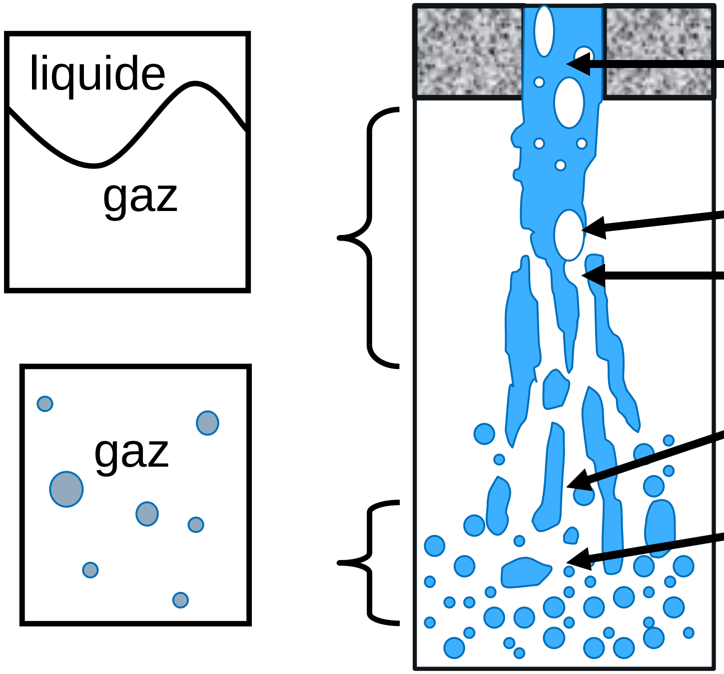
A high order moment method with mesh movement for the description of a polydisperse evaporating spray

Damien KAH, Huy Tran (IFP), Marc MASSOT (ECP), Stéphane JAY (IFP), Frédérique LAURENT (CNRS)

International Conference on Multiphase Flow, Tampa 2010

General context: injection in engines

- Sprays in internal combustion engines
- Numerical simulation of reactive multiphase flow



- Cavitation
- Primary atomization
- Turbulence in surrounding gas due to drag force exerted by the liquid
- Secondary atomization
- Evaporation, drag, heat exchange
- Collisions, coalescence

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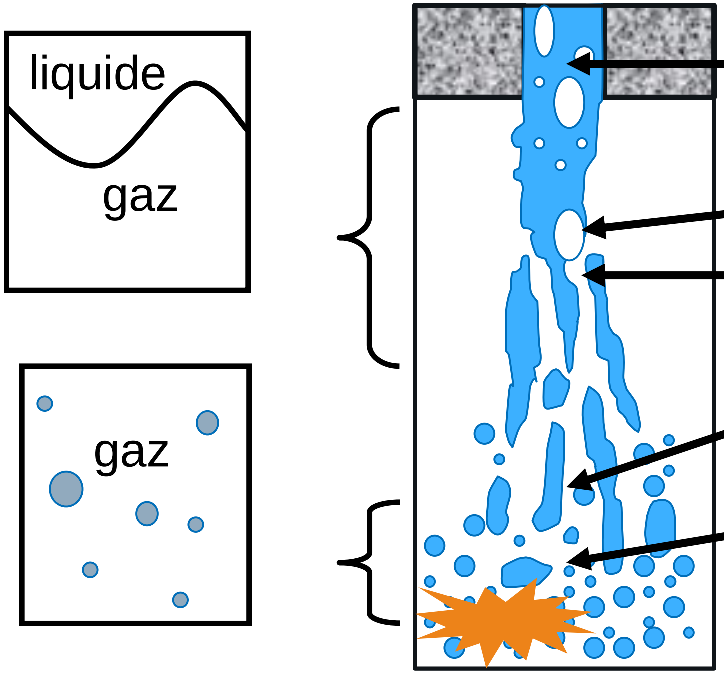

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Better predict fuel fraction in gas before combustion description of polydispersity

General objective

- CFD code IFP-C3D *(Bohbot et al., OGST 09)*
  - Reactive flow with spray (Lagrangian) in engines
  - Studies towards Eulerian two-fluid models,
    - Baer & Nunziato model *(Baer and Nunziato, IJMF 86)*
    - Volume fraction : α
    - Interfacial area density : Σ

    (Jay et al., Comb. And Flame 06)

    Mean diameter : $d = \frac{6\alpha}{\Sigma}$
  - Moving computational geometry, ALE methods *(Donea et al., ECM 04)*

- Objective
  - **Introduce description of polydispersity in IFP-C3D**

General objective

- Statistical approach
  - Spherical droplets (1-100 μm): no interface problem
  - Number density function (NDF) $f(t, \mathbf{x}, \boldsymbol{v}, S)$
  - Williams-Boltzmann Equation *(Williams, Physics of Fluids, 1958)*

$$\boxed{\partial_t f + \partial_{\mathbf{x}} \boldsymbol{v} f + \partial_{\boldsymbol{v}} \boldsymbol{F} f + \partial_S R f = 0}$$

- Eulerian framework
  - Complete resolution with Finite Volume expensive *(Laurent and Massot, Comb. Th. Model. 01)*
  - Size moments $m_k = \int_{S_{min}}^{S_{max}} \int_{\mathbb{R}} S^k f \, \mathrm{d}\boldsymbol{v} \mathrm{d}S$

Objective

- 2 classes of models
  - Sectional methods: multi-fluid model
    (*Tambour, Comb. and Flame 1985*) , (de *Chaisemartin, PhD Thesis 09*)
  - High order moment methods *(Fox Laurent Massot, J. Comp. Phys., 08)*
    Difficulties:
    - stability
    - accuracy
- Objective of this work
  - Design a high order size moment method ...
    - with one size section
    - generic, describing any NDF

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- Objective of this work
  - Design a high order size moment method ...
    - with one size section
    - generic, describing any NDF
  - ... with numerical schemes adapted to the ALE formalism

Outline

- High order size moment method for the description of polydispersity
- Arbitrary Lagrangian Eulerian (ALE) formalism
- High order moment method and ALE
  - Feasibility study
  - Implementation in IFP-C3D

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High order size moment method / Equation system

$$\partial_t m_0 + \nabla_{\mathbf{x}} \cdot m_0 \mathbf{u} = -Rn(t, \mathbf{x}, S = 0)$$

$$\vdots$$

$$\partial_t m_N + \nabla_{\mathbf{x}} \cdot m_N \mathbf{u} = -N m_{n-1}$$

$$\partial_t m_0 \mathbf{u} + \nabla_{\mathbf{x}} \cdot m_0 \mathbf{u} \otimes \mathbf{u} = \underbrace{-Rn(t, \mathbf{x}, S = 0)\mathbf{u}}_{\text{Evaporation}} - \nabla_{\mathbf{x}} P + \underbrace{\boldsymbol{D}}_{\text{Drag}}$$

Innovation Energy Environment

High order size moment method / Equation system

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- $P = 0 \quad \Longleftrightarrow \quad f = n(t, \mathbf{x}, S)\delta(\boldsymbol{v} - \mathbf{u}(t, \mathbf{x}, S))$

(Laurent and Massot, Comb. Th. Model. 01) (Massot et al., Lecture Series VKI, 09)

