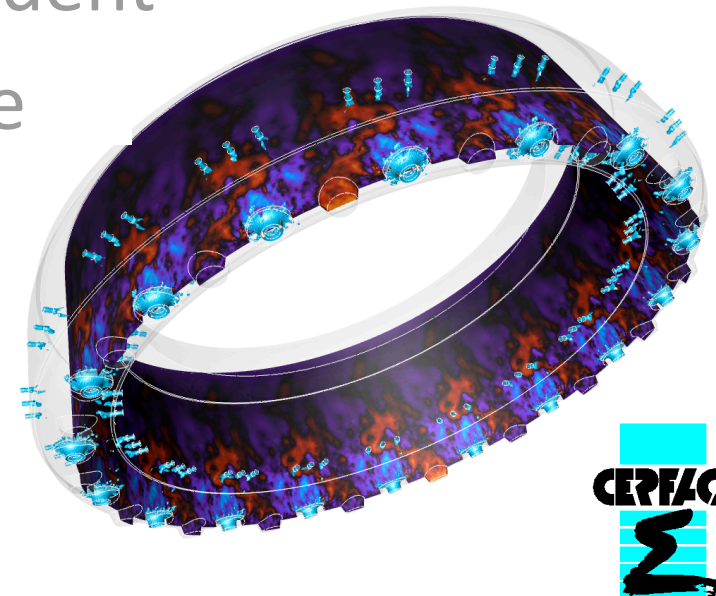
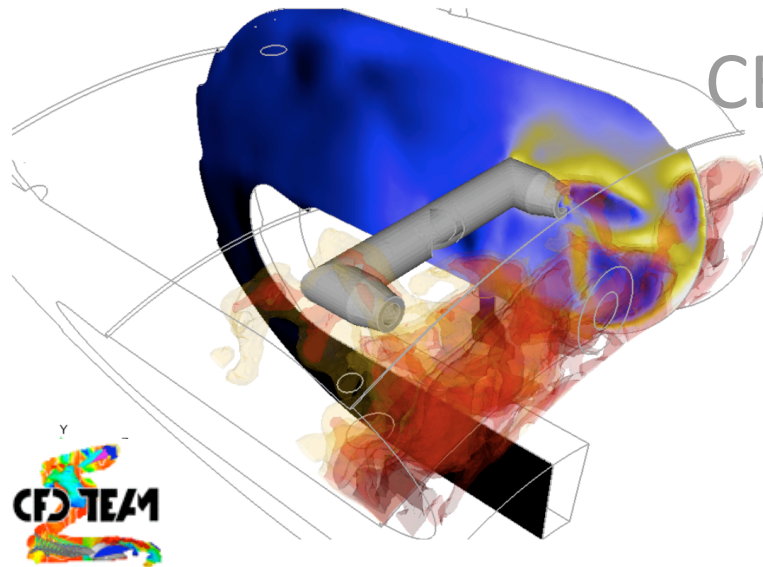


