# Moment methods and realizable numerical methods for polydisperse sprays and particle-laden flows

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In collaboration with
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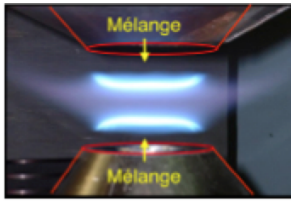
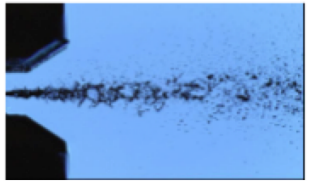
Workshop on Moment Methods in Kinetic Theory II - Fields Institute - Toronto

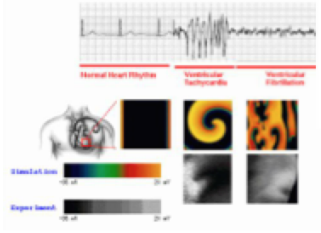
# A mathematics team in an engineering laboratory

➢ **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**
- Separated and disperse two-phase flows, polydisperse spray flows for **combustion chambers in automotive, aeronautic and solid propulsion applications.**





## Mathematics fields of research (EDP, Numerical Analysis,HPC)

- Moment methods for kinetic equations describing disperse two-phase flows, realizable high order numerical methods and asymptotic limits (border of the moment space)
- Adaptation in time and space, with error control based on operator splitting methods and multiresolution analysis for the propagation of stiff reaction fronts
- Derivation of thermodynamically consistant and well-posed fluid models for weakly ionized plasma flows out of thermal and chemical equilibrium using kinetic theory

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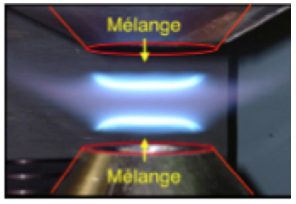


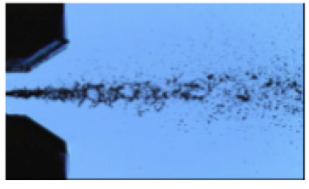

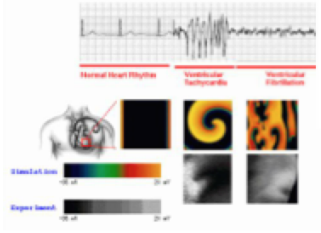

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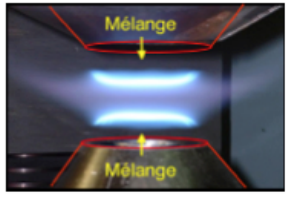
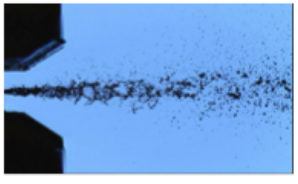
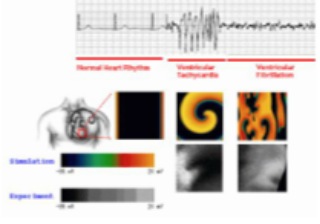
- Membre associé de la Fondation Mathématique Jacques Hadamard, Université Paris-Saclay




Fondation mathématique FMJH Jacques Hadamard

Campus Paris Saclay
Fondation de Cooperation Scientifique





# Context

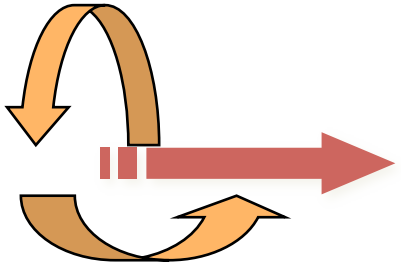
## Industrial applications

- Liquid propulsion: aeronautic or automotive combustion chambers,
- Solid propulsion: solid rocket motor (alumina droplets),

Liquid injection

Source: C. Dumouchel CORIA Rouen

Evaporation + Partial mixing



Swirl of oxydant

Combustion


Source: Pr Edwards, Stanford

**Combustion of polydisperse evaporating sprays**

- Atomization of the liquid phase
- Mixing of the fuel and the air in the vapor phase
- Combustion regimes and dynamics

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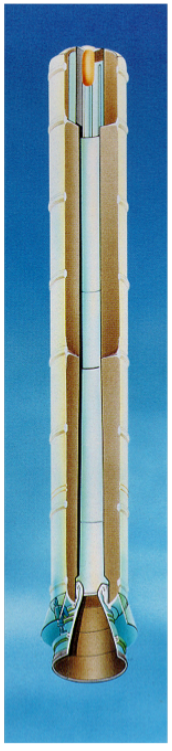

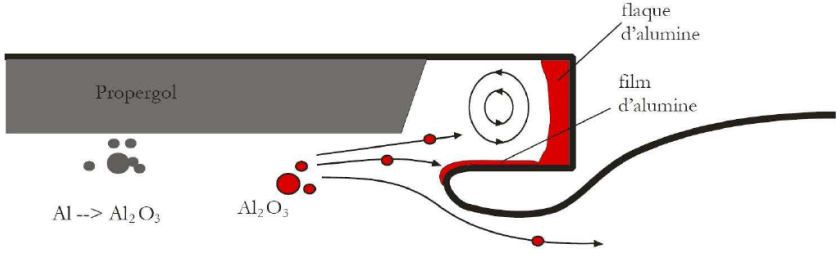



Propellant is aluminized to increase specific impulse $\Rightarrow$ droplets of liquid aluminum oxide

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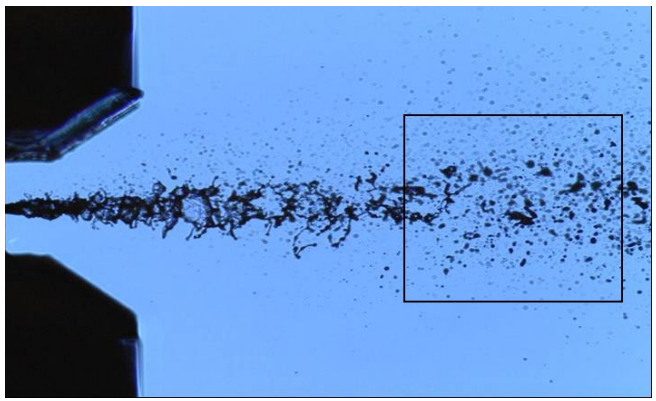
## Industrial applications

- Liquid propulsion: aeronautic or automotive combustion chambers,
- Solid propulsion: solid rocket motor (alumina droplets),

## Presence of a disperse liquid phase: droplets with a large size spectrum

- Droplets-gaz interactions
  drag force, evaporation, heat transfer
- Droplets-droplets interactions
  collision, breakup

**Key parameter**: droplet size



- Neglected volume fraction (source term for gaz equations)
- The flow around the droplets is not resolved
- Spherical droplets

# Modelization of the disperse phase

## Kinetic model

$f(\boldsymbol{x}, \boldsymbol{u}, S, T; t)$ : number density function (NDF)

Transport equation of Boltzmann type [Williams 1958],

$$\underbrace{\partial_t f + \partial_{\boldsymbol{x}} \cdot (\boldsymbol{u} f)}_{\text{free transport}} - \underbrace{\partial_S(\mathrm{K} f)}_{\text{evaporation}} + \underbrace{\partial_{\boldsymbol{u}}(\boldsymbol{F} f)}_{\text{forces}} + \underbrace{\partial_T(E f)}_{\text{heat exchanges}} = \underbrace{\Gamma(f,f)}_{\text{collisions}} + \underbrace{Q(f)}_{\text{breakup}}$$

- evaporation and heating : $d^2$ law ($K$ =cste, $E = 0$), infinite conductivity, ...
- drag and gravity : $F = \dfrac{\boldsymbol{U_g} - \boldsymbol{u}}{\tau_p}\left(1 + \frac{\mathrm{Re}^{2/3}}{6}\right) + g$
- coalescence : $\Gamma(f,f) = -\displaystyle\int_{S^*}\int_{\boldsymbol{u}^*} f\, f^* \beta(S, S^*)|\boldsymbol{u} - \boldsymbol{u}^*| \mathrm{d}S^* \mathrm{d}\boldsymbol{u}^*$
  $+\dfrac{1}{2}\displaystyle\int_{S^* \in [0,S]}\int_{\boldsymbol{u}^*} f^\diamond\, f^* \beta(S^\diamond, S^*)|\boldsymbol{u}^\diamond - \boldsymbol{u}^*| J \mathrm{d}S^* \mathrm{d}\boldsymbol{u}^*$
- rebounds : $\Gamma(f,f) = \displaystyle\int_{\mathbb{R}} \beta(S, S^*) \int_{\mathbb{R}^d}\int_{S^+} [f' f'^* - f f^*]|(\boldsymbol{u} - \boldsymbol{u}^*) \cdot \boldsymbol{n}| \mathrm{d}\boldsymbol{n}\, \mathrm{d}\boldsymbol{u}^* \mathrm{d}S^*$
- secondary breakup PhD [Dufour, 2005, Doisneau, 2013]

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## Lagrangian description

particular discretization - Monte-Carlo methods

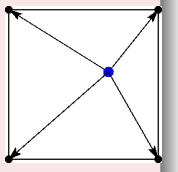
[O'Rourke, 1981, Dukowicz, 1980, Bird, 1994]

## advantages

- usable in most cases
- no numerical diffusion

## disadvantages

- slow convergence
- difficulties for parallelization
- coupling with the Eulerian description of the gas