Pressureless gas dynamics *(Bouchut, Ser. Adv. Math. Appl., 94)*

High order size moment method / Equation system

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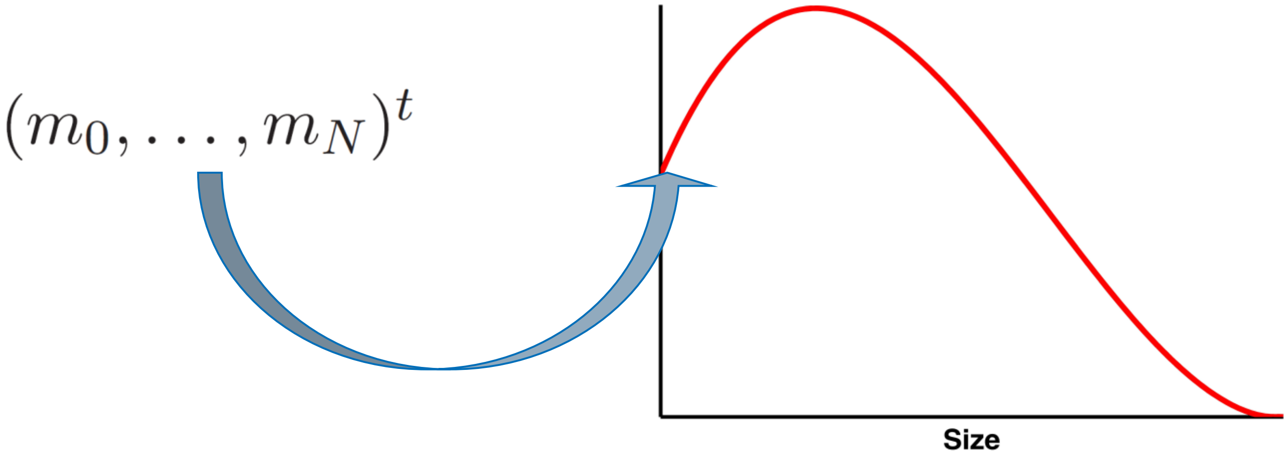
  Pressureless gas dynamics *(Bouchut, Ser. Adv. Math. Appl., 94)*

- Unclosed term $Rn(t, \mathbf{x}, S = 0)$ from $(m_0, \ldots, m_N)^t$

High order size moment method
Closure of the evaporation term

- $Rn(t, \mathbf{x}, S = 0)$ = Evaporation flux



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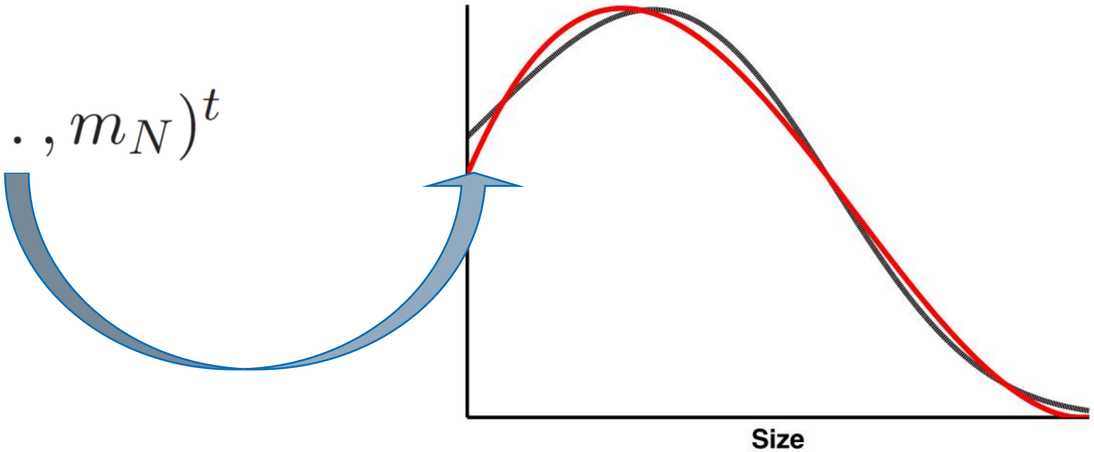
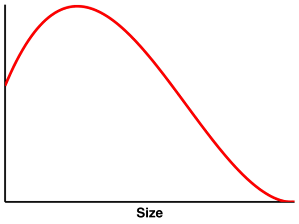
$$(m_0, \ldots, m_N)^t$$



- **Entropy Maximization** *(Mead et al., J. Math. Phys., 1984)*

High order size moment method
Numerical scheme

- 2 requirements for the numerical scheme
  - Stability
    - Realizability condition $(m_0, \dots, m_N)^t$



    - Capture singularities due to pressureless gas
  - Accuracy
- Main features of the schemes
  - Finite volume
  - Explicit exact temporal integration
  - Elements from moment space theory *(Dette et Studden, 1997)*

Second order in space and time

- Evaporation *(Massot et al., SIAM J. Appl. Math. 2010)*
- Transport *(Kah et al., ICLASS, 2009)*

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ALE / General principles

- **Aim**: write a numerical scheme with a moving computational geometry, due to piston movement

- Two referentials:
  - the **spatial** referential : $R_{\boldsymbol{x}}$
  - the **mesh** referential : $R_{\boldsymbol{\chi}}$

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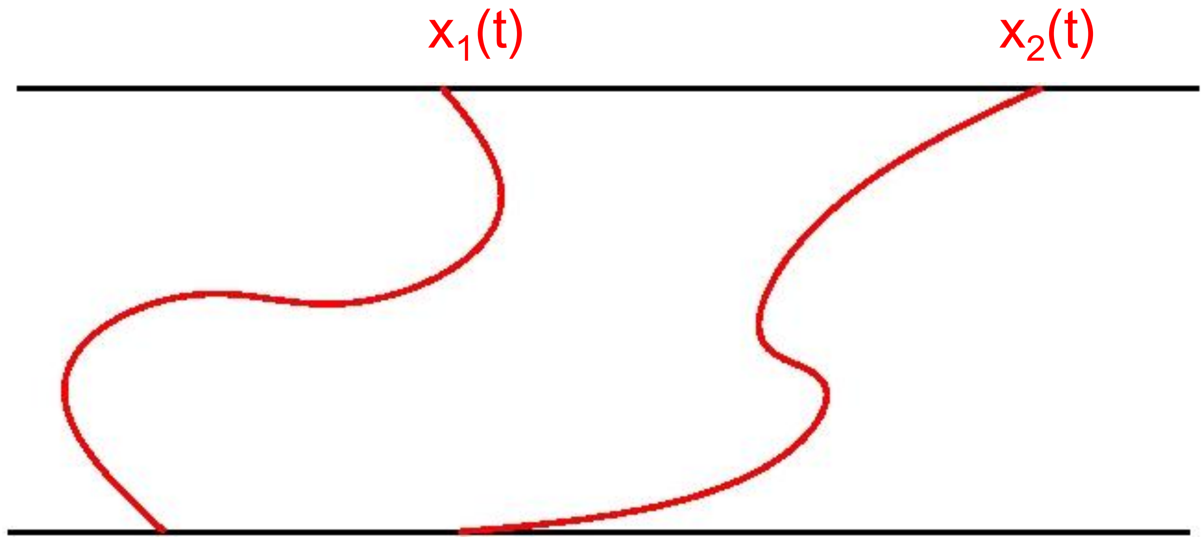

