Modeling and high performance computing (HPC) of two-phase reactive flows with particular application to aircraft and rocket engines

O. Simonin

Institut de Mécanique des Fluides de Toulouse (IMFT)
Particles, Spray and Combustion Research Group
UMR CNRS/INPT/UPS
Université de Toulouse
Application example: the aircraft combustion chamber
Research objectives and methods

- Explore and model local interactions and medium scale behavior in reactive and/or multiphase flows with dispersed phases of solid particles or droplets by using experiments and “full” direct numerical simulations.

- Develop numerical modeling approaches for full-scale predictions of reactive particulate multiphase flows in the general frame of kinetic theory of particulate flows:
  - fluid-particle joint probability density function (PDF) equation,
  - "n-fluid" (or moment) and stochastic Lagrangian (or Monte Carlo) methods coupled with RANS fluid equations,
  - Euler-Lagrange and Euler-Euler large-eddy simulation (LES) approaches

- Full scale prediction of industrial (and environmental) flows:
  + Evaluation of available numerical modeling approaches (comparison with experimental results),
  + Optimization and scale-up of existing processes,
  + Support for development of new processes.
Industrial research projects

+ Ground transportation:
  - Injection in IC engine
  - Droplet deposition

+ Air and space transportation:
  - Aircraft turbines
  - Cryogenic engine
  - Solid fuel rocket booster

+ Energy and safety:
  - Particle transport and deposition
  - Spray into the enclosure of a nuclear reactor
  - Coal boiler for CO2 capture: "chemical looping"

+ Process engineering:
  - Fluid catalytic cracking column (FCC)
  - Fluidized bed chemical reactor (UF₄ fluoration, Zirconium chloration, olefin polymerization)
  - Glass melting furnace
  - Hydrocyclone,
  - …
Modeling challenges

+ 3D unsteady flows in complex geometries (URANS or LES approaches)
+ Poly-dispersed particle mixture
+ Gaseous and heterogeneous combustion
+ Splashing/deposition, bouncing/resuspension
+ Non-spherical or deformable particles
+ Radiative transfer, electrostatic effect
+ ....
Industrial partners

+ Ground transportation:
  - RENAULT, PEUGEOT, SIEMENS, GDF, IFP, CSTB

+ Air and space transportation:
  - SNECMA, SME, ONERA

+ Energy and safety:
  - ALSTOM, EDF, CEA, IRSN, INRS

+ Process engineering:
  - TOTAL, INEOS, AREVA, Air Liquide, SAINT GOBAIN, IFP
**Numerical Tools**

- **VOF type method**: Thétis (TREFLE, Bordeaux)

- **Euler-Lagrange approaches**:
  + "DNS"-DPS: JADIM (Interface-IMFT), NTMIX (CERFACS)
  + LES-DPS: JADIM (Interface-IMFT), AVBP (CERFACS)

- **n-Eulerian RANS-PDF or LES model**:
  + NEPTUNE_CFD (EDF R&D) → dilute and dense particulate reactive flows (parallel multi-phase code, implicit, unstructured VF), NEPTUNE project (CEA, EDF, IRSN and AREVA-NP )
  + AVBP (CERFACS) → dilute droplet flows with turbulent combustion
We thank 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, as well as GENCI and CINES for their computational support.
NEPTUNE CFD HPC efficiency

Simple granular shear flow

Full scale polymerization reactor

38,000,000 cells

3,150,716 cells

ref = 128 cores

ref = 8 cores
Outlines

- Two-fluid simulation of gas-liquid turbulent flow in complex geometry

- RANS-PDF modeling approaches in gas-particle flows

- Euler LES modeling approaches in two-phase reactive flows
Numerical simulation of a 3D unsteady two-phase flow in the filling cavity in oxygen of a cryogenic rocket-engine

M.-C. GAUFFRE, H. NEAU, O. SIMONIN, R. ANSART, N. MEYERS, S. PETITOT
Oxygen filling cavity simulation

- **Context of the study:**
  - To control the ignition phase of the cryogenic upper-stage rocket-engine (LOX / LH2) in both void and microgravity.
  - Necessity to know the transient flow within the injection cavity to provide the correct boundary conditions to simulate accurately the ignition phase.