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## Eulerian description

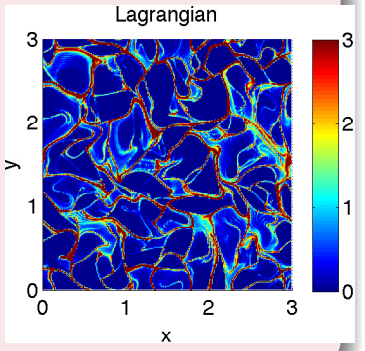
- Moments of the NDF: $M_{i,\boldsymbol{j},k}(t, \boldsymbol{x}) = \int\int S^i \boldsymbol{u}^{\boldsymbol{j}} T^k f(\boldsymbol{x}, \boldsymbol{u}, S, T; t) \mathrm{d}T \mathrm{d}\boldsymbol{u} \mathrm{d}S$
- System of conservation equations on moments

## advantages

- more easy to parallelize
- natural coupling with the Eulerian description of the gas

## disadvantages

- model (closures)
- adapted numerical schemes (hypercompressibility, vacuum zones)



# Modelization of the disperse phase: a simplified case

## Simplified and dimensionless kinetic model

$f(\boldsymbol{x}, \boldsymbol{u}, S, \cancel{\mathcal{T}}; t)$ : number density function (NDF)

Transport equation of Boltzmann type [Williams 1958],

$$\underbrace{\partial_t f + \partial_{\boldsymbol{x}} \cdot (f\,\boldsymbol{u})}_{\text{free transport}} - \underbrace{\partial_S (Kf)}_{\text{evaporation}} + \underbrace{\partial_{\boldsymbol{u}} \left( \frac{\boldsymbol{U_g} - \boldsymbol{u}}{\mathrm{St}(S)} f \right)}_{\text{Stokes drag}} + \cancel{\underbrace{\partial_{\mathcal{T}} (E f)}_{\text{heat exchanges}}} = \cancel{\underbrace{\Gamma(f, f)}_{\text{collisions}}} + \cancel{\underbrace{Q(f)}_{\text{breakup}}}$$

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$$S \in [0, 1]$$
$$\boldsymbol{u} \in \mathbb{R}^d$$

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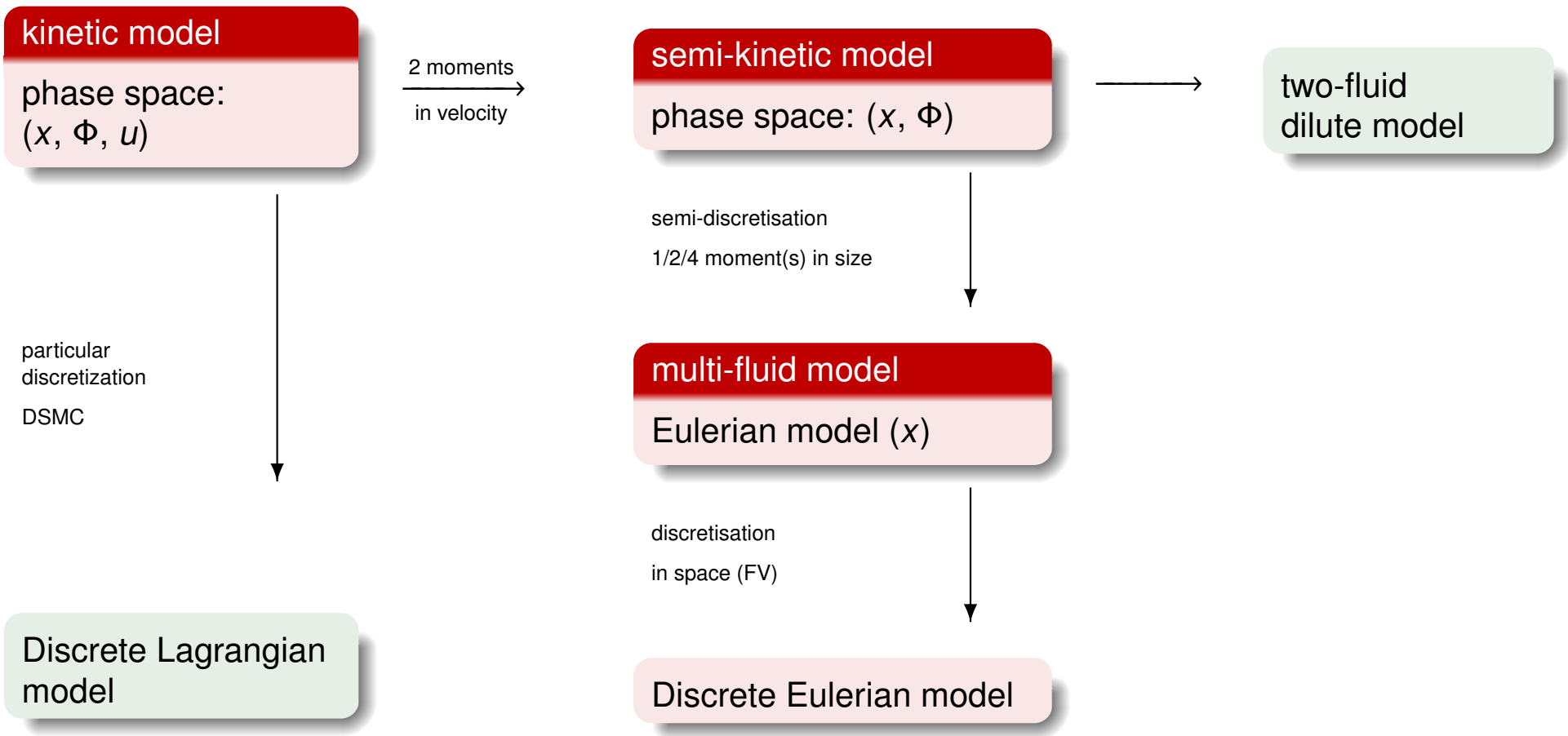
# Discretization Strategies for Polydisperse sprays

**Size polydispersion and evolution has been successfully handled**

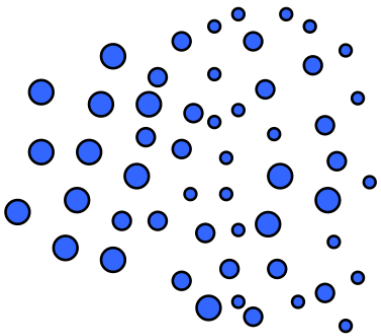
PhD de Chaisemartin 2009, Fréret et al 2009, 2010, 2012, Kah, 2010 (SMAI/GAMNI - ECCOMAS), Doisneau 2013, Massot et al. SIAP 2010, Kah et al. JCP 2012, Vié et al. JCP 2013, Doisneau et al. JCP 2013, Doisneau et al. JPP 2014

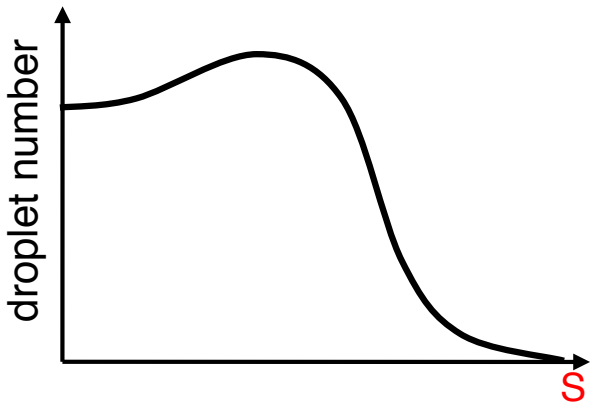


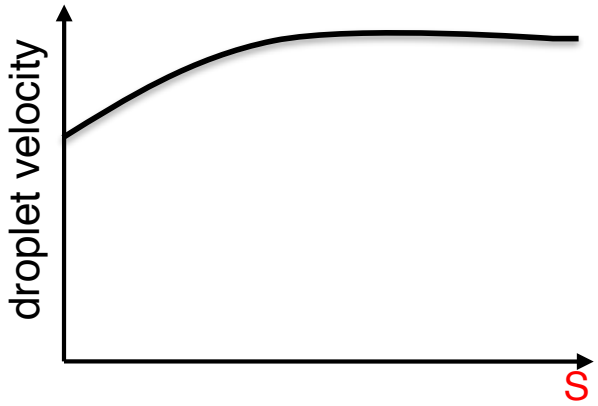
# Eulerian multi-fluid models

## Principle of the method (simplified case)

A conservation law system for each size interval (section)






**Assumptions :**

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

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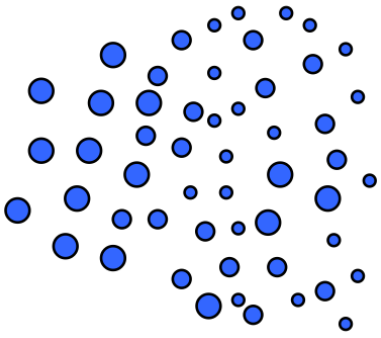