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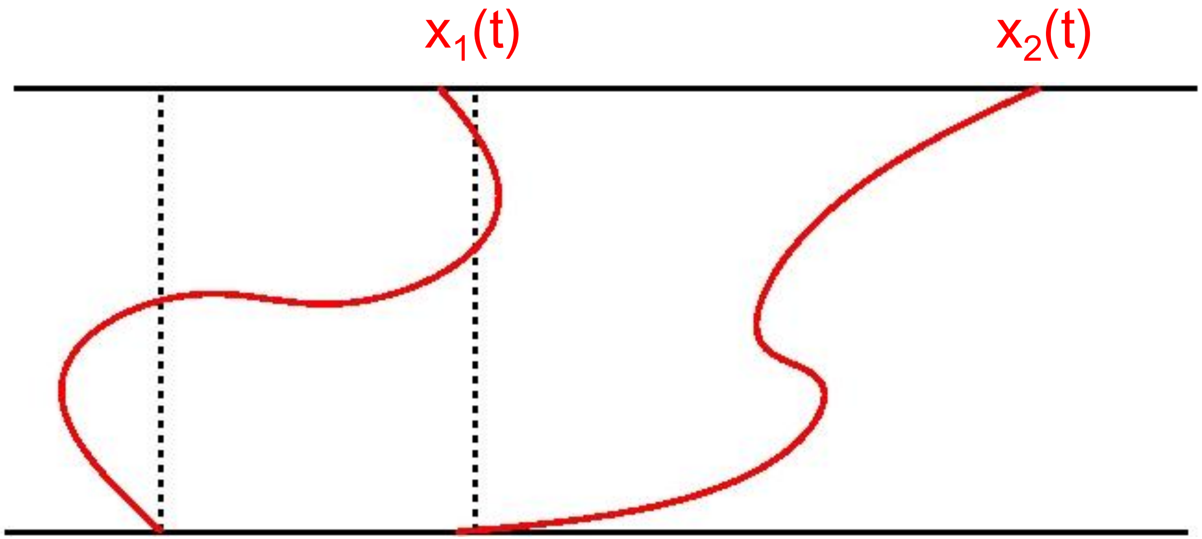

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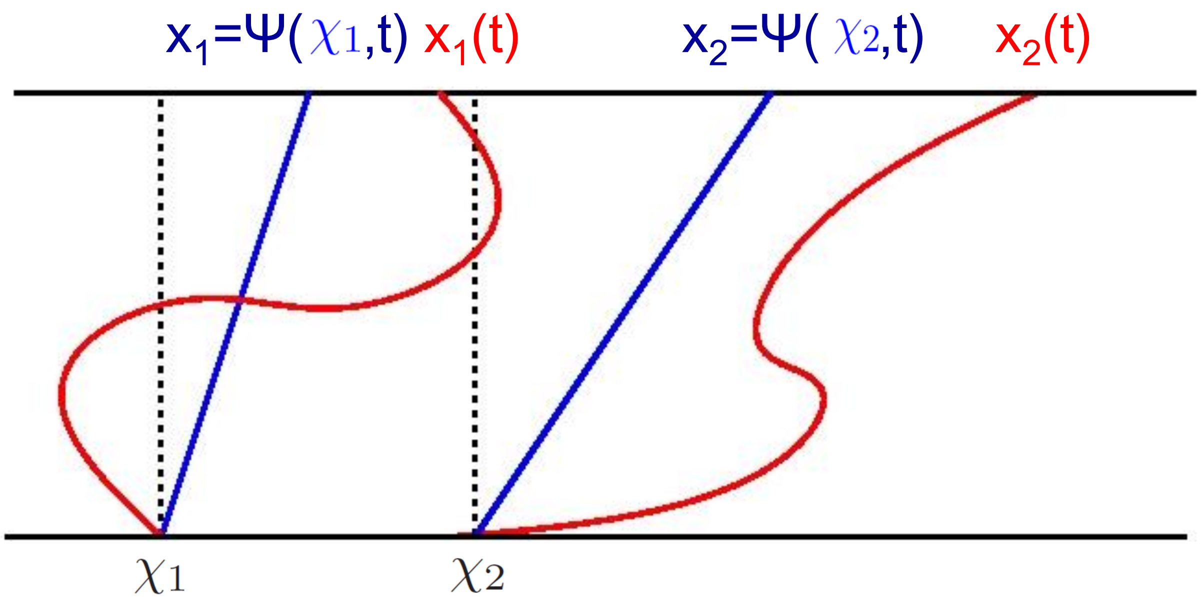

ALE / Algorithm

- **Principle**: Combination of *(Donea et al., ECM, 04), (Farhat et al., J. Comp. Phys. 01)*
  - Accurary of Lagrangian methods
  - Robustness of Eulerian methods
- Operator splitting algorithm
  - Phase A: source terms

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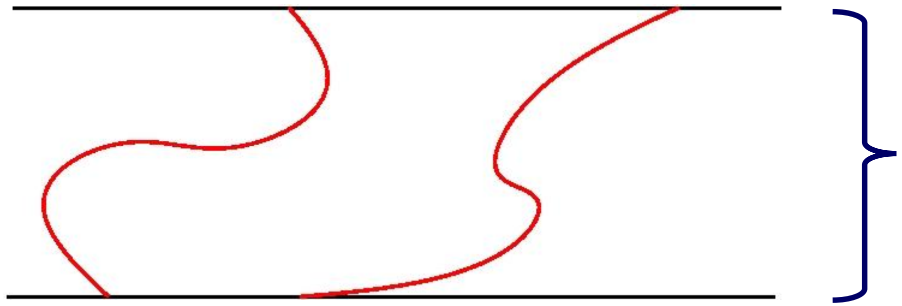

Lagrange step

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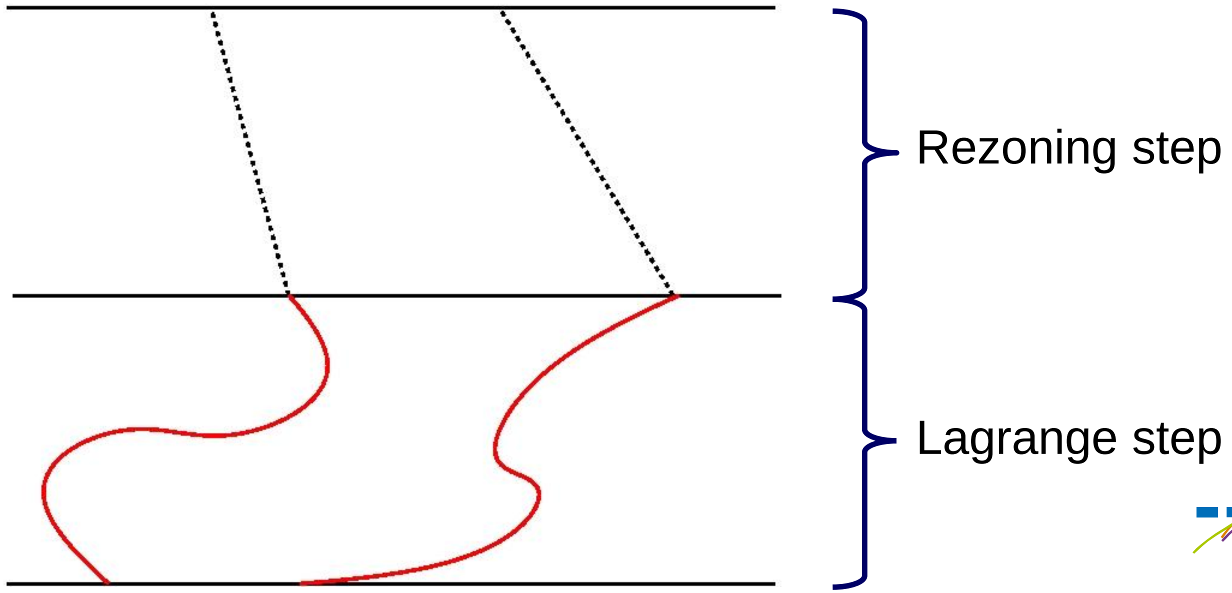
  - Phase C / Eulerian : Advection terms / Rezoning step



