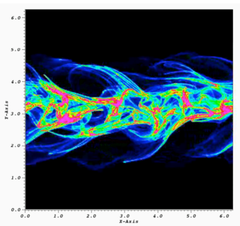
Mathematical modeling and numerical methods for HPC of multi-scale two-phase flow and combustion engineering applications



Marc Massot

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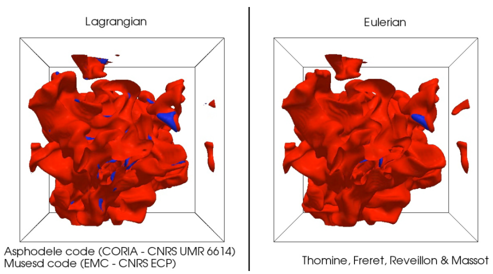
CentraleSupélec (ex- Ecole Centrale Paris)

Laboratoire EM2C - UPR CNRS 288

-



Fédération de Mathématiques

de l'Ecole Centrale Paris

FR CNRS 3487

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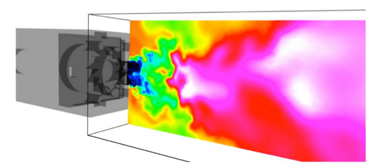
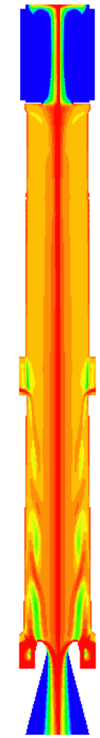
Visiting Professor

Center for Turbulence Research - Stanford University 2011-2012

-

Scientific Adviser ONERA – Palaiseau - DEFA

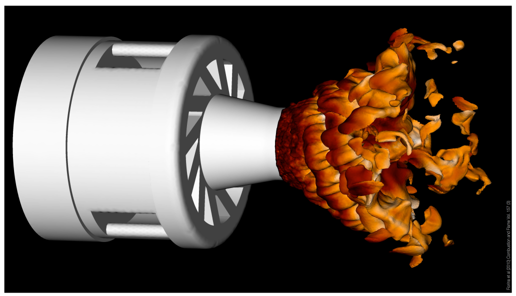




EM2C Laboratory – CentraleSupélec – Paris

Energy, Propulsion and Aerospace

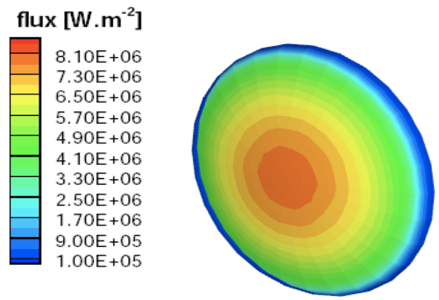
Combustion



EM2C Lab., numerical combustion

Numerical simulation of a stabilized flame in an aircraft engine combustion chamber

Heat transfer



Radiative flux at the wall heat shield for a terrestrial re-entry.

Plasmas

Stabilisation of a propane/air flame by a pulsed plasma discharge

Applied Mathematics team

Numerical analysis / Multi-scale modeling / HPC

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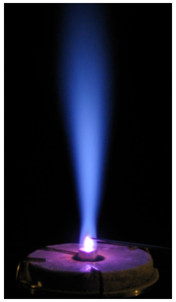
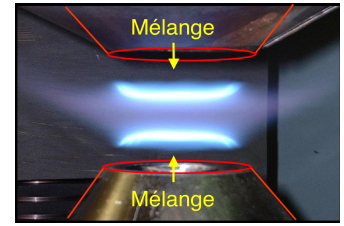
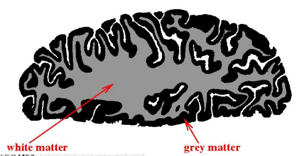
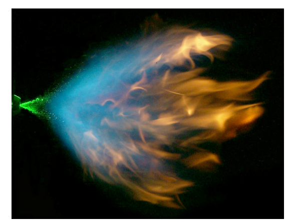


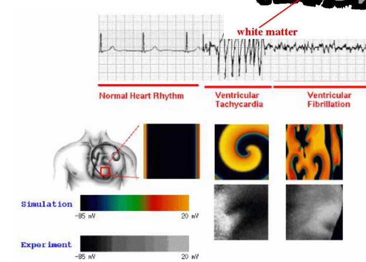
A mathematics team in an engineering laboratory



- **Four fields of applications** :
  - Flame Dynamics, homogeneous and two-phase **combustion**
  - Multi-scale reaction fronts in **Nonlinear chemical dynamics and biomedical engineering** (spiral and scroll waves, strokes, ...)
  - **Astmospheric pressure discharges** (Streamers) for flame stabilization and out of thermal and chemical equilibrium weakly ionized plasma flows for **atmospheric re-entry and solar physics**
  - Separated and disperse two-phase flows, polydisperse spray flows for **combustion chambers in automotive, aeronautic and solid propulsion applications.**

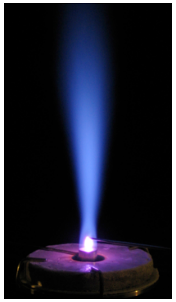






Mathematical subjects

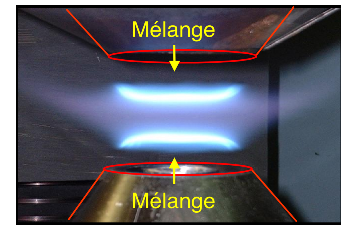
- Mathematical modeling and analysis (PDEs, dynamical systems)
- Numerical analysis, scientific computing, HPC



A mathematics team in an engineering laboratory

2015 - Creation of Université Paris-Saclay

- Part of the "Fédération de Mathématiques de l'Ecole Centrale Paris" FR CNRS 3487

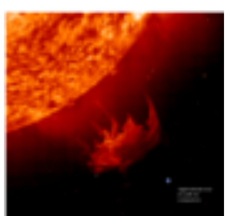


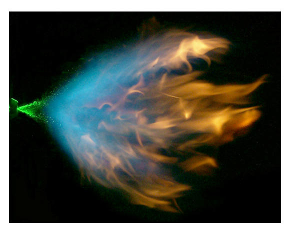
- Associate member of Fondation Mathématique Jacques Hadamard, Université Paris-Saclay

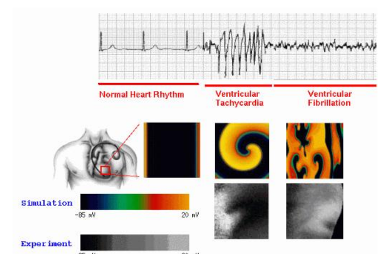
Fondation mathématique FMJH Jacques Hadamard

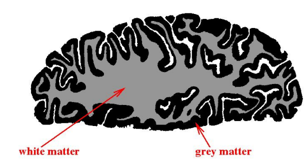
Campus Paris Saclay
FONDATION DE COOPERATION SCIENTIFIQUE

université PARIS-SACLAY









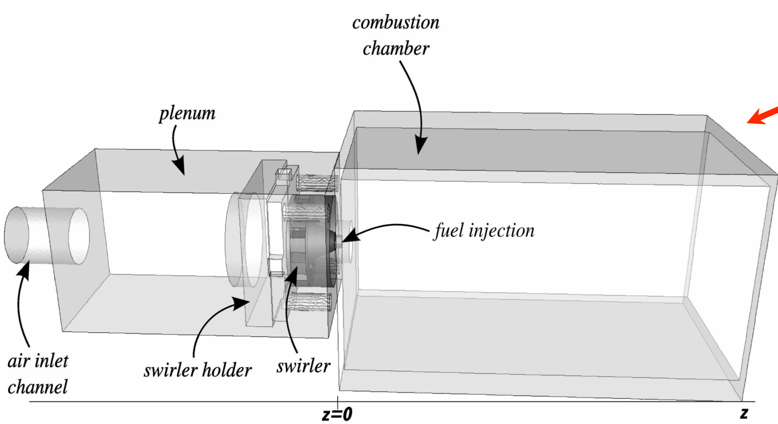
INTRODUCTION

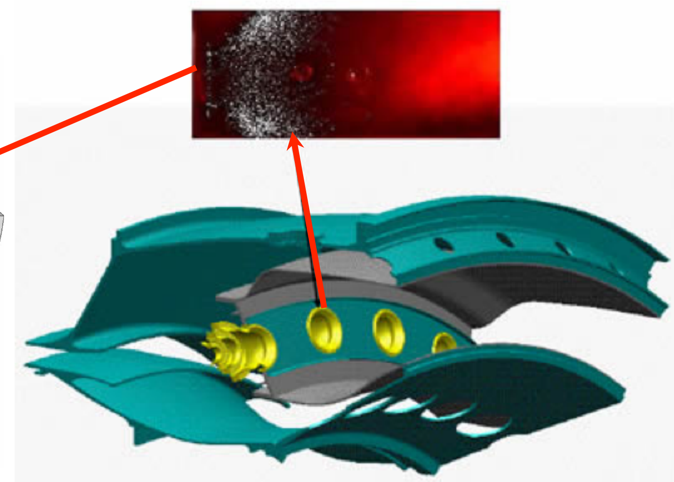
Injection of fuel in Aeronautical Engines (Source ONERA).

Annular Combustion chamber

one sector reproduced in the MERCATO Experiment

(Source Prof. Bowman, Stanford)

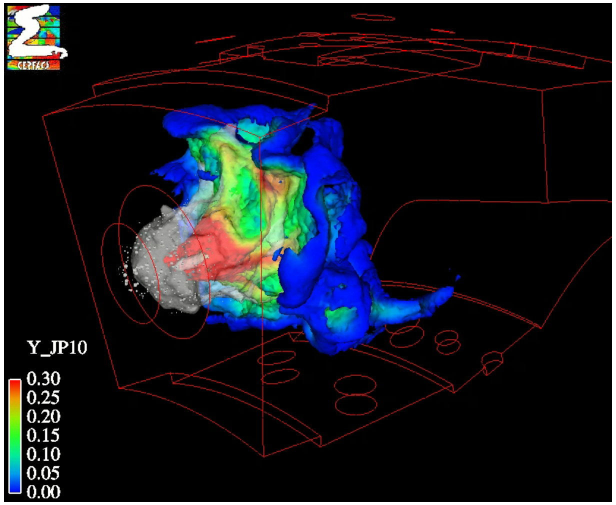




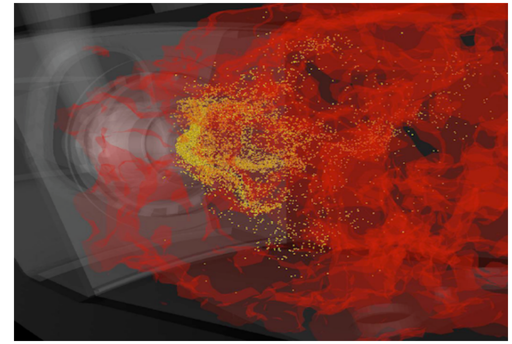
Various phenomena

- Injection
- Primary atomization
- Secondary break-up
- Turbulent dispersion
- Droplet/droplet interaction
- Droplet/wall interaction
- Evaporation
- Combustion

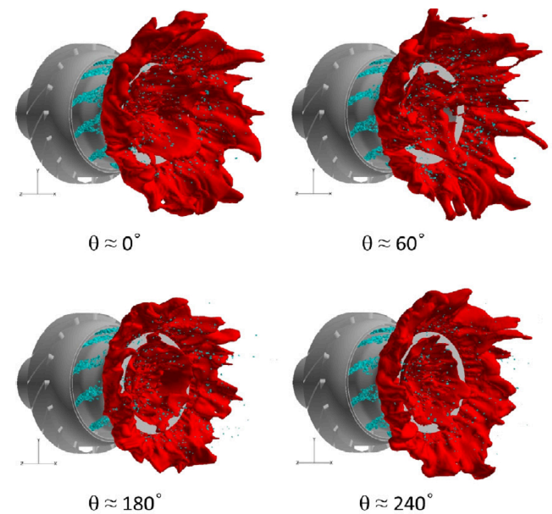
LES of Two-phase flows



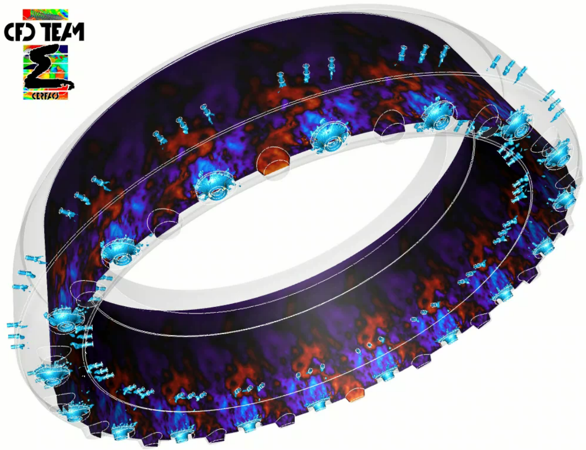
Two-phase flow LES of the steady regime of one sector of an annular aeronautical combustor, 2005, S. Pascaud , CERFACS and Turbomeca (SAFRAN group)



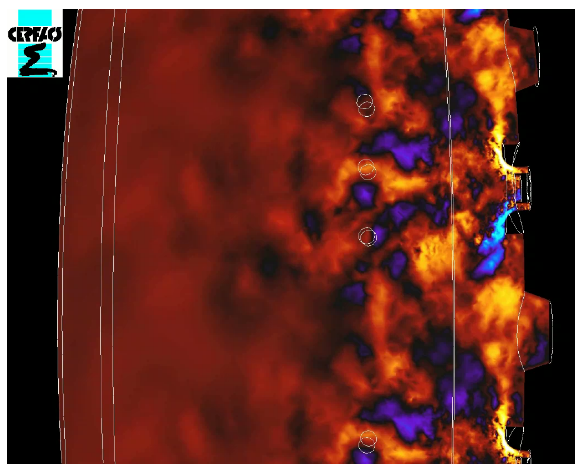
Cascade technology, Pratt & Whitney gas turbine



Tachibana et al, C&F 2015 - Time evolution of three-dimensional iso-thermal surfaces at 1500 K (in red) and main fuel droplet distributions (in light blue) – JAXA – Kyoto Univ.

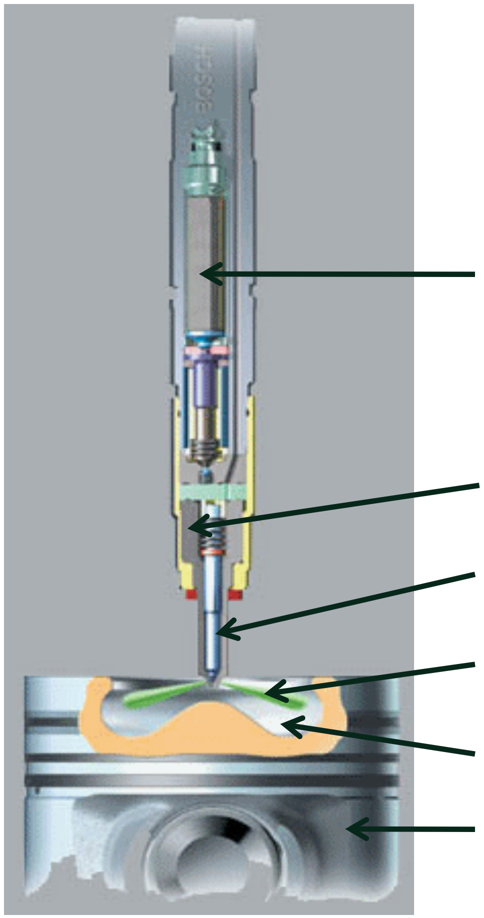


Flame front propagation in the LES of the ignition of a full helicopter combustor, 2007, M. Boileau, G. Staffelbach, CERFACS and Turbomeca (SAFRAN group)



Flame front propagation in the LES of the ignition of a full helicopter combustor, 2007, M. Boileau, CERFACS and Turbomeca (SAFRAN group)

Fuel injection



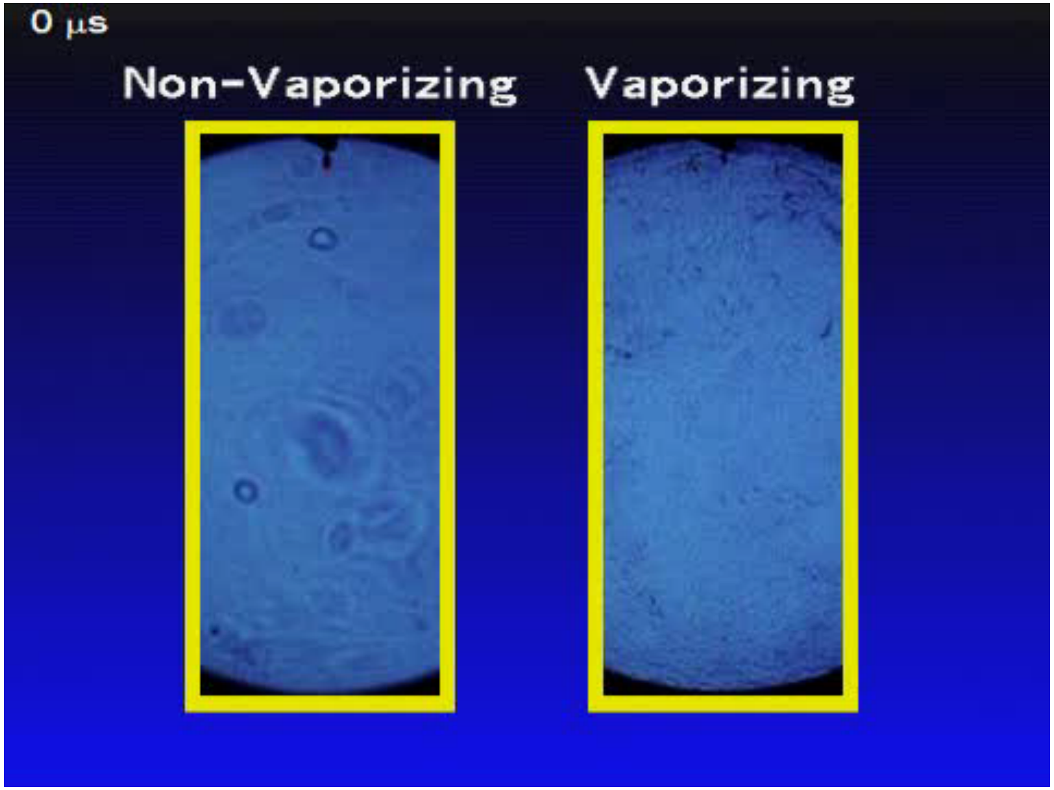
Multiphase flow involved

Fig: Dumouchel, Coria

Injection parameters

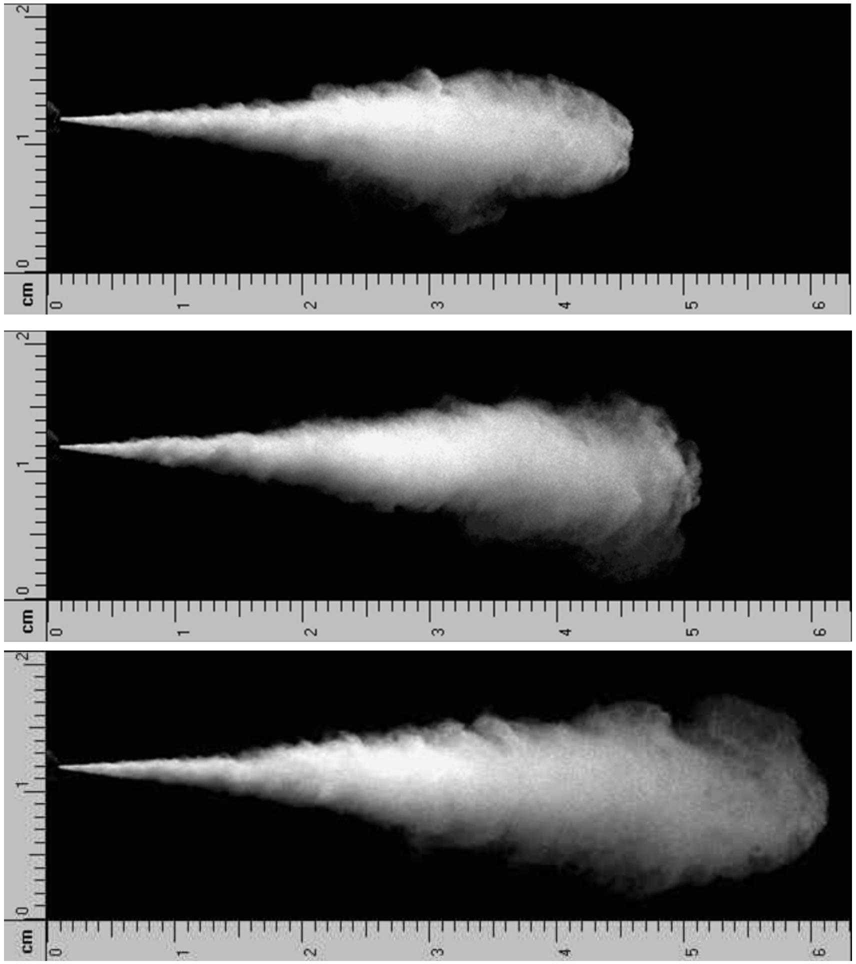
- Injection pressure: 2000 bar
- Injection velocity: 600 $m.s^{-1}$
- Injection time : 2ms

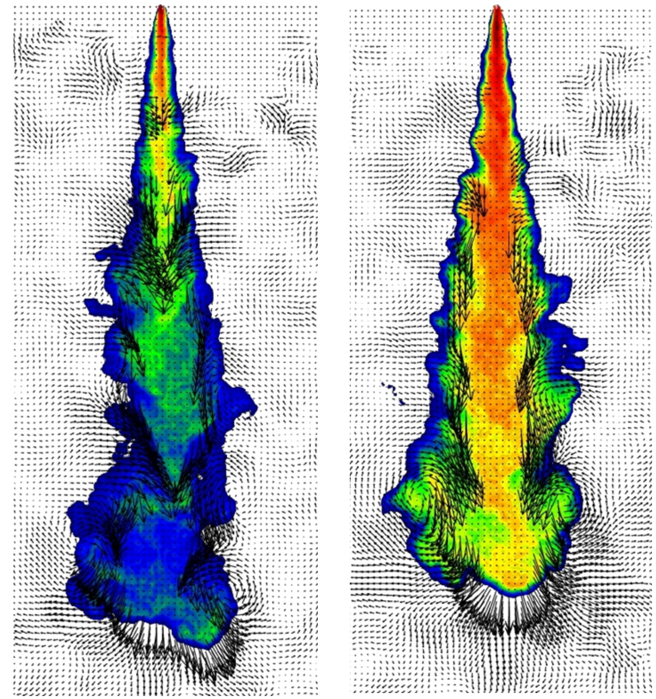
Experimental visualizations



Source : Sandia National Labs

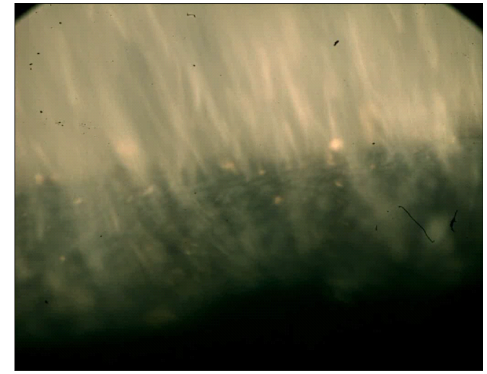
Experimental visualizations (Back light – PIV/LIEF)





Source : IFP Energies nouvelles, France

Solid propulsion for rocket boosters

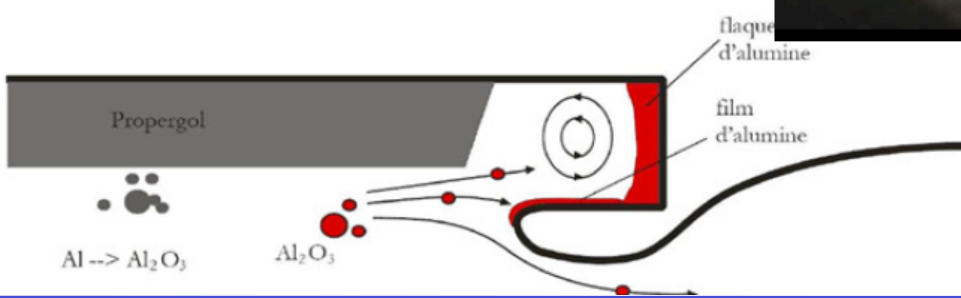


Solid Rocket Motor (boosters, missiles...) :

- Aluminum $\Rightarrow$ higher specific impulse
- Combustion $\Rightarrow$ liquid aluminum oxide (Al_2O_3)
- **Polydisperse droplets** (below 200μm)
- Interaction with flow $\Rightarrow$ performance deterioration

Issues :

- Influence on chamber **instabilities**
- Specific impulse loss in the nozzle
- Aluminum oxide slag accumulation
- Insulation erosion
- Jet signature



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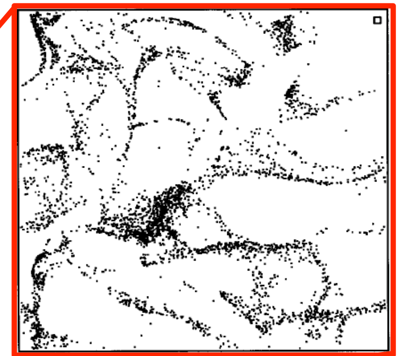
Other examples of environmental particle flows

Preferential concentration of cloud droplets by turbulence



Shaw et al. (1998)

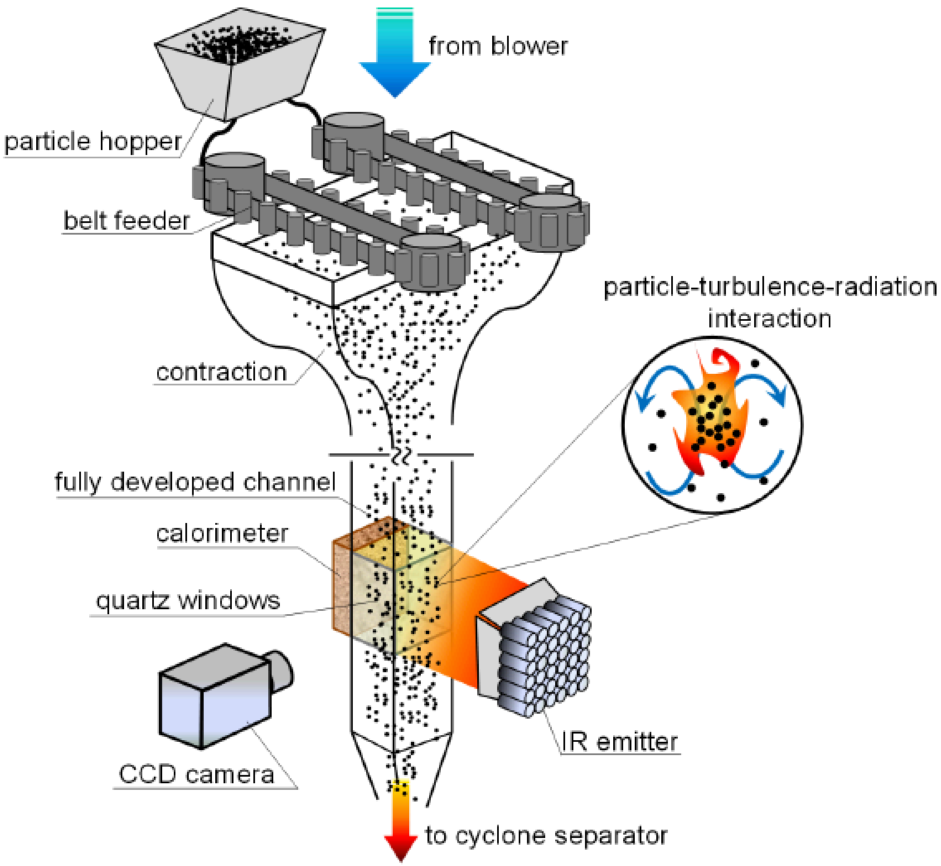
Atmospheric dispersion

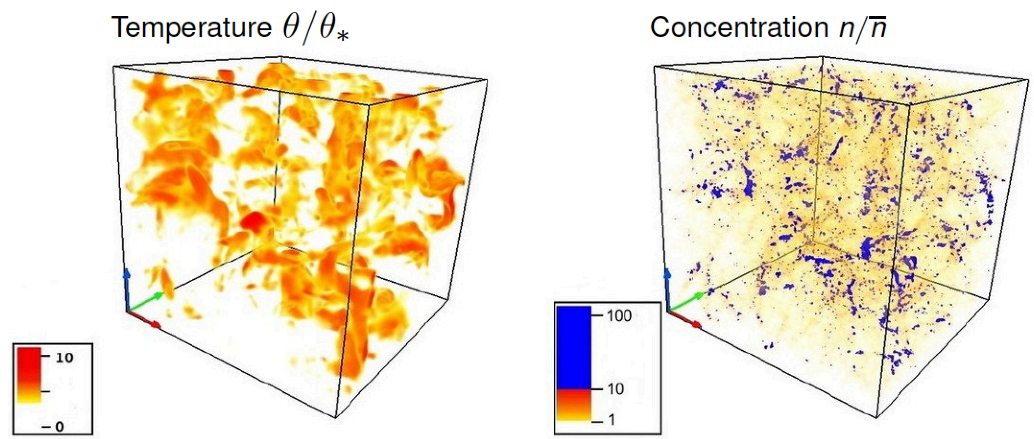
Dry avalanches

Sand dunes

Coupling of radiative heating / spray dynamics / turbulence
PSAAP2 project CTR Stanford – Solar Harvesting

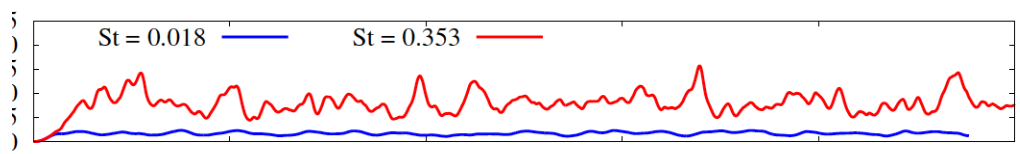
Zamansky, Coletti, Massot, Mani, PoF 2014





Large fluctuations

CLUSTERS



IN ALL THESE APPLICATIONS, WE ARE INTERESTED IN THE

POLYDISPERSE SPRAY DYNAMICS

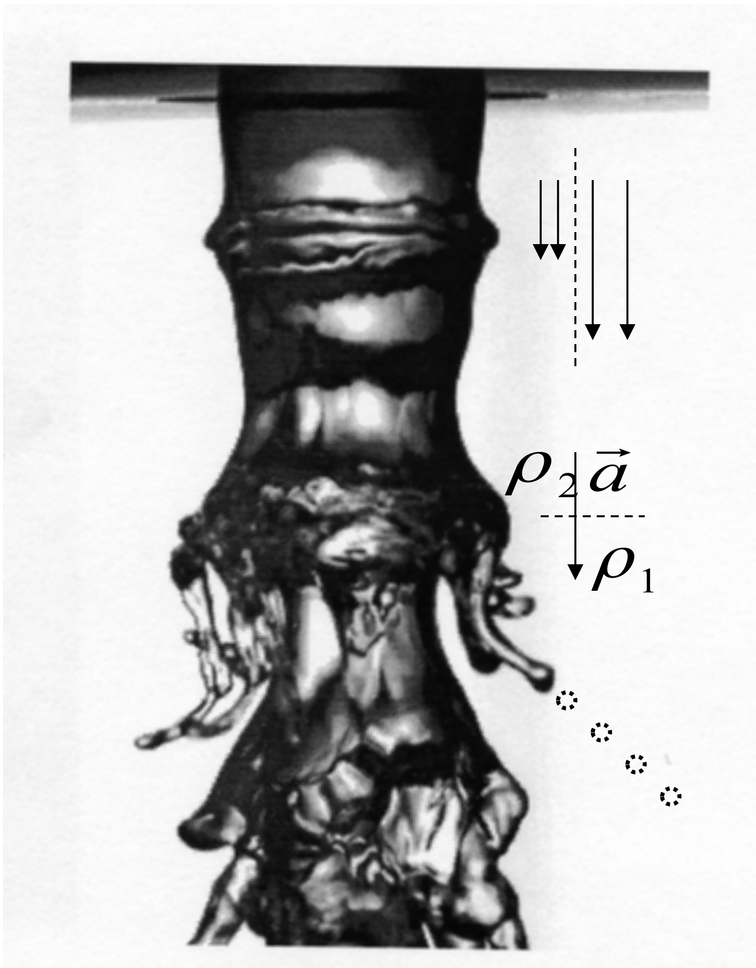
WHICH WILL GOVERN THE PHYSICS OF THE PROBLEM

COMBUSTION / INTERACTION OF ALUMINA PARTICLES WITH THE FLOW FIELD AND ACOUSTICS

Coming back to combustion chambers

Can we resolve the whole process from the injection of the liquid fuel?

Various physical phenomena and instabilities leading to primary atomization

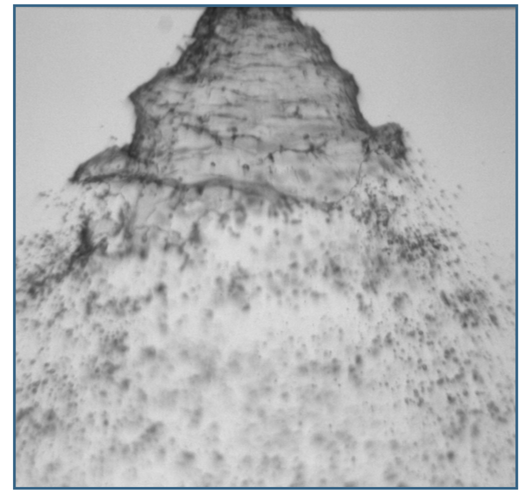


Kelvin-Helmholtz

Rayleigh-Taylor

Rayleigh-Plateau

- Pressure Swirl injector

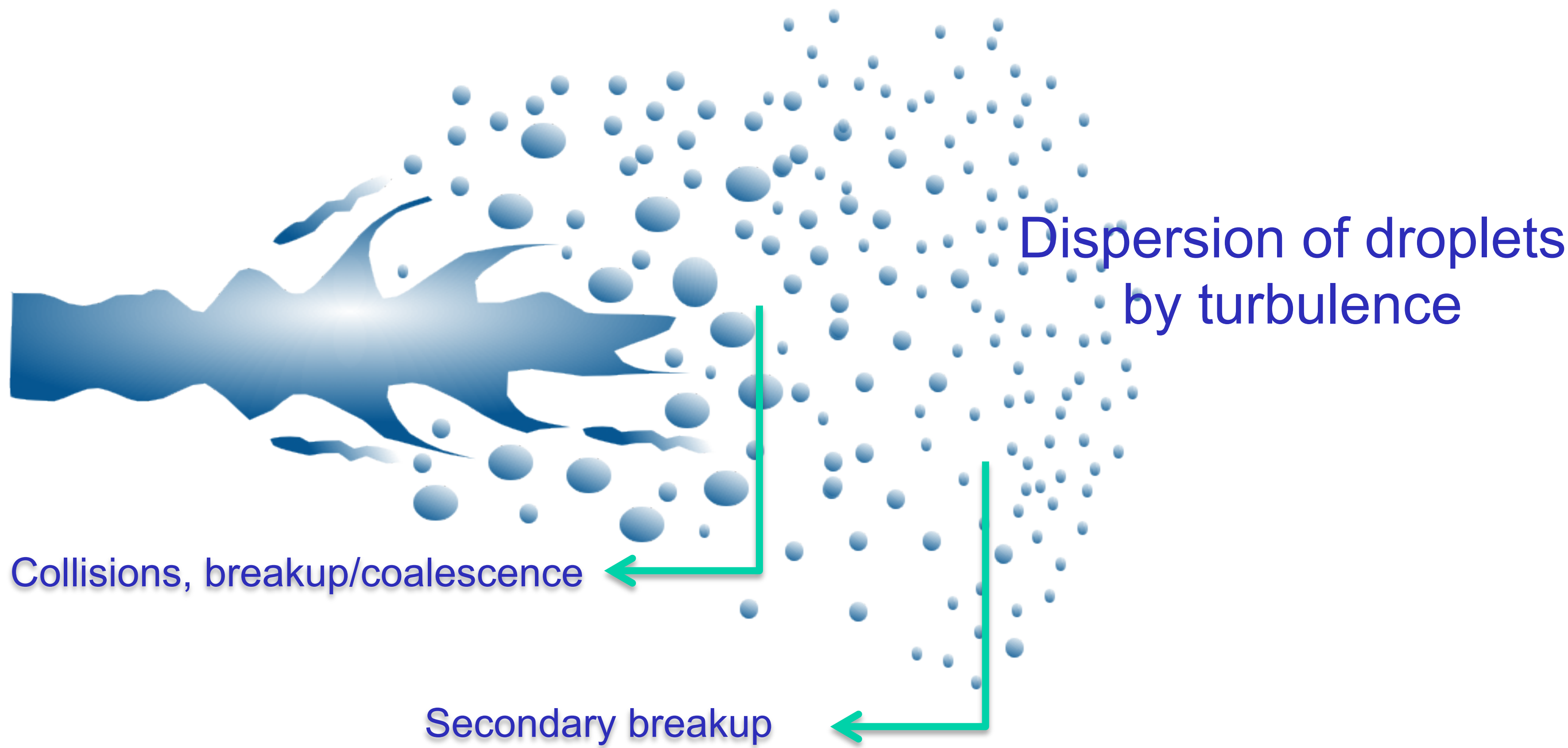


- *Lasheras, Villermaux, Hopfinger, JFM (1998)*
- *Lasheras, Hopfinger, Annual Review of Fluid Mechanics (2000)*

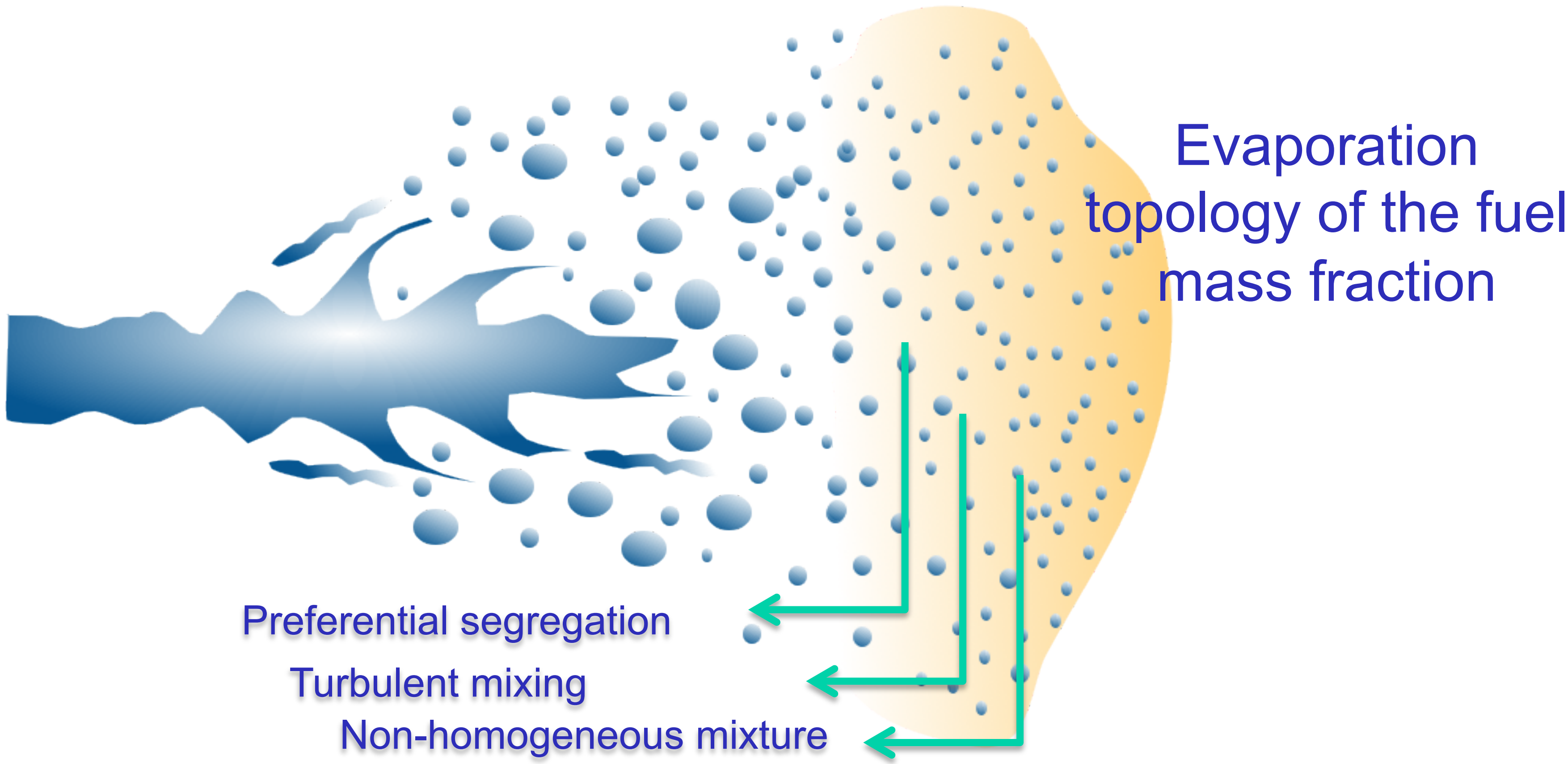
Source

- J. Reveillon (CORIA- Rouen France)

Combustion chamber



Combustion chamber



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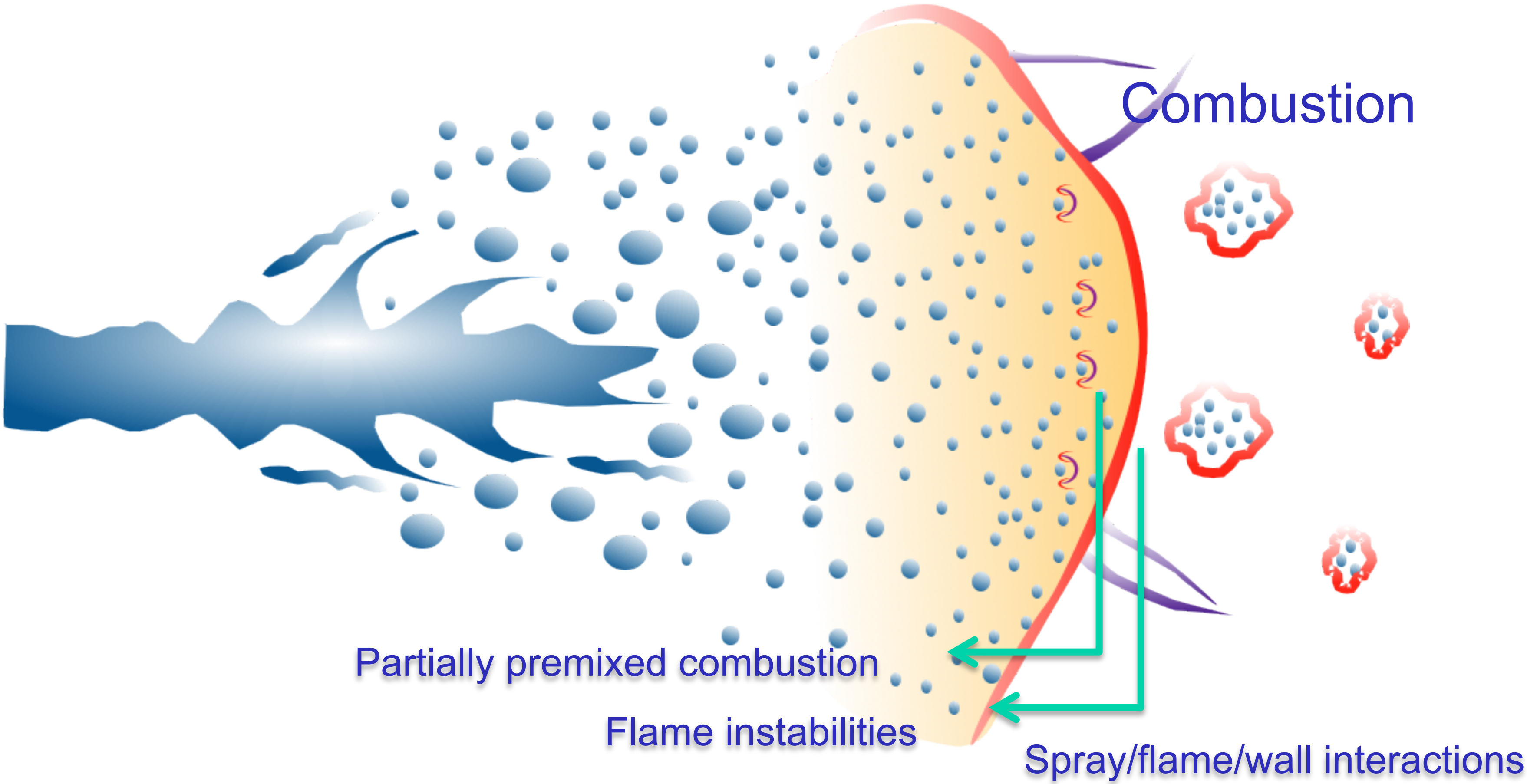
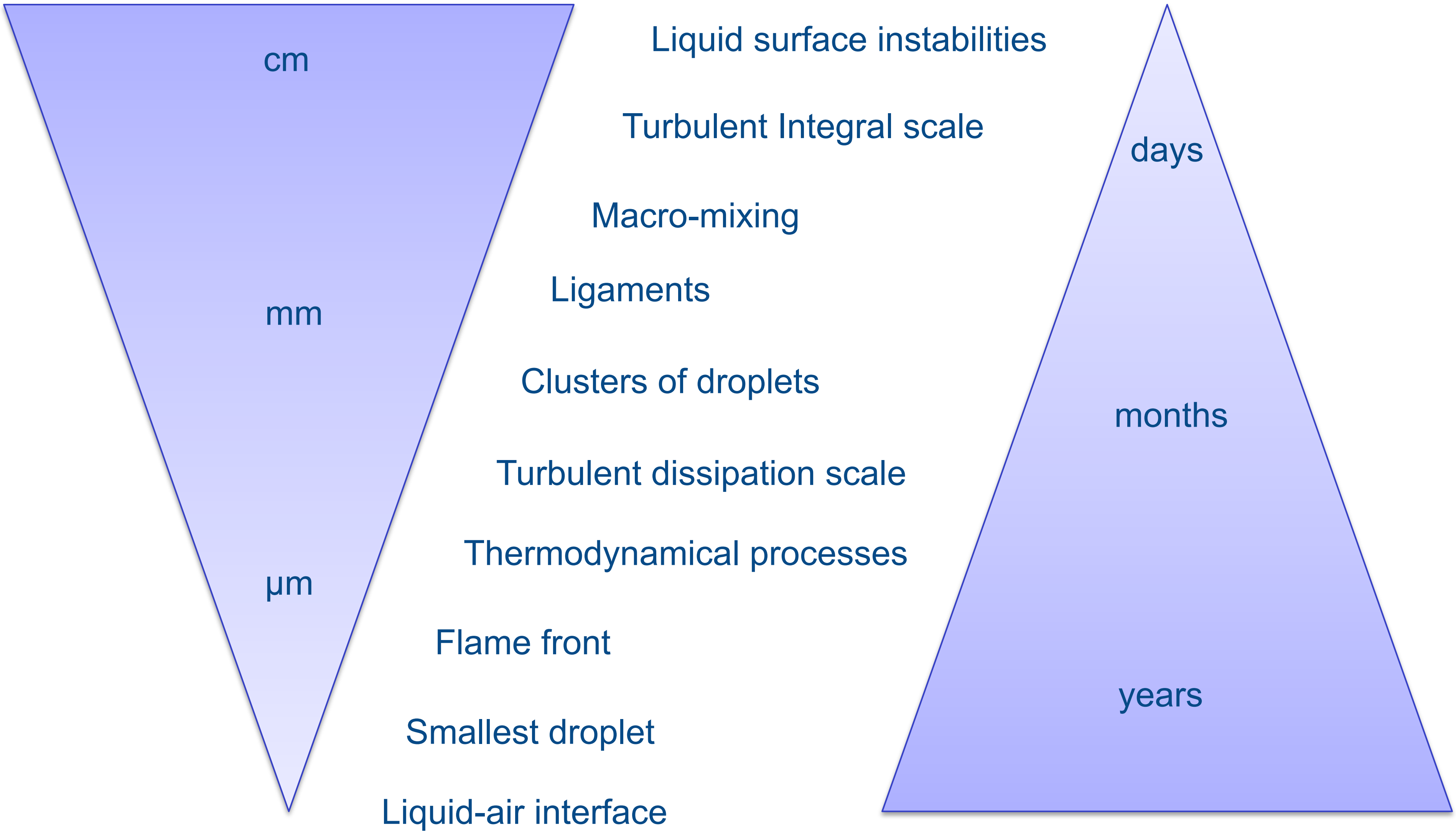
Combustion chamber

