Accélération de Flamme en mélange non uniforme

Journée des Doctorants LIMSI

5 juin 2019

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Groupe : Mecanique
Financement : CEA

Context

Hydrogen combustion

- Wide range of flammability limits and low ignition energy
- High combustion speed and excessively generated over-pressure

Overpressure depends of various local conditions

- Fuel/air concentration
- Interaction with turbulence
  - Flame velocity
  - Stretching (impact of obstacles)

FIGURE 1 – Hydrogen explosion at Fukushima Daiichi nuclear power plant

Resulting different possible scenarios Flame acceleration (FA) or Deflagration-to-Detonation Transition (DDT)

Impact for nuclear industry

- In case of incident, possible generation of hydrogen inside the reactor (Zircaloy-water reactions)
- Potential ignition and acceleration up to supersonic speeds (damage components)

CFD model for hydrogen ignition

Navier-Stokes equation

$$\mathbf{w}_t + \nabla \cdot (\mathbf{f}^E(\mathbf{w}) - \mathbf{f}^V(\mathbf{w}, \nabla \mathbf{w})) = \mathbf{S}(\mathbf{w}), \text{ with } \mathbf{w} = (\rho, \rho \mathbf{u}, \rho E)^T \quad (1)$$

Problematics

- Multi-scale phenomena (reaction, shock-wave propagation, species diffusion...)
  $\Rightarrow$ stiff equations, small time step and fine mesh
- Large geometry and computational field
  $\Rightarrow$ significant costs

MR_CHORUS solver

- LIMSI compressible solver build to be able to capture discontinuities with adaptive multiresolution
- Dynamical graded tree data structure : computation on the most pertinent refinement level [1] [2]
- Strang splitting to solve independantly each part of the Navier Stokes equation
  - Euler part with Roe Solver [3] [4]
  - Viscous part with RK2 solver
  - Source term with implicit scheme and adaptive time step [5] (to develop)

Objectives

MR_CHORUS Development

- Complete MR_CHORUS solver to compute multispecies and reactive flow
- Capture flame/turbulence interaction with moderate ressources
- Validation with CEA experiments

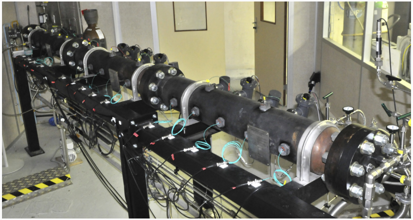

FIGURE 2 – Structures Submitted to an EXplosion of HYdrogen experiment

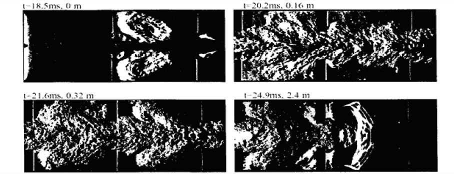

FIGURE 3 – Flame propagation through obtacles (SORIN (2005))

Multispecies implementation

Multispecies

- New conservatives variables $\mathbf{w} = (\rho Y_1, \cdots, \rho Y_N, \rho \mathbf{u}, \rho E)^t$
- Species diffusion with Hirshfelder and Curtiss approximation [6]
- use of Agath : 1D solver to compute thermodynamic and transport properties of the mixing
  - Thermodynamic : constant or polynomial specific heat capacities
  - Transport : computation of transport coefficients from binary diffusion coefficients with CHEMKIN methods [7]
- Extension of Roe solver for equilibrium flow [8]

Test Cases

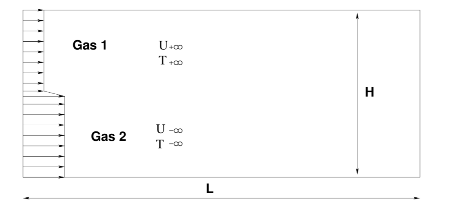

FIGURE 4 – Mixture Layer Air/H2

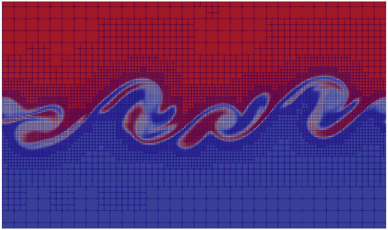

FIGURE 5 – Mixture of Air/H2

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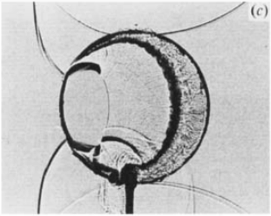

FIGURE 4 – Shock/Bubble interaction experiment [9]

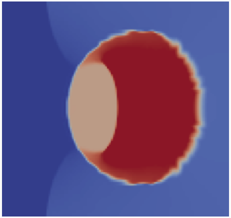

FIGURE 5 – Shock/Bubble interaction simulation

Immersed boundary technique [10]

Objectives

- Add some obstacles in the flow to generate turbulences
- Managing cut-cells in the cartesian mesh

Flow around a cylinder

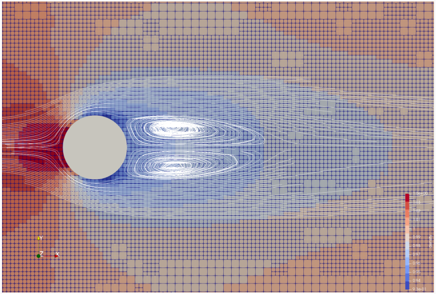

FIGURE 6 – Laminar case $Re_D = 40$

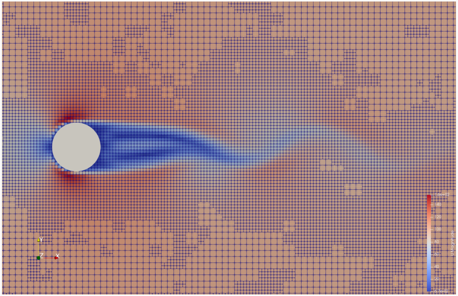

FIGURE 7 – Turbulent case $Re_D = 1000$

Immersed boundary technique [10]

Objectives

- Add some obstacles in the flow to generate turbulences
- Managing cut-cells in the cartesian mesh

Flow around a square

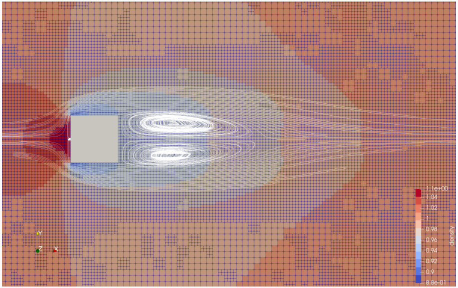

FIGURE 6 – Laminar case $Re_D = 40$

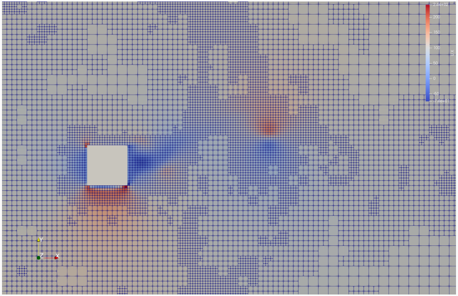

FIGURE 7 – Turbulent case $Re_D = 1000$

Conclusion and Perspectives

Conclusion

- Multispecies implementation
  - Diffusion model
  - Coupling with Agath 1D solver library
  - Roe solver adapted for equilibrium real gas mixture
- Integration of embedded boundary methods

Perspectives

- Implicit reactive source term with adaptive Splitting time step (see DUARTE 2015)[5]
- Comparison between embedded boundary methods
- 3D geometry
- Boundary layer
- Parallelisation

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