Diagram of the rocket-engine
Computational study

- **Unstructured 3D mesh:**
  - equivalent to the experimental mock-up,
  - result of the merging of non coincident mesh,
  - composed of 1,124,200 cells

Experimental mock-up at LEGI

Mesh for the simulations
Computational study

- **CFD code: NEPTUNE_CFD V1.08**
  - Developed in the framework of the NEPTUNE project
  - Financially supported by CEA (Commissariat à l’Énergie Atomique), EDF (Électricité de France), IRSN (Institut de Radioprotection et de Sûreté Nucléaire), and AREVA-NP
  - Finite Volume Eulerian multi-phase solver parallelized designed for nuclear engineering

- **Calculations performed at CALMIP (Centre de CAlcuL Midi-Pyrénnées)**
  - with the Super computer HYPERION:
    - 352 nodes – 8 cores per node – 2816 cores
    - Intel "Nehalem" EP quad-core.
  - Physical time: 1.2 s
    - Local CPU Time: 32 hours on 128 cores
Model and initial conditions

- **Physical models: Injection of water in a mock-up initially filled with air**
  - Incompressible two-phase flow (with water and air) for each phase, without mass and energy transfer
  - $k$-$\varepsilon$ turbulence model activated for both phases:
  - Equations solved for each phase:
    - Mass balance equation
    - Momentum balance equation
  - Coupling between the two phases by the Simmer-like law (phase separated drag model depending on the volume fraction).

- **Initial conditions: Dome initially filled with air**
  - Air density $\rho = 1.2 \text{ kg/m}^3$
  - Dynamic viscosity $\mu = 1.85 \times 10^{-5} \text{ Pa.s}$
**Inlet conditions: valve opening modelisation**

- Evolution of the opening angle $\theta$ and of the opening surface area of the bushel valve respected.

- Evolution compared of the experimental and numerical inlet mass flow rates of water:

\[
\left| \frac{Q_{Exp} - Q_{Num}}{Q_{Exp}} \right| \times 100 < 1\%
\]
- Evolution of the mass flow rates and of the mass of water in dome

- Dome filling phase
- Dome emptying phase

- 90% of the dome volume occupied by water at the maximum
- Evolution of the dome pressure

![Graph showing the evolution of dome pressure over time with numerical and experimental pressures compared to valve position.]

- Experimental pressure
- Numerical pressure
- Valve position
- Volume fraction of liquid

Time = 0.000 s
Conclusion

3D unsteady CFD simulations (NEPTUNE_CFD) of the experiments at LEGI with substitution fluids (air and water):

- Incompressible two-phase flow without energy and mass transfer
- Complex industrial geometry equivalent to the experimental mock-up
- Major impact of the drag law
  - globally on the outlet mass flow rate of water, on the mass of water in dome and on the dome pressure
  - locally on the wet injectors
- Lack of robustness of the numerical method: gas-liquid interface + mesh distortion
Outlines

- Two-fluid simulation of gas-liquid turbulent flow in complex geometry

- RANS-PDF modeling approaches in gas-particle flows

- Euler LES modeling approaches in two-phase reactive flows
**Kinetic theory of particulate flows**

Derivation and closure of the kinetic transport equation on the single particle PDF based on a Lagrangian modelling of particle-fluid, particle-particle and particle-wall interactions.

- Lagrangian stochastic modeling approach based on discrete numerical particles computation using stochastic gas turbulence model and Monte Carlo simulation method

  or

- Eulerian approach based on PDF moment equations (number density, velocity, temperature, random motion kinetic energy, kinetic stresses…) and transport properties (viscosity, diffusivity).