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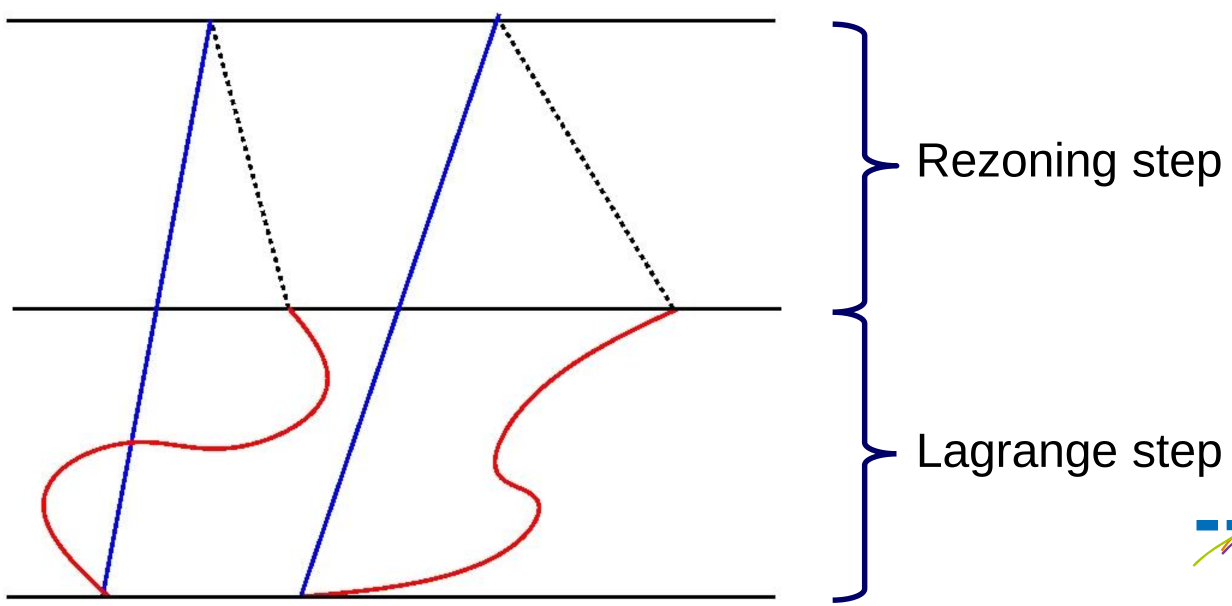

Outline

- High order size moment method for the description of polydispersity
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- High order moment method and ALE
  - Feasibility study on a Structured Grid
  - Implementation in IFP-C3D

High order moment method and ALE / Feasability study on a structured grid

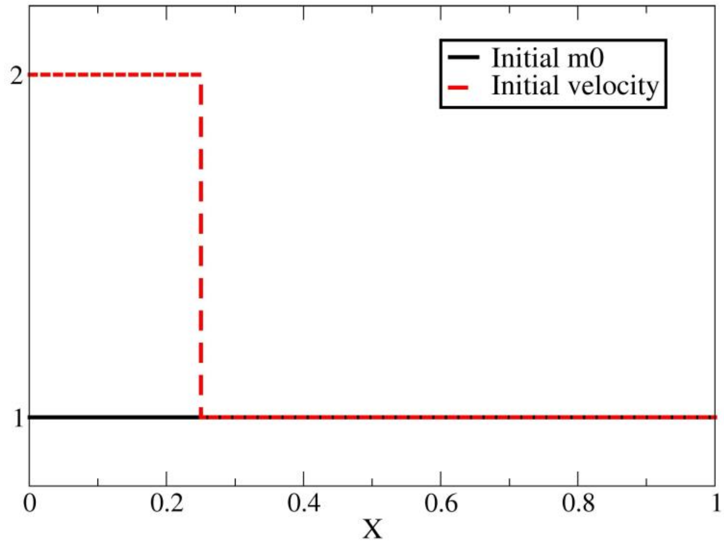
- Advection of the moments
  - Adaptation of Eulerian scheme in the rezoning step
  - Preservation of the properties
    - Stability
    - Accuracy

- Advection of velocity
  - Nodal definition of the velocities
  - Cell volume change
  - Conservation of momentum / Discrete maximum principle for velocity *(Larrouturoux, J. Comp. Phys, 2004)*

⇨ Second order in time and space on a moving grid

High order moment method and ALE / Feasibility study on a structured grid / test case

- Riemann problem
- Initial condition : 4 moments (N=3)

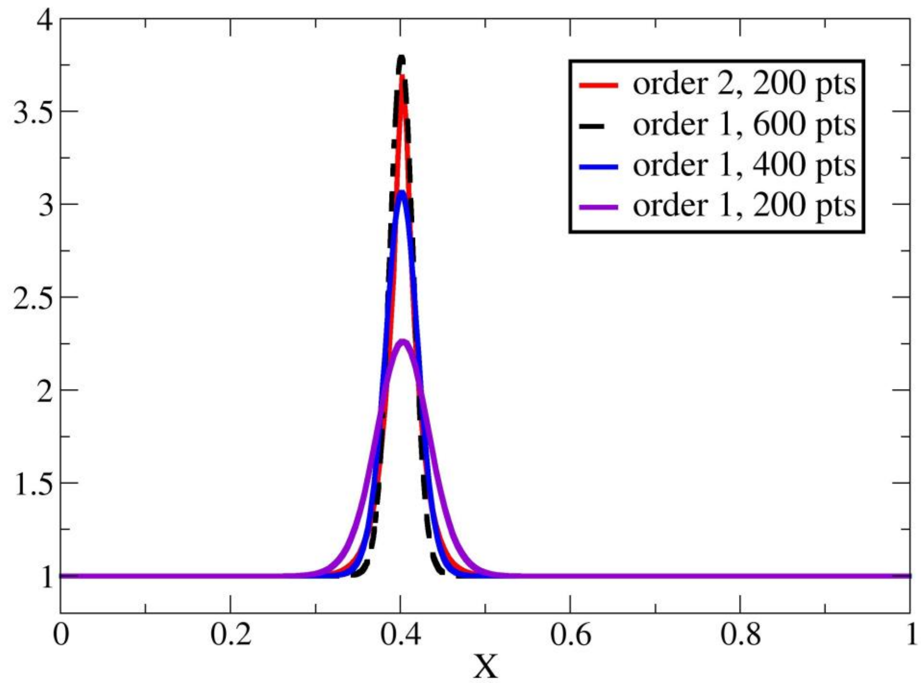


Size distribution

- Moving grid : $x(t) = 0.2\sin(2\frac{\pi}{0.1}t)$
- Results for m_0
- Results at time t=0.1

High order moment method and ALE / Feasibility study on a structured grid / test case

- Results at time t=0.1



- Resolution of shock dynamic coupled to mesh movement
- Validation of the developments

High order moment method and ALE / Implementation in IFP-C3D

- IFP-C3D numerical software
  - A hexahedral unstructured solver devoted to internal CFD with spray and combustion modelling
  - The conservation equations of mass, mass species, momentum and energy for compressible and reactive flows with spray are solved on moving grids
  - The equations are solved using a finite volume method extended with the ALE (Arbitrary Lagrangian Eulerian) method. The temporal integration scheme is implicit.
  - The k-ε turbulence model is used (RANS)