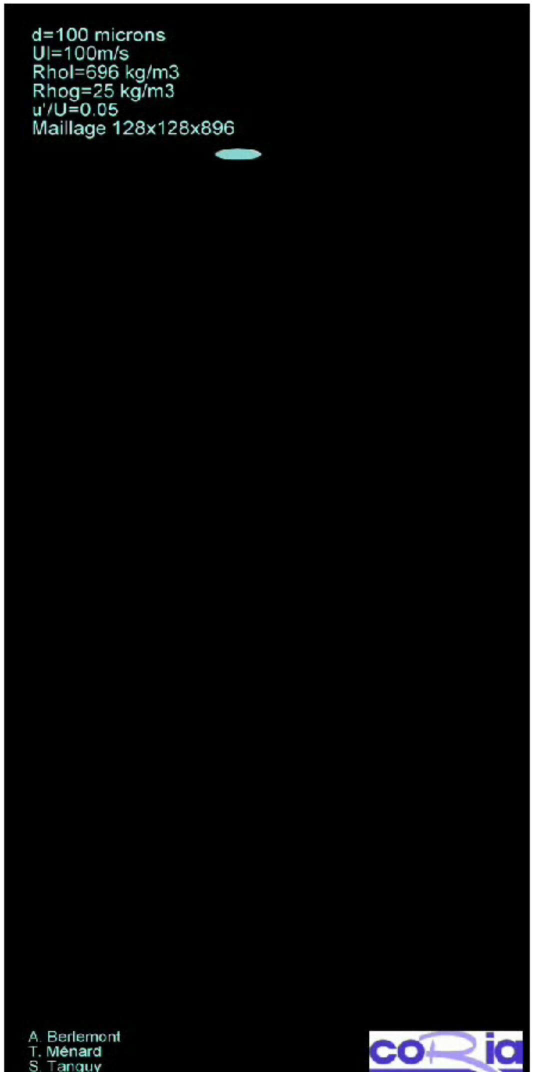


A wide range of scales

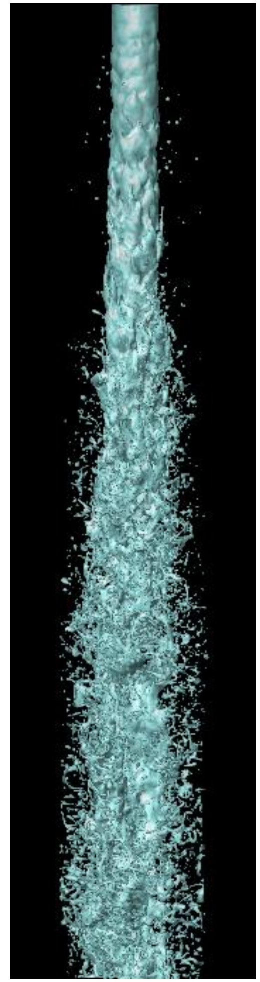


Source T. Ménard

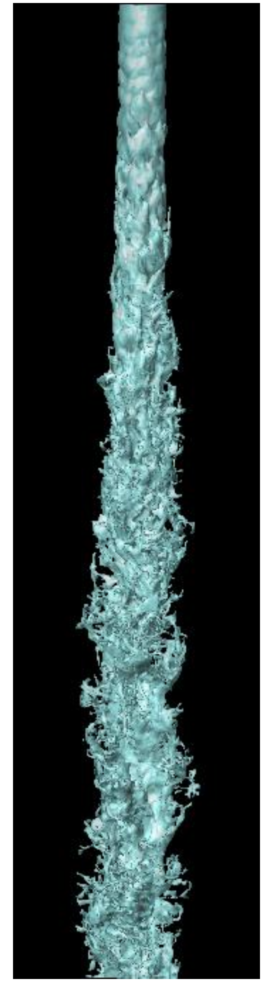
CORIA- Rouen France



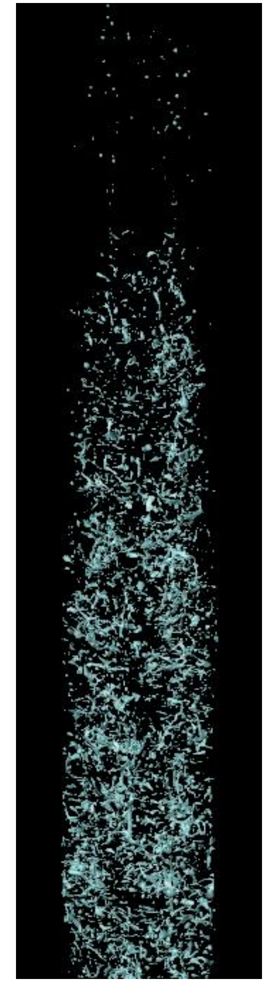
Full

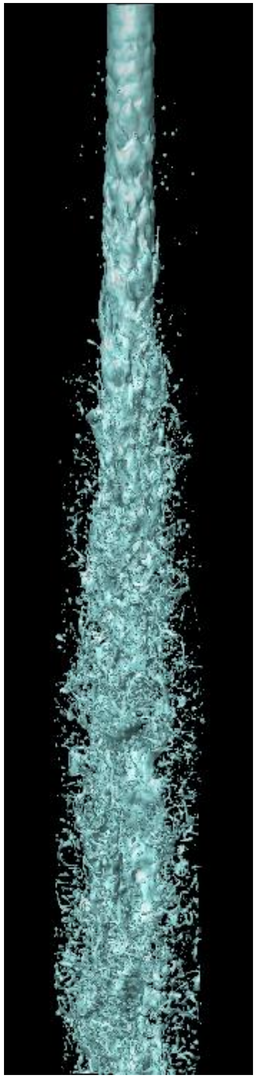


Attached



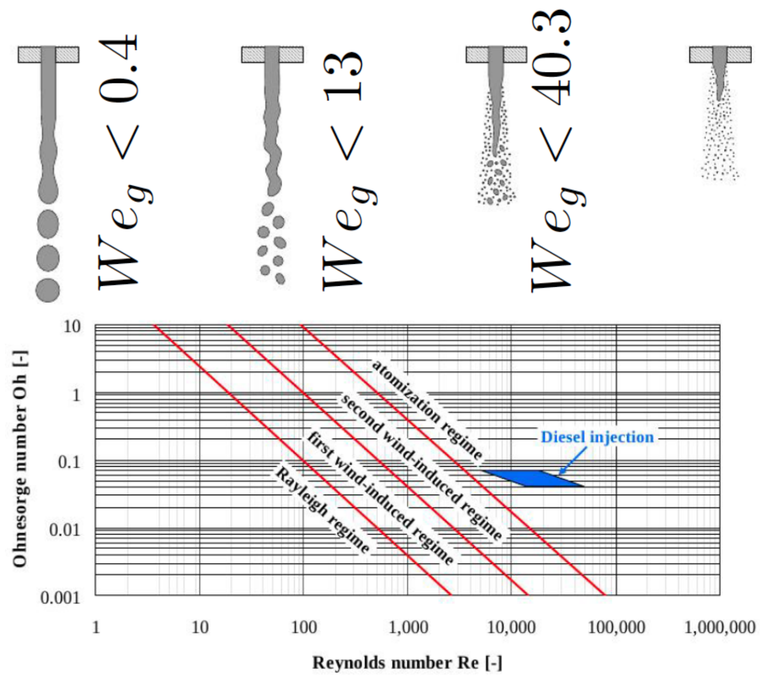
Detached



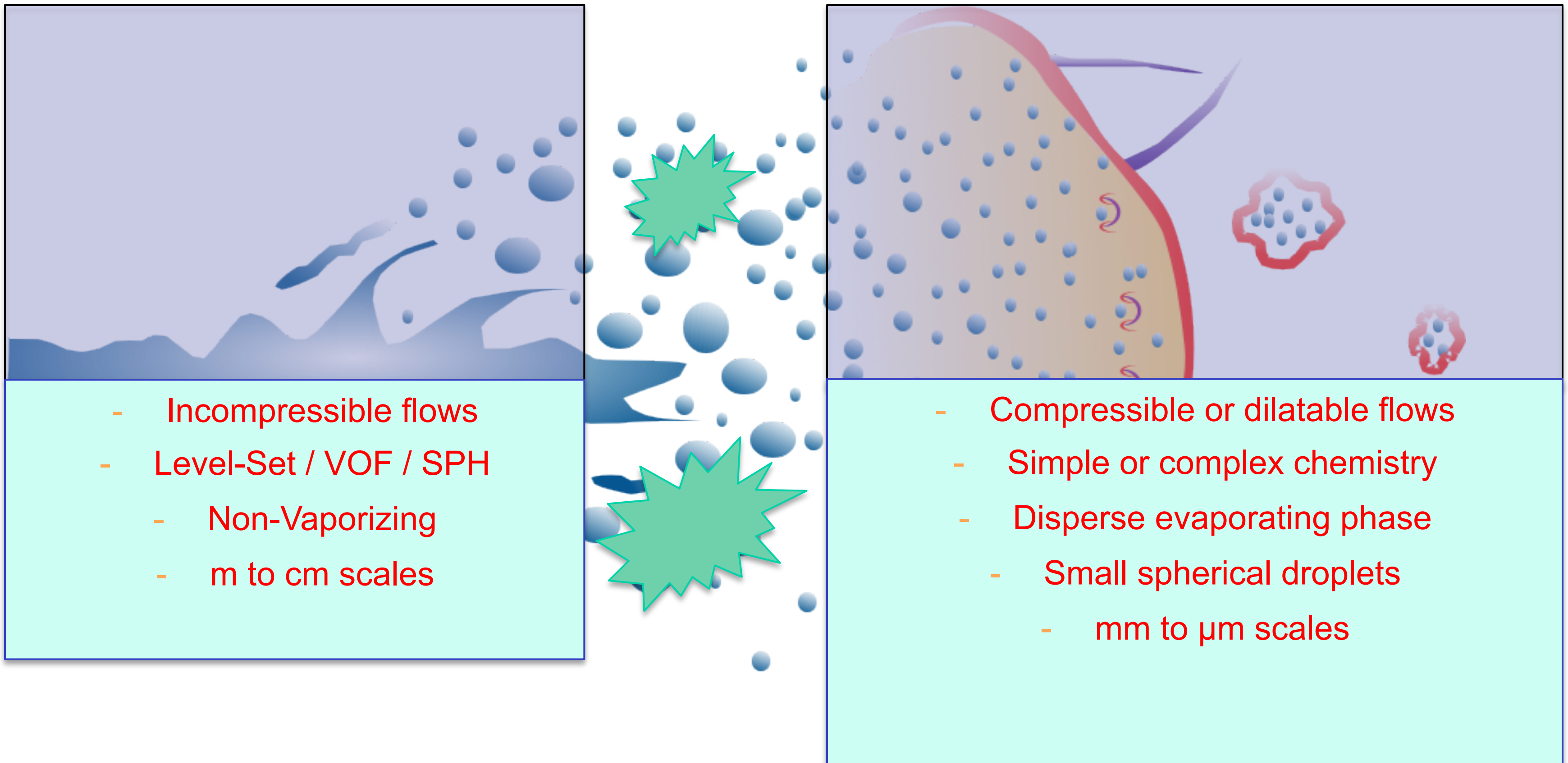


- In the region where the liquid phase occupies a volume of the same order at the one of the gas (separated phase two-phase flows), a branch of the scientific community has developed powerful and efficient solvers in order to resolve the dynamics of such interfacial flows, using incompressible Navier-Stokes Equations in both gas and liquid.

- However, the accuracy of such solvers to fully resolve the generation of the polydisperse spray obtained after primary and secondary atomization for realistic Reynolds and Weber numbers is questionable, thus limiting their range of validity in the atomization process.



No unified model treating the whole jet consistantly

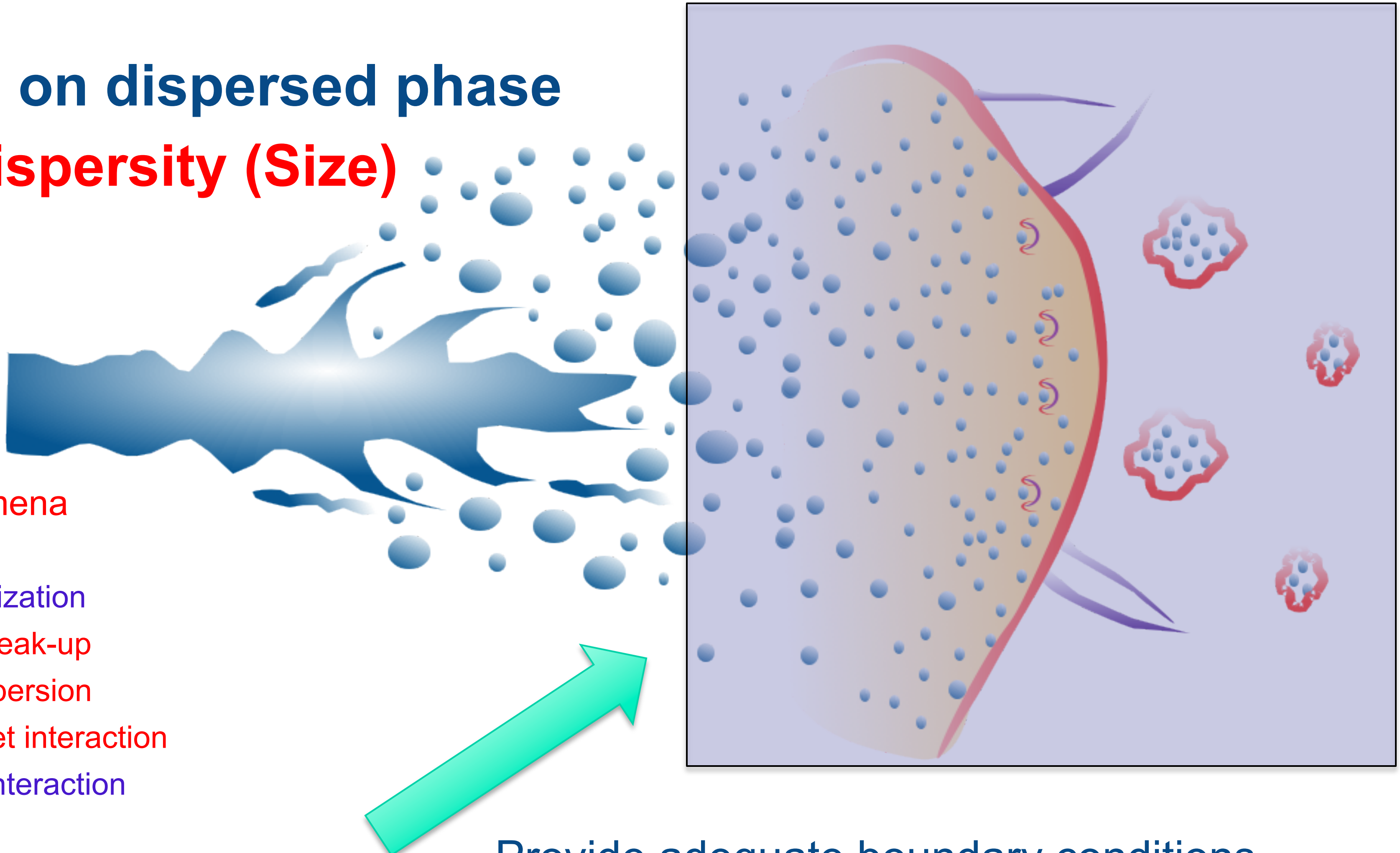


Different numerical methods, physical outcomes and communities !!!

→ Junction stumbling block – hot research topic

Focus on dispersed phase

Polydispersity (Size)



Various phenomena

- Injection
- Primary atomization
- Secondary break-up
- Turbulent dispersion
- Droplet/droplet interaction
- Droplet/wall interaction
- Evaporation
- Combustion

Provide adequate boundary conditions

New combustion chambre concepts ➡ unsteadyness

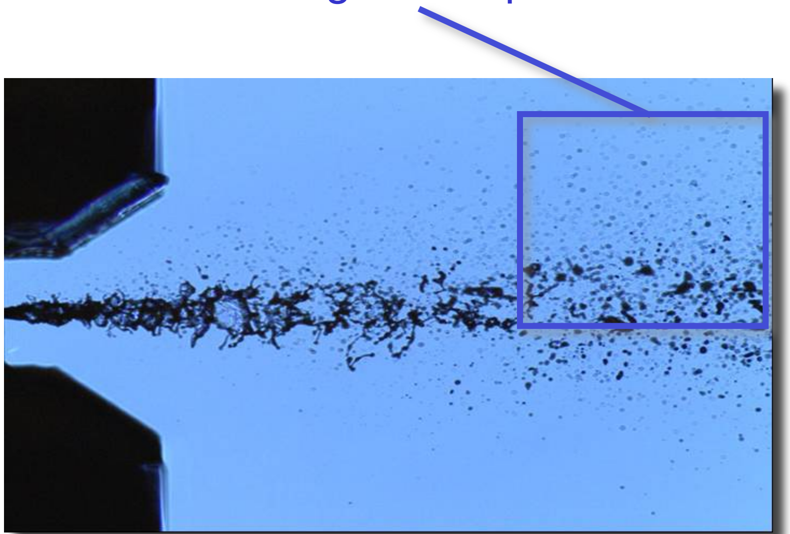
Dispersed liquid phase

+

Large size spectrum

➡

- Mixing of fuel vapor mass fraction and gaseous air
- Stabilization
- Combustion regimes



(Source C. Dumouchel, CORIA Rouen)

(Source Prof. Bowman, Stanford)

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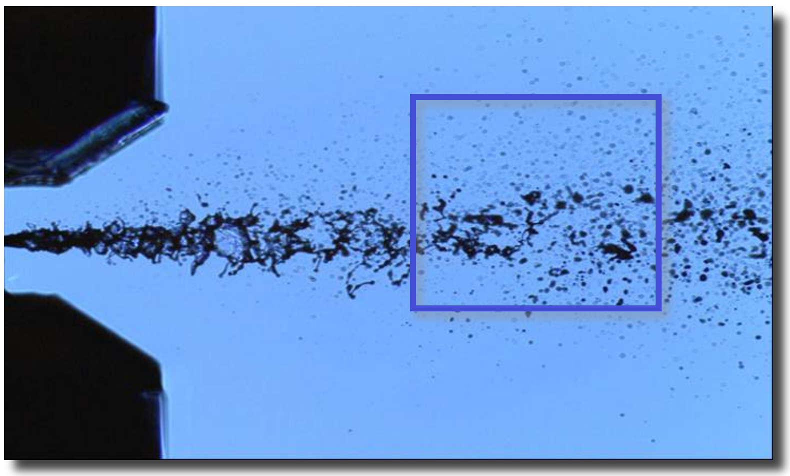
Modeling of the polydisperse spray

- **Droplet - gas interactions**
  → evaporation, drag and heat transfer
- **Droplet - droplet interactions**
  → coalescence, break-up, …

Key parameter : size



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Two existing approaches in the applications:

LAGRANGIAN approach: following droplets

- Accurate resolution of spray dynamics
- Difficulty to couple to gaseous phase equation / Grid convergence
- Hard to parallelize efficiently

Eulerian approach: system of conservation equations

- Efficient coupling with gaseous carrier phase
- High scalability and efficiency for massively parallel computing
- Modeling difficulties (closure) / singularities
- Hard to have accurate and robust numerical methods (diffusion)

Relying on rigorous mathematical modeling and kinetic theory knowledge we look for:

EULERIAN FLUID MODELING AND SIMULATION

MOMENT METHODS HIERARCHY

-

NEW MODEL AND NUMERICAL METHODS

-

EULERIAN / ROBUST / ACCURATE

HIGHLY PARALLELIZABLE

-

cope with asympotic limits !

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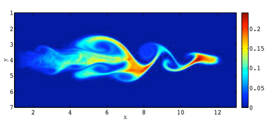
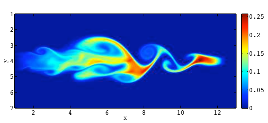
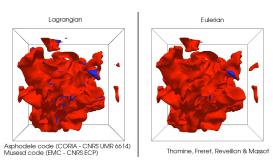
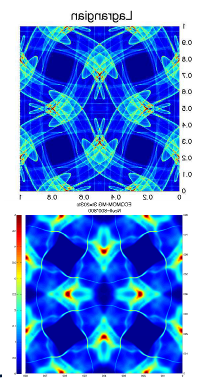
Eulerian models for the description of polydisperse sprays: from fundamental issues to industrial applications and HPC

Outline of the presentation :



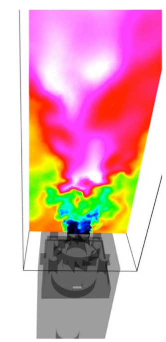


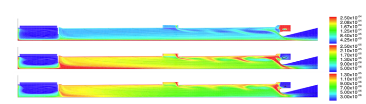




- **Introduction**
  - Application context : Aeronautical/Automotive engines / Rocket Boosters / Counter-flow flames
  - Difficulty to model and simulate the whole process – focus on polydisperse spray region
- **Multi-fluid modeling and simulation – new model and numerical methods**
  - Focus on disperse liquid phase : evaporating sprays - Context and modeling at mesoscopic level – Williams Boltzmann Equation - Fundamentals of Multi-fluid model
  - Detailed study in the config. of a free jet (MUSES 3D Euler/Euler vs. Euler/Lagrange)

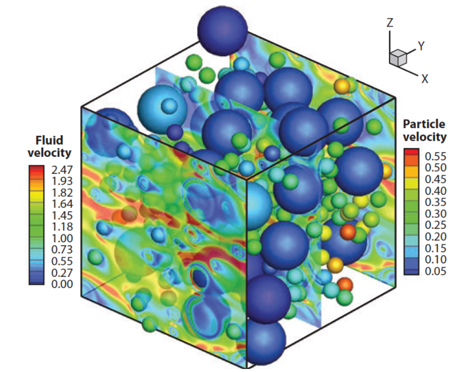
    Thesis of S. de Chaisemartin (2009)
  - Verification - detailed comparisons with Lagrangian simulations (Evap/Combustion)
- **Extensions :**
  - High order moment methods Ph.D. Theses of D. Kah, O. Emre, M. Essadki (IFPEn),
  - Droplet trajectory crossing - A. Vié (DIGITEO, Stanford), M. Sabat (SAFRAN Tech)
  - Coalescence and secondary break-up - Ph.D. F. Doisneau, A Sibra, V. Dupif (ONERA)
- **Implementation in industrial codes AVBP / IFPC3D / CEDRE**
- **Conclusions, Perspective, Validation**



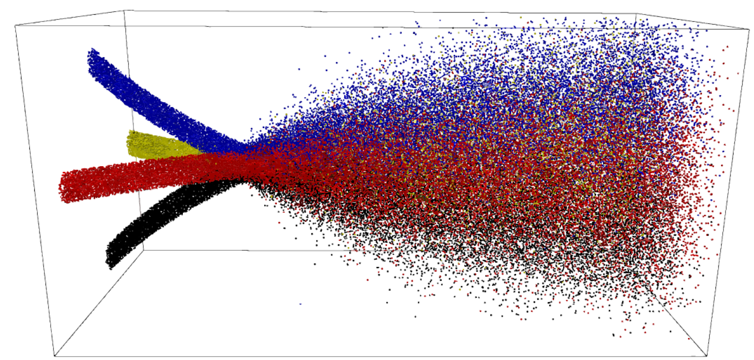


Three levels of modeling of the spray of droplets:

- Full Direct Numerical Simulation of each droplet/particle with its interface evolution for liquid droplets



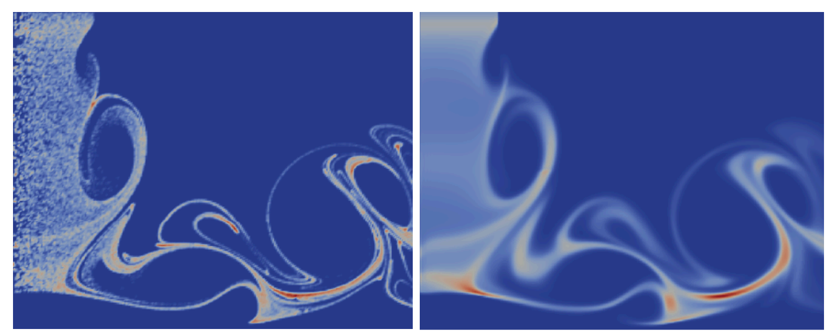
- Discrete Particle Simulation – each droplet is represented by a numerical particle (collision detection due to finite size for example – Ph.D. O. Thomine)



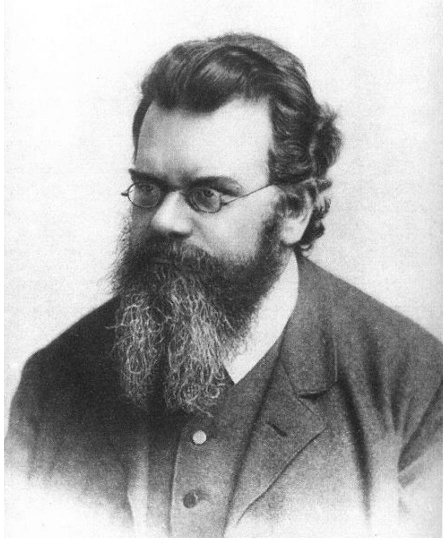
- Statistical description of a spray through an ensemble average equation in phase space (size, temp., velocity…)

POINT PARTICLES / KINETIC THEORY

Stochastic particle discretiszation / reduced deterministic – Moments methods



Modeling of the polydisperse spray



- **Droplet - gas interactions**
  $\rightarrow$ evaporation, drag and heat transfer
- **Droplet - droplet interactions**
  $\rightarrow$ coalescence, break-up, …

$f^{\phi}(t, x, \phi, \mathbf{u_l}, \mathbf{T_l})$: droplet number density (NDF)

Transport equation of Williams-Boltzmann type (Williams 1958):

$$\underbrace{\partial_t f^{\phi} + \partial_x \cdot (u_l f^{\phi})}_{\text{Free transport}} + \partial_{\phi}(R_{\phi} f^{\phi}) + \partial_{\mathbf{u_l}} \cdot (F f^{\phi}) + \partial_{\mathbf{T_l}}(E f^{\phi}) = \Gamma$$

evaporation

drag

heat transfer

coalescence and break-up integral operator

Coupled to the Navier-Stokes equations for the gas (source terms)

« kinetic model »
Phase space :
(x, size, vel.)

moments in velocity.

Semi-kinetic model
Phase space :
(x, size)

moment in size

Two-fluid dilute model

Particular discretization DSMC

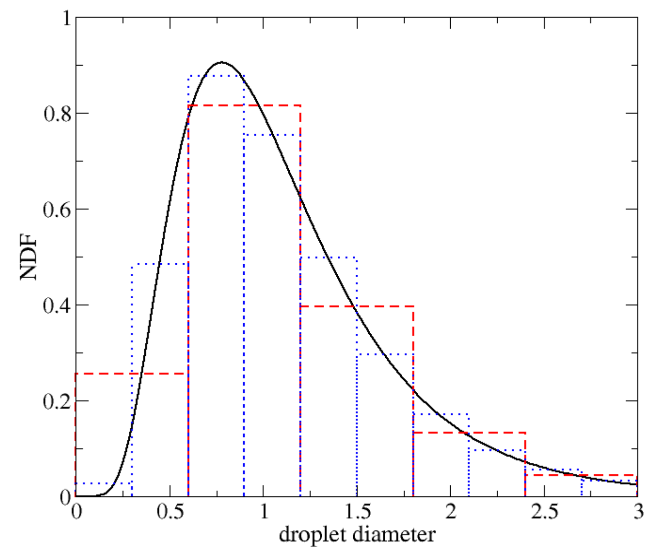
semi-discretization finite volume in size

multi-fluid « model »
Eulerian

discretization in space

discrete “model”
Lagrangian

Discrete “model”
Eulerian



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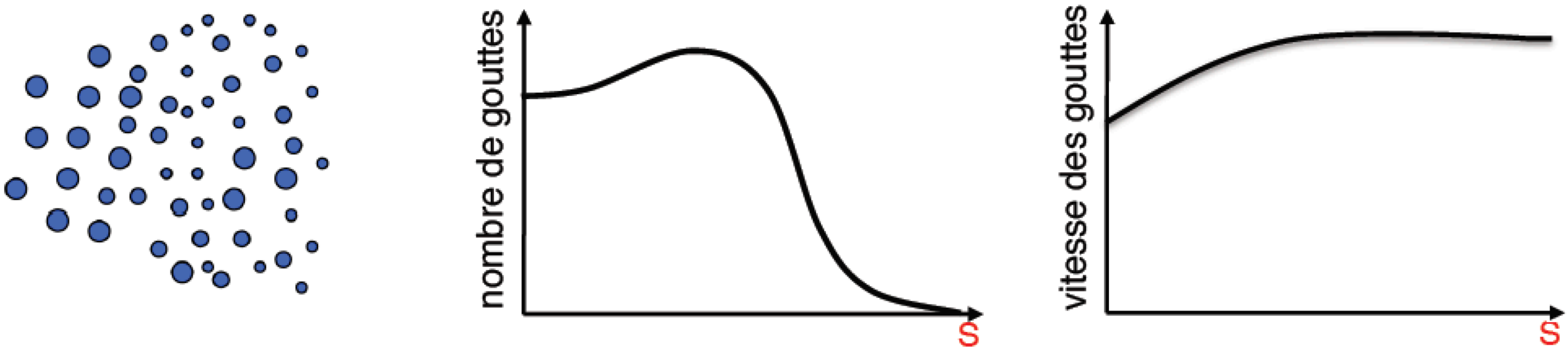
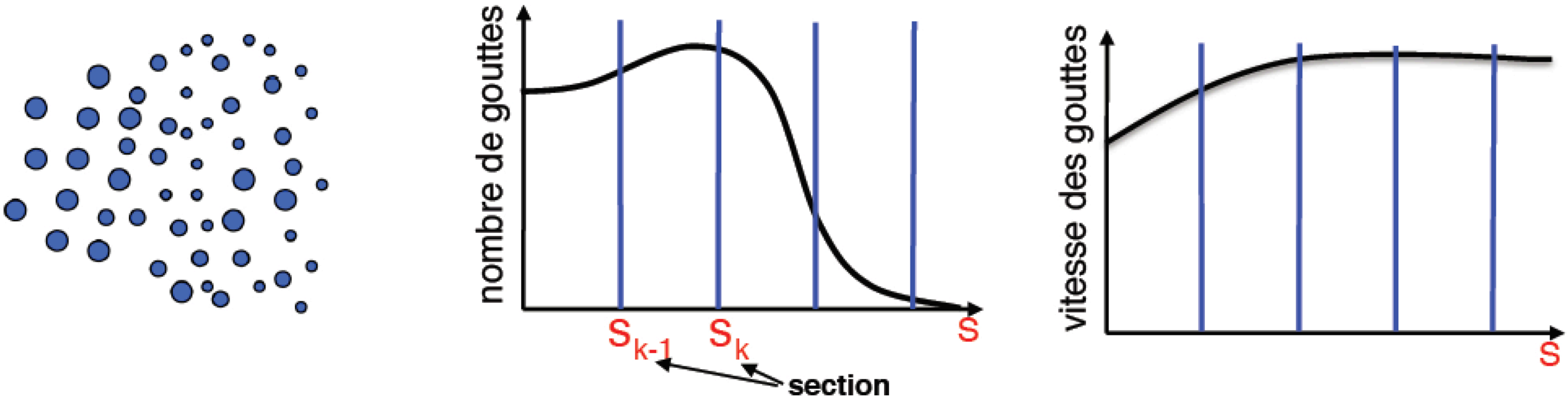


Assumption on velocity closure conditioned in size:

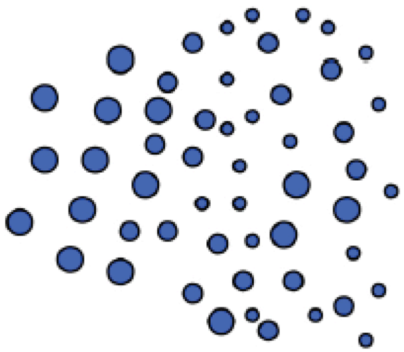
$$f(t, \boldsymbol{x}, \boldsymbol{u}, S) = n(t, \boldsymbol{x}, S)\delta(\boldsymbol{u} - \boldsymbol{u_d}(t, \boldsymbol{x}, S))$$

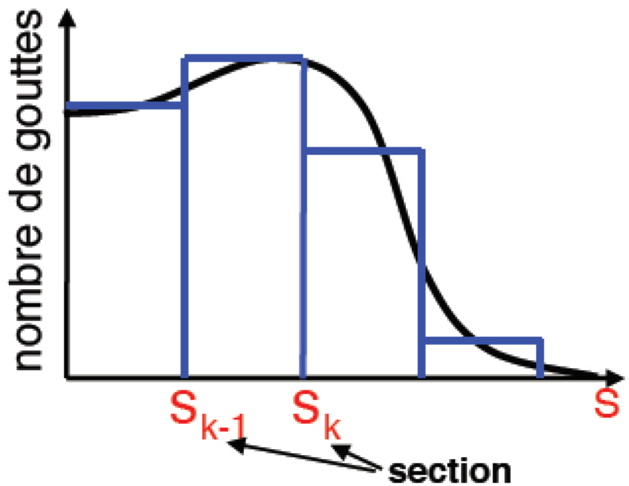


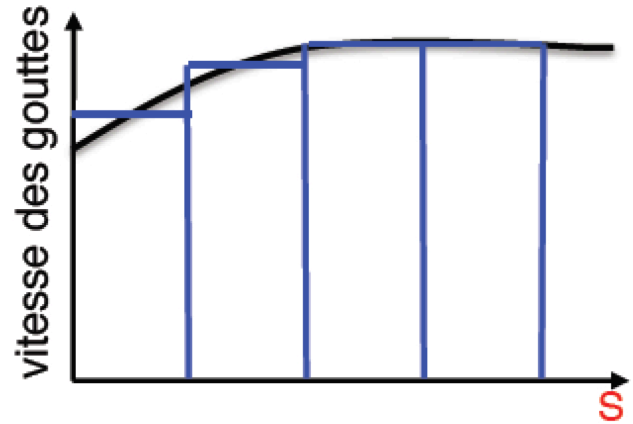
One size mass moment per section

$$m^{(j)}(t, \boldsymbol{x}) = \int_{S_{j-1}}^{S_j} S^{3/2} \int f(t, \boldsymbol{x}, \boldsymbol{u}, S)\, d\boldsymbol{u} dS$$

$$m^{(j)} u^{(j)}(t, \boldsymbol{x}) = \int_{S_{j-1}}^{S_j} S^{3/2} \int \boldsymbol{u} f(t, \boldsymbol{x}, \boldsymbol{u}, S)\, d\boldsymbol{u} dS$$







Presumed size NDF inside each section (FV):

$$n(t, \boldsymbol{x}, S) = m^{(k)}(t, \boldsymbol{x})\kappa^{(k)}(S)$$
$$\boldsymbol{u_d}(t, \boldsymbol{x}, S) = \boldsymbol{u_d}^{(k)}(t, \boldsymbol{x})$$

Eulerian Multi-fluid model - Conservation equations for "fluid" corresponding to each size interval:

$$\partial_t m^{(j)} + \partial_x \cdot (u_d^{(j)} m^{(j)}) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} + E_1^{(j+1)} m^{(j+1)}$$

$$\partial_t (m^{(j)} u_d^{(j)}) + \partial_x \cdot (m^{(j)} u_d^{(j)} \otimes u_d^{(j)}) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} u_d^{(j)} + E_1^{(j+1)} m^{(j+1)} u_d^{(j+1)} + m^{(j)} F^{(j)}$$

- **Mono-kinetic assumption at given size, location and time**
  Equivalent to Pressureless Gas Dynamics (PGD) HYPERCOMPRESSIBILITY

Eulerian Multi-fluid model - Conservation equations for "fluid" corresponding to each size interval:

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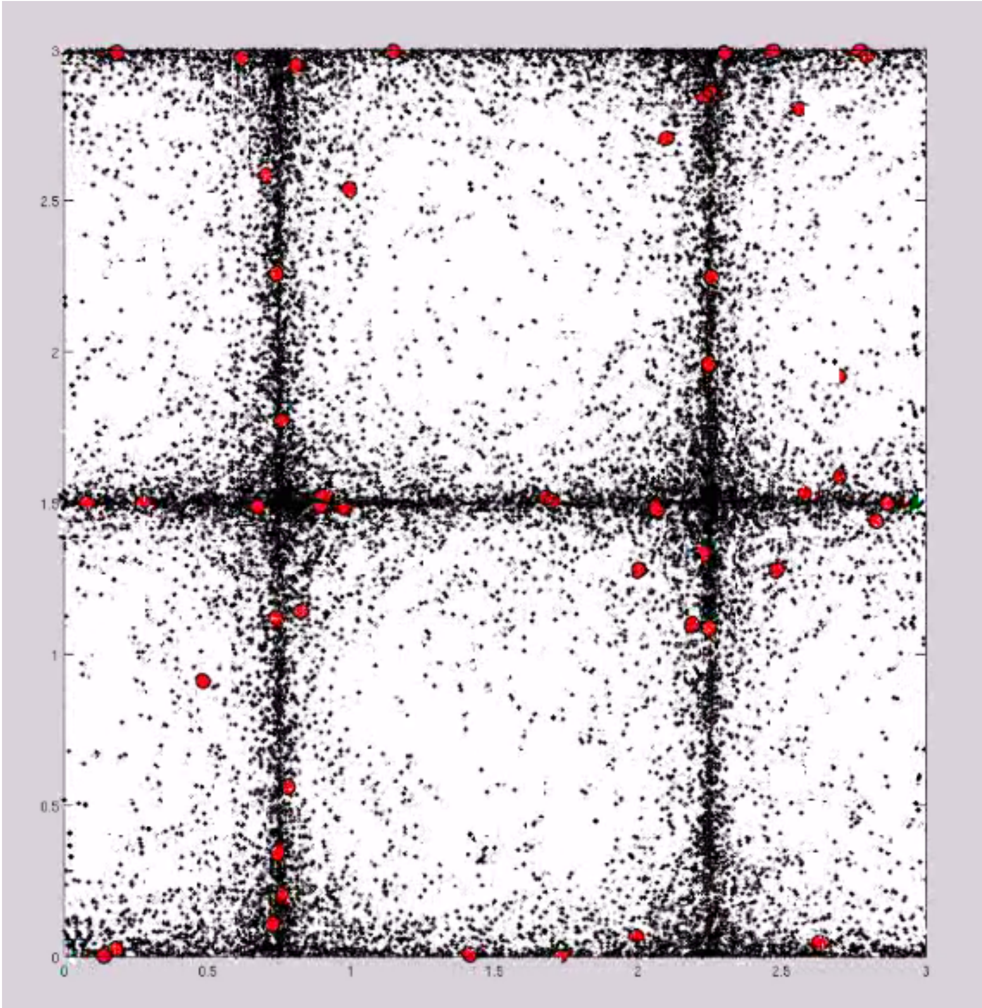
- **Mono-kinetic assumption at given size, location and time**
  Equivalent to Pressureless Gas Dynamics (PGD) HYPERCOMPRESSIBILITY

Hyper-compressibility due to preferential segregation

- Taylor-Green Vortices (4 contra-rotating vortices with periodic boundaries) and related Lagrangian particles dynamics
- Small Stokes – Particles remain in their own vortex in the lattice cells. (Stokes = 0.03)



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- **Mono-kinetic assumption at given size, location and time**
  Equivalent to Pressureless Gas Dynamics (PGD) HYPERCOMPRESSIBILITY

- **Dedicated numerical methods : combination of operator splitting techniques and kinetic finite volume schemes on structured grids allow second order in time and space with very limited numerical diffusion AND robustness (de Chaisemartin 09)**

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Comparison with other Eulerian models

kinetic model

pdf equation on $f^\phi(t, x, \phi, u_l)$

$$f^\phi(t, x, \phi, u_l) = \sum_{n=1}^{N} w_n \delta(\phi - \phi_n)\delta(u_l - u_n)$$

presumed pdf in velocity

conditioned by size

$$f^\phi(t, x, \phi, u_l) = n^\phi(t, x, \phi)\, \varphi_\sigma(u_l - u_d(t, x, \phi))$$

moments in velocity

at sampled size

semi-kinetic model

conservation equations on $n^\phi(t, x, \phi)$ $u_d(t, x, \phi)$

presumed pdf in size

$u_d(\phi)$ given form

presumed pdf in size

and correlations

for each section

Moment Methods DQMOM

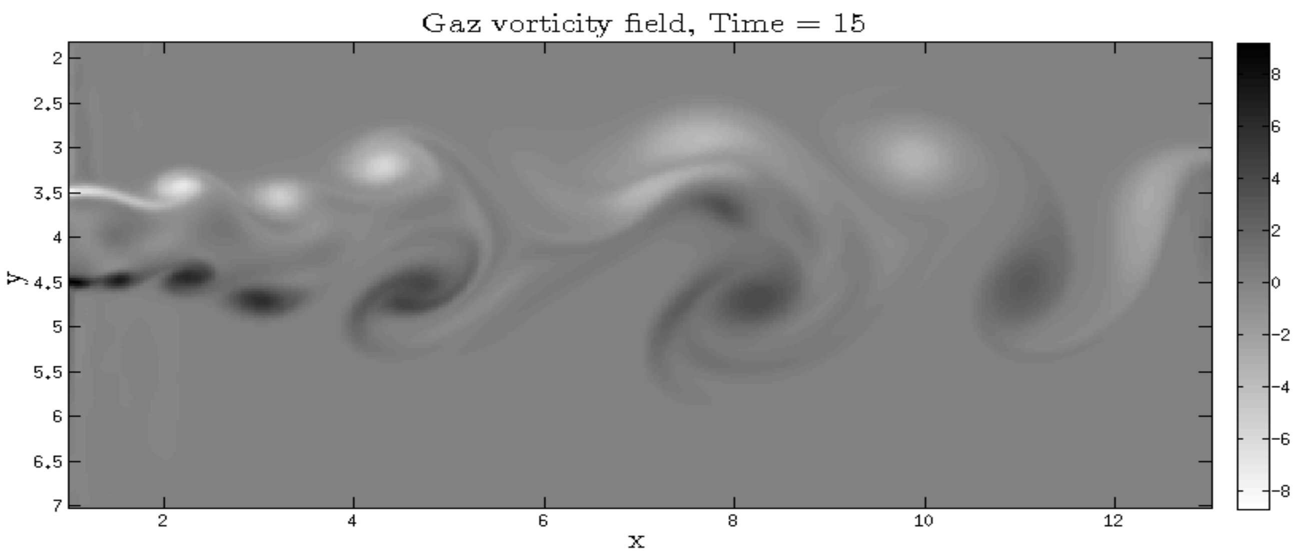
Two-fluid model

Presumed pdf method

Eulerian multi-fluid

Free jets with polydisperse spray injection and evaporation

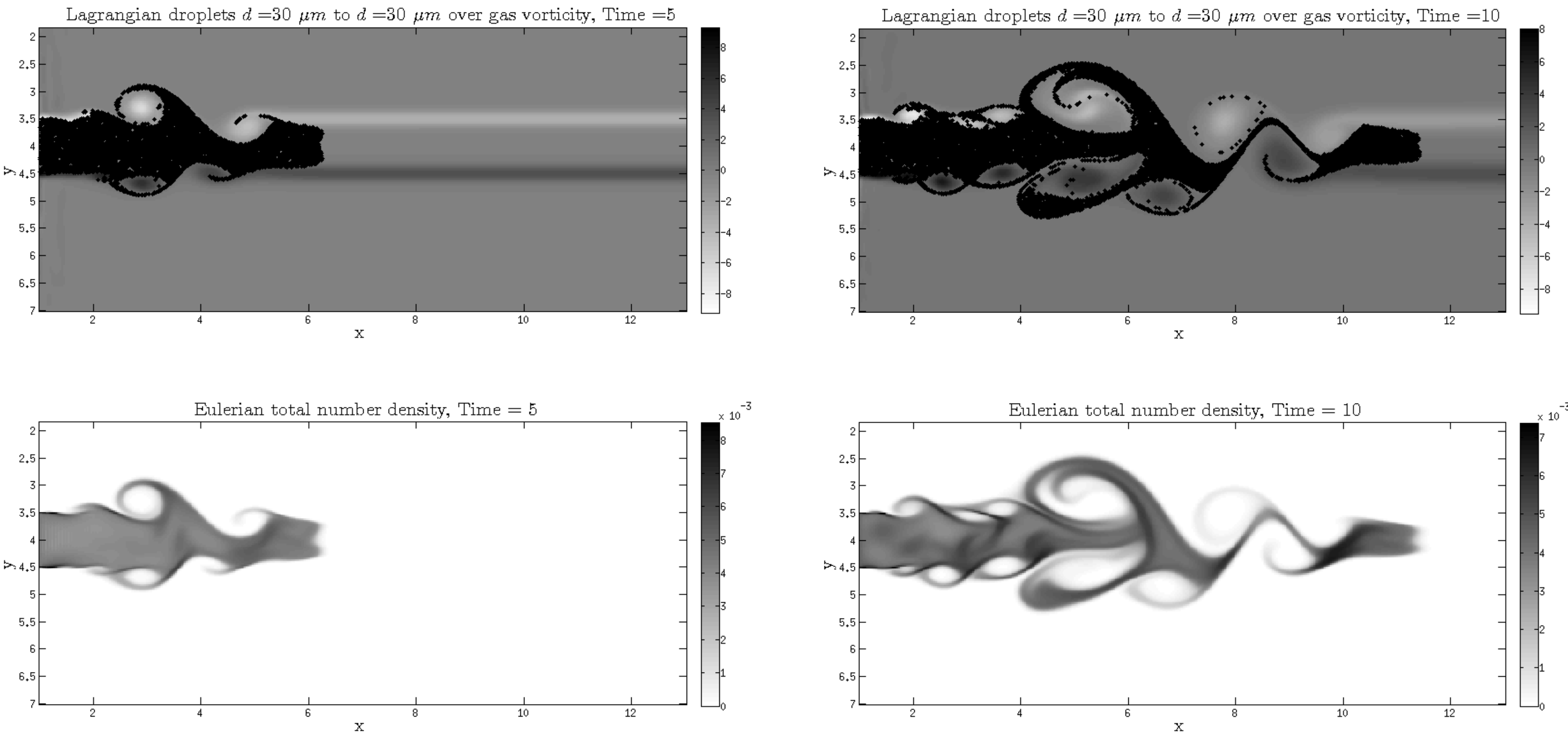
- Coupling Multi-Fluid with Euler-Lagrange code **ASPHODELE** (J. Reveillon - CORIA)
- Injection of a polydisperse spray in the center of the jet
- Re=1000 with a low level turbulence injection for destabilization purposes. Klein's method with 10% of fluctuations
- Droplet distribution between Stokes = 0.03 and 1.34 divided in sections
- Discretization in 400*200*10 sections (overnight on 1 computer)



MUSES 3D – Multi-Fluid Spray Eulerian Solver (Dev. S. de Chaisemartin)

Free jets with polydisperse spray injection and evaporation

Achievement : Eulerian multi-fluid model (at equilibrium – Thesis of S. de Chaisemartin, EM2C) captures the droplets dynamics and evaporation for relative **low Stokes : 0.12**



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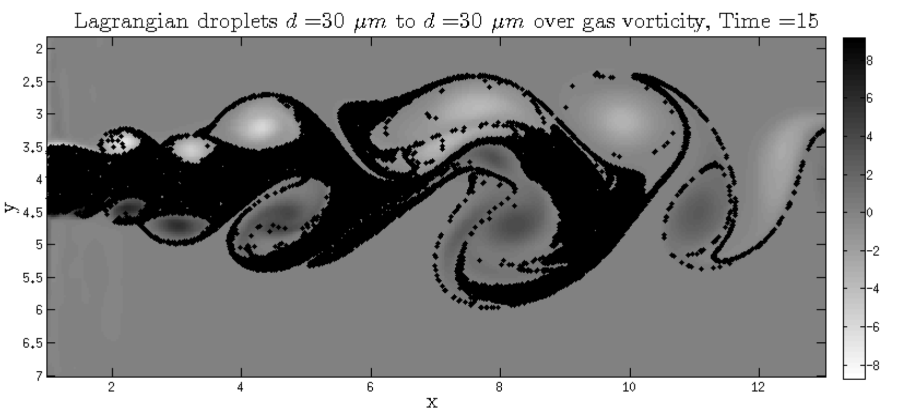
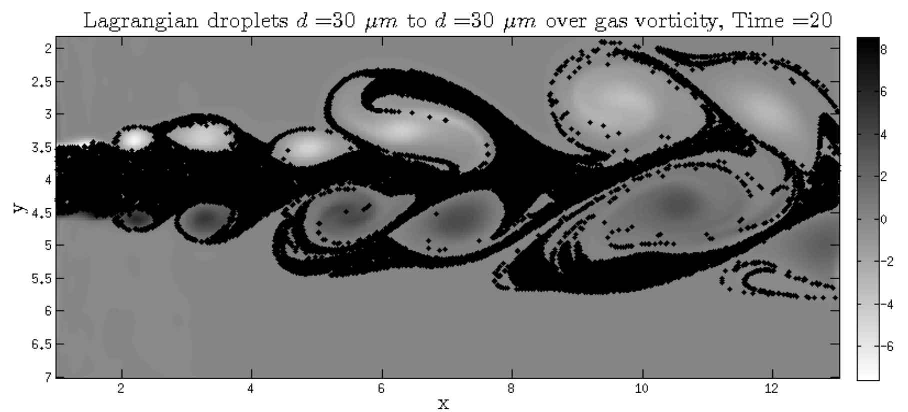
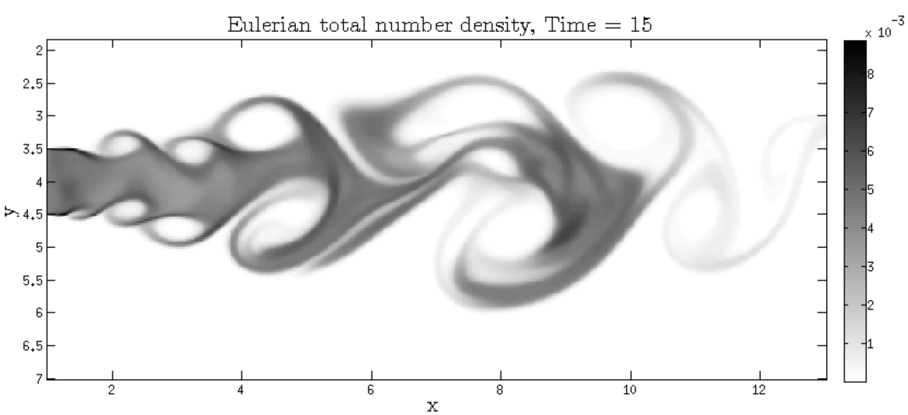
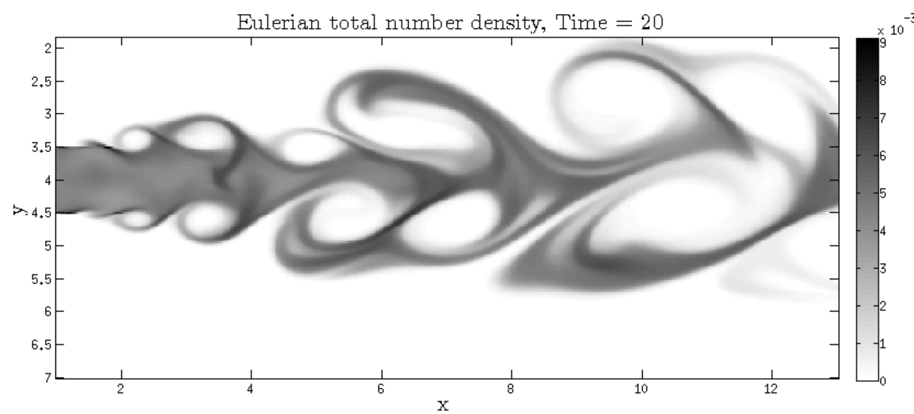


