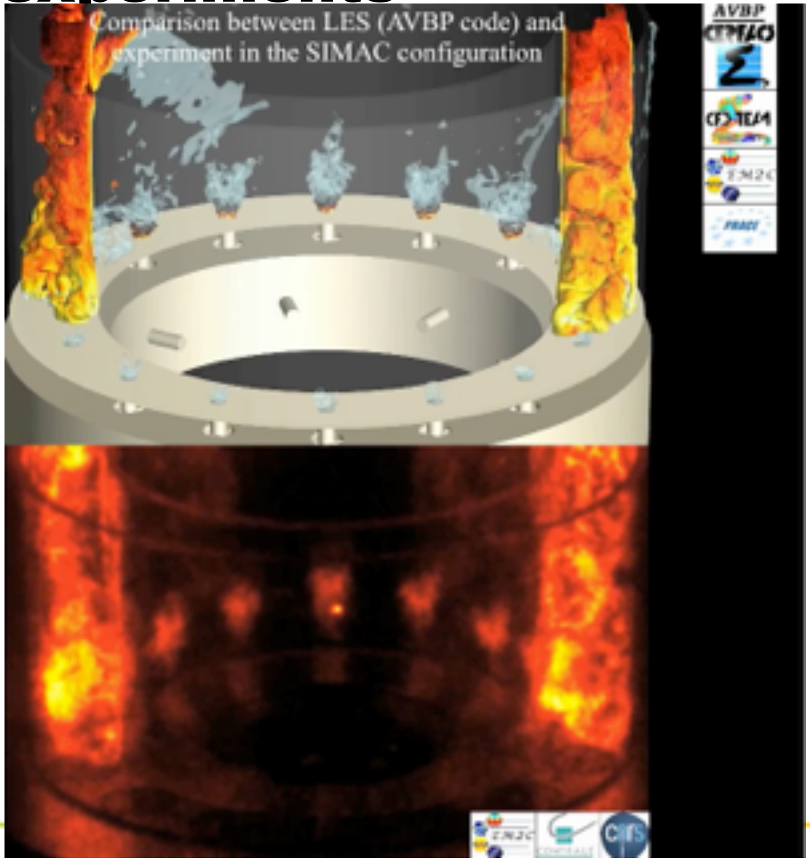
Ignition on an annular burner

15 million hours CURIE TTGC GENCI

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





E. Riber, B. C… elin, M.
Boileau, M. P…

Simulation of … stor
injector and …

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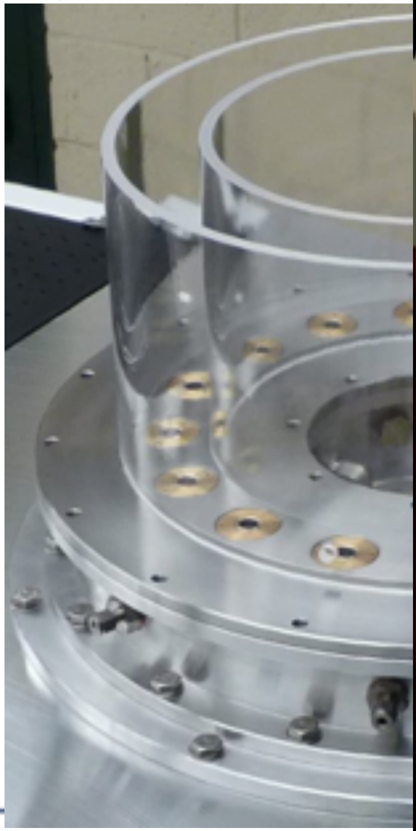
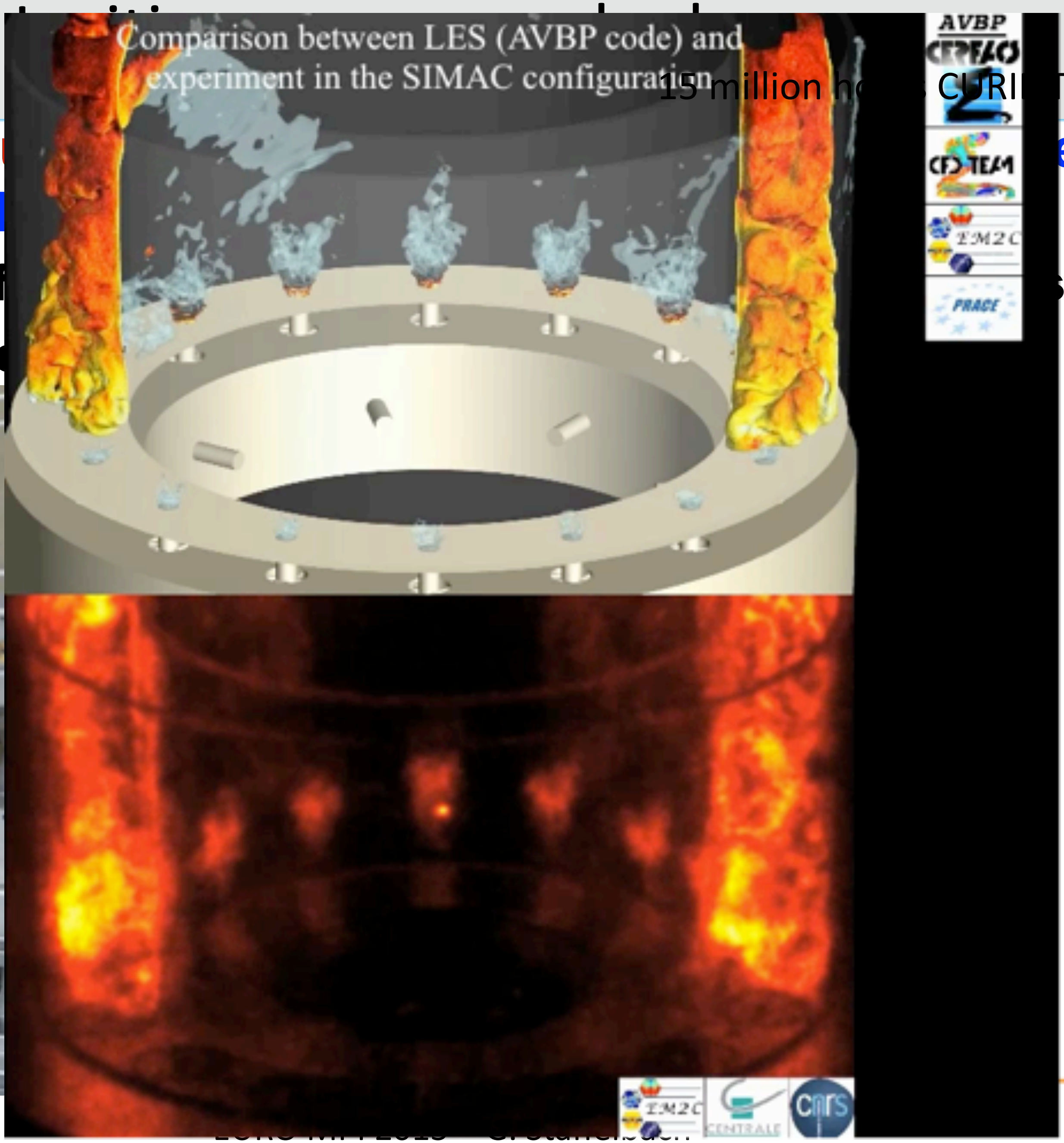


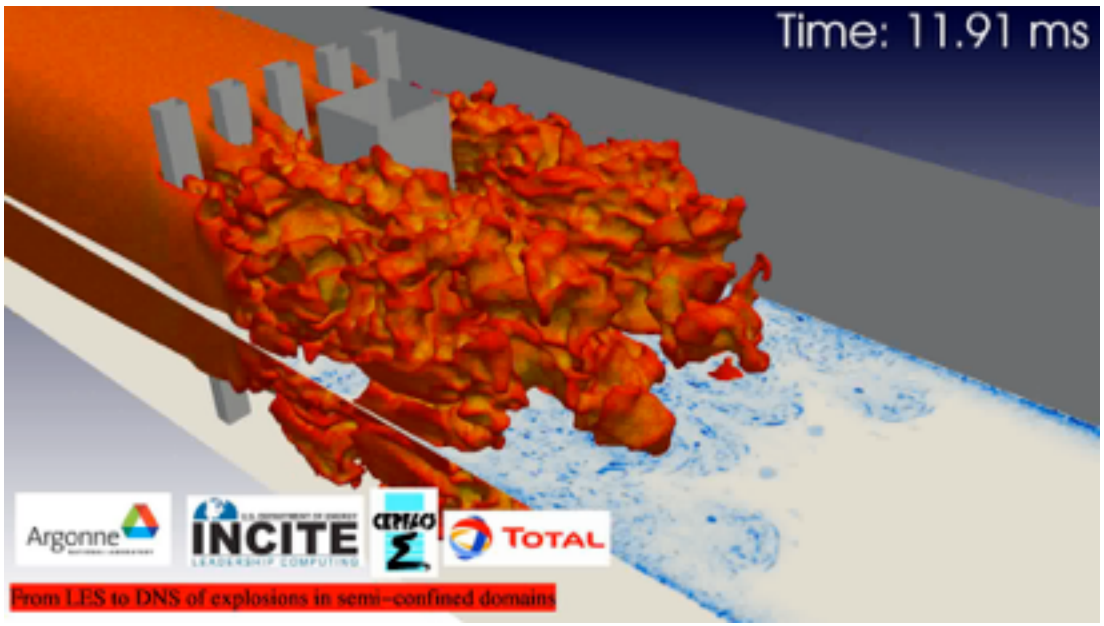


From LES to DNS of expositions in semi-confined domains

Understand the physical phenomena involved in confined space explosions and validate the methodology for multiple scales

Sydney experiment, Masri et al

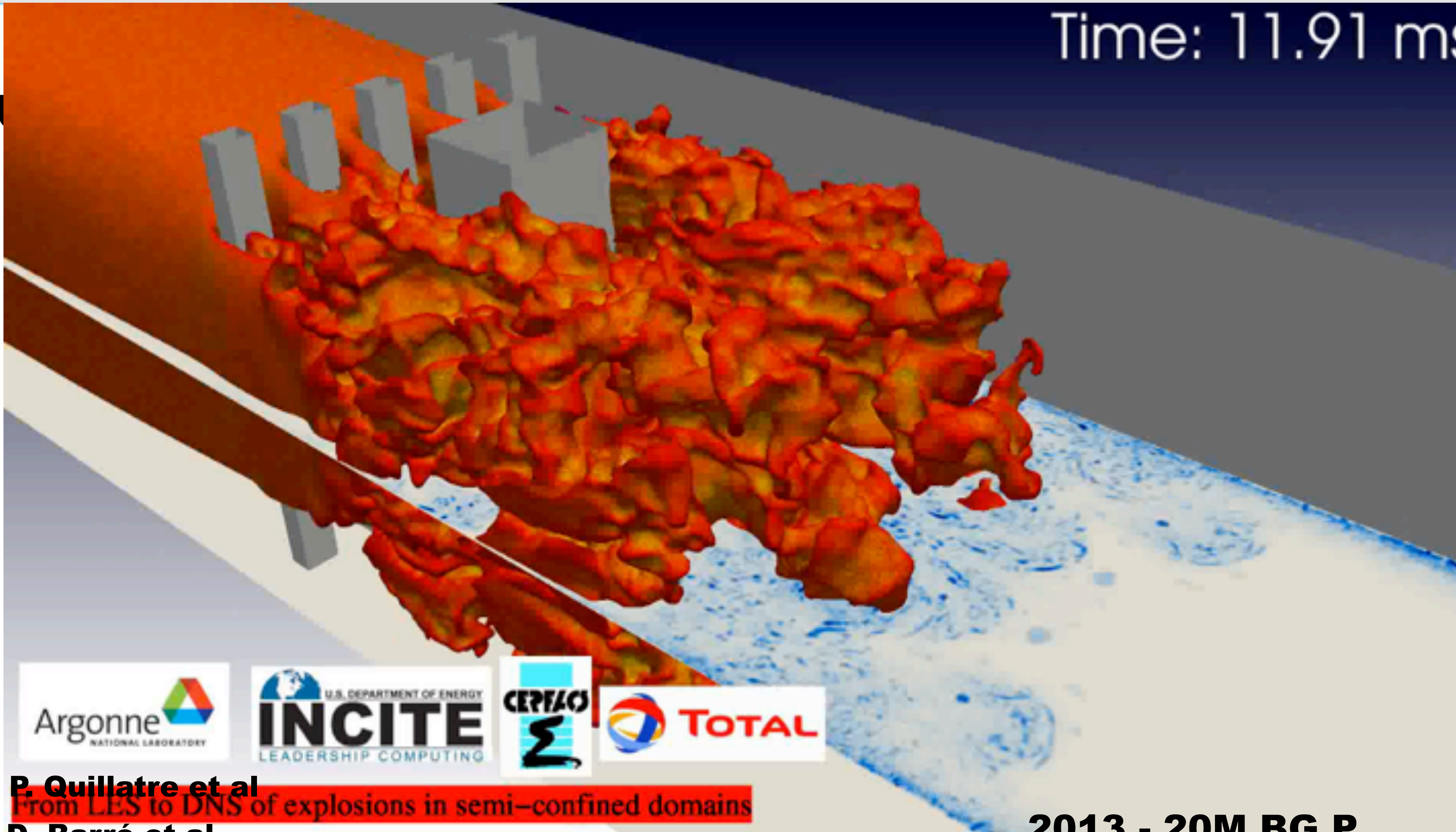
25cm length
LES and DNS (1Be elements)



P. Quillatre et al
D. Barré et al

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

Using simulation for safety applications



P. Quillatre et al

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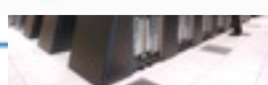

2013 - 20M BG P

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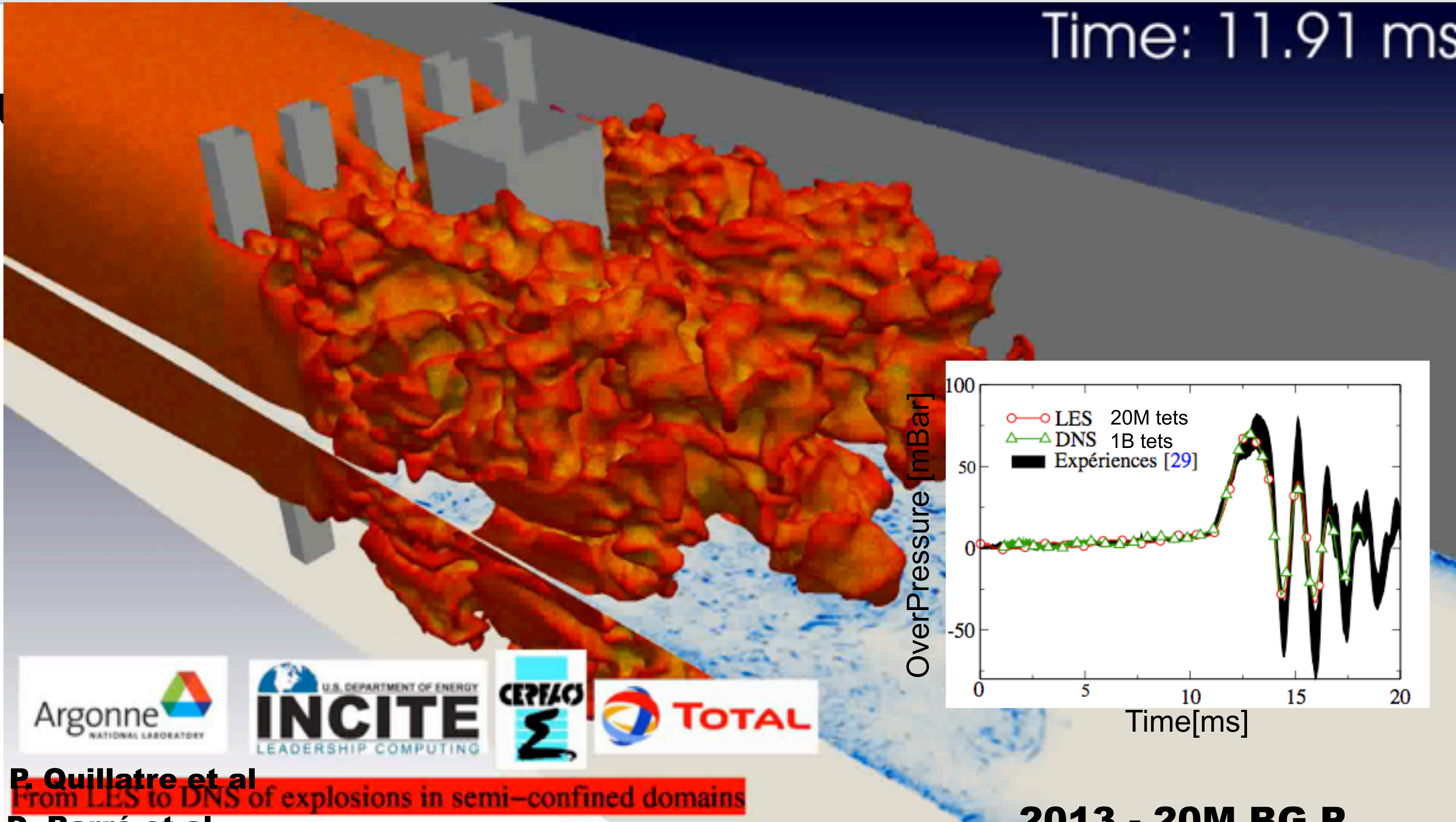
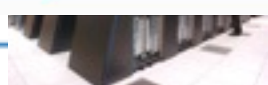


P. Quillatre et al

From LES to DNS of explosions in semi–confined domains

D. Barré et al



2013 - 20M BG P

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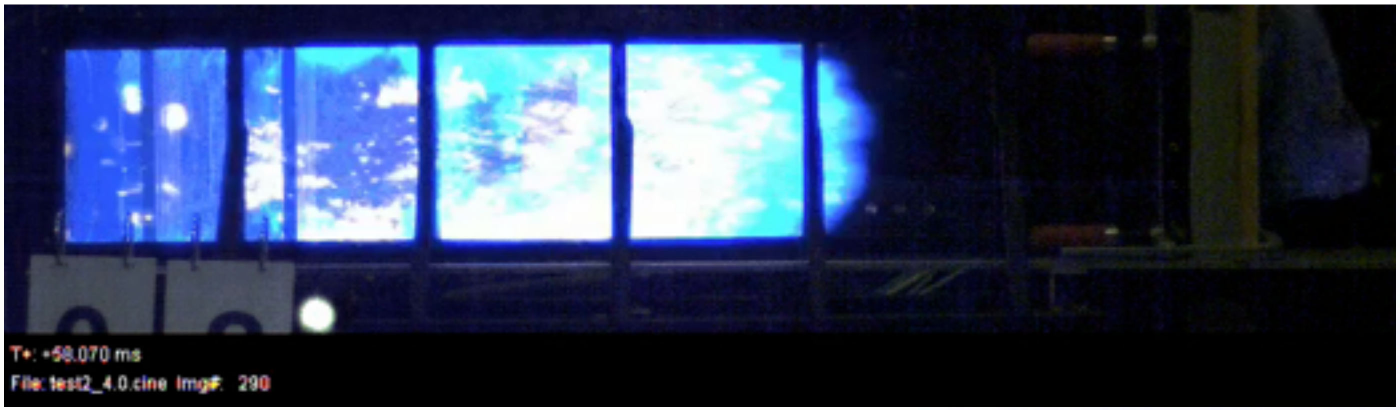
Using simulation for safety applications

Large Eddy Simulation of the 1.5m configuration versus experiment



Experiment performed by Gexcon

Large Eddy Simulation

P. Quillatre et al

P. Quillatre

Using simulation for safety applications

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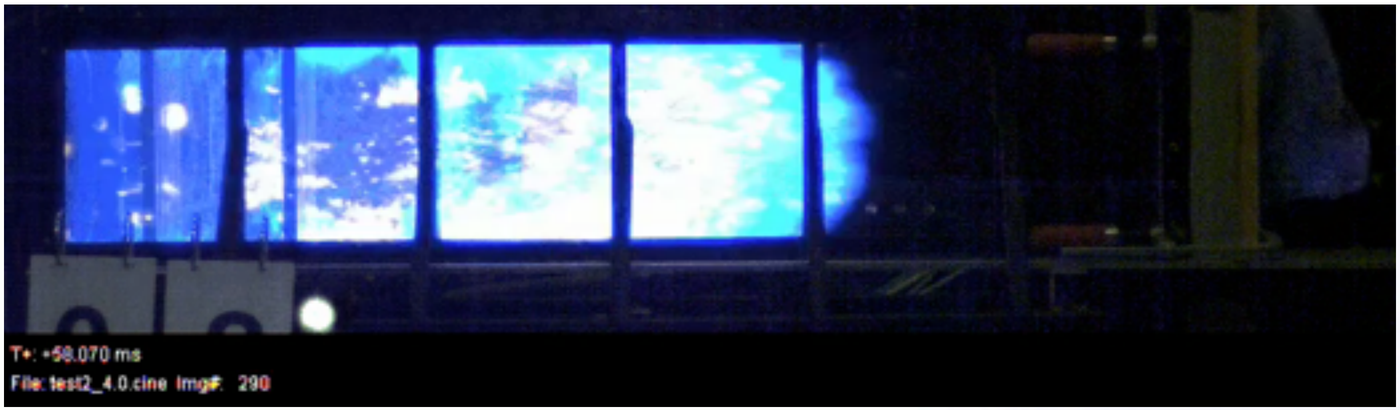