HPC challenges for aerothermal predictions in aeronautical engines

4th SciDAC CScADS Summer Workshop

B. Franzelli, PhD student

CERFACS, France



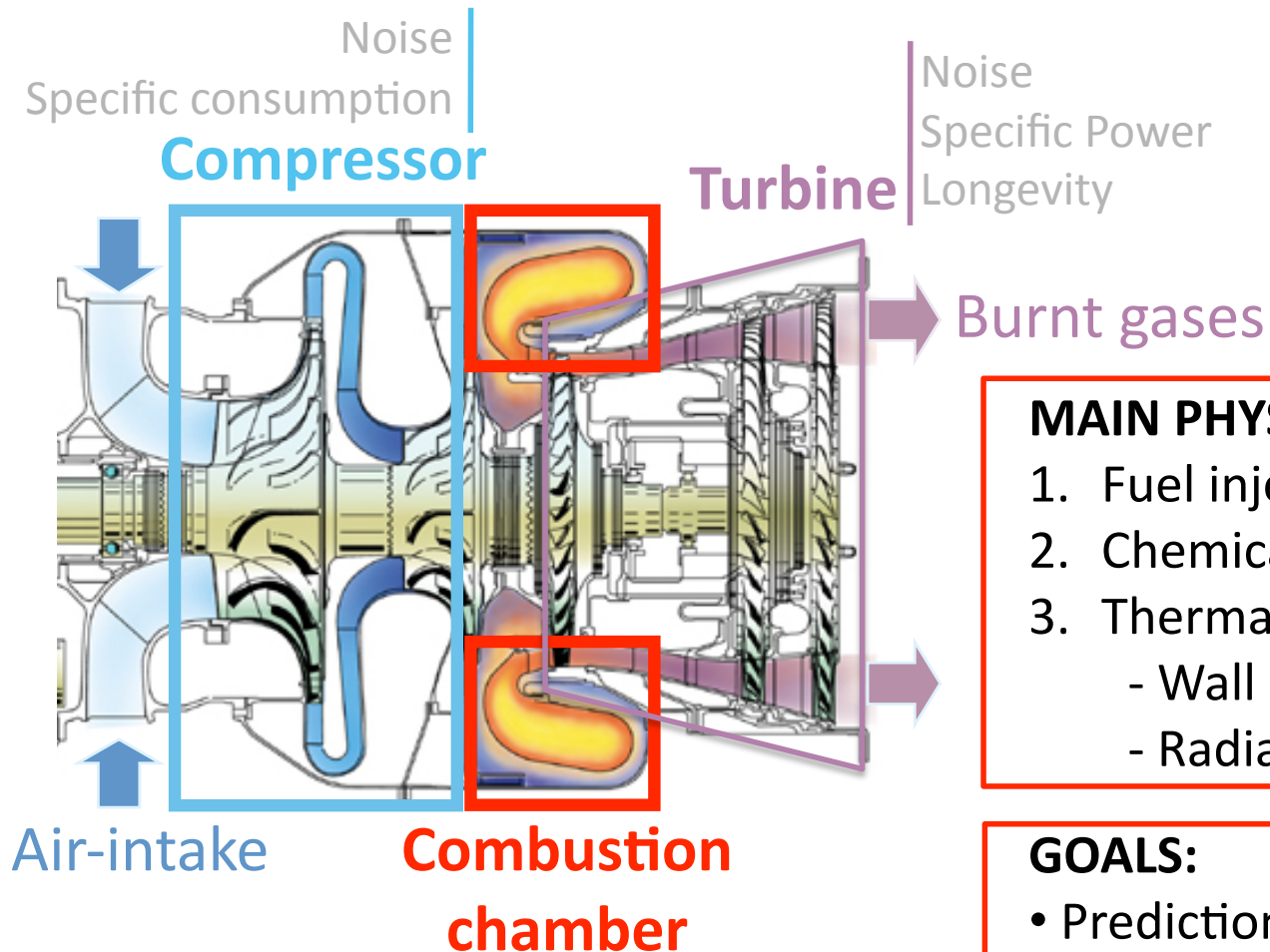


CERFACS



- European Center for Research and Advanced Training in Scientific Computing
- Research civil society
- 7 shareholders: CNES, EDF, Météo-France, ONERA, EADS, SAFRAN, TOTAL
- 110 people, 90 researchers and engineers coming from more than 10 countries
- Main research fields:
 - Aerodynamics
 - Climate and environment
 - Code coupling
 - Combustion
 - Data assimilation
 - Electromagnetism
 - Parallel algorithms

Combustion in aeronautical engines



MAIN PHYSICAL PHENOMENA :

1. Fuel injection (two-phase flow)
2. Chemical Kinetics
3. Thermal transfers:
 - Wall heat transfer
 - Radiative heat transfer

MULTIPHYSICS

GOALS:

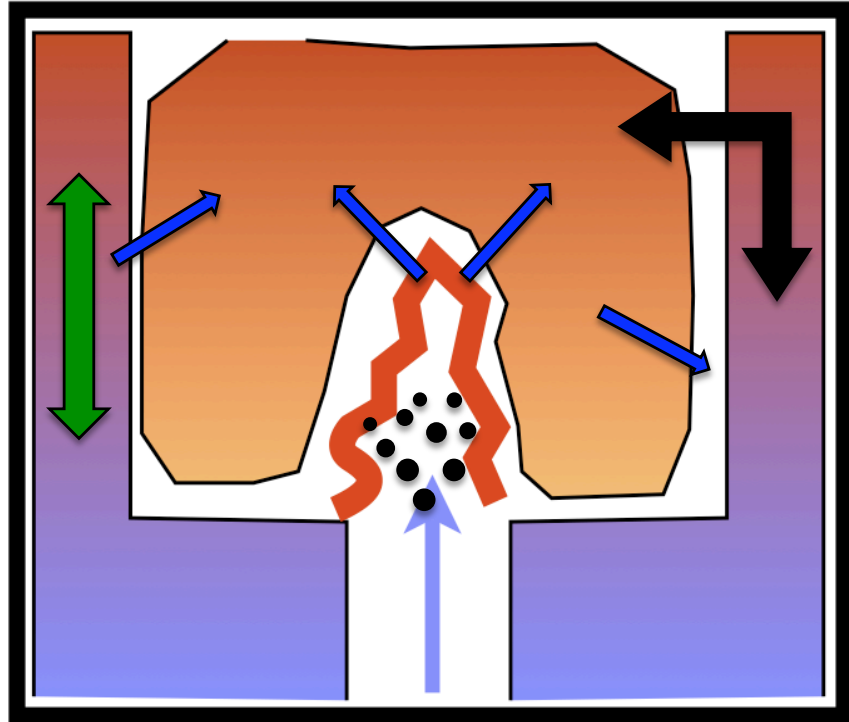
- Prediction of pollutants (CO, Nox, Soot)
- Temperature profile at combustor exit (an increase of 20K at the exit divides the shelf life of the engine by 2)



The full thermal problem

The objective is to describe a two-phase reactive flow in a complex geometry taking into account:

- Combustion & soot production
- Conduction
- Radiation
- Convection



STRATEGY = MULTIPHYSICS COUPLING

The full thermal problem is resolved coupling three codes dedicated to each separate phenomenon via a parallel dynamic coupler.

Outline

- Description of the codes developed
- Examples of partitioning problems
 - Efficient partitioning algorithms for two-phase flow simulations using a Lagrangian approach
 - Storage of huge chemical databases for tabulation methods
 - Parallelization of the radiative code
- Tomorrow challenge: the full thermal problem