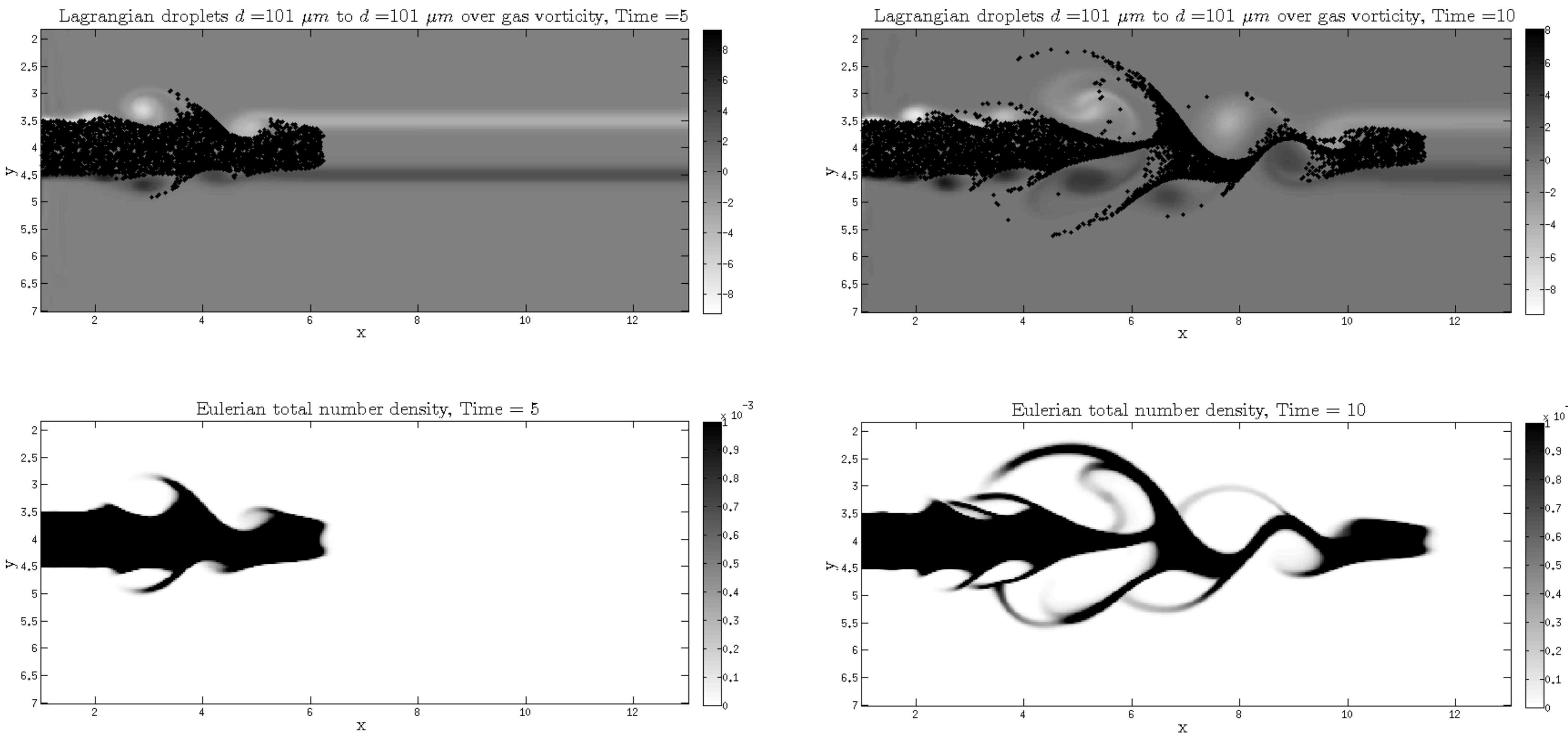






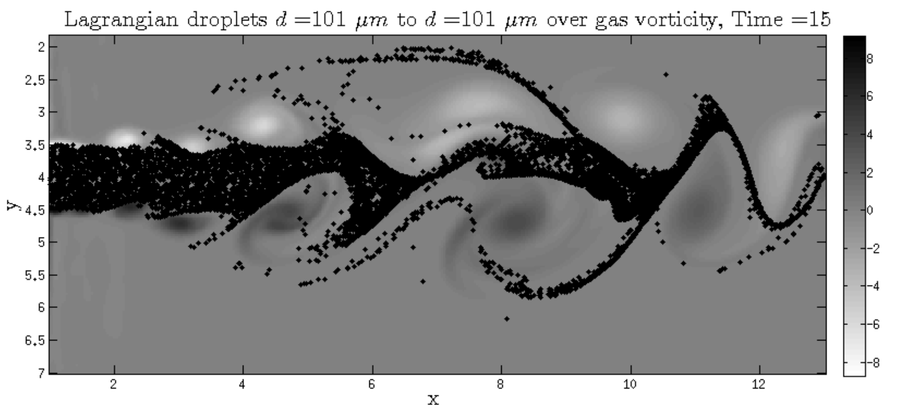
Free jets with polydisperse spray injection and evaporation

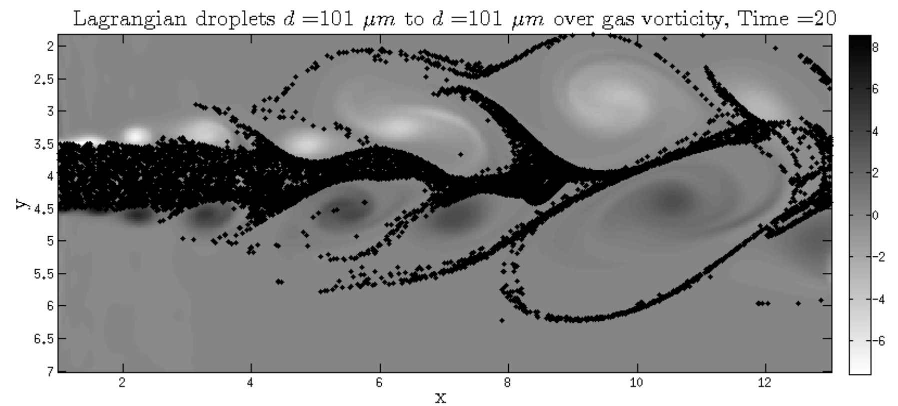
Achievement : Eulerian multi-fluid model (at equilibrium – Thesis of S. de Chaisemartin, EM2C) captures the droplets dynamics and evaporation for relative **low Stokes : 1.34**

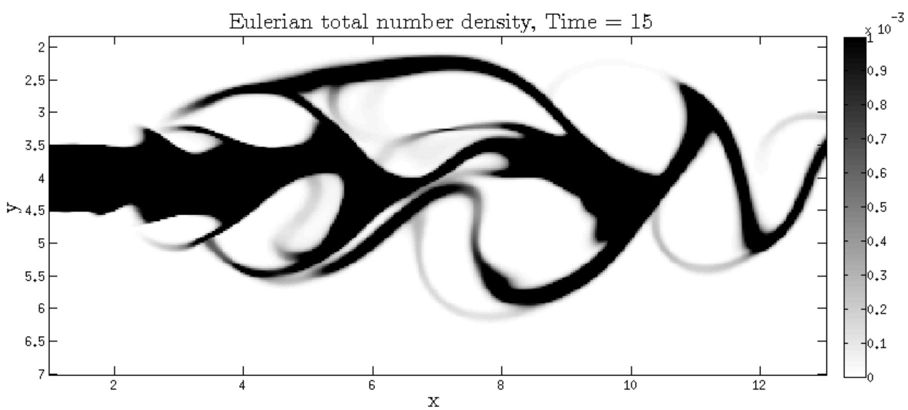


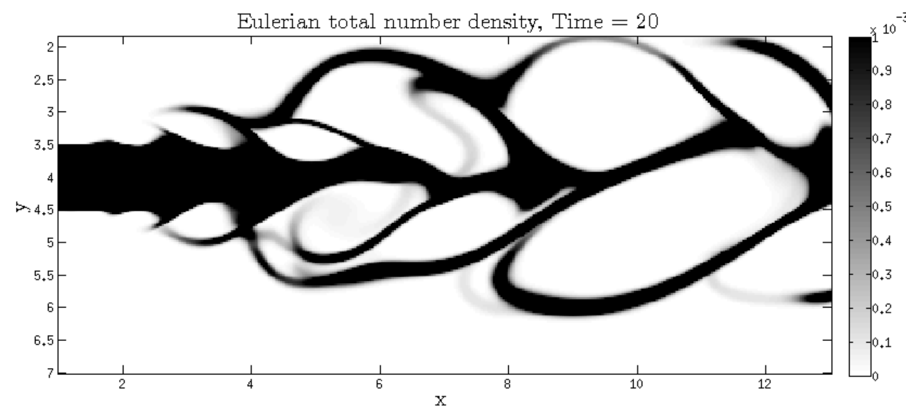
Free jets with polydisperse spray injection and evaporation

Achievement : Eulerian multi-fluid model (at equilibrium – Thesis of S. de Chaisemartin, EM2C) captures the droplets dynamics and evaporation for relative **low Stokes : 1.34**



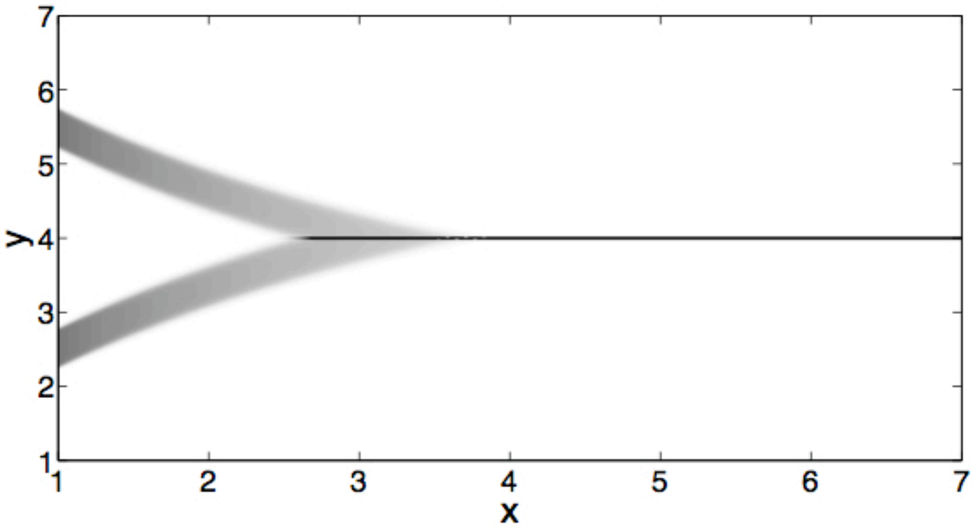




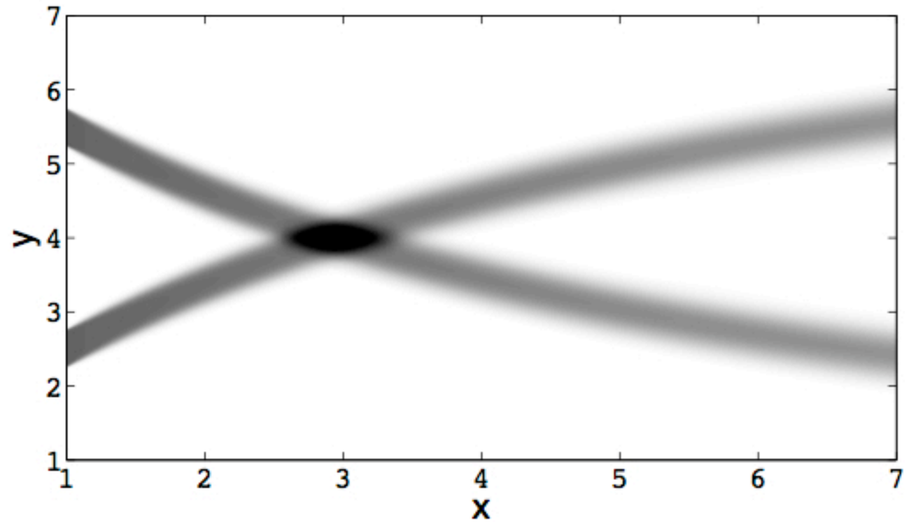


➢Crossing jets at infinite Knudsen number : negligible collision frequency

- ➢Development of a Eulerian model out of equilibrium able to reproduce the effect of particle crossing trajectories (at mesoscopic scale) Test/validation configurations



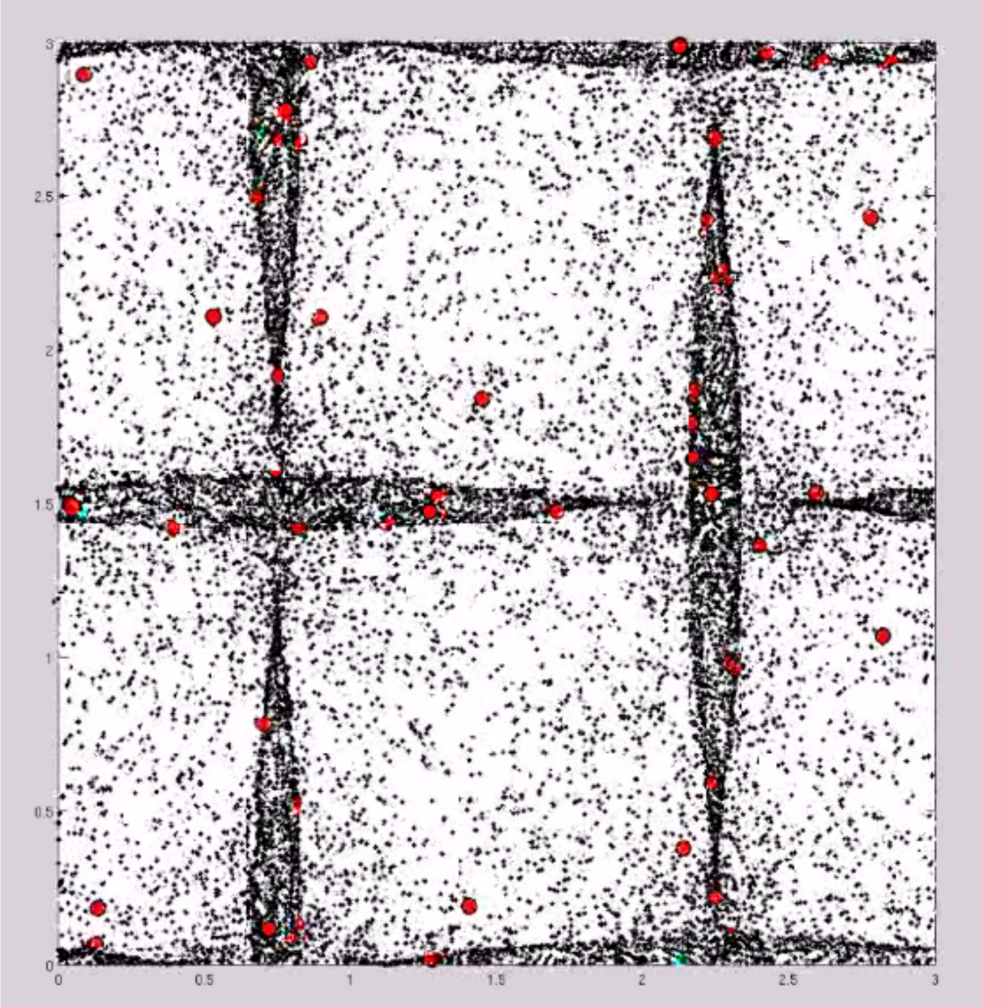
(a) Multi-Fluid.



(b) Multi-velocity.

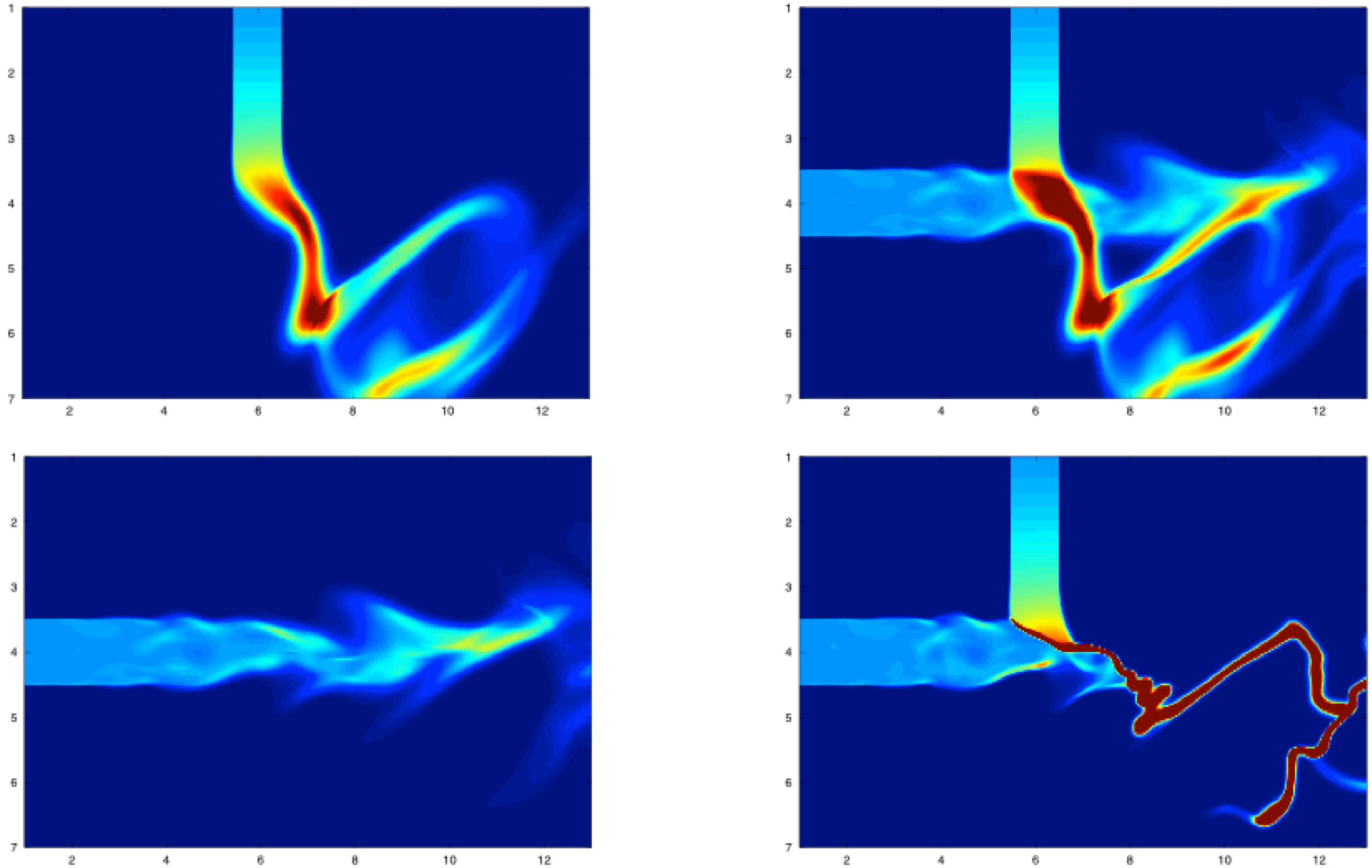
Hyper-compressibility due to preferential segregation

- Taylor-Green Vortices (4 contra-rotating vortices with periodic boundaries) and related Lagrangian particles dynamics
- Larger Stokes – Particles are ejected from the vortices in the lattice cells. (Stokes = 0.3)



- **Free jets with polydisperse spray injection – effect of droplet crossing – FTC 2010**

Ph.D D. Kah – SMAI (France) and ECCOMAS (Europe) prize 2010



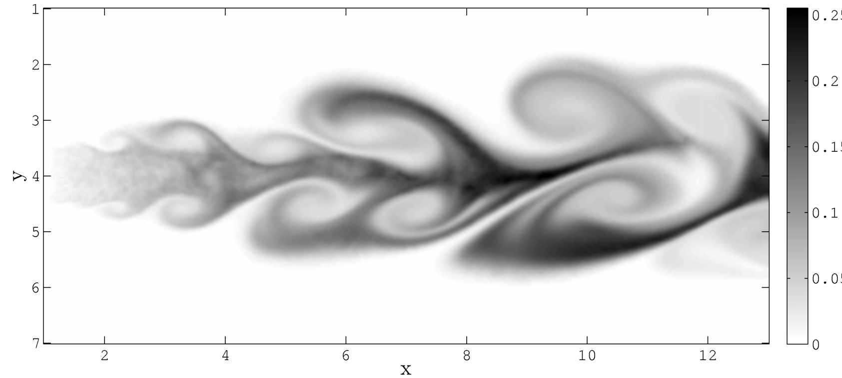
- Free jets with polydisperse spray injection and evaporation
- Log normal distribution with 10 sections

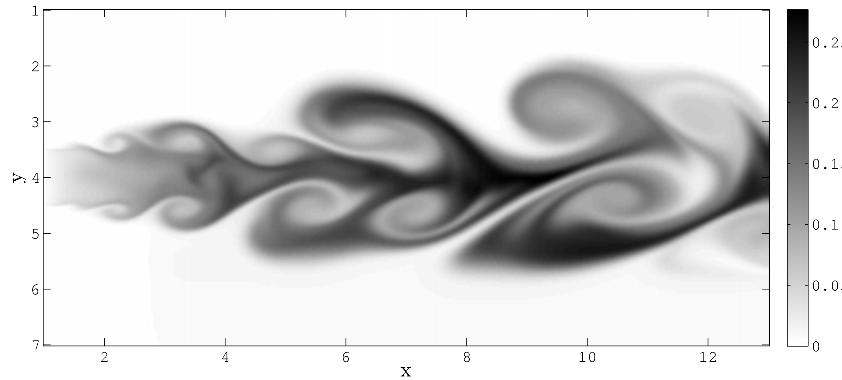
Excellent agreement

for the fuel mass fraction

Top : Lagrangian

Bottom : Eulerian





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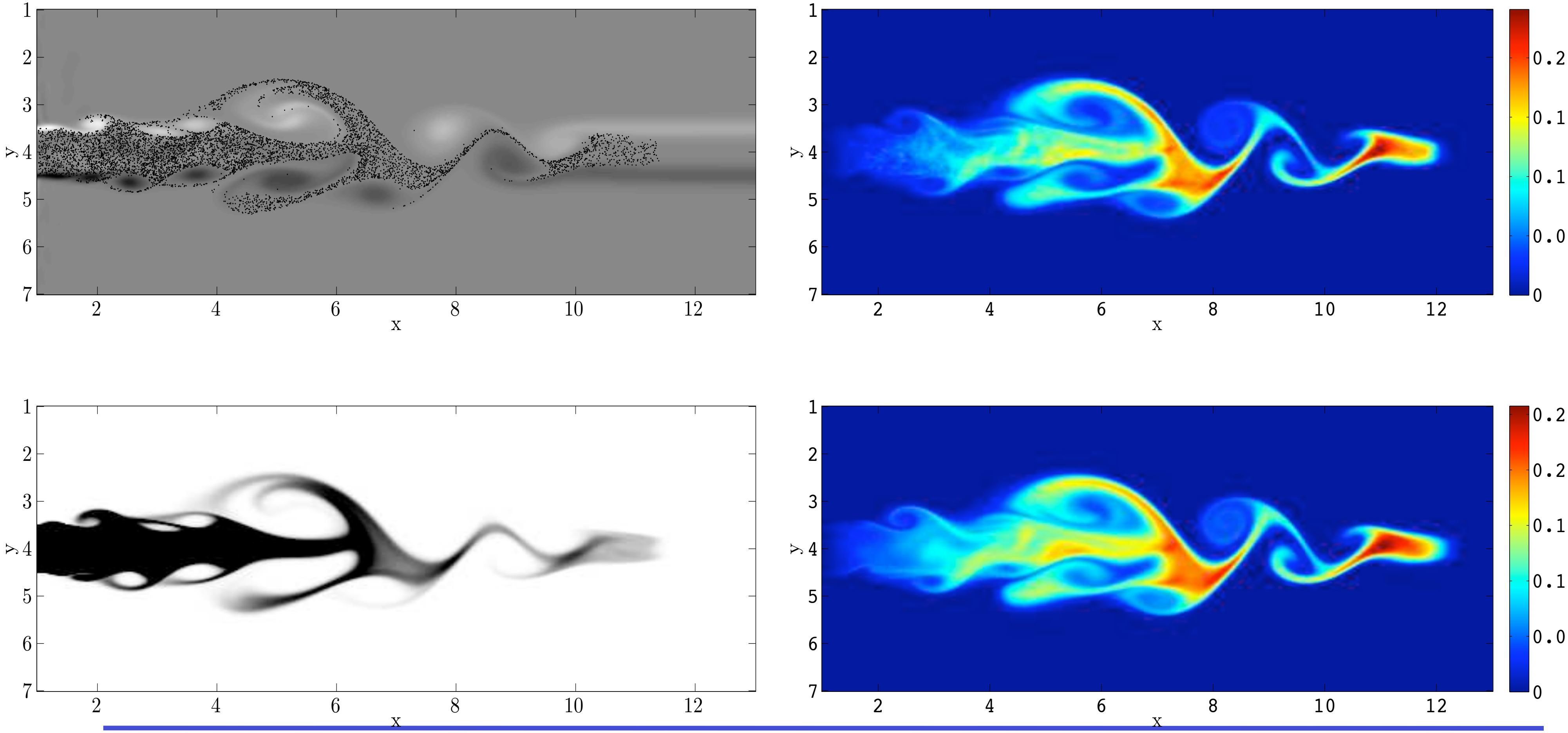
- **Free jets with polydisperse spray injection and evaporation**
- **Log normal distribution with 10 sections**



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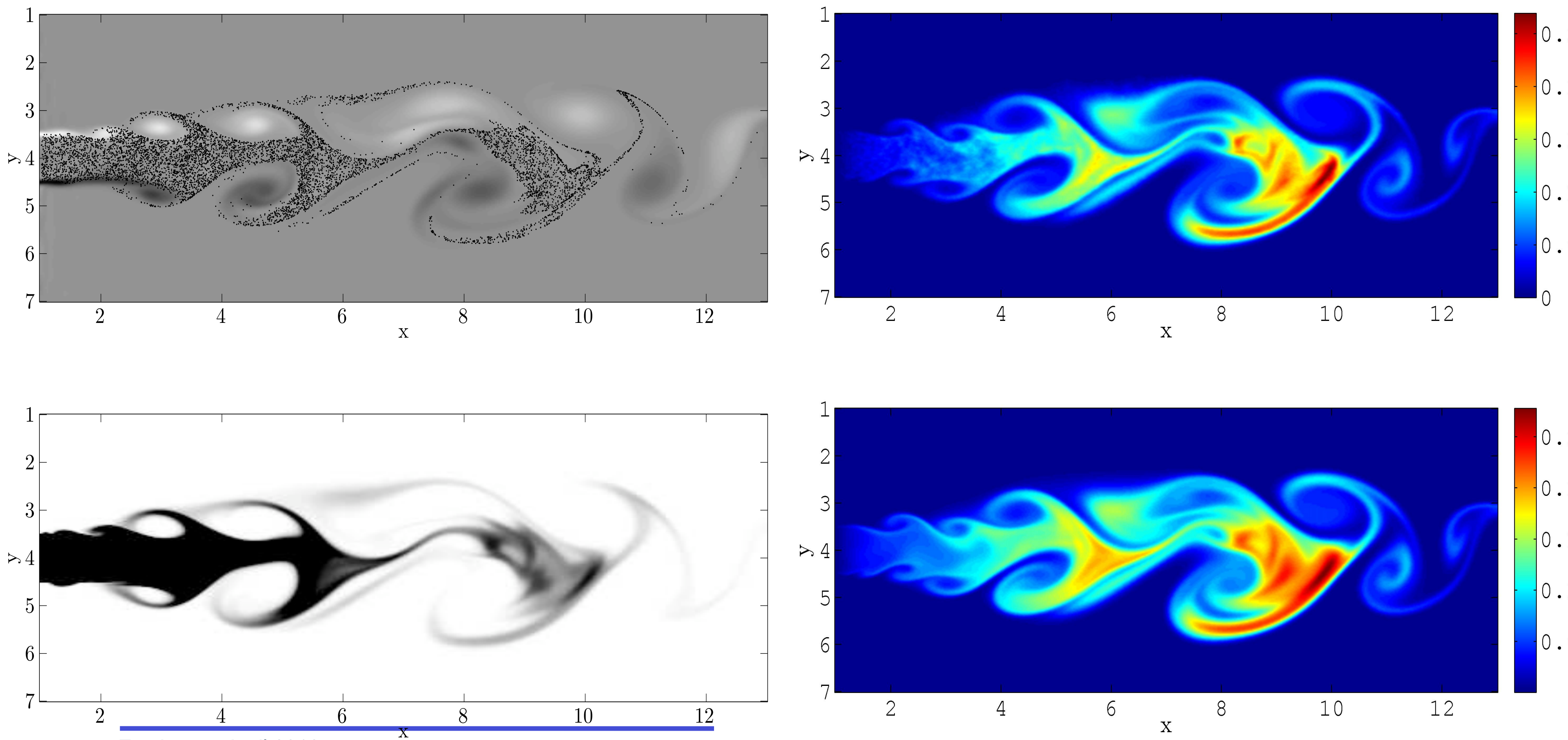
- Free jets with polydisperse spray injection and evaporation
- Log normal distribution with 10 sections



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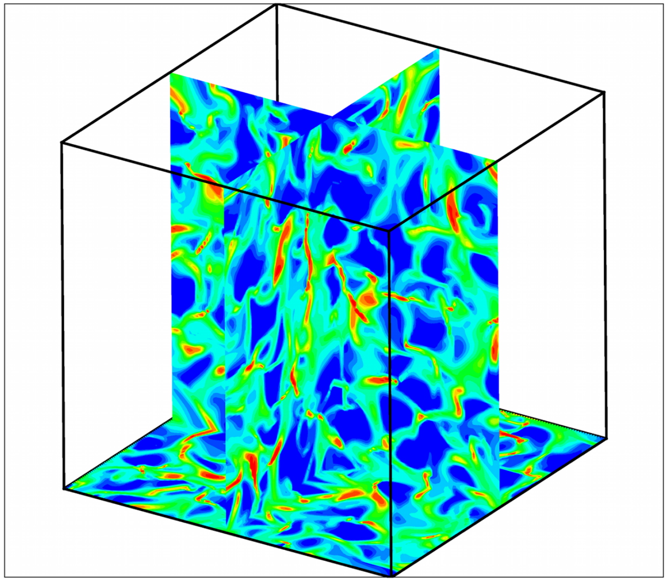
- **Eulerian multi-fluid description of the polydisperse evaporating spray**
- **MUSES 3D - Typically 128^3 to 512^3 with 10 sections**
  - **Numerical method : finite volumes on a structured grid coupled with an operator splitting technique as far as transport in physical space and transport in phase space are concerned – dimensional splitting for the transport in physical space. Globally : highly parallelizable algorithm or order 2 in space and time**
  - **Domain decomposition with MPI Library**
  - **Scalability of the code : efficiency of 1 up to 1024 processors (CERTAINTY – CTR - Stanford and IDRIS/ CINES projects France, CentraleSupélec Mesocenter)**
  - **Typical time of simulation 256^3 with 10 sections over 2 eddy turn over time on 100 processors is 6h (4D unsteady simulation with about 16 millions of cells and 800 millions variables)**



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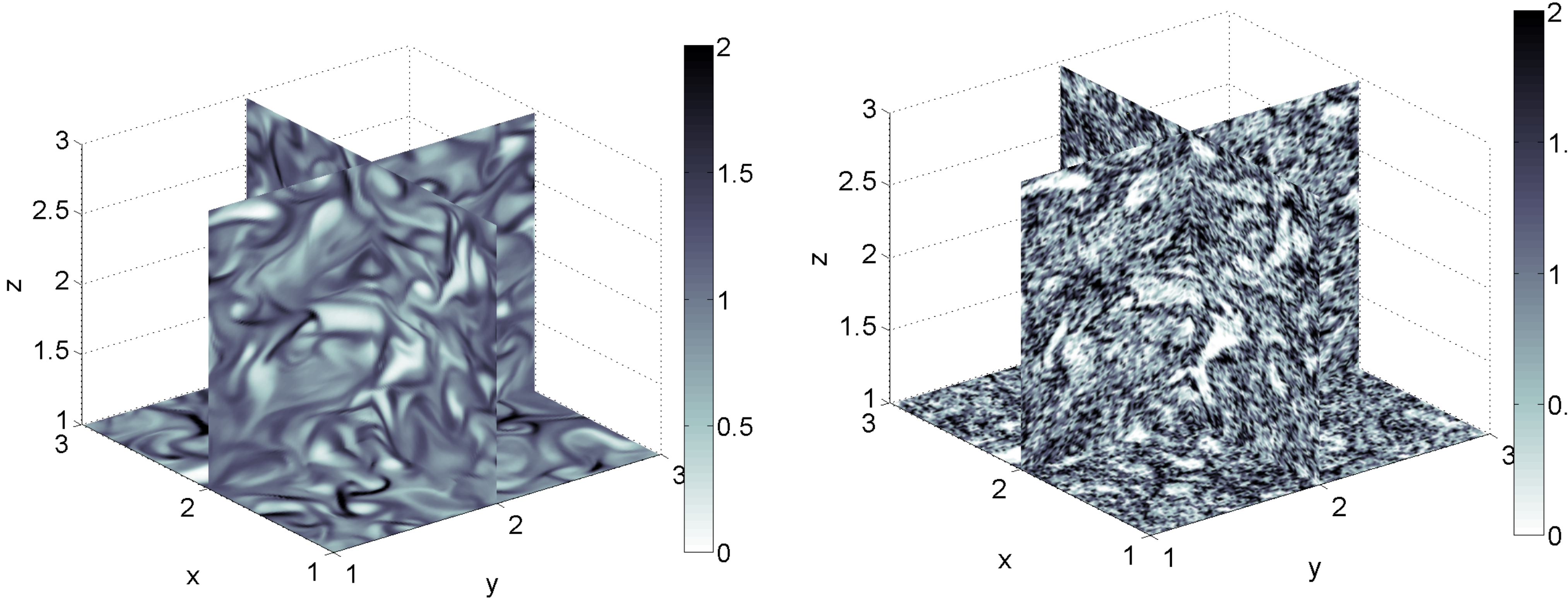
Coupling of ASPHODELE Code of CORIA with MUSES3D - Forced HIT

- **Eulerian multi-fluid description of the polydisperse spray**
- **Stokes = 0.17**



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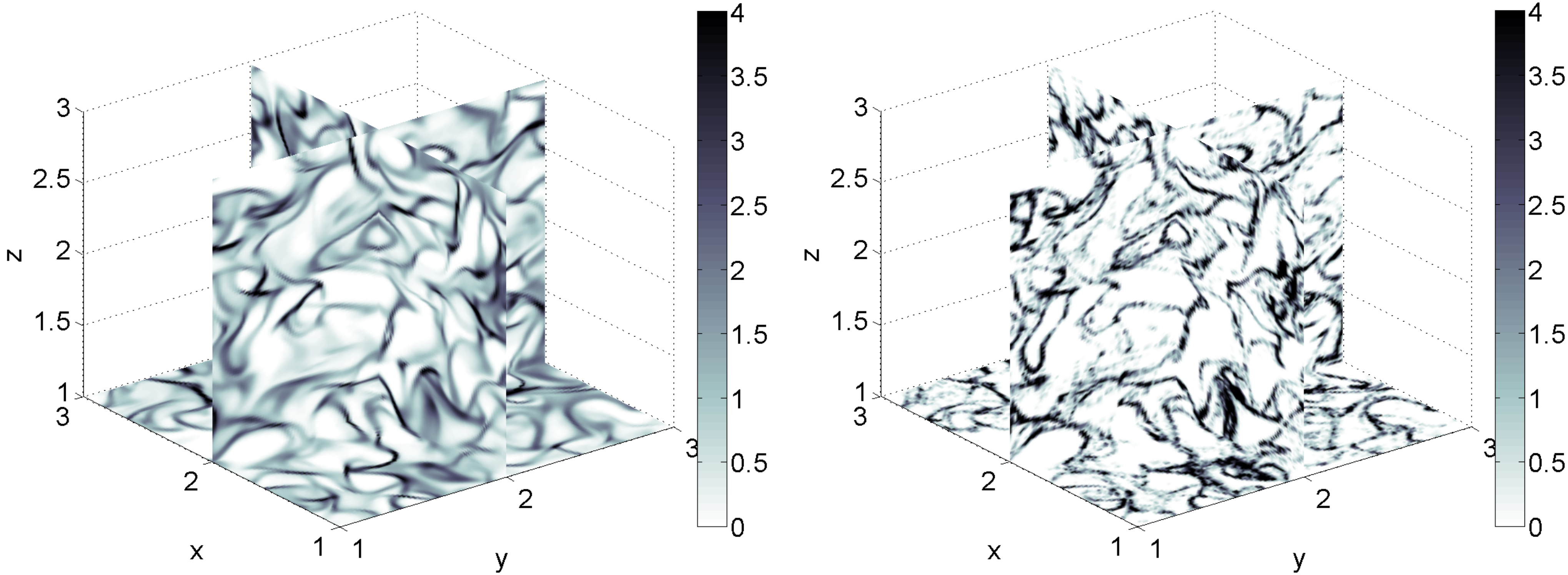
Coupling of ASPHODELE Code of CORIA with MUSES3D - Forced HIT

- **Eulerian multi-fluid description of the polydisperse spray**
- **Stokes = 1.05**



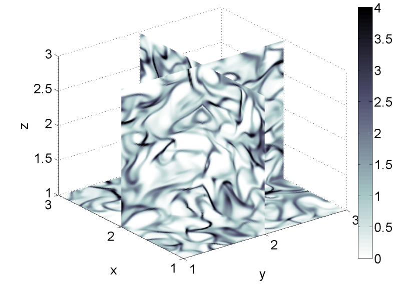
Eulerian Multi-Fluid versus Lagrangian spray flames

EM2C - MUSES3D Code

- Mono-kinetic assumption as a closure $f(t, \mathbf{x}, \mathbf{u}, S) = n(t, \mathbf{x}, S)\delta\left(\mathbf{u} - \overline{\mathbf{u}}(t, \mathbf{x}, S)\right)$

  => **DNS at limited Stokes** numbers

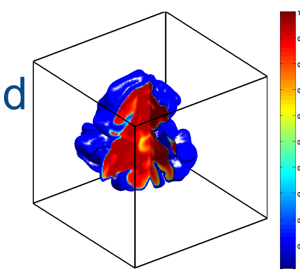
- Polydispersity by discretizing the droplet size phase space
- Accurate and robust numerical schemes
- Fully parallelized (efficiency one on Certainty up to 512 cores)



Fully coupled during CTR Summer Program and parallelized –flame dynamics comparison

CORIA – ASPHODELE Code

- Spectral forcing and resolution of the gaseous flow field



CONSTANT DENSITY FLAME Configuration

Polydisperse spray flame dynamics

- Polydispersity and droplet crossing naturally handled by Lagrangian method

Eulerian Multi-Fluid versus Lagrangian spray flames

- EM2C - **MUSES3D Code**
  - Mono-kinetic assumption as a closure

    => **DNS at limited Stokes** numbers
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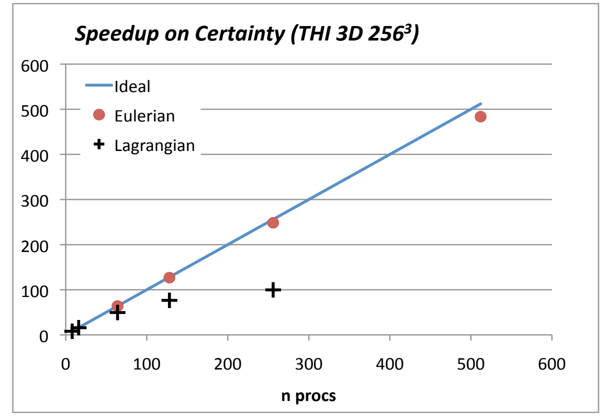

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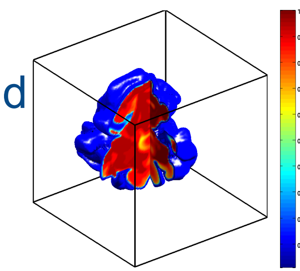
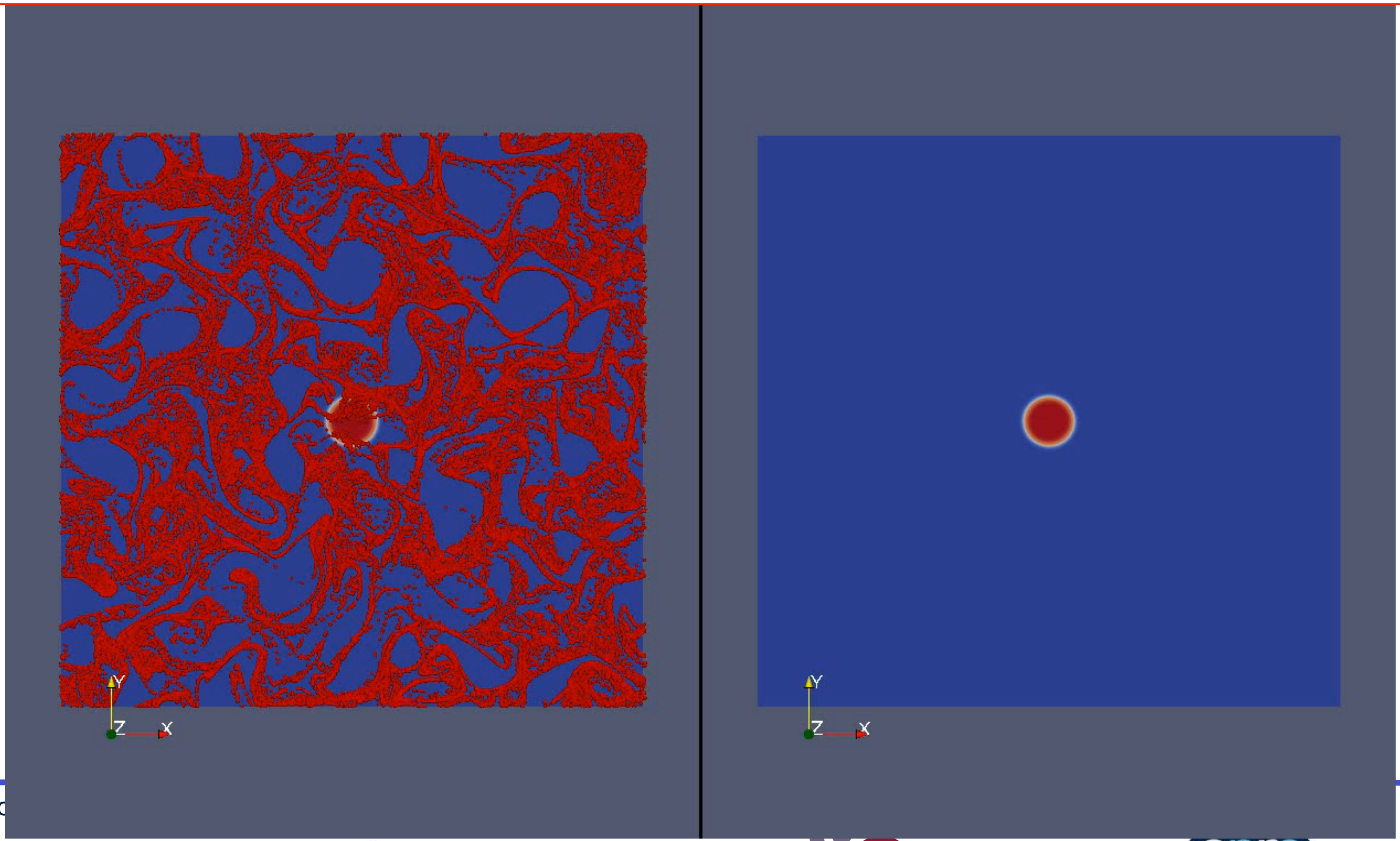


- Polydispersity and droplet crossing naturally handled by Lagrangian method

Polydisperse spray flame dynamics – detailed comparison

- Most difficult case : the spray is already segregated at Stokes 0.2 in 2D – initially monodisperse (handled with Eulerian multi-fluid using ten sections)



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Polydisperse spray flame dynamics – detailed comparison