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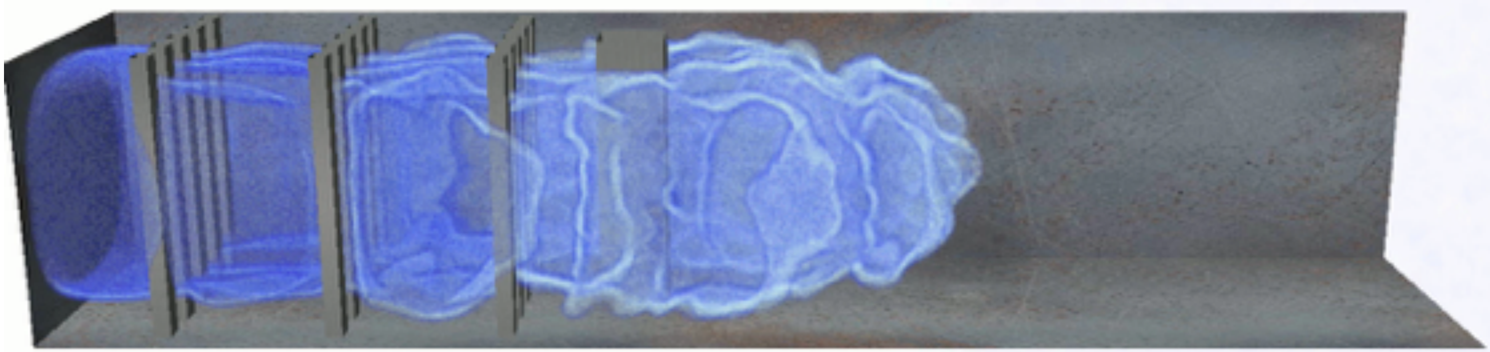


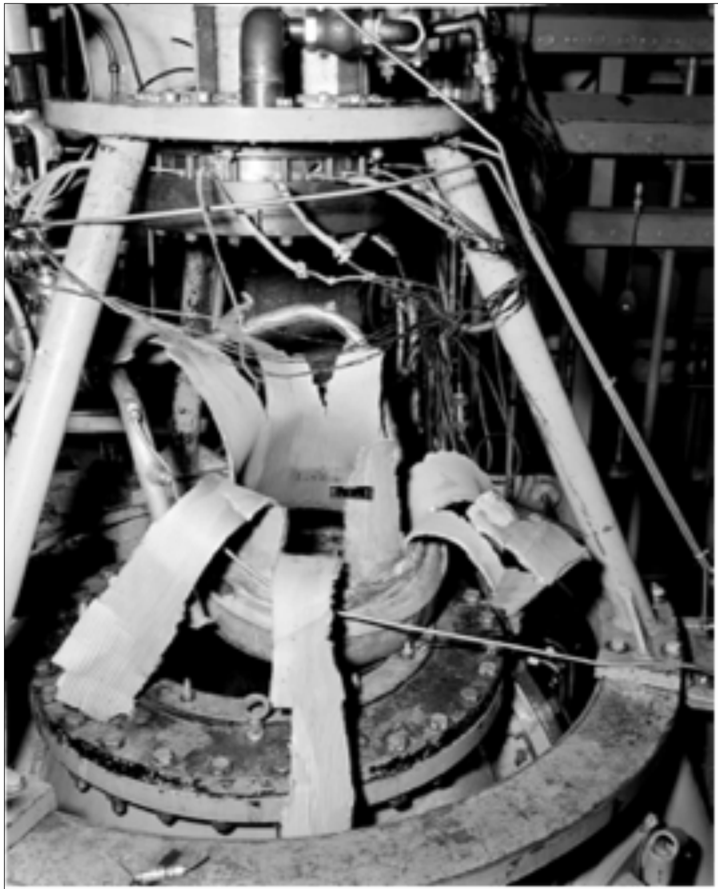
Large Eddy Simulation

P. Quillatre et al

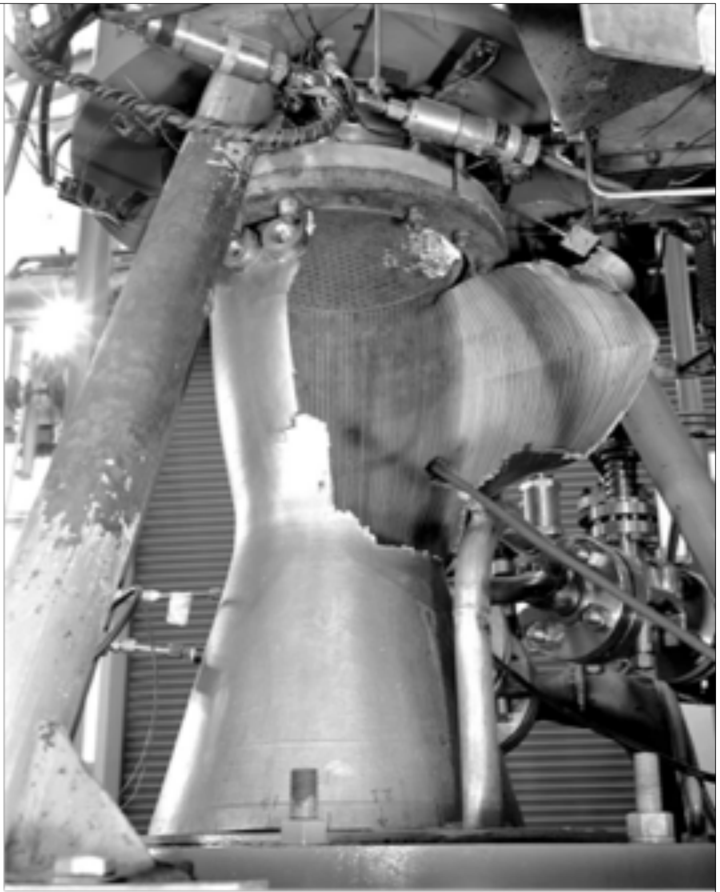
Time: 58.0

P. Quillatre

The 10 M$ failure(s)



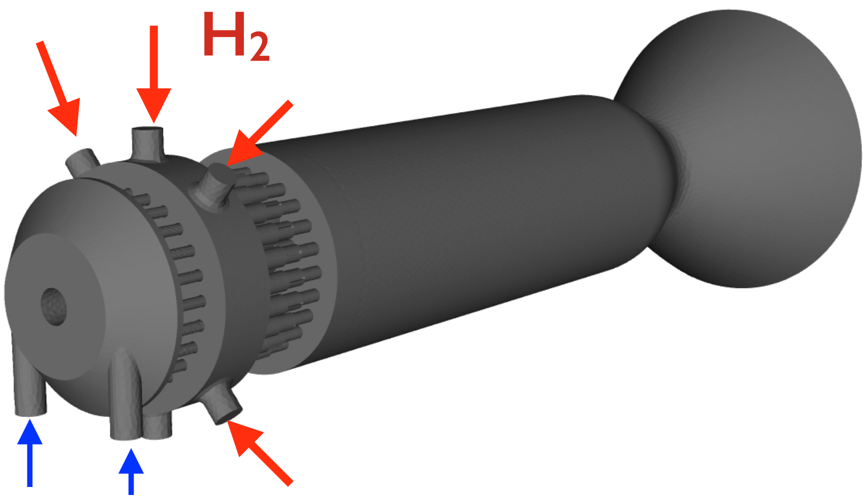
Liquid rocket engine (NASA 1957)

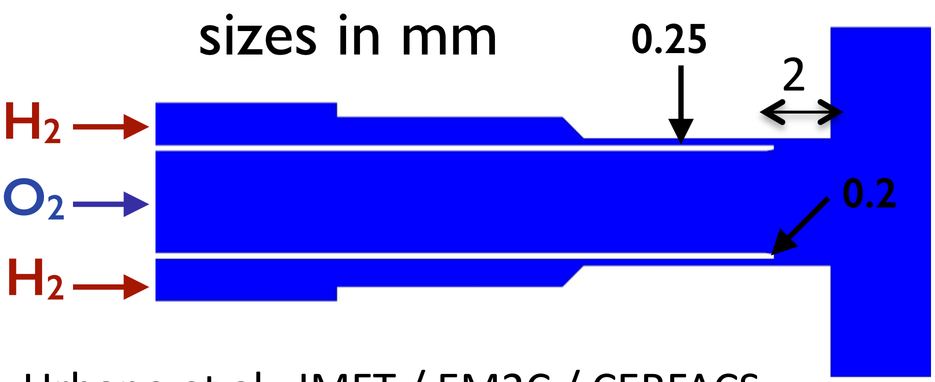


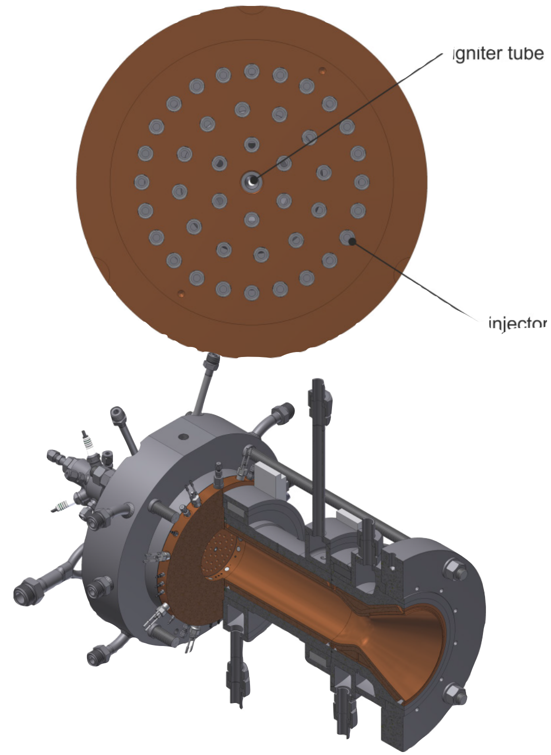
Liquid rocket engine (NASA 1963)

➡ DLR LAMPOLDSHAUSEN HF7 BKD

Full engine: 42 coaxial injectors
Cryogenic O_2/H_2 propellants
Pressure range: 50-80 bar





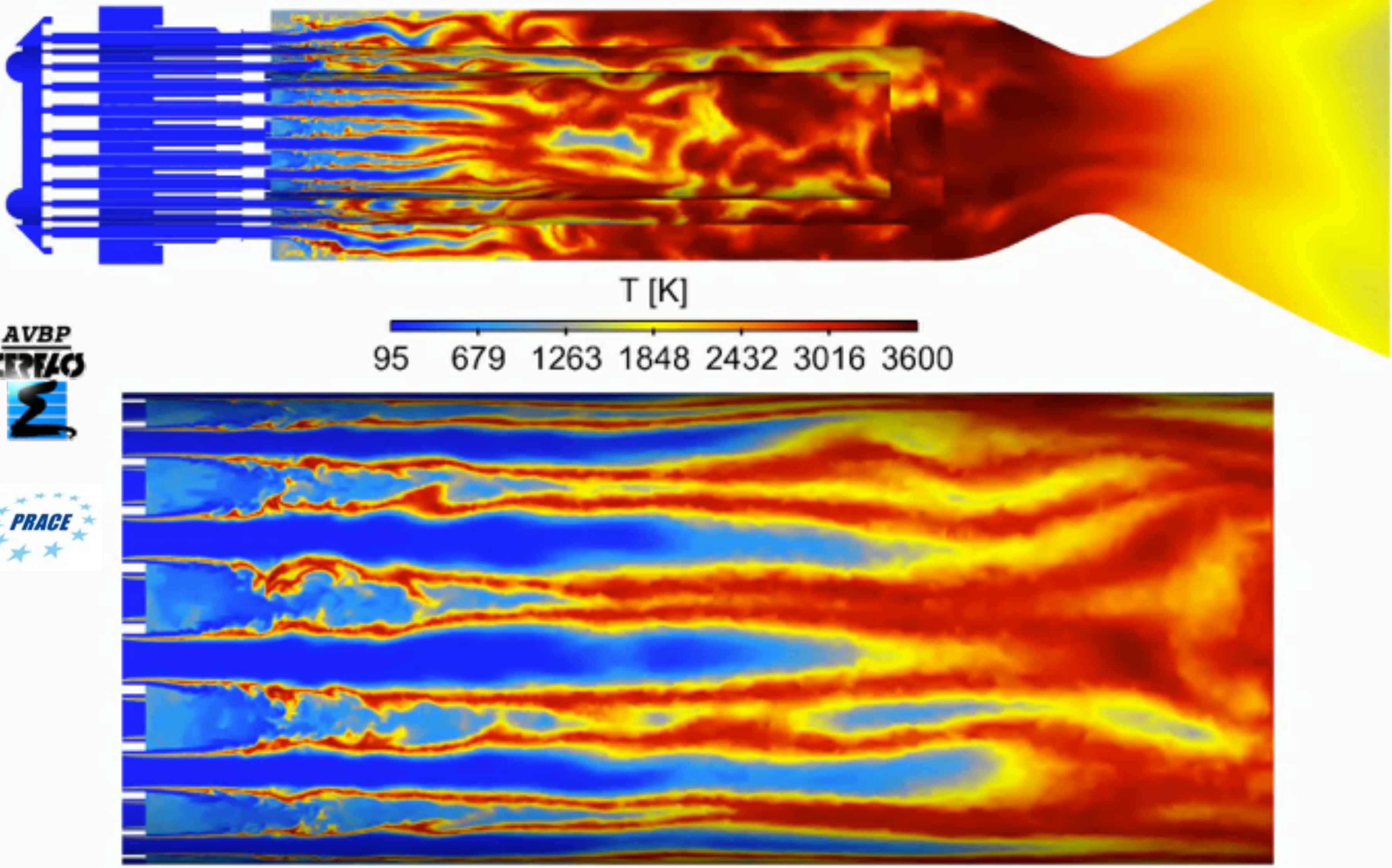


A. Urbano et al. IMFT / EM2C / CERFACS

power ~ 100 MW

80 M hours on FERMI (cineca IT) , 9th Prace CALL

40k Euros Simulation !



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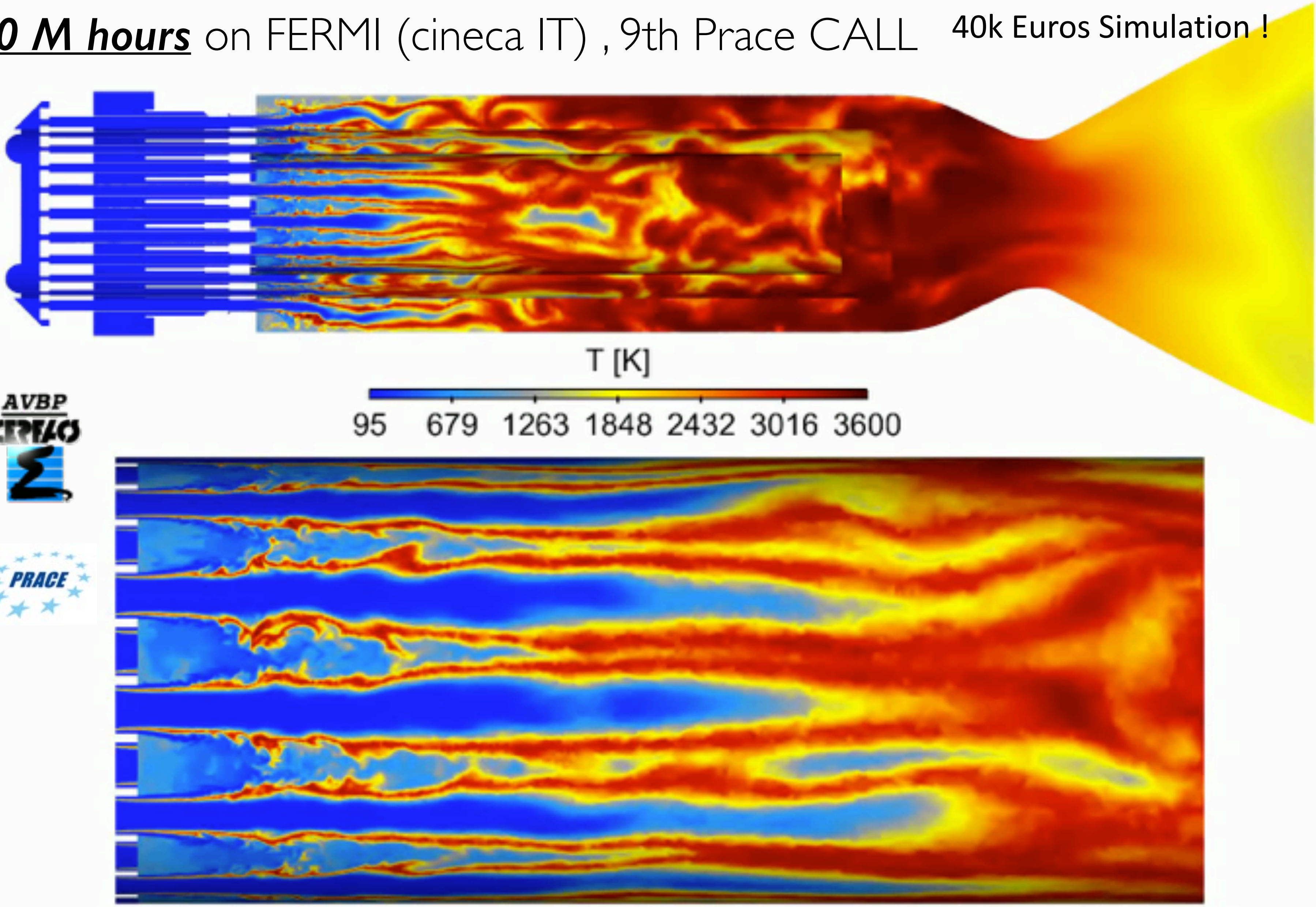


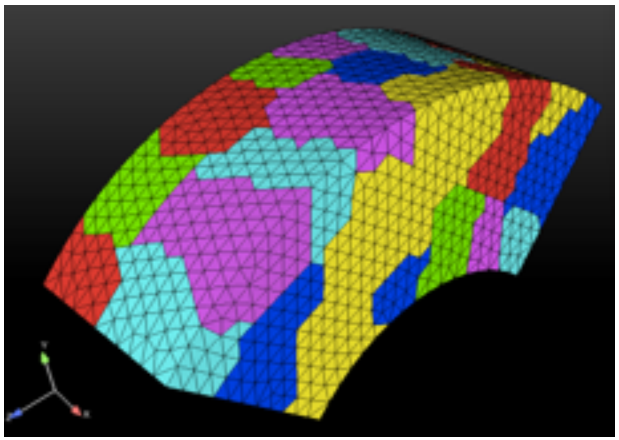
A. Urbano et al. IMFT / EM2C / CERFACS

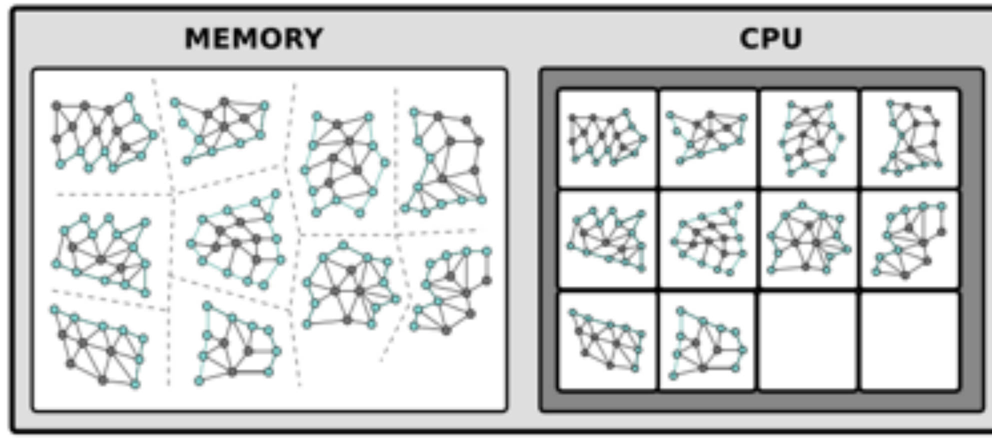
HPC and Combustion

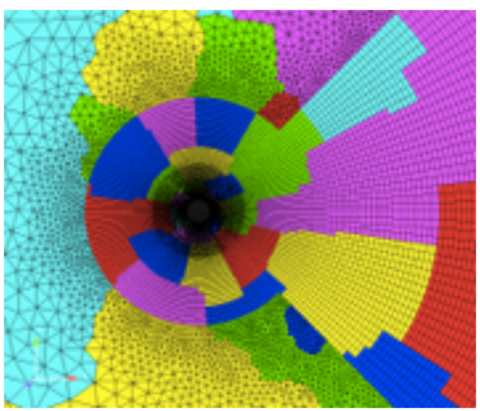
- These highly complex systems require large amount of computing power and large simulation times.
- At CERFACS we strive to keep the code as simple and portable as possible while trying to optimise the code as best we can on multiple architecture ..
- However sometimes physics and HPC do not get along …

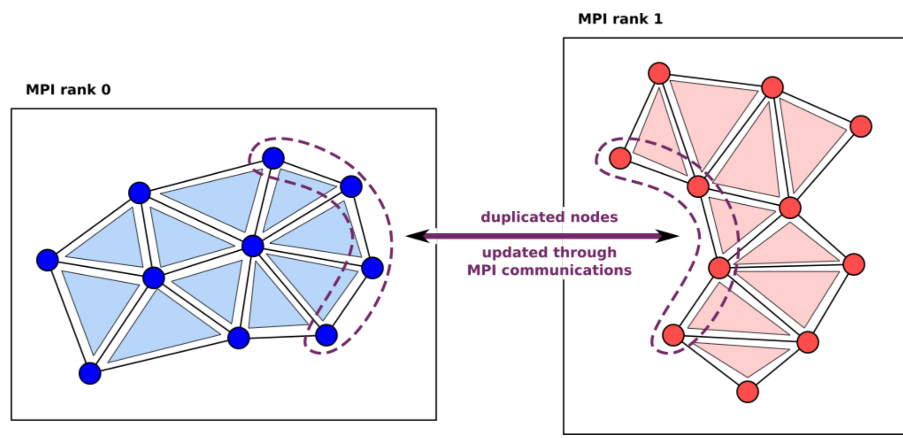
Parallelisation

- AVBP parallelism relies on MPI non blocking ISEND IRECV with a single node overlapping domain decomposition