- Implementation of the high order moment method in IFP-C3D validated on 2 test cases:
  - Moving piston
  - Interaction with Taylor-Green vortices

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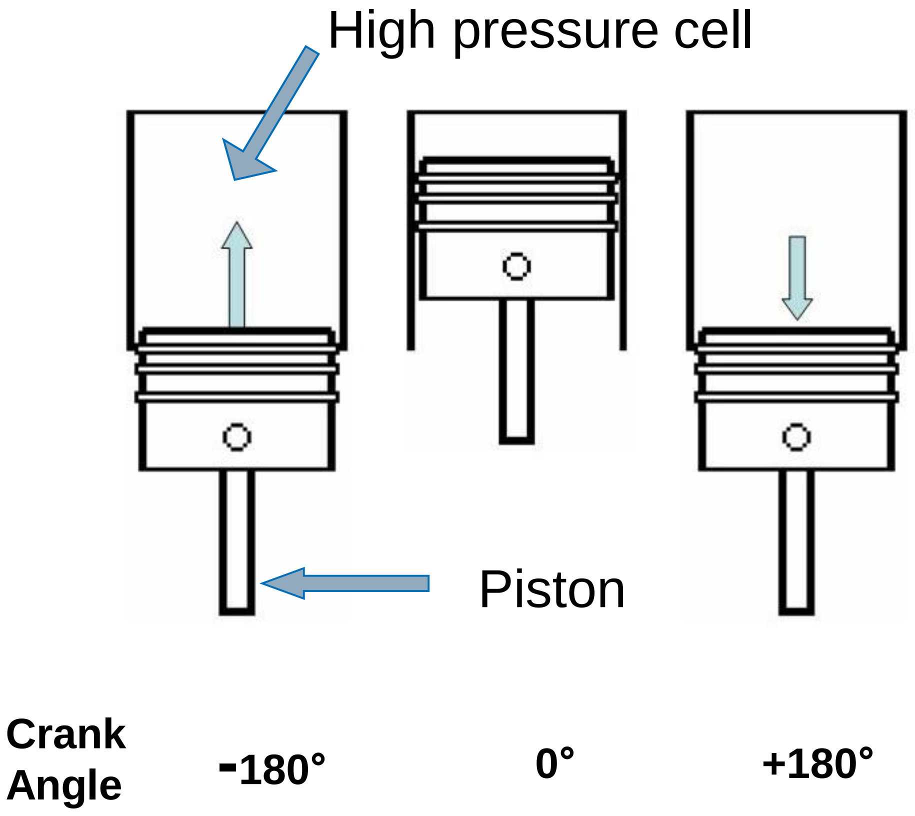
High order moment method and ALE / Implementation in IFP-C3D

- Moving piston (rpm=1200)