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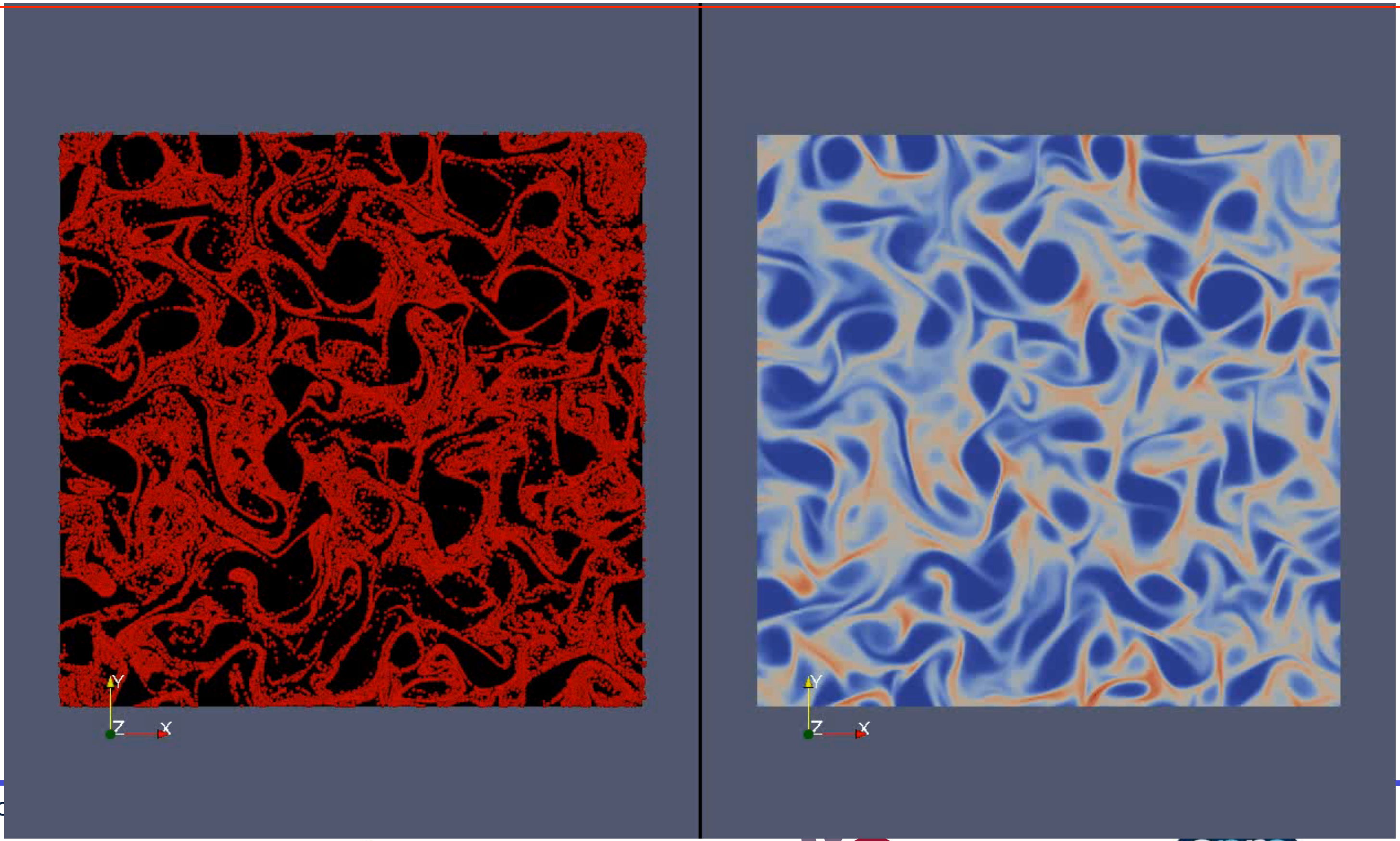
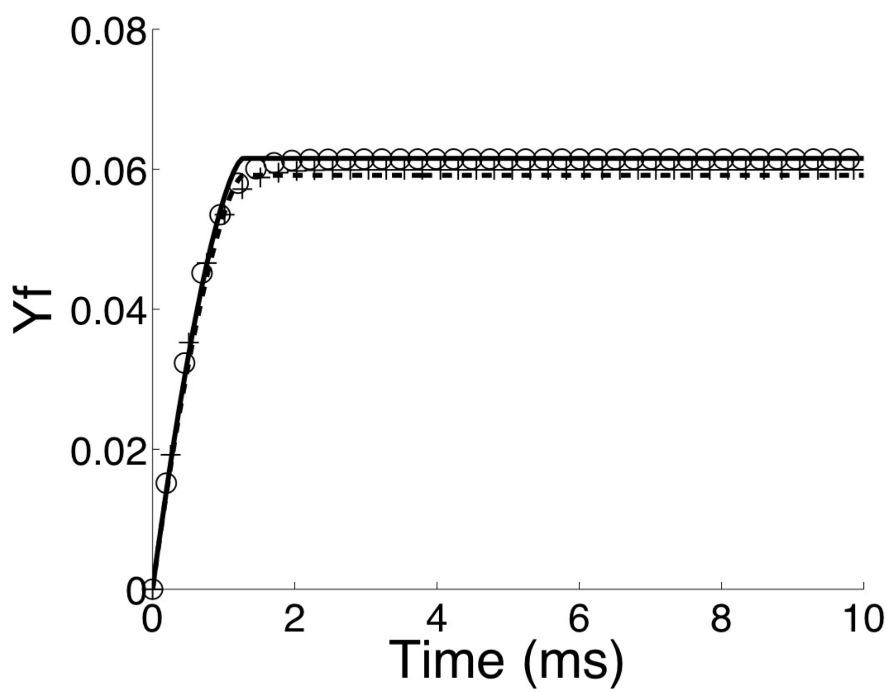
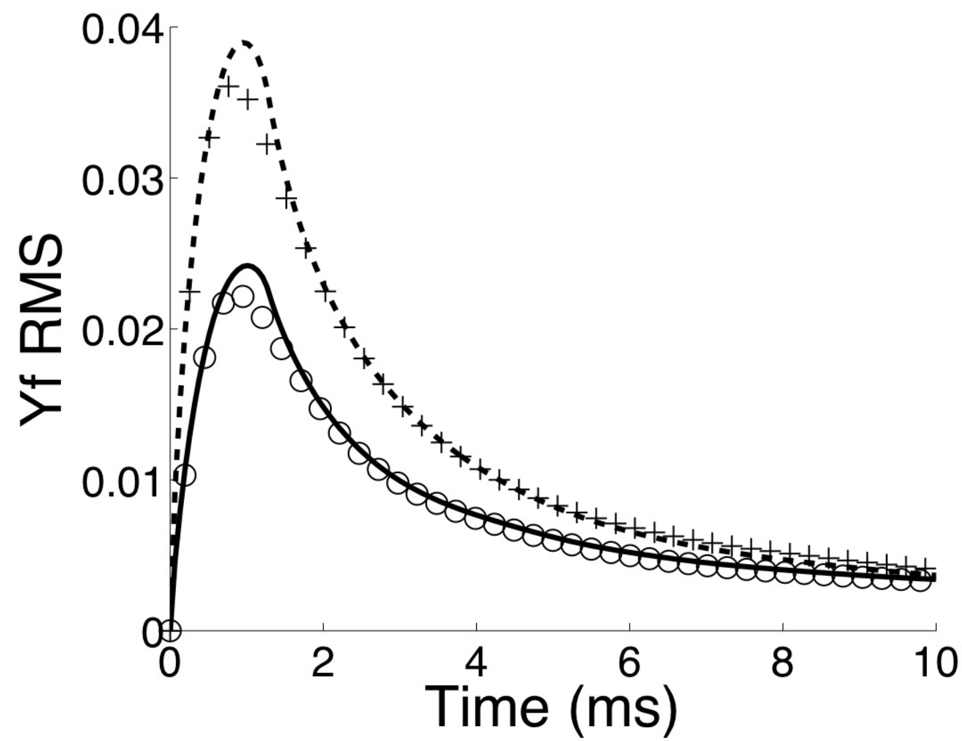


Polydisperse spray flame dynamics – detailed comparison

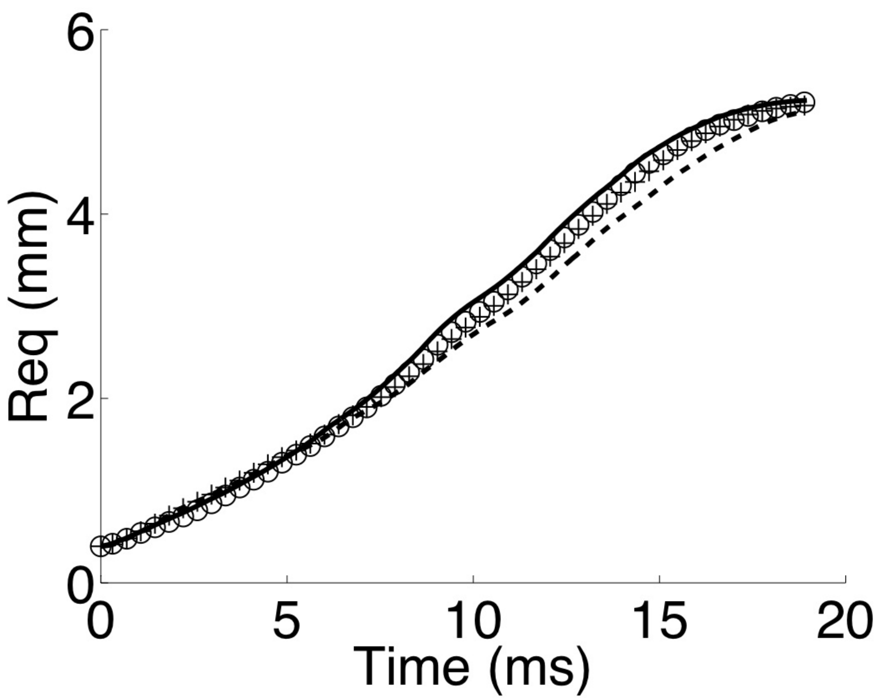
- Time evolution of the fuel mass fraction and its rms
- Lines: Lagrangian – Symbols: Eulerian

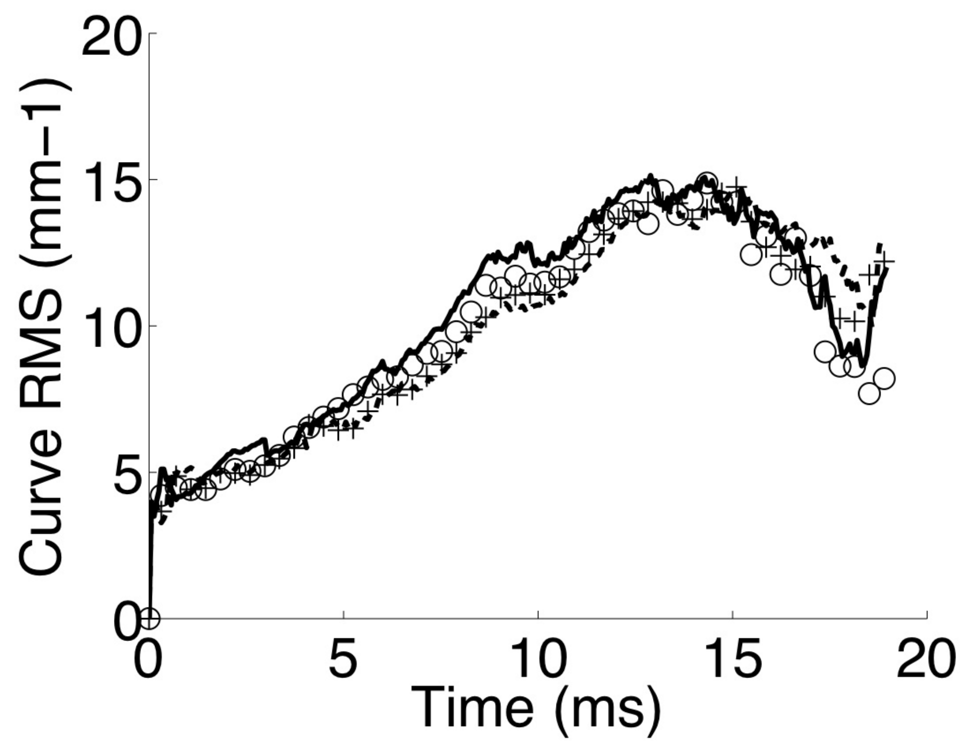




Polydisperse spray flame dynamics – detailed comparison

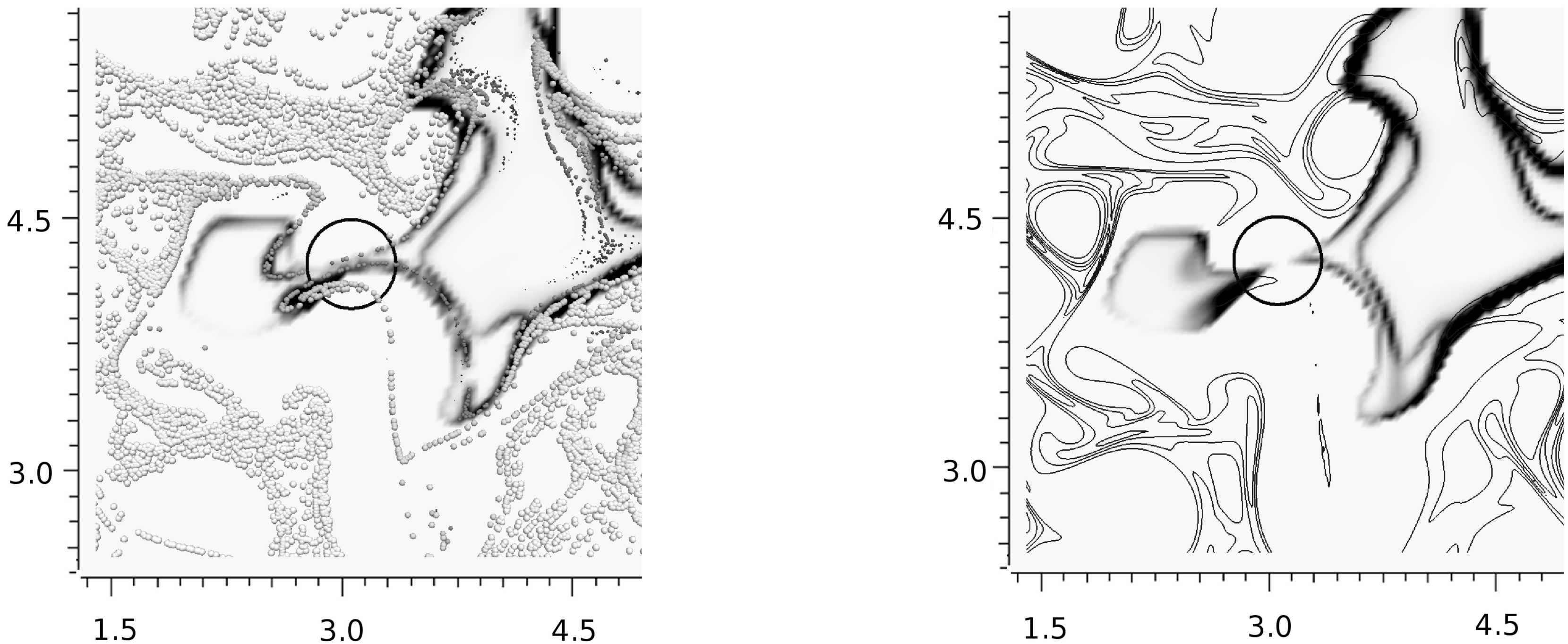
- Flame mean radius evolution and curvature of the flame





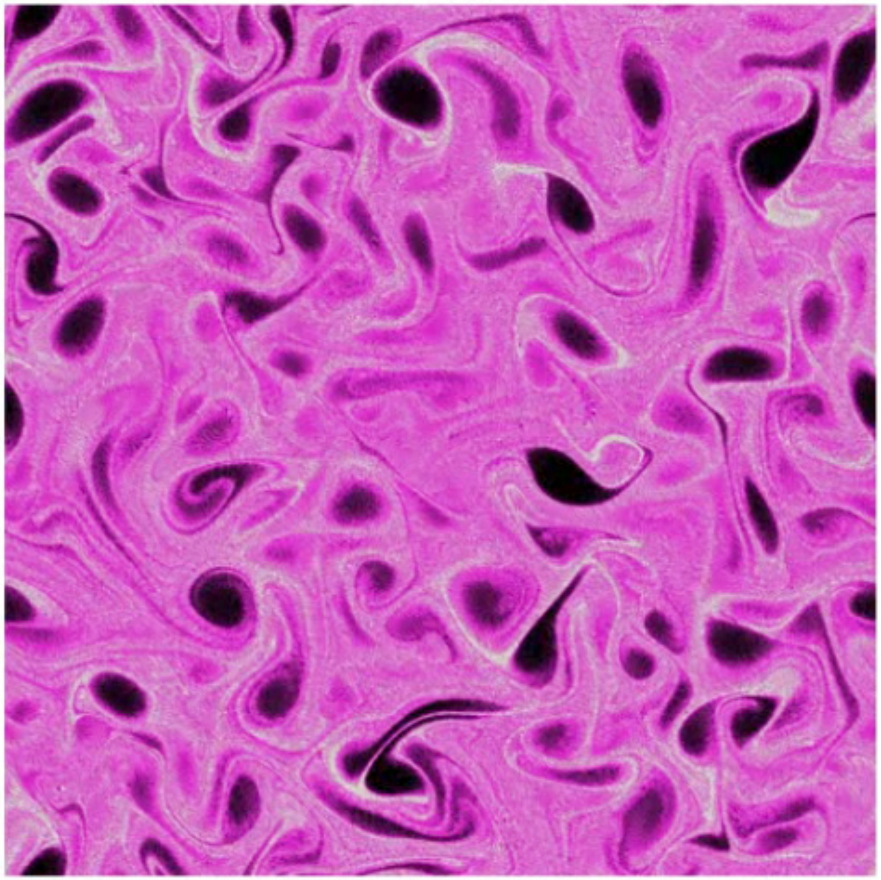
Polydisperse spray flame dynamics – detailed comparison

- Flame dynamics – extinction zone – double flame structure
  - Lagrangian on the left / Eulerian on the right



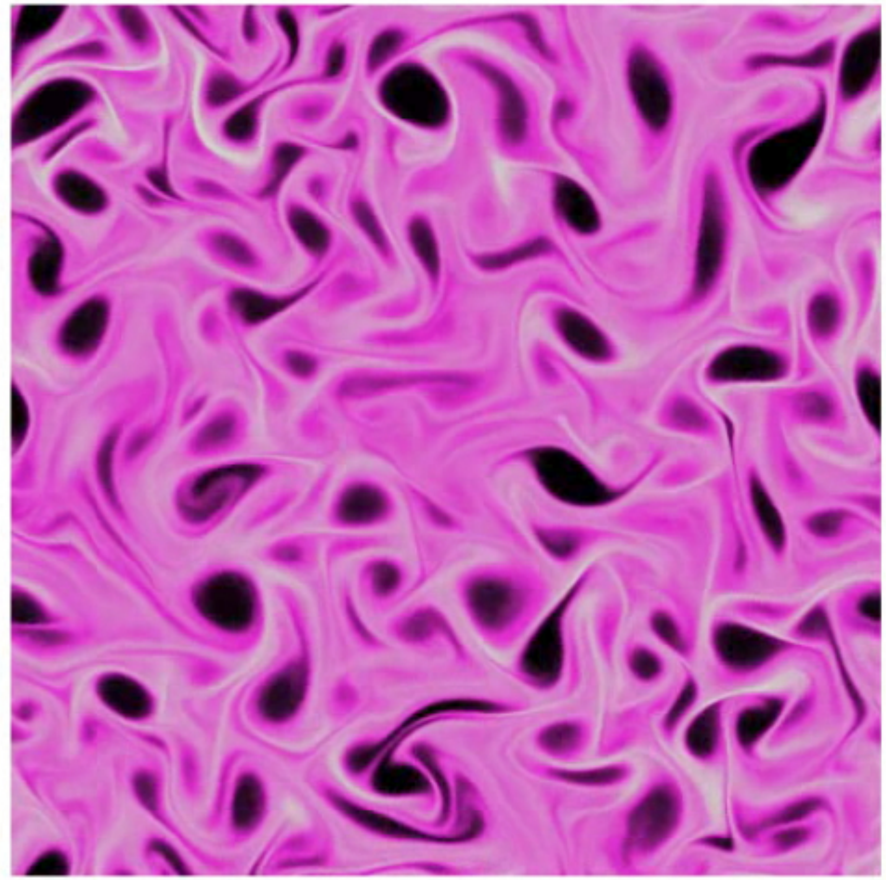
Polydisperse spray dynamics – detailed comparison

Lagrangian



Asphodele code (CORIA - CNRS URM 6614)
Muses3d code (EM2C - CNRS ECP)

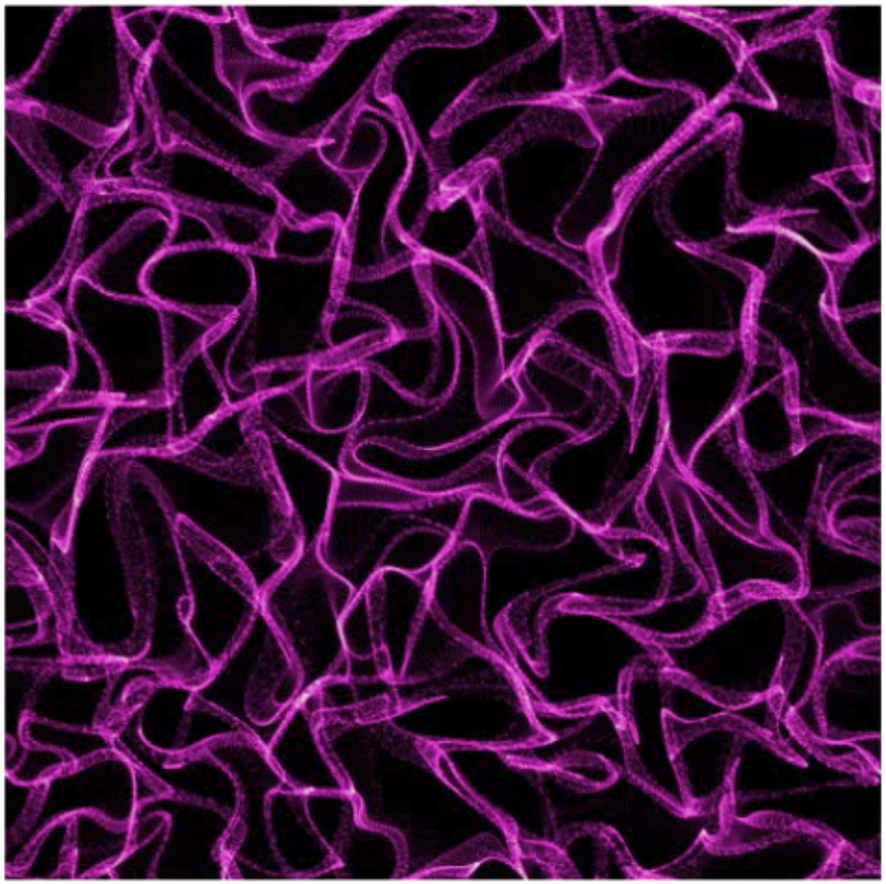
Eulerian



Thomine, Freret, Reveillon & Massot

Polydisperse spray dynamics – detailed comparison

Lagrangian



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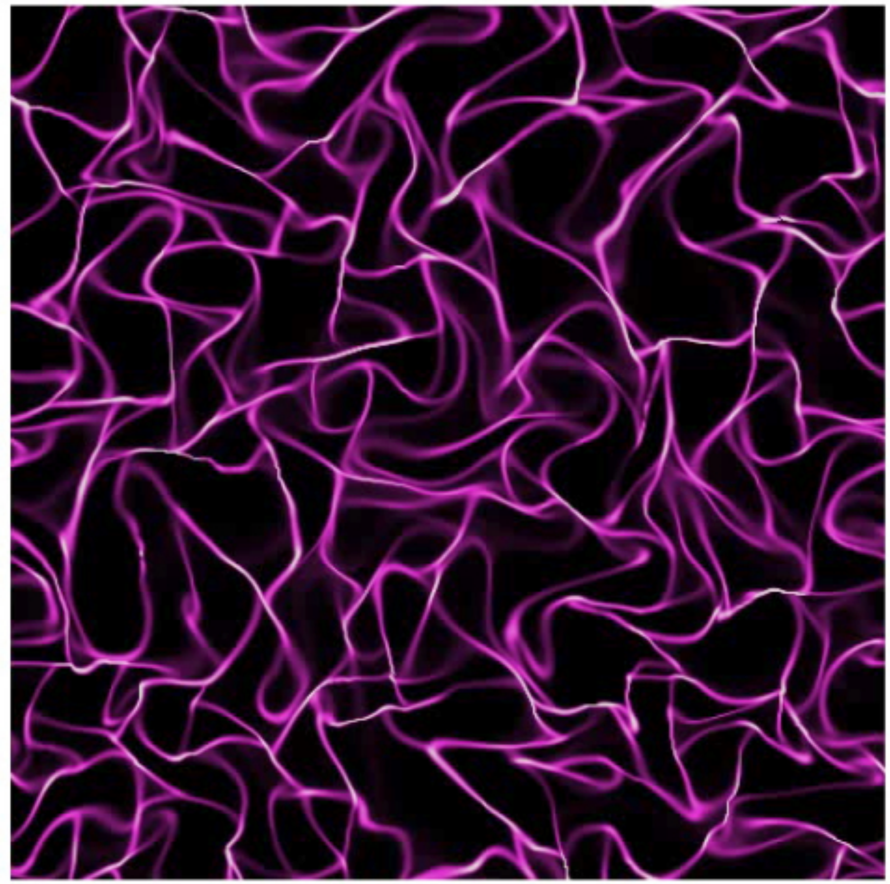
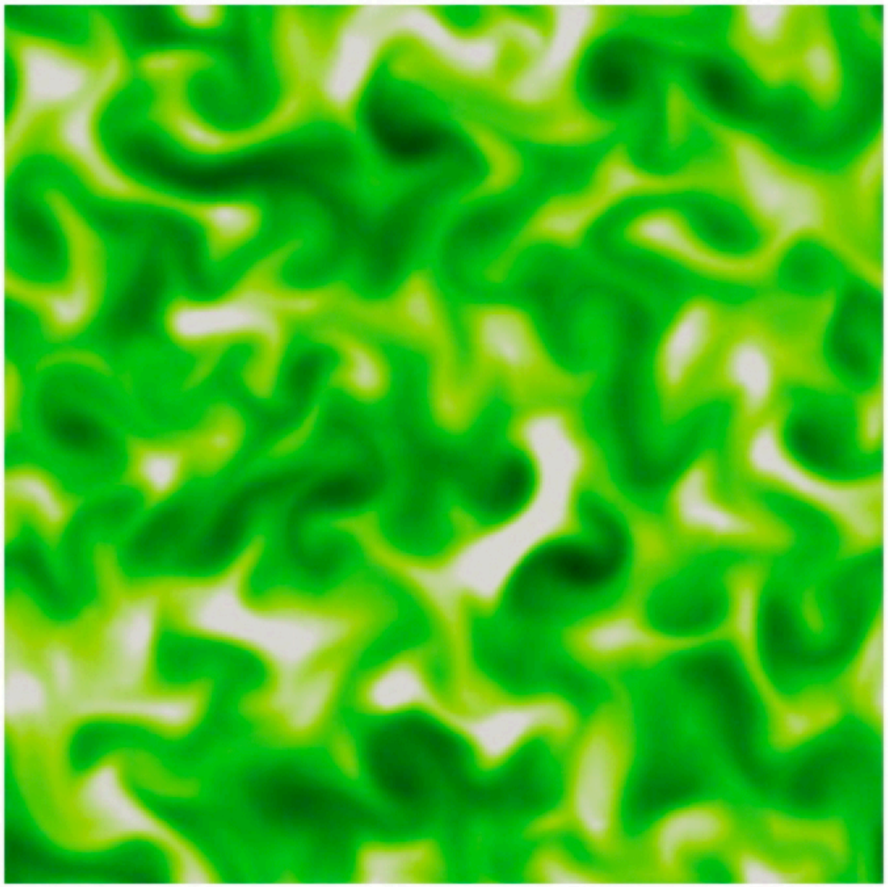


Thomine, Freret, Reveillon & Massot

Polydisperse spray flame dynamics – detailed comparison

Lagrangian



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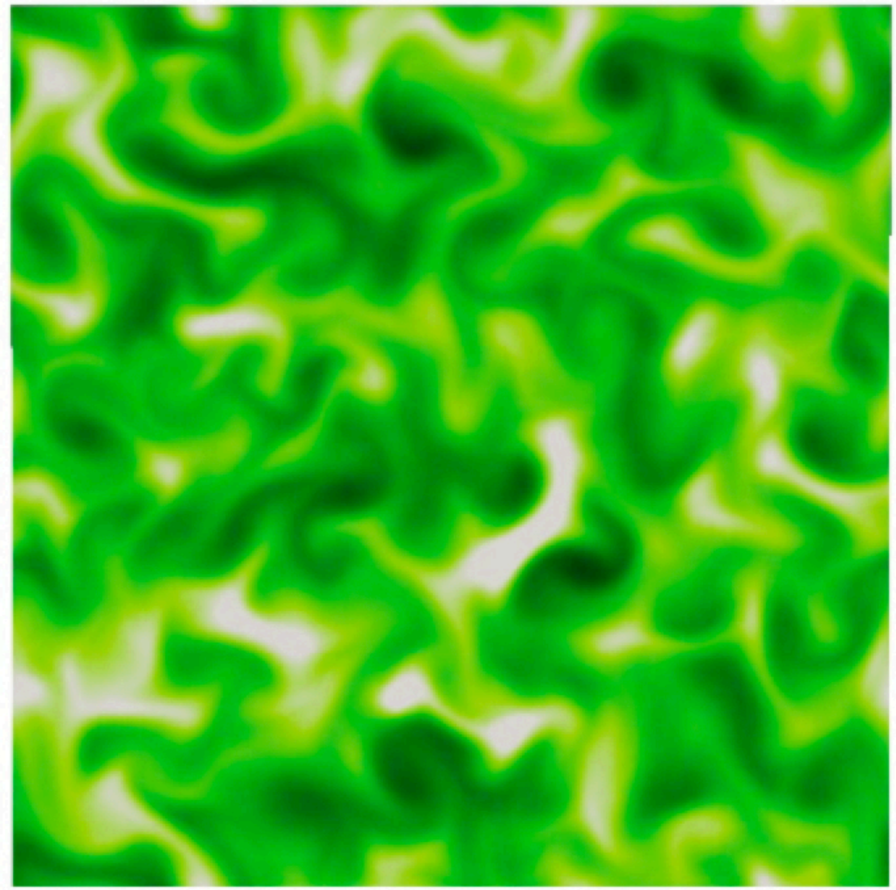
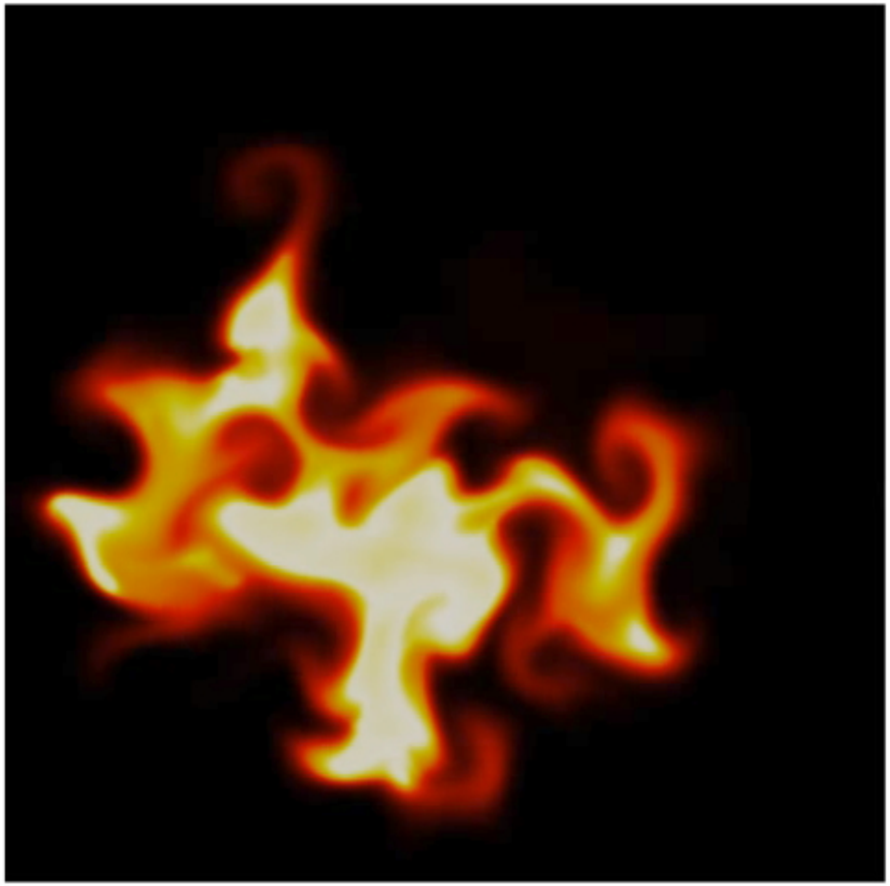


Thomine, Freret, Reveillon & Massot

Polydisperse spray flame dynamics – detailed comparison



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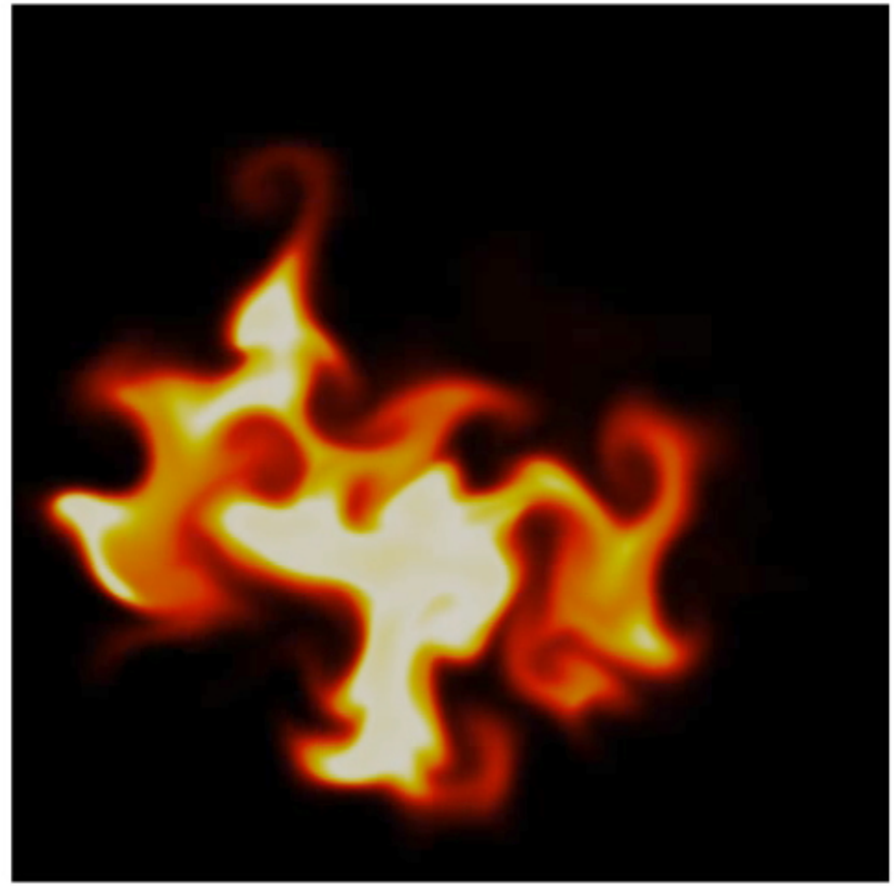

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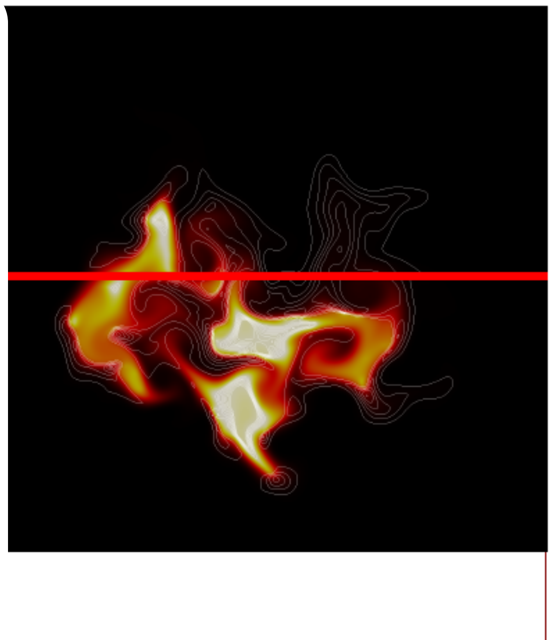
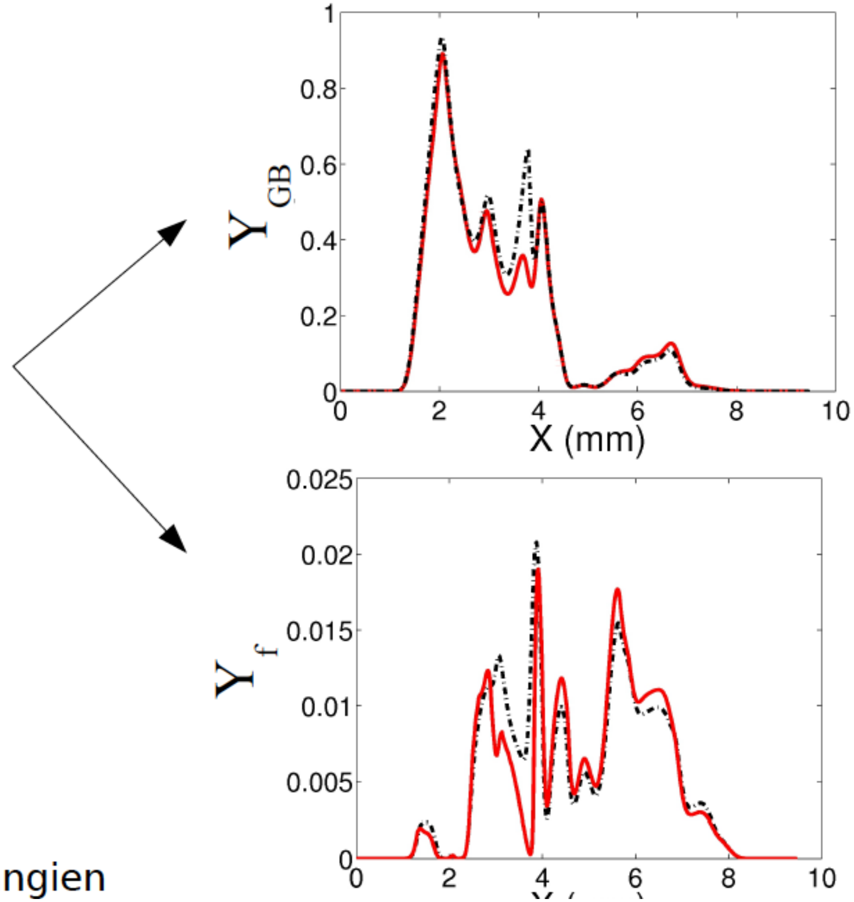
Combustion : propagation d'un front de flamme dans le domaine (iso-contours de Y_{GB} et Y_f).

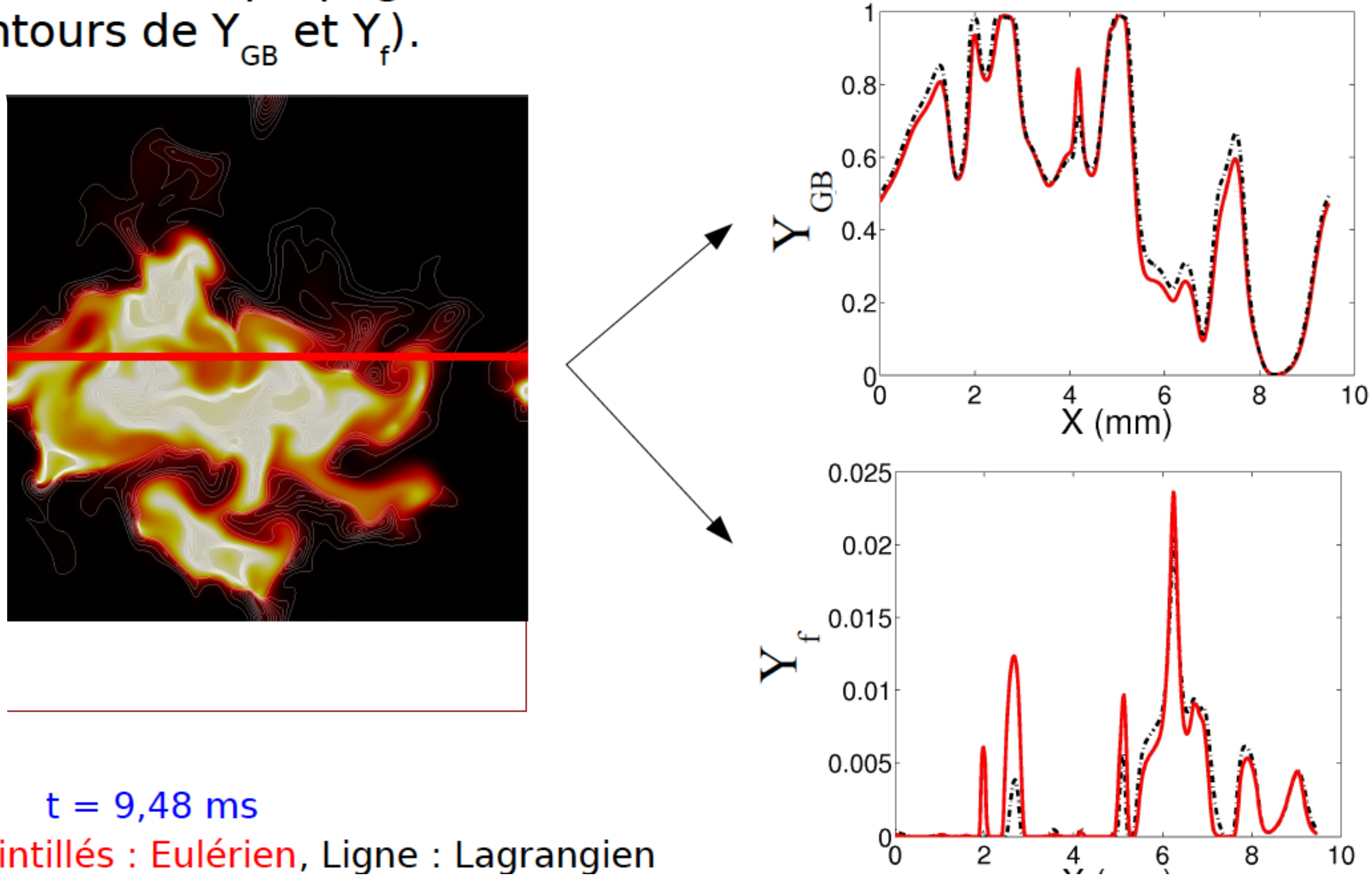




t = 6,31 ms

Pointillés : Eulérien, Ligne : Lagrangien

Combustion : propagation d'un front de flamme dans le domaine (iso-contours de Y_{GB} et Y_f).

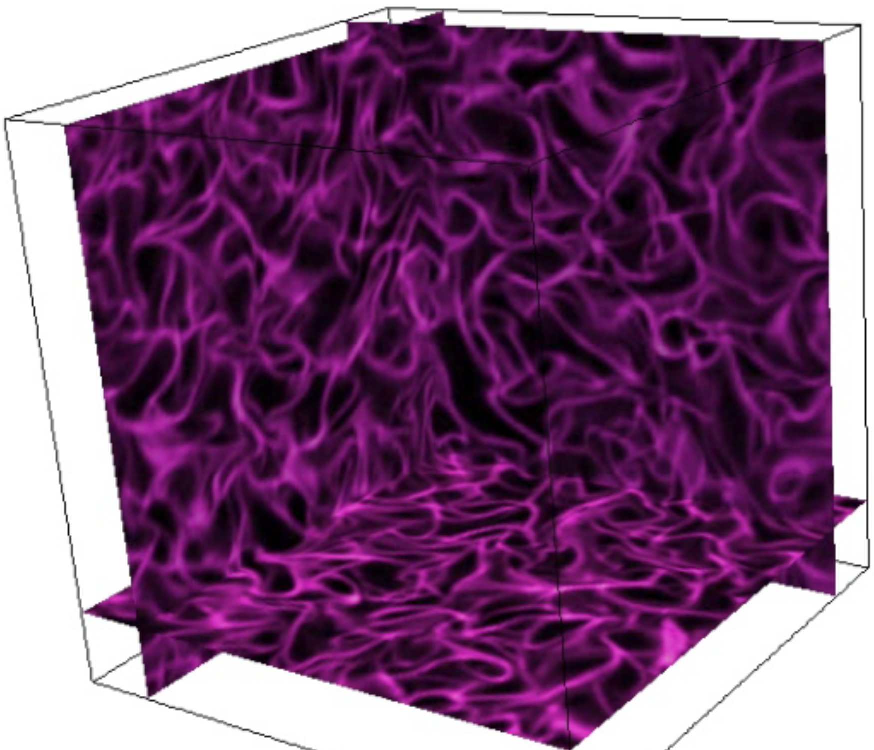


t = 9,48 ms

Pointillés : Eulérien, Ligne : Lagrangien

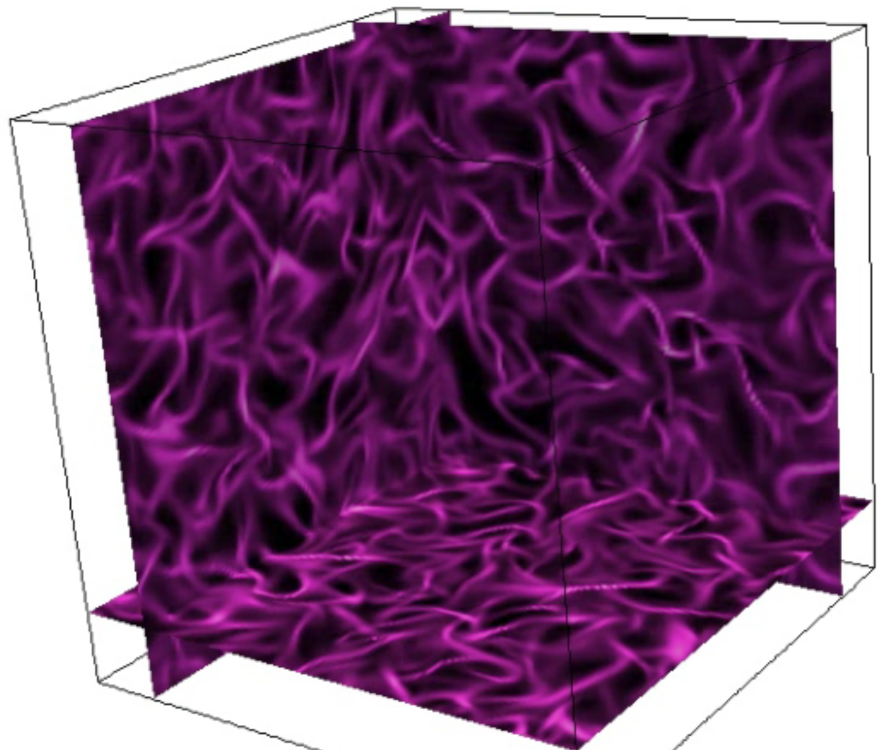
Polydisp. 3D spray flame – detailed dynamics comparisons

Lagrangian



Asphodele code (CORIA - CNRS UMR)
Muses3d code (EM2C - CNRS ECP)