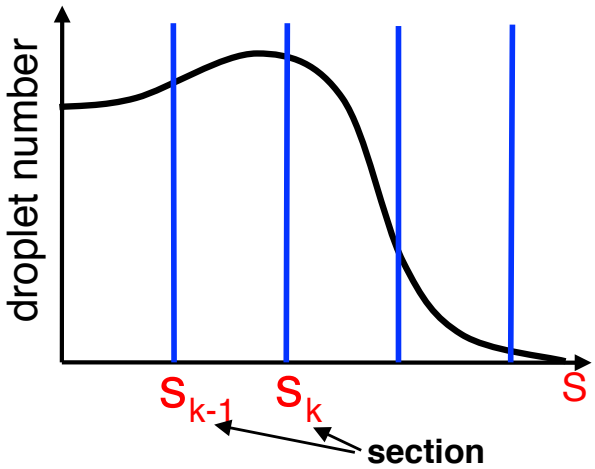


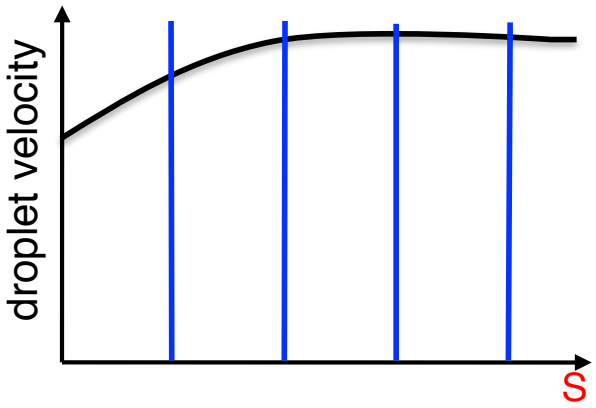


**Considered moments:**

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

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

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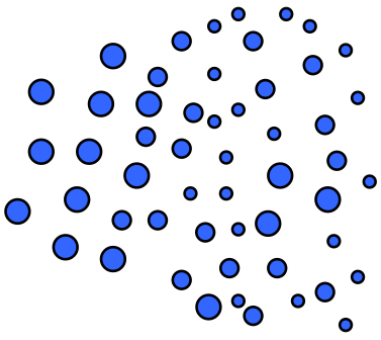

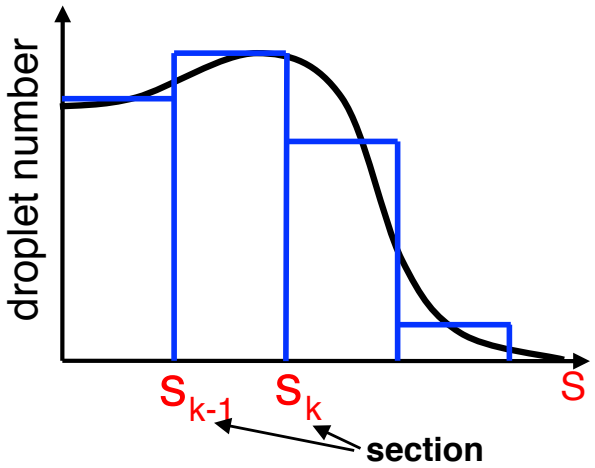


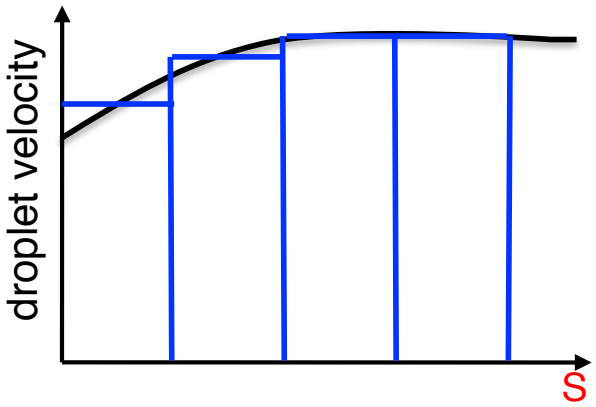


**presumed pdf** in each section $k$

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

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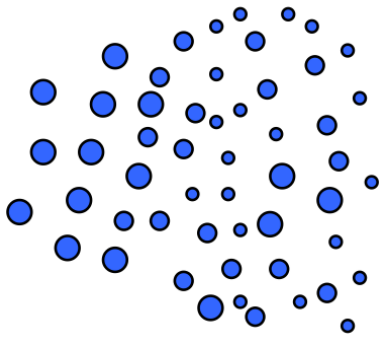
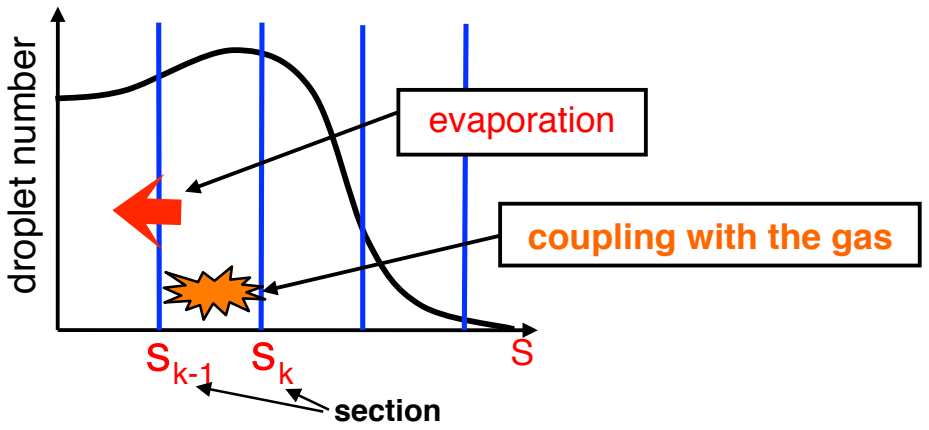





**Equations:** [Laurent and Massot, 2001]

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

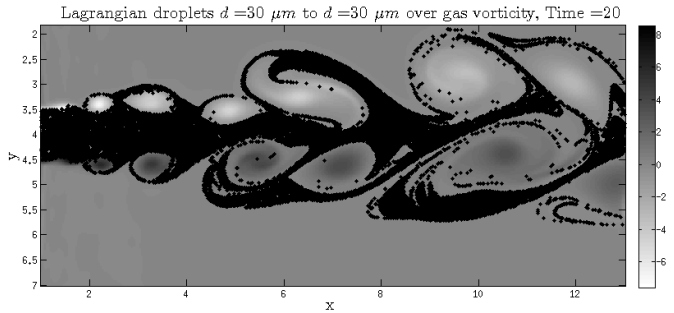
$$\partial_t(m^{(k)} u^{(k)}) + \partial_x \cdot (m^{(k)} u^{(k)} \otimes u^{(k)}) = -(E_1^{(k)} + E_2^{(k)}) m^{(k)} u^{(k)} + E_1^{(k+1)} m^{(k+1)} u^{(k+1)} + m^{(k)} F^{(k)}$$

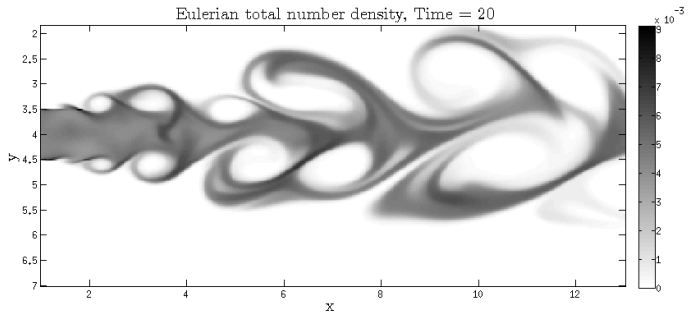
# Eulerian multi-fluid models

## Eulerian multi-fluid models

- Very good agreement with the Lagrangian model [de Chaisemartin, 2009]
- Validation through comparisons with experiments

  [Freret et al., 2008]
- Efficient parallelization [Fréret et al., 2010]



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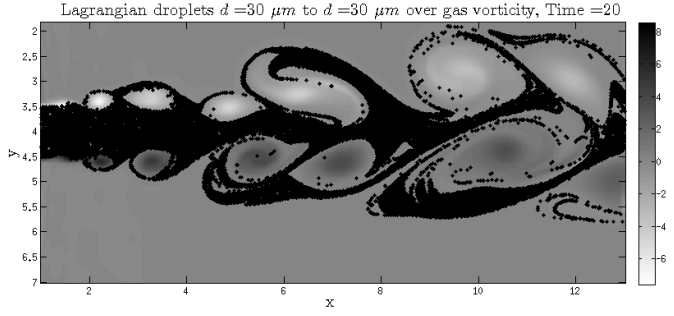