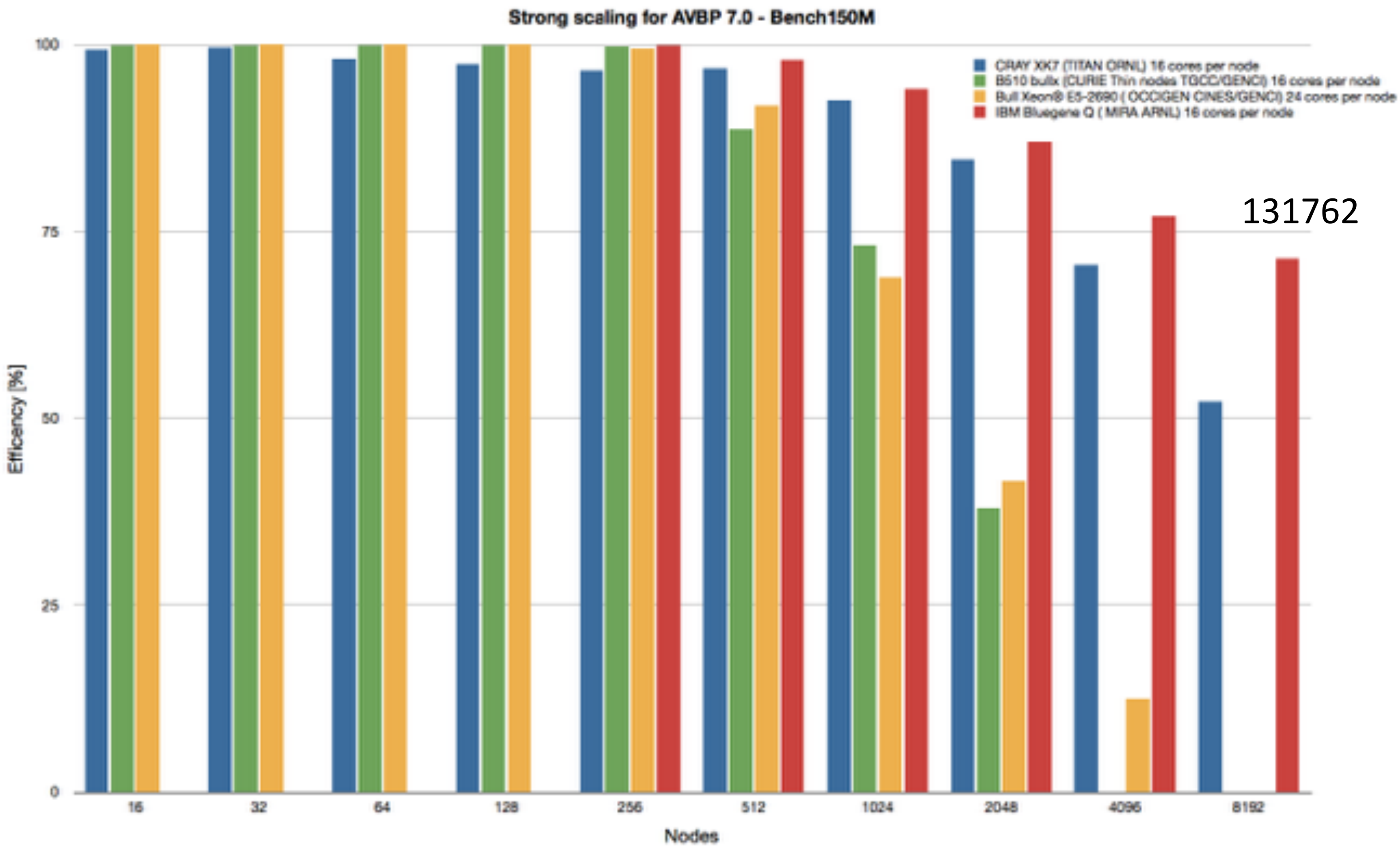




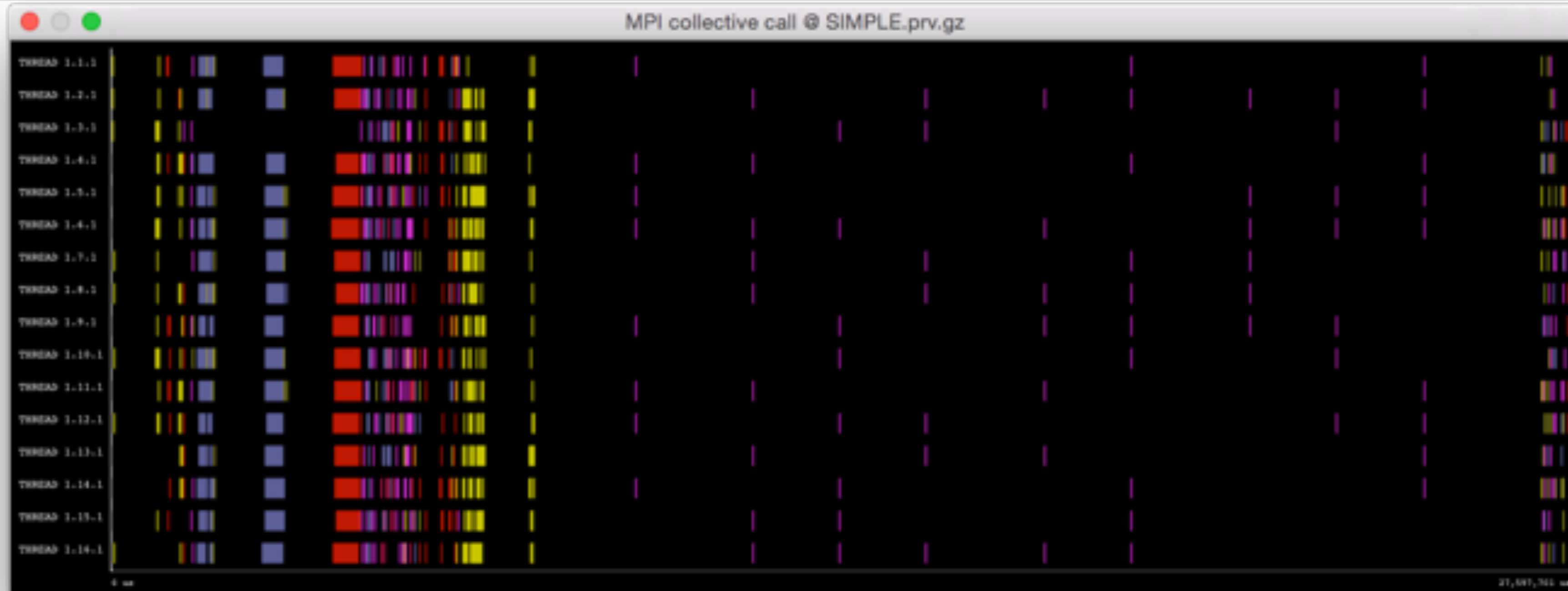




Parallel performance



Collective Calls

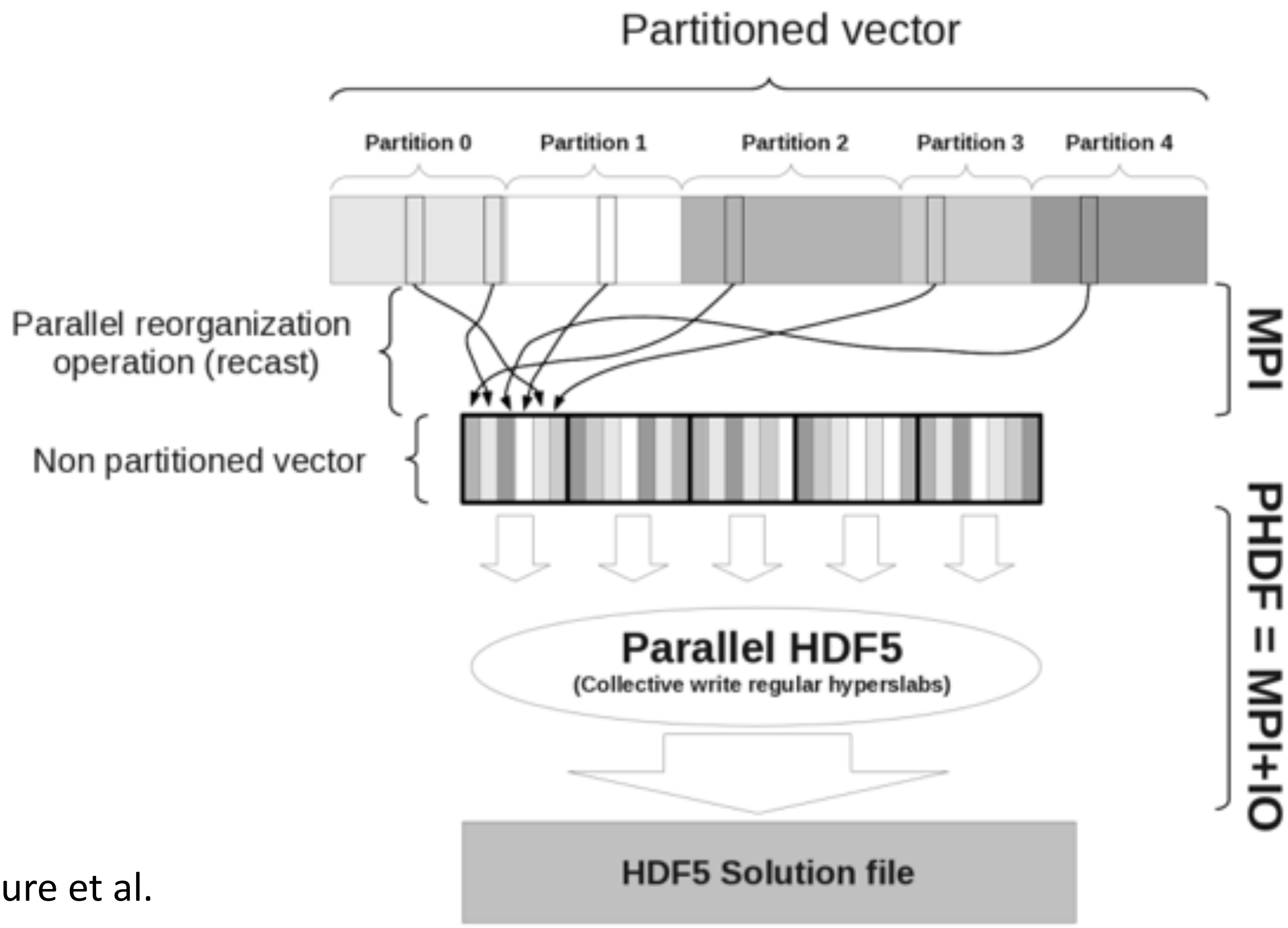


- MPI_BCAST
- MPI_BARRIER
- MPI_ALLTOALL
- MPI_ALLREDUCE

➡ High usage of collectives

- Physics
- Monitoring
- I/O

Parallel I/O



Jaure et al.

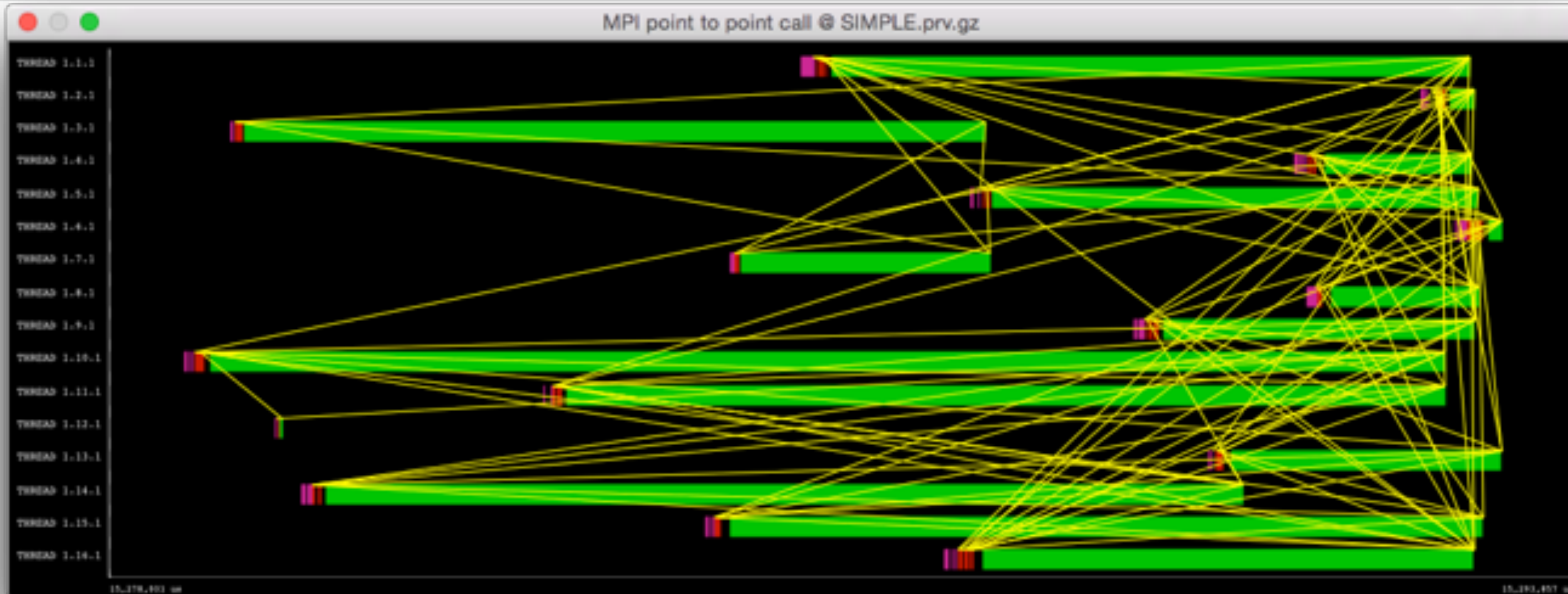
Point to Point

MPI_WAITALL

MPI_IRECV

MPI_ISEND

Point to Point

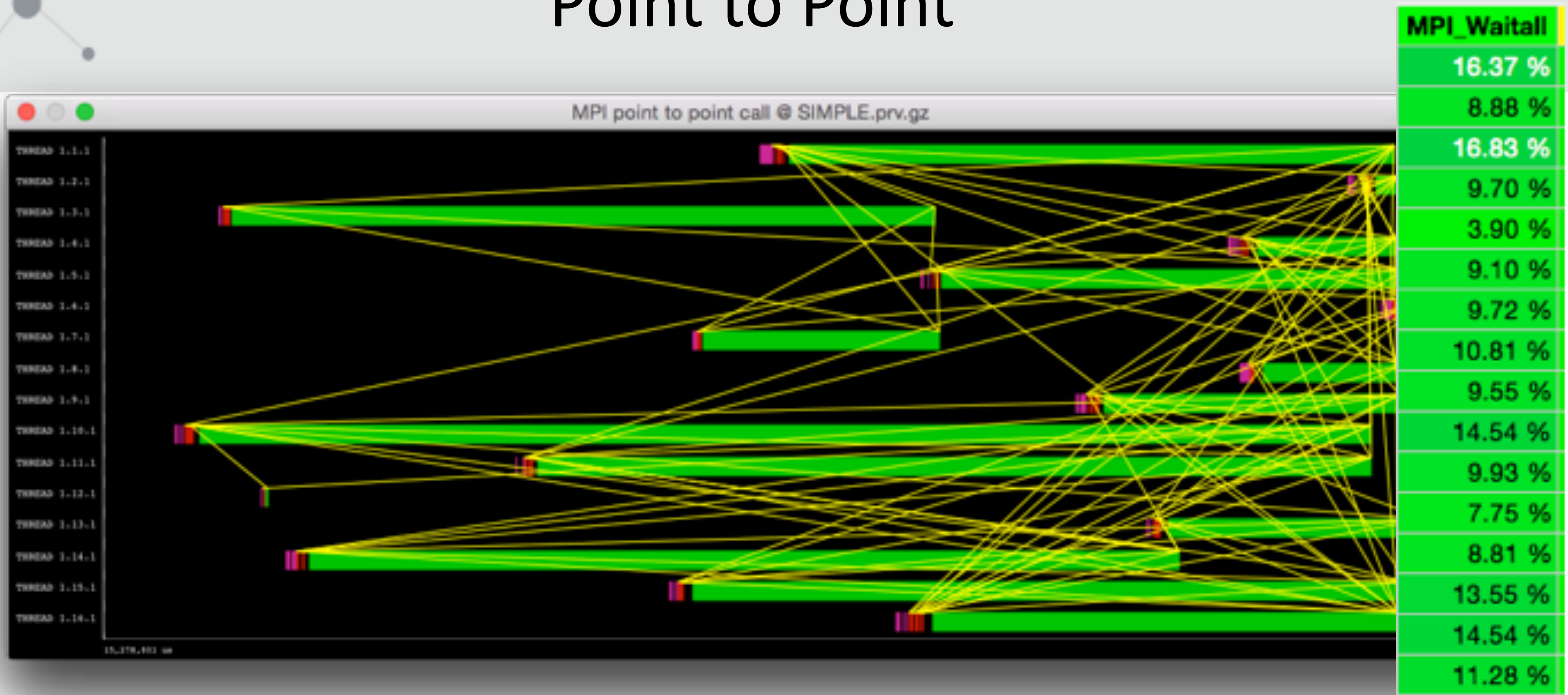


MPI_WAITALL

MPI_IRECV

MPI_ISEND

Point to Point



- MPI_WAITALL
- MPI_IRECV
- MPI_ISEND

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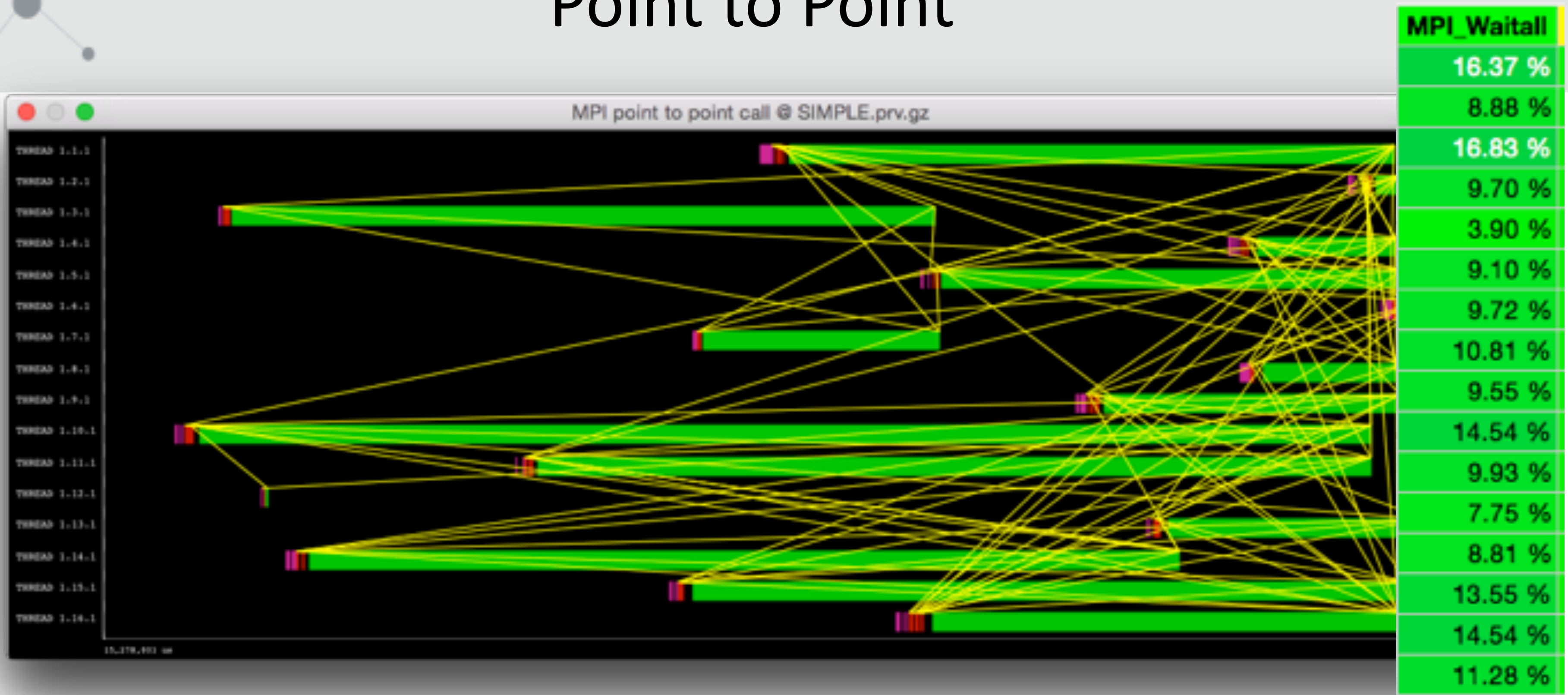

