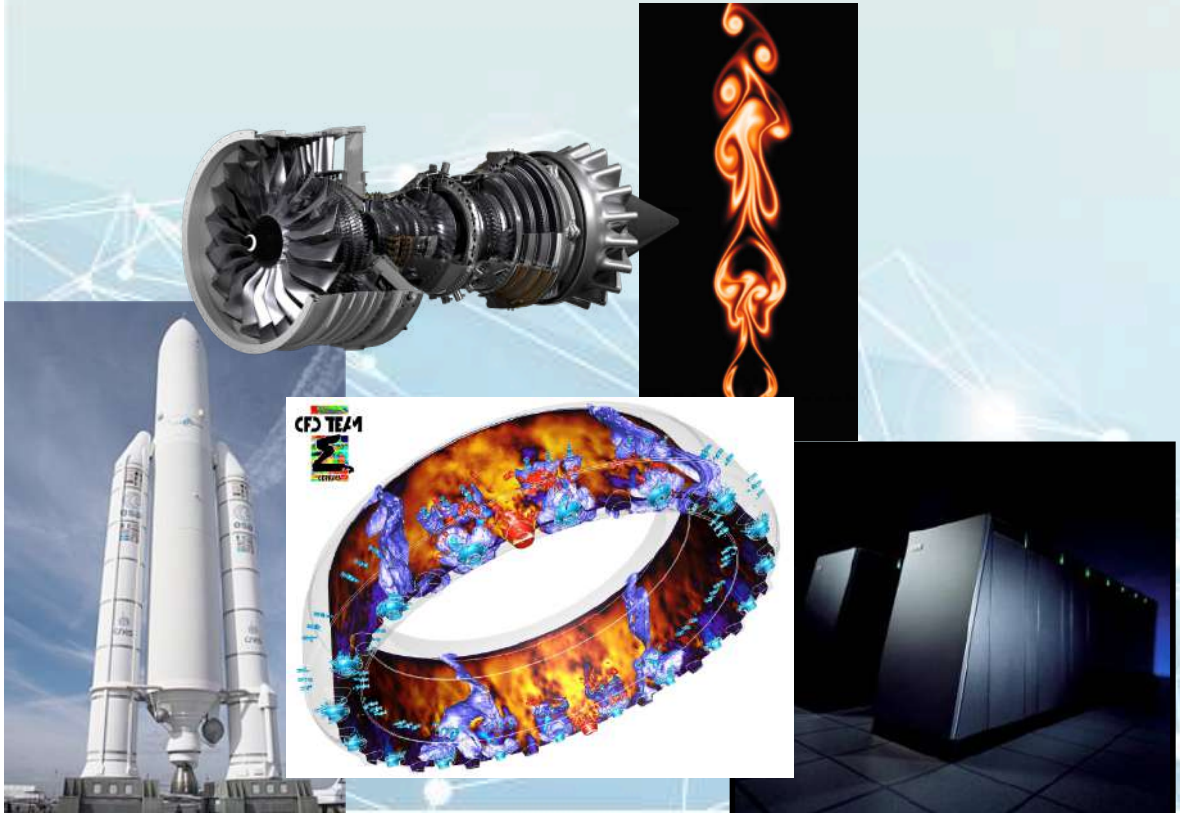
CERFACS

EUROPEAN CENTRE FOR RESEARCH AND ADVANCED TRAINING IN SCIENTIFIC COMPUTING

Numerical Simulation of Turbulent Combustion



B.Cuenot & the CFD Team

www.cerfacs.fr

Combustion is (almost) everywhere ...

Furnaces

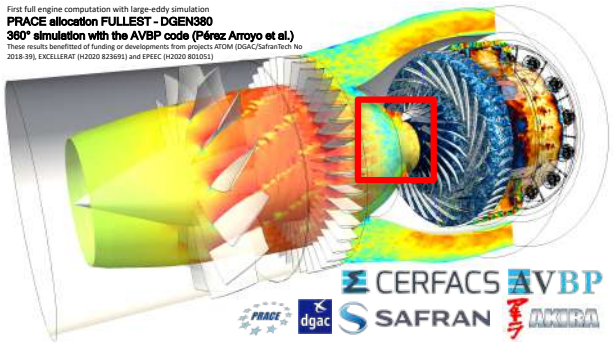
Transport

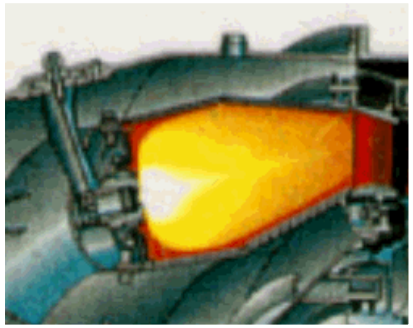
Fires

Why study Turbulent Combustion?

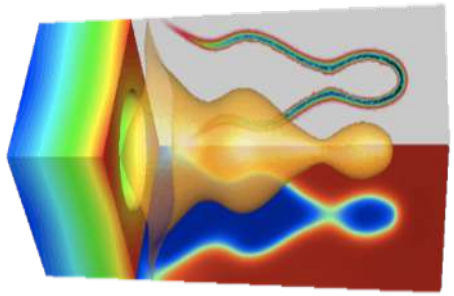
Practical combustion systems

complex geometry





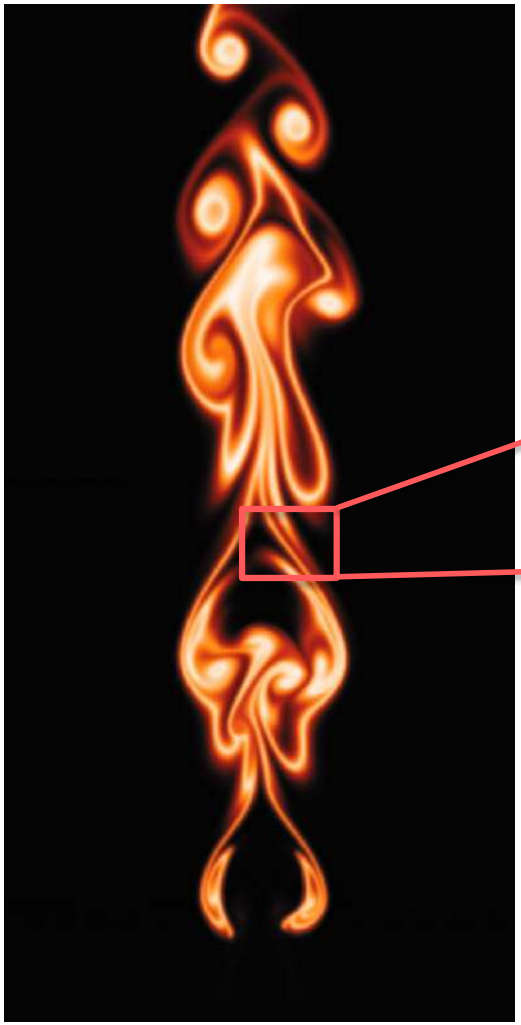
kinetics
turb/chem
spray
emissions



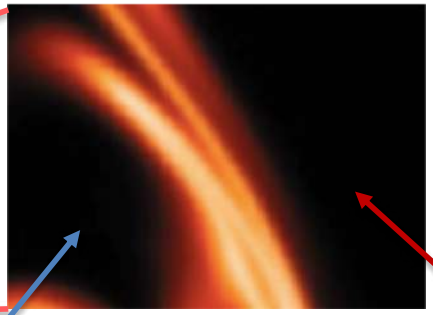
acoustics/comb

Advanced CFD and ***Massively parallel*** computer architectures offer a clear potential for time and cost reductions of the design process by providing ***accurate predictions***

What is a flame?



A flame is the combination of thermochemical processes and transport (mixing)



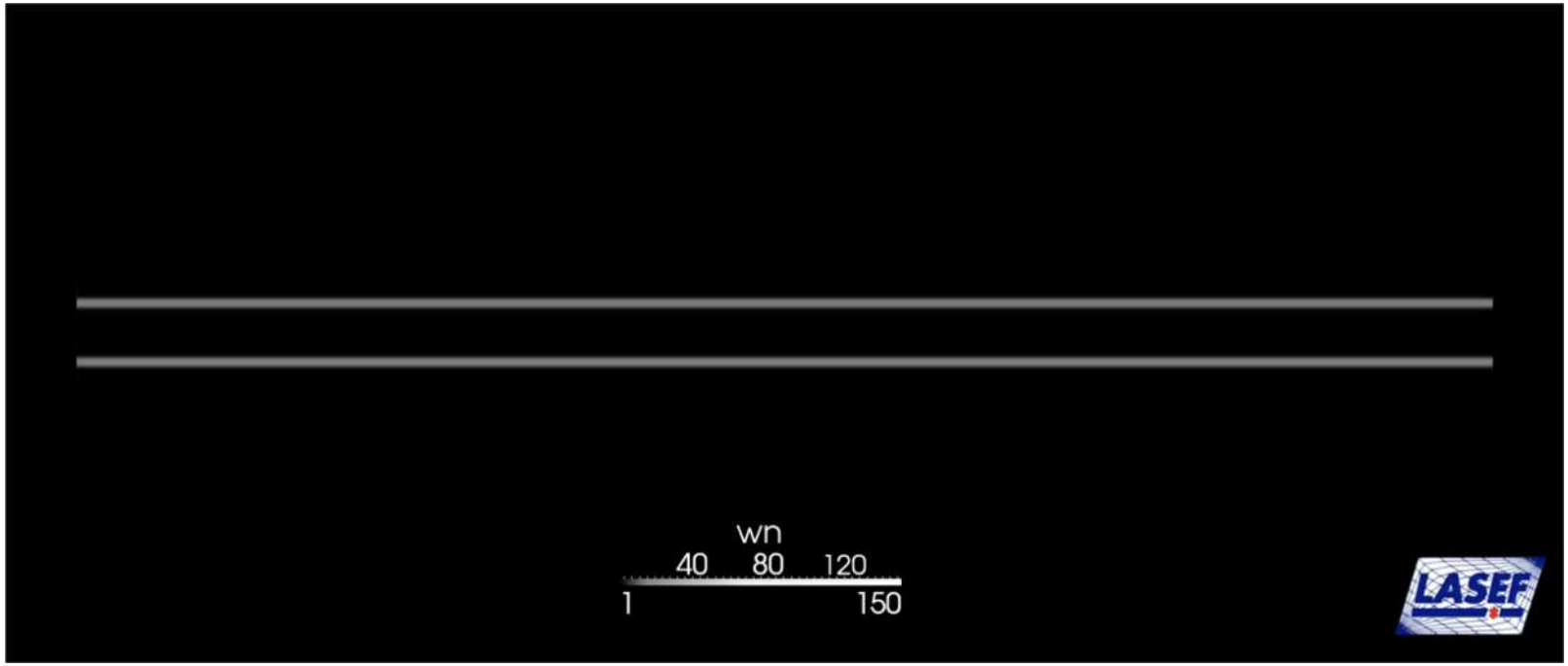
Reactants

flame zone

Products + Heat release

Flow model:
- variable density
- multi-species
- chemical source terms

What is turbulence?