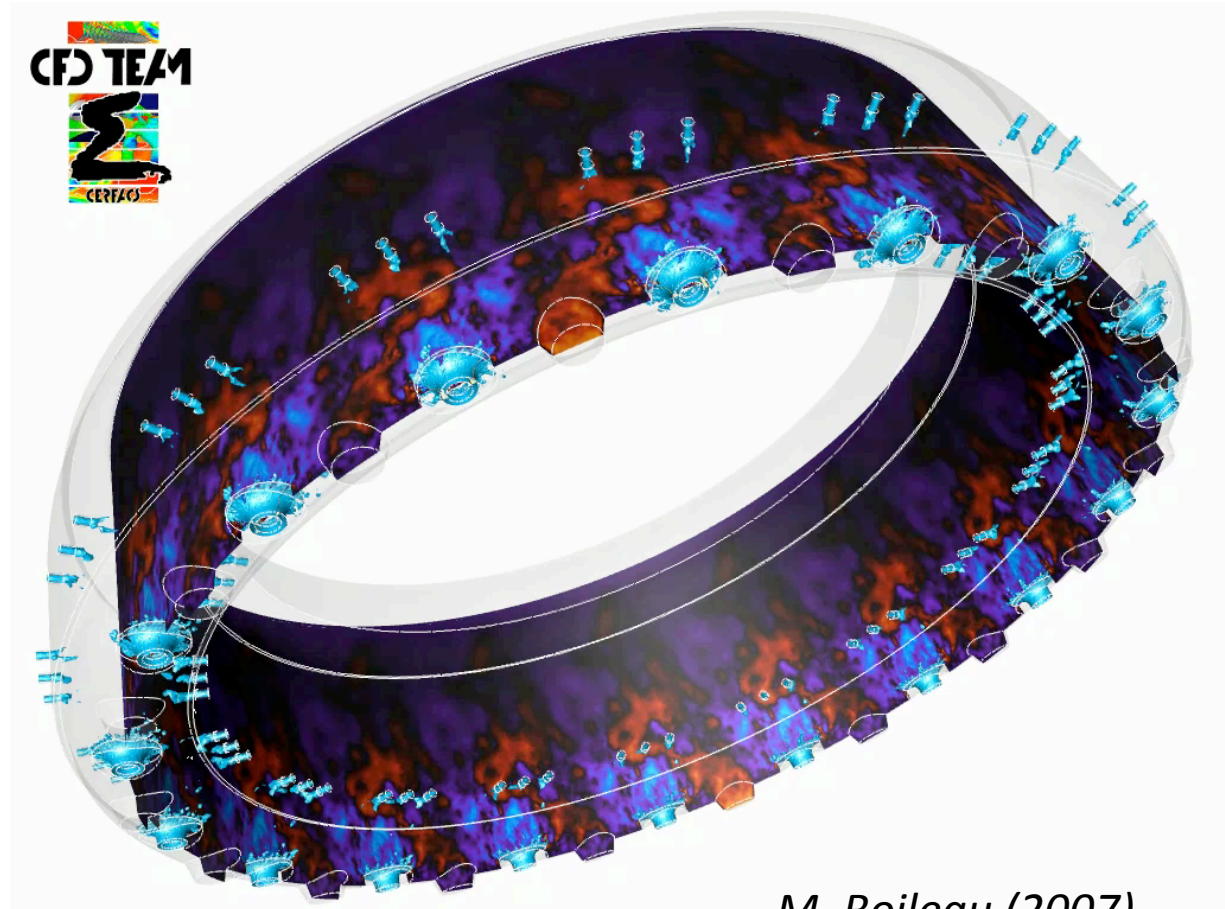
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AVBP code main characteristics

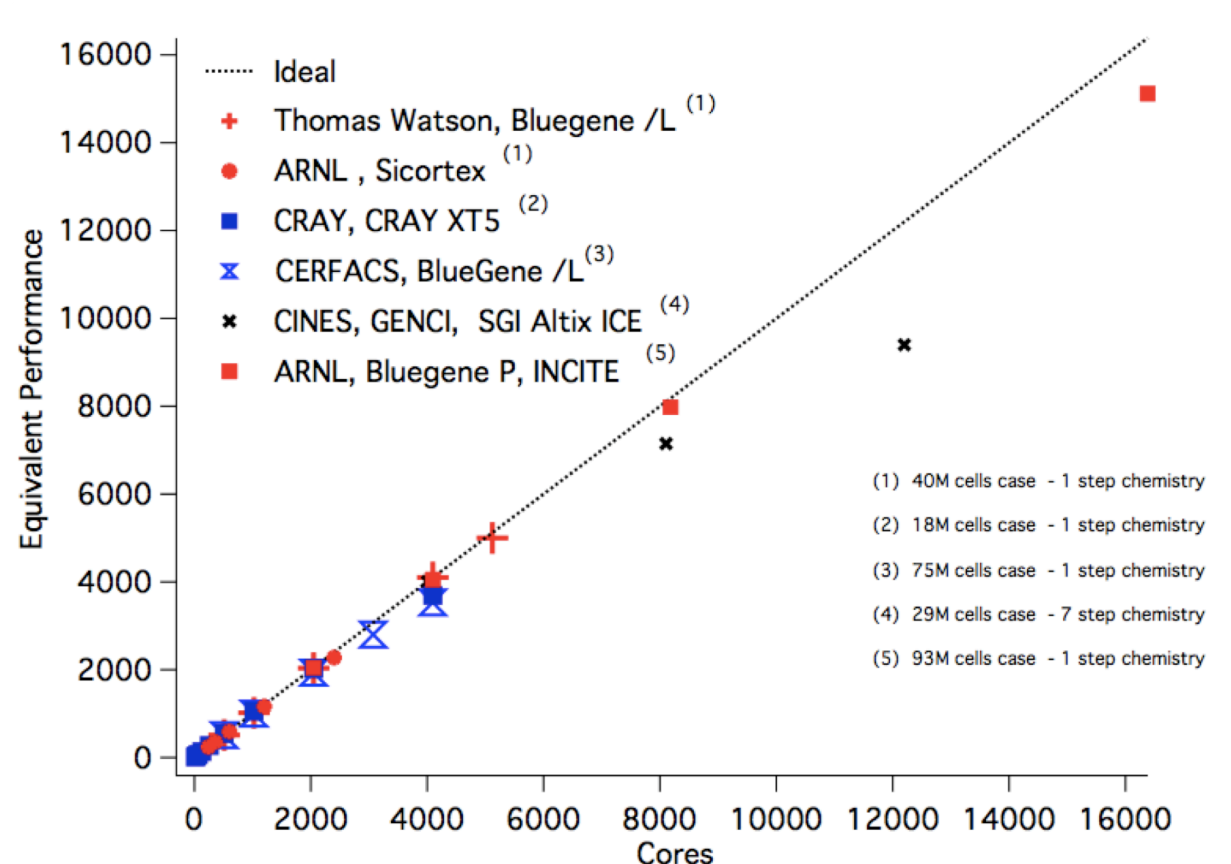
- Started in 1993
- Compressible reactive NS equations
- Explicit in time
- Unstructured/hybrid meshes
- Moving meshes
- Centred schemes
 - Finite Volume/Finite Element (2nd/3rd order)
 - + controlled local artificial viscosity
- Massively Parallel
- Machine Independent