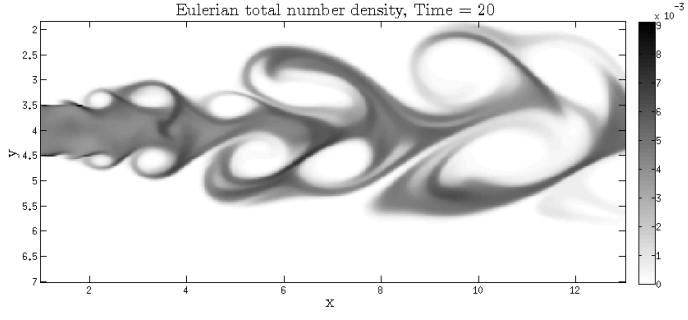


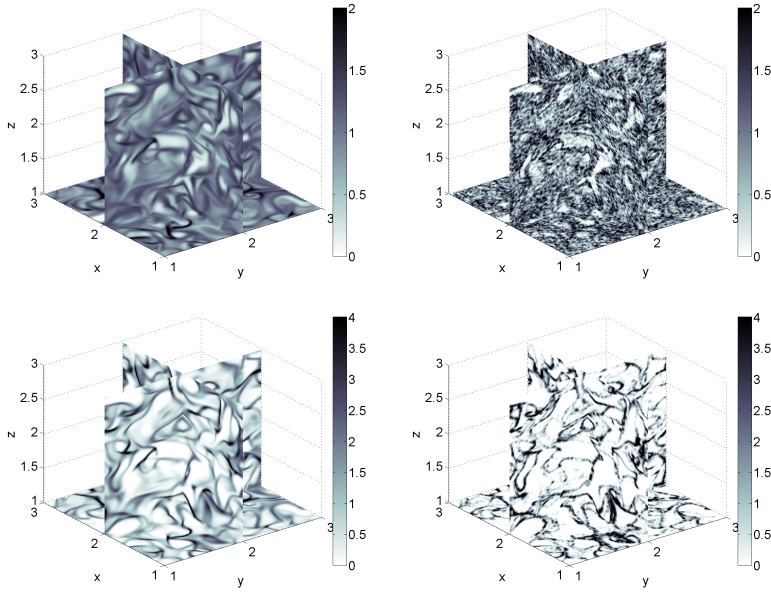

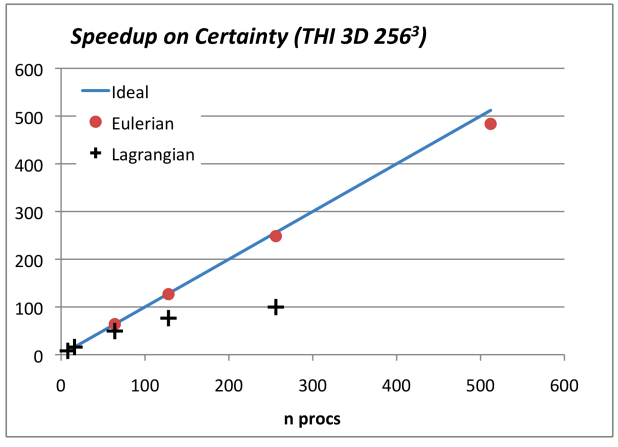

# Eulerian multi-fluid model

## Code MUSES3D - S. de Chaisemartin, L. Fréret

Conservation equations for each size interval:

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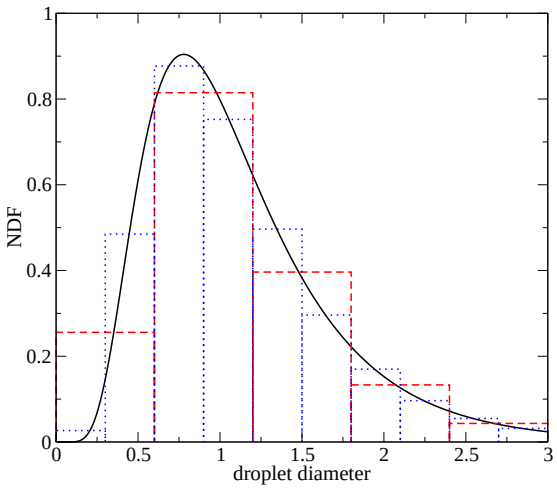
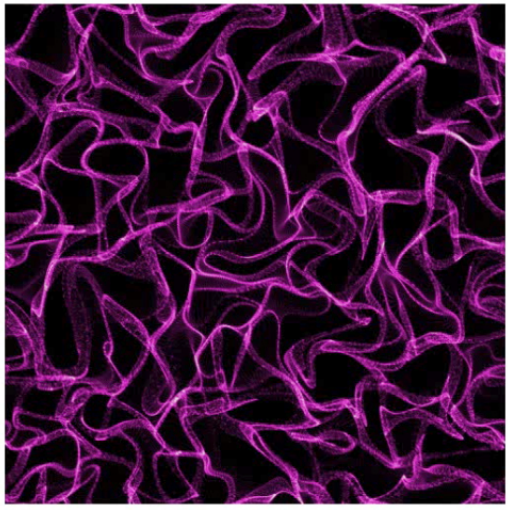
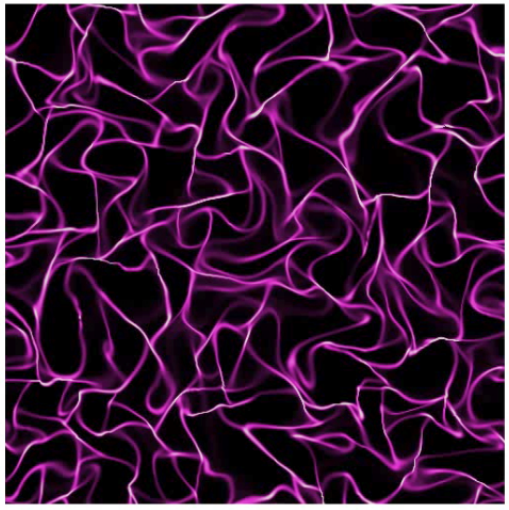



Lagrangian



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

Eulerian



Thomine, Freret, Reveillon & Massot

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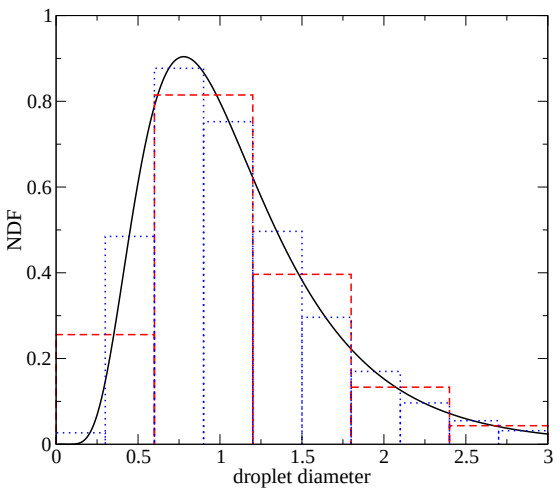


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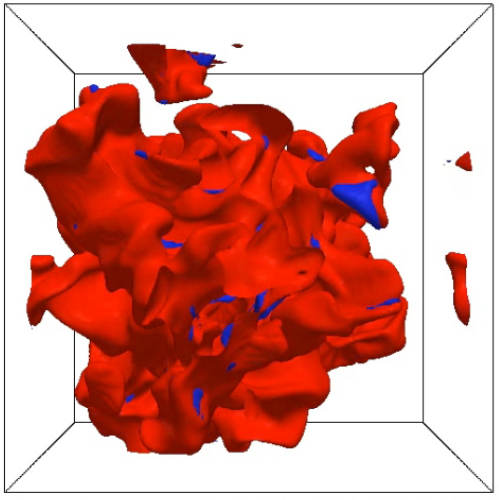

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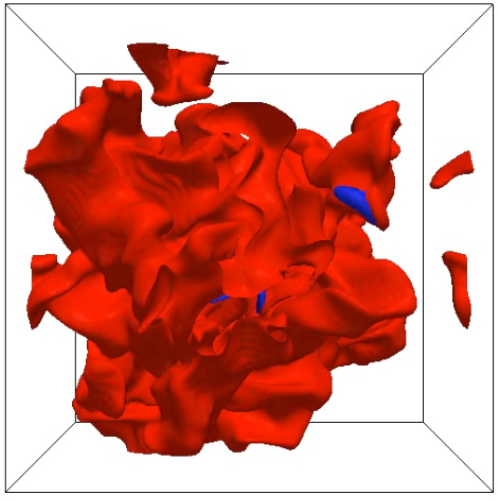

Thomine, Freret, Reveillon & Massot

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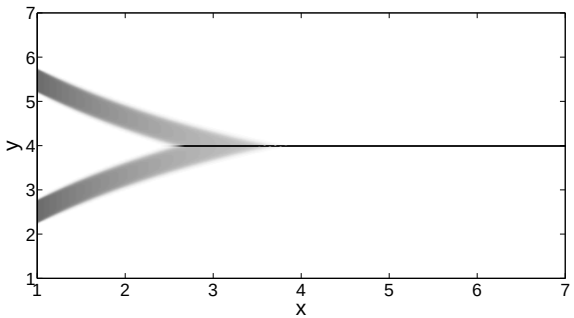
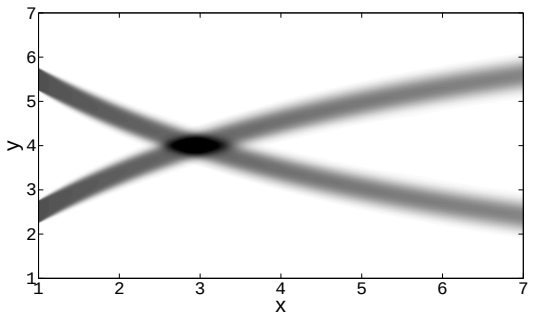
- mono-kinetic assumption at a given size, location and time
  Equivalent to pressureless gas dynamics
  For DNS and Low Stokes numbers

multi-fluid model




multi-velocity model




Key issue : accurate schemes in space and time

# Eulerian multi-fluid model

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- one-moment per section leads to a first order moment method
  strong numerical diffusion in size phase space
  several sections needed for an accurate resolution of evaporation

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- one-moment per section leads to a first order moment method

  strong numerical diffusion in size phase space

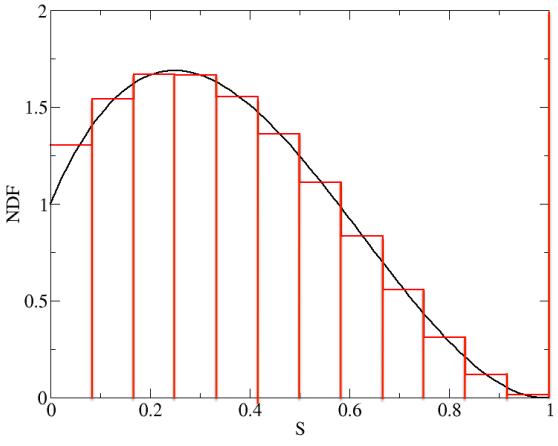
  several sections needed for an accurate resolution of evaporation