Reynolds number UL / ν

What are the equations?

Navier-Stokes equations:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

- steady / unsteady
- compressible / low-mach

Species conservation equations

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho(u_i + V_{k,i})Y_k}{\partial x_i} = \dot{\omega}_k$$

- thermodynamic and transport properties
- chemical kinetics

Energy equation

$$\rho\frac{DE}{Dt} = -\frac{\partial q_i}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij}u_i) - \frac{\partial}{\partial x_i}(Pu_i) + \dot{\omega}_T + \dot{\Omega}$$

4 + Nspec conservation equations

What are the equations?

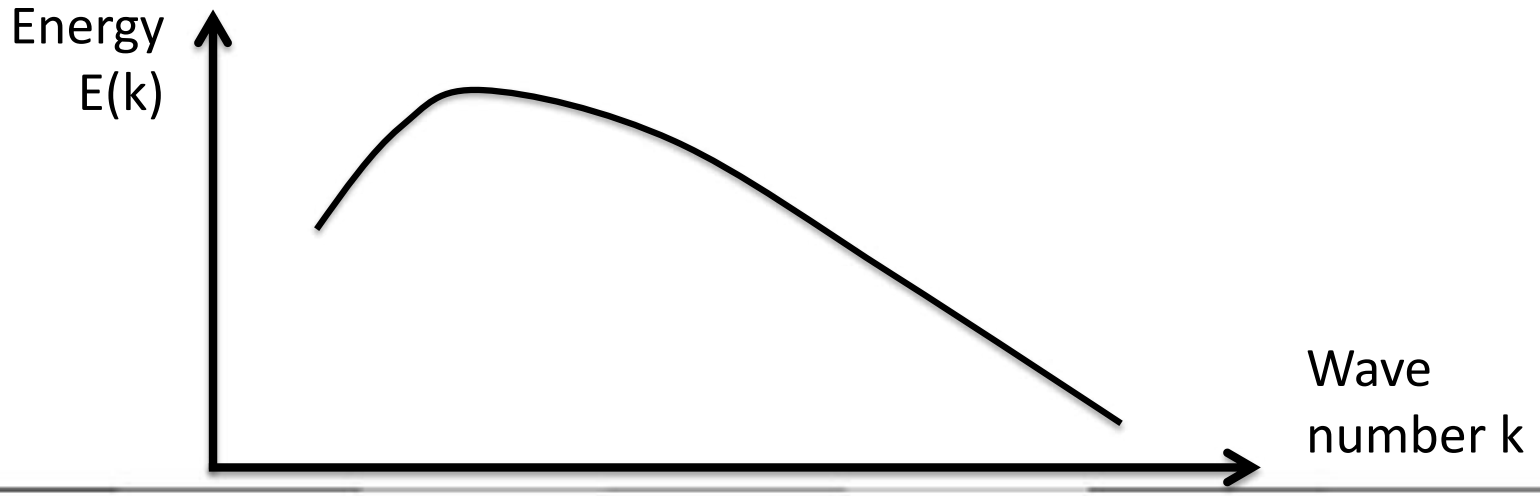
Navier-Stokes equations:

$$\frac{\partial(\rho u_i)}{\partial t} + \boxed{\frac{\partial(\rho u_i u_j)}{\partial x_j}} = -\frac{\partial P}{\partial x_i} + \boxed{\frac{\partial \tau_{ij}}{\partial x_j}}$$

Production / destruction terms of turbulence:

- Non-linear
- Large frequency spectrum

MODELLING !



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Combustion terms

The Arrhenius law

The progress rate of the j^{th} reaction is given by:

$$Q_j = K_j^f \prod_{k=1}^{n} \left[\frac{\rho Y_k}{W_k}\right]^{\nu'_{kj}} - K_j^b \prod_{k=1}^{n} \left[\frac{\rho Y_k}{W_k}\right]^{\nu''_{kj}}$$

Reverse rate of reaction

Forward rate of reaction

The essential problem of chemists is to provide these two rates. They usually rely on the Arrhenius law:

$$K_j^f = A_j^f T^{\beta_j} \exp(-E_j / RT)$$

Collision frequency:
- Pre-exponential Cst
- Temp. modulation

Activation energy

and equilibrium constants:

$$K_j^r = \frac{K_j^f}{(P_a/RT)^{\sum_{k=1}^{n}(\nu'_{kj}-\nu''_{kj})}} \exp\left(\frac{\Delta S_j^0}{R} - \frac{\Delta H_j^0}{RT}\right)$$

Entropy and enthalpy changes of j^{th} reaction (from the thermodynamics table)

The Arrhenius law

The progress rate of the j^{th} reaction is given by:

Reverse rate of reaction

$$Q_j = \ldots \prod_{k=1}^{n} \left[\ldots\right]^{\nu'_{kj}} \ldots \prod_{k=1}^{n} \left[\ldots\right]^{\nu''_{kj}}$$

Non-linear turbulent transport

+

Non-linear chemistry

⇒

Complex chemistry / turbulence interaction

⇒ MODELLING !

The essential pro … s. They usually rely on the Arrhe … s:

$$K_j^f = A_j^f \, T^{\beta_j} \ldots K_j^f \left(P_a / RT\right)^{\sum_{k=1}^{n}\left(\nu'_{kj}-\nu''_{kj}\right)} \exp\left(\frac{\Delta S_j^0}{R} - \frac{\Delta H_j^0}{RT}\right)$$

Collision frequency:
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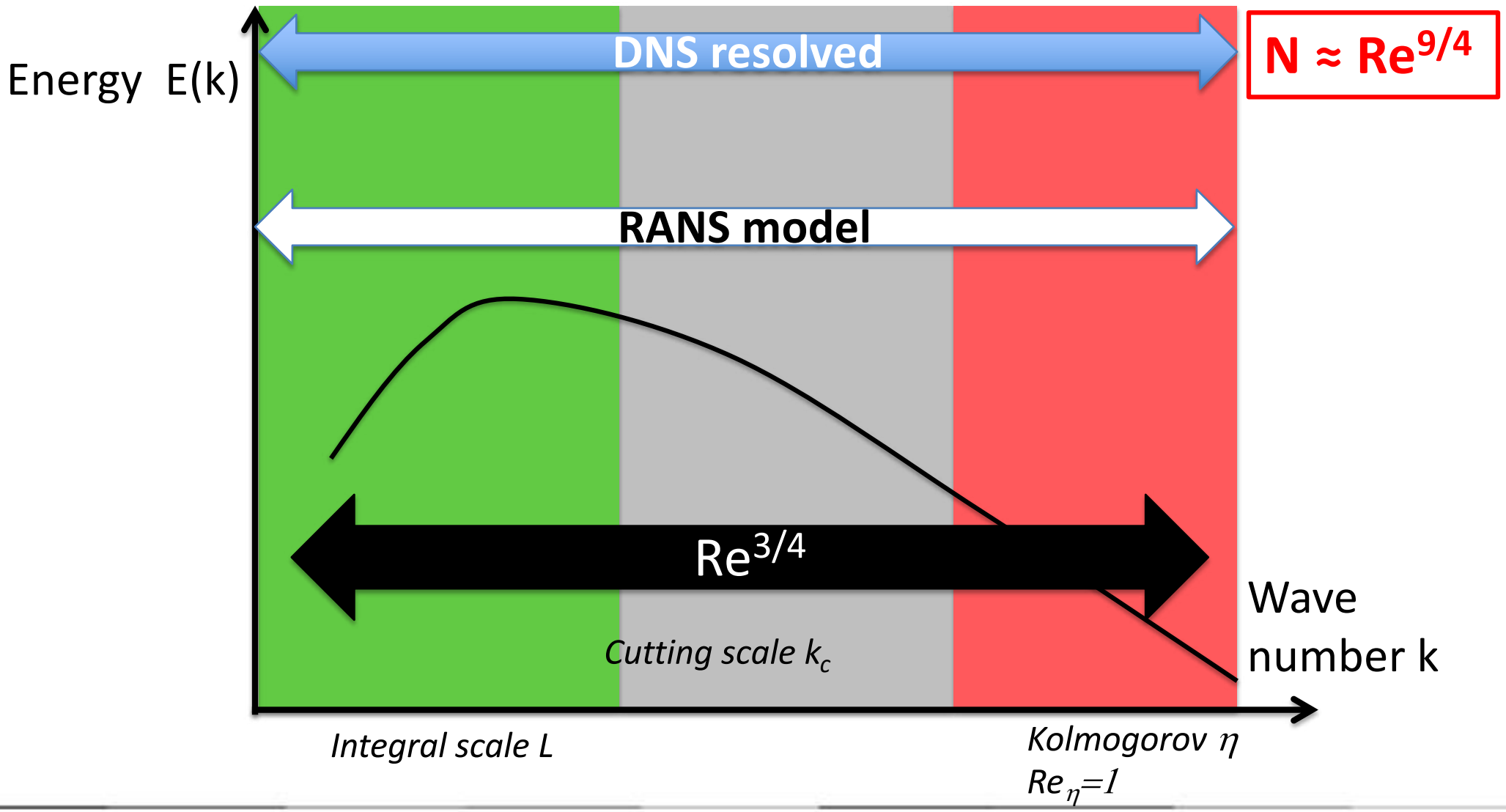
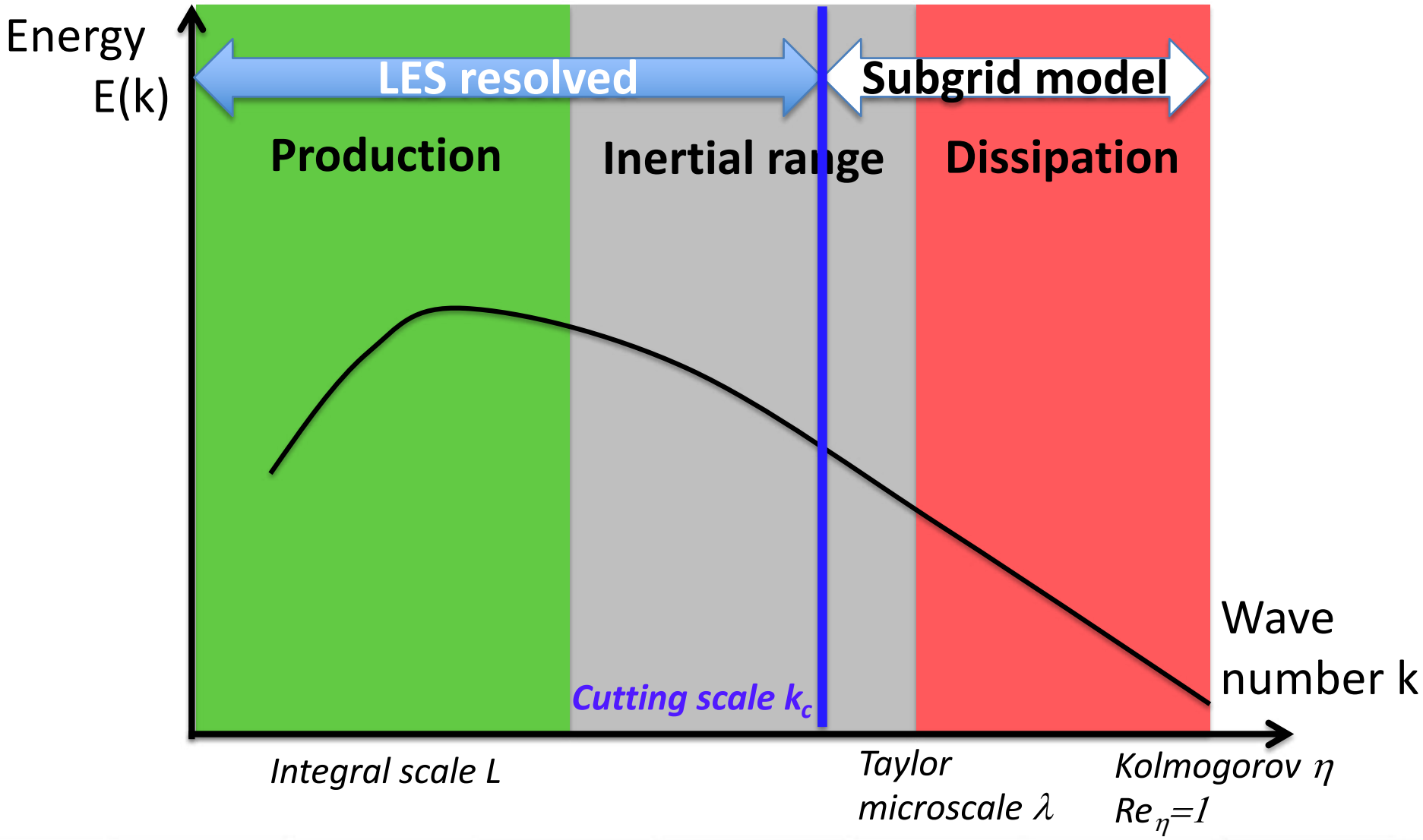
Activation energy