- Cray XT3 (Rochester, US)	- Consumption : 112 000 h CPU
- AMD bi-core Opteron 2.4 Ghz	- Execution time : 160 h
- 700 processors	- Physical time : 50ms

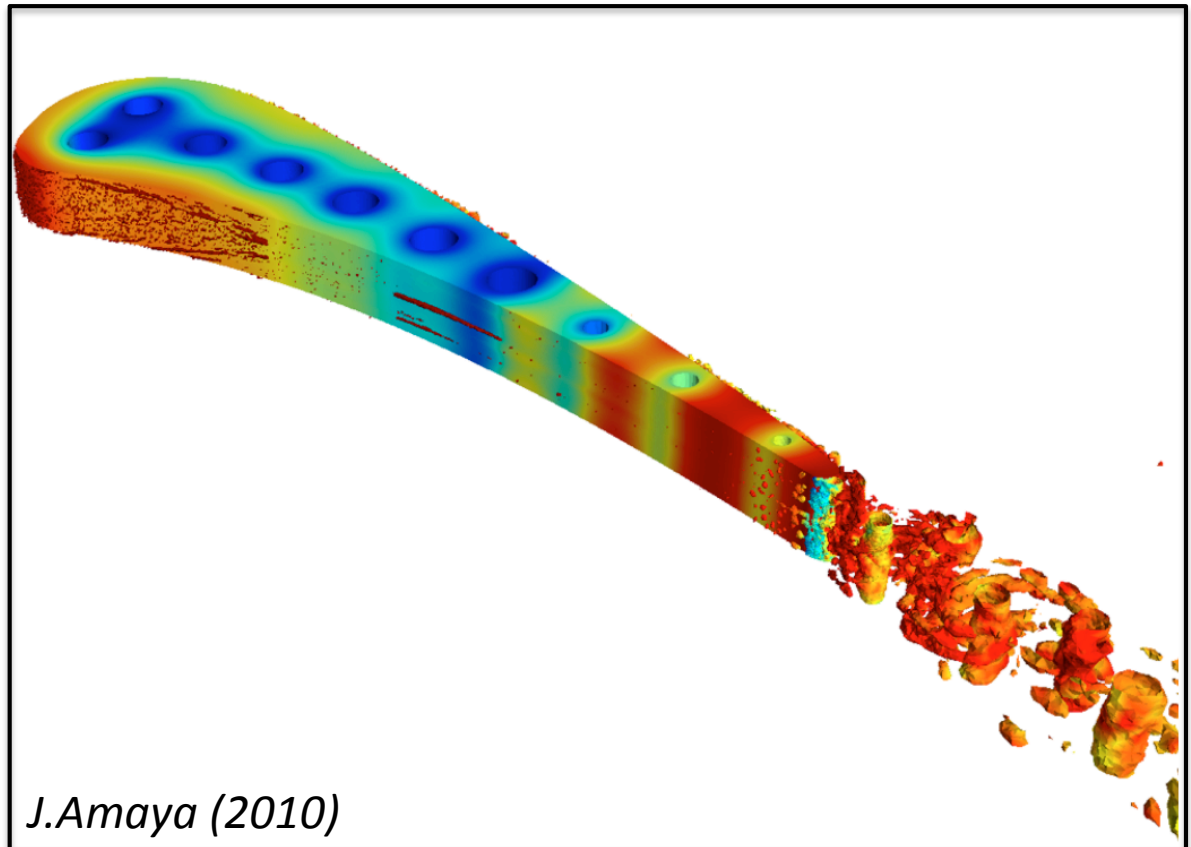
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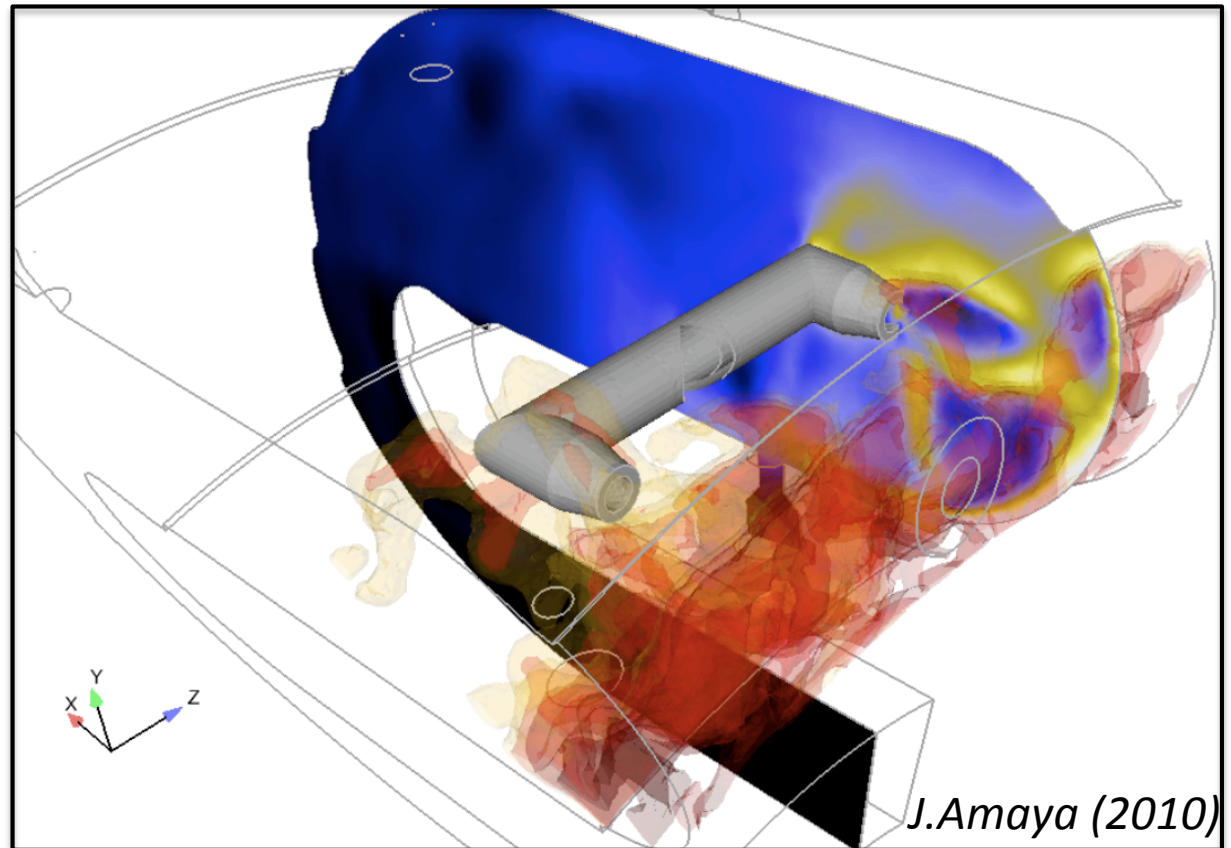
AVTP code main characteristics