**General objectif : design higher order moment methods in size and velocity which preserve realizability**
**and built-in realizability preserving numerical methods - high order**

# Outline

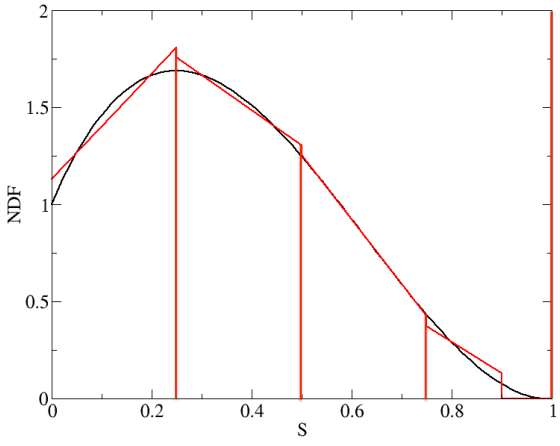
# Evolution of the Eulerian multi-fluid models

1 moment/section



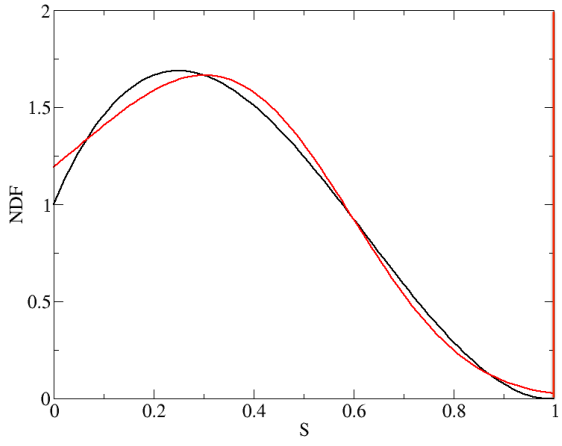

[Laurent and Massot, 2001]

2 moments/section




[Laurent, 2006, Doisneau et al 2013]

4 moments/section




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

increasing the number of size moments per section

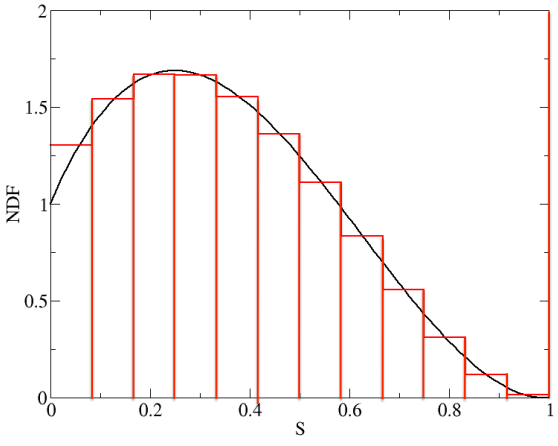
decreasing the number of sections

decreasing the cost

increasing the model complexity

# Evolution of the Eulerian multi-fluid models

1 moment/section

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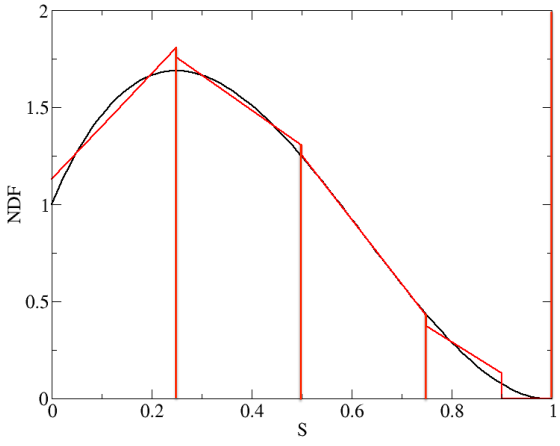


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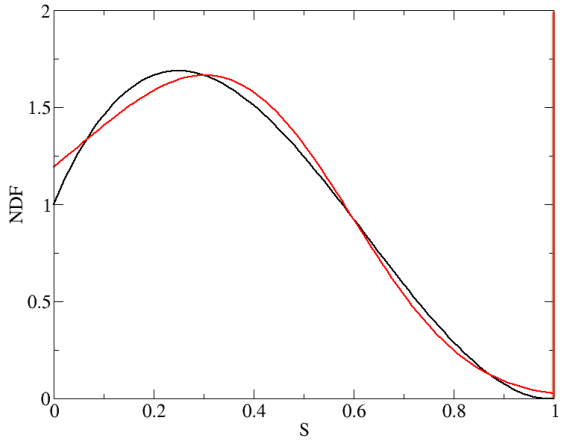


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increasing the number of size moments per section

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decreasing the cost

increasing the model complexity

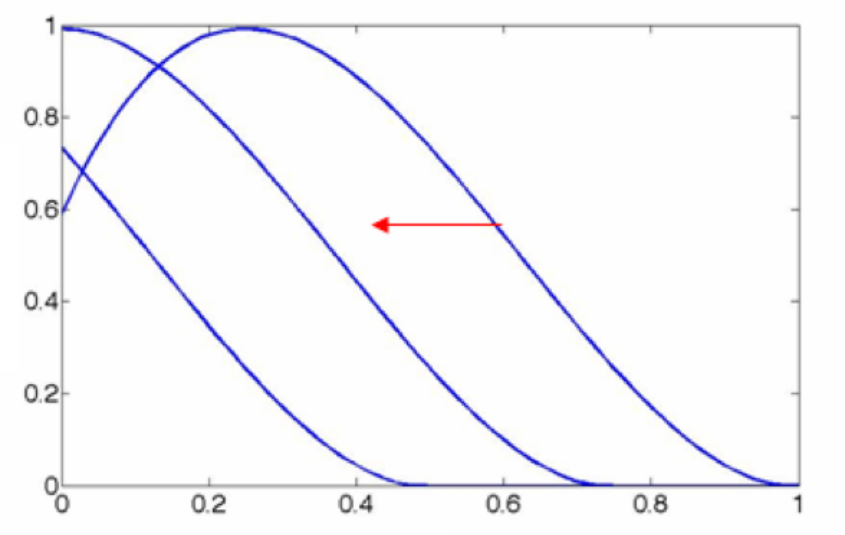
# Moment method for purely evaporating case

## Kinetic model for purely evaporating case, $d^2$ law, dimensionless

$$\begin{cases} \partial_t f - \partial_S(K f) = 0, & t \in \mathbb{R}^+, S \geq 0 \\ f(0,S) = f_0(S), & S \geq 0 \end{cases}$$

with $K = \mathbb{1}_{[0,+\infty[}(S)$

solution: $f(t,S) = \left(\int_0^t f_0(\sigma)\mathrm{d}\sigma\right)\delta_0(S) + f_0(S+t)$




Moments: $\mathcal{M}_k = \int_0^1 S^k f(S)\mathrm{d}S,\ k = 0,\ldots,N$

System to solve:

$$d_t\mathcal{M} = -A\,\mathcal{M} - \phi_-, \qquad \mathcal{M} = (\mathcal{M}_0,\ldots,\mathcal{M}_N)^t$$

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with

$$\phi_- = f(t,0) \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \qquad A = \begin{bmatrix} 0 & & & & \mathbf{0} \\ 1 & 0 & & & \\ & 2 & \ddots & & \\ & & \ddots & \ddots & \\ \mathbf{0} & & & N & 0 \end{bmatrix}.$$

- closure problem: pointwise values of $f$ from its moments
- realizability problem: $\mathcal{M}$ has to stay in the moment space

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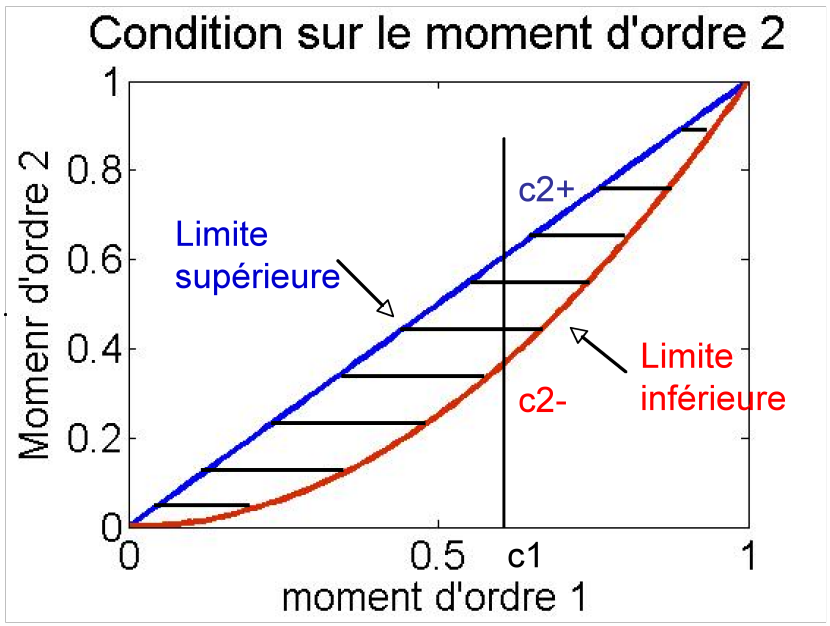
# Moment space