Entropy and enthalpy changes of j^{th} reaction (from the thermodynamics table)

Numerical Strategies to solve turbulence



Numerical Strategies to solve turbulence : Large Eddy Simulation



$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial}{\partial x_i}(\overline{\rho}\widetilde{u}_i\widetilde{u}_j) + \frac{\partial \overline{p}}{\partial x_j} = \frac{\partial}{\partial x_i}\left[\overline{\tau}_{ij} - \overline{\rho}\left(\widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j\right)\right]$$

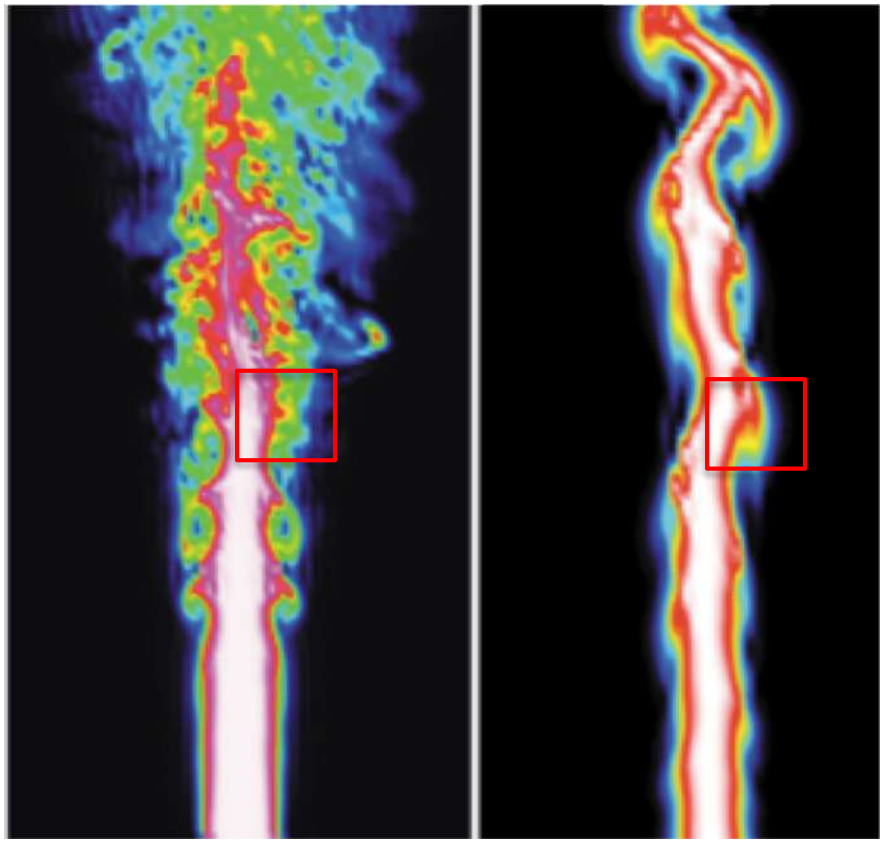
$$\mathcal{T}_{ij} = \widetilde{u_i u_j} - \widetilde{u}_i\widetilde{u}_j = \frac{\delta_{ij}}{3}\mathcal{T}_{kk} - 2\nu_t\left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{3}\widetilde{S}_{kk}\right)$$

$$\nu_t = (C_s\Delta)^2\sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}}$$

– Smagorinsky model
– Germano dynamic model
– WALE model
– Structural models
– …and others

Modeling combustion in LES
The **filtered** source term

DNS LES



Loss of subgrid-scale wrinkling → longer flame

Two major approaches

- PDF-based

$$\widetilde{\Phi} = \int_{c*}^{\cdot} \int_{Z*}^{\cdot} \Phi(c^*, Z^*) P(c^*) P(Z^*) dc^* dZ^*$$

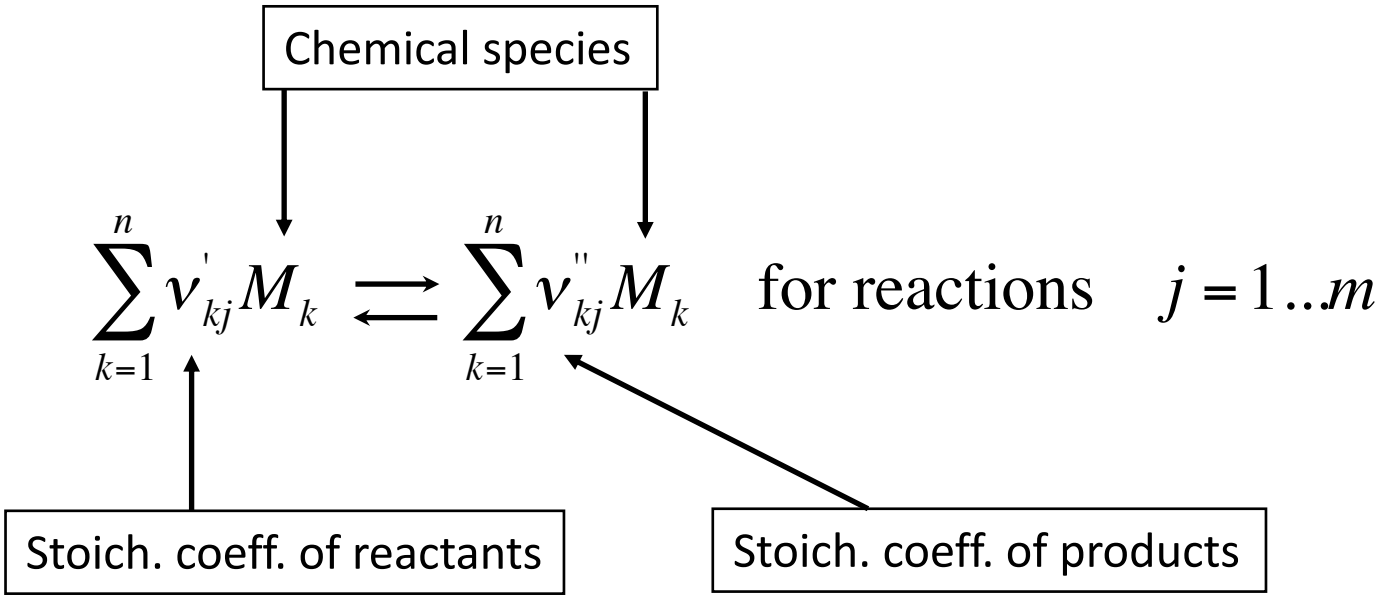
Given flame structure

- Thickened flame

Resolved flame structure

A word about chemistry

Stoichiometric relationships for an arbitrarily complex set of *m* reactions involving *n* species, may be written:



Nb	Reaction
1	$H_2 + O_2 \rightleftharpoons 2OH$
2	$OH + H_2 \rightleftharpoons H_2O + H$
3	$H + O_2 \rightleftharpoons OH + O$
4	$O + H_2 \rightleftharpoons OH + H$
5[a]	$H + O_2 + M \rightleftharpoons HO_2 + M$
6	$H + O_2 + O_2 \rightleftharpoons HO_2 + O_2$
7	$H + O_2 + N_2 \rightleftharpoons HO_2 + N_2$
8	$OH + HO_2 \rightleftharpoons H_2O + O_2$
9	$H + HO_2 \rightleftharpoons 2OH$
10	$O + HO_2 \rightleftharpoons O_2 + OH$
11	$2OH \rightleftharpoons O + H_2O$
12[b]	$H_2 + M \rightleftharpoons H + H + M$
13	$O_2 + M \rightleftharpoons O + O + M$
14[c]	$H + OH + M \rightleftharpoons H_2O + M$
15	$H + HO_2 \rightleftharpoons H_2 + O_2$
16	$HO_2 + HO_2 \rightleftharpoons H_2O_2 + O_2$
17	$H_2O_2 + M \rightleftharpoons OH + OH + M$
18	$H_2O_2 + H \rightleftharpoons HO_2 + H$
19	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$

Reduced chemical schemes

- Detailed schemes (GRImech~500 reactions) are produced from very large size schemes developed by chemists and are able to accurately describe oxidation of most hydrocarbons
- A first reduction step leads to skeletal mechanisms (~50-100 reactions) that keep most of the performances of detailed schemes
- A second reduction step (QSS) leads to analytical schemes (~10-30 reactions) having reduced but still reasonable performances
- Finally, optimally fitted global or semi-global schemes (1 to 4 steps) often require on-line adjustment of constants with P, Φ, etc

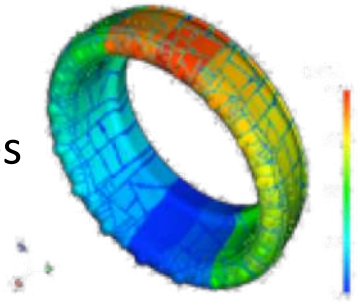
In addition, complex fuels are simplified and described with surrogate fuels

	Surrogate 1		Surrogate 2	
Component	mole [%]	vol. [%]	mole [%]	vol. [%]
n-heptane	22.0	23.5	66.8	74.1
iso-octane	44.8	53.6	0.4	0.5
benzene	13.0	10.0	24.8	20.0
toluene	20.2	12.9	7.9	5.3
Avg. formula	$C_{7.32}H_{14.0}$		$C_{6.75}H_{12.9}$	