- Heat Equation solver for a non-homogenous non-isotropic solid medium
- Data structure and numerical methods inherited by AVBP
- Unstructured/hybrid meshes



PRISSMA code main characteristics

- Radiative Transfert Equation (RTE) solver
- Based on the Discrete Ordinates Method (DOM)
- Unstructured/hybrid meshes
- Different global and narrow-band models for the spectral integration
- Radiation properties of combustion gases (CO, CO₂, H₂O) and soot



Outline

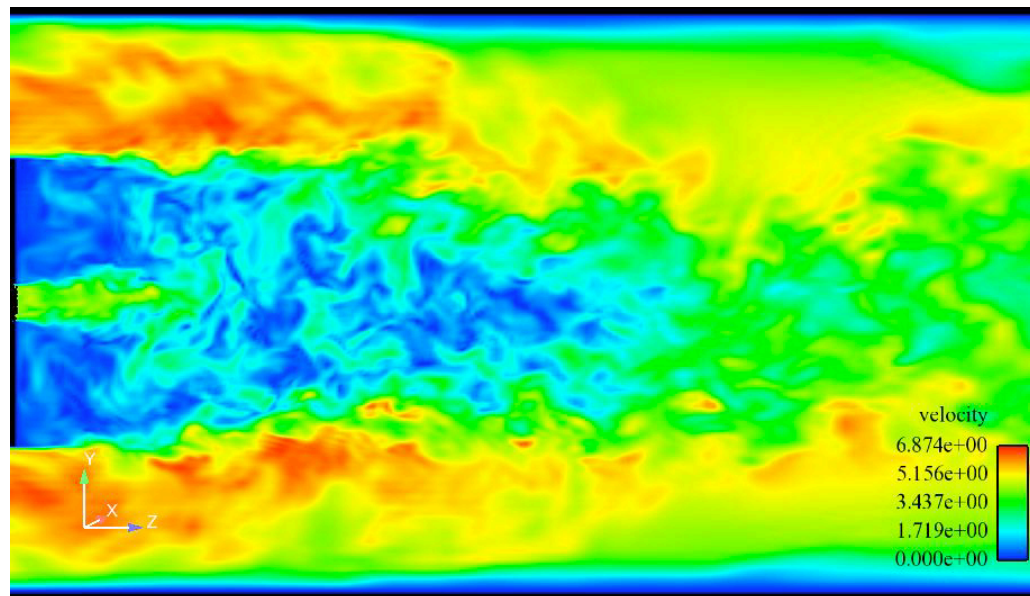
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1. Two-phase flow and HPC

Development of 2 solvers in AVBP:

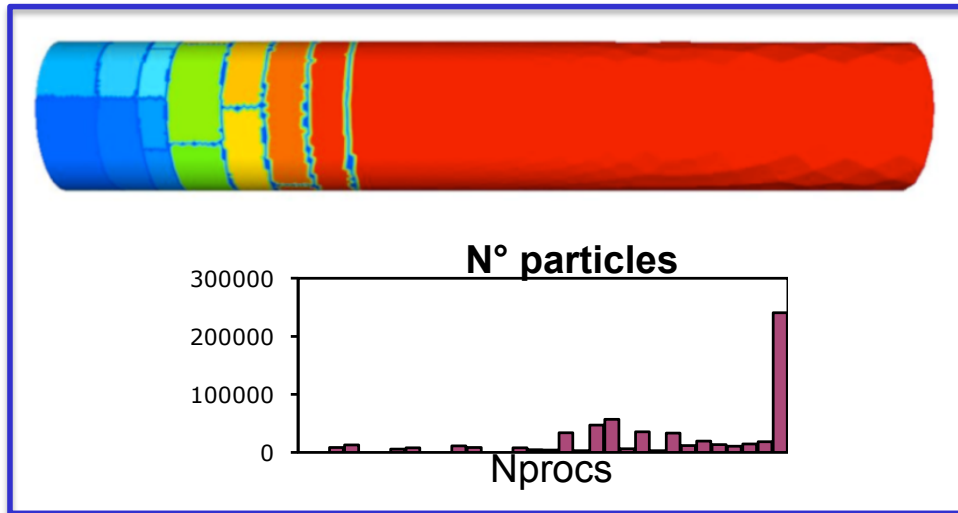
- Gas phase: Euler solver
- Liquid phase: Lagrange solver
 - ✗ There are millions of fuel droplets to be tracked downstream from the injector
 - ✗ Need for efficient two-constraint partitioning algorithms