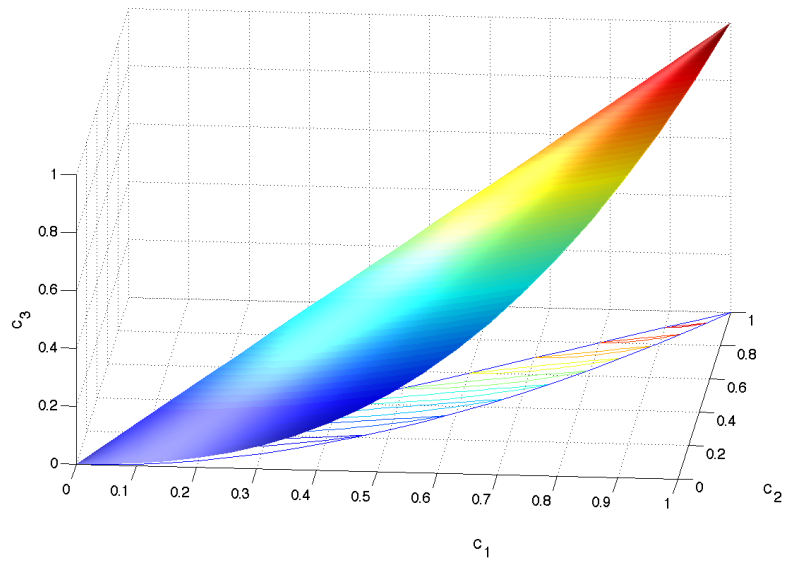
## $N^{th}$ moment space of probability measures on $[0, 1]$

$$\widetilde{\mathcal{M}}_N = \{\mathbf{c}_N(\mu) | \mu \in \mathcal{P}\}, \quad \mathbf{c}_N(\mu) = (c_1(\mu), \dots, c_N(\mu))^t, \quad c_k(\mu) = \int_0^1 x^k \, d\mu(x).$$

→ convex space but “complex" geometry




$c_1^2 < c_2 < c_1$




$\widetilde{\mathcal{M}}_3$

⇒ the numerical methods have to preserve this space

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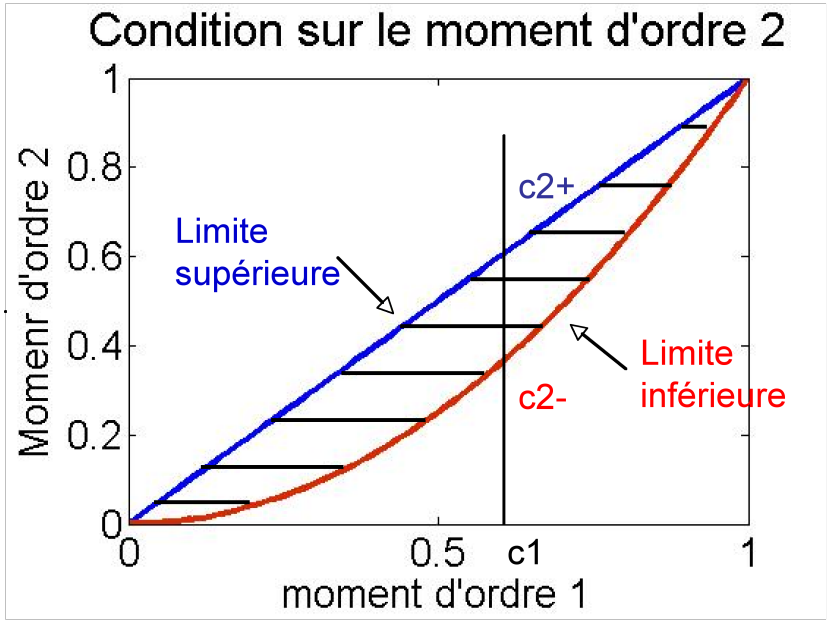


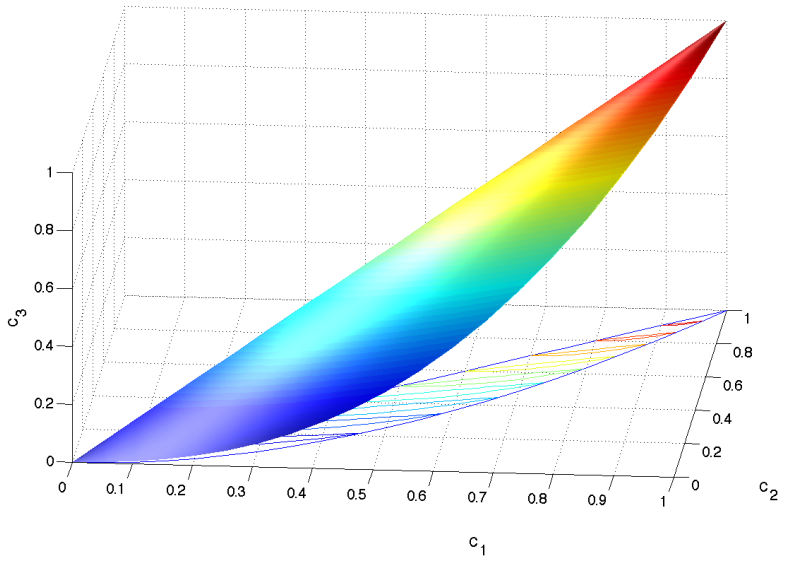


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**Hankel determinants:**

$$\underline{H}_{2m+d} = \begin{vmatrix} c_d & \cdots & c_{m+d} \\ \vdots & & \vdots \\ c_{m+d} & \cdots & c_{2m+d} \end{vmatrix} \quad \overline{H}_{2m+d} = \begin{vmatrix} c_{1-d} - c_{2-d} & \cdots & c_m - c_{m+1} \\ \vdots & \vdots & \vdots \\ c_m - c_{m+1} & \cdots & c_{2m-1+d} - c_{2m+d} \end{vmatrix}$$

$$\mathcal{M} = (c_1, \ldots, c_N) \in \widetilde{\mathcal{M}}_N \Leftrightarrow \underline{H}_i \geq 0 \text{ and } \overline{H}_i \geq 0 \text{ for } d = 0, 1 \text{ and } i = 0, \ldots, N.$$

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**Canonical moments** [Dette and Studden, 1997]:

$$p_1 = c_1, \quad p_2 = \frac{c_2 - c_1^2}{c_1(1 - c_1)}, \quad p_3 = \frac{(1 - c_1)(c_1 c_3 - c_2^2)}{(c_2 - c_1^2)(c_1 - c_2)}, \quad \ldots$$

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for fixed $\boldsymbol{c}_{k-1} = (c_1, \ldots, c_{k-1})^t \in \mathring{\widetilde{\mathcal{M}}}_{k-1}$, $c_k \in [c_k^-(\boldsymbol{c}_{k-1}), c_k^+(\boldsymbol{c}_{k-1})]$ and one denotes

$$p_k = \frac{c_k - c_k^-(\boldsymbol{c}_{k-1})}{c_k^+(\boldsymbol{c}_{k-1}) - c_k^-(\boldsymbol{c}_{k-1})} \in [0,1],$$

$$p_1 = c_1, \qquad p_2 = \frac{c_2 - c_1^2}{c_1(1-c_1)}, \qquad p_3 = \frac{(1-c_1)(c_1 c_3 - c_2^2)}{(c_2 - c_1^2)(c_1 - c_2)}, \qquad \ldots$$

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bijection between the interior of $\widetilde{\mathcal{M}}_N$ and $]0,1[^N$

# Reconstruction

## Finite Hausdorff moment problem for the moment vector $\mathcal{M}$

find a non-negative real function $f_{\mathcal{M}}$ defined on $[0,1]$ and such that

$$\mathcal{M} = \int_0^1 f_{\mathcal{M}}(x) \begin{pmatrix} 1 \\ x \\ \vdots \\ x^N \end{pmatrix} dx$$

Let us assume that $\mathcal{M}$ belongs to the interior of $\mathcal{M}_N$ → infinity of solutions

- **quadrature** solution as a sum of Dirac delta functions
- **polynomial** reconstruction [Laurent, 2006]
- reconstruction with a **sum of beta PDF** [Yuan et al., 2012]
- **Shannon's Entropy maximization** $H[f] = -\int_0^1 f(x) \ln f(x) dx$

  [Mead and Papanicolaou, 1984, Tagliani, 1999, Massot et al., 2010]

$$\Rightarrow f(x) = \exp\left(-\sum_{j=0}^{N} \xi_j x^j\right)$$

The interior of the moment space is entirely attained (in theory).
Calcul of the $\xi_j$ by an iterative Newton method
Calcul of the integrals by a Gauss-Legendre quadrature

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Let us assume that $\mathcal{M}$ belongs to the interior of $\mathcal{M}_N$ → infinity of solutions

- **quadrature** solution as a sum of Dirac delta functions
  → unique lower principale representation (minimization of $M_{N+1}$)
  → not adapted for the computation of pointwise values or integrals on intervals strictly included in $]0,1[$
- **polynomial** reconstruction [Laurent, 2006]
- reconstruction with a **sum of beta PDF** [Yuan et al., 2012]
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- **quadrature** solution as a sum of Dirac delta functions
- **polynomial** reconstruction [Laurent, 2006]
  → $N+1$ order of accuracy
  → Need more work for positivity preserving (done in the case $N=1$ with a bi-affine reconstruction)
- reconstruction with a **sum of beta PDF** [Yuan et al., 2012]
- **Shannon's Entropy maximization** $H[f] = -\int_0^1 f(x) \ln f(x) dx$