AVBP – An unstructured LES solver

developed by CERFACS

- External, internal flows
- Fully compressible turbulent reacting flows (ideal & real gas thermo.)
- DNS / LES approach



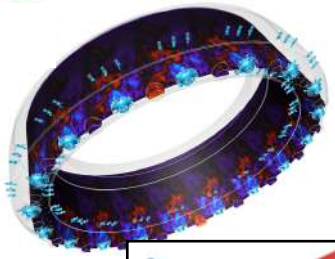
- Unstructured hexaedral, tetraedral, prisms & hybrid meshes
- Massively parallel, SPMD approach
- Explicit in time
- **Centered schemes**

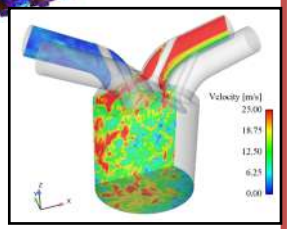
  Finite Volumes / Finite Elements (2nd/3rd order[a])

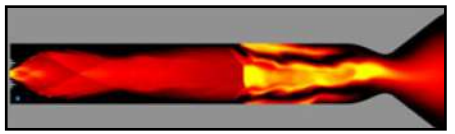
- SGS models : Smagorinsky(dynamic)/WALE[b]
- NSCBC[c] boundary cond. + wall laws
- Reduced[d] or tabulated[e] chemical kinetics
- Thickened flame turb. combustion model (TFLES)[f]
- Multi-phase solvers (Lagrangian & Eulerian)

Applications

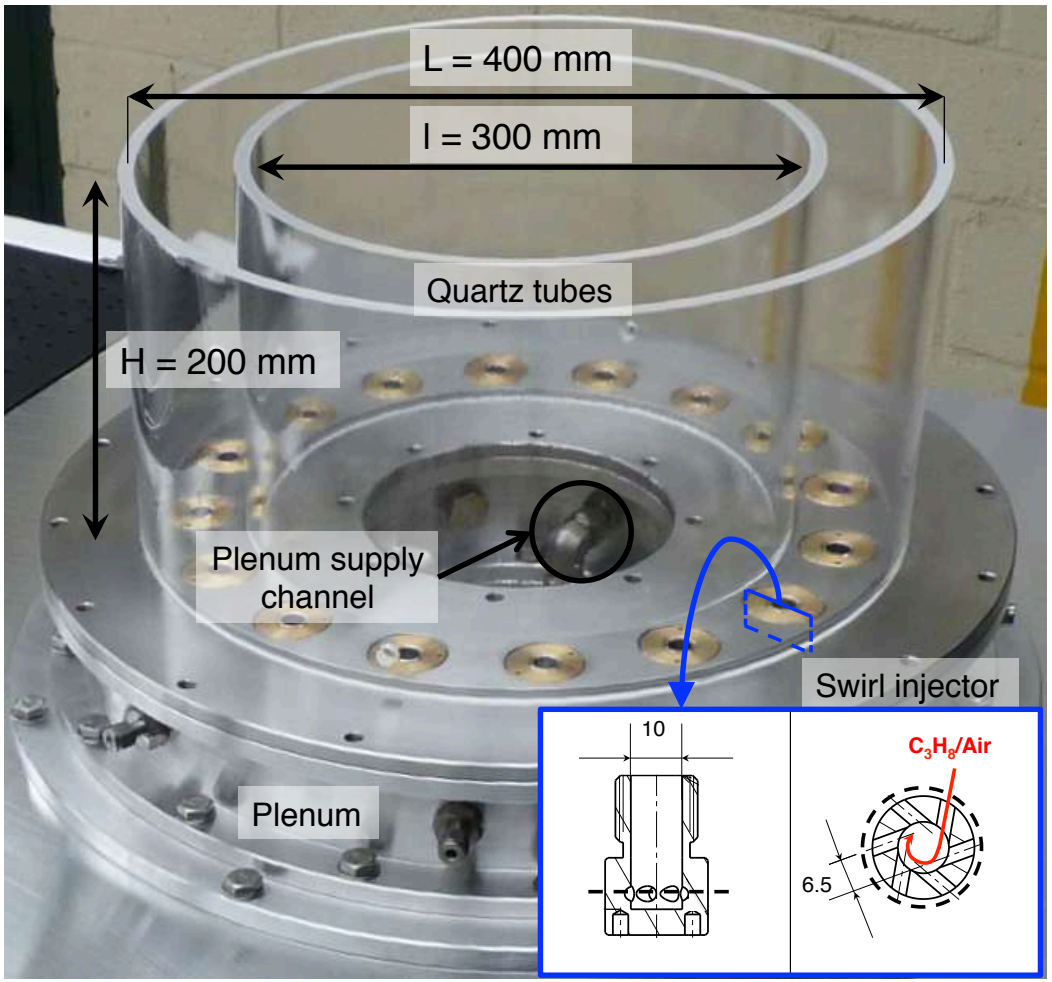
- Gas turbines
- Aeronautical engines
- Piston engines
- Statoreactor
- Rocket engines
- Furnaces
- Heat exchangers







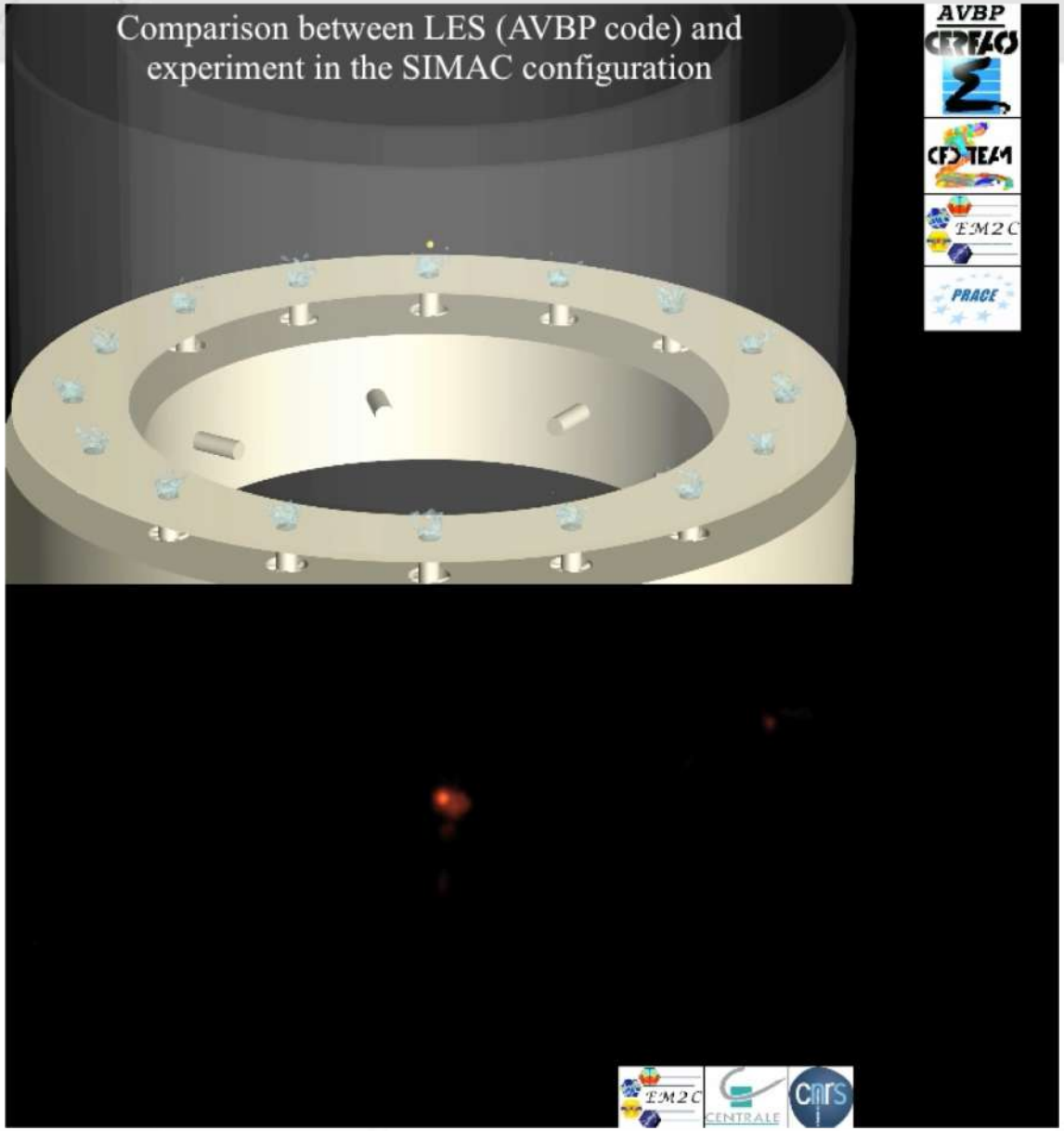
Ignition of the MICCA burner of EM2C



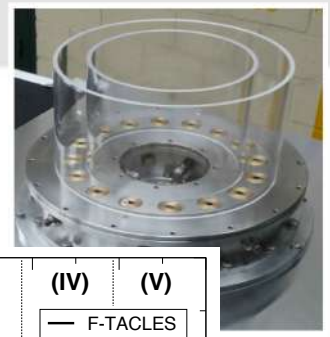
MICCA (EM2C) (*Durox et al*)

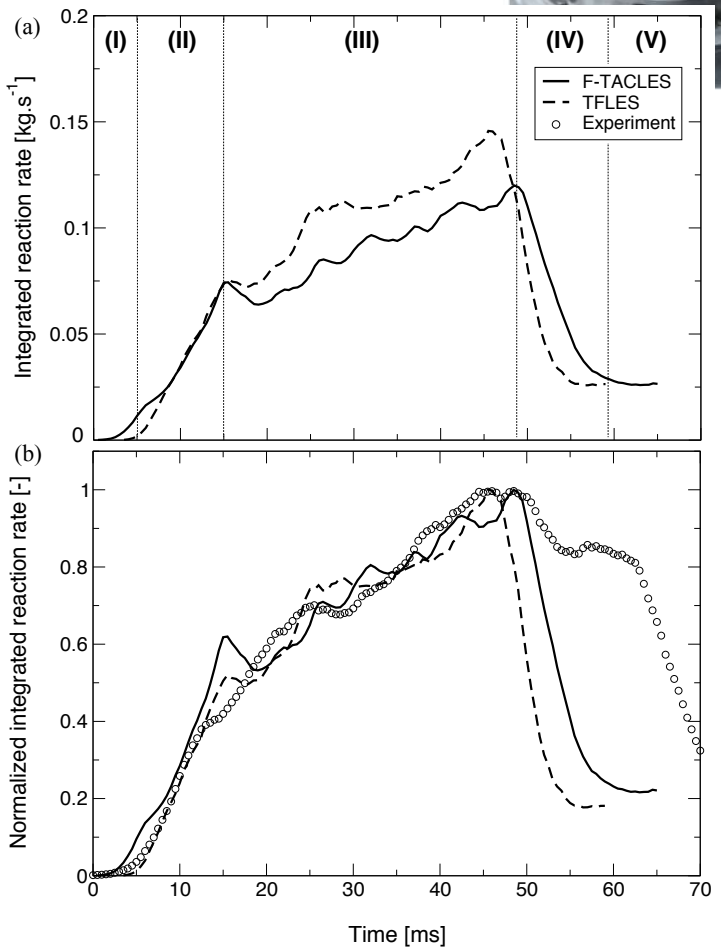
- Annular chamber
- 16 swirled injectors
- propane
- transparent walls