Validation from "*Euler-Lagrange numerical experiments*"

→ Implementation in CFD codes and comparison of model predictions with experimental measurements (laboratory, pilot and industrial scales).
**Particle PDF microscopic equation**

\[ f_p^{(1)}(\mathbf{c}_p, \mathbf{x}, t) \] single particle PDF (Probability Density Function)

Probability distribution of local instantaneous number of particles with a translation velocity \( \mathbf{u}_p^{(n)} = \mathbf{c}_p \)

\[
\frac{\partial}{\partial t} f_p^{(1)}(\mathbf{c}_p, \mathbf{x}, t) + \frac{\partial}{\partial x_j} \left[ c_{p,j} f_p^{(1)} \right] + \frac{\partial}{\partial c_{p,j}} \left[ \frac{F_{p,j}}{m_p} |\mathbf{c}_p| f_p^{(1)} \right] = \left( \frac{\partial}{\partial t} f_p^{(1)} \right)_{\text{coll}}
\]

\[
F_{p,j} = -\frac{m_p}{\tau_p} \left[ c_{p,j} - u_f @ p, j \right] + m_p g_j \quad \text{external force acting on a particle}
\]

\[
\left( \frac{\partial}{\partial t} f_p^{(1)} \right)_{\text{coll}} \quad \text{interparticle collision effect}
\]
Lagrangian Stochastic Modeling

Methodology

Tracking of discrete particles in a fluid turbulent flow predicted using RANS (k-epsilon, Rij-epsilon) approach

Generation of the instantaneous turbulent fluid properties (velocity, temperature) from RANS predictions using a random process (eddy-life time model, Langevin equation) for the computation of the interphase transfers

Monte-Carlo simulation of the particle-particle interaction process (collision)

Back effect towards the fluid RANS equations (two-way coupling)

Strengths and weaknesses

(+ ) Extensively implemented in industrial CFD codes (Fluent, StarCD, CFX,…)

(+ ) Very efficient (and reasonably accurate) in dilute turbulent dispersed two-phase flows

(+ ) Allows to implement easily complex local physical phenomena endured by the particles (heat and mass transfer, wall-particle interaction, coalescence and break-up, … )

(- ) Modelling and numerical limitations for high dispersed phase loading

(- ) Some open physical modelling questions: fluid turbulent velocity random generation in strongly sheared flow (wall boundary layer), inter-particle correlation effect on the collision mechanism, ….
NUMERICAL SIMULATION OF COALEScing DROPLETS SUSPENDED IN HOMOGENEOUS ISOTROPIC TURBULENCE

STOCHASTIC LAGRANGIAN MODELLING

D. Wunsch$^{1,2}$, R. Belt$^{1,2}$, P. Fede$^{1,2}$, O. Simonin$^{1,2}$, P. Villedieu$^3$

$^1$Université de Toulouse; INPT, UPS ; IMFT ; 31400 Toulouse, France
$^2$CNRS; Institut de Mécanique des Fluides de Toulouse ; 31400 Toulouse, France
$^3$ONERA ; 31400 Toulouse, France
We stretching separation

Reflexive separation

Permanent coalescence

\[ X = \frac{2\delta}{d_p + d_q} \]

\[ We = \frac{\rho d_p w_r^2}{\sigma} \]

Source: Ashgriz & Poo, JFM 221/Qian & Law JFM 331
RANS + Lagrangian stochastic modelling of the particle laden turbulent flow in a segmented solid rocket booster

Turbulent kinetic energy of the gas in the booster

Schematic view of the flow in the aft end of a segmented solid propellant motor
RANS + Lagrangian stochastic modelling of the particle laden turbulent flow in a segmented solid rocket booster

Positions of the “test” sections

Correlated collision model

Uncorrelated collision model

Section 2
Evolution of the droplet size distribution
DPS of coalescing droplets coupled with DNS

Coalescence treatment

- Deterministic algorithm detection
- Only binary interaction (dilute)
- Permanent coalescence (2 drops → single drop)

\[ m^* = m_{p1} + m_{p2} \]
\[ m^*_p u^*_p = m_{p1} u_{p1} + m_{p2} u_{p2} \]