MPI_WAITALL

MPI_IRECV

MPI_ISEND

➡ Small communication pattern

- High imbalance

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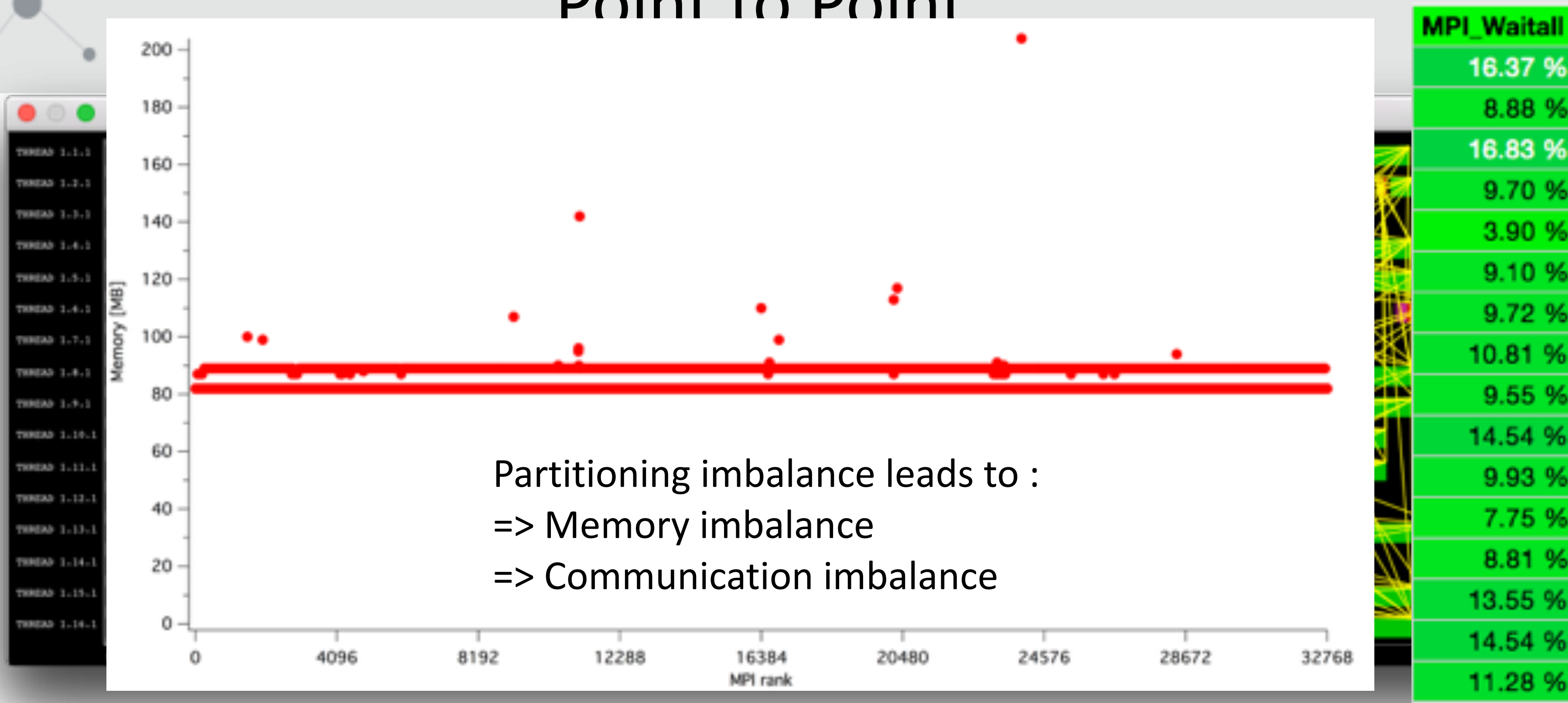


MPI_WAITALL

MPI_IRECV

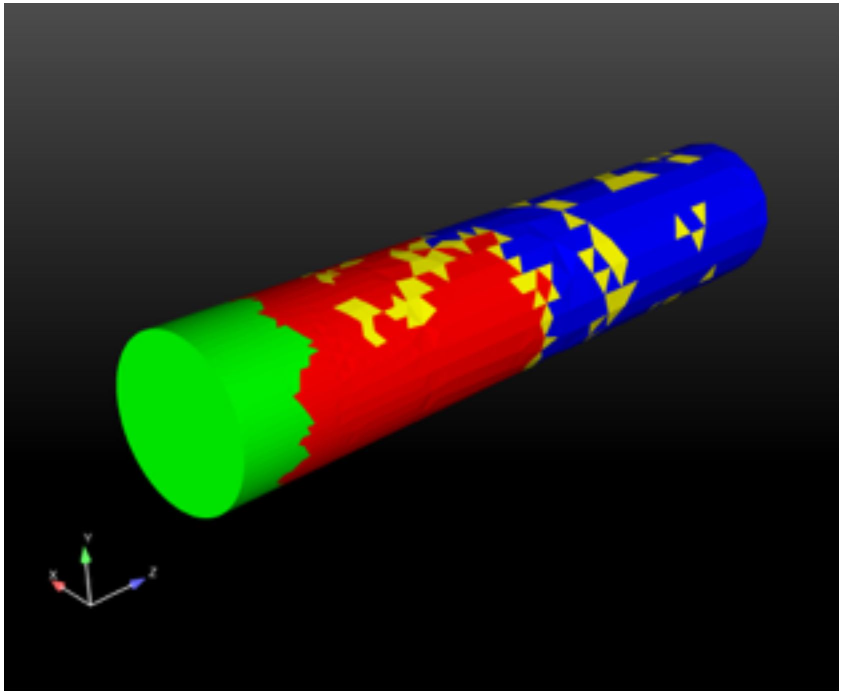
MPI_ISEND

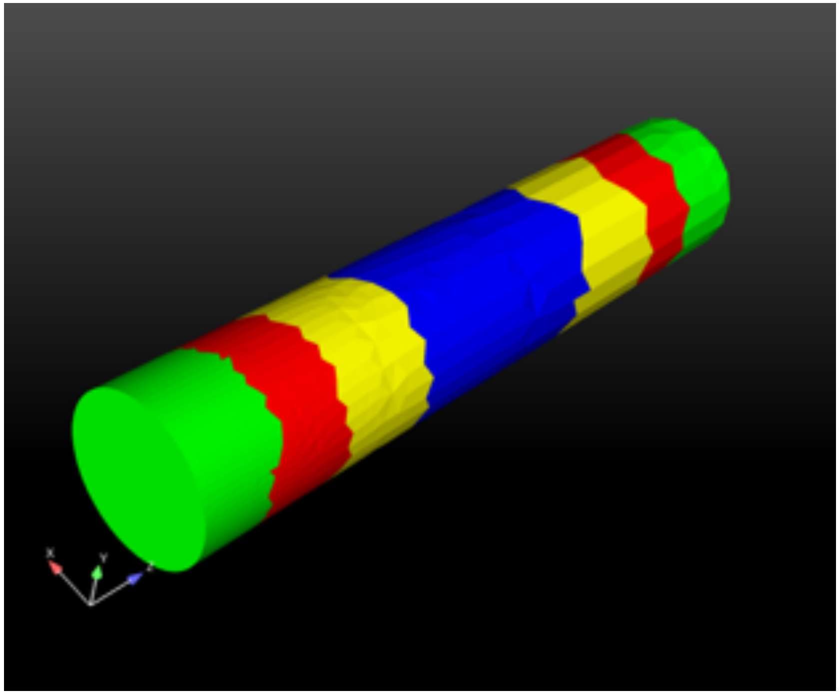
➡ Small communication pattern

- High imbalance

Balanced partition does not mean balance communications …

- Simple Cylinder on 4 domains …

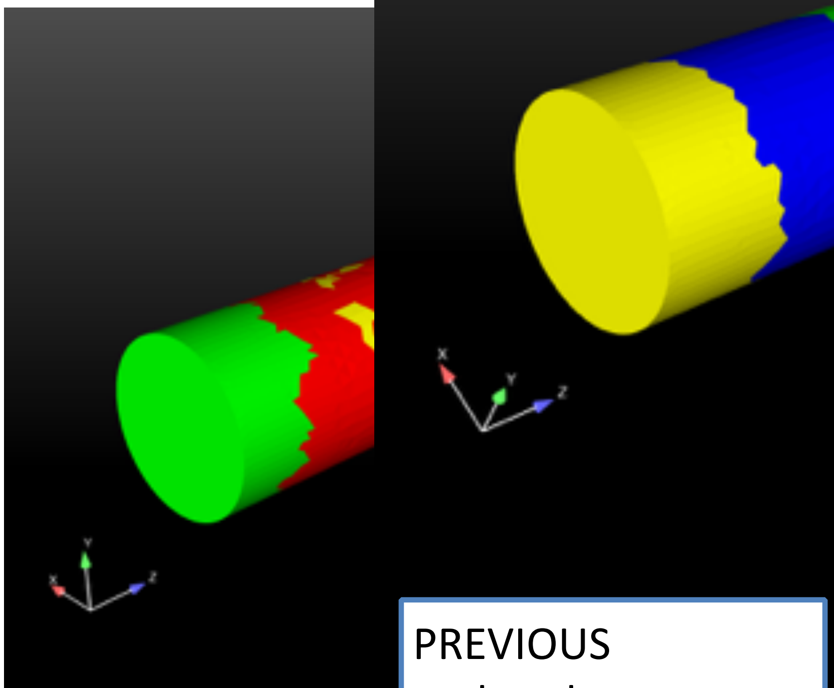


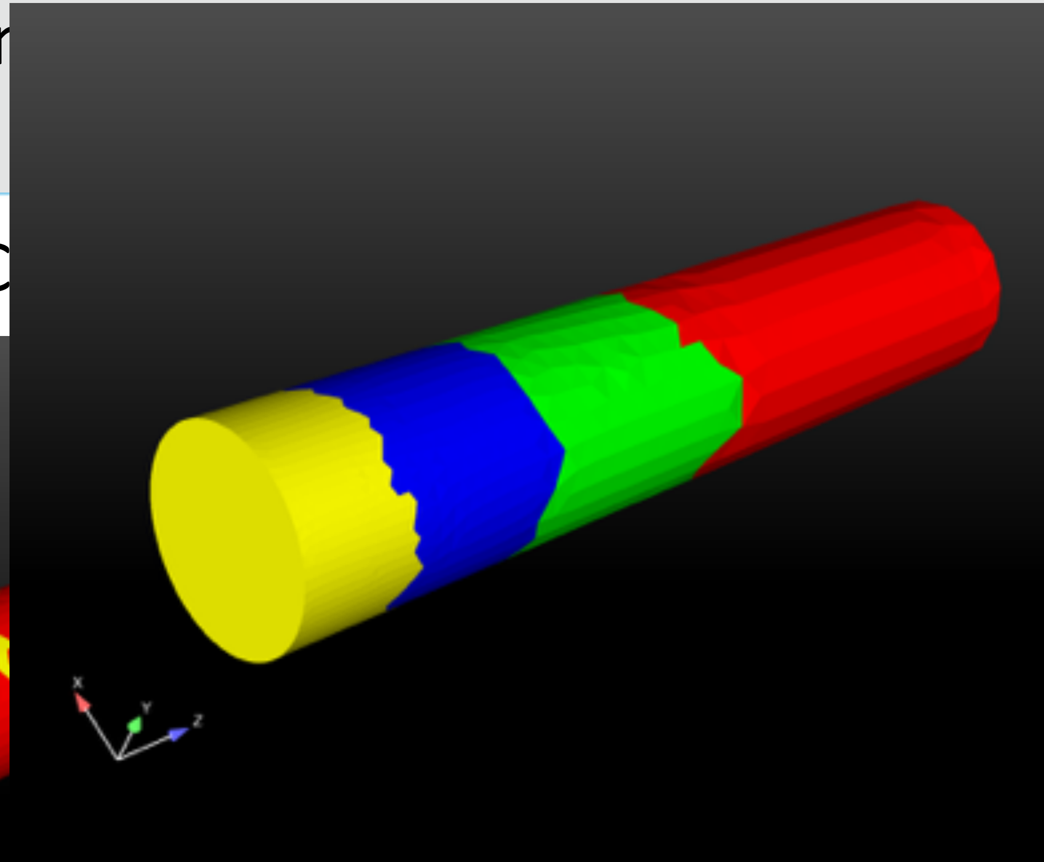


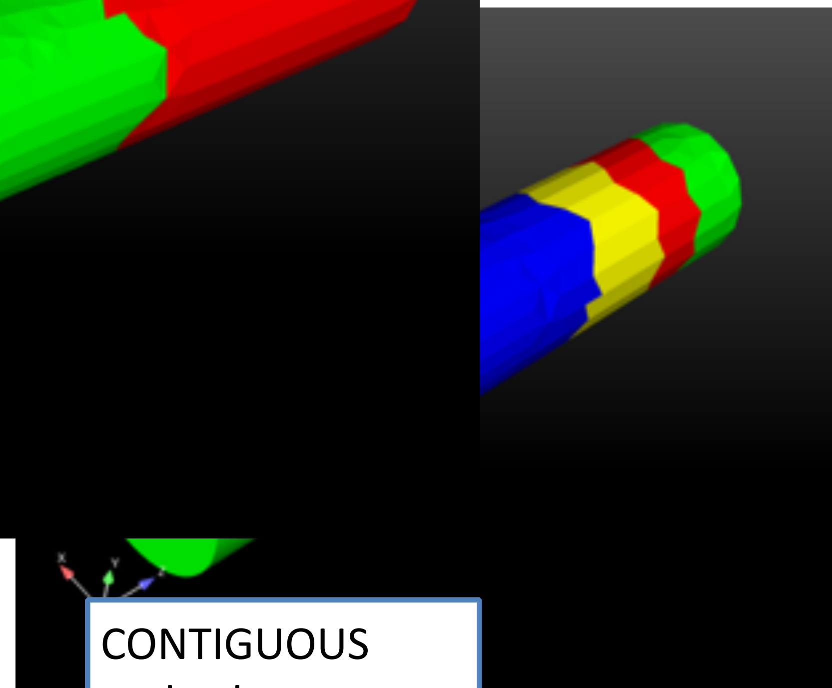
rank	elements
1	18949
2	19011
3	18997
4	19011

Bala ... ance

- Simple C







PREVIOUS

rank	elements
1	18949
2	19011
3	18997
4	19011

CONTIGUOUS

rank	elements
1	38050
2	16336
3	16979
4	4603

Current Challenges

- Imbalance can be somewhat compensated by Communication/Computation overlap
  - Contiguous partitioning
    - Reduces the number of neighbours !
    - Is not 'fully balanced' : imbalanced vertices/task
- High usage of collective leads to radical differences depending on the implementations.
  - Collectives are extremely important for CFD applications
- Overlap of (MPI) I/O and computation

Current frontier Science : MPMD coupling/Multiphysics

- One code all the science .... Not realistic (Optimisation, physical models , Complexity of maintaining the tool)
- Solution : MPMD code coupling
- Use optimize code for each physics and use a coupler to handle the interaction

- CERFACS and ONERA develop the Open source coupler

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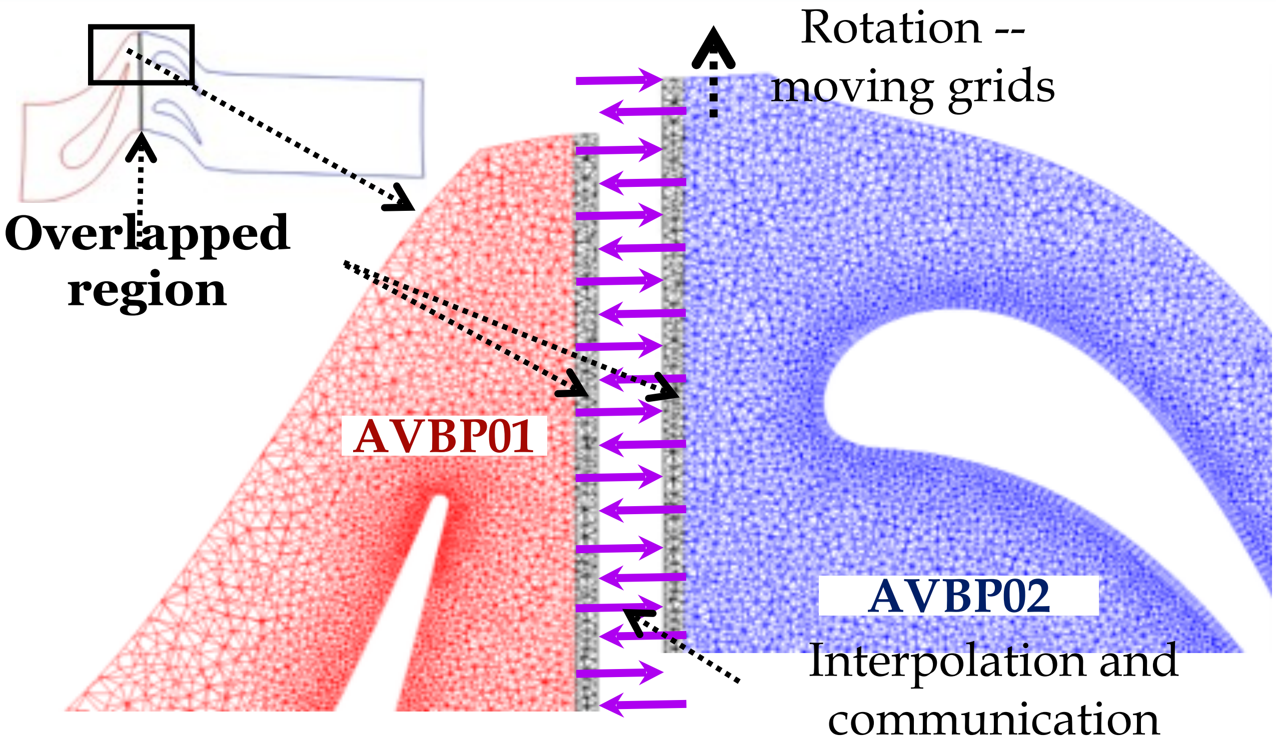
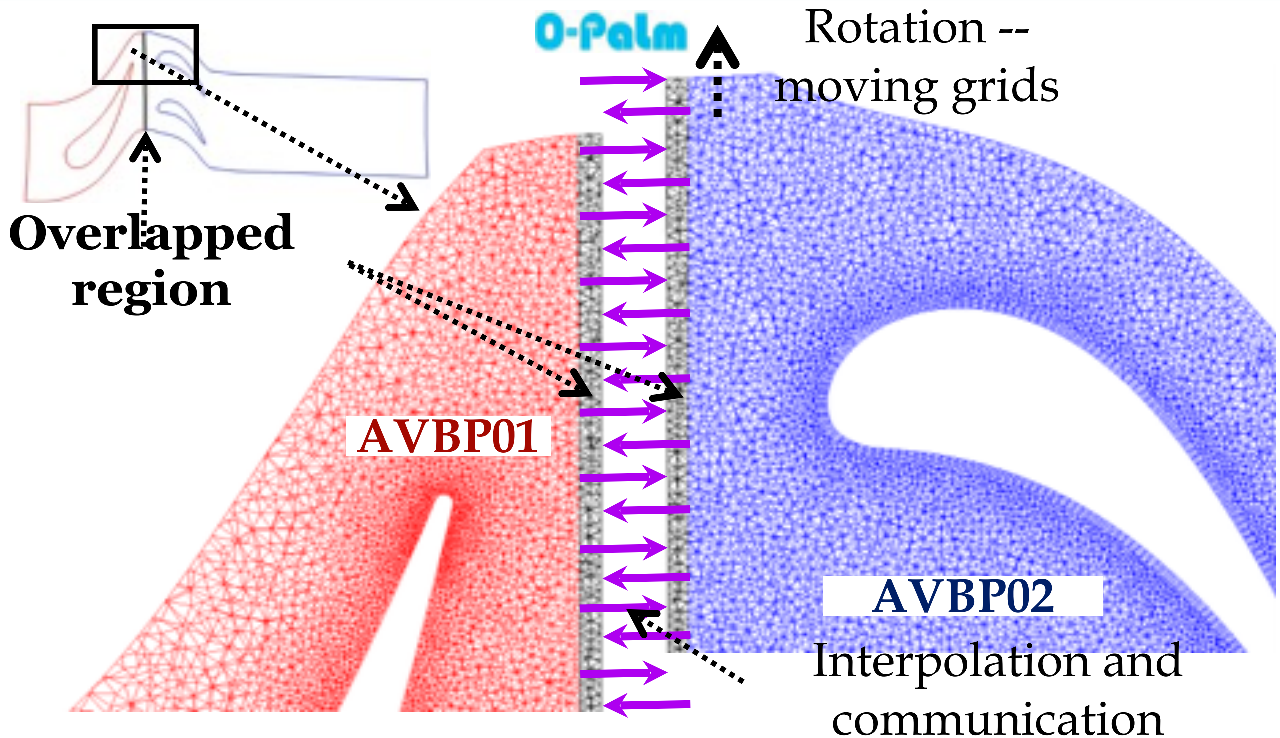
Example of code coupling method for moving parts



- Characteristics are similar to the sliding mesh approach (Francois, ISABE 2011):
- Overlapping section width depends on numerical stencil 2nd and 3rd order interpolation available (Linear and Hermite-type)

Example of code coupling method for moving parts



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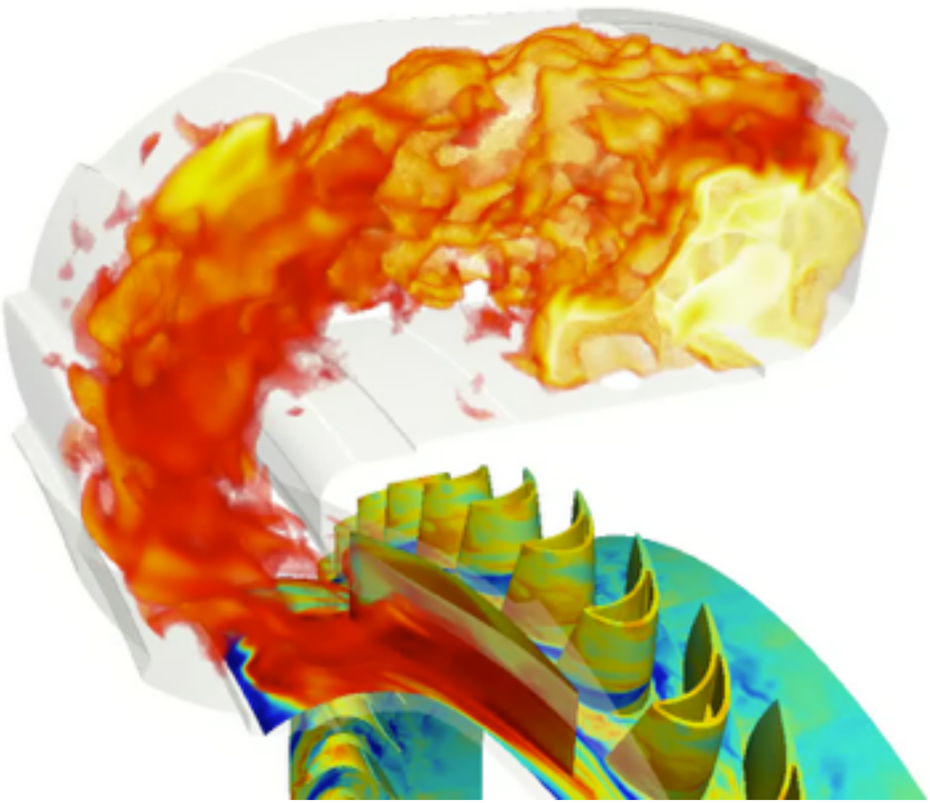
Combustion chamber / Turbine Simulation

➡ First LES of combustion and first turbine stage



- Possibility to perform each simulation separate before doing the coupled case
- Hand made load balancing between the two instances.