Ignition of the MICCA burner of EM2C



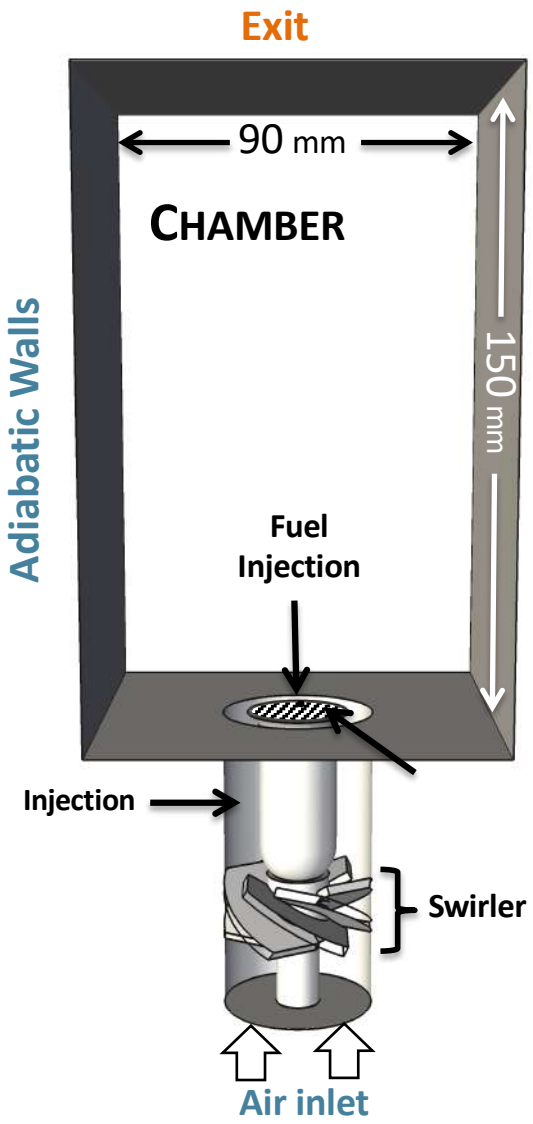
Philip et al, ASME 2013

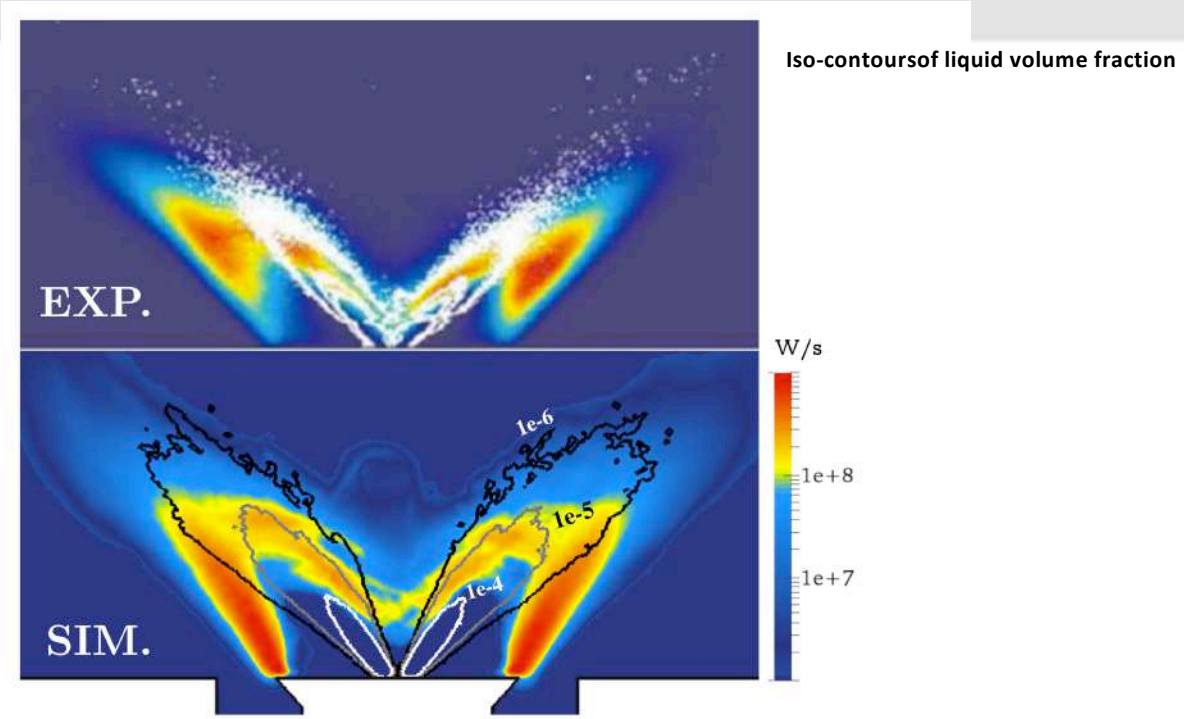


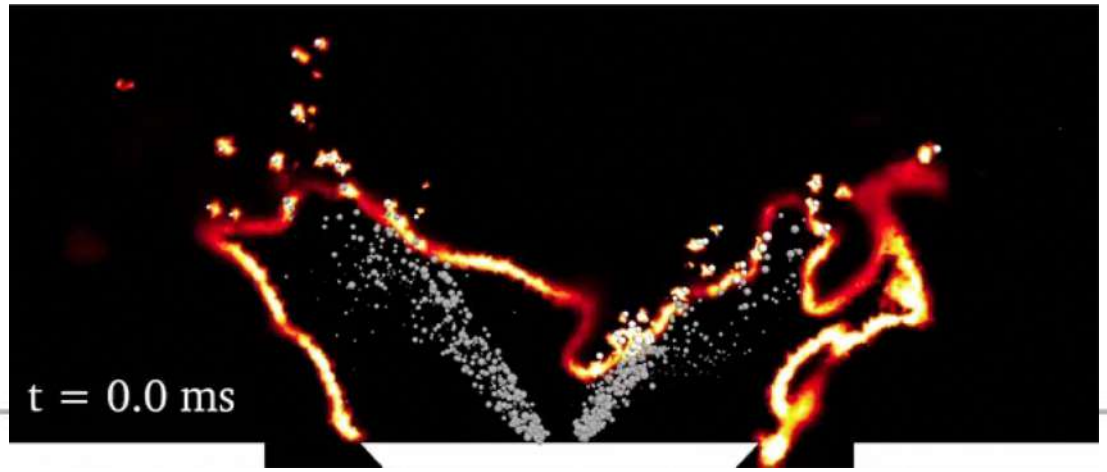


Adding two-phase flow : liquid fuel

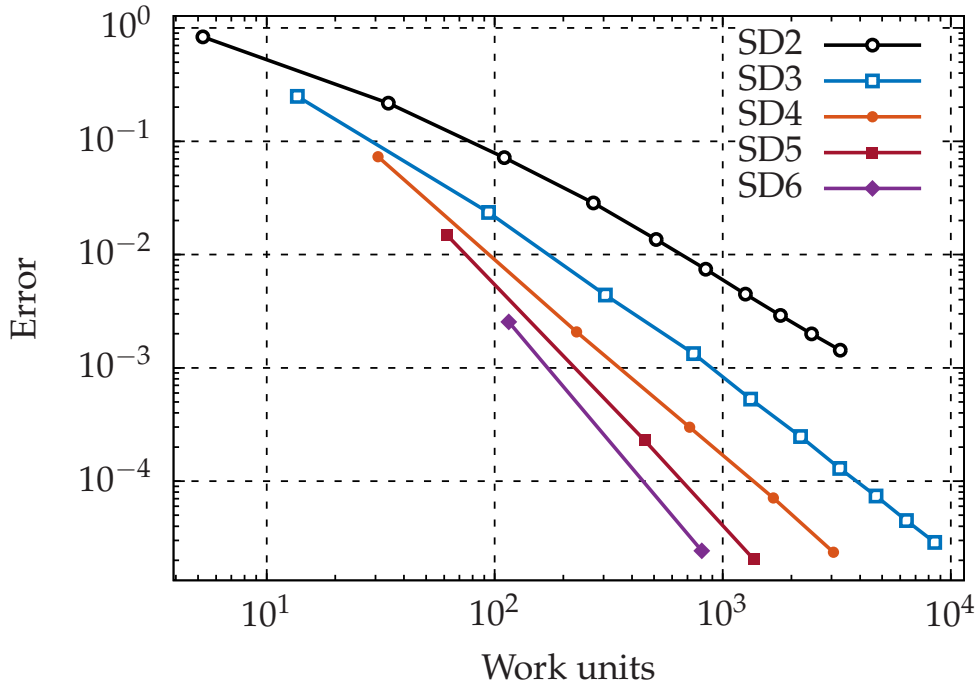
Experiment of Cambridge university





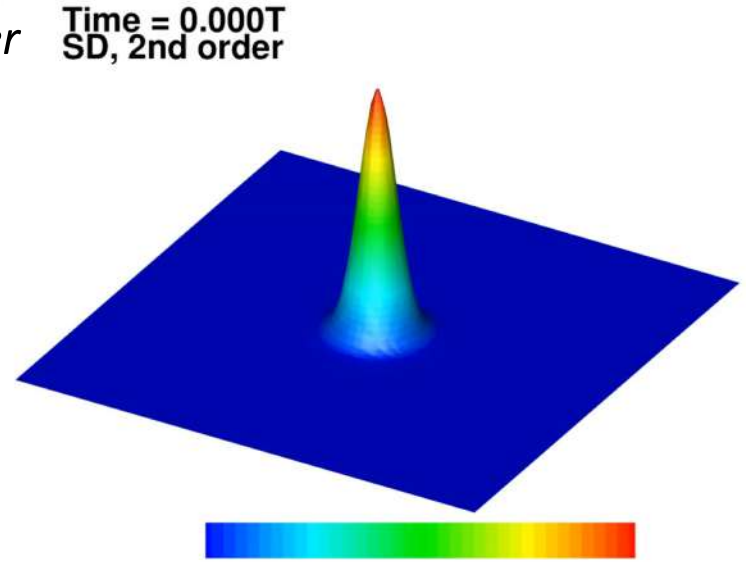


High order methods

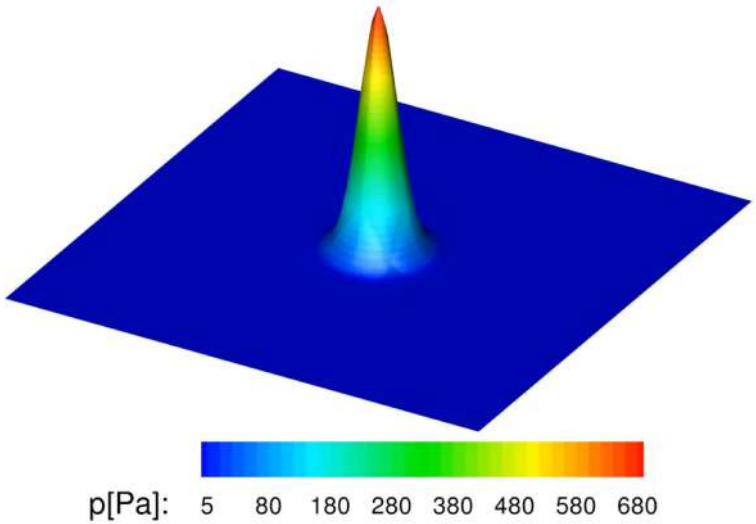


For a given precision, high order methods are computationally efficient

Low order



High order



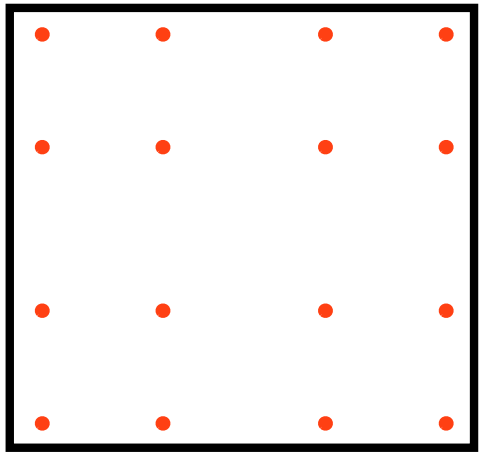
Spectral discontinuous approach

Assumptions:

- Unknowns are represented **locally** (inside a cell) as a **polynomial of degree *p***
- **No continuity** is assumed **at the interface between two adjacent cells**
- Compute an **interface flux polynomial** using (approximated) **Riemann solvers** as in **Finite Volume Method**

Several techniques:

- Solve the *weak* form of the equation locally
  ⇔ **Discontinuous Galerkin method**
- Solve the *strong* form of the equation locally
  ⇔ **Spectral Difference method**



One high-order 2D cell

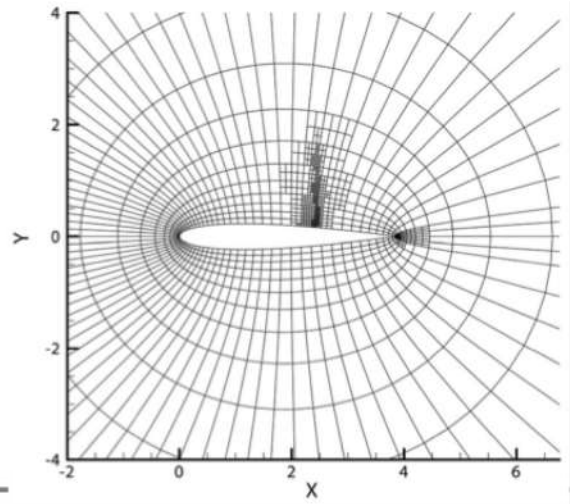
Spectral discontinuous approach

Promising techniques for LES and DNS

- **Accuracy:** control by the polynomial degree p chosen by the user
- **Local treatment:**
  - Algorithm can easily be written in term of **matrix/vector product ⇔ Good vectorization**
  - **Very compact stencil ⇔High Parallel Efficiency**
- **Compatible with Unstructured grids**

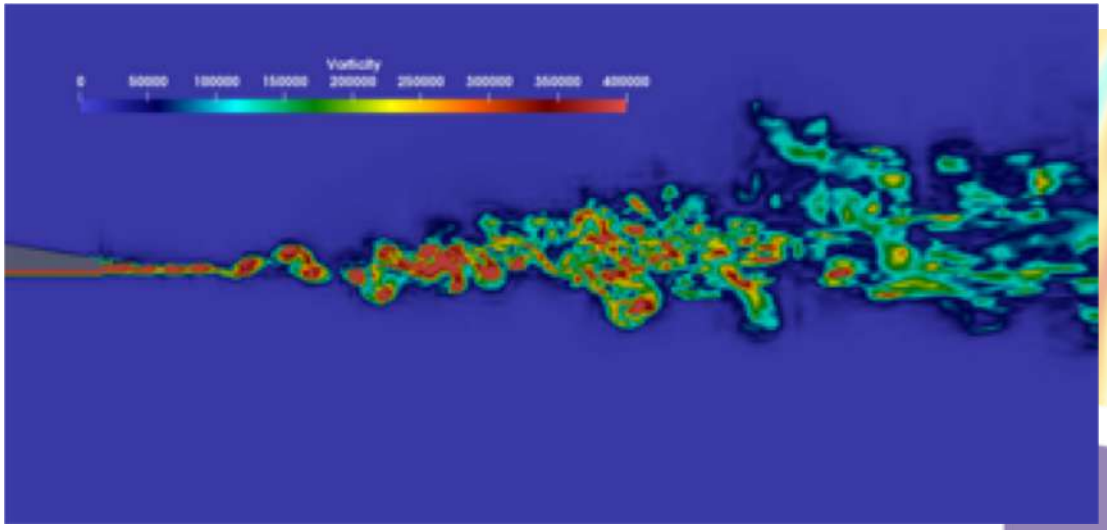
hp-adaptation

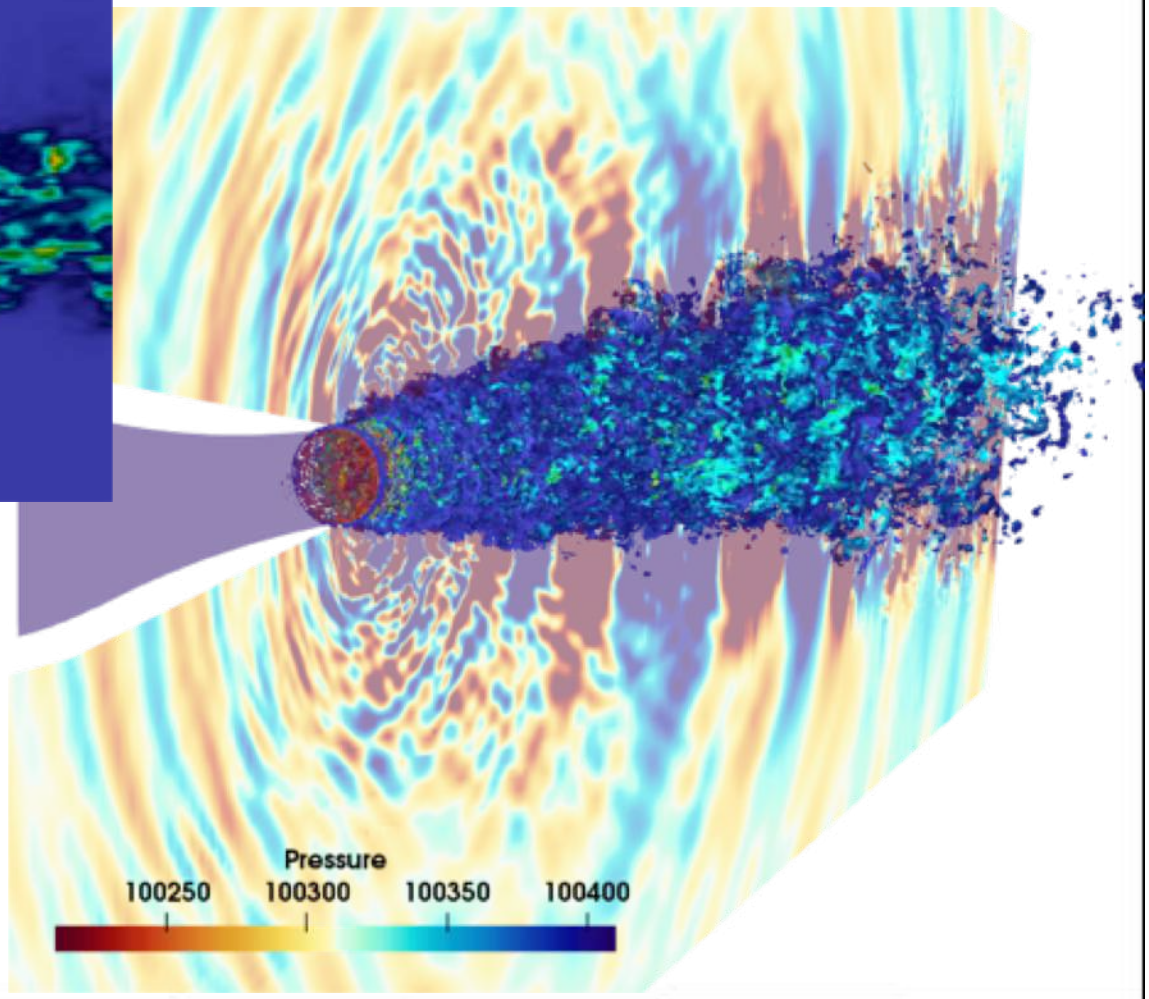
- Change **local refinement** (size h of the cell)
- Change **solution accuracy** (degree p of the polynomial representation)



Spectral discontinuous approach

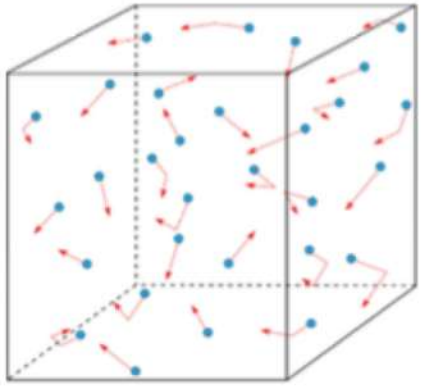
Example : jet noise simulation





Lattice Boltzman Method (LBM)

Can we avoid meshing complex geometries ?



Boivin et al. , M2P2

Lattice Boltzmann equation

$$\frac{\partial f}{\partial t} + \xi_\beta \frac{\partial f}{\partial x_\beta} + F_\beta \frac{\partial f}{\partial \xi_\beta} = \Omega(f)$$

$$-\frac{1}{\tau}(f - f^0)$$

BGK

Maxwell-Boltzmann distribution function

$$f^{(0)} = \frac{\rho}{(2\pi c_T^2)^{D/2}} \exp\left(\frac{-(\vec{\xi} - \vec{u})^2}{2c_T^2}\right)$$

Continuum-statistical variables

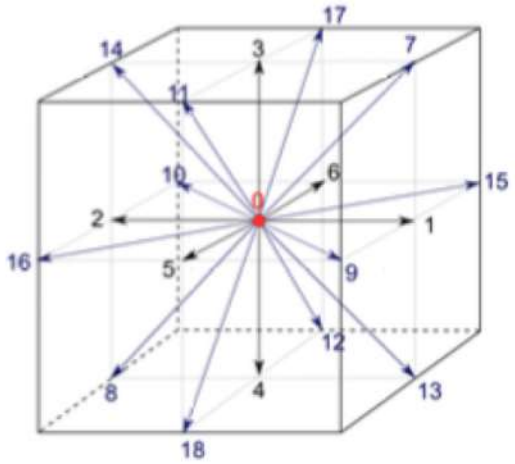
$$\rho(x,t) \equiv mn(x,t) = m\int f dv$$

$$\rho u(x,t) = m\int f v dv$$

$$\rho e(x,t) = \frac{1}{2}m\int f|\underbrace{v-u}_{c}|dv$$

Lattice Boltzman Method (LBM)

Can we avoid meshing complex geometries ?