DPS of coalescing droplets coupled with DNS

Droplet properties

<table>
<thead>
<tr>
<th>$d_p$</th>
<th>50µm</th>
<th>100µm</th>
<th>200µm</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d_p/\eta_K$</td>
<td>0.16</td>
<td>0.34</td>
<td>0.68</td>
</tr>
<tr>
<td>$S_t (g=0)$</td>
<td>0.17</td>
<td>0.63</td>
<td>2.18</td>
</tr>
<tr>
<td>$S_t (g=9.81)$</td>
<td>0.17</td>
<td>0.58</td>
<td>1.67</td>
</tr>
</tbody>
</table>

$\rho_p = 1000 \text{kg/m}^3$

$S_t = \frac{\tau_p}{\nu_f}$

Simulation methodology

Initialization Fluid  | Statistics Fluid  | Initialization Droplet  | Statistics Droplet  | Coalescence

$\langle u_iu_i \rangle$  | $\langle u_pu_p \rangle$

$St_2 > St_1$
Collision kernel modeling

The collision kernel can be written as:

\[
\left( \frac{\partial f_p}{\partial t} \right)_{\text{coll}} = K^+ (c_p, \mu_p, x, t) - K^- (c_p, \mu_p, x, t)
\]

Permanent coalescence

The rate of vanishing droplets

\[
K^- (c_p, \mu_p; x, t) = \int_{w_{pq} \cdot k_{pq} < 0} f_p^{(2)} (c_p, \mu_p, c_q, \mu_q; x, x + d_{pq} k_{pq}, t) |w_{pq} \cdot k_{pq}| d^2_{pq}
\]

\[
\times d c_q d \mu_q d k_{pq}
\]

Model for the pair particle PDF is needed
Instantaneous particle and fluid velocity distributions from ‘DNS’ (one-way coupling) in homogeneous isotropic turbulent flow, particle relaxation time to fluid Lagrangian integral time scale ratio $St = 0.13$. 
Instantaneous particle and fluid velocity distributions from ‘DNS’ (one-way coupling) in homogeneous isotropic turbulent flow, particle relaxation time to fluid Lagrangian integral time scale ratio $St = 2.17$. (fluid and particle velocity vectors obey different scaling)
Effect of turbulence on coalescence kernel

Collision frequency:
\[ f_{col} = \pi d_p^2 n_p^2 g_0 < w_r > \]

Light (small) particles: \( \tau_p \ll \tau_K \) Saffman & Turner, 1956

Relative velocity proportional to the local fluid velocity gradient \( \rightarrow \)
\[ < w_r > = d_p \sqrt{\frac{2 \epsilon_f}{15 \pi v_f}} \]

Heavy (large) particles: \( \tau_L \ll \tau_p \) Abrahamson, 1975

Uniform particle distribution \( \rightarrow \) \( g_0 = 1 \)

Relative velocity related to particle agitation \( \rightarrow \)
\[ < w_r > = \sqrt{\frac{8 q_p^2}{\pi}} \]

Molecular chaos assumption
\[ f^{(2)}_p (c_p, c_q; x, x + d_{mn} k_{mn}, t) = g_0 f_p (c_p; x, t) f_p (c_q; x + d_{mn} k_{mn}, t) \]
Effect of turbulence on coalescence kernel

Intermediate régime: \( \tau_p \approx \tau_L \)

Non-uniform particle distribution \( \Rightarrow g_0 > 1 \)

Williams & Crane, 1983; Kruis & Kuster, 1997; Laviéville et al., 1997; Pigeonnau, 1998; Fede & Simonin, 2003; Zaichik et al, 2006

Laviéville et al. (1997) take into account this effect of the turbulence by using the joint fluid-particle pair pdf to close the collision kernel:

\[
f^{(2)}_{fp}(c_p, c_{f,p}, c_q, c_{f,q}) \approx g_0 f^{(2)}_f(c_{f,p}, c_{f,q}) f_p(c_p, c_{f,p}) f_p(c_q, c_{f,q})
\]