Eulerian



Thomine, Freret, Reveillon & Massot

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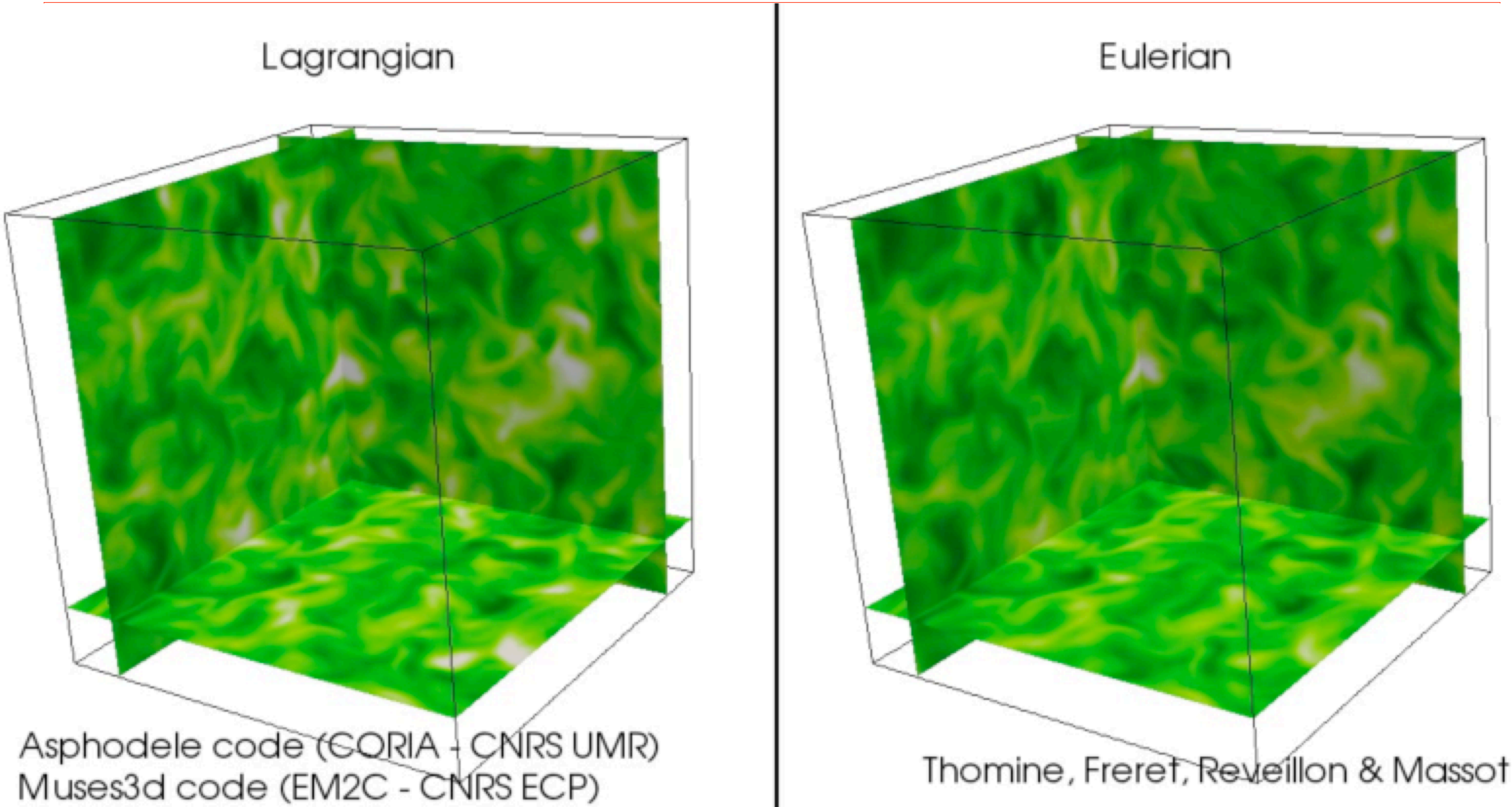
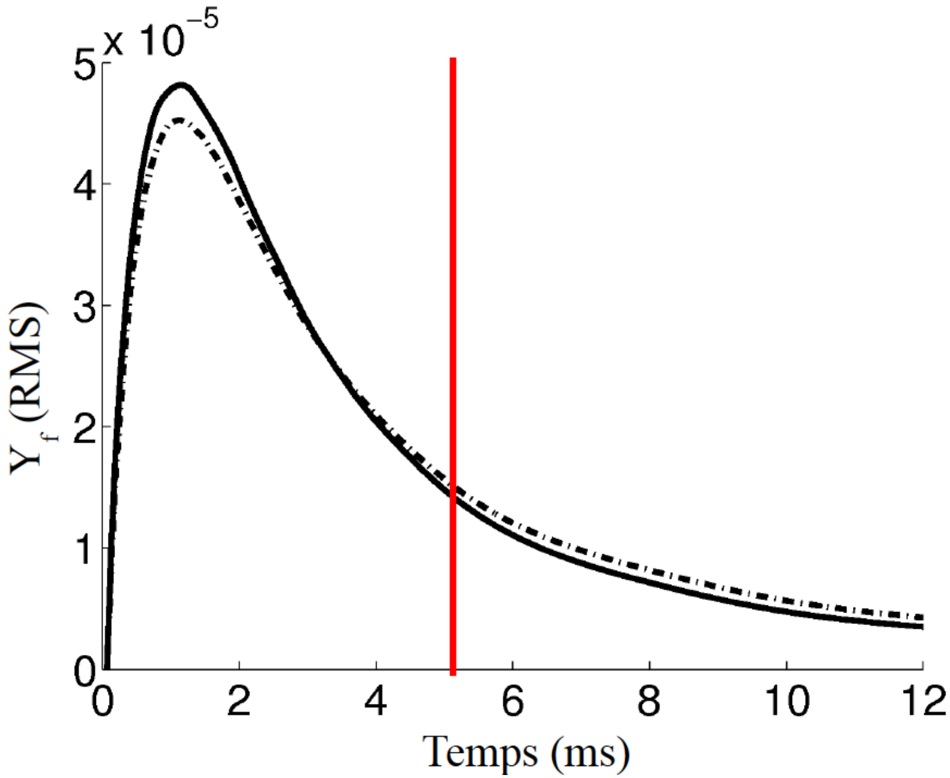
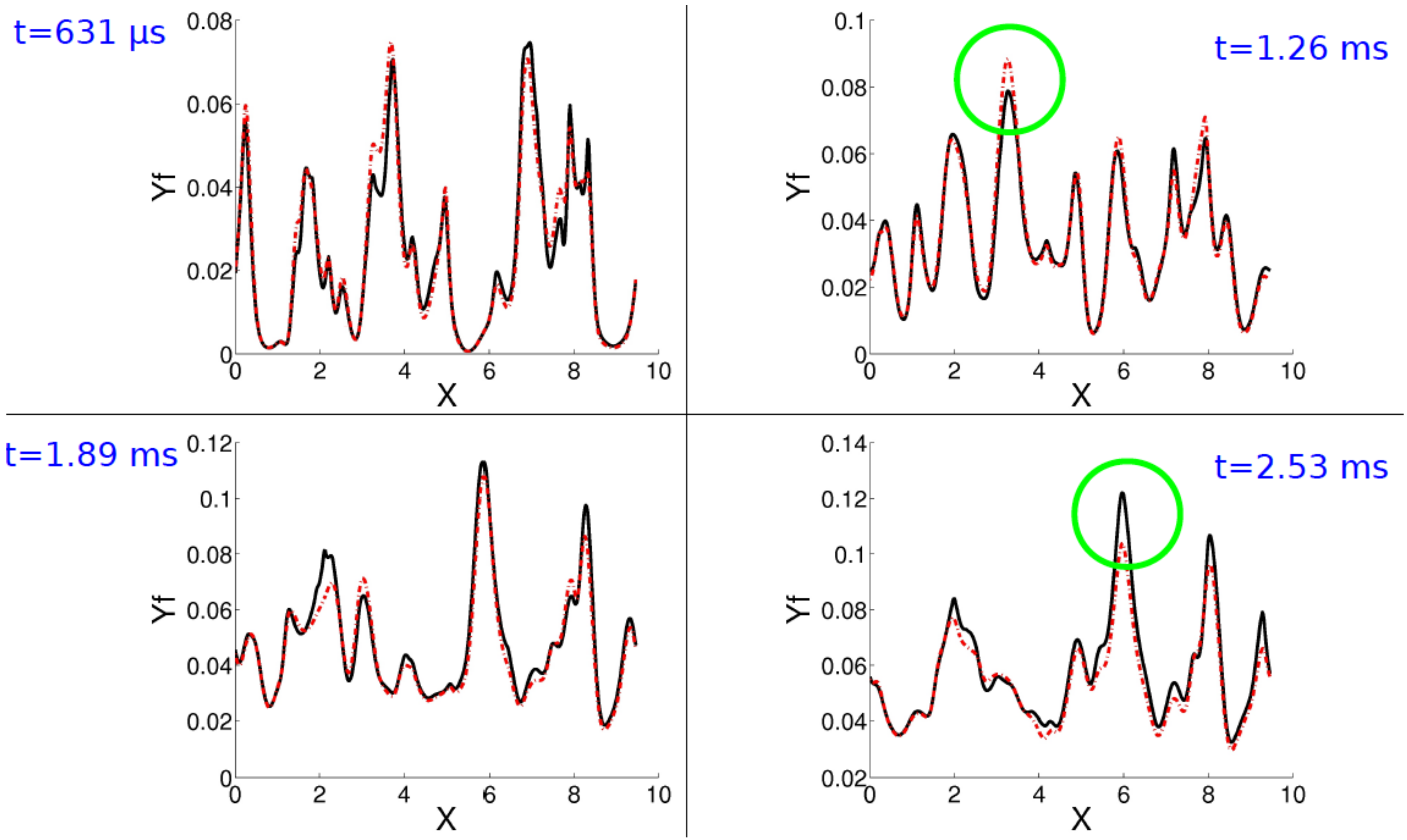
Polydisp. 3D spray flame – detailed dynamics comparisons



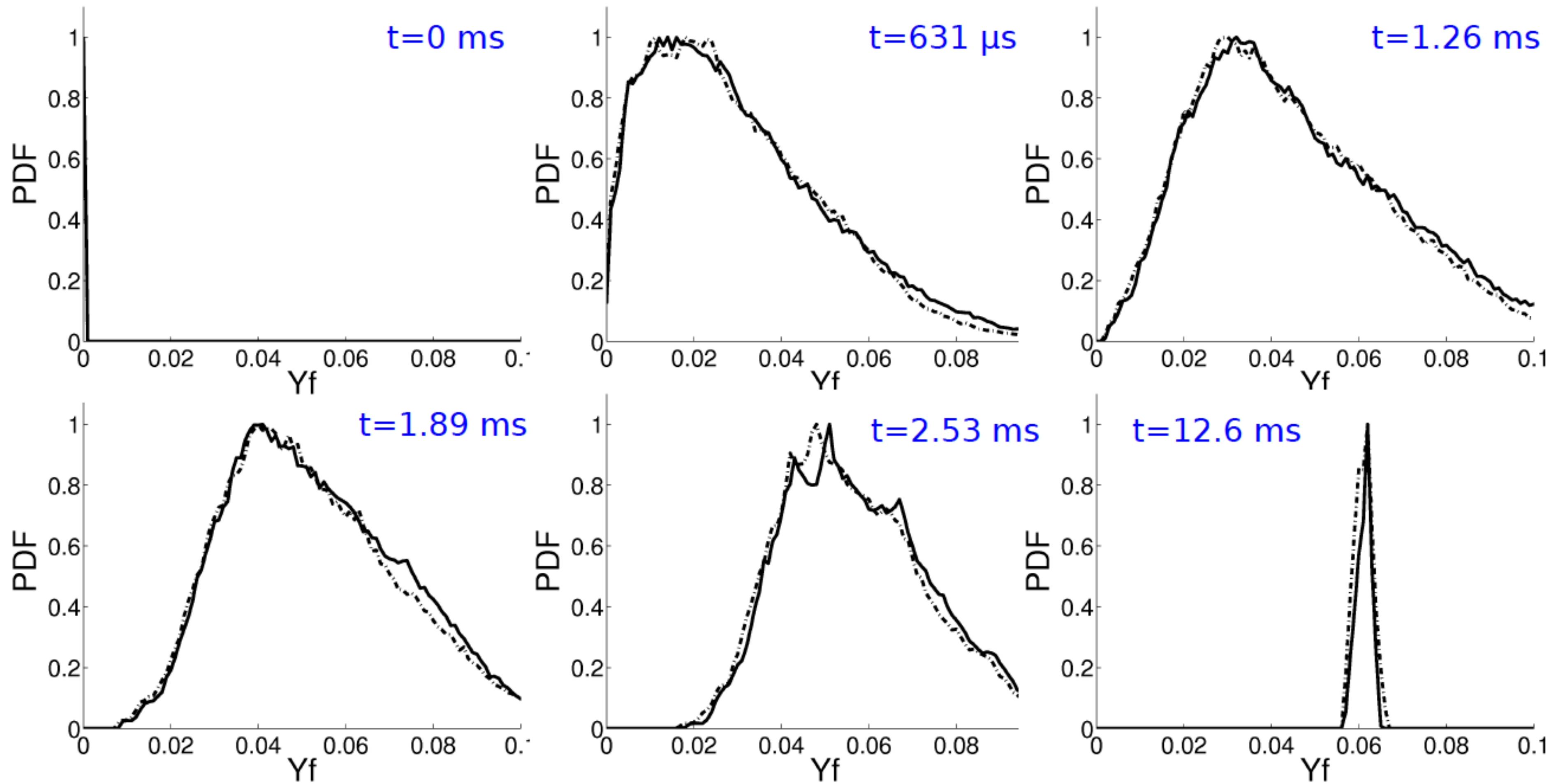


Pointillé: Eulérien

Ligne : Lagrangien



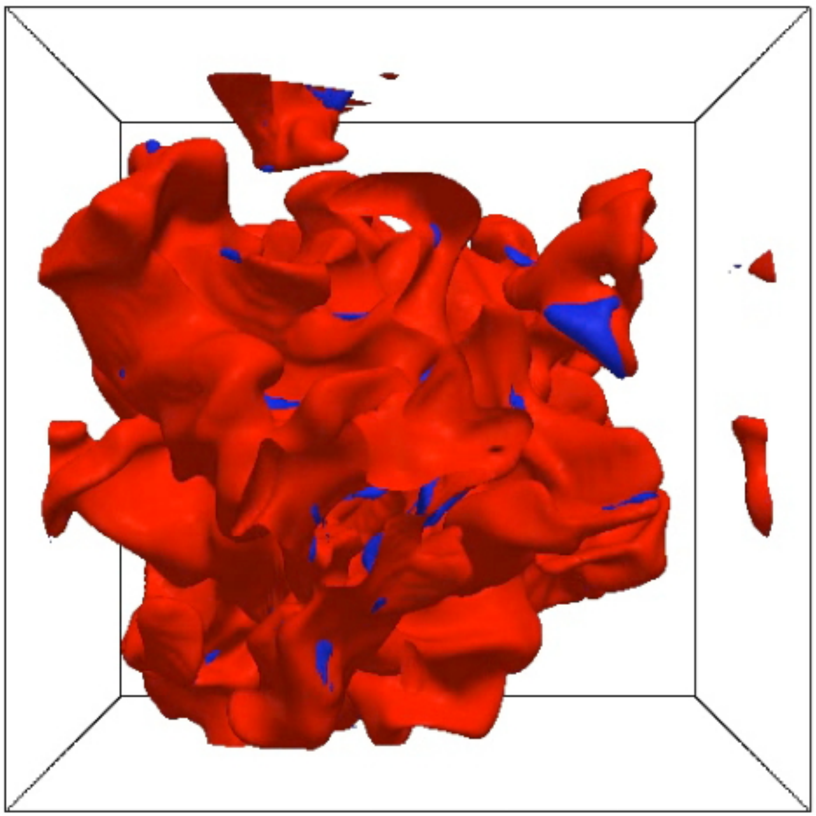
t=631 µs
t=1.26 ms
t=1.89 ms
t=2.53 ms
Yf
X
0.08
0.06
0.04
0.02
0
0.1
0.12
0.14
0
2
4
6
8
10


t=0 ms
t=631 µs
t=1.26 ms
t=1.89 ms
t=2.53 ms
t=12.6 ms
PDF
Yf
0
0.2
0.4
0.6
0.8
1
0.02
0.04
0.06
0.08
0.1

Polydisp. 3D spray flame – detailed dynamics comparisons

Euler-Euler - 3D – **Polydisperse** – Flame front (iso – T) – iso YF

Lagrangian



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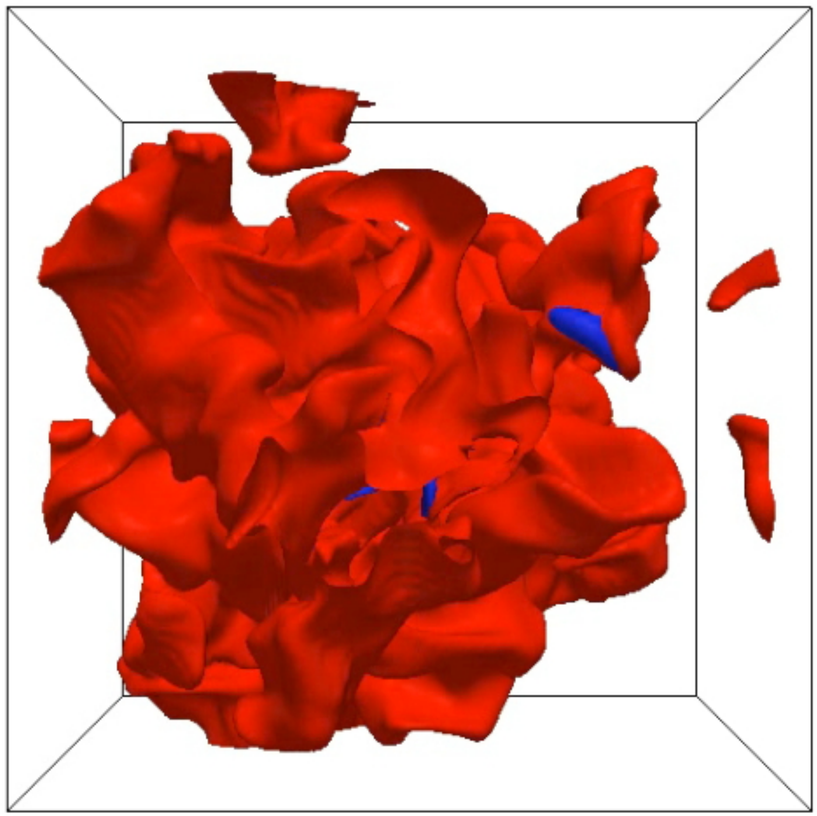
Eulerian



Thomine, Freret, Reveillon & Massot

Achievements – Low Stokes numbers

- Development of the parallel version of the coupled code ASPHODELE/MUSES3D
- Simulations on the CTR Cluster and CNRS National Centers IDRIS and CINES up to 1024 cores for 256^3 / 512^3 with 10 sections in polydisperse simulations with efficiency 1

- Excellent level of comparison for the dynamics of the spray for various Stokes numbers as well as

Polydisperse spray Combustion dynamics

Proper level of modeling coupled to robust / accurate / highly parallelizable numerical schemes

---

- Validation of the numerical method for the Eulerian model able to cope with singularities (hyper-compressibility) with a very limited amount of numerical diffusion

EXTENSIONS

1- Polydispersity with high order moment methods for computational cost

PhD of D. Kah (2010) – A. Vié (2011-2013)

PhD of O. Emre (2014) and M. Essadki (2017) - IFPEn

2- Particle trajectory crossing and Eulerian modeling hierarchy of high order moments - A. Vié, A. Larat, F. Laurent, C. Chalons, R.O. Fox

PhD of M. Sabat (2016) and D. Mercier (2018) - IMFT

3- Coalescence / Break-up and alumina particle in Rocket Boosters

PhD of F. Doisneau (2013) – PhD of V. Dupif (2017) – F. Laurent - ONERA

Evaporation / Combustion of aluminum particles

Thesis of A. Sibra (2014) – F. Laurent - ONERA

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Eulerian Multi-Size Model: Modeling (Thesis D. Kah 2010)

High order moment model : 4 size moments per section

Switch from several sections (10) where one mass moment is transported, to a single / few sections where 4 surface moments are conserved and transported:

! **Realizability condition – notion of moment space**

$$m_k(t,x) = \int_{S_{\min}}^{S_{\max}} S^k n(t,x,S)\mathrm{d}s$$

Evaporation leads to a disappearance flux at lower boundary

- We must reconstruct the flux at zero size from the knowledge of moments
- Entropy Maximization
- Design of dedicated numerical schemes for evaporation

EMSM model - General resolution strategy

Moment equation system

We aim at solving the following system:

$$\begin{aligned}
\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) &= -Kn(t, \boldsymbol{x}, S = 0) \\
&\vdots \\
\partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) &= -KN m_{N-1} \\
\partial_t m_1 \boldsymbol{u}_p + \underbrace{\nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p)}_{\text{advection}} &= \underbrace{-K m_0 \boldsymbol{u}_p}_{\text{evaporation}} - \nabla_{\boldsymbol{x}} P + \underbrace{\boldsymbol{D}}_{\text{drag}}
\end{aligned}$$

EMSM model - General resolution strategy

Moment equation system

We aim at solving the following system:

$$\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) = -K n(t, \boldsymbol{x}, S = 0)$$

$$\vdots$$

$$\partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) = -K N m_{N-1}$$

$$\partial_t m_1 \boldsymbol{u}_p + \underbrace{\nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p)}_{\text{advection}} = \underbrace{-K m_0 \boldsymbol{u}_p}_{\text{evaporation}} - \nabla_{\boldsymbol{x}} P + \underbrace{\boldsymbol{D}}_{\text{drag}}$$

Unclosed terms

- $f(t, \boldsymbol{x}, S, \boldsymbol{u}) = n(t, \boldsymbol{x}, S)\delta(\boldsymbol{u} - \boldsymbol{u}_p)$ $\Rightarrow$ $P = 0$ (velocity dispersion)
- $n(t, \boldsymbol{x}, S = 0) = \Phi(m_0, ..., m_N)(t, \boldsymbol{x})$ pointwise value of the size NDF

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EMSM model - General resolution strategy

- Operator splitting strategy *(Descombes and Massot 04)*

to treat each operator with a dedicated scheme: limit diffusion

- Successive resolution of
  - Evaporation
  - Advection
  - Drag

$$\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) = -Kn(t, \boldsymbol{x}, S = 0)$$

$$\vdots$$

$$\partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) = -Km_{N-1}$$

$$\partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) = -Km_0 \boldsymbol{u}_p + \boldsymbol{D}$$

EMSM model - General resolution strategy

- Operator splitting strategy *(Descombes and Massot 04)* to treat each operator with a dedicated scheme: limit diffusion
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  - Drag

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$$\vdots$$

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Topics discussed during this presentation

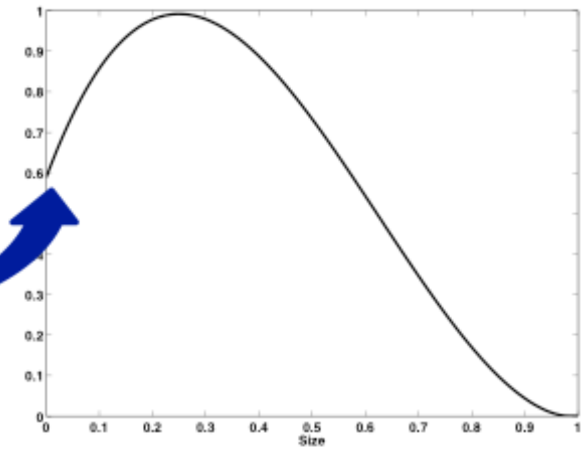
- **EMSM model: Modeling and numerical tools**
  - General resolution strategy
  - Evaporation term resolution
  - Advection term resolution

- **Evaluation of the EMSM model**
  - Quantitative validation
  - Comparison with the MF model

Continuous problem

- Closure of $Kn(t, \boldsymbol{x}, S = 0)$ = evaporation flux
- The challenge is to reconstruct, from the data of the moments, a point-wise value of the size NDF

$$\boldsymbol{m}_N = (m_0, \ldots, m_N)^t$$



- Stability condition : moment space preservation

Moment space

- The vector $\boldsymbol{m}_N = (m_0, \ldots, m_N)^t$ belongs to moment space $\mathbb{M}_N$
- $\mathbb{M}_N$ has a complex geometry

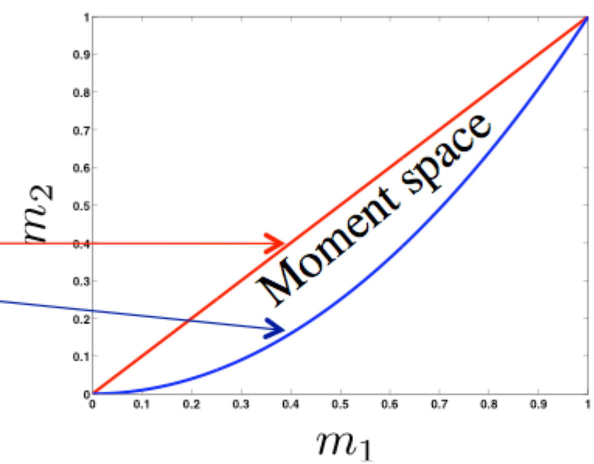
Example of moment space geometry

- Set of PDF such as $m_0 = \int_0^1 n \, \mathrm{d}S = 1$, on [0,1]
- Condition on m_1 and m_2

$$m_1 = \int_0^1 S \, n \, \mathrm{d}S, \quad 0 < m_1 < 1$$

$$m_2 = \int_0^1 S^2 \, n \, \mathrm{d}S, \quad \underbrace{m_1^2}_{\text{low border}} < m_2 < \underbrace{m_1}_{\text{high border}}$$

Moment space structure



- **Realizable condition**

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Continuous problem

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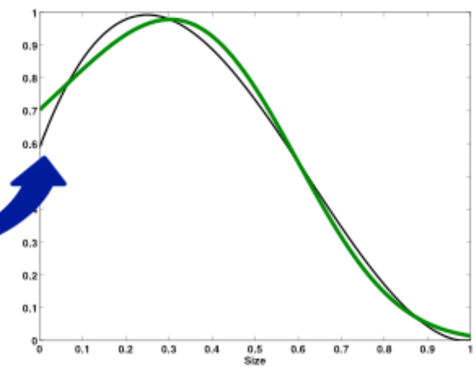


- Stability condition : moment space preservation:

Realizable condition

Solution

Approximation of the size NDF by **Maximization of Entropy** *(Mead 84)*

$$\boldsymbol{m}_N = (m_0, \ldots, m_N)^t \Rightarrow \tilde{n}_{ME}$$

Challenge for the discrete problem

Evaporation system **cannot** be solved by ODE solvers

⚠ **Realizable condition**

Solution

- Finite volume scheme
- Exact temporal integration
- Flux calculation: kinetic scheme

- The kinetic scheme lies on the equivalence between the two equations:
  - kinetic (or semi-kinetic): $\partial_t n - \partial_S (K\, n) = 0$
  - macroscopic: $$\mathrm{d}_t \boldsymbol{m}_N = -\mathbf{A}\, \boldsymbol{m}_N - \boldsymbol{\phi}_-$$

Principle of a kinetic scheme

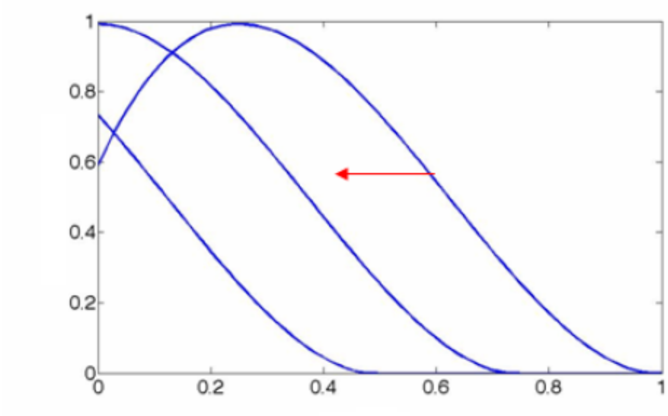
$$\begin{array}{ccc} \boldsymbol{m}_N(0) & & \boldsymbol{m}_N(\Delta t) \\ \downarrow & & \uparrow \\ \tilde{n}_{ME}(0,S) & \xrightarrow[\Delta t]{\text{exact evolution}} & \tilde{n}_{ME}(\Delta t, S) \end{array}$$

- $\tilde{n}_{ME}$ is reconstructed from $\boldsymbol{m}_N$
- $\tilde{n}_{ME}(\Delta t, S)$ is computed from $\tilde{n}_{ME}(0,S)$ through the kinetic equation
- Fluxes of $\boldsymbol{m}_N$ are computed using $\tilde{n}_{ME}(\Delta t, S)$

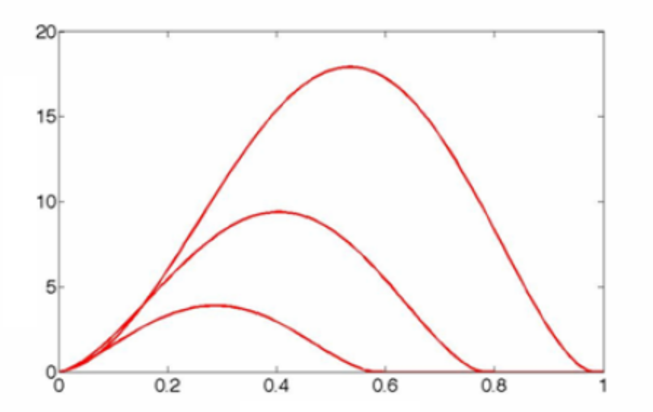
EMSM model: Evaporation Verification

Solved kinetic equation : $\partial_t n + \partial_S R_S n = 0$, with $R_S = -1$

- Analytical solution :



number density



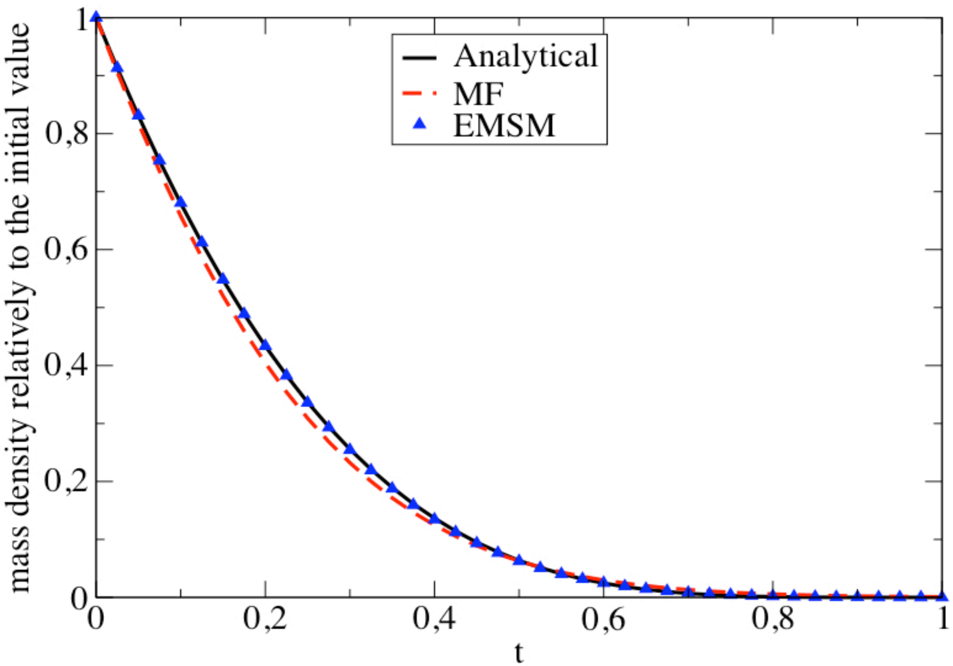
mass density

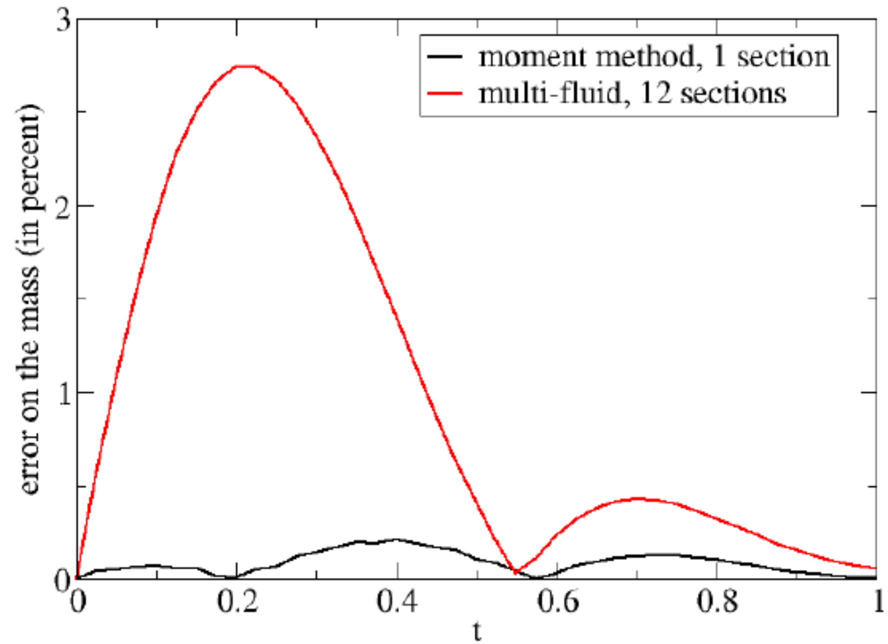
Comparison between EMSM and MF models

- MF model: $m_{3/2}$ - 1 moment and 12 sections
- EMSM model: $m_k, k = 0, \ldots, 3$ - 4 moments and 1 section

EMSM model: Evaporation Validation

- **Results**





- Very good level of comparison (less than 1% error on the 4 moments)

EMSM with 1 section more precise than MF with 12 sections

EMSM: Evaporation Conclusion

- **Stable and accurate scheme for evaporation flux**

  Design of

  - **theoretical tool (Maximization of Entropy)**
  - **numerical tool (kinetic scheme)**

- **EMSM model with 1 section more precise than the MF model with 12 sections**

- **EMSM model and numerical tools extendable to**
  - **arbitrary evaporation laws**
  - **formalism with several sections**

EMSM model: Advection term resolution

Purpose

Design a high order advection scheme for the system:

$$\begin{aligned}\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) &= 0\\ &\vdots\\ \partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) &= 0\\ \partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) &= 0\end{aligned}$$

dimensional splitting

Resolved system

1D system:

$$\begin{aligned}\partial_t m_0 + \partial_x(m_0 u_p) &= 0\\ &\vdots\\ \partial_t m_N + \partial_x(m_N u_p) &= 0\\ \partial_t m_1 u_p + \partial_x(m_1 u_p^2) &= 0\end{aligned}$$

Challenges

- Pressureless gas dynamics (PGD)– delta choc, vacuum zones

  Dedicated scheme designed in *(de Chaisemartin, PhD 09)* from the kinetic scheme *(Perthame 02, Bouchut 03)* and using dimensional splitting
- **Realizability condition**

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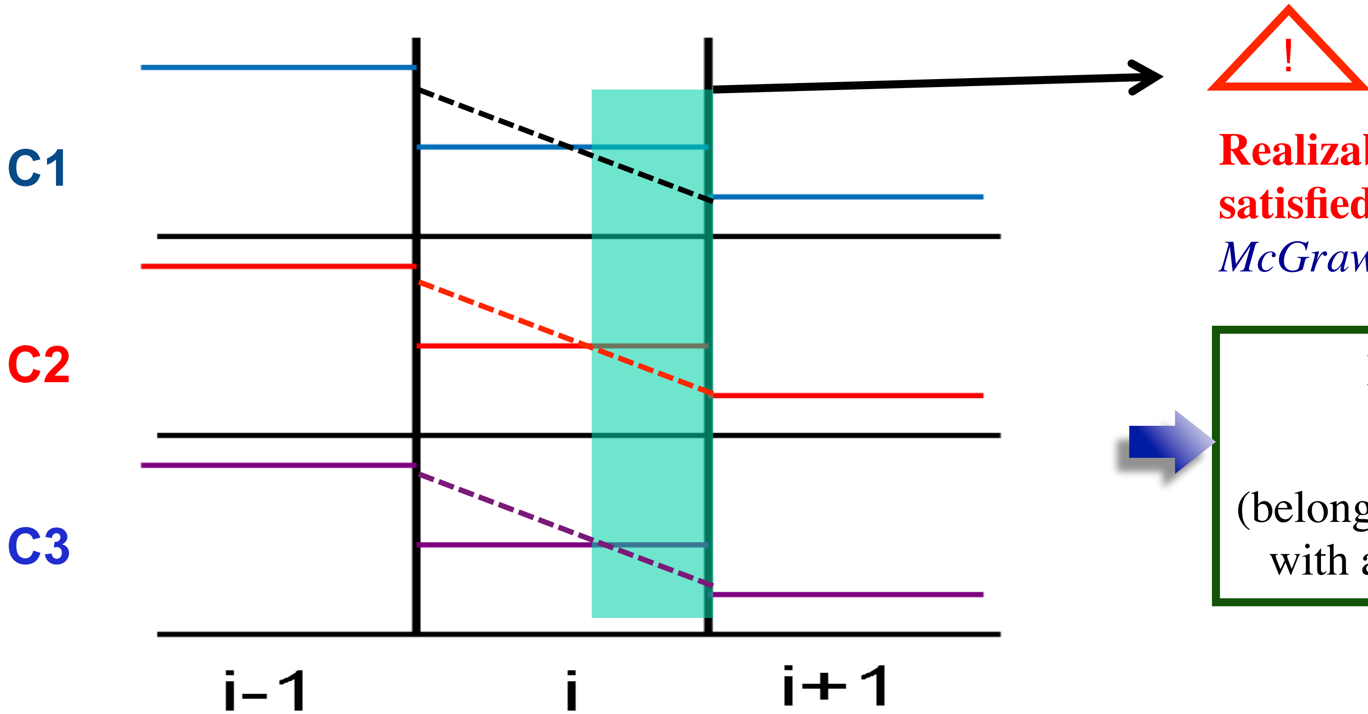
EMSM model: Advection term resolution

Realizability condition

- **Considering normalized moments** $$c_k = \frac{m_k}{m_0}, \; k = 1, \ldots, N$$
  the ck are transported quantities as they verify $$\partial_t c_k + u_p \partial_x c_k = 0$$
- **Independent reconstruction of the c_k , with slope limiters**



Realizability condition might not be satisfied in the whole cell *(Wright 07, McGraw 07)*

Moment space theory

Canonical moments

(belong to canonical moment space, with a cubic geometry $[0, 1]^N$)

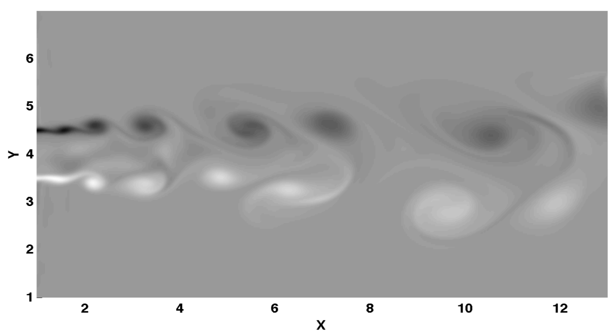
Comparison with the MF model : Free jet test case

Case run with Muses3D coupled with Asphodele *(Reveillon 07)*

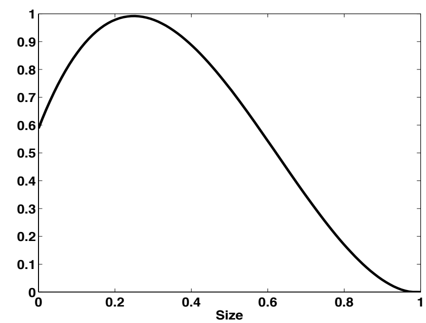
- Complex case: injected turbulence in the gas phase
- Time resolved dynamics, compared to the MF model

Presentation of the configuration

- Gas vortices field at time t=20



- Size NDF for the droplet



- $\mathrm{St}_{max} = 0.75$
- Comparison of $m_{3/2}, Y_F$ (evaporated fuel mass fraction)

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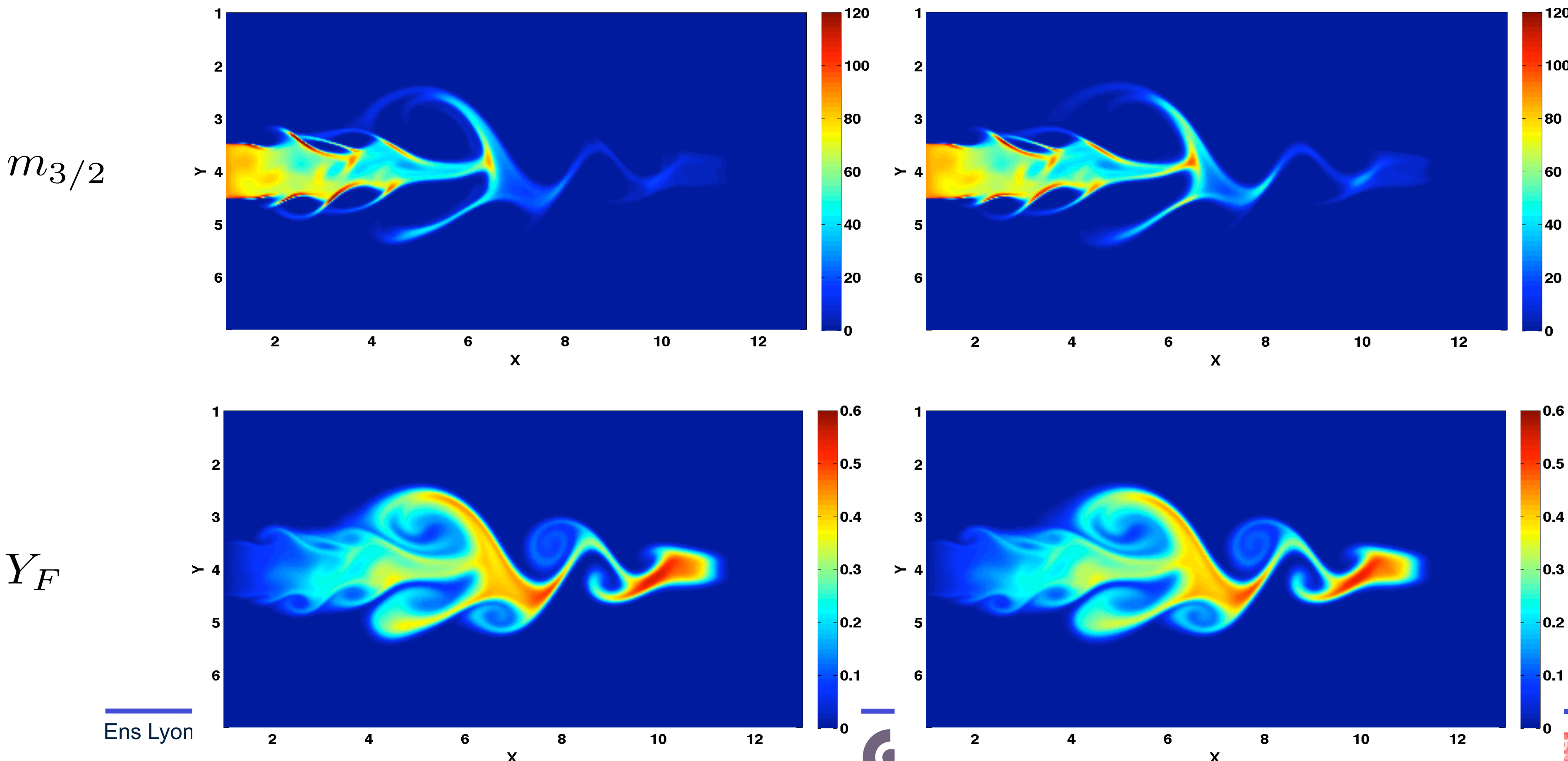
Comparison with the MF model : Free jet test case

Results at t =10

EMSM model

MF model



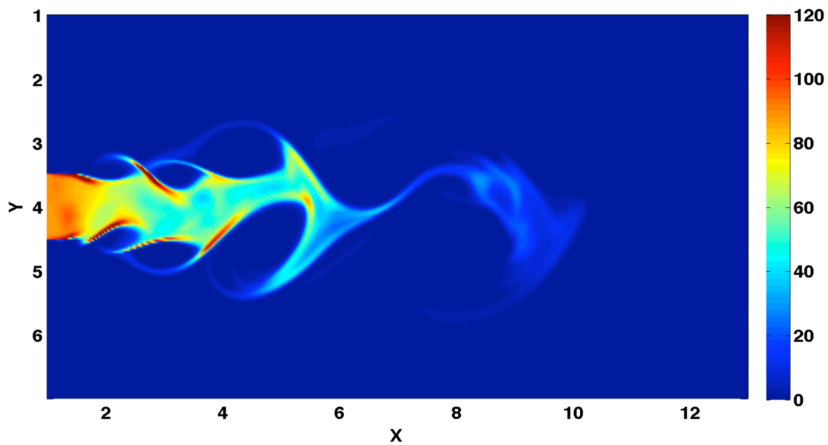
Comparison with the MF model : Free jet test case

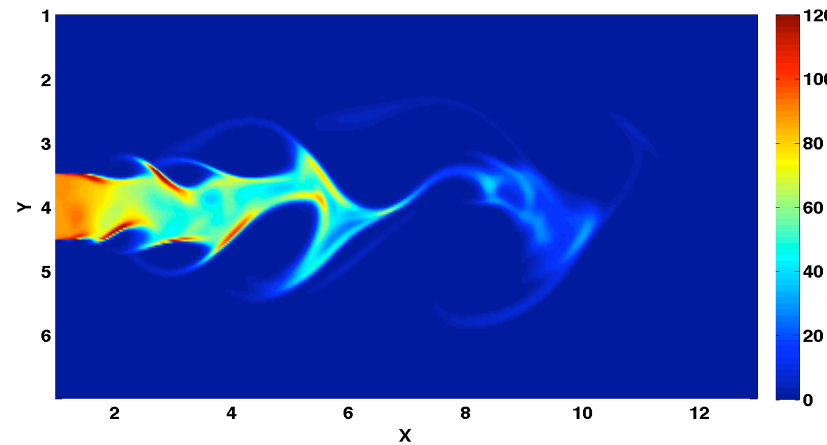
Results at t =15

EMSM model

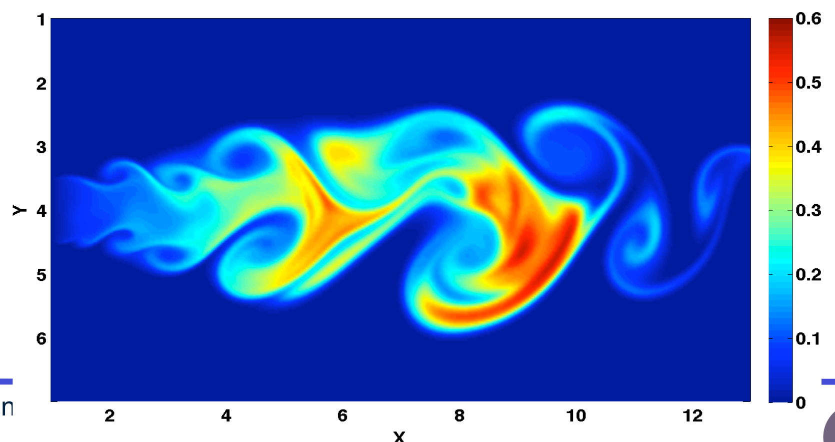
MF model

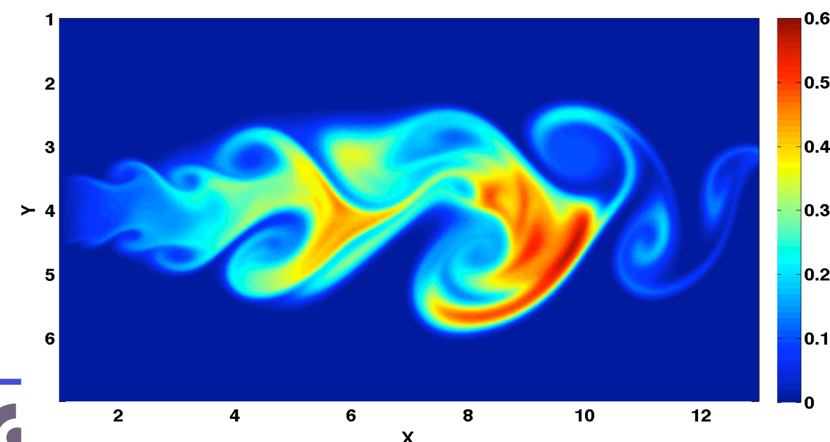
$m_{3/2}$





Y_F





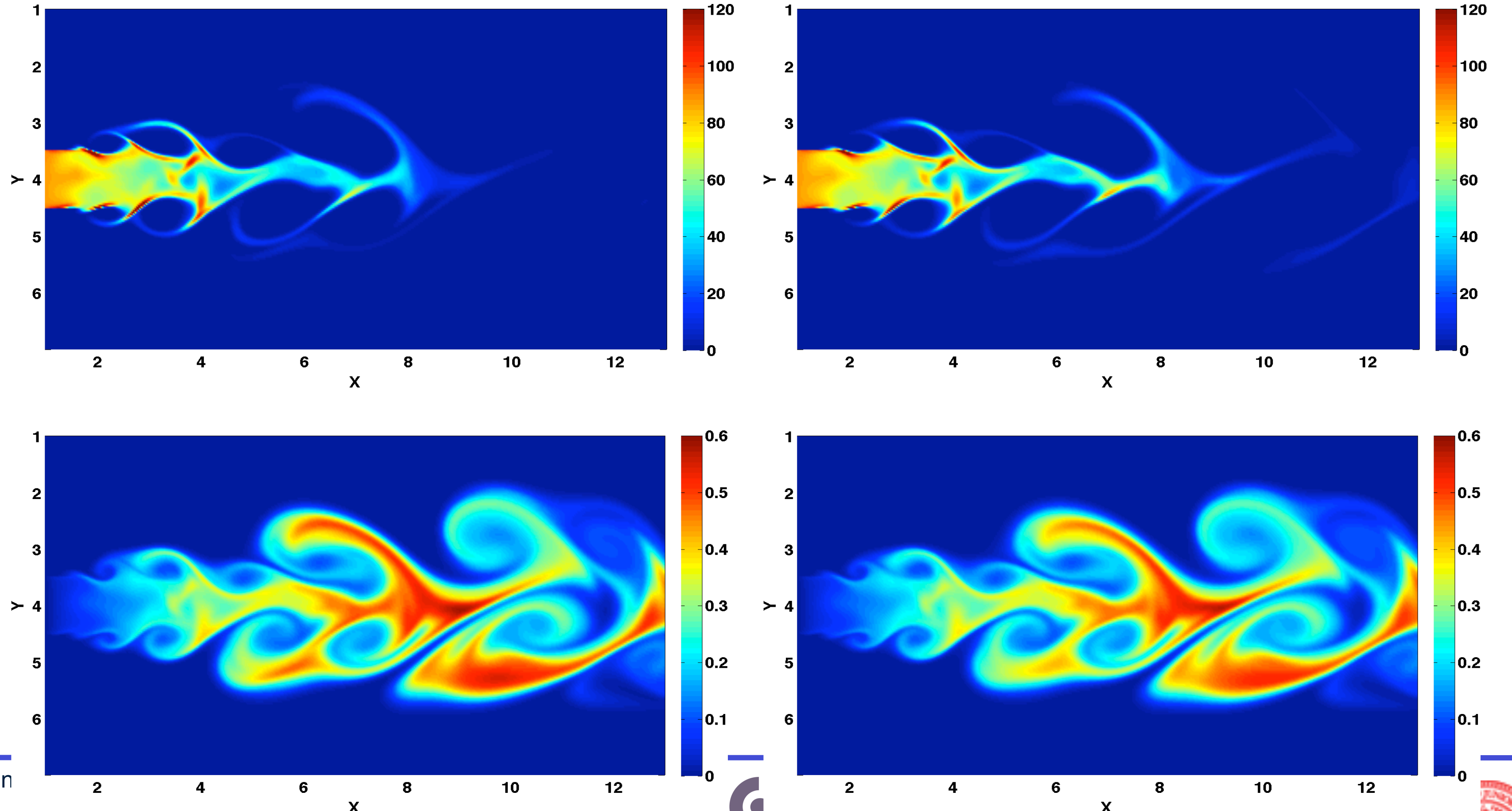
Comparison with the MF model : Free jet test case

Results at t =20

- **EMSM model**
- **MF model**

$m_{3/2}$

Y_F



Free jet case : Conclusions

- **Jet dynamics resolved with ONE section**
  - High order moment method, with
  - high order advection scheme

➡ **Transport of a moment set enforcing the realizability condition**

this difficulty has been stated in *(wright07, mcgraw07)* ***Kah et al. JCP 2012***

- Excellent level of comparison with the MF model

➡ **Verification of the EMSM model and numerical tools**

- In terms of CPU time

  2D case of evaporating spray dynamics in Taylor-Green vortices

➡ **EMSM 4 times faster than Multi-Fluif in 2D – Computationally efficient**

- **Efficient, accurate and robust approach for automotive engines**

Kah, et al *IJMF 2015* - Emre et al *A&S 2015*

Automotive engines (fruitful collaboration with IFPEn)