Lattice Boltzmann equation

$$f_i(\boldsymbol{x} + \boldsymbol{c}\delta t, t + \delta t) - f_i(\boldsymbol{x}, t) = -\frac{1}{\tau}[f_i(\boldsymbol{x}, t) - f_i^{eq}(\boldsymbol{x}, t)]$$

Streaming — Collision

Maxwell-Boltzmann distribution function

$$f_i^{eq} = \rho w_i \left[1 + \frac{\boldsymbol{c}_i \cdot \boldsymbol{u}}{c_s^2} + \frac{(\boldsymbol{c}_i \cdot \boldsymbol{u})^2}{2c_s^4} - \frac{\boldsymbol{u}^2}{2c_s^2}\right]$$

Boivin et al. , M2P2

Lattice Boltzman Method (LBM)

Can we avoid meshing complex geometries ?

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \left[\rho\nu(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T)\right]$$

→ **LBM**

$$\frac{\partial T}{\partial t} + u_\alpha \frac{\partial}{\partial x_\alpha} T = \frac{1}{\rho}\frac{\partial}{\partial x_\alpha}(\rho D_T \frac{\partial T}{\partial x_\alpha}) + \frac{\omega_h}{\rho c_p}$$

+

$$\frac{\partial Y_k}{\partial t} + u_\alpha \frac{\partial}{\partial x_\alpha} Y_k = \frac{1}{\rho}\frac{\partial}{\partial x_\alpha}(\rho D_k \frac{\partial Y_k}{\partial x_\alpha}) + \frac{\omega_k}{\rho}$$

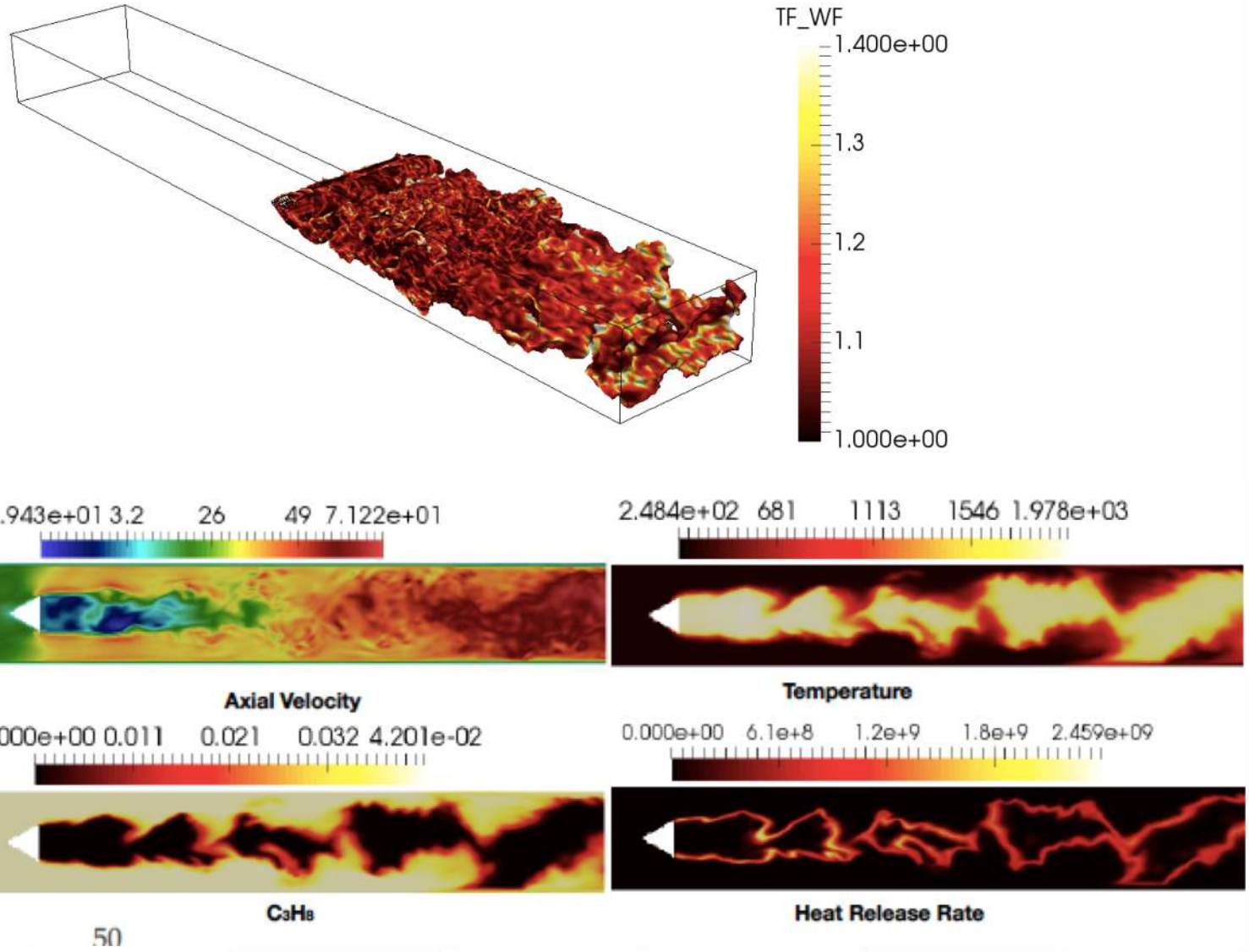
→ **Finite differences**

Boivin et al. , M2P2

Lattice Boltzman Method (LBM)