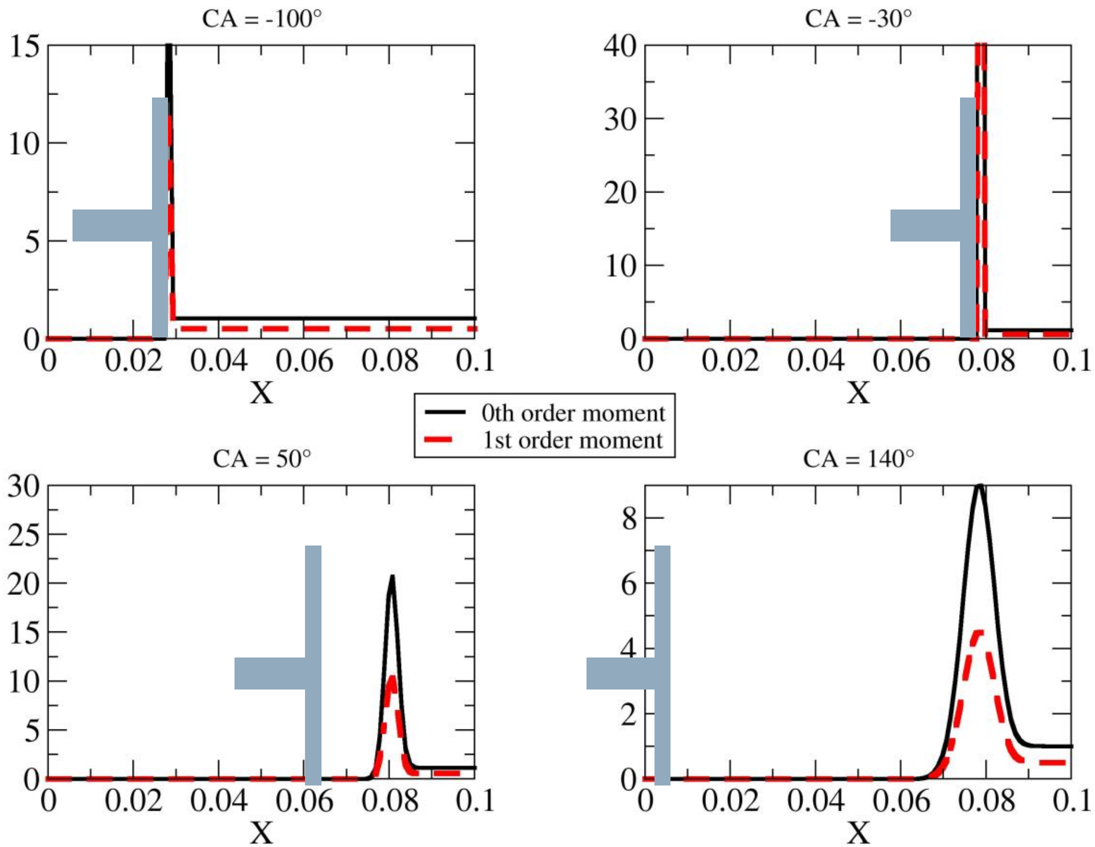
- Size distribution

- Homogeneous field

  Initial velocity = 0
- Homothetic cell volume variation

High order moment method and ALE / Implementation in IFP-C3D

- Spray

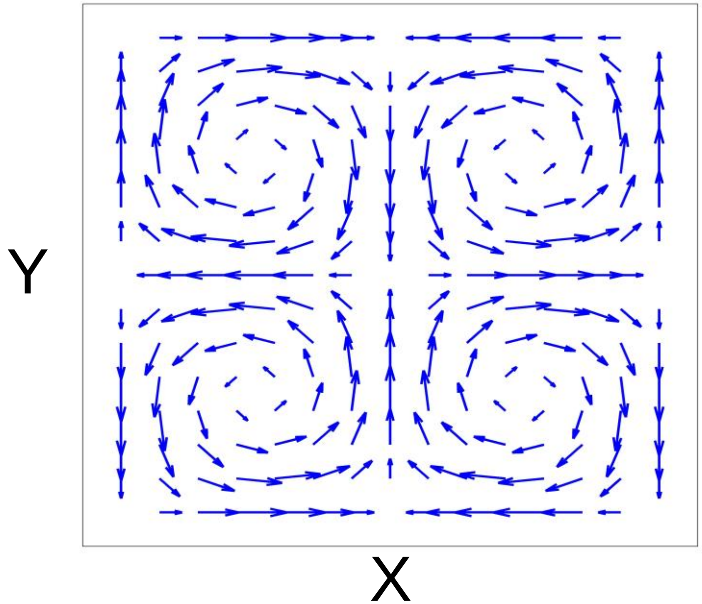


- Singularity dynamic preserved with piston boundary condition

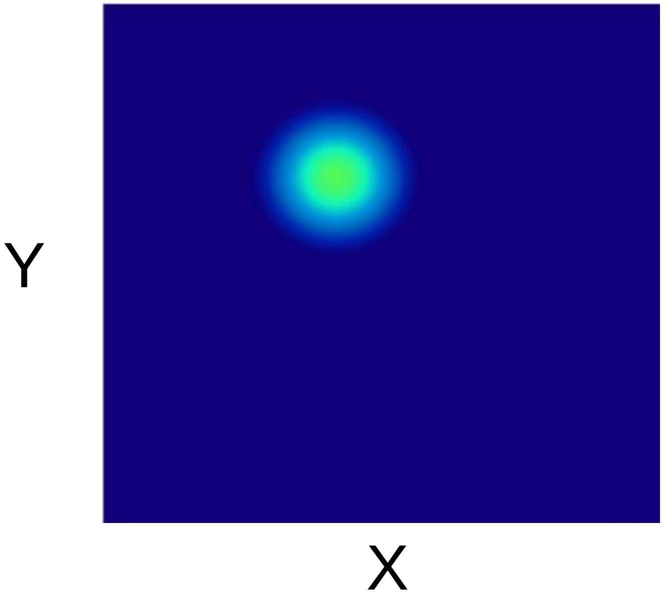
High order moment method and ALE / Implementation in IFP-C3D

- 2D test with evaporation and drag

Taylor-Green vortices for gas flow

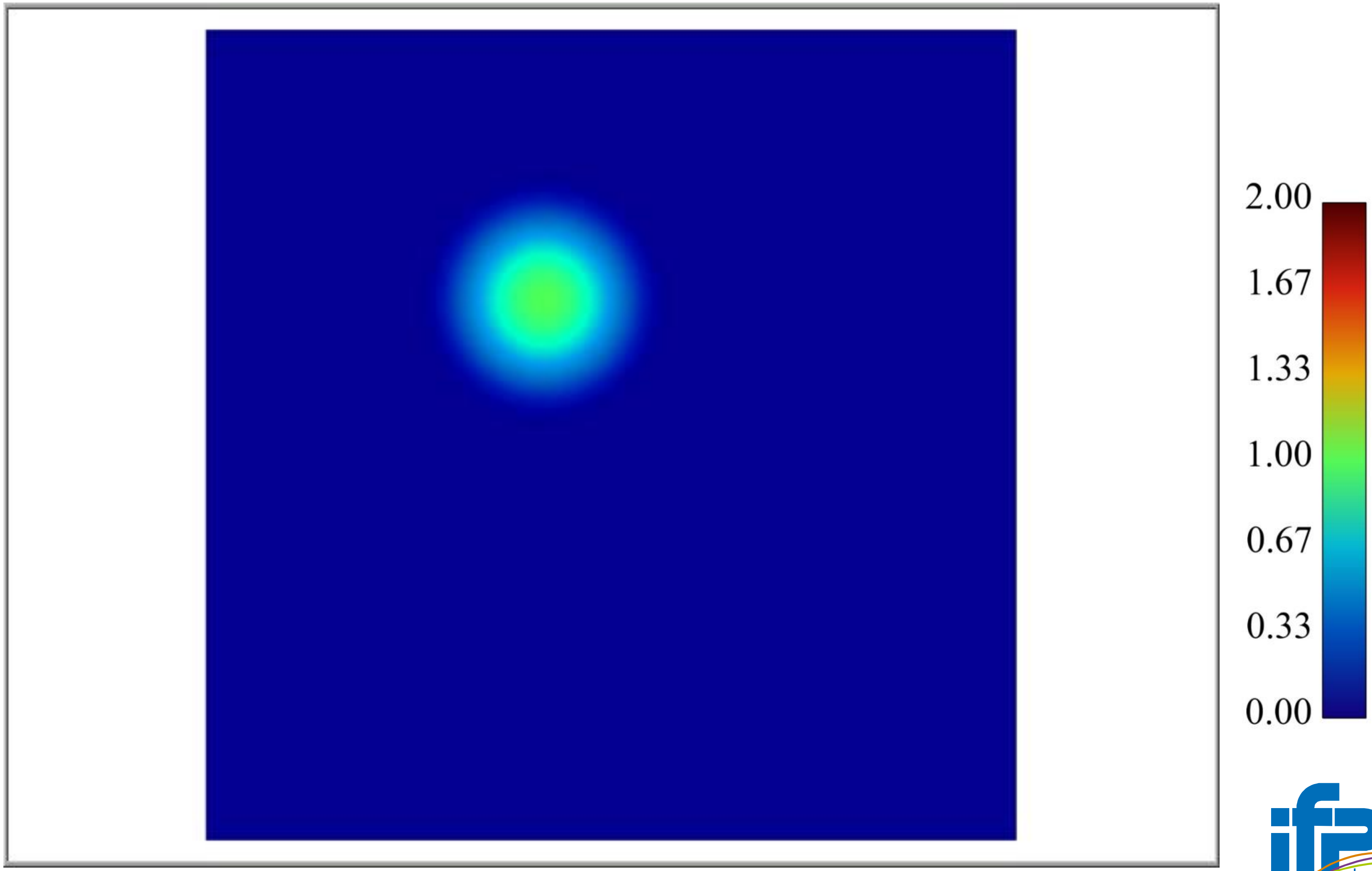


Initial condition for the spray



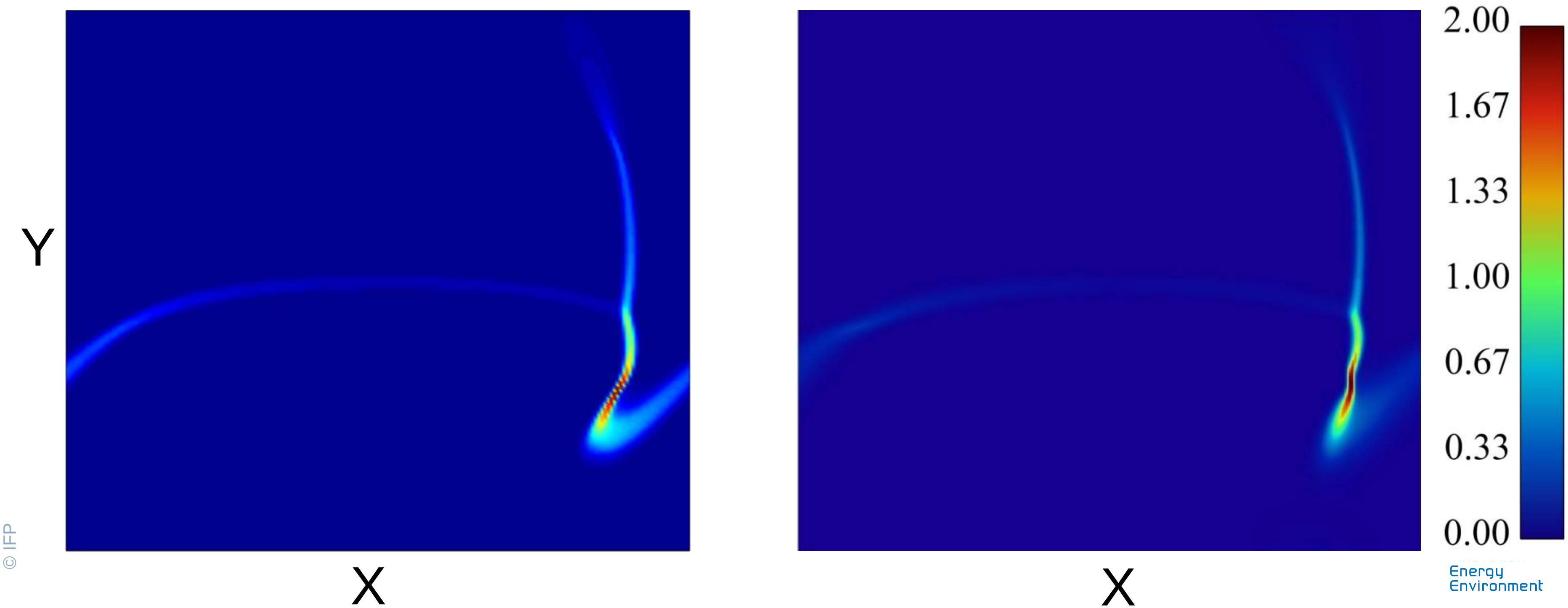
- Periodic Boundary conditions
- Drag: Maximum Stokes = 2.81
- Evaporation: R = 0.21
- Final time = 2