- **Extended to Unstructured meshes and moving grids**

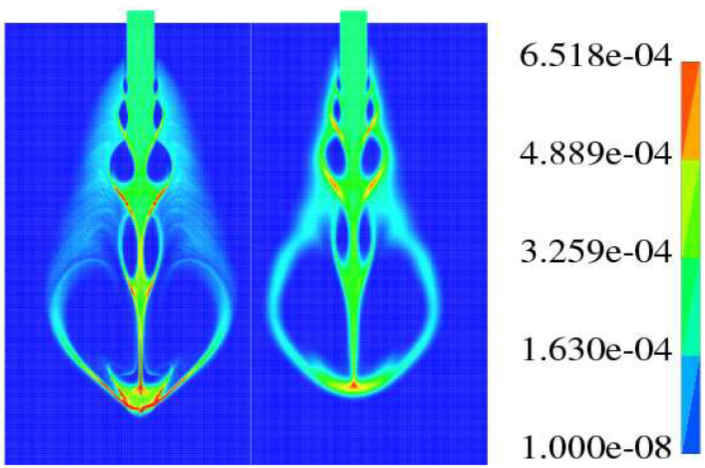
Kah et al. ICMF 2010, Kah, et al IJMF 2015

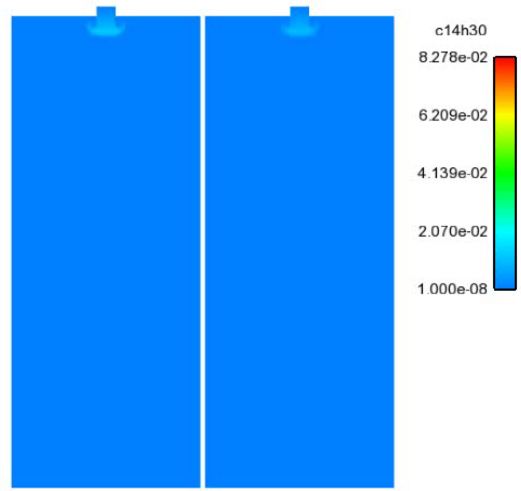
- **Extended to RANS modeling with consistent two-way coupling**

Emre FTC 2014 - Emre et al. JCP 2015

- **Implemented in IFPC3D Code at IFPEn**

Emre FTC 2014 - Emre et al. A&S 2015





EXTENSIONS

1- Polydispersity with high order moment methods for computational cost

PhD of D. Kah (2010) – A. Vié (2011-2013)

PhD of O. Emre (2014) and M. Essadki (2017) - IFPEn

2- Particle trajectory crossing and Eulerian modeling hierarchy of high order moments - A. Vié, A. Larat, F. Laurent, C. Chalons, R.O. Fox

PhD of M. Sabat (2016) and D. Mercier (2018) - IMFT

3- Coalescence / Break-up and alumina particle in Rocket Boosters

PhD of F. Doisneau (2013) – PhD of V. Dupif (2017) – F. Laurent - ONERA

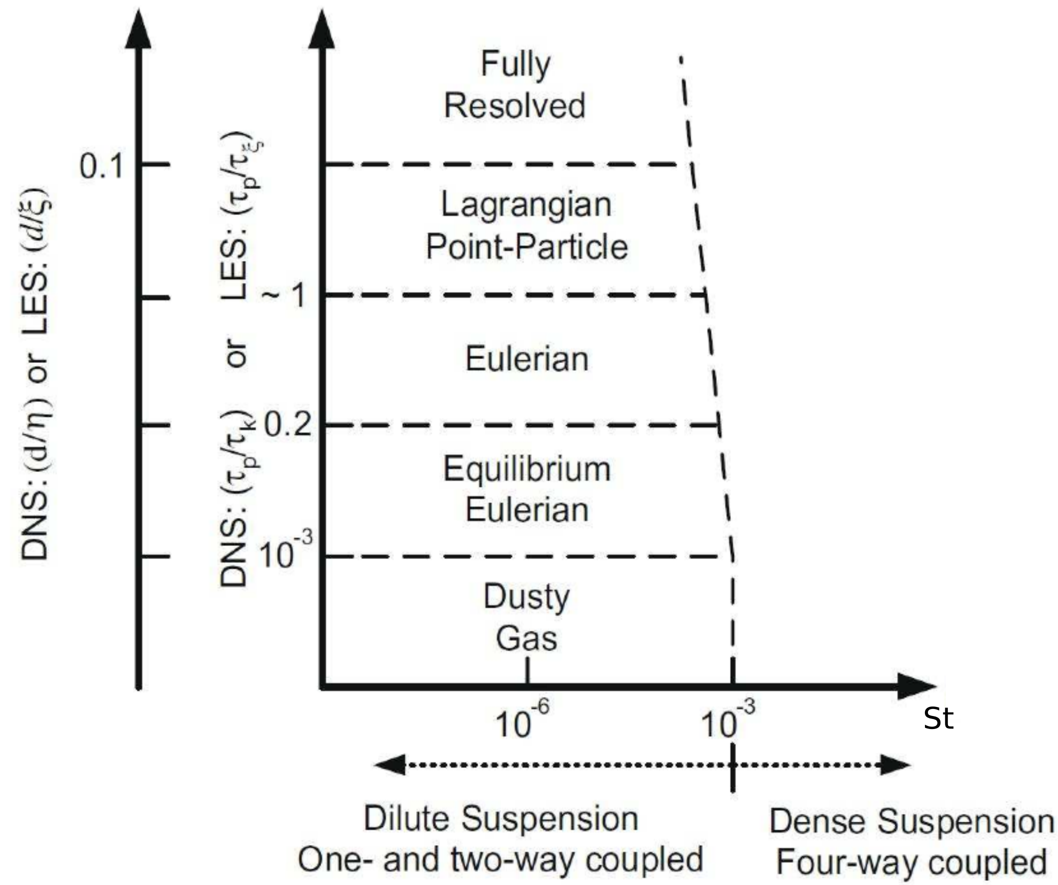
Evaporation / Combustion of aluminum particles

Thesis of A. Sibra (2014) – F. Laurent - ONERA

Turbulent particulate flows: modeling strategies

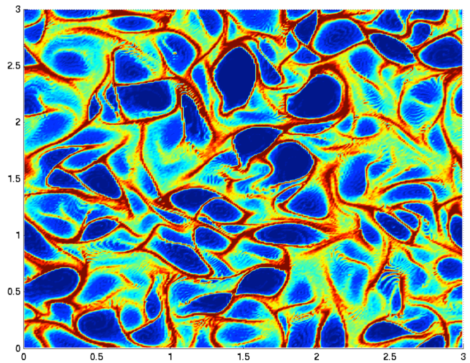
- **Following Balachandar and Eaton, Eulerian methods are suitable only for small Stokes number**

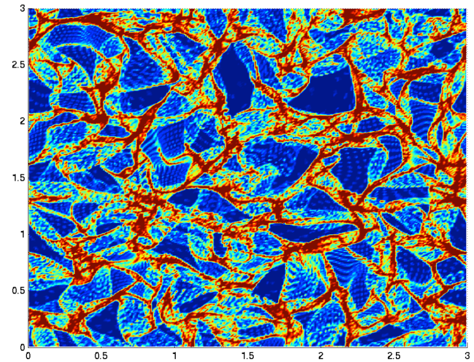
- **The limitation is due to the occurrence of particle trajectory crossings**

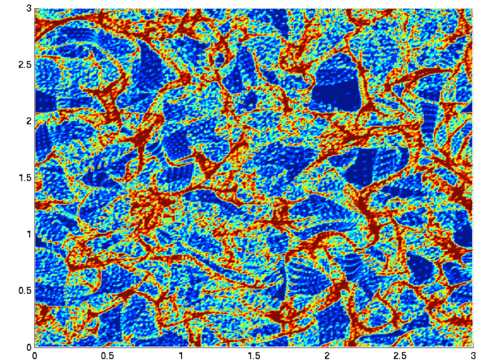


S. Balachandar and J.K. Eaton, Annual Review of Fluid Mechanics, 42, pp. 111-133, 2010

Turbulent particulate flows modeling: PTC







0 | 1 | 10 | **Stokes Number**

No trajectory crossing	Small-scale trajectory crossing	Large-scale trajectory crossing
Eulerian multi-fluid model Equilibrium Eulerian	ACBMM KBMM – ANISO	KBMM-CQMOM KBMM-Multi-Gaussian

CTR Summer Program 2012

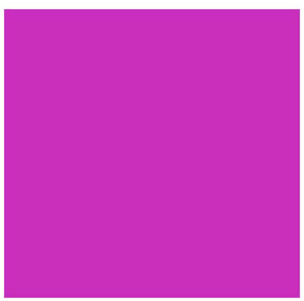
Comparison of the strategies developed at IMFT and at EM2C - A. Vié, et al.

Turbulent particulate flows modeling: PTC

0 — 1 — 10 — St

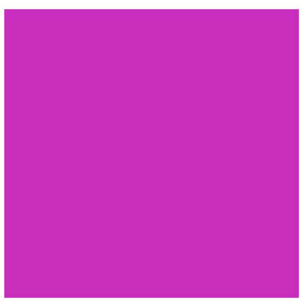
St < 1	1 < St < 10	St > 10
No trajectory crossing	Small-scale modeled trajectory crossing	Large-scale trajectory crossing
Eulerian multi-fluid model	ACBMM (IMFT) Anisotropic Gaussian (EM2C)	CQMOM Multi-Gaussian

Lagrangian



Asphodele code (CORIA - CNRS URM 6614)
Muses3d code (EM2C - CNRS ECP)

Eulerian



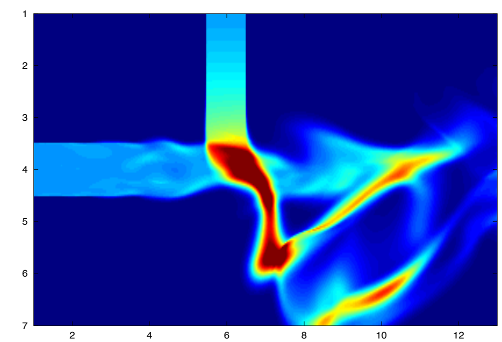
Thomine, Freret, Reveillon & Massot

Lagrangian

Asphodele code (CORIA - CNRS URM 6614)
Muses3d code (EM2C - CNRS ECP)

Eulerian

Thomine, Freret, Reveillon & Massot



Eulerian modeling of sprays

Simplified population balance equation:

$$\partial_t f + \mathbf{c}_p \cdot \partial_{\mathbf{x}} f + \partial_{\mathbf{c}_p} \cdot (\mathbf{F} f) = 0$$

$f(t, \mathbf{x}, \mathbf{c}_p)$ = the number density function which lies in a 4D space

$\mathbf{F} = \frac{1}{\mathrm{St}\tau_\eta}(\mathbf{u}_g - \mathbf{c}_p)$ = acceleration due to fluid drag

Eulerian approach

Track the moments of the NDF

$$M_{i,j} = \int c_{p,1}^{i} c_{p,2}^{j} f(t, \mathbf{x}, \mathbf{c}_p) \mathrm{d}\mathbf{c}_p$$

Solve a system of conservation laws

$$\partial_t M_{i,j} + \partial_{\mathbf{x}} \cdot \begin{pmatrix} M_{i+1,j} \\ M_{i,j+1} \end{pmatrix} = \frac{[i u_{\mathrm{g}} M_{i-1,j} + j v_{\mathrm{g}} M_{i,j-1} - (i+j) M_{i,j}]}{\mathrm{St}\tau_\eta}$$

Eulerian modeling of sprays

$$\partial_t M_{i,j} + \partial_{\mathbf{x}} \cdot \begin{pmatrix} M_{i+1,j} \\ M_{i,j+1} \end{pmatrix} = \frac{[iu_{\mathrm{g}} M_{i-1,j} + jv_{\mathrm{g}} M_{i,j-1} - (i+j)M_{i,j}]}{\mathrm{St}\tau_\eta}$$

Two major choices determine the Eulerian method

- *The number of moments to solve:* define the level of accuracy on the integral evaluation, i.e. on the NDF
- *The closure law for the unknown higher order moments:* define the behavior of the PDE system (physics, hyperbolicity, singularities…)

M00	**M10**	**M20**	**M30**	M40
M01	**M11**	**M21**	M31	
M02	**M12**	M22		
M03	M13			
M04				

A hierarchy of modeling approaches

M00	M10	M20	M30	M40
M01	M11	M21	M31	M41
M02	M12			
M03	M13			
M04	M14			

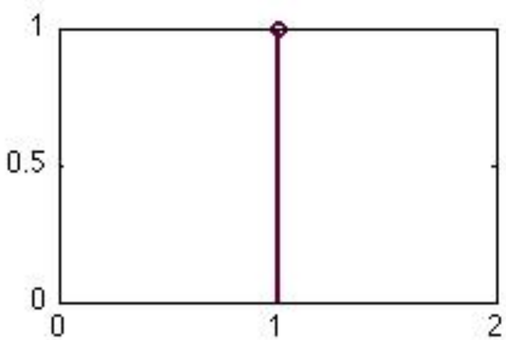
StK=0 **StK=1** **StL=1** *Stokes number*

Zeroth order

Equilibrium Eulerian

First order

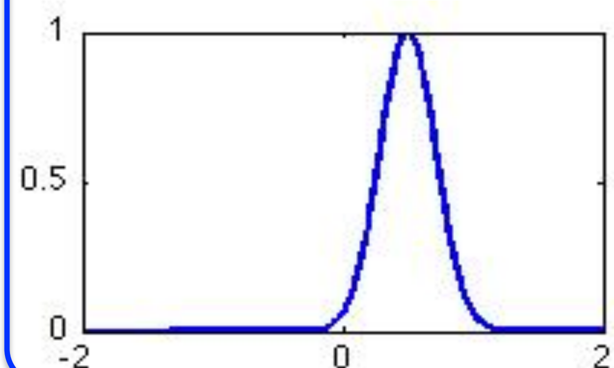
Monokinetic Assumption



Second order

2-Phi-EASM

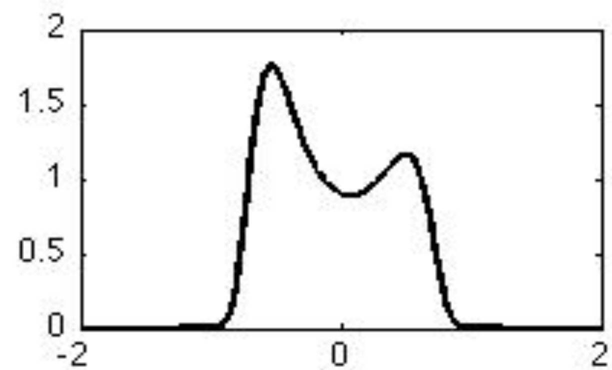
Anisotropic Gaussian



Third and fourth order moments

CQMOM

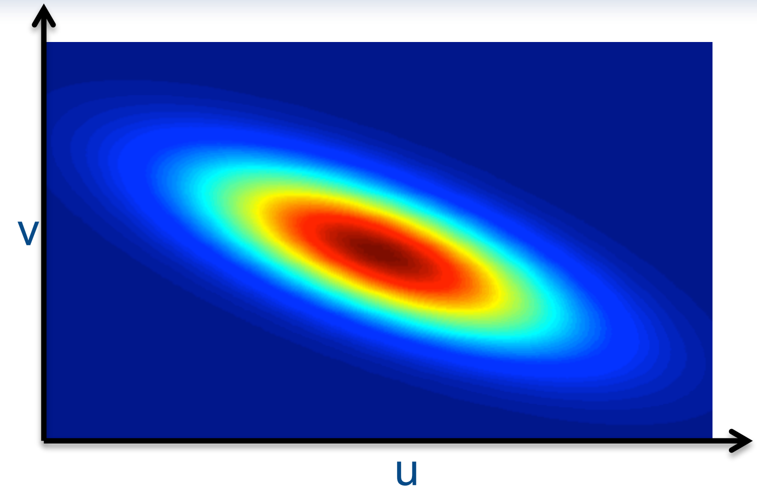
Multi-Gaussian



1 **3** **4** **6** **12** **17** *Moment number*

Second Order Moments

M00	**M10**	**M20**	M30	M40
M01	**M11**	M21	M31	
M02	M12	M22		
M03	M13			
M04				



- *The number of moments to solve:* ***6***

  all zero-to-second order moments

- *The closure law for the unknown higher order moment*:

  Anisotropic Gaussian Closure

$$f_G(t, x, \mathbf{c}_p) = \frac{n_p}{2\pi\sqrt{|\mathbf{R}_p|}} \exp\left(-(\mathbf{c}_p - \mathbf{u}_p)^T \mathbf{R}_p^{-1} (\mathbf{c}_p - \mathbf{u}_p)\right)$$

Vié et al., Communications In Computational Physics, 2015

Inversion algorithm and realizability conditions

INVERSION ALGORITHM

$$M_{00} = n_p$$

$$M_{10} = n_p u_p$$

$$M_{01} = n_p v_p$$

$$M_{20} = n_p \left(u_p^2 + R_{p,11} \right)$$

$$M_{11} = n_p \left(u_p v_p + R_{p,12} \right)$$

$$M_{02} = n_p \left(v_p^2 + R_{p,22} \right)$$

Simple relationships between moments and parameters of the distribution

REALIZABILITY CONDITIONS

$$n_p > 0$$

$$R_{p,11} > 0$$

$$R_{p,22} > 0$$

$$R_{p,11} R_{p,22} - R_{p,12}^2 > 0$$

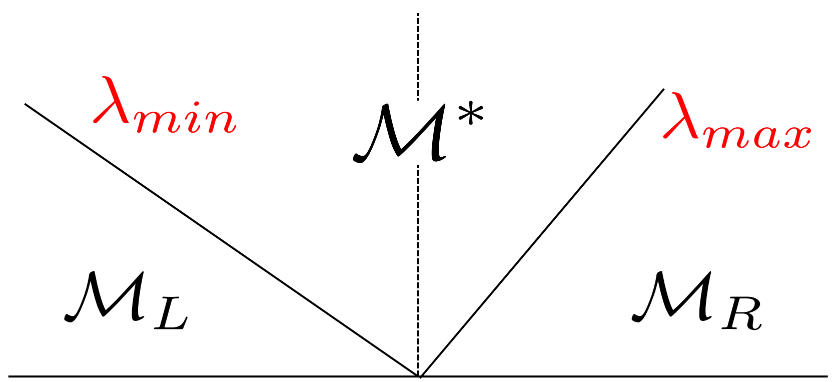
Positivity of the density, the energies and the determinant of the Gaussian distribution

A Second Order Transport scheme

$$\partial_t \mathcal{M} + \partial_{x_m} \mathcal{F}_m(\mathcal{M}) = 0$$

- **Hyperbolic system of equations**
- **Dimensional splitting**
- **Approximate Riemann solver : HLL scheme**

$$\mathcal{M}^* = \frac{\mathcal{M}_L - \mathcal{M}_R - (\mathcal{F}(\mathcal{M}_L) - \mathcal{F}(\mathcal{M}_R))}{\lambda_{min} - \lambda_{max}}$$



A Second Order Transport scheme

- **Second order approximation : MUSCL strategy**

$$\mathbf{U} = (n_p, u_p, v_p, R_{11}, R_{12}, R_{22})^T$$

- **Limited conservative and realizable linear reconstruction of central moments - Realizable**

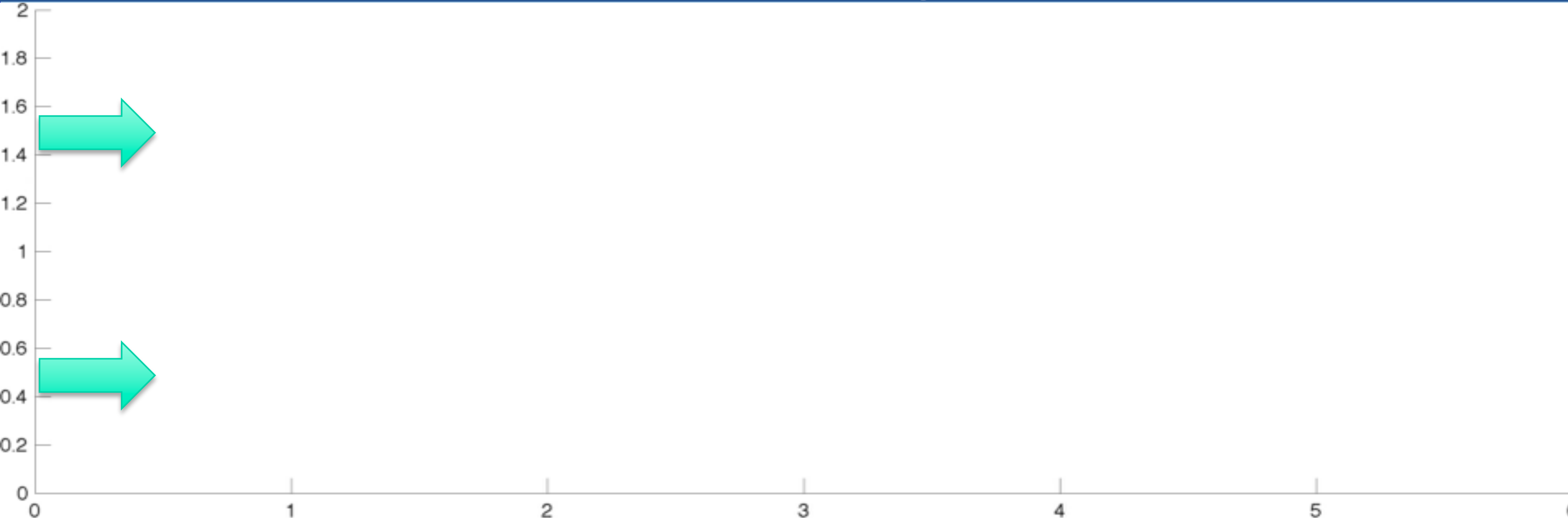
$$\mathbf{U}_j(x) = \overline{\mathbf{U}}_j + \mathbf{D}_{\mathbf{U}} x$$

- **2nd order Runge-Kutta time integration**

$$\mathcal{M}_j^{n+1/2} = \mathcal{M}_j^n - \frac{1}{2}\frac{\Delta t}{\Delta x}\left(\mathcal{F}_{j+1/2}^n - \mathcal{F}_{j-1/2}^n\right)$$

$$\mathcal{M}_j^{n+1} = \mathcal{M}_j^n - \frac{\Delta t}{\Delta x}\left(\mathcal{F}_{j+1/2}^{n+1/2} - \mathcal{F}_{j-1/2}^{n+1/2}\right)$$

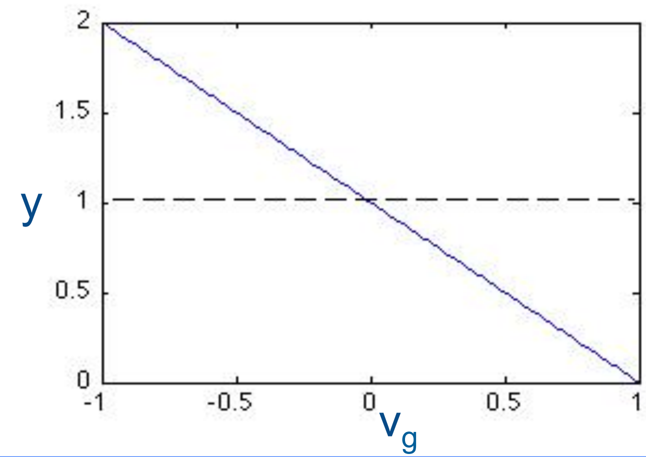
Two-jet configuration



- Gaseous compressive field

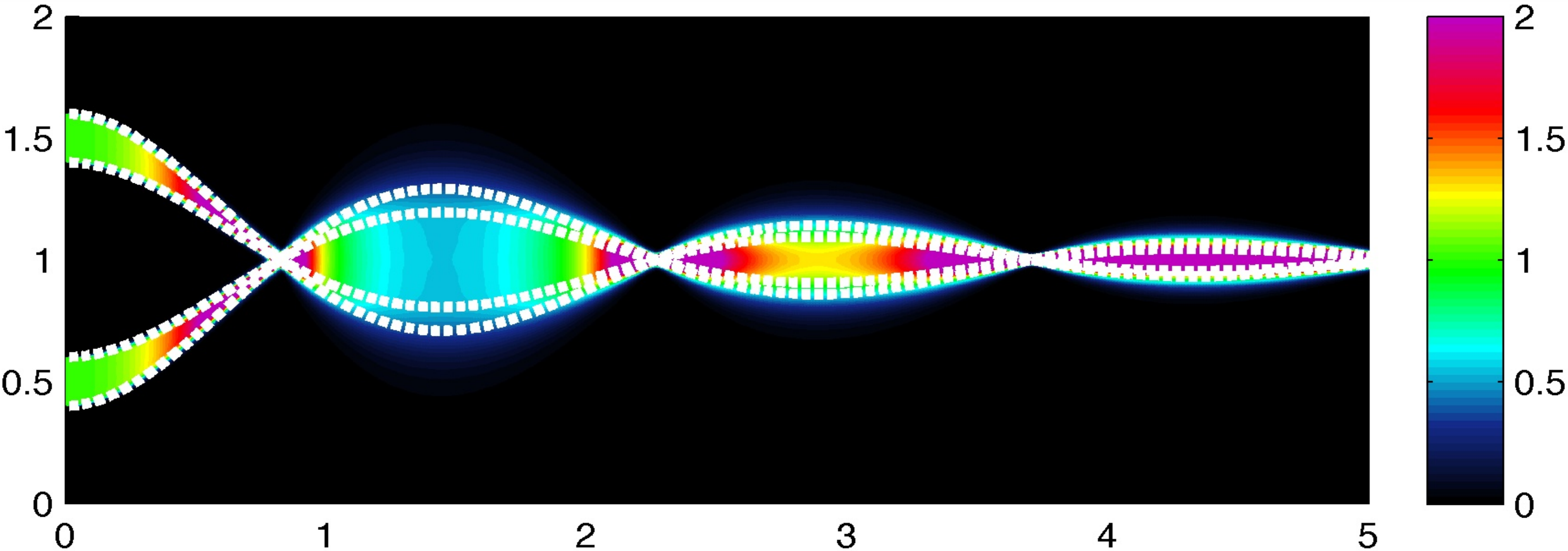
- Injection of two jets at each side of the center line with zero gas velocity

$$u_g = 0.2, v_g = -(y-1)$$



Two-jet configuration

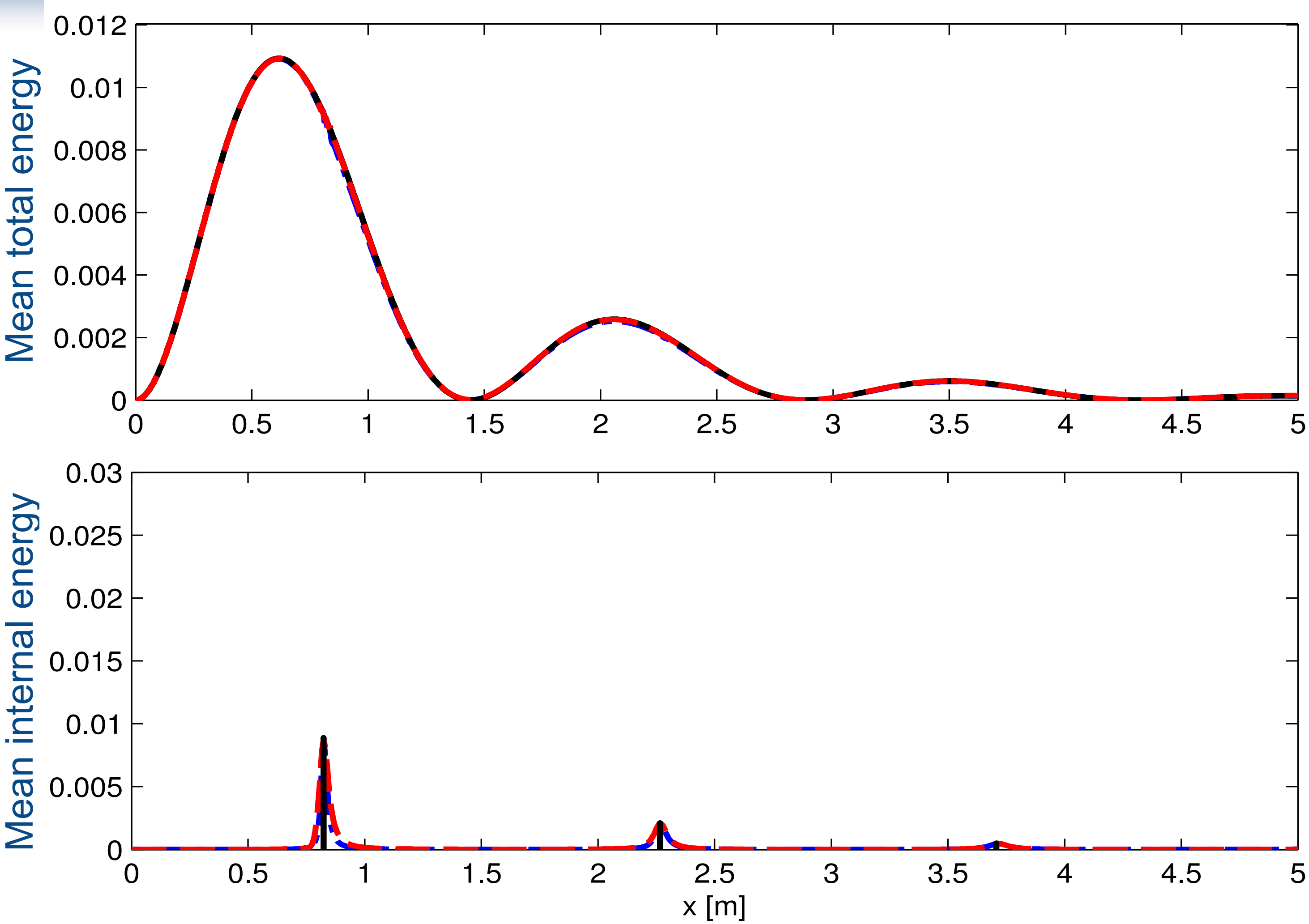
Number Density



white lines = lower and upper limits for the Lagrangian solution

- Before the first crossing, Lagrangian and Eulerian solutions are overimposed
- After the first crossing, the Eulerian solution is spread
- However the Eulerian solution captures the width of the crossing event

Two-jet configuration



Black line

=Lagrangian

Red line

=Anisotropic Gaussian

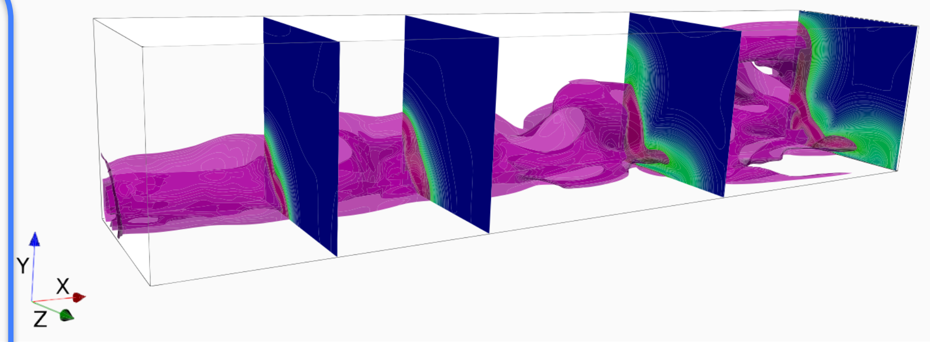
- The Eulerian solution captures the energetic behavior of the two jet configuration

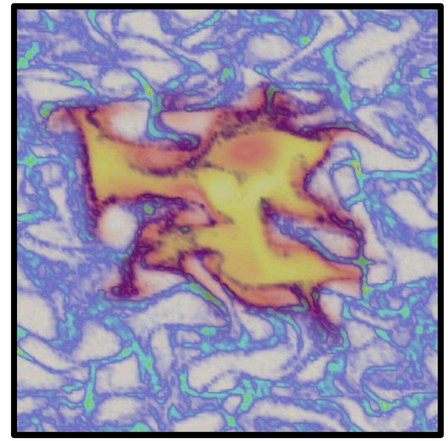
3D Results: HPC

Asphodele solver from CORIA

- Initially developed by J. Reveillon
- Parallel Low-Mach dilatable multi-species solver - Combustion
- Lagrangian solver for particles

- Current developers:
  - O. Thomine (CORIA then CEA)
  - J. Brandle de Motta (EM2C then CORIA)



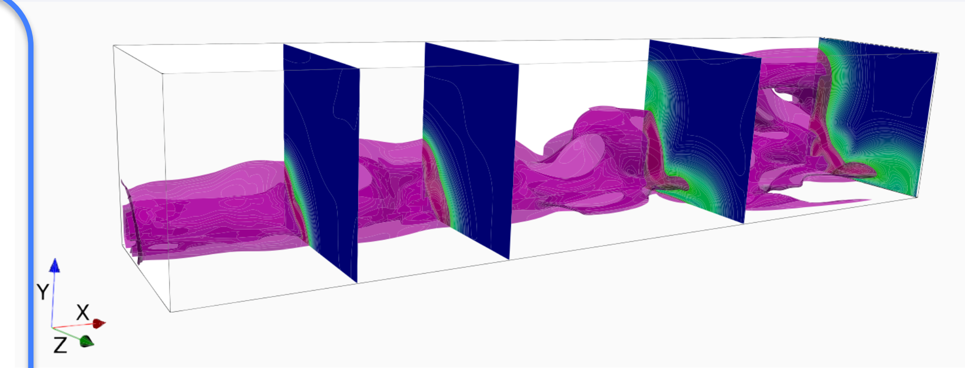


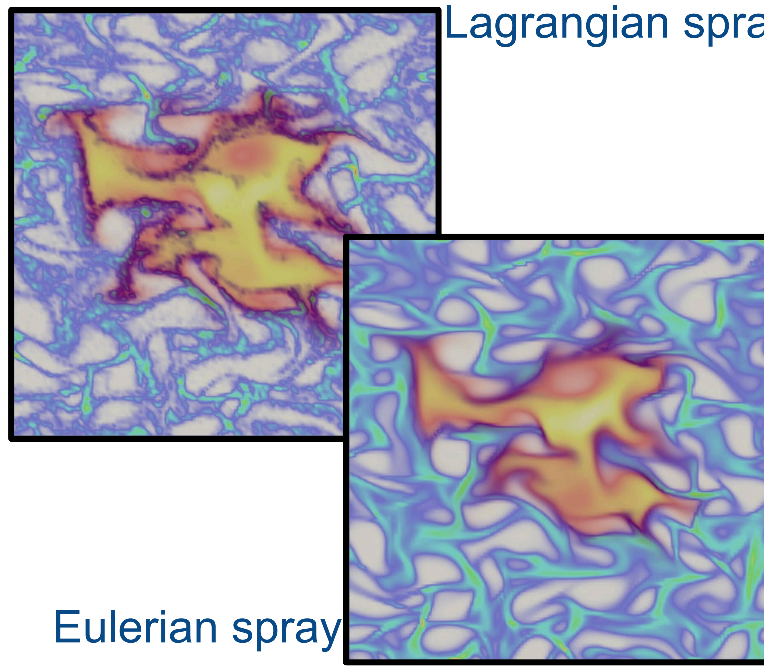
Lagrangian spray

3D Results: HPC

MUSES3D solver from EM2C

- Initially developed by S. de Chaisemartin (EM2C, now at IFPen)
- Eulerian solver for disperse phase (polydisperse, polykinetic)
- Current developers:
  - M. Sabat (EM2C)
  - J. Brandle de Motta (EM2C then CORIA)





Lagrangian spray

Eulerian spray

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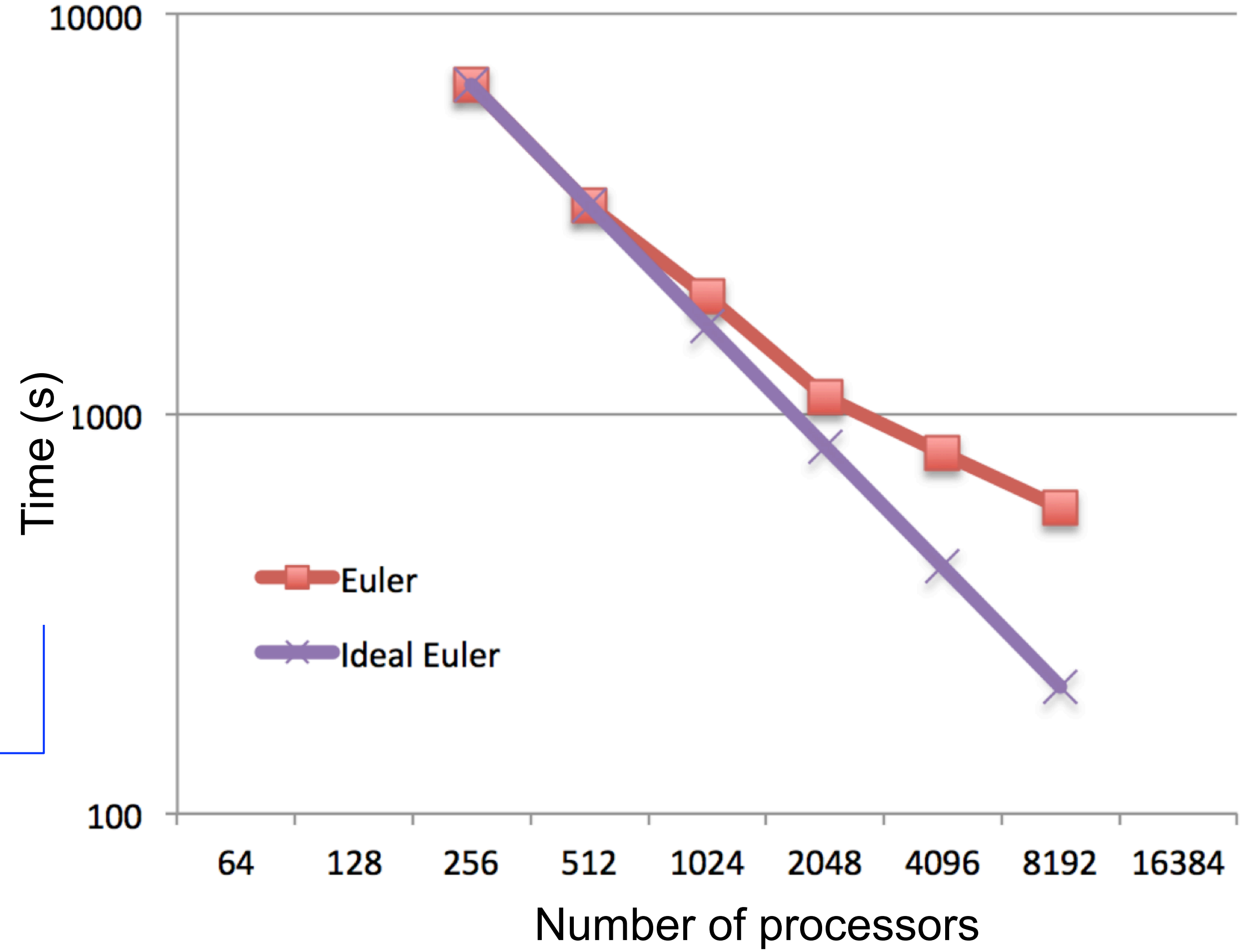
3D Results: HPC

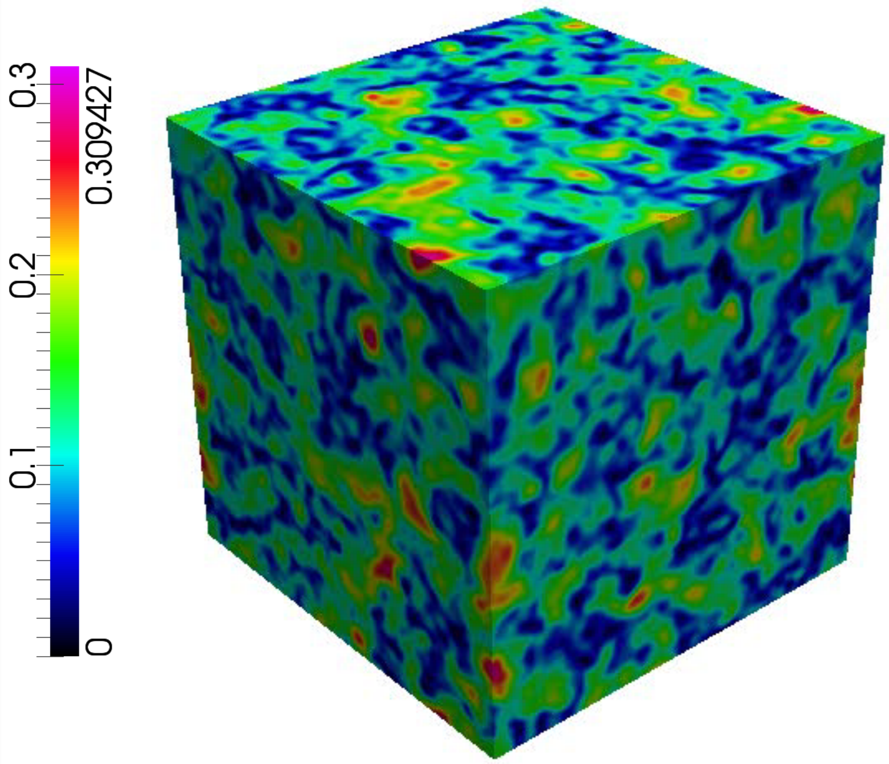
Performance of MUSES3D on OCCIGEN, CINES

- Performance evaluated on a 3D Homogeneous Isotropic Turbulence test case
- Mesh for the spray in MUSES3D is 512^3

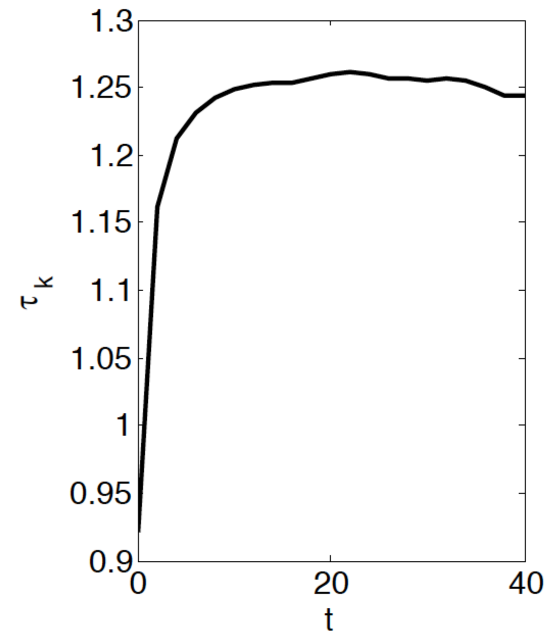


3D Homogeneous Isotropic Turbulence

- Carrier phase: 3D HIT box



- Homogeneous spray at t=0



Spectral initialisation and forcing

- Deterministic forcing scheme of Guichard et al. 2004
- Reynolds number based on Taylor scale $Re_\lambda = 21.5$

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3D Homogeneous Isotropic Turbulence

Disperse phase simulations

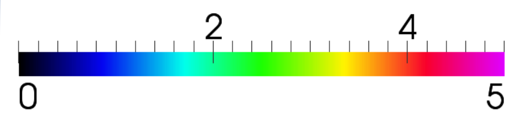
- Homogenous distribution at initial time
- Zero initial velocity
- Three models
  - Lagrangian simulation with fixed grid
  - Eulerian simulation for 64^3, 128^3, 256^3 and 512^3 meshes
    - Mono-Kinetic model
    - Anisotropic Gaussian model
- Various Stokes number from 0.05 to 15

Results

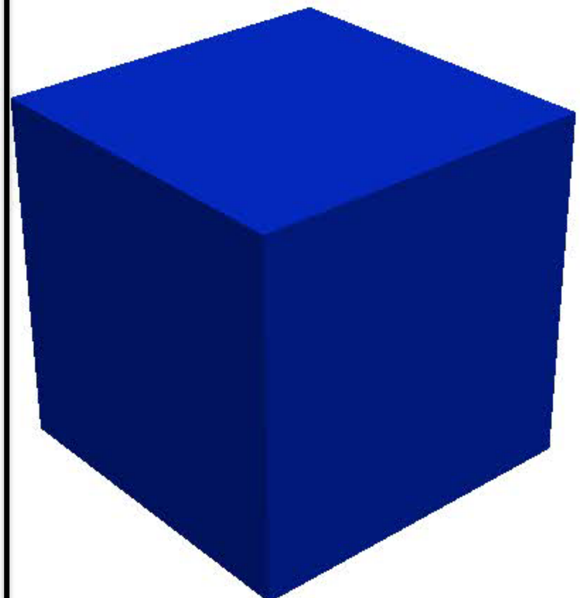
- Qualitative comparison
  - Number density
  - Velocity
  - Covariance matrix elements
- Quantitative:
  - Statistical results
  - Distribution function

3D HIT St=0.5

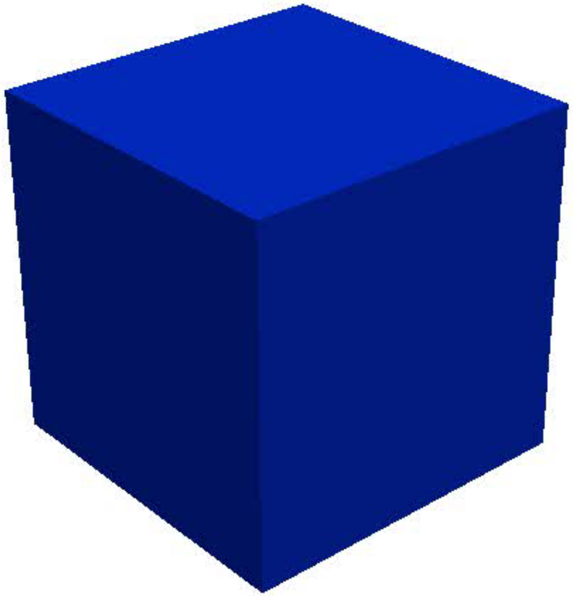
Number Density



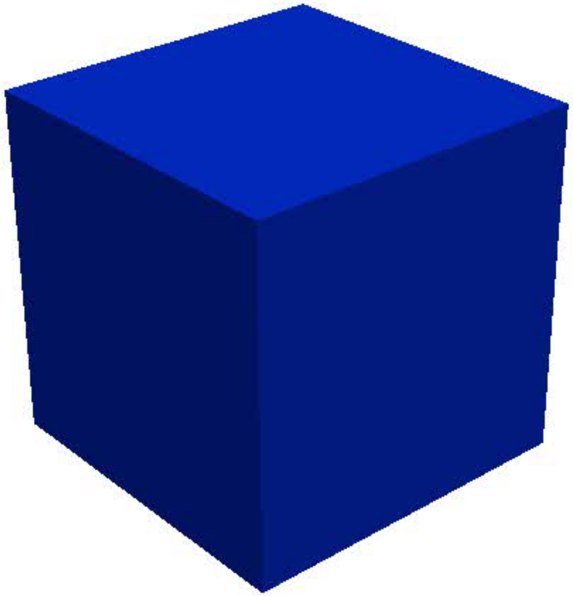
Lagrangian



Mono-Kinetic



Anisotropic Gaussian



MK and AG : qualitatively matches the Lagrangian results

118

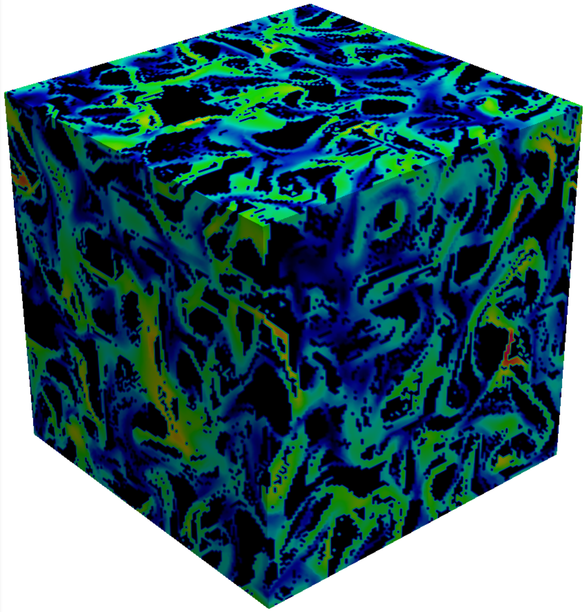
3D HIT St=0.5

Velocity

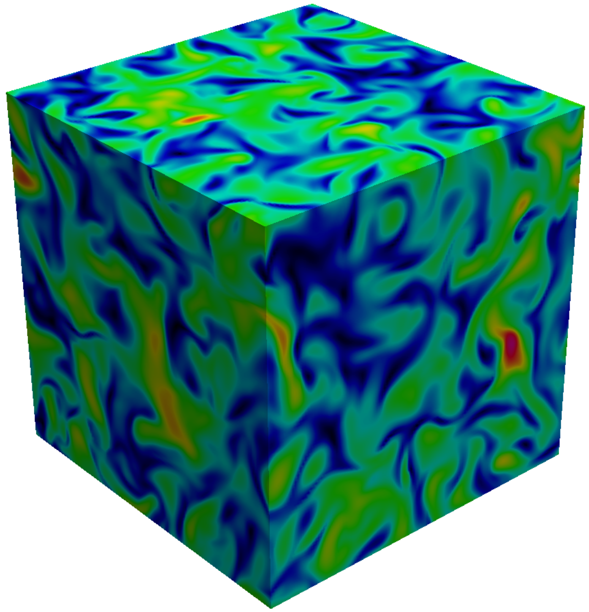
0.1 0.2 0.3

0 0.309427

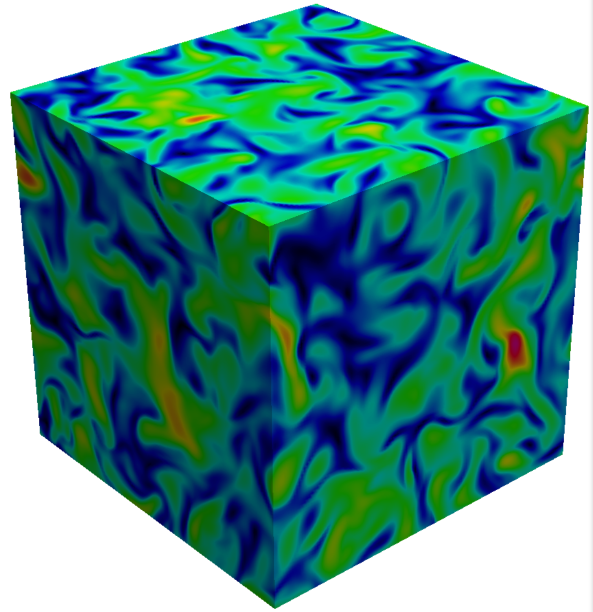
Lagrangian



Mono-Kinetic

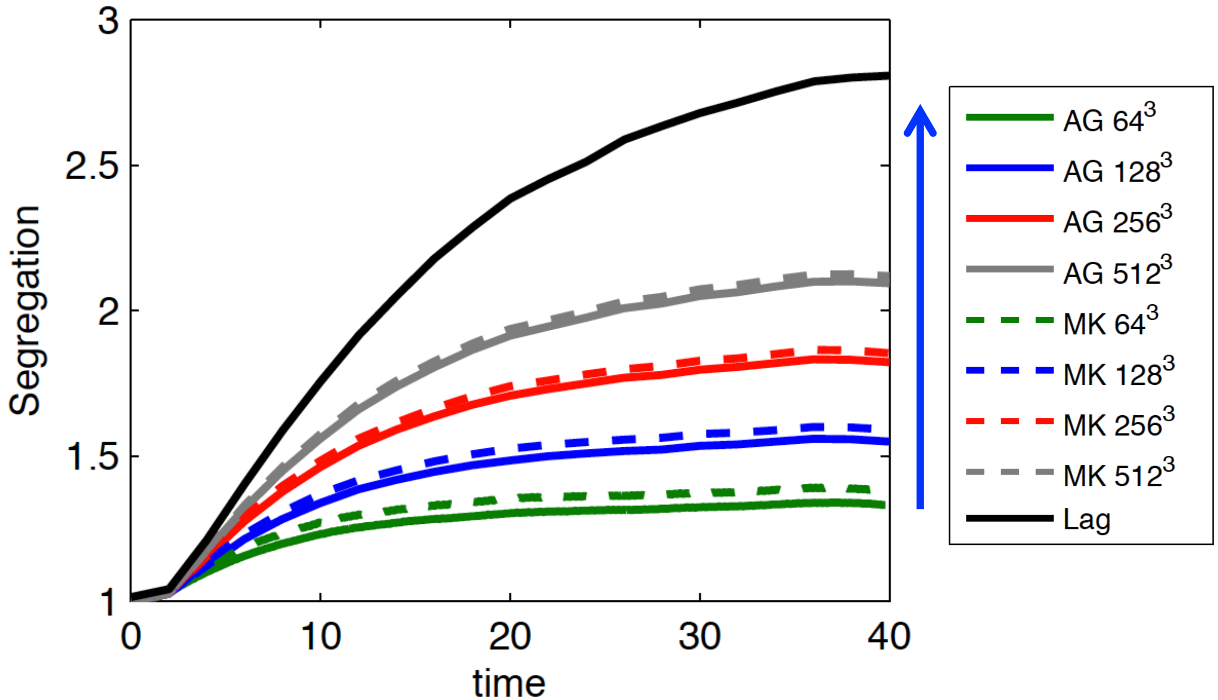


Anisotropic Gaussian



MK and AG : qualitatively matches the Lagrangian results

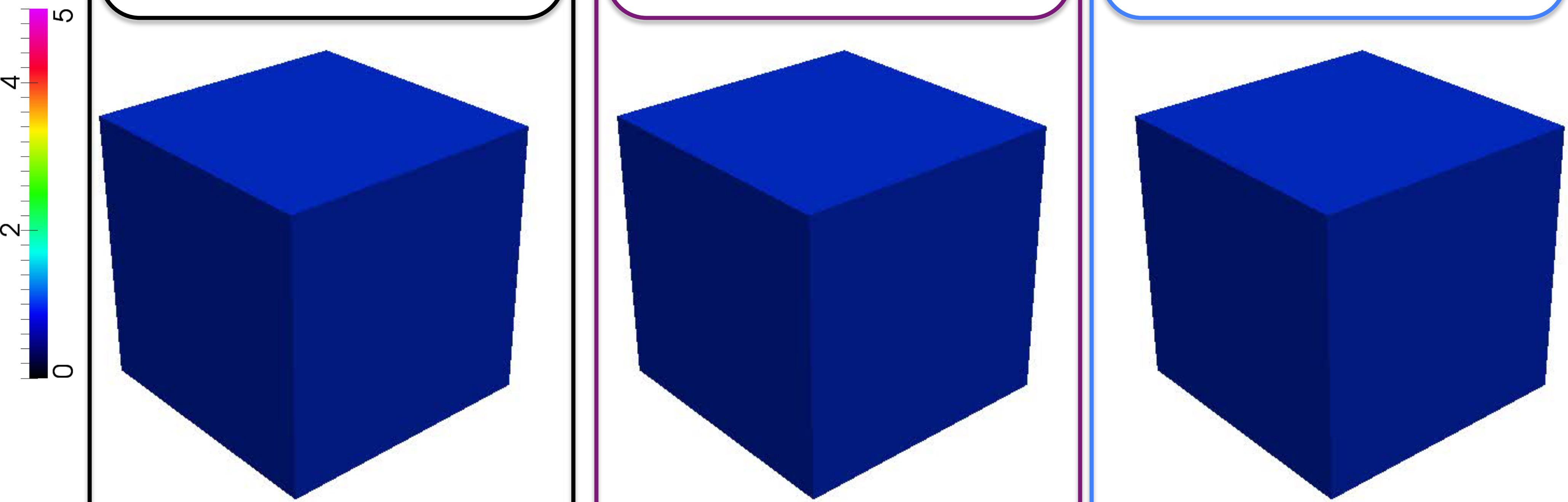
3D HIT St=0.5, Segregation



- For low inetria particles, both the MonoKinetic and Anisotropic Gaussian models
  - Have the right statistical behavior compared to the segregation of the Lagrangian result
  - converges towards the Lagrangian solution with mesh refinement
- In this case, no significant particles trajectory crossing occurs.