D. Papadogianis et al

Combustion chamber / Turbine Simulation

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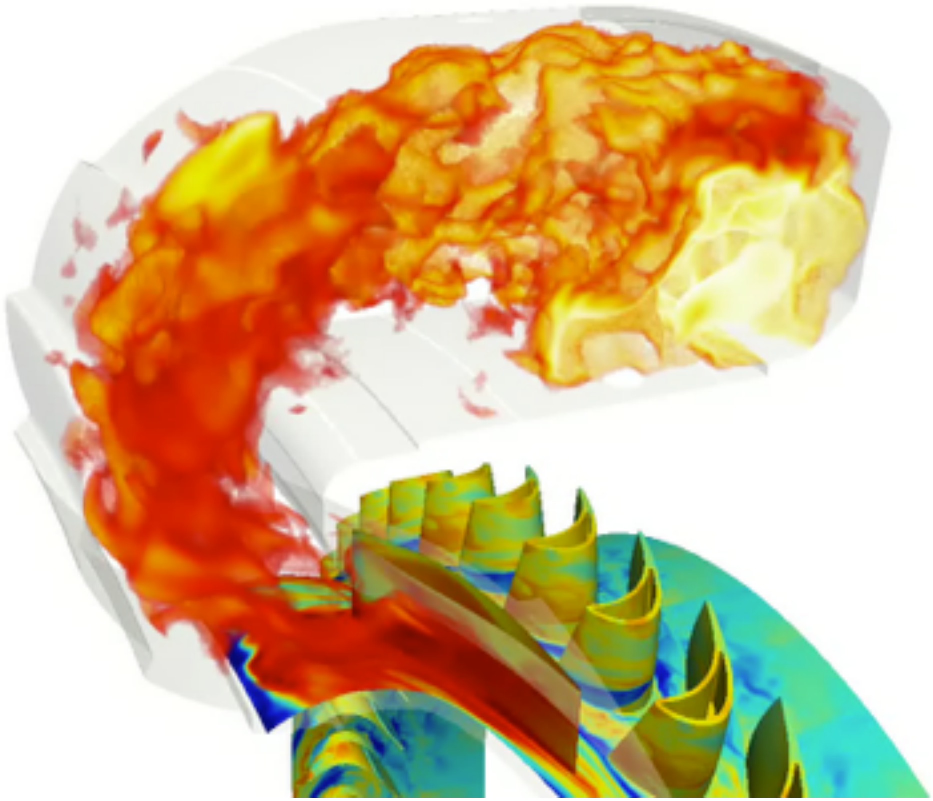

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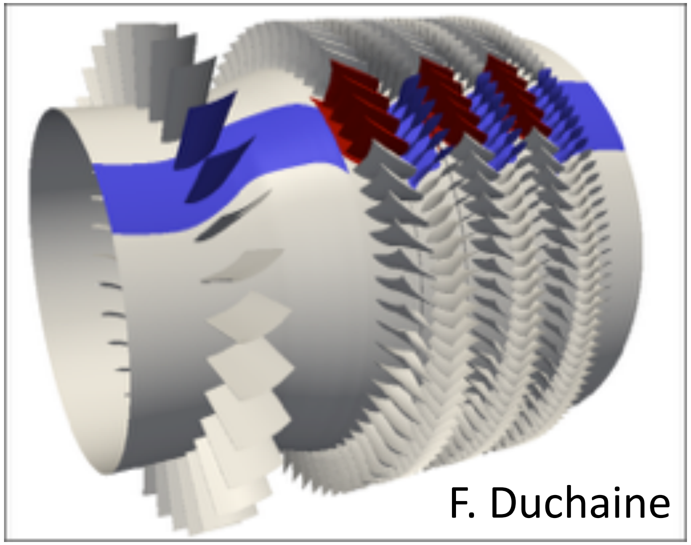
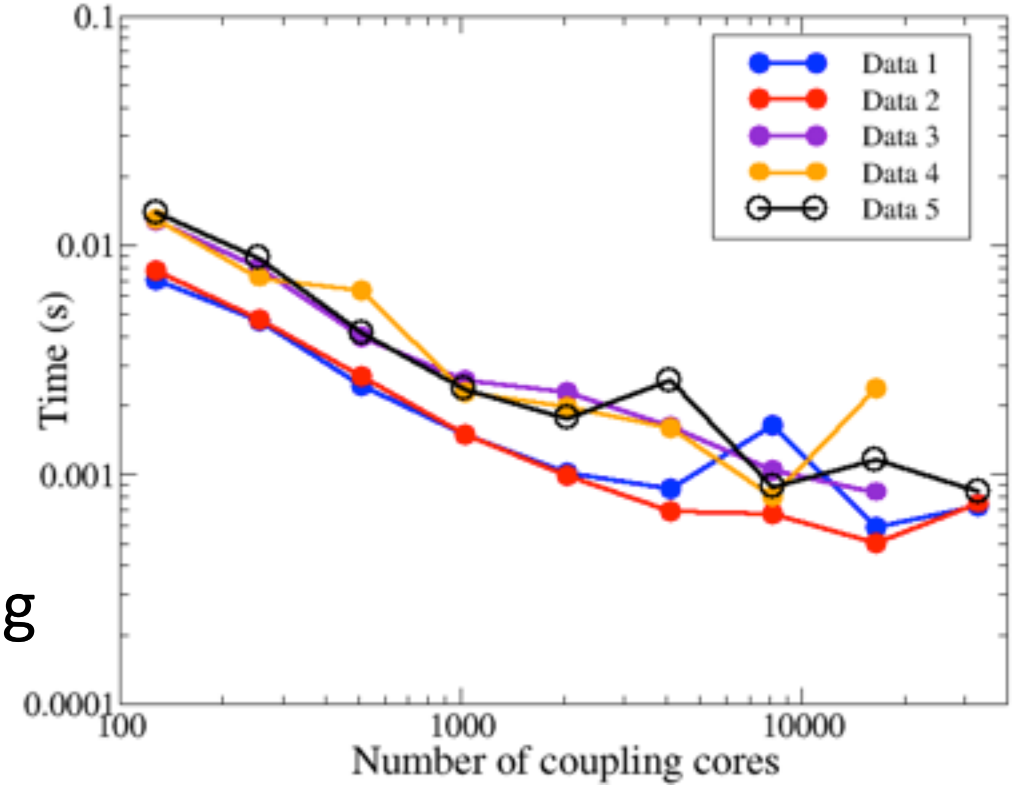
D. Papadogianis et al

Duchaine et al.



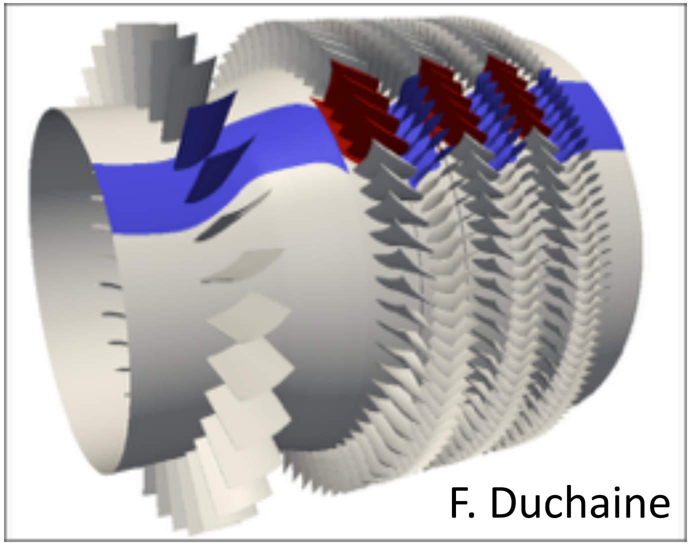
Exchanges time for TITAN CRAY (ORNL)



- Multiple stage coupling
- Two AVBP instances

Full compressor LES

Duchaine et al.



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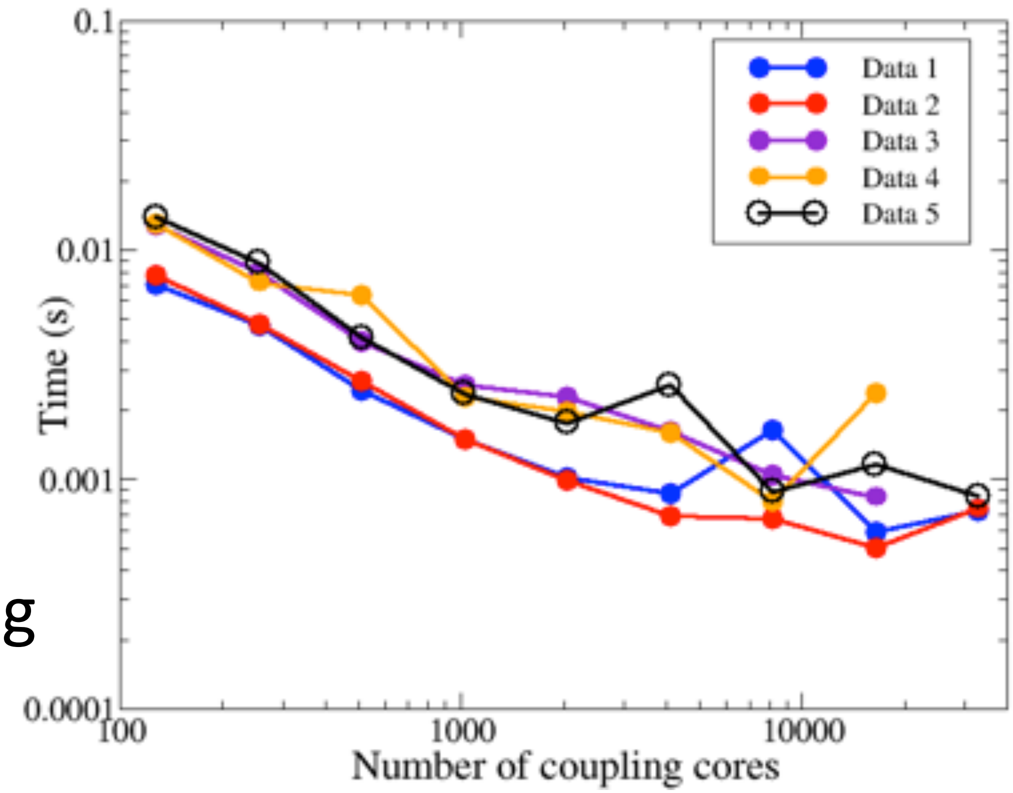
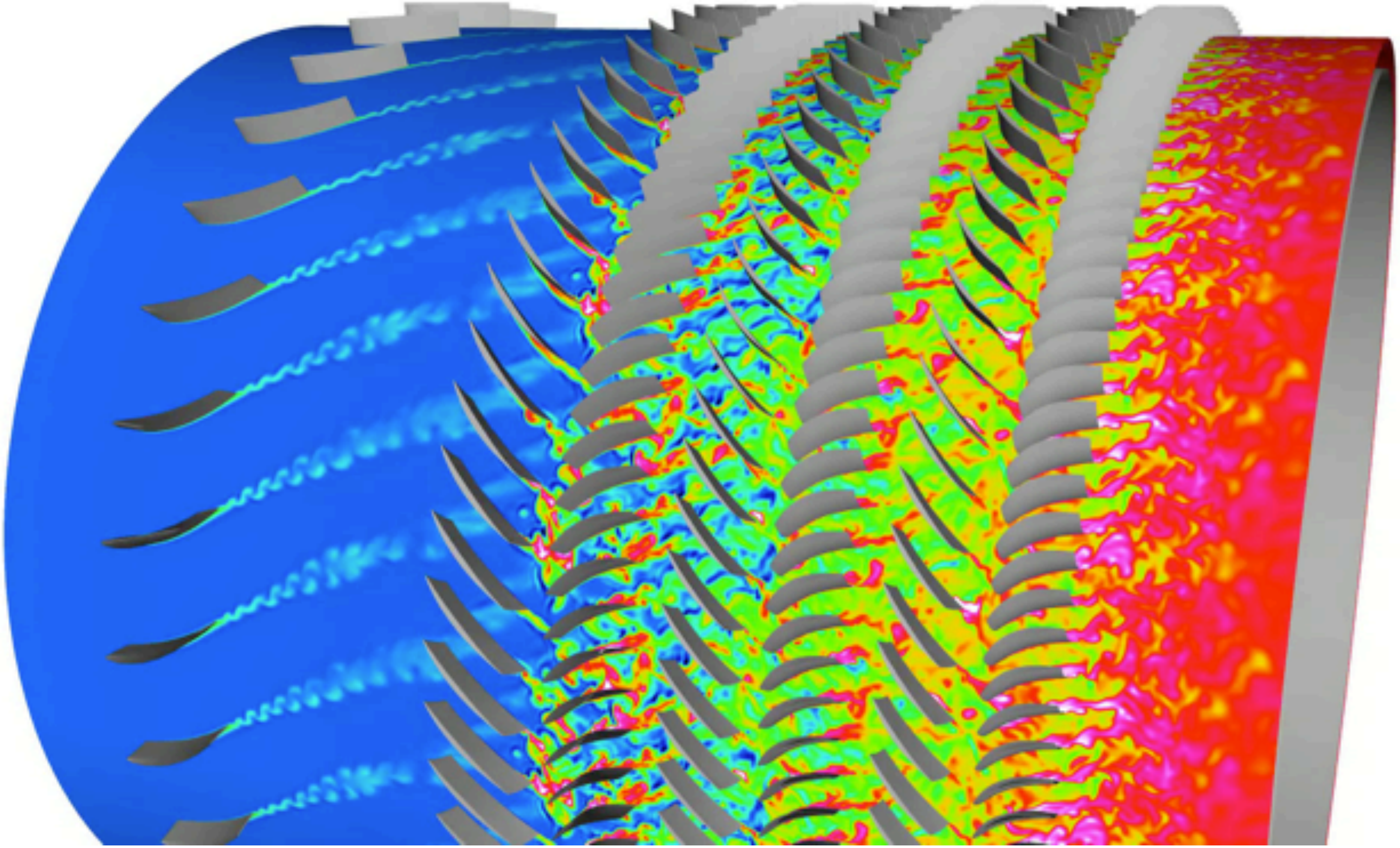


- Multiple stage coupling
- Two AVBP instances

<u>Need for co-partitititioning methods :</u>

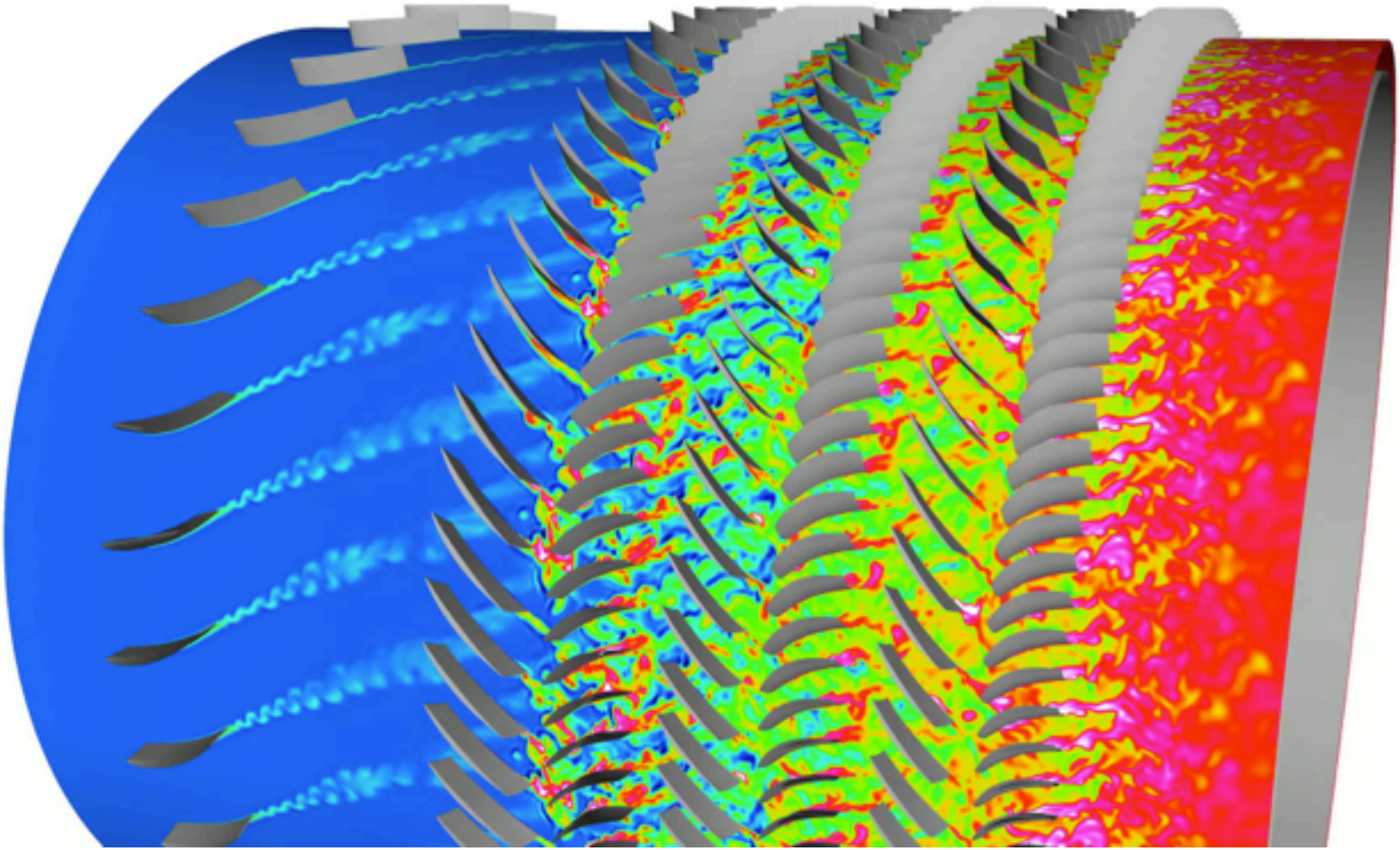
<u>=> Partition instance 2 based on instance 1 to limit exchanges</u>

Full compressor LES



Multi-Stage Gas Turbine Computation. Grand Challenge OCCIGEN. GENCI/CINES. 7680 Haswell Cores.
IDRIS Grand Challenge 6144 MPI tasks
J. Delaborderie, F. Duchaine, L. Gicquel, G. Staffelbach