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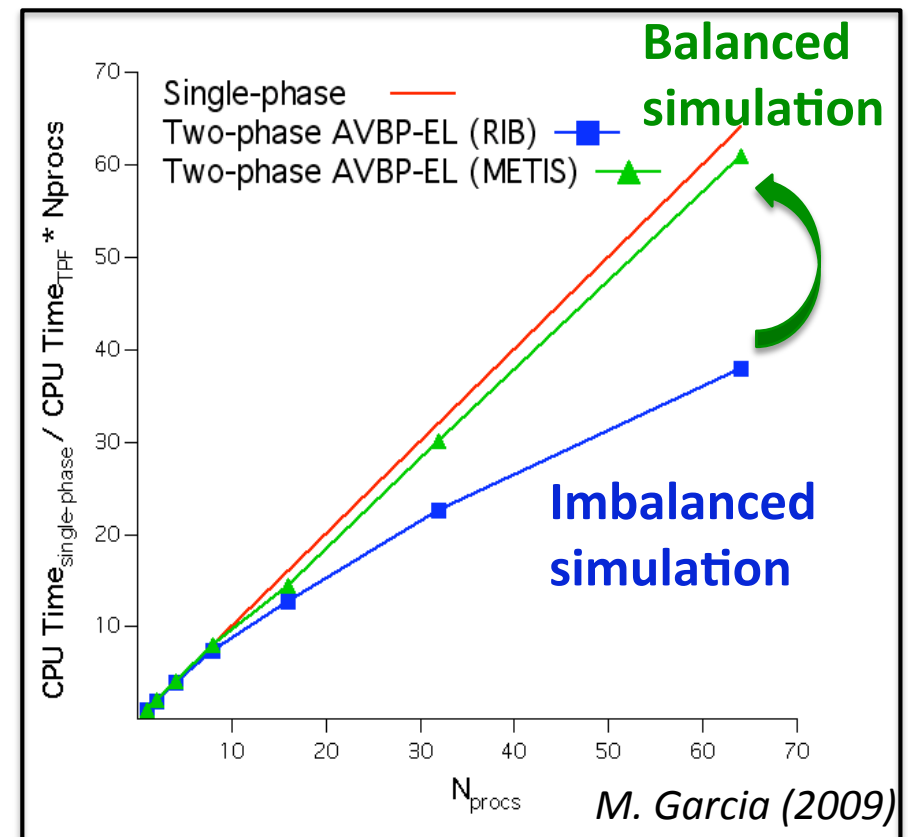
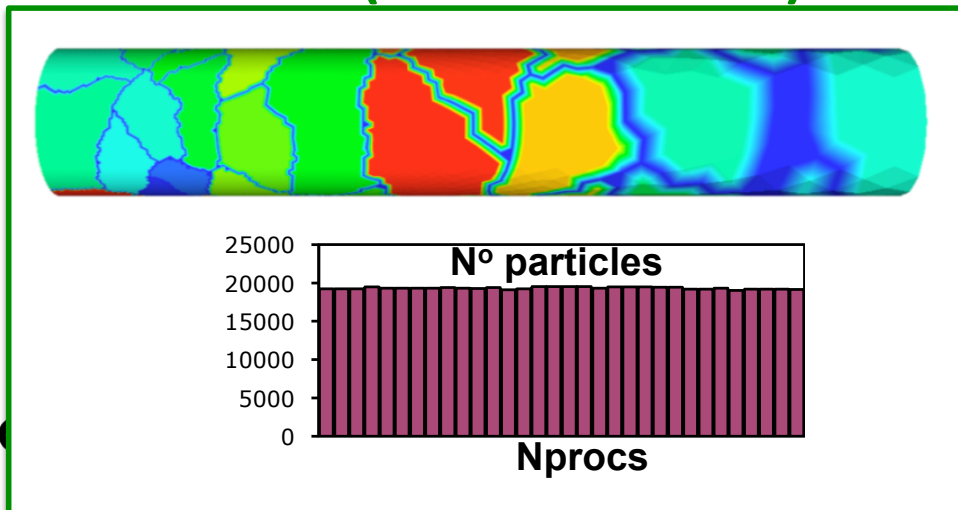
1. Two-phase flow and HPC

RIB (one-constraint)



For two-phase flows where particles are non-uniformly located, two-constraint partitioning algorithms are required to avoid load imbalancing.

METIS (two-constraint)



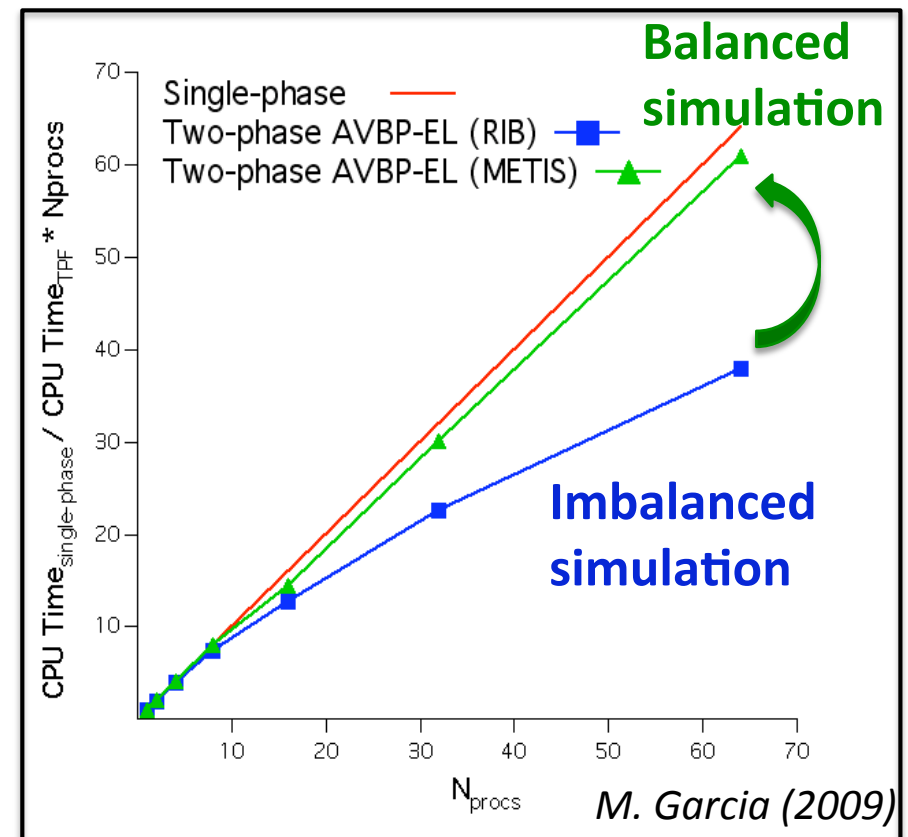
1. Two-phase flow and HPC

OPEN QUESTIONS:

During the calculation of an unsteady case, particles do not remain at the same place:

- How to modify the partitioning with time in order to preserve a correct particles balance??
- Which criteria should be used to determine when and how to modify the partitioning???

For two-phase flows where particles are non-uniformly located, two-constraint partitioning algorithms are required to avoid load imbalancing.



2. Chemical kinetics and HPC

- In order to correctly describe intermediate species, pollutants and soot in a turbulent reactive flow, an accurate description of the chemical kinetics is required.
- **Tabulation methods are widely worked on:** a database of relevant chemical terms (mass fractions and temperature) based on simulations of simple combustion problems is used to rebuild the chemical source terms in a complex 3D calculation.

An *a priori* partitioning of the database is impossible: in an unsteady computation, each grid node must be able to access any part of the database at each timestep.

POTENTIAL SOLUTIONS:

- **Read the whole database on each processor:** a large amount of memory per processor is then required, which is contrary to the tendency of the new generation machines.
- **Reduce the database size:** some information could be neglected or single precision floating-point format could be used, which would decrease the accuracy of the chemical description.
- **Read dynamically and partially the database on each processor:** a very quick I/O communication is then required.



3. Radiation and HPC

Radiative source term depends on the **photon frequency** and the **angular direction**.

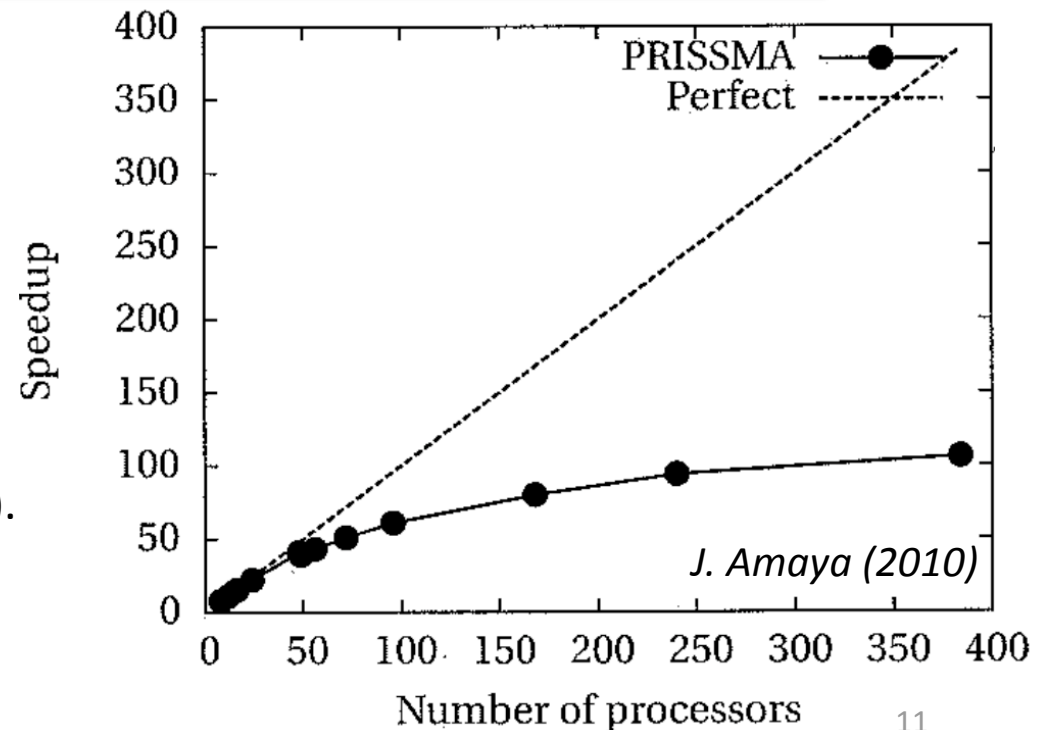
$$S_r(\mathbf{x}) = \int_0^\infty \kappa_\nu \left[4\pi L_\nu^0(\mathbf{x}) - \int_{4\pi} L_\nu(\mathbf{x}, \mathbf{u}) d\Omega \right] d\nu$$

FREQUENCY INTEGRATION:

quantities depend on local properties => **good subdomain parallelism**.

ANGULAR DIRECTION:

includes data from ALL the points of the domain (long distance iterations). Sequential algorithm => **problem for subdomain parallelism**.