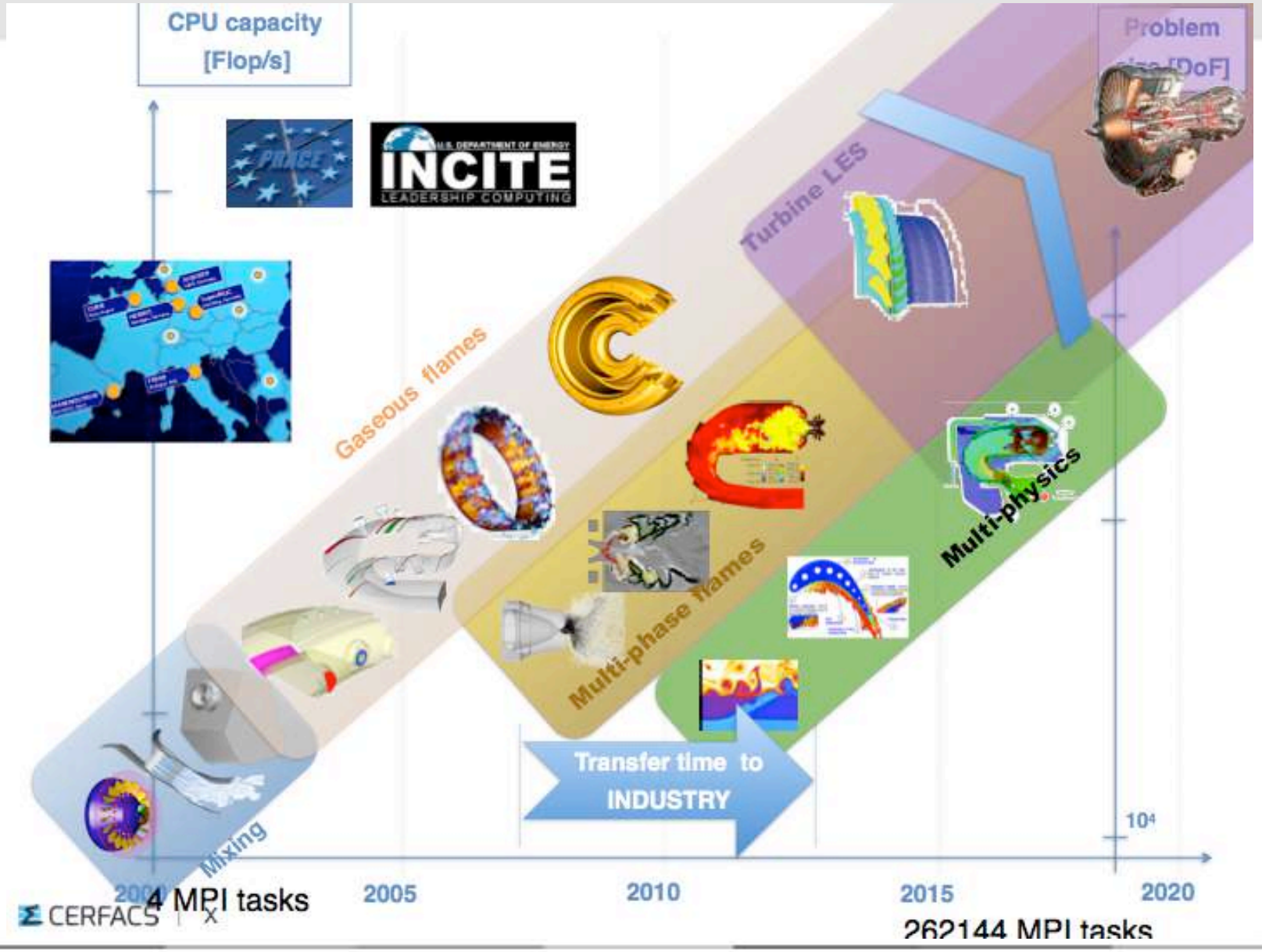
VOLVO case

Sjunnesson et al., 1991

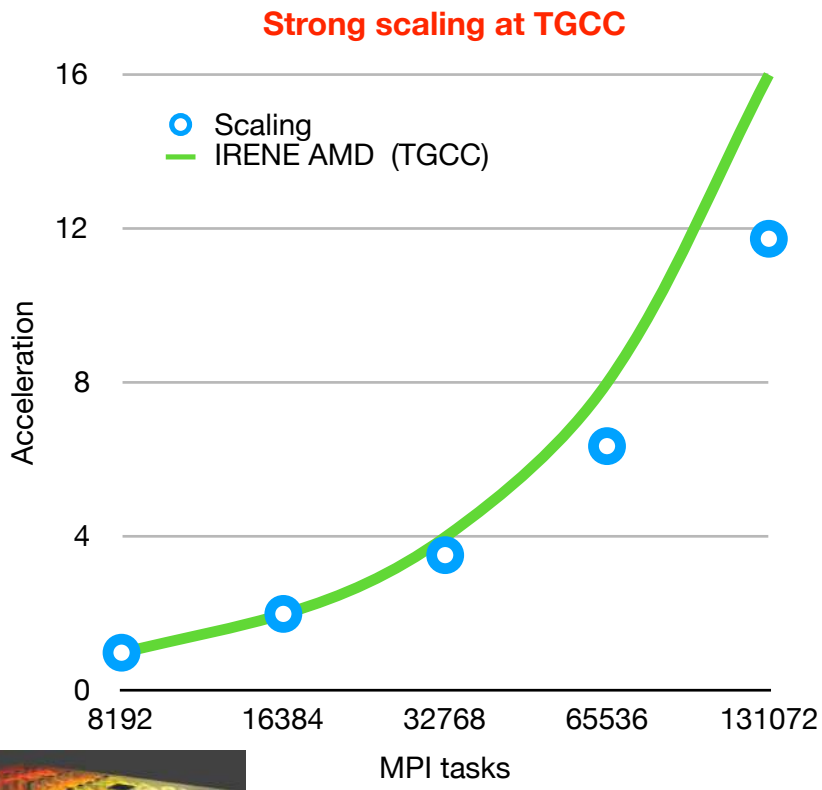


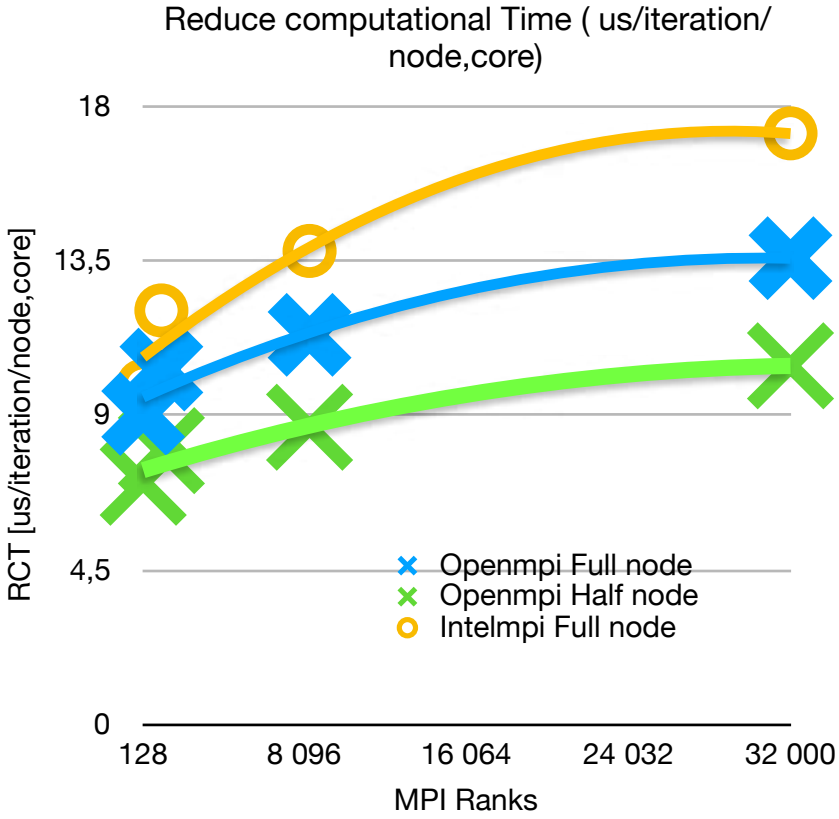
Boivin et al. , M2P2

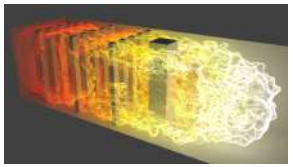
High Performance Computing



- Scaling: Strong i.e faster result (left) and weak i.e finer mesh (right)

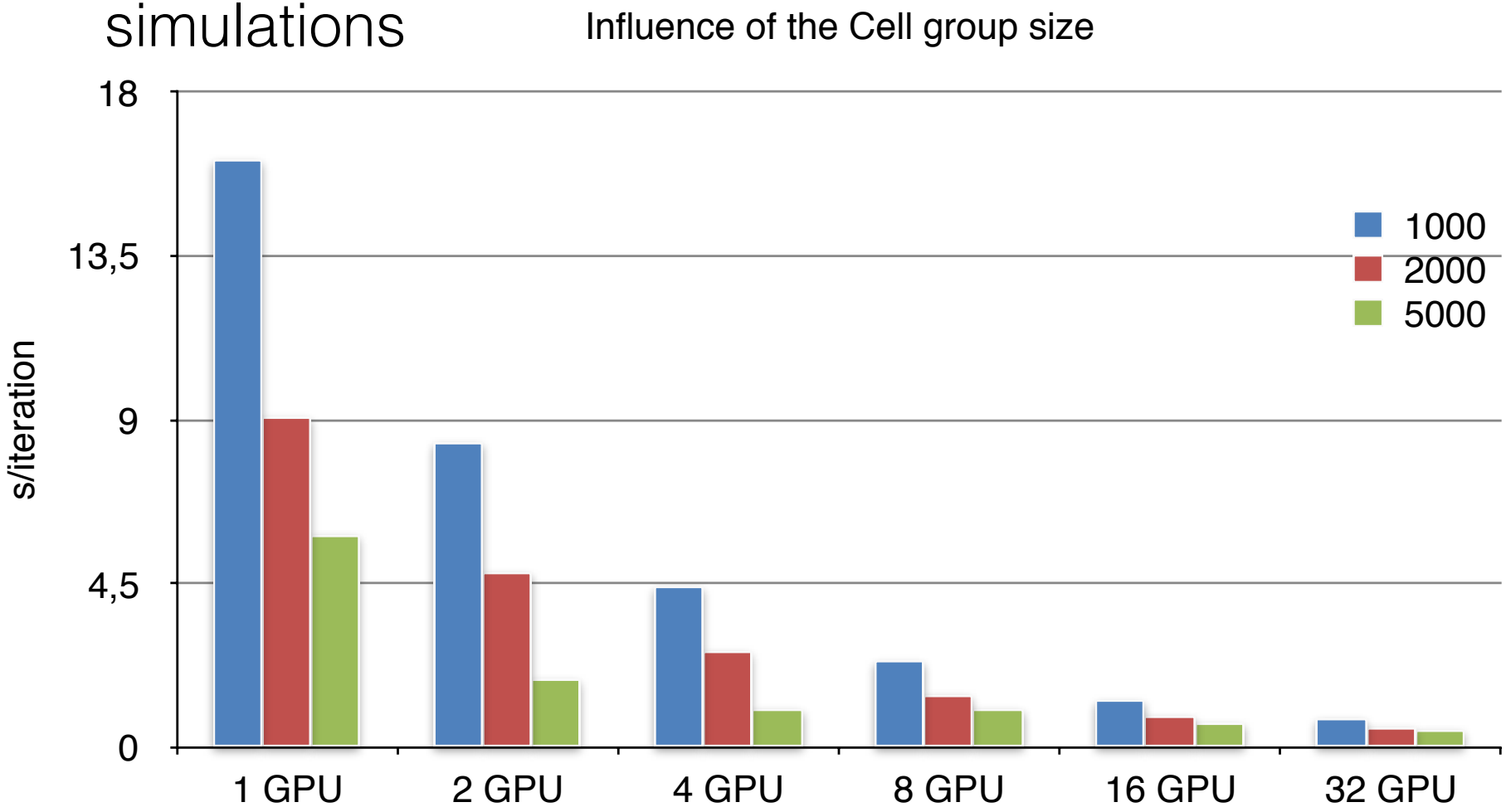






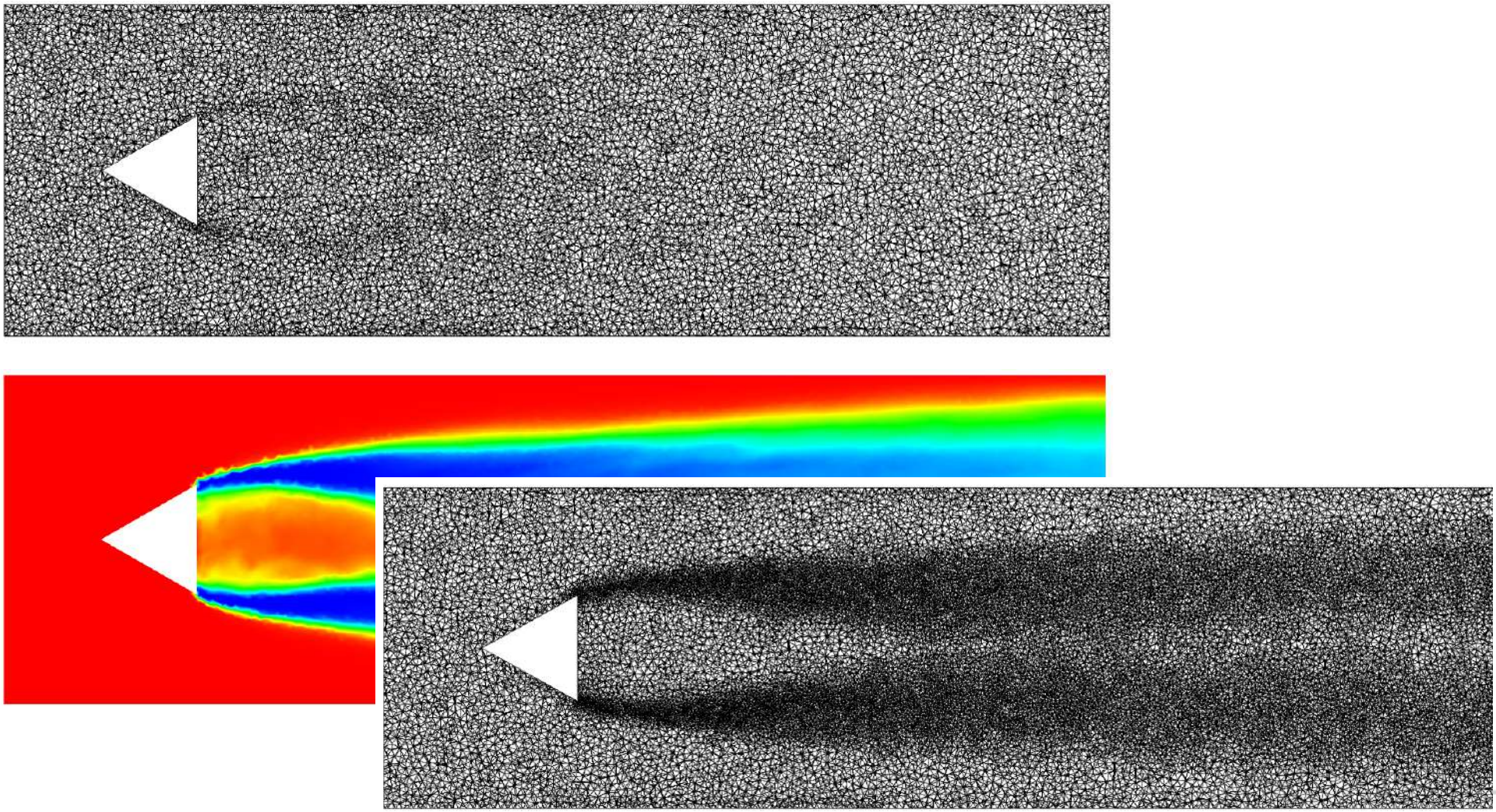
Scaling on GPUs

- Excellent strong scaling performance
- Additional cache optimisations accelerate the simulations



Mesh adaptation

- Adaptation using Grad C/C



Conclusion

Key ingredients for accurate and reliable numerical simulation of turbulent combustion:

- High-quality, adapted mesh
- High order integration schemes
- Parallel efficiency

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