Full compressor LES



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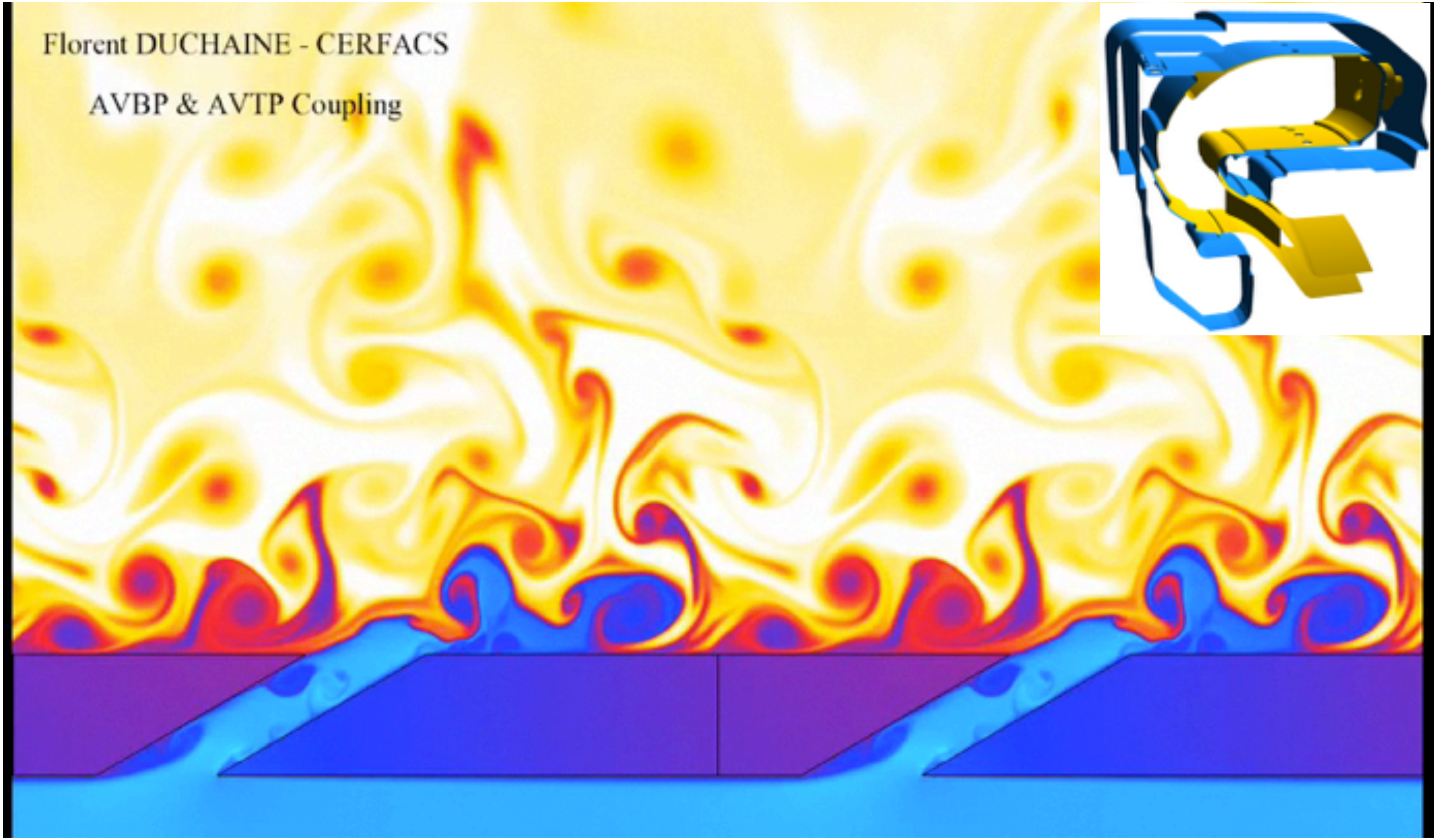
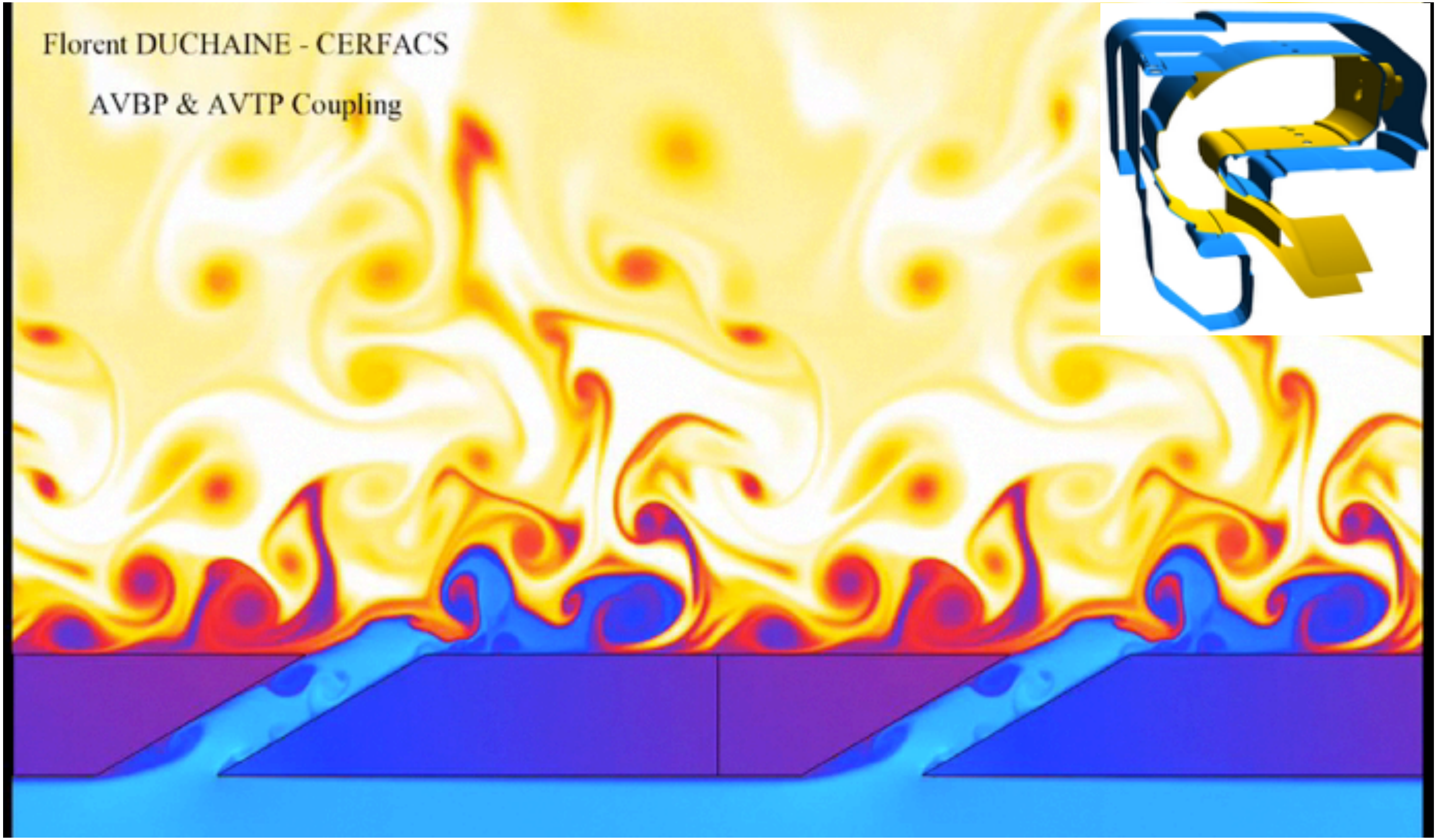
J. Delaborderie, F. Duchaine, L. Gicquel, G. Staffelbach

Fluid / Solid thermal conduction



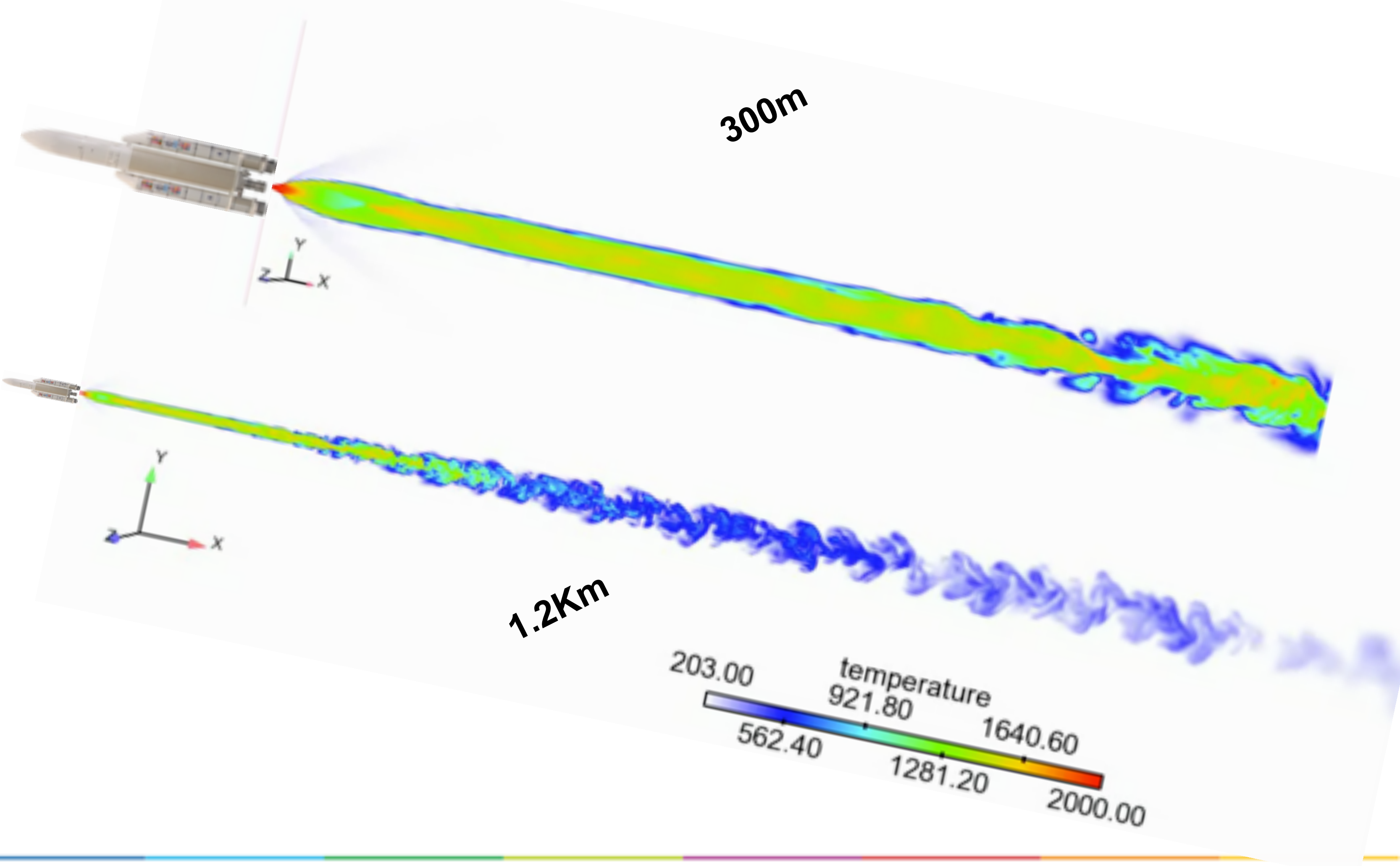
Fluid / Solid thermal conduction



Fun application: 3D Large Eddy Simulation of a booster trail.

A. Poubeau R. Paoli

Booster trail simulation



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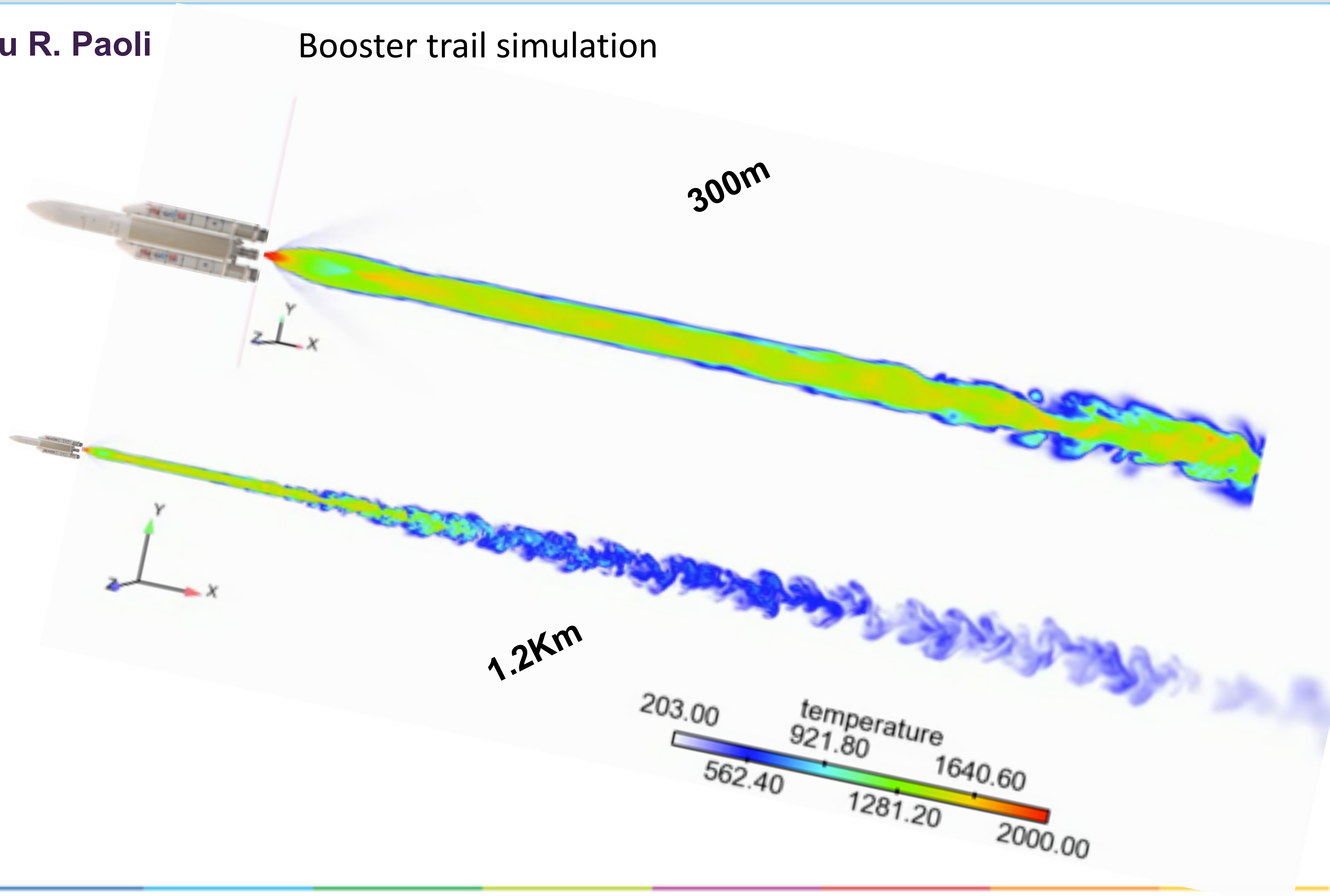

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A. Poubeau R. Paoli

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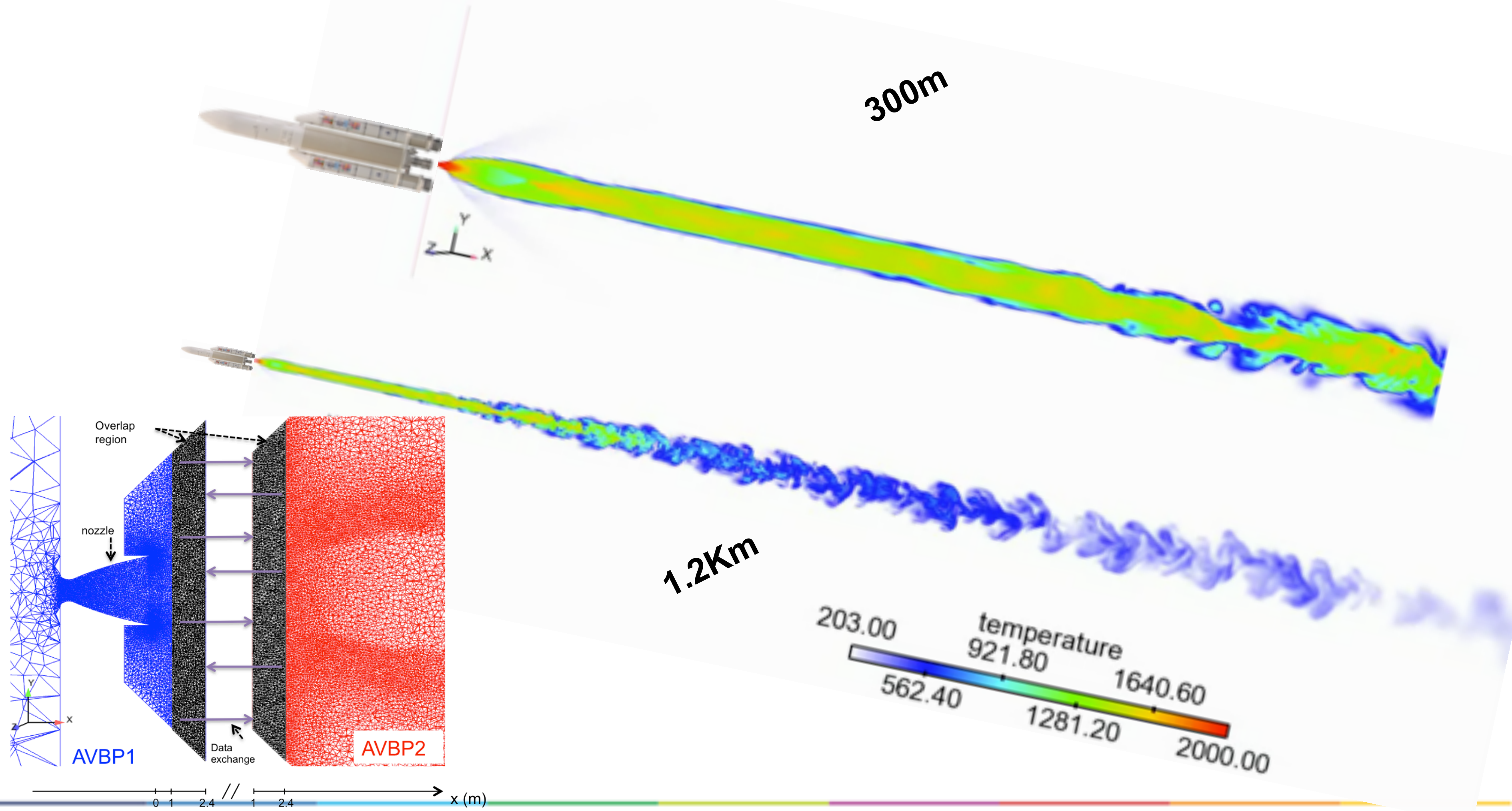
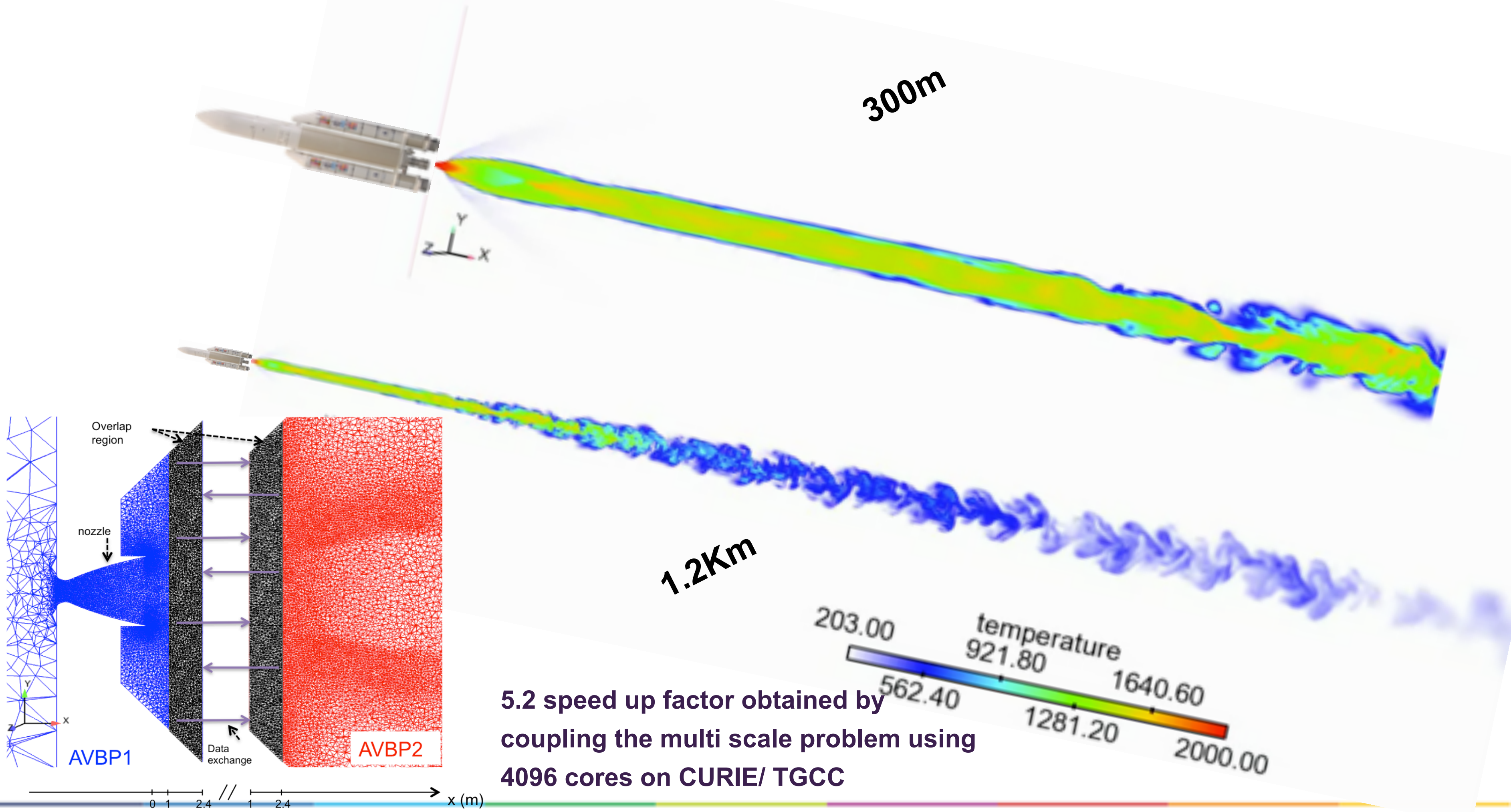


Cut of the domain showing the grids around the coupling zone

Fun application: 3D Large Eddy Simulation of a booster trail.