Fede et al. (IJMF, 2015) proposed a collision algorithm for Lagrangian Stochastic simulation (Monte-Carlo Simulation) based on the closure proposed by Laviéville et al. \( \Rightarrow \) Bird algorithm with collision conditioned by the fluid velocity viewed by the particles
Lagrangian stochastic modelling of droplet coalescence in an homogeneous isotropic turbulent gas flow

$Re_A=32.9, \text{ St}=0.10$: 

\begin{itemize}
  \item Molecular-Chaos assumption
  \item Droplet velocity correlation closure
\end{itemize}

Time evolution of the dimensionless number of particles and mean Sauter diameter: comparison between Monte-Carlo predictions and DNS+DPS results
Re$_A$ = 32.9, St = 0.95:

- Molecular-Chaos assumption
- Droplet velocity correlation closure

Lagrangian stochastic modelling of droplet coalescence in an homogeneous isotropic turbulent gas flow

Time evolution of the dimensionless number of particles and mean Sauter diameter: comparison between Monte-Carlo predictions and DNS+DPS results
Lagrangian stochastic modelling of droplet coalescence in an homogeneous isotropic turbulent gas flow

\( \text{Re}_\Delta = 32.9, \text{St}=2.43: \)

- - - Molecular-Chaos assumption

\[ \text{Droplet velocity correlation closure} \]

Time evolution of the dimensionless number of particles and mean Sauter diameter: comparison between Monte-Carlo predictions and DNS+DPS results
Outlines

- Two-fluid simulation of gas-liquid turbulent flow in complex geometry

- RANS-PDF modeling approaches in gas-particle flows

- Euler LES modeling approaches in two-phase reactive flows
The general framework of the methodology

Overview of existing UNSTEADY Eulerian modeling approaches

The general framework of the methodology

Overview of existing UNSTEADY Eulerian modeling approaches

In this study

Kaufmann et al. (2008)

Moreau et al. (2010)
Particle Euler LES equation derivation

Local instantaneous particle moment equations derived from the Boltzmann type equation governing the particle PDF (conditioned by the fluid flow realization)

Particle number density equation:
\[
\frac{\partial}{\partial t} n_p + \frac{\partial}{\partial x_i} n_p u_{p,i} = 0 \quad \alpha_p \approx n_p \frac{\pi d_p^3}{6}
\]

Particle mesoscopic velocity equation:
\[
\frac{\partial}{\partial t} n_p u_{p,i} + \frac{\partial}{\partial x_j} n_p u_{p,i} u_{p,j} = n_p g_i - \frac{n_p}{\bar{\tau}_p} \left[ u_{p,i} - u_{f,i} \right] - \frac{\partial}{\partial x_j} n_p \delta\sigma_{p,ij}
\]

In dilute flows, \(\delta\sigma_{p,ij}\) represents the kinetic stress due to “microscopic” particle random motion (granular temperature):

\[
\delta\sigma_{p,ij} = < \delta u_{p,i} \delta u_{p,j} | H_f >_p
\]

Particle random kinetic energy equation:
\[
\frac{\partial}{\partial t} n_p \delta\theta_p + \frac{\partial}{\partial x_i} n_p u_{p,i} \delta\theta_p = -\frac{n_p}{\bar{\tau}_p} \delta\theta_p - n_p \delta\sigma_{p,ij} \frac{\partial u_{p,i}}{\partial x_j} - \frac{\partial}{\partial x_j} n_p Q_{p,ij} - n_p \delta\varepsilon_p
\]
**Particle Euler LES equation derivation**

Favre spatial filtering

\[
\bar{n}_p(x,t) = \int G_\Delta(y - x) n_p(y,t) dy
\]

\[
\bar{u}_p(x,t) = \frac{1}{\bar{n}_p(x,t)} \int G_\Delta(y - x) n_p(y,t) u_p(x,t) dy
\]

Particle filtered number density equation :

\[
\frac{\partial}{\partial t} \bar{n}_p + \frac{\partial}{\partial x_i} \bar{n}_p \bar{u}_{p,i} = 0
\]