High order moment method and ALE / Implementation in IFP-C3D



High order moment method and ALE / Implementation in IFP-C3D

- **Muses3D**
  - Structured
  - Eulerian
  - 2nd order
- **C3D**
  - Unstructured
  - ALE
  - 1st order



Conclusions-Perspectives

- Conclusions
  - Design of a high order moment method describing polydispersity without discretizing the size phase space
  - Adaptation of this method to the ALE formalism
    - Preservation of the scheme’s property (stability and accuracy) in a structured grid
    - Feasibility of implementation in an industrial unstructured grid
- Perspective
  - Injection cases
  - Improvement of scheme accuracy for an unstructured grid
  - Comprehensive model including descriptions of spray and of two-fluid models

Thank you for your attention

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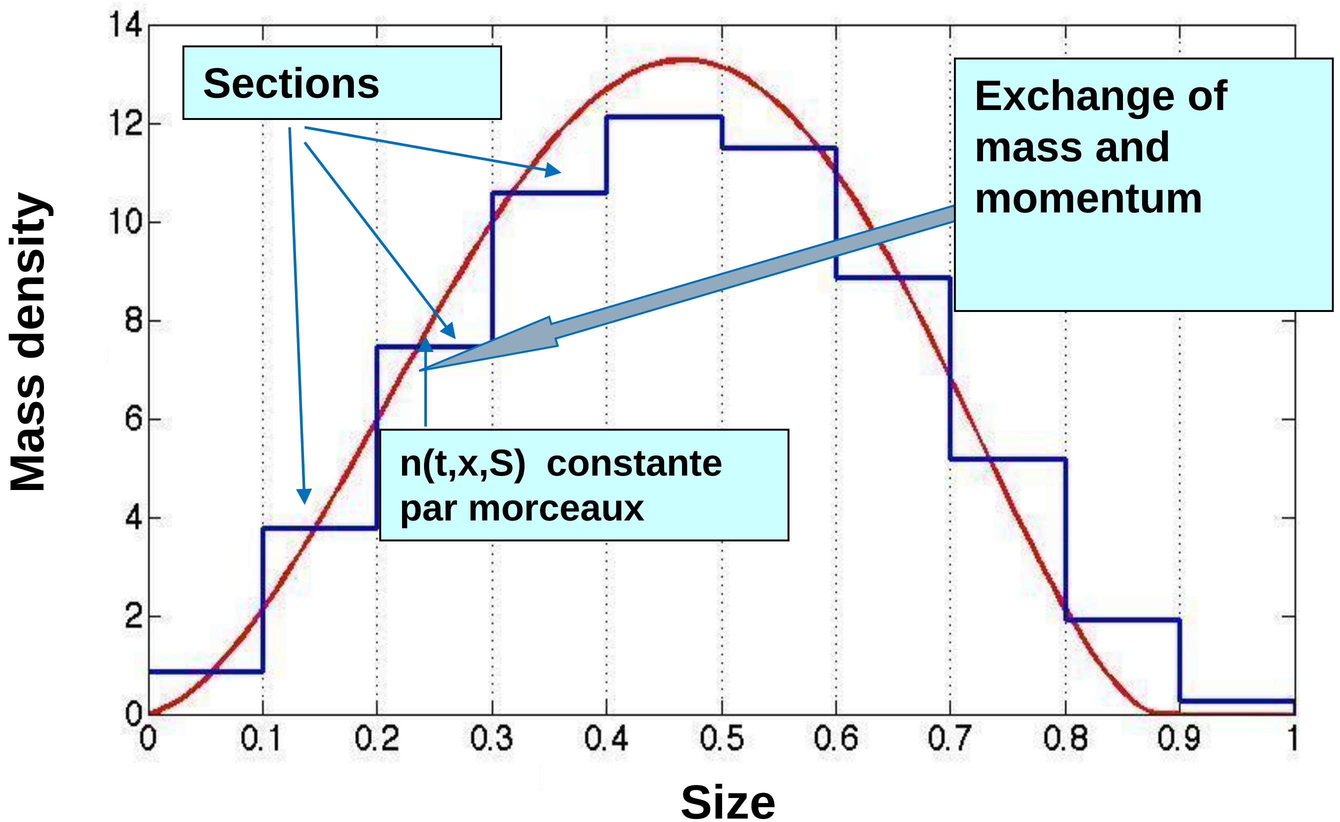
Multi-fluid method

- Several sections, section $[S_i, S_{i+1}]$
- Evolution of $m_{3/2,i}, m_{3/2,i} u_i$ in a section
- Reconstruction: $n(t, x, S) = \kappa_i(S) m_{3/2,i}(t, x)$



Equations in a moving frame

- **Aim**: write a numerical scheme with a moving computational geometry, due to piston movement
- Two referentials:
  - the **spatial** referential : $R_{\boldsymbol{x}}$
  - the **mesh** referential : $R_{\boldsymbol{\chi}}$

$$\left.\begin{aligned} &\mathbf{x} = \Phi(\boldsymbol{\chi}, t), \;\; J(\boldsymbol{\chi}, t) = det(\nabla_{\boldsymbol{\chi}}\mathbf{x}), \\ &\boldsymbol{u}_{\boldsymbol{\chi}}(\boldsymbol{\chi}, t) = \partial_t \mathbf{x}|_{\boldsymbol{\chi}} \end{aligned}\right\}$$

- The transport equation in $R_{\boldsymbol{x}}$

$$\partial_t \alpha + \nabla_{\mathbf{x}} \alpha \mathbf{u} = \nabla_{\mathbf{x}} \boldsymbol{\sigma} + S$$