A. Poubeau R. Paoli

Booster trail simulation

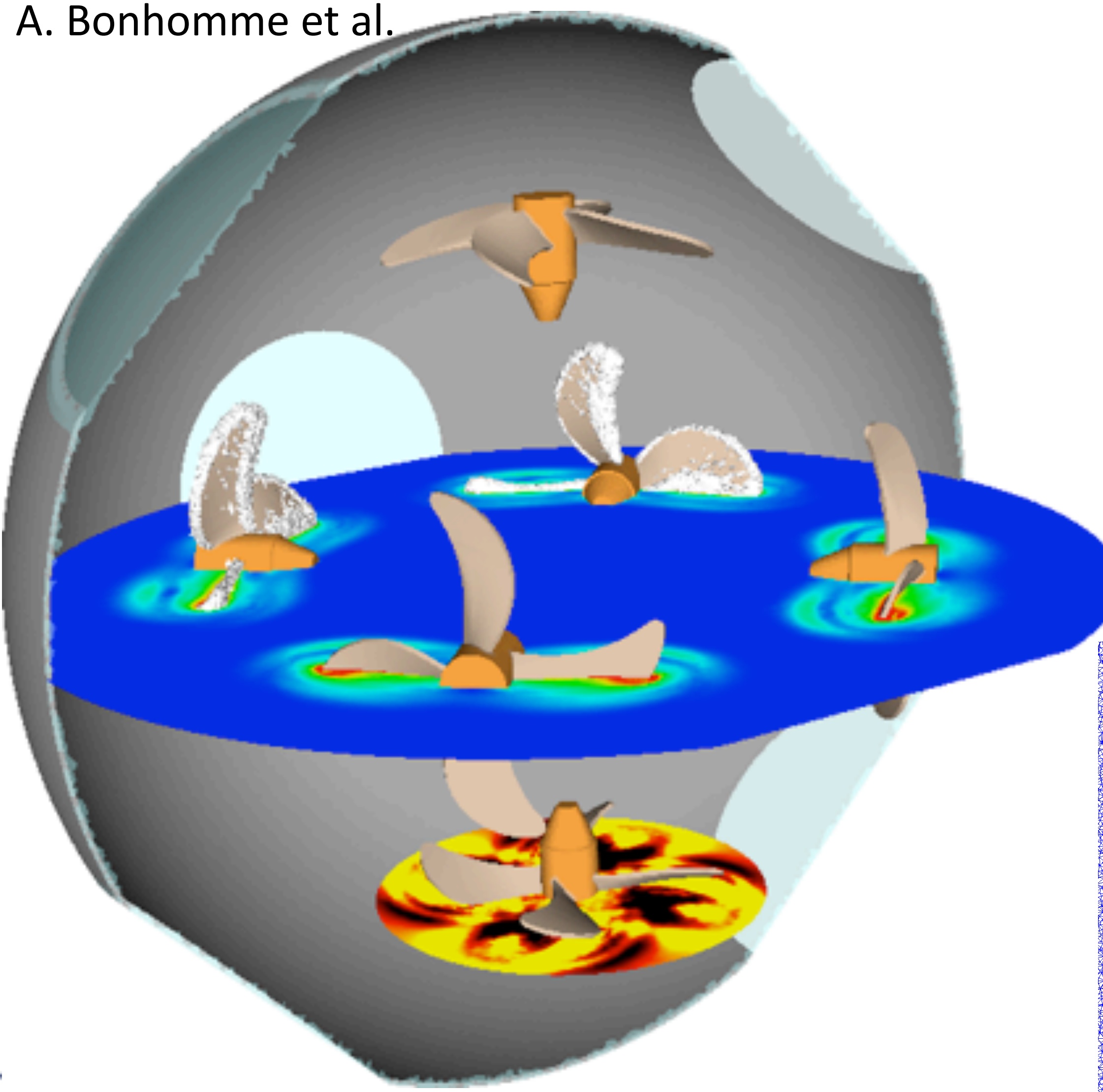


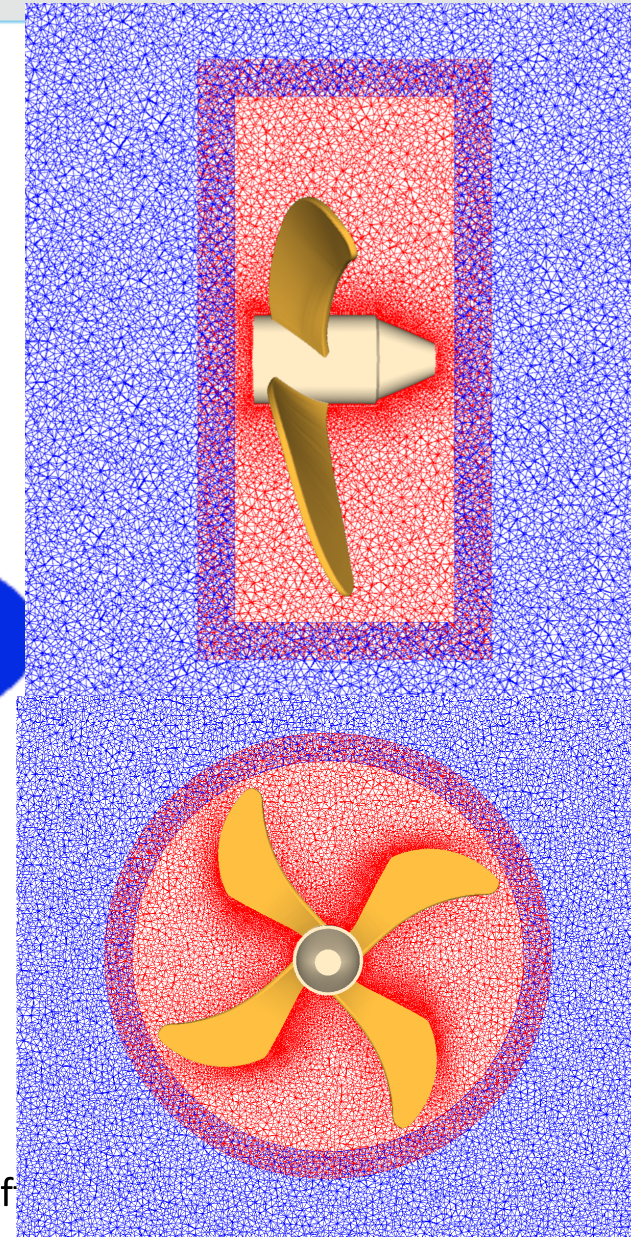
Cut of the domain showing the grids around the coupling zone

5.2 speed up factor obtained by coupling the multi scale problem using 4096 cores on CURIE/ TGCC

Fun application

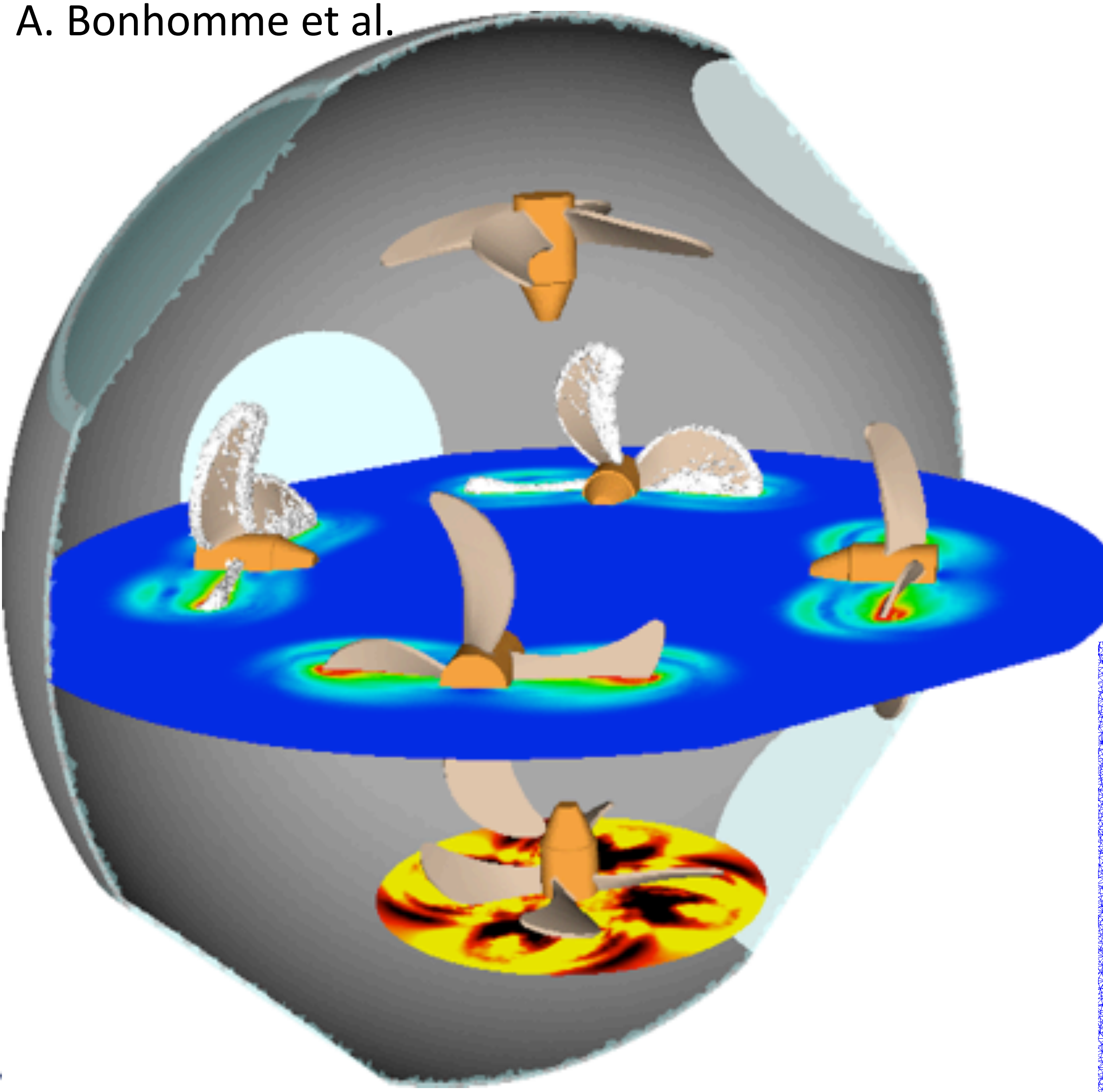
A. Bonhomme et al.

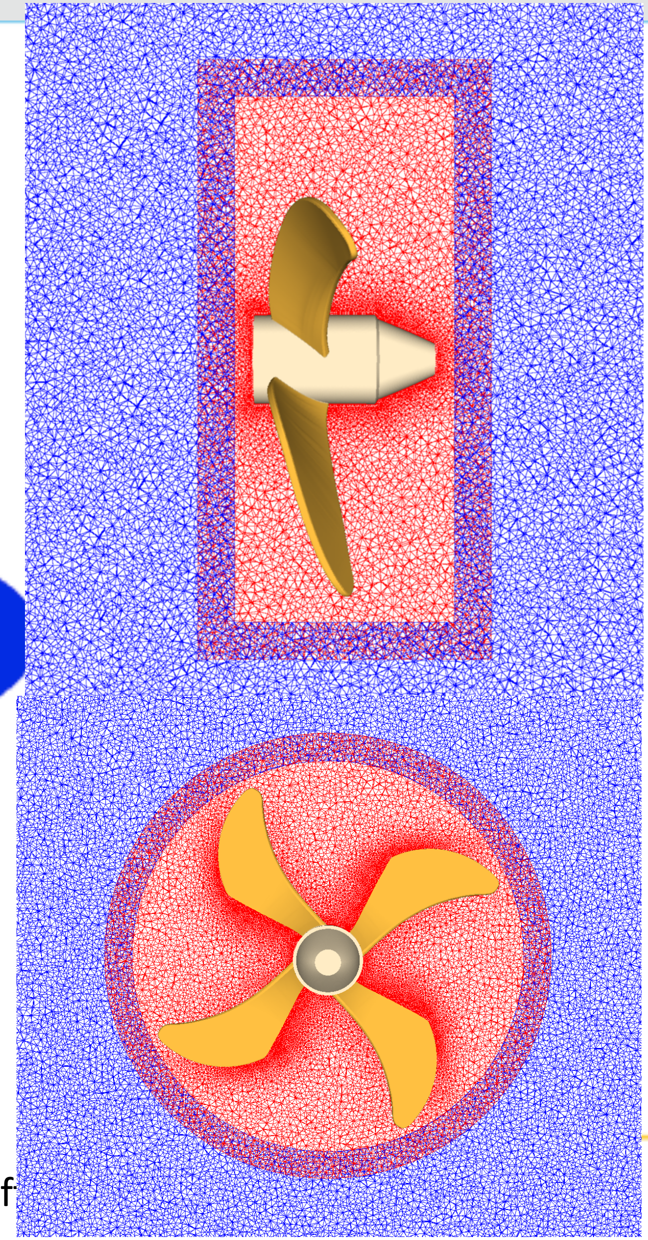




Fun application

A. Bonhomme et al.





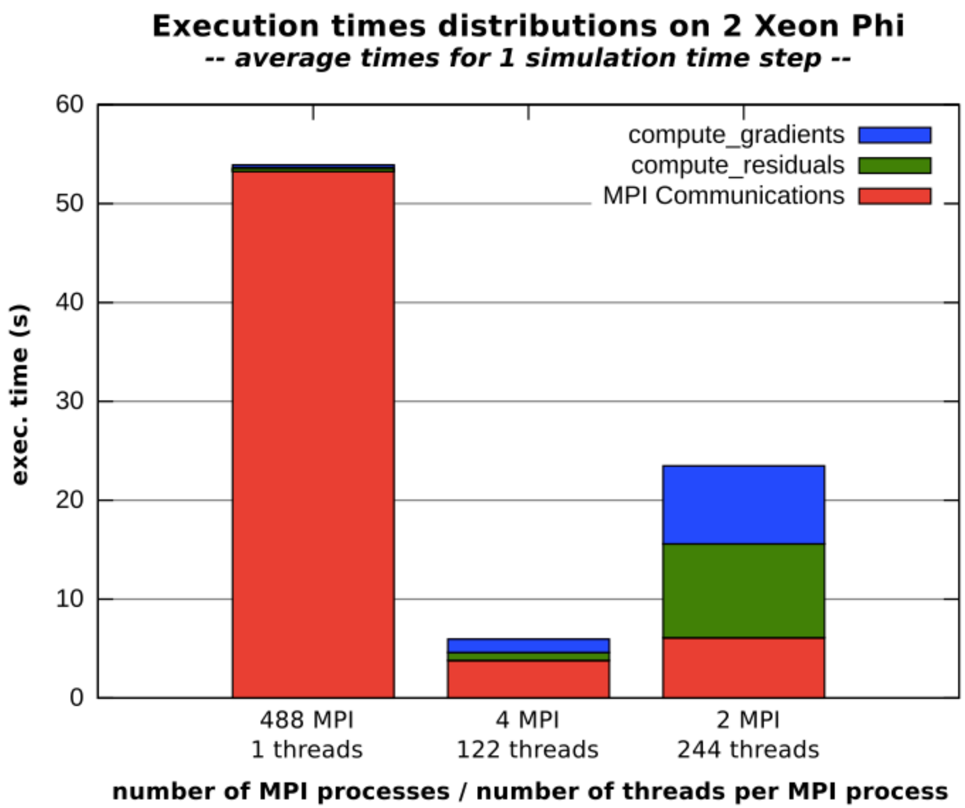
CFD MPI challenges

- High usage of collectives ..
  - Physics likes maxima/Sums … Not optimised on all implementations.
  - For code coupling .. reductions on sub-communicators is 100 times slower than on MPI_COMM_WORLD (BG \Q , CRAY) ….
- Enormous dependency on partitioning .. Most balanced work is not always the best approach ..

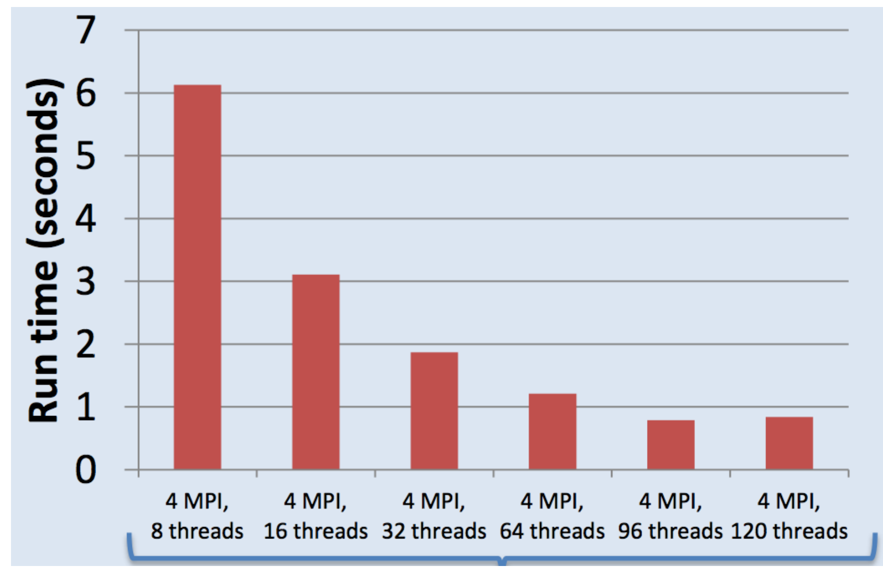
- How to handle heterogeneous machines with only MPI ?

MPI limitations on Heterogeneous MIC systems

- MPI execution times is highly dominated by MPI ….



Intel PCC



XEON PHI

➡ Possible to avoid hybrid approach via runtime or MPI put/get implementation ?

Code modernisation : MPI+OPENMP4

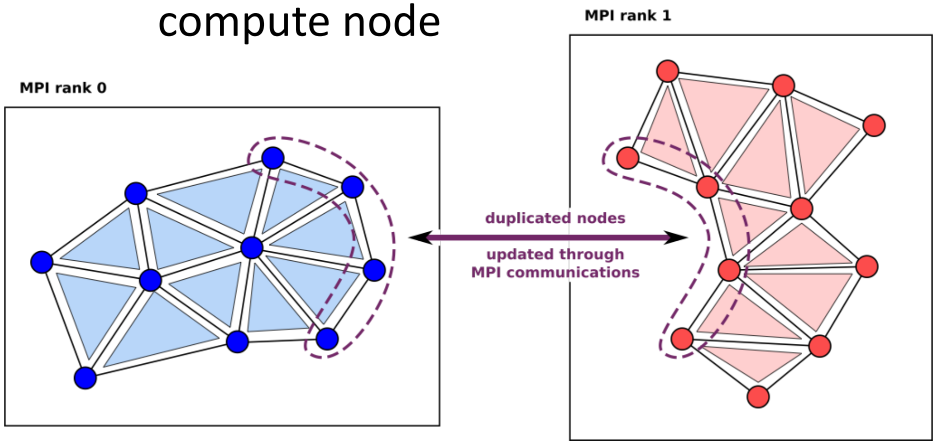
➡ Introduction of a second level of decomposition