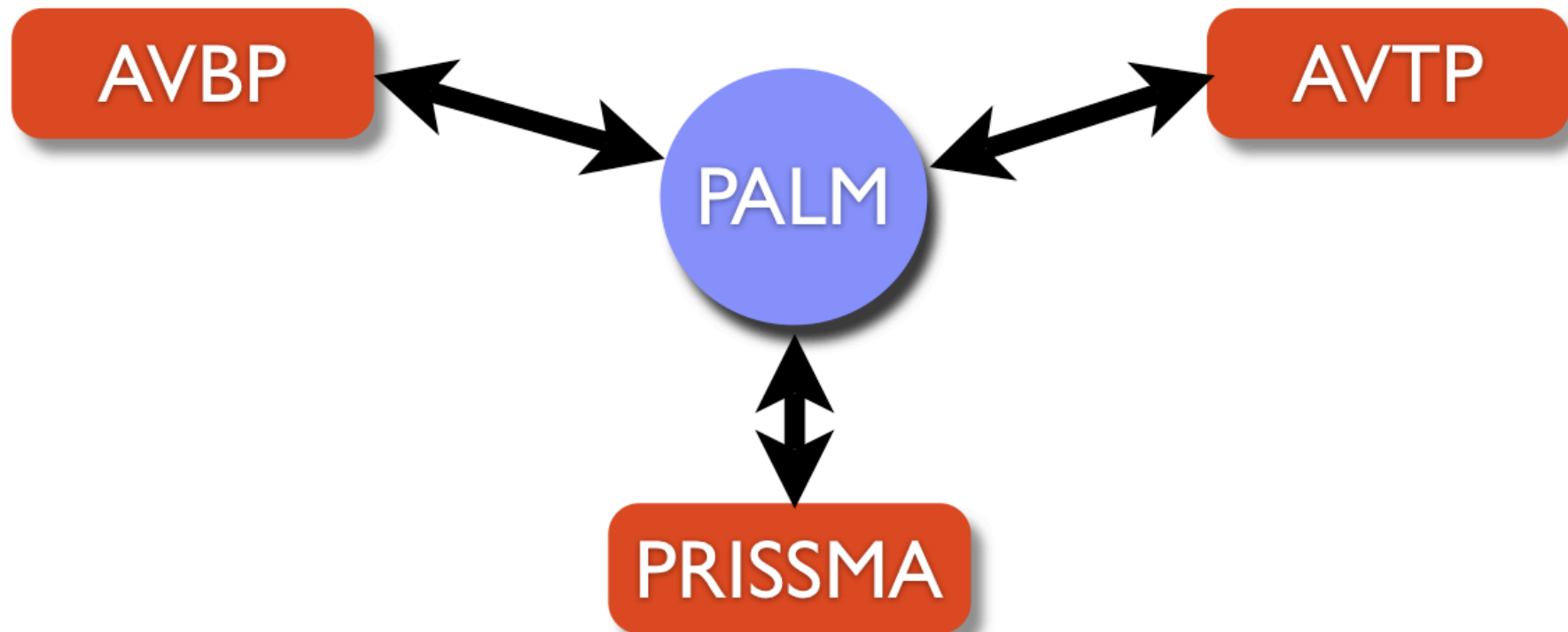
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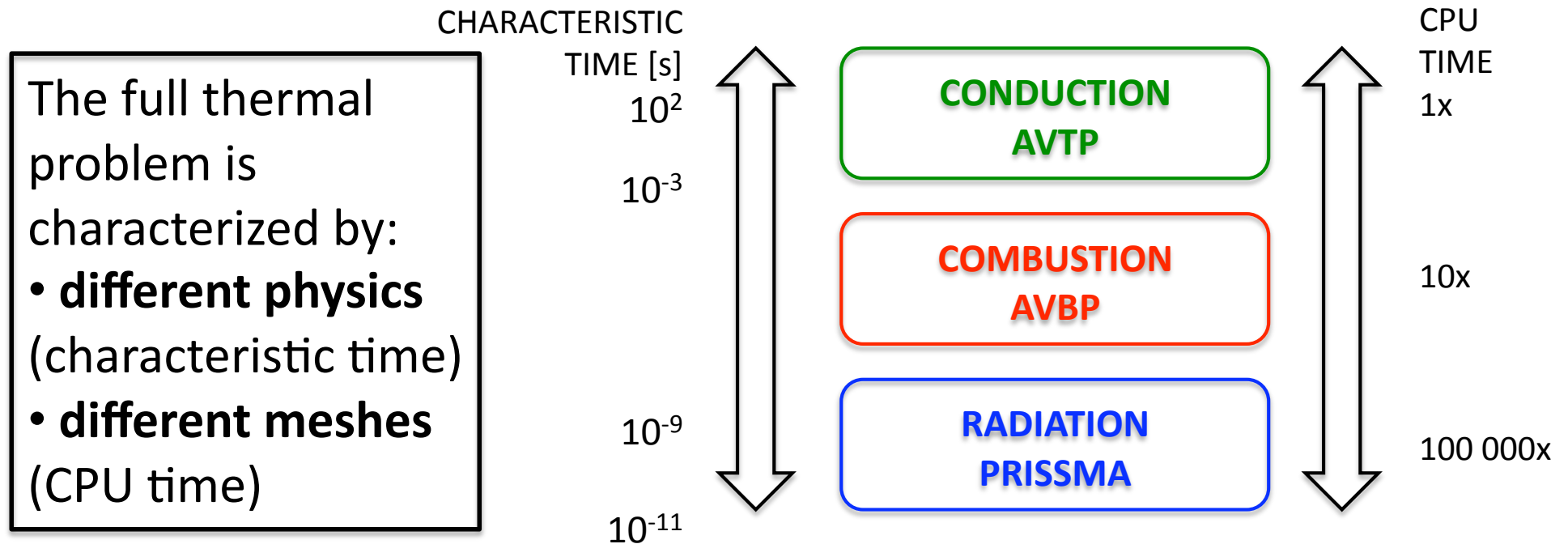
The full thermal problem

The full thermal problem is resolved using specialized codes for each transfer mode.



A coupler (PALM) is used to exchange data between the codes.

The full thermal problem



Different computational resources and restitution times of calculations must be managed by the coupler: difficult to achieve the optimum on a massively parallel machine.

The full thermal description and HPC

- **Multi code problem:** how could the coupler manage the huge amount of information required and calculated by the three codes in a massively parallel way (memory and synchronisation problems)?
- **Multi machine problem:** how to manage the communication of 3 codes running on different machines ?
- **Dynamical distribution of processors:** how could processors be dynamically distributed between the different codes (i.e. unsteady cases or moving meshes).





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