3D HIT St=3 , Number density

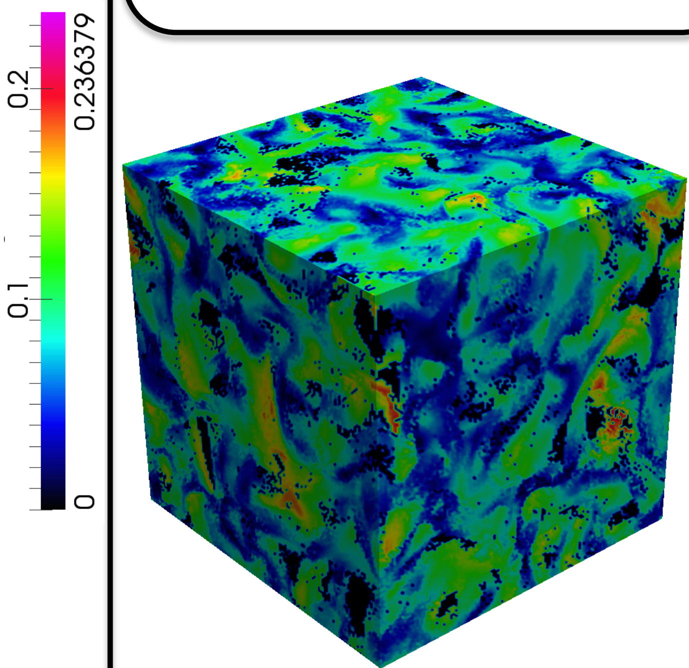
Lagrangian | **Mono-Kinetic** | Anisotropic Gaussian



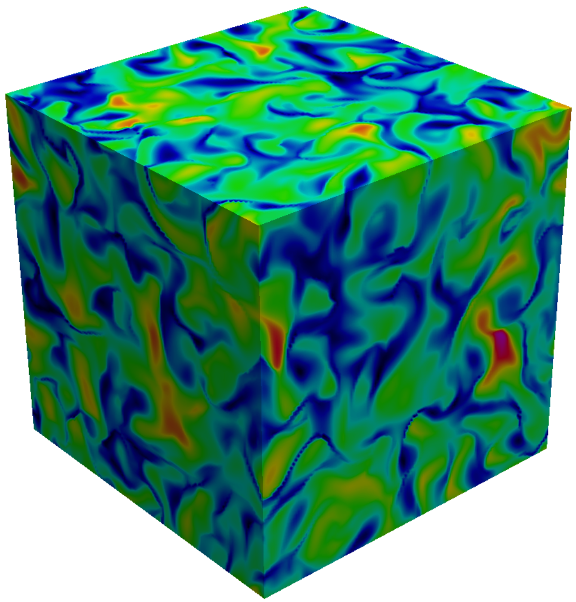
MK: generate δ-shocks, overestimates the accumulations, and shrink the structures
AG: qualitatively matches the Lagrangian results

3D HIT St=3 , Velocity

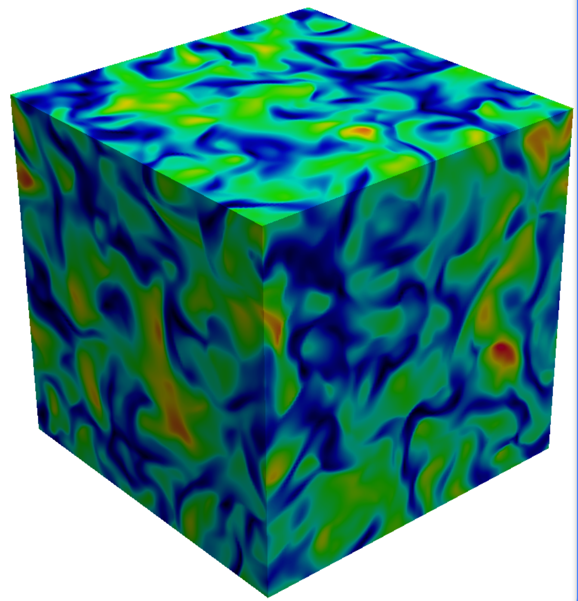
Lagrangian



Mono-Kinetic



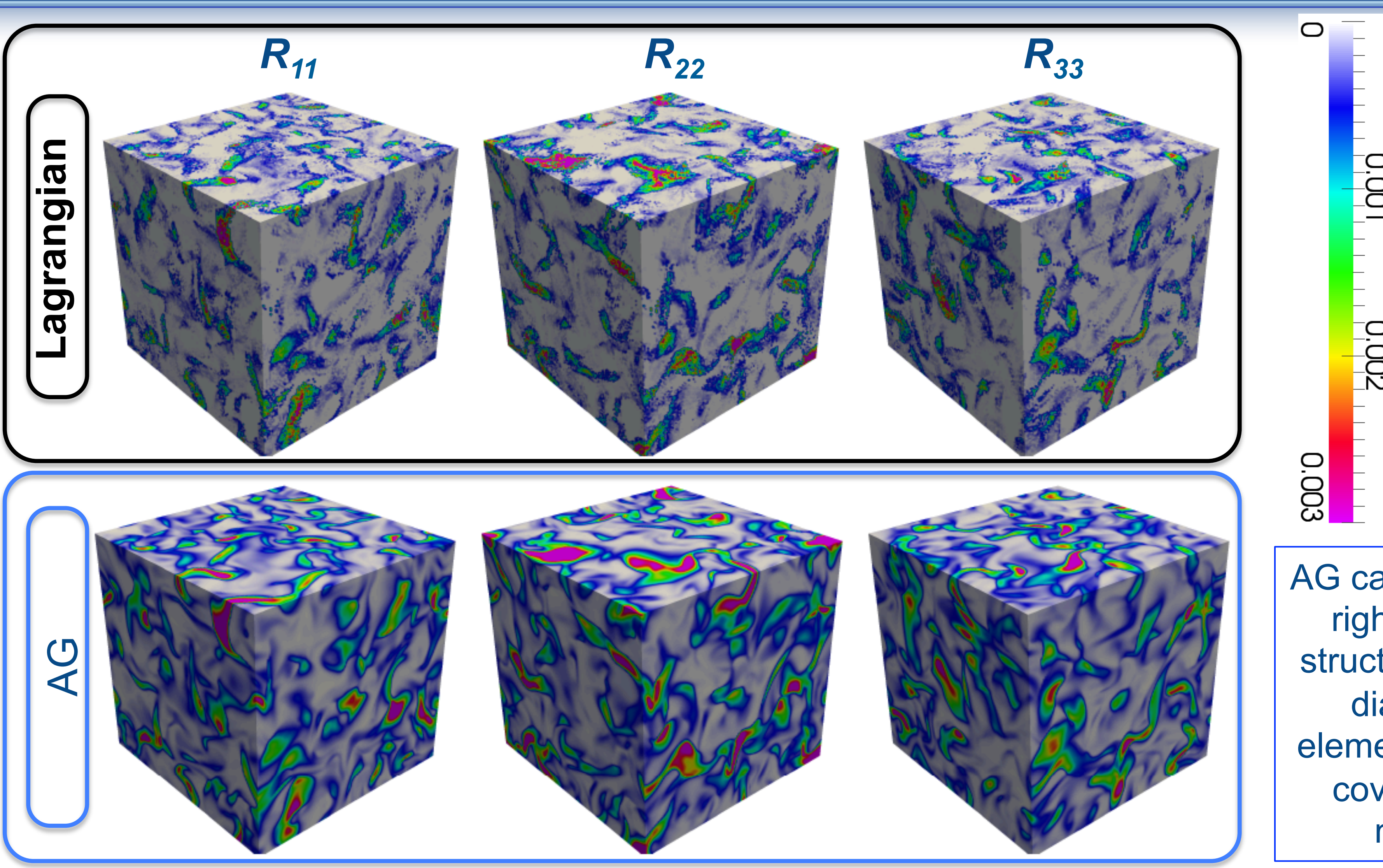
Anisotropic Gaussian



MK: overestimates the velocity
AG: qualitatively matches the Lagrangian results

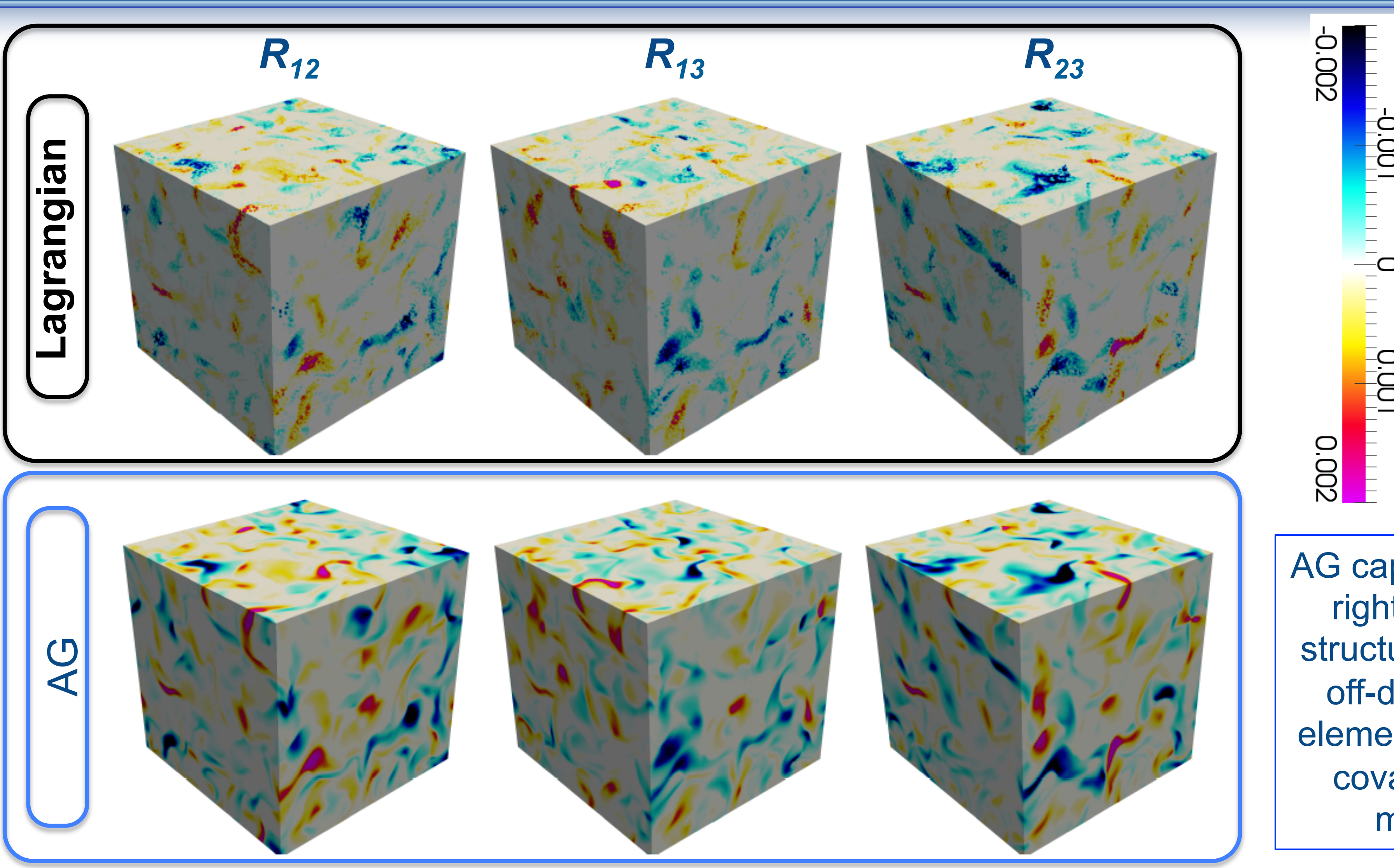
122

3D HIT St=3 , Velocity dispersion



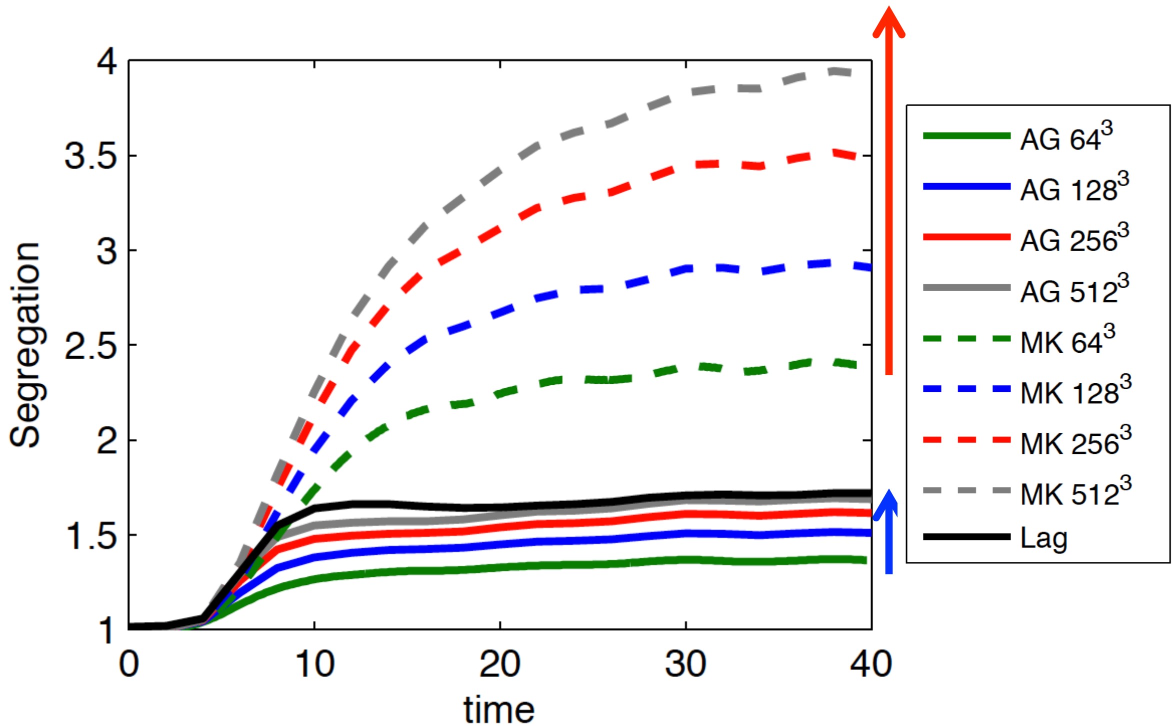
AG captures the right global structure of the diagonal elements of the covariance matrix

3D HIT St=3 , Velocity dispersion



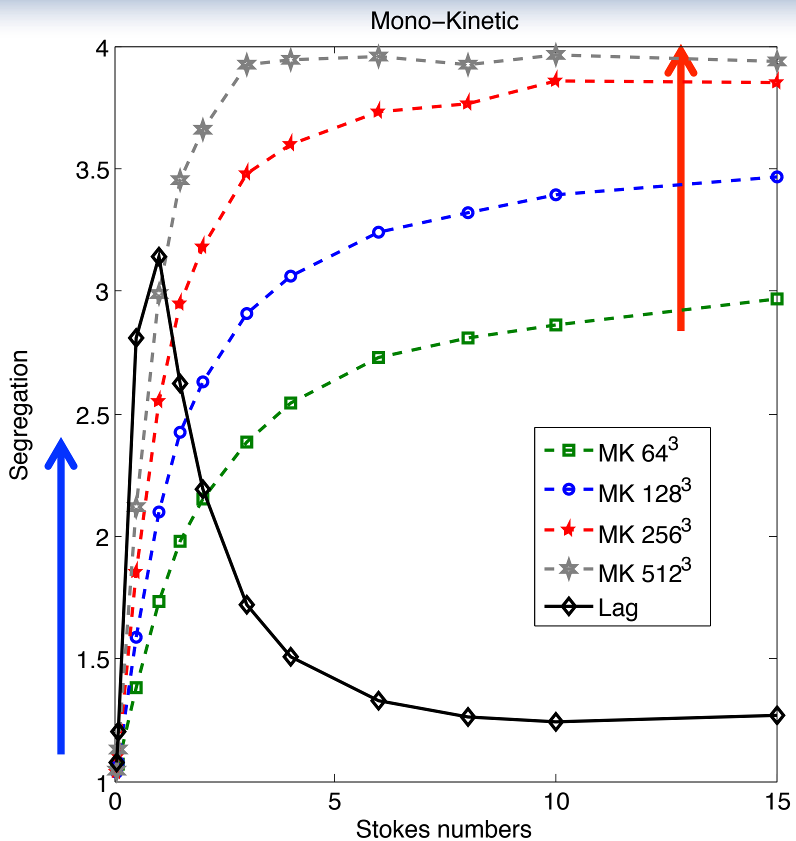
AG captures the right global structure of the off-diagonal elements of the covariance matrix

3D HIT St=3, Segregation



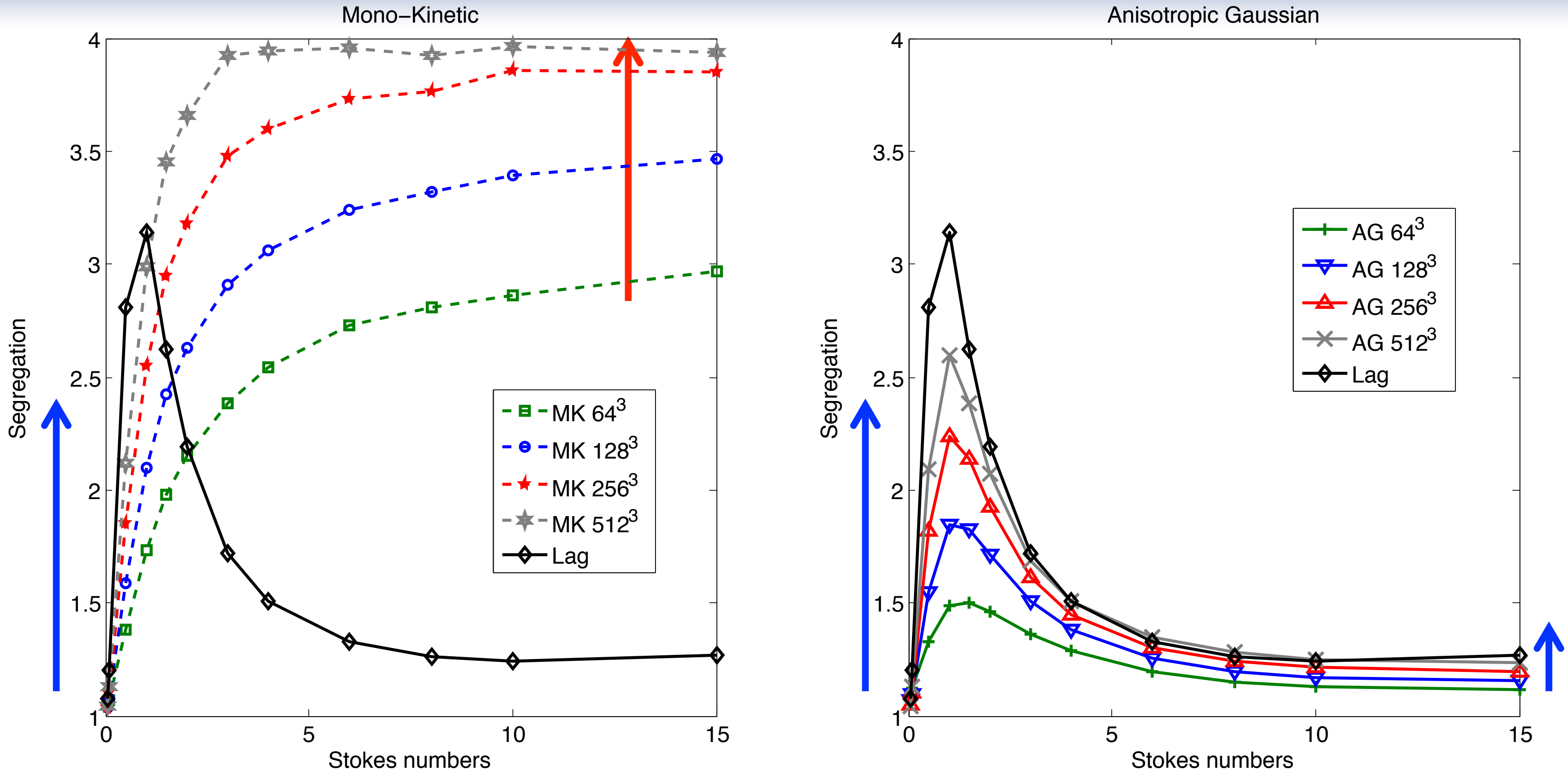
- Mono-Kinetic:
  - overestimates the segregation
  - Does not converge to the lagrangian solution with mesh refinement
- Anisotropic Gaussian:
  - Right statistical behavior compared to the segregation of the Lagrangian result
  - converges towards the Lagrangian solution with mesh refinement

3D HIT, segregation vs. Stokes number



- Mono-Kinetic:
  - overestimates the segregation for moderately inertial to inertial particles
  - Does not converge to the Lagrangian solution with mesh refinement for high Stokes

3D HIT, segregation vs. Stokes number



- Anisotropic Gaussian:
    - Right statistical behavior for the studied Stokes numbers
    - converges towards the Lagrangian solution with mesh refinement

Conclusions on 2nd Order Methods

- The Anisotropic Gaussian closure is able to capture the characteristic width of the crossing events, either in two-jet configuration or in Taylor-Green vortices

- In 2D Homogeneous Isotropic Turbulence, the Anisotropic Gaussian closure is proven to be accurate

- In 3D Homogeneous Isotropic Turbulence, the Anisotropic Gaussian results matchs qualitatively and quantitatively the Lagrangian results:
  good candidate for complex applications

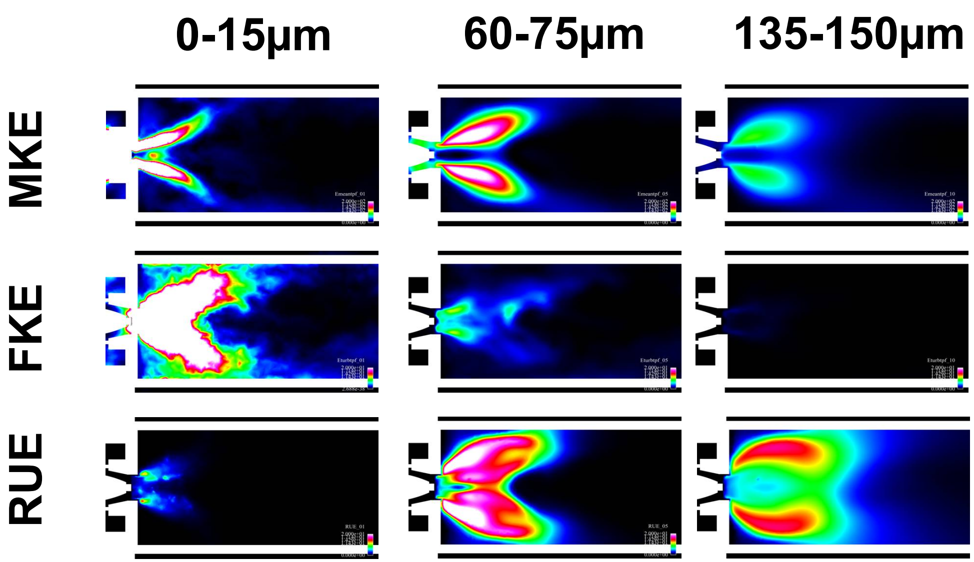
- **Extension to LES and unstructured meshes (DG – with A. Larat) conducted in the Ph.D. of M. Sabat 2016, Sabat et al 2016**

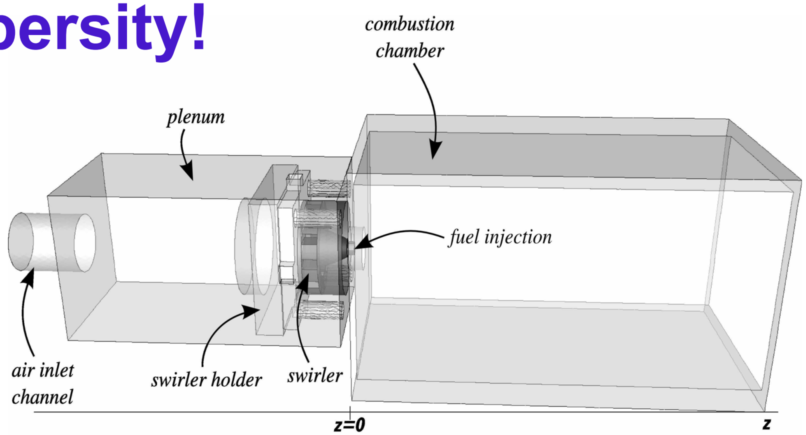
IMPLEMENTATION IN INDUSTRIAL CODE AVBP – A. VIÉ

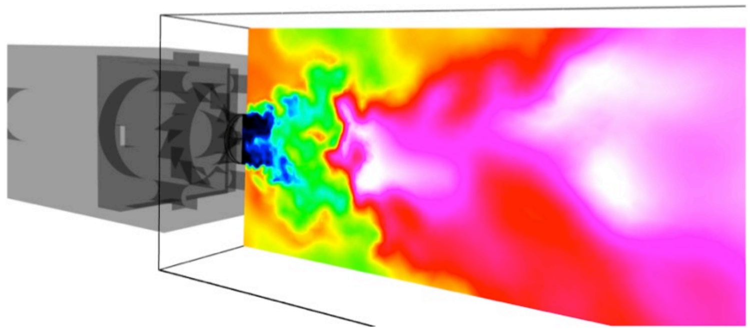
Aeronautical engines : polydispersity!

MERCATO Configuration

A. Vié et al, ICMF 2010 and FTC 2013







EXTENSIONS

1- Polydispersity with high order moment methods for computational cost

PhD of D. Kah (2010) – A. Vié (2011-2013)

PhD of O. Emre (2014) and M. Essadki (2017) - IFPEn

2- Particle trajectory crossing and Eulerian modeling hierarchy of high order moments - A. Vié, A. Larat, F. Laurent, C. Chalons, R.O. Fox

PhD of M. Sabat (2016) and D. Mercier (2018) - IMFT

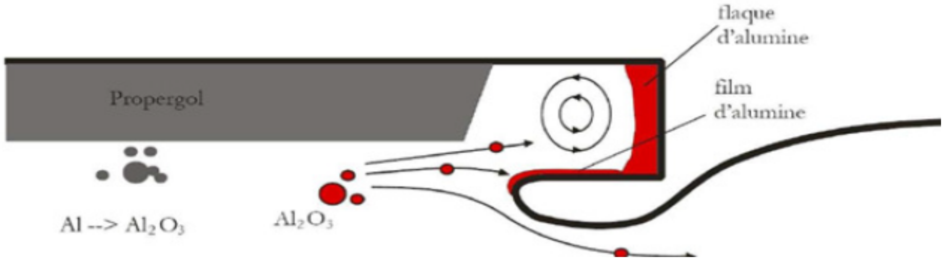
3- Coalescence / Break-up and alumina particle in Rocket Boosters

PhD of F. Doisneau (2013) – PhD of V. Dupif (2017) – F. Laurent - ONERA

Evaporation / Combustion of aluminum particles

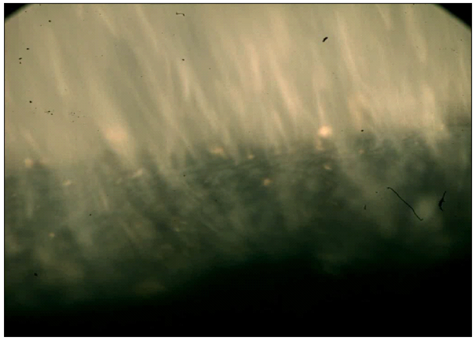
Thesis of A. Sibra (2014) – F. Laurent - ONERA

Solid Rocket Motor Context - ONERA CEDRE Code



Combustion chamber flow

- **Combustion** of aluminum particles
- **Polydisperse** droplets of alumina
- High mass fraction and **two-way** coupling
- **Size evolution** (Coalescence, break-up)



PhD contributions ⇔ ONERA / App. Math. Team (EM2C lab.) collaboration
Solid propulsion simulations of instabilities – HPC / Splitting

Evaporating polydisperse sprays (only sampling)

Mono-component droplet

Simplified combustion models

« Weak » two-way coupling with a single-species gas

Numerical developments

Evaporating polydisperse sprays (sampling & MF)

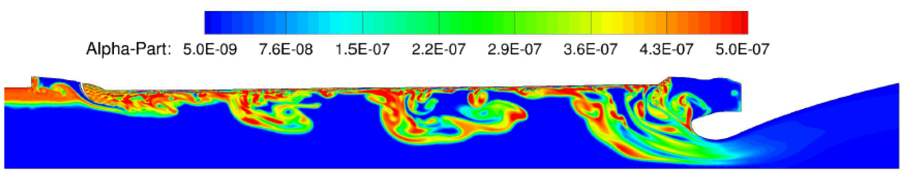
Coalescence – Break-up

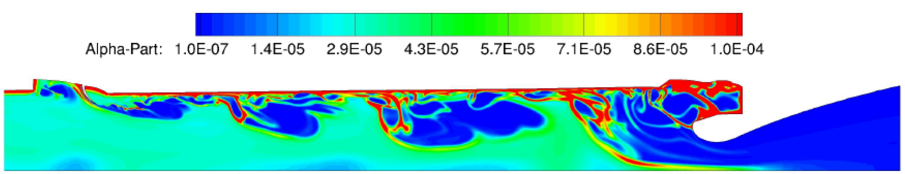
Bi-component droplet

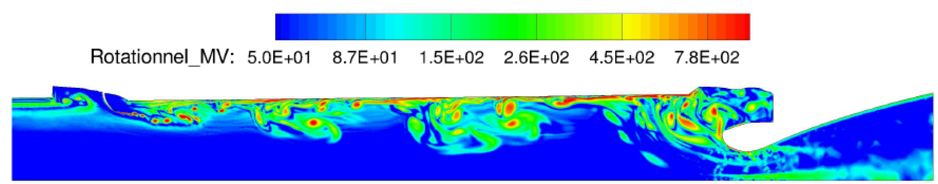
Realistic combustion models

« Robust » **two-way coupling** with a multi-species gas

Numerics accuracy/stability







Doisneau et al JCP 2013, CRM 2013, JPP 2014, Sibra et al AIAA 2013, JCP 2014, Sibra PhD 2015

Dupif et al, EUCASS 2015, ICMF 2016

Conclusion – Take home message

Eulerian modeling effort coupled to scheme development / HPC – Robust/accurate

Academic configurations → Industrial codes

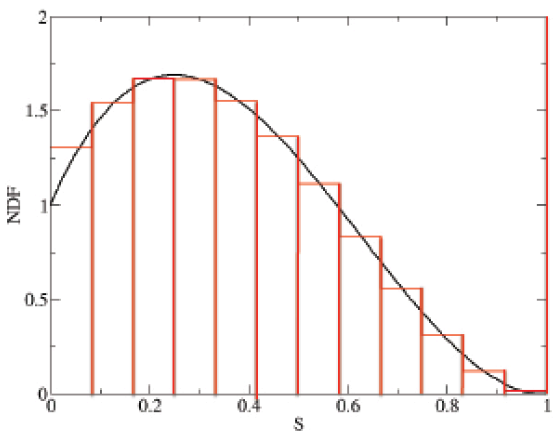
- **Polydisperse simulations is ESSENTIAL for combustion applications since the fuel mass fraction is really piloted by the polydispersion (SRM same)**
- **Particle Trajectory crossing taken into account for inertial droplets – also allows to include subgrid modeling (KBMM – AG – LES – PhD M. Sabat 2016)**
- **High order accurate and robust numerical schemes: Key issues are related to high order methods for the transport in physical space and phase space.**

Polydisperse spray Combustion dynamics

Eulerian models and methods mature for DNS and LES of complex flows

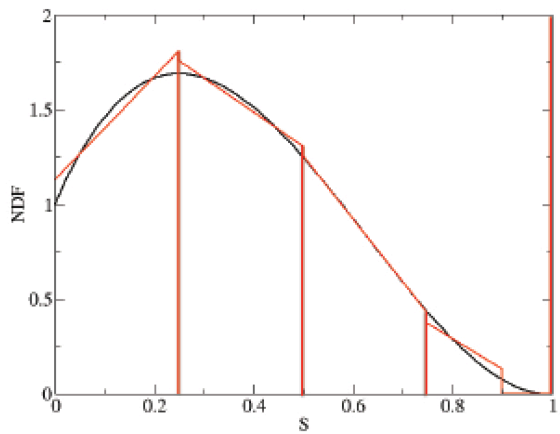
Treatment of polydispersion: physics dependent

1 moment/section



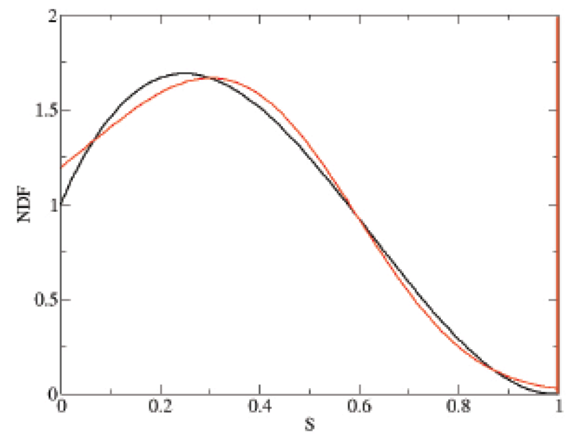
[Laurent and Massot, 2001]

2 moment/section



[Laurent, 2006, Doisneau et al., 2013]

4 moment/section



[Massot et al., 2010, Kah et al., 2012]

Increase the number of moments per section / hybrid

Lower the number of sections for accurate simulation

Lower cost

Increase of the model complexity and algebra

Take home message – towards industrial codes

- Coalescence / break-up = complex size dynamics / multi-modal – second order affine moment method (Laurent M2AN 2006, Doisneau JCP 2013, Doisneau JPP 2014, Sibra JCP 2015, Laurent CICP 2015)

  → ONERA CEDRE Code – F. Doisneau – A. Sibra – V. Dupif

- Polydispersion in automobile and aeronautical (RANS/LES) engines leads to "simple" size distributions – Hybrid high order moment methods – 1 to 3 sections

  → IFP-C3D Code – D. Kah, O. Emre

  → AVBP code – A. Vié

Size-velocity (size-temperature) correlations (CSVM – Vié, JCP 2013)

Take home message

- Choice of “closure” in velocity piloted by the need for hyperbolic systems (or at least weakly hyperbolic) with an entropic structure in order to **treat singularities** (Chalons, Kah, Massot, CMS 2012, Vié, Doisneau Massot CICP 2015, Larat 2015)

- Has a strong impact on the numerical schemes – key issue: **high order** methods for the transport part (splitting strategy in order to cope with stiffness)

  → Convexity preserving DG methods → A. Larat
  (Sabat, JCP 2016, ICMF 2013, JCMF 2014)

- Depending on the zones Stokes numbers can vary → **model coupling** (Boileau, Chalons, Massot, SIAM SISC 2015) and since size evolution and large spectrum → **AP schemes** (LES : Vié et al SIAM MMS 2015, Sabat et al 2015).

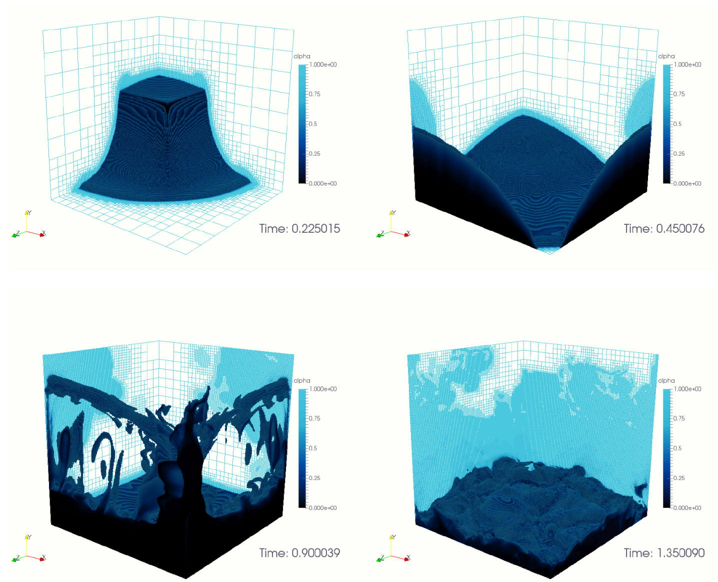
- Lots of “local” computations (quadrature / reconstruction) – **Hybrid Parallelism**

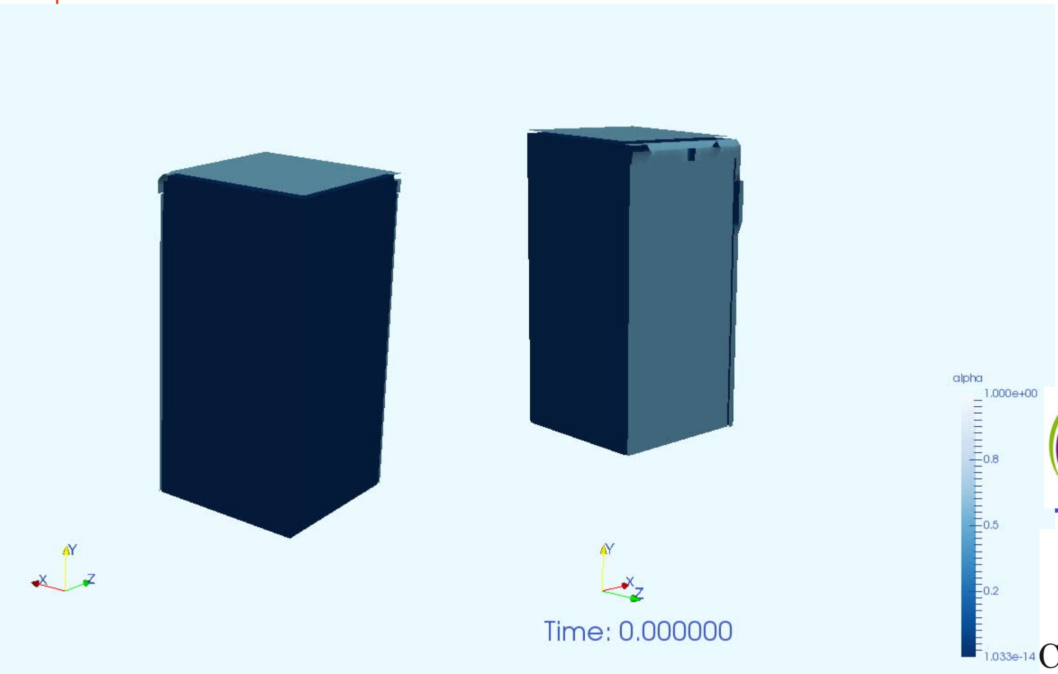
Further developments – Separated phases / spray coupling

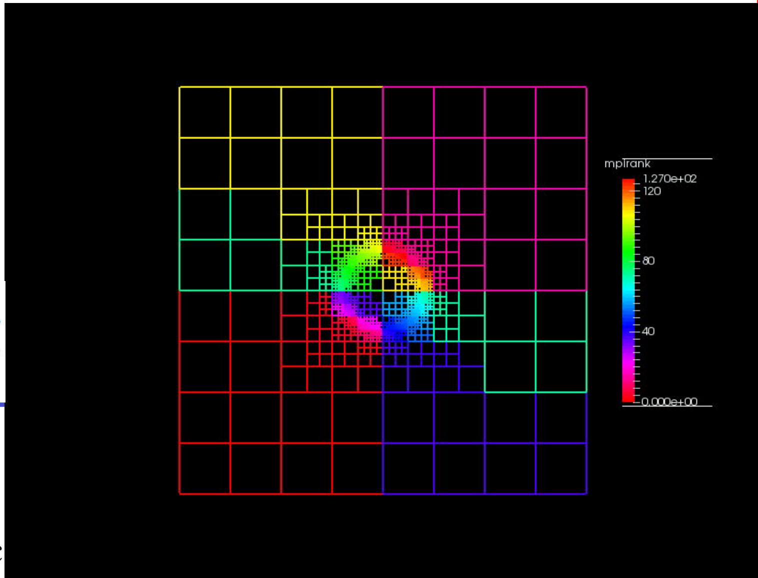
PhD Florence Drui (EM2C – MdlS – DGA/CEA)

(Coll. S. de Chaisemartin. M. Essadki, P. Kestener, S. Kokh, A. Larat)

- Diffuse interface modeling with proper mathematical derivation and a hierarchy of models involving various physics
- Numerical scheme to handle multi-scale character of the whole hierarchy – Asymptotic preserving schemes
- Development of **CanoP** code (**p4est** library) with cell-based AMR and scalability on massively parallel architectures