compute node

MPI decomposition

Parmetis / Ptscotch

all ranks



task

Group decomposition

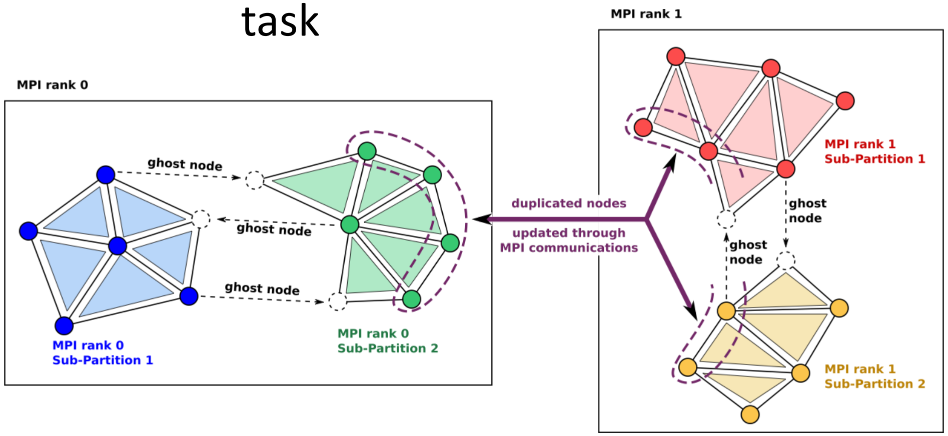
…

…

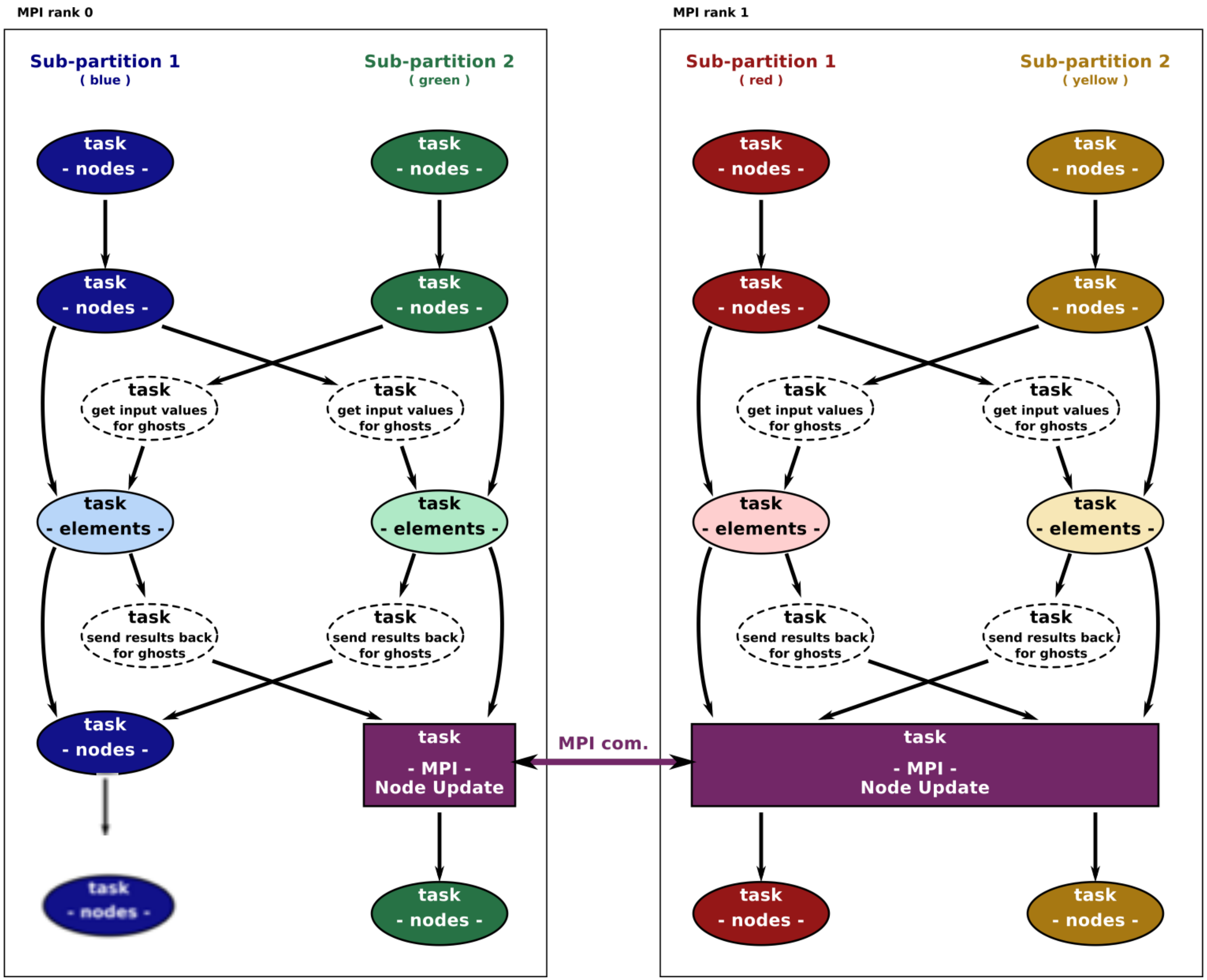
…

METIS

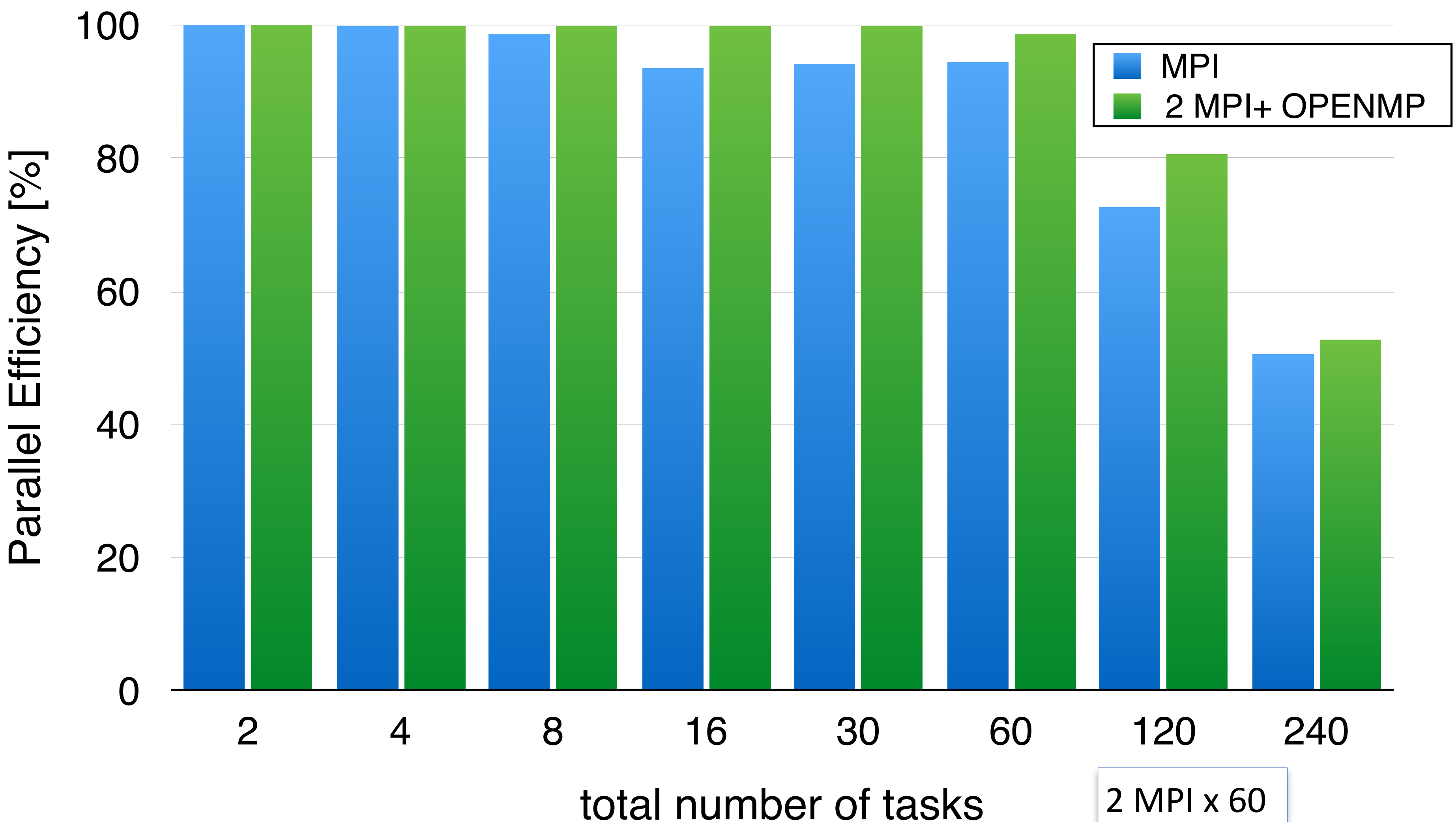
task decomposition



MPI+OPENMP4 tasks

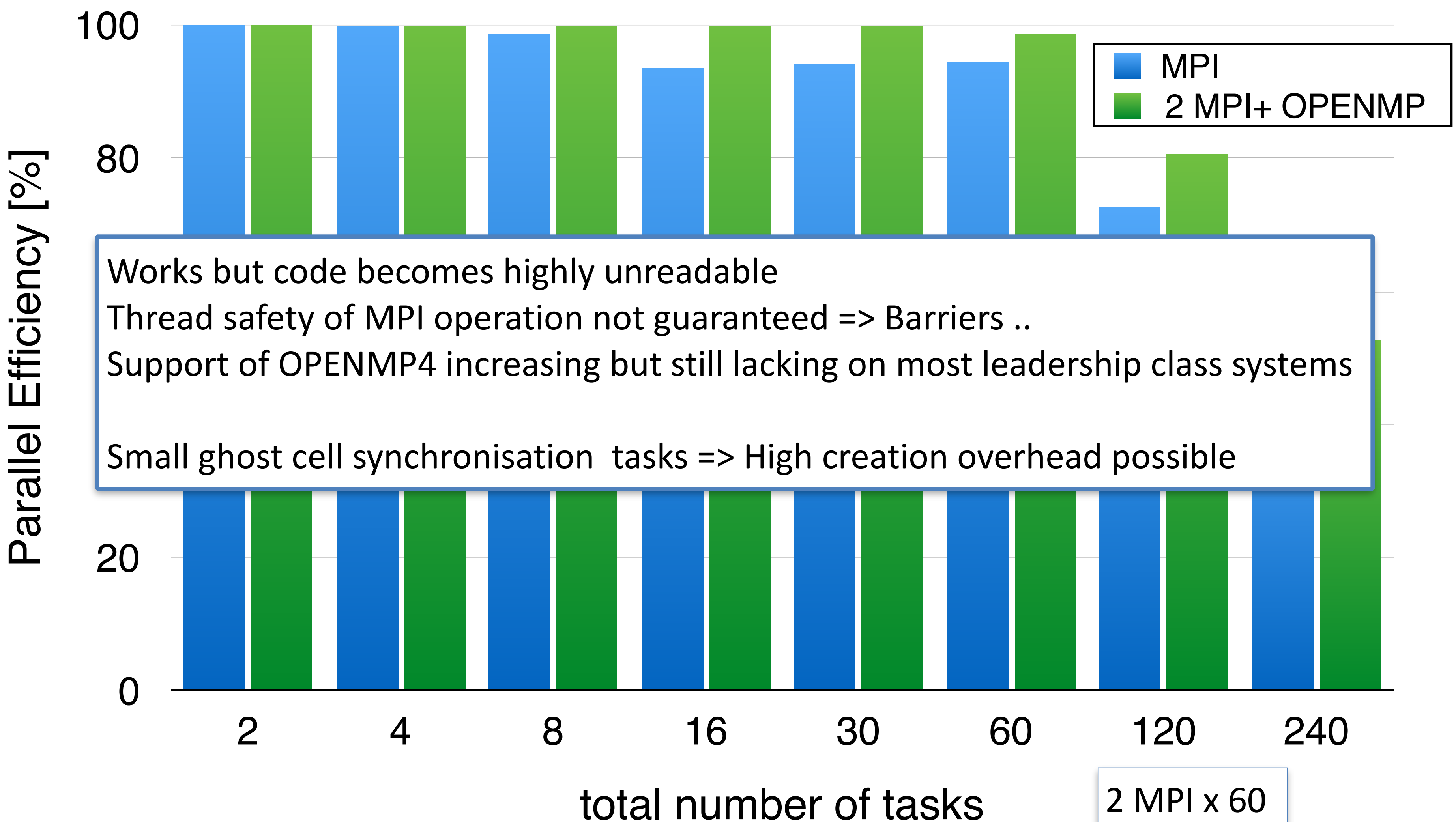


Parallel efficiency on a single Xeon with 60 cores on a small test case



2 MPI x 60 tasks per MPI

Parallel efficiency on a single Xeon with 60 cores on a small test case



Works but code becomes highly unreadable
Thread safety of MPI operation not guaranteed => Barriers ..
Support of OPENMP4 increasing but still lacking on most leadership class systems

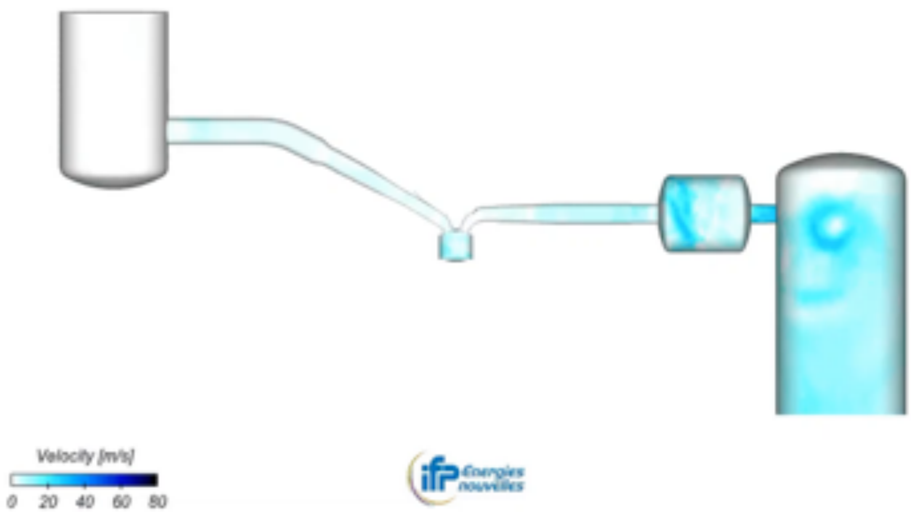
Small ghost cell synchronisation tasks => High creation overhead possible

2 MPI x 60 tasks per MPI

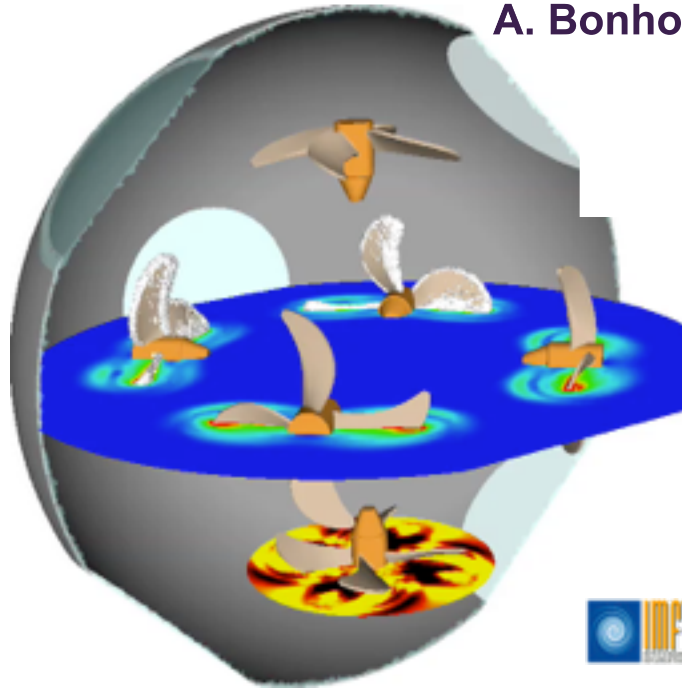
THANK YOU

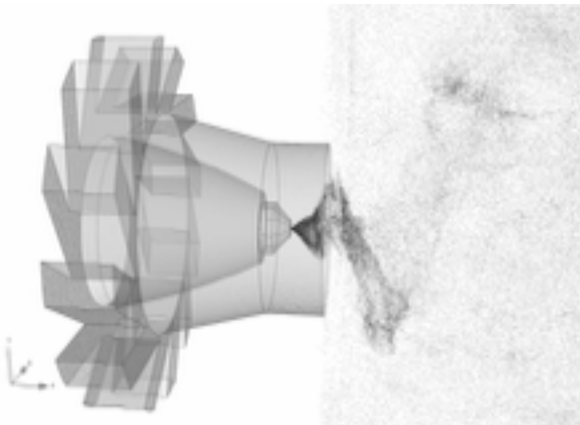
ICAMDAC **A. Misdaris**

2070 CA

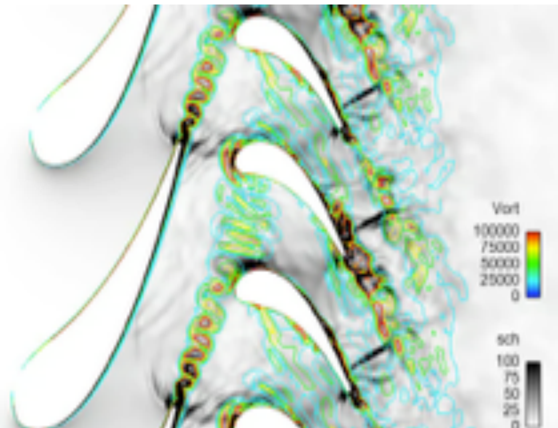


A. Bonhomme

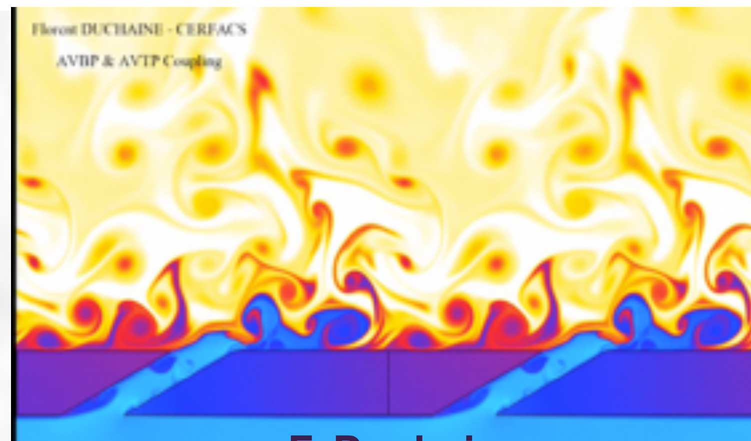




J.M. Senoner



D. Papadogianis

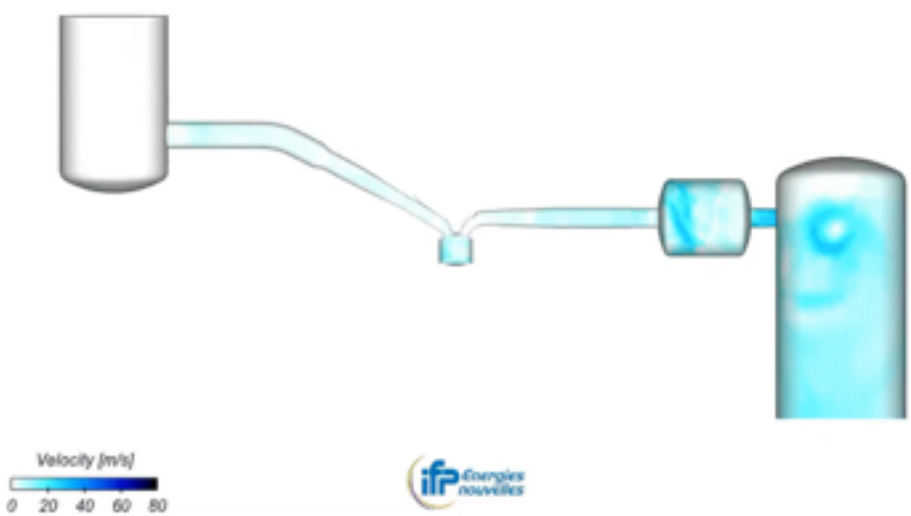


F. Duchaine

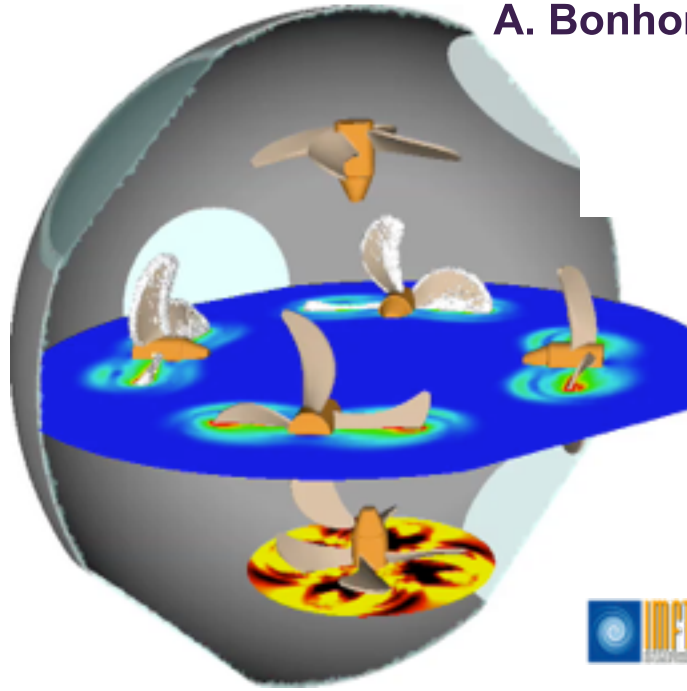
THANK YOU

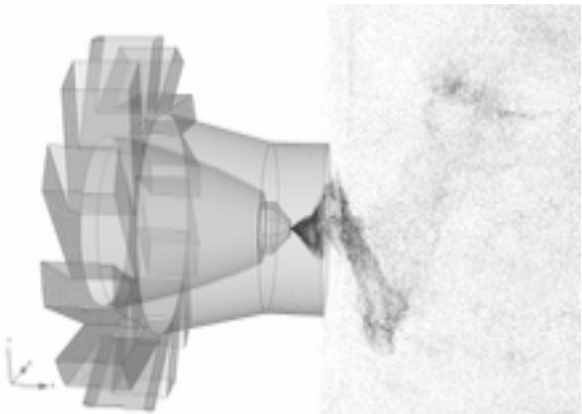
ICAMDAC
2070 CA

A. Misdaris

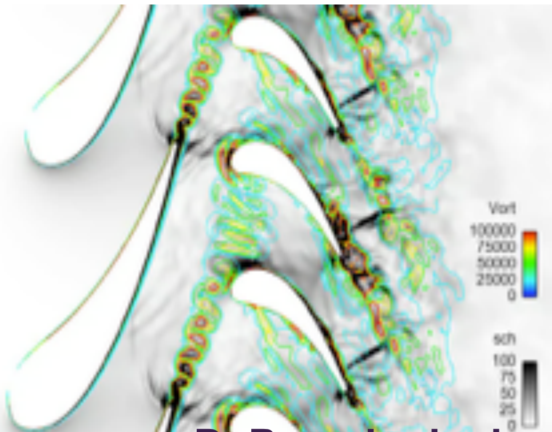


A. Bonhomme





J.M. Senoner



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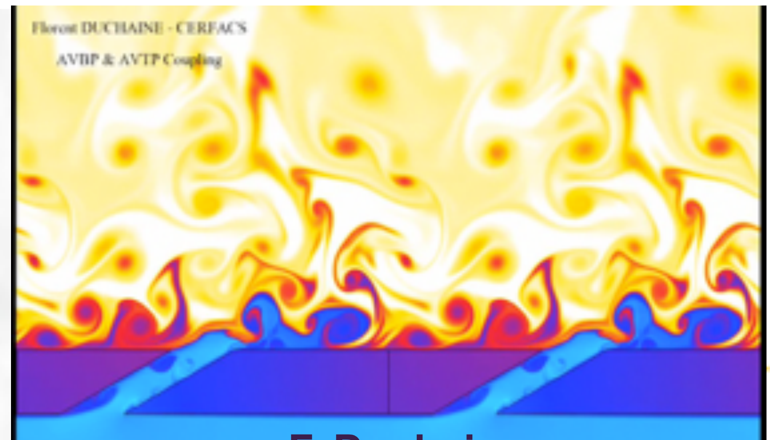

F. Duchaine