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Let us assume that $\mathcal{M}$ belongs to the interior of $\mathcal{M}_N$ → infinity of solutions

- **quadrature** solution as a sum of Dirac delta functions
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- reconstruction with a **sum of beta PDF** [Yuan et al., 2012]

$$f(\xi) = \sum_{\alpha=1}^{n} w_\alpha \frac{\xi^{\frac{\xi_\alpha}{\sigma}-1}(1-\xi)^{\frac{1-\xi_\alpha}{\sigma}-1}}{B\left(\frac{\xi_\alpha}{\sigma}, \frac{1-\xi_\alpha}{\sigma}\right)}$$

→ one recover the quadrature when $\sigma \to 0$
→ eventually “lose" of the last moment

- **Shannon’s Entropy maximization** $H[f] = -\int_0^1 f(x) \ln f(x) dx$

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# Reconstruction

## Finite Hausdorff moment problem for the moment vector $\mathcal{M}$

find a non-negative real function $f_{\mathcal{M}}$ defined on $[0,1]$ and such that

$$\mathcal{M} = \int_0^1 f_{\mathcal{M}}(x) \begin{pmatrix} 1 \\ x \\ \vdots \\ x^N \end{pmatrix} dx$$

Let us assume that $\mathcal{M}$ belongs to the interior of $\mathcal{M}_N$ → infinity of solutions

- **quadrature** solution as a sum of Dirac delta functions
- **polynomial** reconstruction [Laurent, 2006]
- reconstruction with a **sum of beta PDF** [Yuan et al., 2012]
- **Shannon's Entropy maximization** $H[f] = -\int_0^1 f(x) \ln f(x) dx$

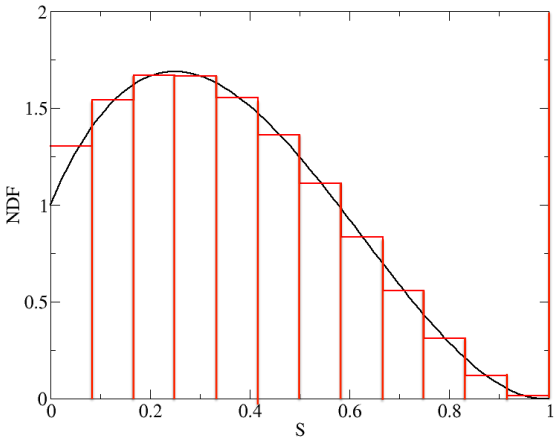
  [Mead and Papanicolaou, 1984, Tagliani, 1999, Massot et al., 2010]

$$\Rightarrow f(x) = \exp\left(-\sum_{j=0}^{N} \xi_j x^j\right)$$

The interior of the moment space is entirely attained (in theory).
Calcul of the $\xi_j$ by an iterative Newton method
Calcul of the integrals by a Gauss-Legendre quadrature

# Examples of reconstructions

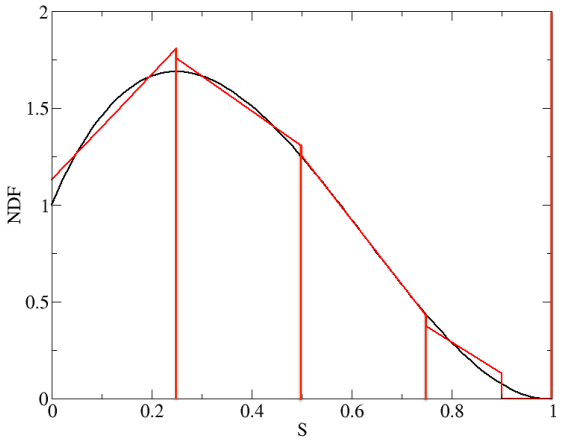
1 moment/section




contant function in the section

12 moments

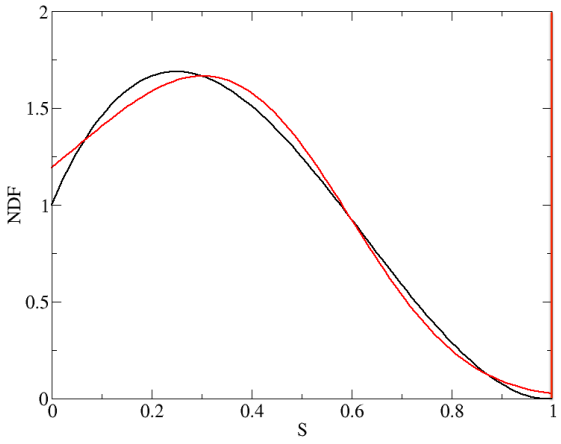
2 moments/section




bi-affine function

8 moments

4 moments/section




entropy maximization

4 moments

increasing the number of size moments per section

decreasing the number of sections

decreasing the cost

increasing the model complexity

# Robust algorithm for the resolution: purely evaporating case

System to solve:

$$d_t \mathcal{M} = -A\,\mathcal{M} - \phi_-, \qquad \mathcal{M} = (\mathcal{M}_0, \ldots, \mathcal{M}_N)^t$$

## Integral version of the system

The integral form of the solution is written :

$$\exp(t\,A)\,\mathcal{M}(t) = \mathcal{M}(0) - \Psi_-(t), \qquad \Psi_-(t) = \int_0^t f(0,\beta) \begin{bmatrix} 1 \\ \beta \\ \vdots \\ \beta^N \end{bmatrix} d\beta.$$

## Algorithm

1. Reconstruction $f_{ME}$ by entropy maximization and flux evaluation
2. Shift in size
3. Projection

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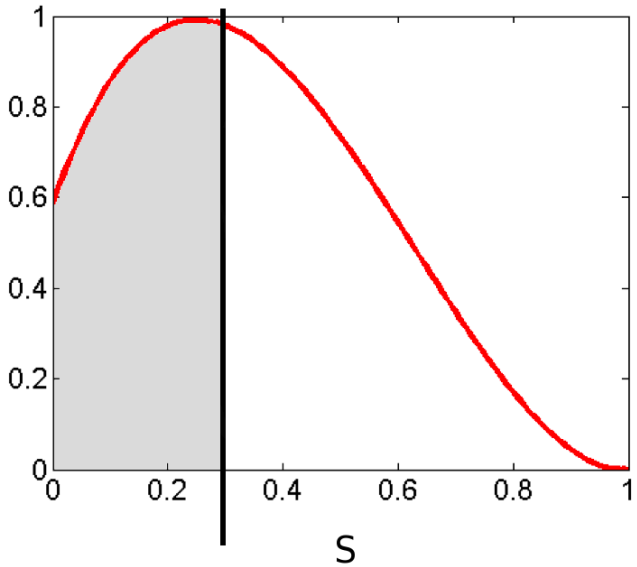

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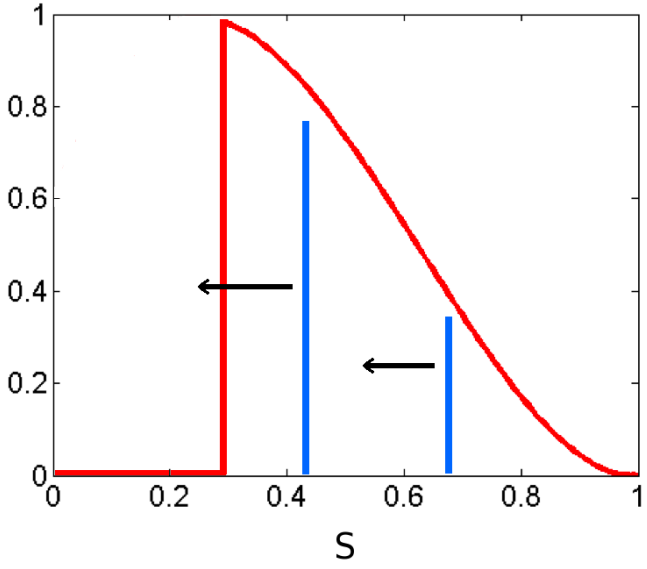
## Algorithm

1. Reconstruction $f_{ME}$ by entropy maximization and flux evaluation
2. Shift in size

$$\mathcal{M}_k(0) - \Psi_{k-}(t) = \sum_{i=1}^{(N+1)/2} w_i(0) S_i(0)^k, \qquad \frac{dS_i}{dt} = -1$$

the abscissas $S_i(0)$ are in $[t, 1+t]$

3. Projection



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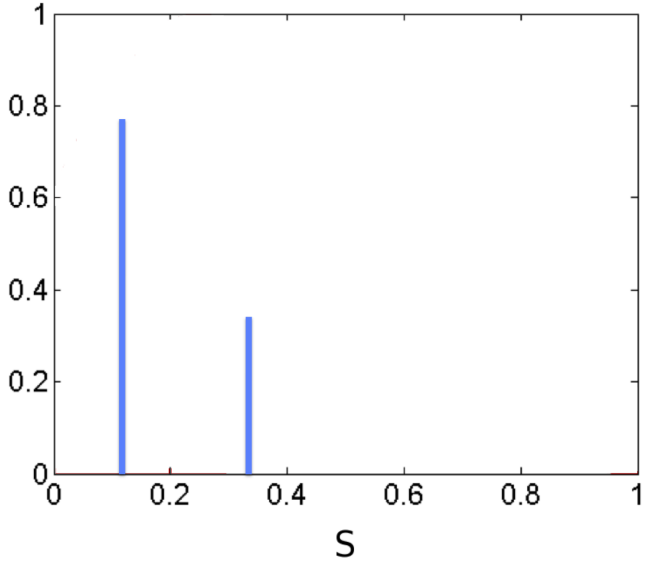
$$\mathcal{M}_k(t) = \sum_{i=1}^{(N+1)/2} w_i(t) S_i(t)^k$$

$\mathcal{M}(t)$ is a moment vector!