DGA

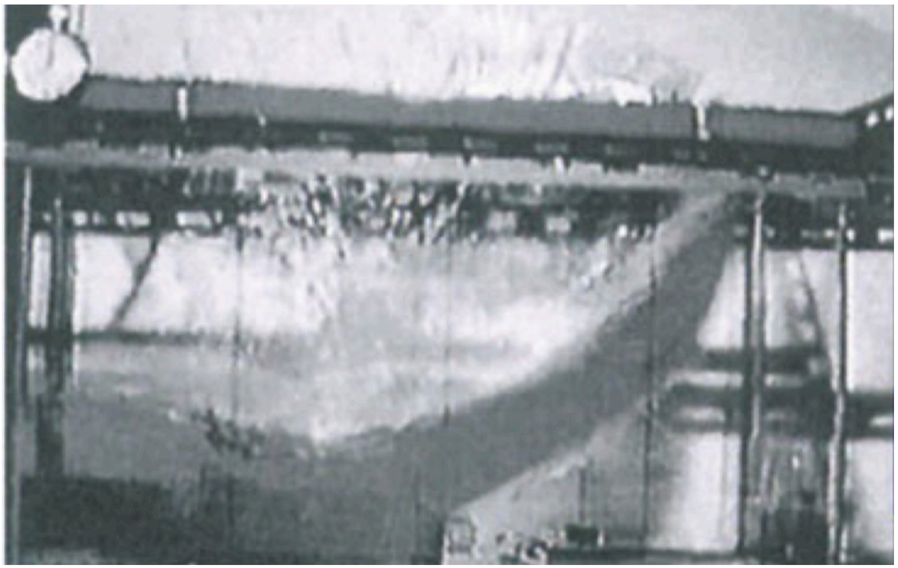
MAISON DE LA SIMULATION

ifp Energies nouvelles

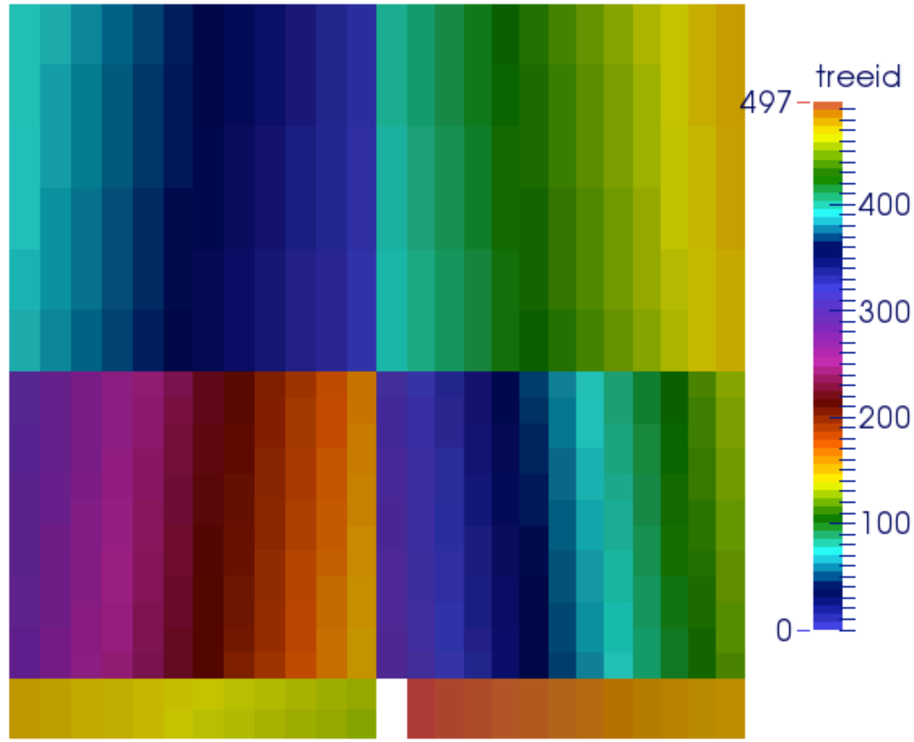
CentraleSupélec

Further developments – Separated phases / spray coupling

- PhD Florence Drui (EM2C – MdlS – DGA/CEA)
- Reproducing experiments



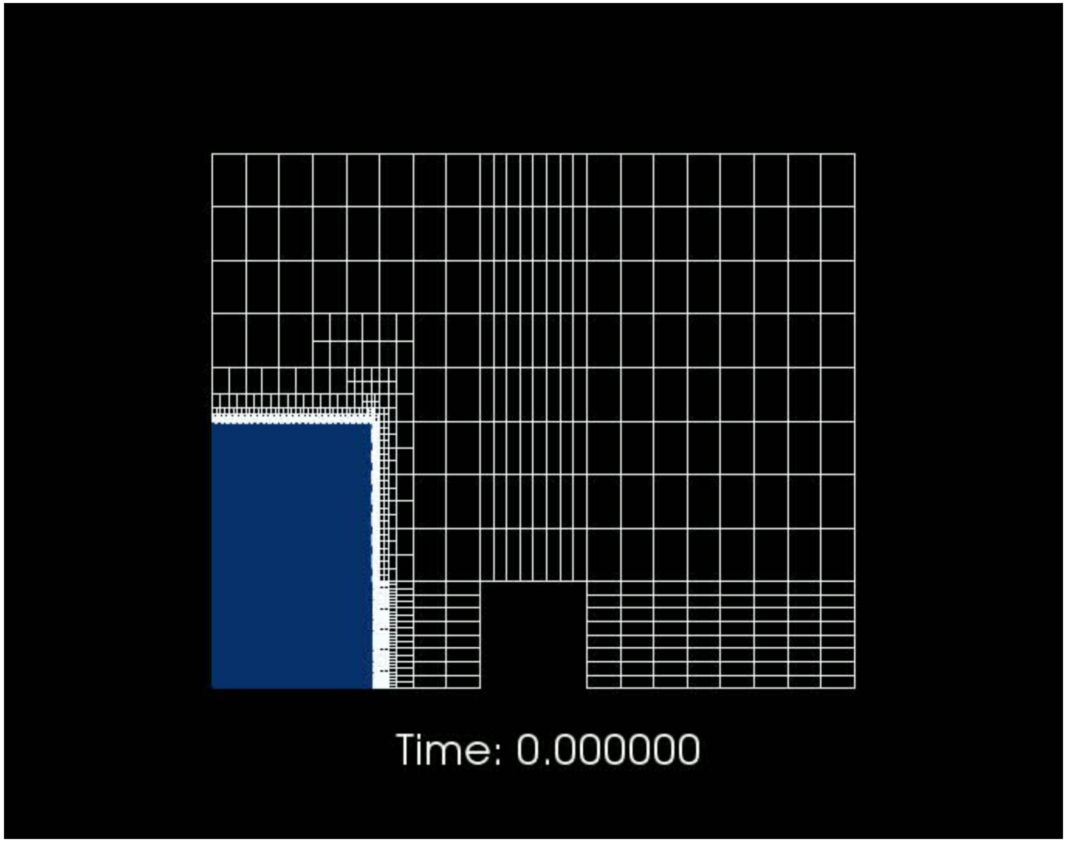
Forest of trees

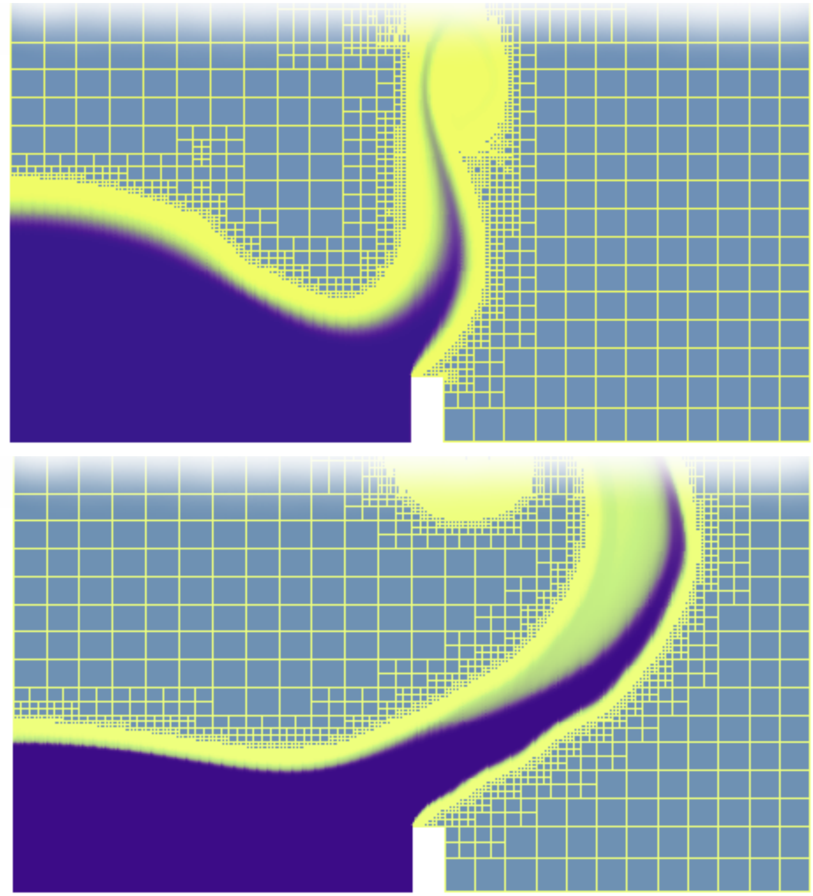


- Bridging the gap between the two descriptions with a single model…

Further developments – Separated phases / spray coupling

- PhD Florence Drui (EM2C – MdlS – DGA/CEA)

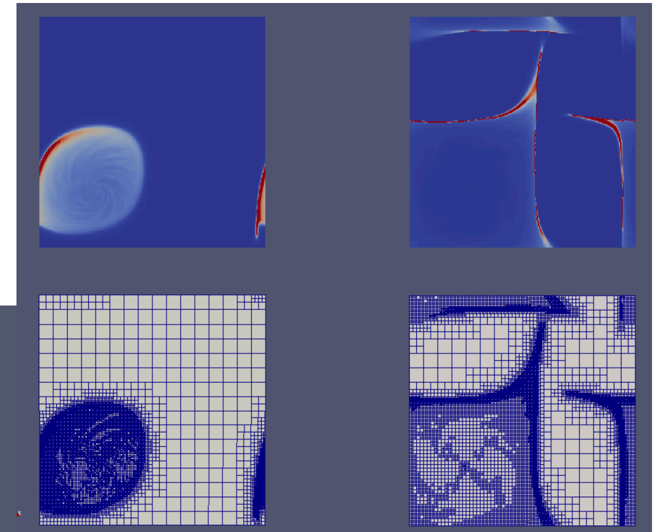


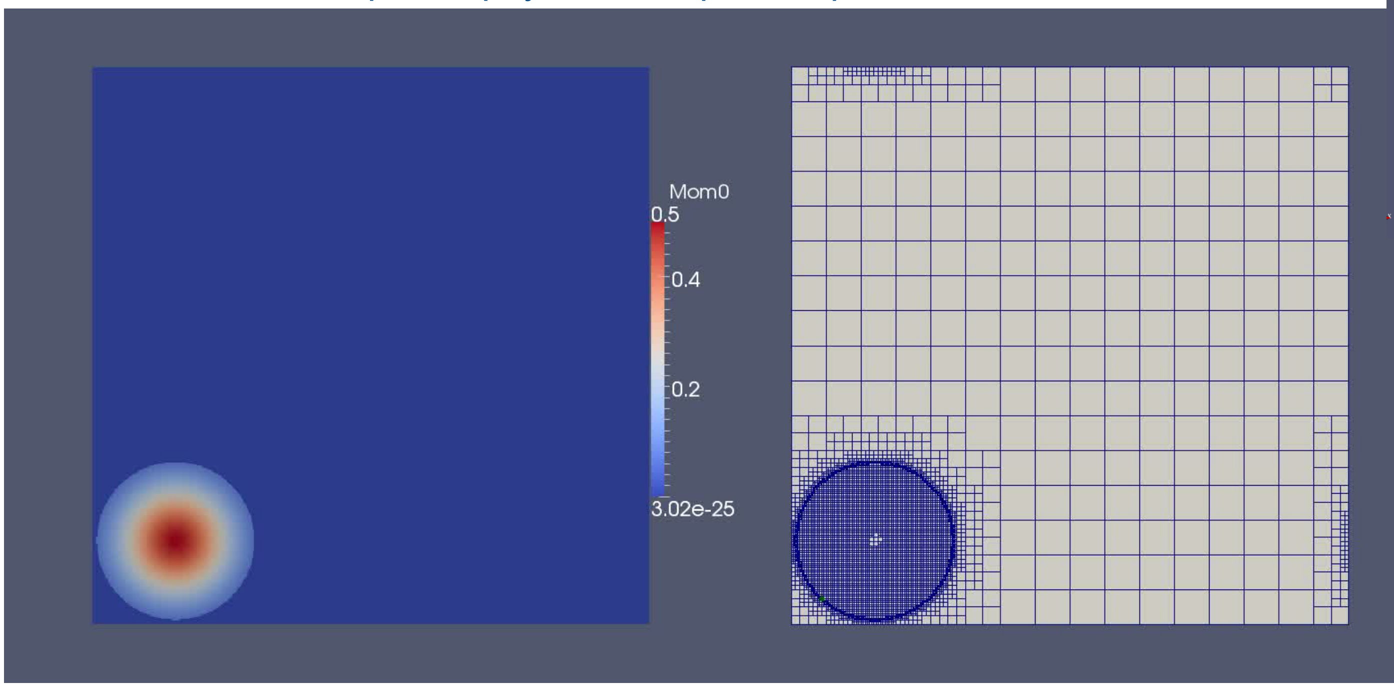


- Bridging the gap between the two descriptions with a single model…

Further developments – Separated phases / spray coupling

- **PhD Mohamed Essadki (IFPEn – EM2C) CanoP**
  - Development of a **geometrical high order moment method** for the coupling to a separate phases modeling of diffuse interface type
  - **Realizability, robustness and accuracy through mesh adaptation** of the transport in physical and phase space





Bridging the gap between the two descriptions with a single model…

(OGST 2016, SIAM 2016, ICMF 2016)

Further developments – Separated phases / spray coupling

PhD Mohamed Essadki (IFPEn – EM2C)

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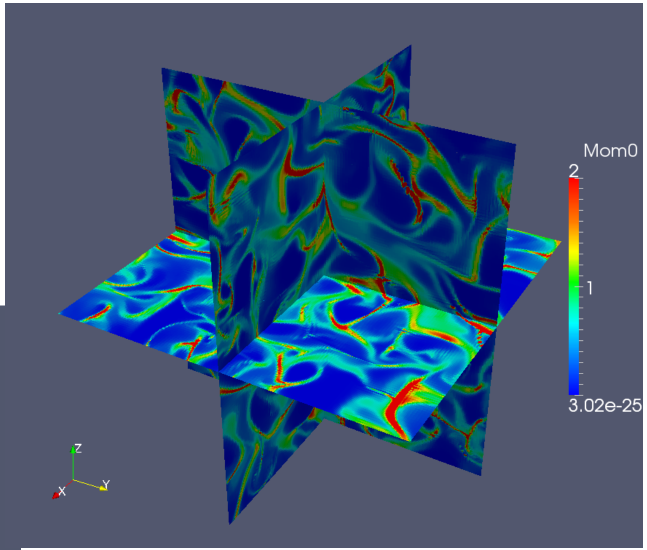

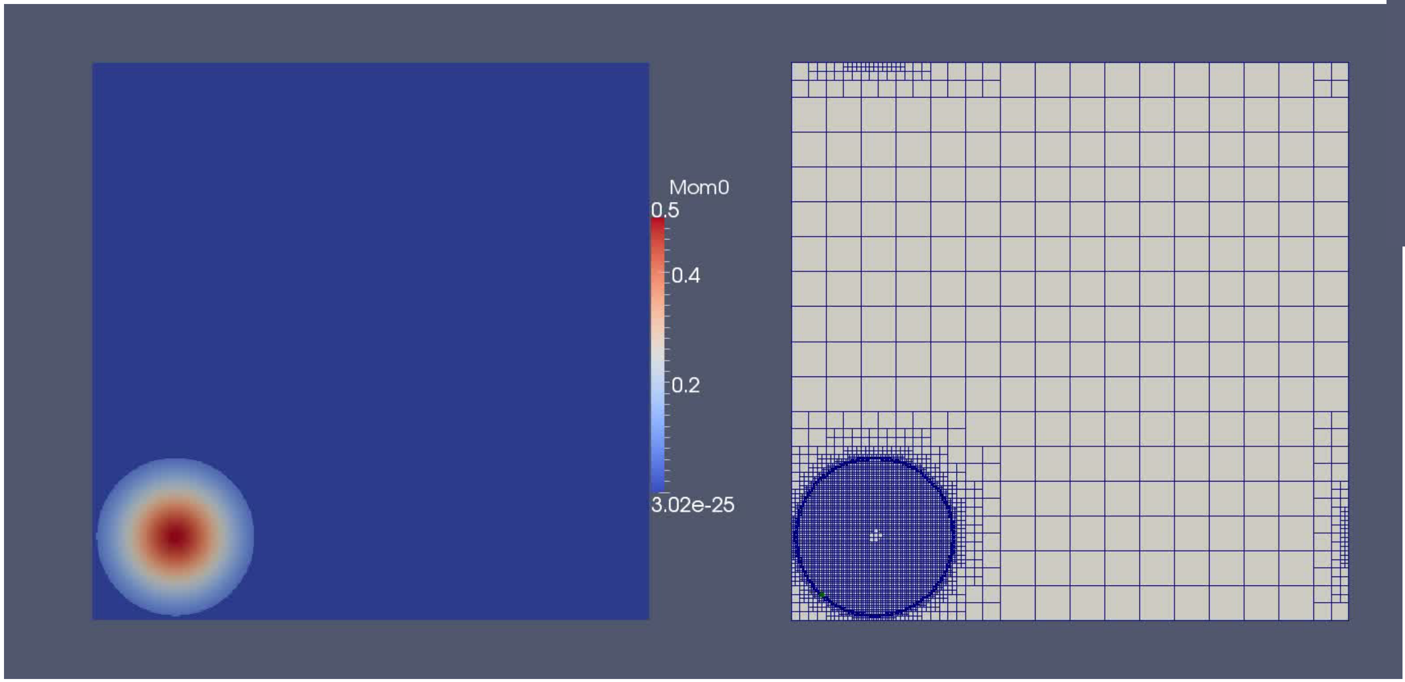

Bridging the gap between the two descriptions with a single model…

(OGST 2016, SIAM 2016, CMF 2016)

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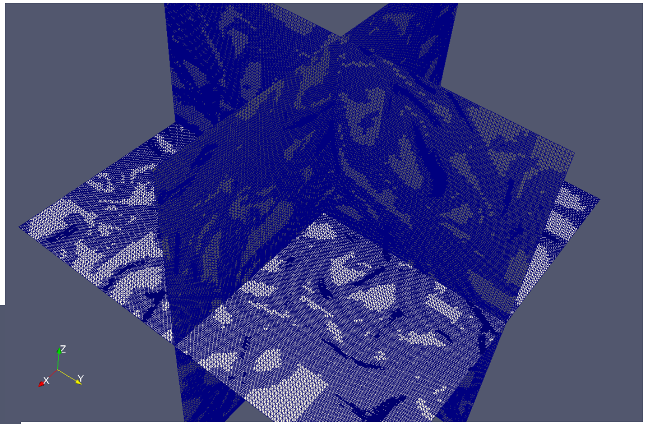
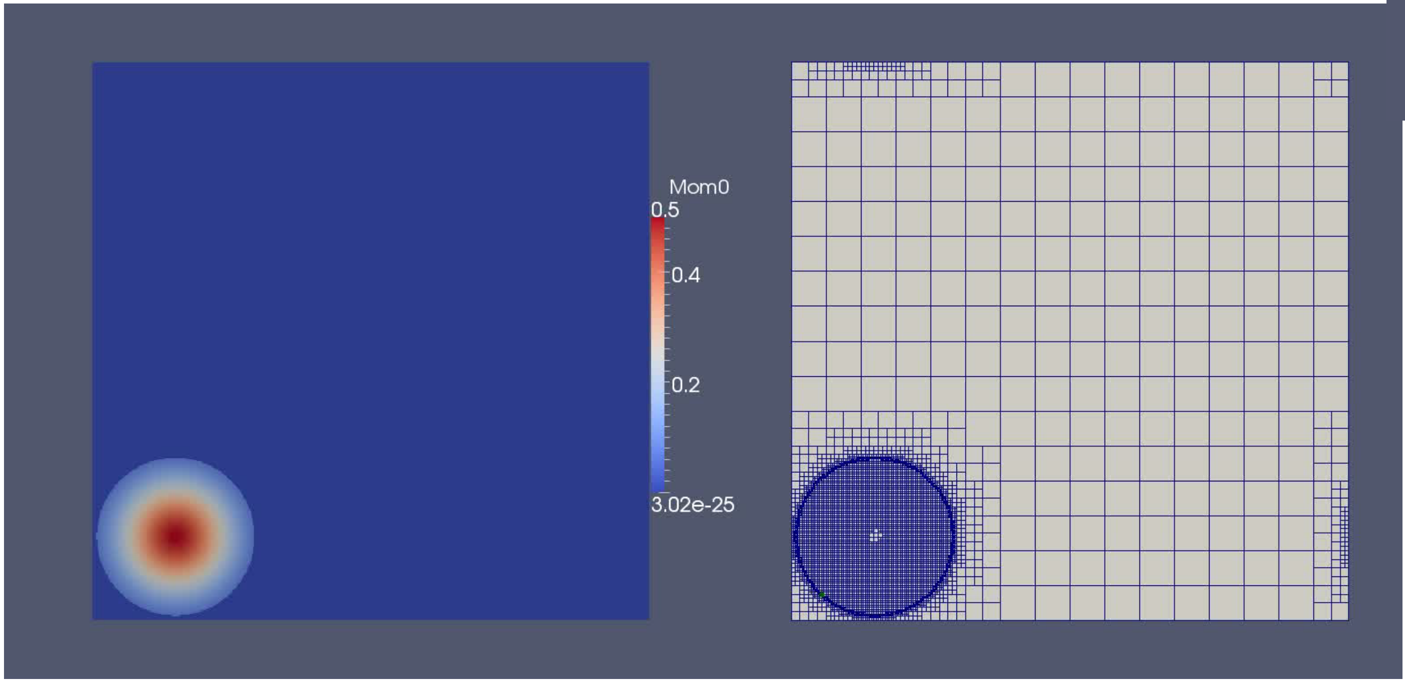




(256^3 - 84% - time/6)

Bridging the gap between the two descriptions with a single model…

(OGST 2016, SIAM 2016, ICMF 2016)

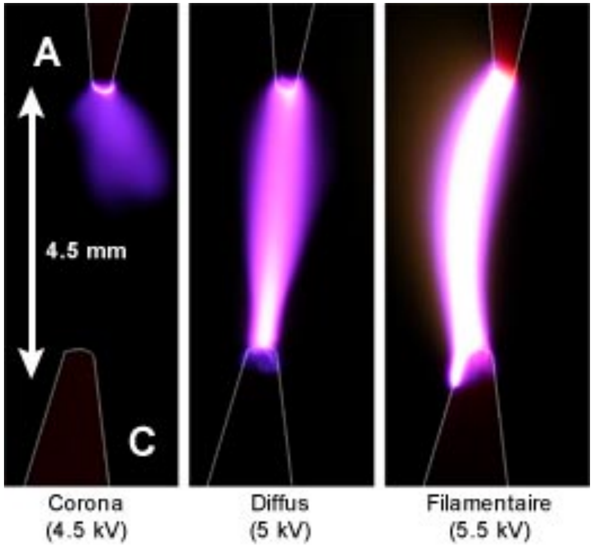
Further developments – reaction waves + MR + error control

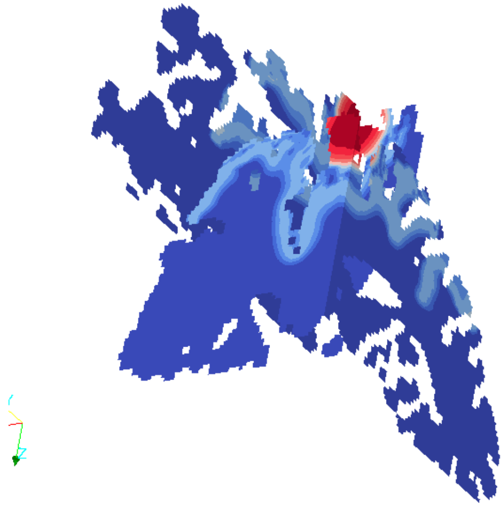
- **PhD Max Duarte** – stiff reaction waves

(Collab. S. Descombes, T. Dumont, V. Louvet, C. Tenaud, S. Candel, T. Guillet)

Adaptation in space and time for reaction-conv-diff. equations with error control.

Operator splitting with time adaptation + Multiresolution analysis





Combution – low swirl

plasma discharges

biomedical engineering - TD

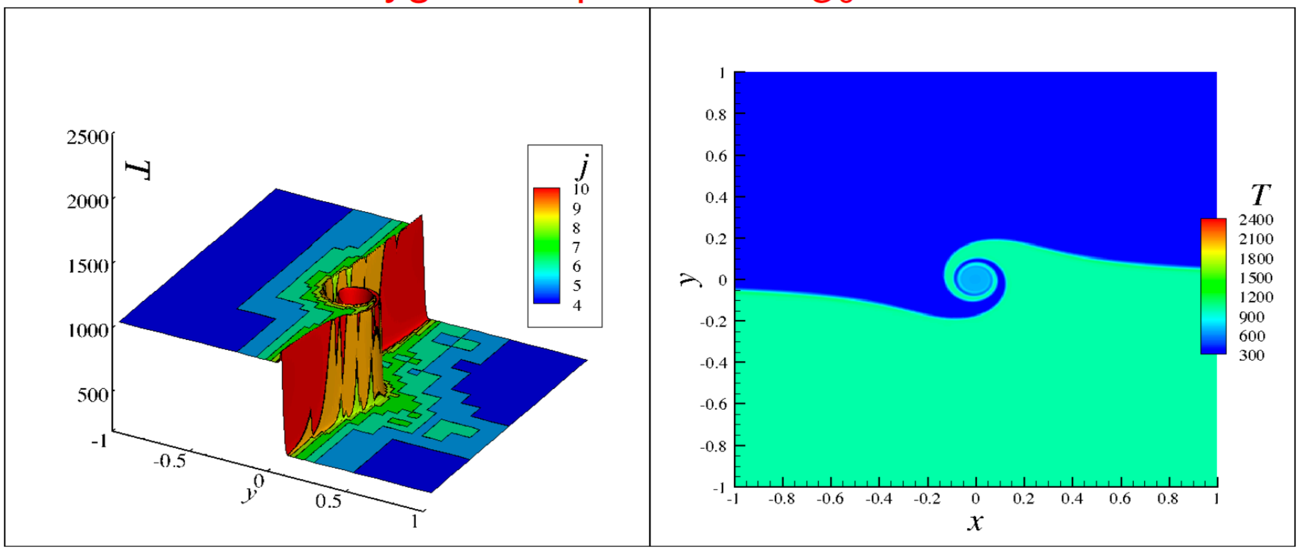
Further developments – reaction waves + MR + error control

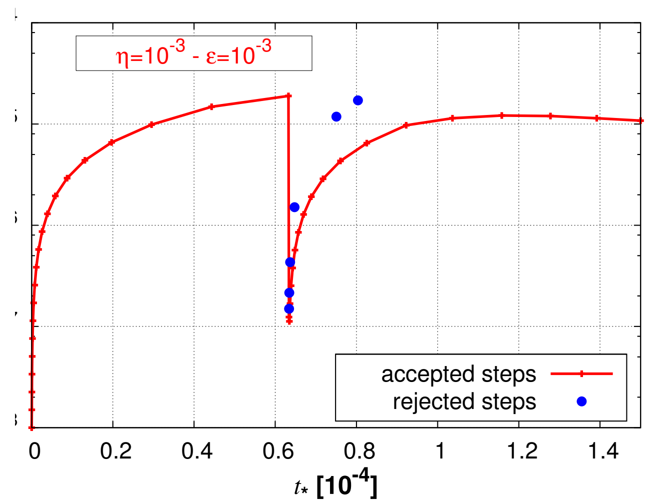
- **PhD Max Duarte + Collab** – reaction waves (combution, plasma, biomedical eng.)

MBARETE Code (MD) **Adaptation in space and time for reaction diffusion equations with error control.**

Numerical Simulations (Re=1000)

Fresh fuel temperature: $T_{F0} = 300\,\mathrm{K}$
Hot oxygen temperature: $T_{O0} = 1000\,\mathrm{K}$





Finest Grid $= 1024^2$ - $\dfrac{\text{Active Grid}}{\text{Finest Grid}} \lesssim 7\%$

$\boxed{\text{CPU time} \sim 3\text{h}28 \quad \Rightarrow \quad \sim 0\text{h}09}$

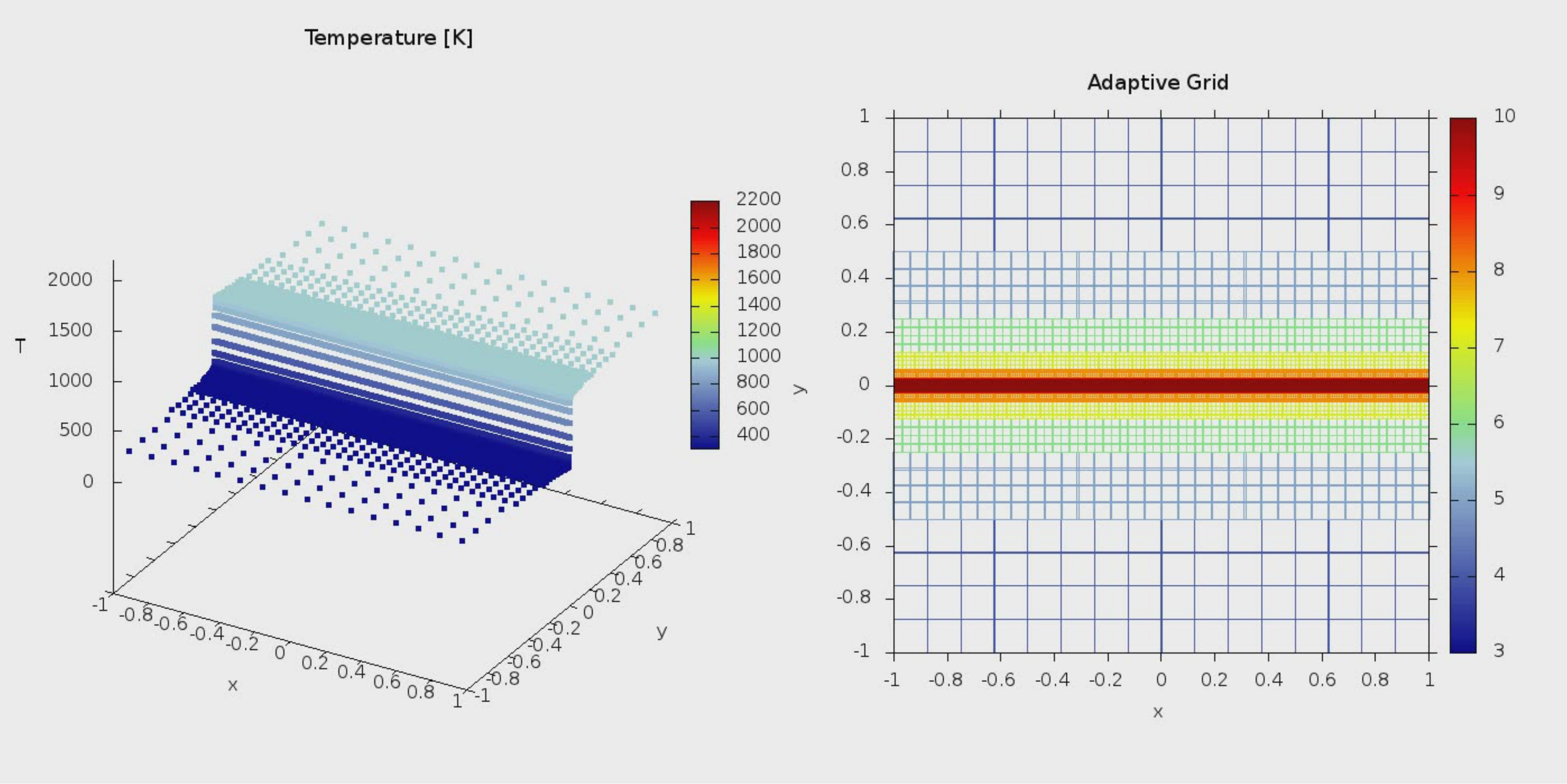
(same time integration solver: adaptive splitting)

CPU time (finest grid/constant splitting of 10^{-7}) $\sim$ 11h15

Further developments – reaction waves + MR + error control

- **PhD Max Duarte + Collab** – reaction waves (combution, plasma, biomedical eng.)

MBARETE Code (MD) **Adaptation in space and time for reaction diffusion equations with error control.**



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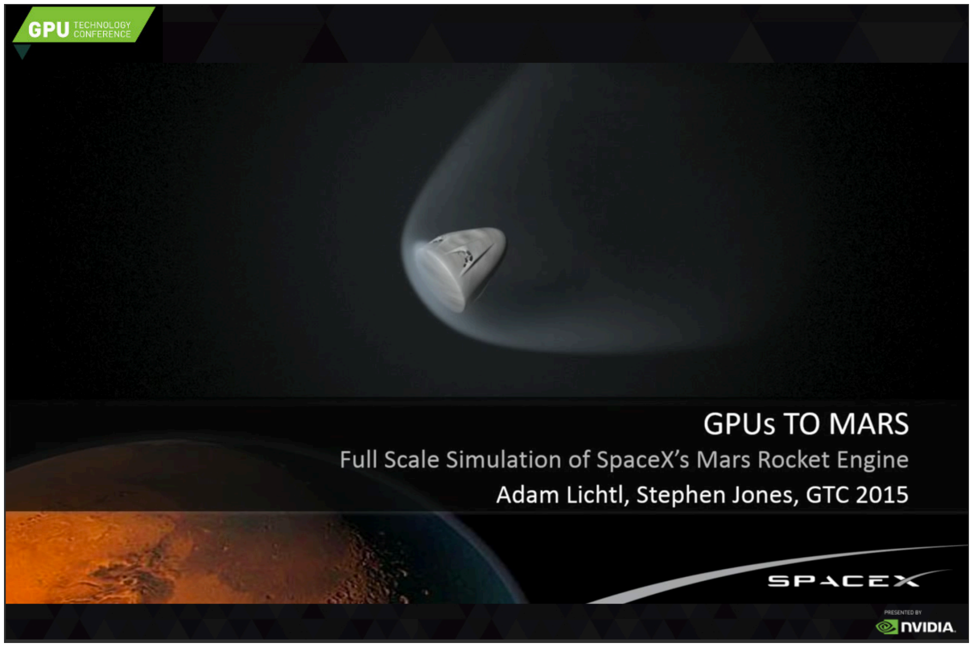

http://on-demand.gputechconf.com/gtc/2015/video/S5398.html

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Further developments – reaction waves + MR + error control

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(Collab. S. Descombes, T. Dumont, V. Louvet, C. Tenaud, S. Candel, T. Guillet)

Adaptation in space and time for reaction diffusion equations with error control.

Operator splitting with time adaptation + Multiresolution analysis

→ Shared memory with recursive tree navigation : proof of concept (MBARETE - MD)

→ Shared memory architecture : Xeon Phi (Z-code – TD)

→ Main challenge : switching to distributed memory with error control and MR

(CM 2011, SIAM SISC 2012, JCP2012, C&F 2013, SIAM NA 2014, JCP 2015, SMAI-JCM 2015)

Advertising – 30th of May – CentraleSupélec

- **“Multiresolution for multiscale PDE and parallelism” – 1:30pm – 6:00pm**

  (Groupe CALCUL – séminaire du Mésocentre – GT Transverse Paris-Saclay)

Petros Koumoutsakos - Chair of Computational Science, ETH Zurich

“Multiresolution Flow Simulations Using Grids and Particles”

Max Duarte - CD-adapco (previously Lawrence Berkeley National Laboratory)

“Dedicated time integration schemes on multiresolution adapted grids for stiff PDEs”

Thierry Dumont - Institut Camille Jordan, Université Claude Bernard Lyon 1

“Task-based adaptive multiresolution for time-space multi-scale reaction-diffusion systems on multi-core architectures”

Thomas Guillet - Intel France

“Understanding the CPU performance of irregular HPC codes”

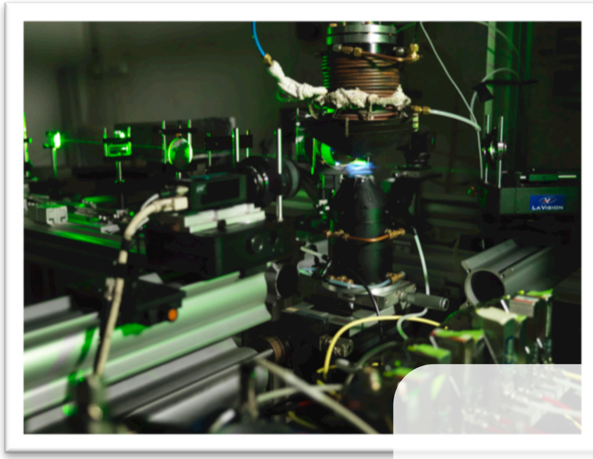
- **Comparisons with experiments esssential for model validation.**

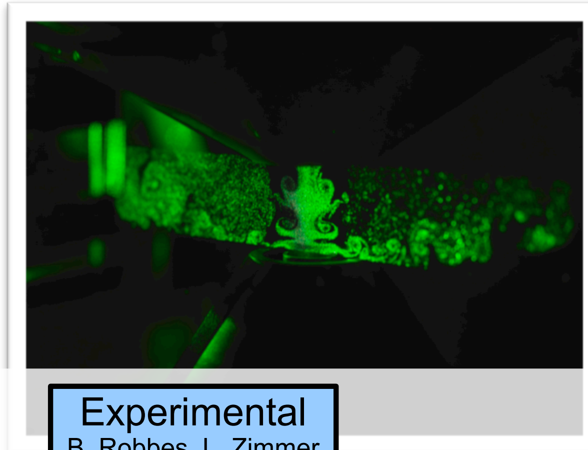
Lacour et al.
Exp. In Fluids
(2011)

-

Fréret et al.
Symposium on
Combustion (2009)

Two-phase counterflow flame: Industrial code validation





NEXTFLAME Project

Photo: C. Oriot

Experimental
B. Robbes, L. Zimmer
EM2C

DNS (Academic)
Present Work
EM2C / CORIA

Unstructured code
F. Shum-Kivan, E. Riber
CERFACS

Chemistry
- KGKAS, Chemkin

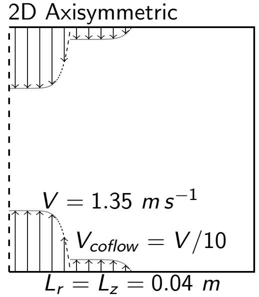
Low Mach Solver

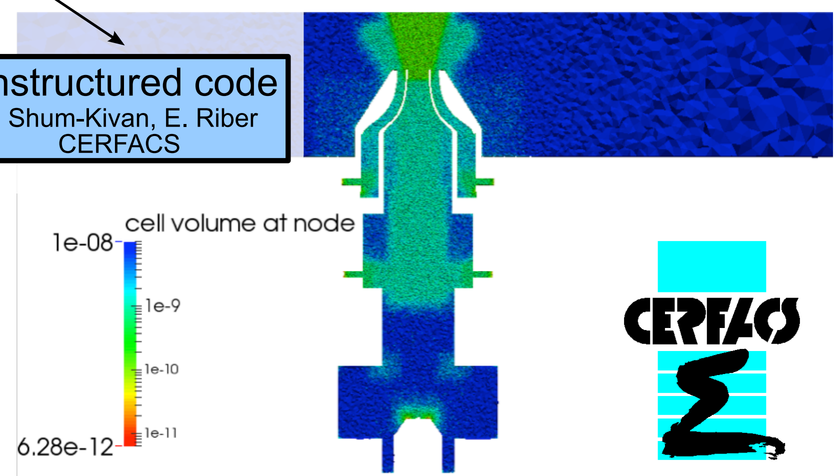
Lagrangian
- Droplet tracking
- Evaporation

Eulerian
- Realizable and robust
- Multi Fluid method
- Evaporation

Asphodele   Muses

2D Axisymmetric





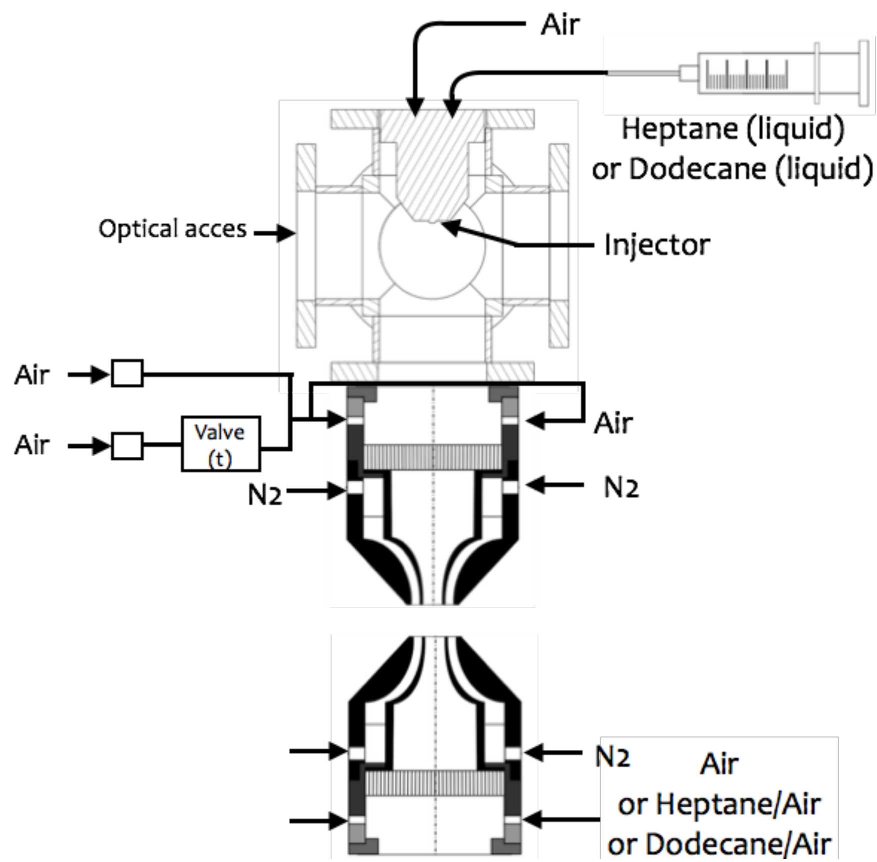
Two-phase counterflow flame: experimental setup

Forcing

- Convective forcing (No acoustics)
- Electronic valve

Measurements

- HWA – Gas Phase
- PIV – Gas Phase
- IPI – Liquid phase
- PIV – Liquid
- PDA – Liquid Phase
- Rainbow – Liquid Phase (Temperature)
- Concentration – liquid fuel
- OH-PLIF – Flame



L. Zimmer, B. Robbes, EM2C

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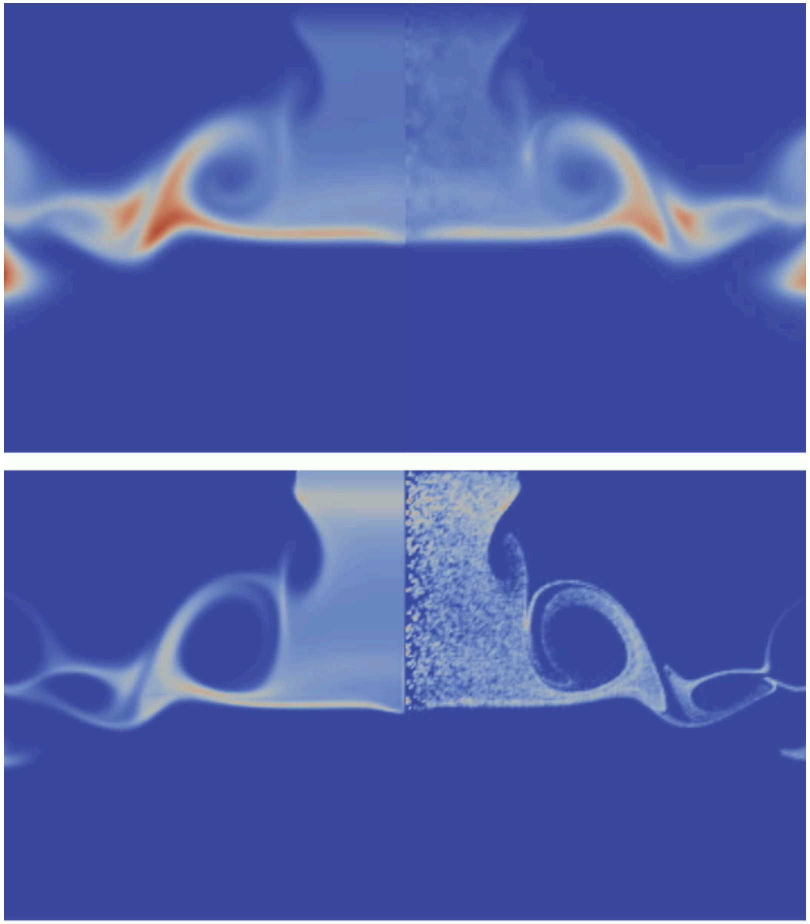
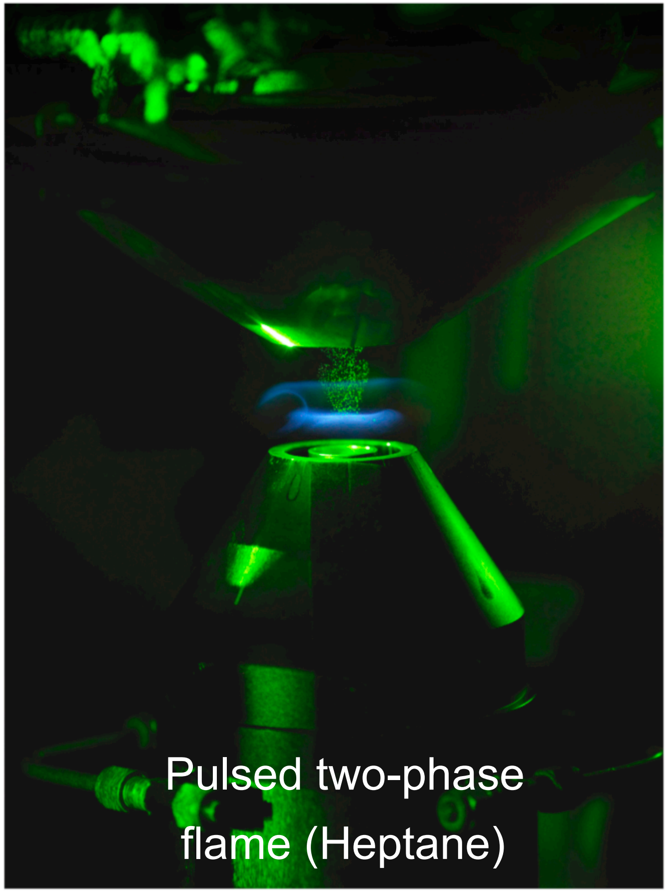
Two-phase counterflow evaporating polydisperse spray: Comparison Eulerian-Lagrangian (d^2 evaporating law)

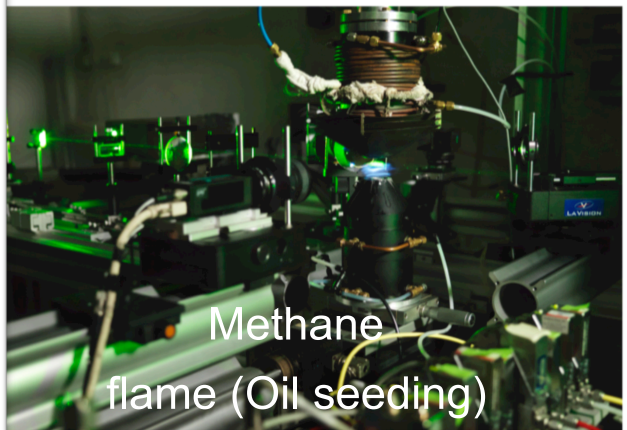
Fuel evaporated mass fraction

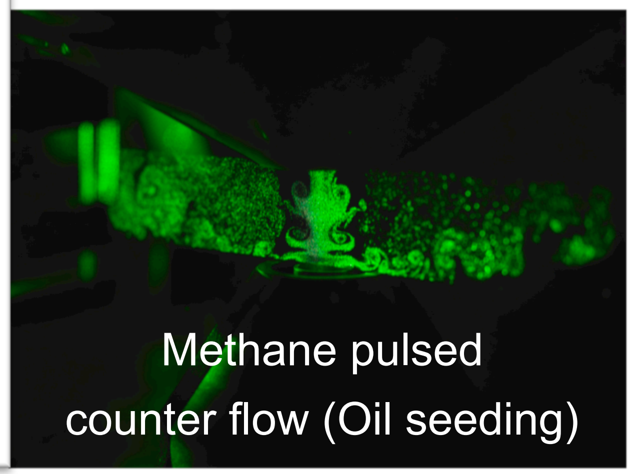
Liquid mass fraction

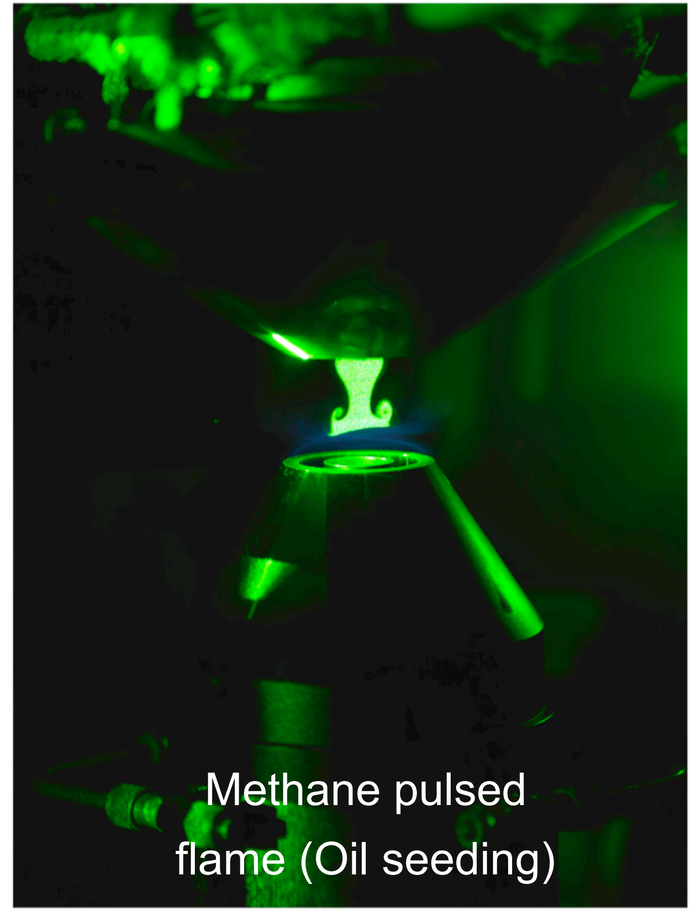


Two phase counterflow flame









L. Zimmer – B. Robbes - Photo : C. Oriot, CentraleSupelec

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