… writes in $R_{\boldsymbol{\chi}}$

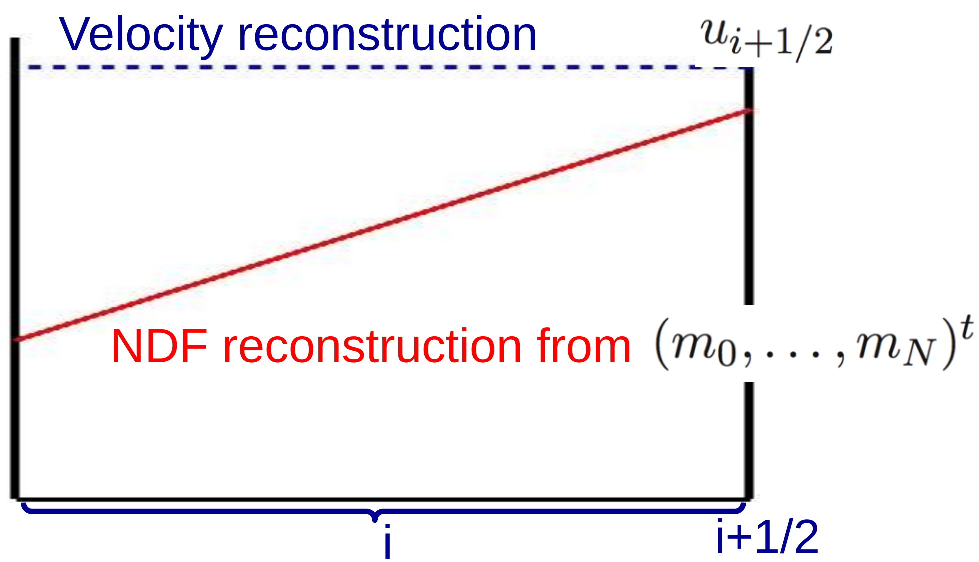
$$\partial_t J = J \nabla_{\mathbf{x}} \boldsymbol{u}_{\boldsymbol{\chi}}$$

$$\partial_t J\alpha|_{\boldsymbol{\chi}} + J\nabla_{\mathbf{x}}\alpha(\mathbf{u} - \boldsymbol{u}_{\boldsymbol{\chi}}) = J\nabla_{\mathbf{x}}\boldsymbol{\sigma} + JS$$

(Hirt 74, Despres 05)

Advection of the moments

- $$\frac{(Jm_1)_i^{n+1} - (Jm_1)_i^n}{\Delta t} + \frac{F_{i+1/2} - F_{1-1/2}}{\Delta x} = 0$$



- Reconstruction of the NDF, like in a fixed Eulerian Grid
- 1st order reconstruction of the velocity to compute the flux using an upwind scheme

$$\Rightarrow \quad F_{i+1/2}, F_{i-1/2}$$

Advection of the velocity:

Preservation of the maximum principle for a cell-centered quantity

- $\partial_t J m_1 + \partial_\chi m_1 u = 0$

  $\partial_t J m_1 Y + \partial_\chi m_1 Y u = 0$

- $$\frac{(Jm_1)_i^{n+1} - (Jm_1)_i^n}{\Delta t} + \frac{F_{i+1/2} - F_{1-1/2}}{\Delta x} = 0$$

  $$\frac{(Jm_1Y)_i^{n+1} - (Jm_1Y)_i^n}{\Delta t} + \frac{G_{i+1/2} - G_{1-1/2}}{\Delta x} = 0$$

- $G_{i+1/2} = (m_1 Y) u_{i+1/2}$

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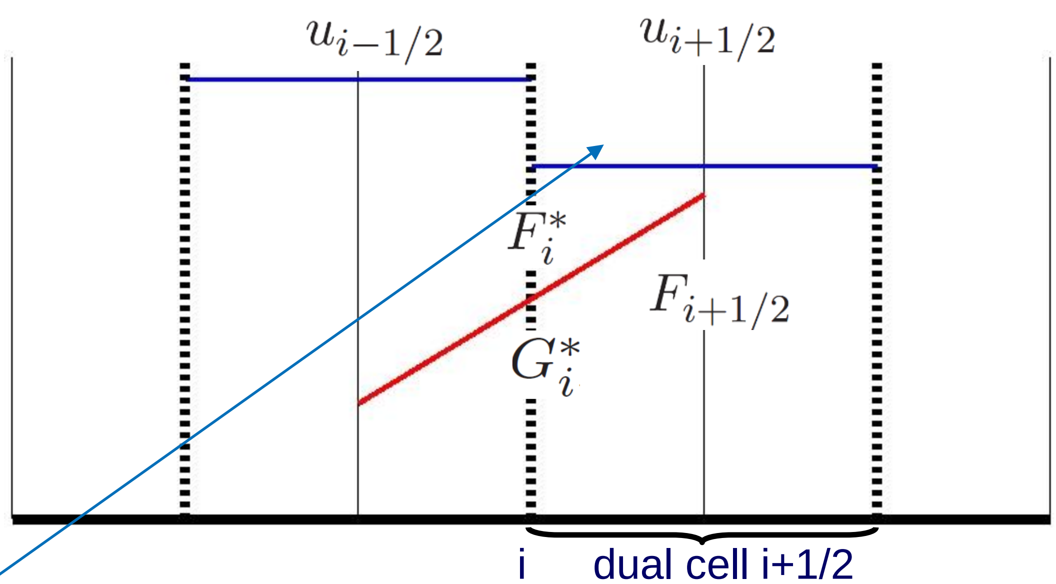
- $$\begin{aligned} G_{i+1/2} &= (m_1 u)_{i+1/2} Y \\ &= F^+_{i+1/2} Y_i + F^-_{i+1/2} Y_{i+1} \end{aligned}$$ *(Larrouturoux)*

Advection of the velocity

Preservation of the maximum principle for the velocity, defined on nodes

- $$\frac{(Jm_1u)^{n+1}_{i+1/2} - (Jm_1u)^{n}_{i+1/2}}{\Delta t} + \frac{G^*_{i+1} - G^*_i}{\Delta x} = 0$$



- $$(Jm_1u)_{i+1/2} = \left(\frac{(Jm_1)_{i+1} + (Jm_1)_i}{J_{i+1} + J_i}\right)u_{i+1/2}$$

Advection of the velocity

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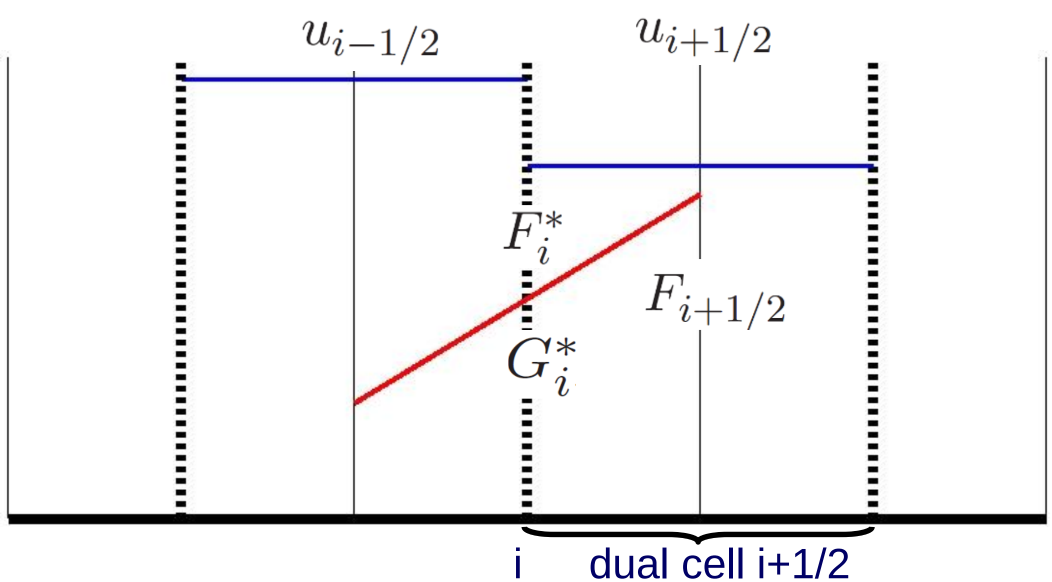

- $$G^*_i = F^{*+}_i u_{i-1/2} + F^{*-}_i u_{i+1/2}$$
- $$F^*_i = 1/2(F_{i+1/2} + F_{i-1/2})$$