Particle filtered mesoscopic velocity equation :

\[
\frac{\partial}{\partial t} \bar{n}_p \bar{u}_{p,i} + \frac{\partial}{\partial x_j} \bar{n}_p \bar{u}_{p,i} \bar{u}_{p,j} = \bar{n}_p g_i - \bar{n}_p \frac{\tau_p}{\bar{u}_{p,i} - \bar{u}_{f \otimes p,i}} \frac{\partial}{\partial x_j} \bar{n}_p \bar{\sigma}_{p,ij} - \frac{\partial}{\partial x_j} \bar{n}_p \bar{\tau}_{p,ij}
\]
Particle subgrid closure problems

Particle filtered mesoscopic velocity equation:

\[
\frac{\partial}{\partial t} \bar{n}_p \bar{u}_{p,i} + \frac{\partial}{\partial x_j} \bar{n}_p \bar{u}_{p,i} \bar{u}_{p,j} = -\bar{n}_p g_i \frac{\partial}{\partial x_j} \left( \bar{u}_{p,i} - \bar{u}_{f@p,i} \right) - \frac{\partial}{\partial x_j} \bar{n}_p \delta \sigma_{p,ij} - \frac{\partial}{\partial x_j} \bar{n}_p \tau_{p,ij}
\]

I \rightarrow Modeling of the subgrid drag effect due to the correlation between the local particle distribution and the subgrid fluid turbulence

\[
\bar{u}_{f@p}(\mathbf{x},t) = \frac{1}{\bar{n}_p(\mathbf{x},t)} \int G_\Delta(\mathbf{y} - \mathbf{x}) n_p(\mathbf{y},t) \mathbf{u}_f(\mathbf{x},t) d\mathbf{y} \quad \bar{u}_{f@p}(\mathbf{x},t) \neq \bar{u}_f(\mathbf{x},t)
\]

II \rightarrow Modeling of the filtered particle kinetic (or collisional) stress in terms of computed variables (transport equation for the filtered particle random kinetic energy)

III \rightarrow Modeling of the particle subgrid (normal and shear) stress (closures developed by analogy with compressible single phase flow LES models)

\[
n_p \tau_{p,ij} = n_p u_{p,i} u_{p,j} - \bar{n}_p \bar{u}_{p,i} \bar{u}_{p,j}
\]
Particle subgrid stress modeling

- Compressible gaseous turbulence subgrid stress models
  - Fluid subgrid stress:
  - Viscosity model:

  \[
  T_{f,ij} = \bar{\rho}(u_{f,i}u_{f,j} - u_{f,i}u_{f,j})
  \]

  \[
  T_{f,ij} = P_{SGS} \delta_{ij} - \nu_{SGS} S_{f,ij}^*
  \]

  \[
  S_{f,ij} = \frac{1}{2} \left( \frac{\partial u_{f,i}}{\partial x_j} + \frac{\partial u_{f,j}}{\partial x_i} \right)
  \]

  \[
  S_{f,ij}^* = S_{f,ij} - \frac{1}{3} S_{f,kk} \delta_{ij}
  \]

  \[
  P_{SGS} = 2C_1 \bar{\rho}_f \Delta_f^2 |S_f|^2
  \]

  \[
  \nu_{SGS} = 2C_s \bar{\rho}_f \Delta_f^2 |S_f|
  \]

  (Moin et al, 1991)

  \[
  C_1 \text{ and } C_s \text{ are dynamically evaluated}
  \]

  \[
  C_1 \in [0.0025-0.009] \text{ and } C_s \in [0.008-0.014]
  \]
**Particle subgrid stress modeling**

A priori testing of particle sub-grid stress models in DNS+DPS HIT

\[ \varepsilon_{SGS}^{I} \]
- DNS+DPS
- Viscosity
- Mixed

\[ \varepsilon_{SGS}^{II} \]
- DNS+DPS
- Viscosity
- Mixed

---

**Cases:**

<table>
<thead>
<tr>
<th>Cases</th>
<th>A</th>
<th>B</th>
<th>C</th>
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<tbody>
<tr>
<td>( \text{Re}_t )</td>
<td>6,6</td>
<td>40</td>
<td>40</td>
</tr>
<tr>
<td>( \text{St} )</td>
<td>1.1</td>
<td>1.1</td>
<td>0.47</td>
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</table>

**Constants:**

<table>
<thead>
<tr>
<th></th>
<th>( C_S )</th>
<th>( C_r )</th>
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</thead>
<tbody>
<tr>
<td>Viscosity</td>
<td>0.02</td>
<td>0.012</td>
</tr>
<tr>
<td>Mixed</td>
<td>0.0085</td>
<td>0.0033</td>
</tr>
</tbody>
</table>
AVBP code main characteristics

- Started in 1993
- Compressible reactive NS equations
- Large Eddy Simulation approach
- Explicit in time
- Unstructured/hybrid meshes
- Centred schemes:
  - Finite Volume/Finite Element (2\textsuperscript{nd}/3\textsuperscript{rd} order)
- (Dynamic)Smagorinsky/Wale SGS models
- NSCBC + Law-of-the-walls
- Reduced & tabulated chemistry (by EM2C)
- Thickened Flame model (TFLES)
- Euler-Lagrange and Euler-Euler approaches
- Massively Parallel

- Co-developed by CERFACS and IFPEN
- Used by many labs in France and Europe
- Industrial version used by SAFRAN, ANSALDO,…
We thank 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, as well as GENCI and CINES for their computational support.
### MERCATO combustion chamber – non reacting case
(test-rig located at ONERA Fauga Mauzac)

Collaboration with:
- ONERA (DMAE)
- Stanford University
- TURBOMECA

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Sanjósé et al. 2011

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<table>
<thead>
<tr>
<th>Case</th>
<th>Pressure</th>
<th>Air temperature</th>
<th>Liquid temperature</th>
<th>Air massflow rate</th>
<th>Fuel massflow rate</th>
<th>Equivalence ratio</th>
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<tbody>
<tr>
<td>Gaseous flow</td>
<td>1 atm</td>
<td>463 K</td>
<td>-</td>
<td>15.</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Two-phase flow</td>
<td>1 atm</td>
<td>463 K</td>
<td>300K</td>
<td>15.</td>
<td>1.</td>
<td>1.</td>
</tr>
</tbody>
</table>

Comparison between Euler-Lagrange and Euler-Euler Simulations
MERCATO – Gas flow topology

[Diagram showing gas flow topology with labels for CRZ, ensemble rotation, high strain rate zone, trace of PVC, interactions, and Q criteria. Dimensions indicated: 6mm, 26mm, 56mm, 86mm, 116mm.]
MERCATO – Gas mean axial velocity

Radial distance (mm)

6 mm  26 mm  56 mm  86 mm  116 mm

$w_{\text{gas, moy.}} \text{ [m/s]}$

- CDP
- AVBP
- LDA
MERCATO – Gas RMS axial velocity

Radial distance (mm)

$w_{gaz, \text{rms}} [\text{m/s}]$

- CDP
- AVBP
- LDA
MERCATO – Qualitative EE/EL comparison

AVBP Euler-Euler

AVBP Euler-Lagrange

Temperature Gaz (K)

Workshop on TPF combustion - EM2C
MERCATO – Quantitative EE/EL comparison

Liquid mean axial velocity

Liquid RMS axial velocity
• LES of two-phase reacting flows in complex geometries are feasible
• Numerous issues still open:
  – Injection: atomisation-dispersion-film
  – ....
  – Liquid phase introduces new flame structures which require new combustion models:
    • Non adiabatic
    • Variable equivalence ratios through the flame
    • Other combustion regimes (isolated droplets)
    • Complex chemistry
Final objective: full industrial systems

- LES of an ignition sequence in an annular chamber

- Temperature field
  - Iso-surface of reaction rate

M. Boileau (2007)

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