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## Algorithm

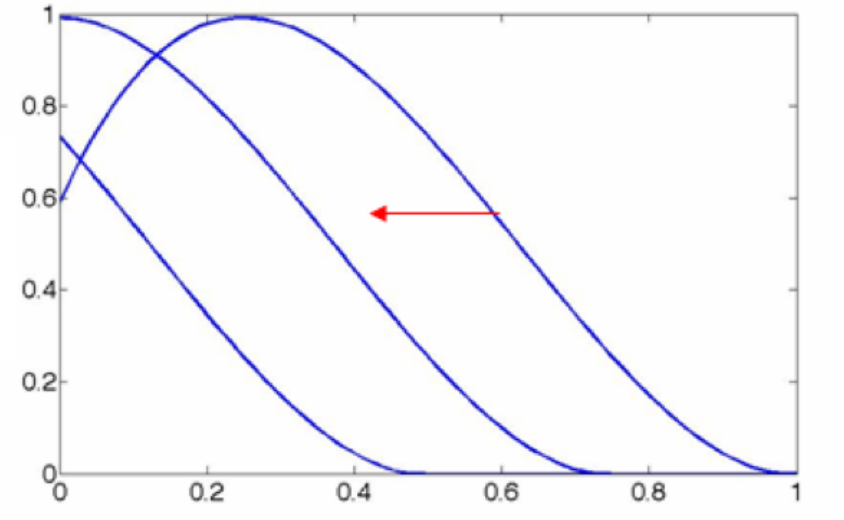
1. Reconstruction $f_{ME}$ by entropy maximization and flux evaluation
2. Shift in size
3. Projection

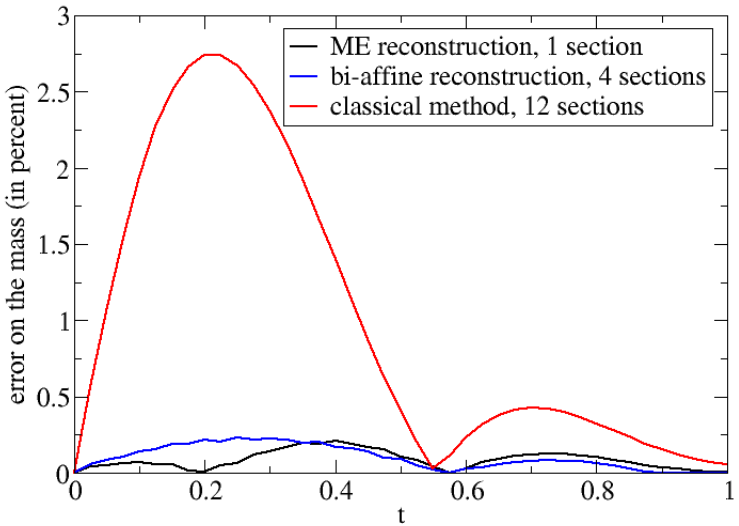
generalized to any $S$ dependent evaporation law

For N=3, the method is called EMSM (Eulerian Multi-Size Model)

[Massot et al., 2010]

# Error on mass evolution




## Error for the purely evaporating case

- EMSM more efficient than the classical method (1 moment/section) with 12 sections
- equivalent error between the second order method with 4 sections (8 moments) and the 4 moment method with 1 section
- EMSM highly decrease the computation cost compared to Multi-fluid model (in 2D, 36 moments for the Multi-fluid method, 6 moments for EMSM)

# Advection scheme

**General method**: splitting between transport in physical space and transport in phase space.

→ the transport part has also to preserve the moment space

## Kinetic model for purely advection case: $f(x, \boldsymbol{u}, S; t)$

$$\partial_t f + \boldsymbol{u} \cdot \partial_x f = 0$$

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

$$\begin{cases} \partial_t(\mathcal{M}) + \partial_{\boldsymbol{x}}(\mathcal{M}\,\boldsymbol{u_d}) = 0, \\ \partial_t(M_1\boldsymbol{u_d}) + \partial_{\boldsymbol{x}}(M_1\boldsymbol{u_d} \otimes \boldsymbol{u_d}) = 0. \end{cases}$$

→ weakly hyperbolic system [Bouchut, 1994]

⇒ Kinetic finite volume scheme [Bouchut et al., 2003]

$\mathcal{M}_j^n, u_j^n$ $\qquad$ $\mathcal{M}_j^{n+1}, u_j^{n+1}$

$\downarrow$ $\qquad$ $\uparrow$

$f(x, u, S; t^n) \xrightarrow[\Delta t]{\text{exact evolution}} f(x, u, S; t^{n+1})$

with

$$f(x, u, S; t^n) = f_{\mathcal{M}^n(x)}(S)\,\delta(u - u^n(x))$$

**Difficulty**: for the second order of accuracy, the $x$-reconstruction is not trivial

→ $x$-reconstruction of canonical moments [Kah et al 2012]

and use of a symbolic algebra software to determine the fluxes

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$$\begin{array}{ccc} \mathcal{M}_j^n, u_j^n & & \mathcal{M}_j^{n+1}, u_j^{n+1} \\ \downarrow & & \uparrow \\ f(x, u, S; t^n) & \xrightarrow[\Delta t]{\text{exact evolution}} & f(x, u, S; t^{n+1}) \end{array}$$

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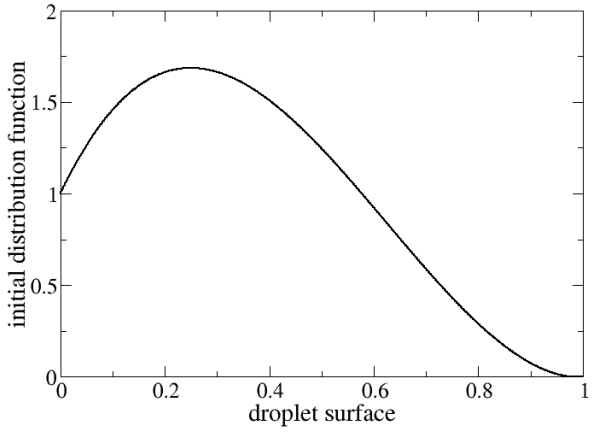
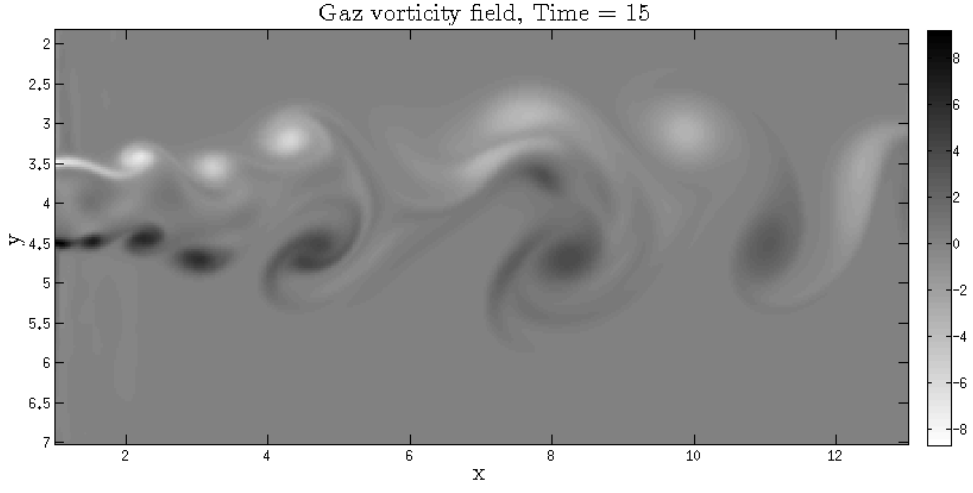
# Configuration

## Free jets with polydisperse spray injection and evaporation [de Chaisemartin et al., 2009]

- Injection of a polydisperse spray in the center of the jet
- Re=1000 with a low level turbulence injection for destabilization purposes.
- Droplet distribution between Stokes = 0.03 and 0.75



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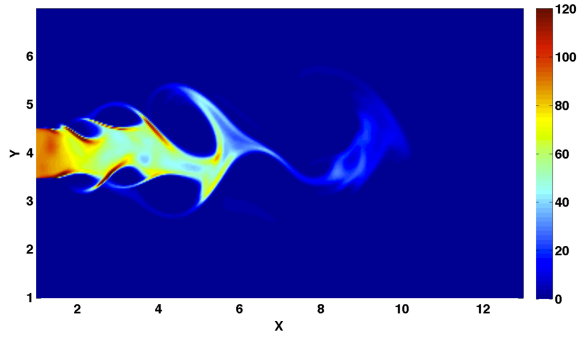
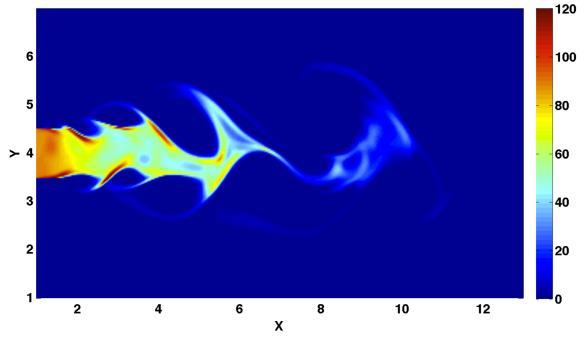
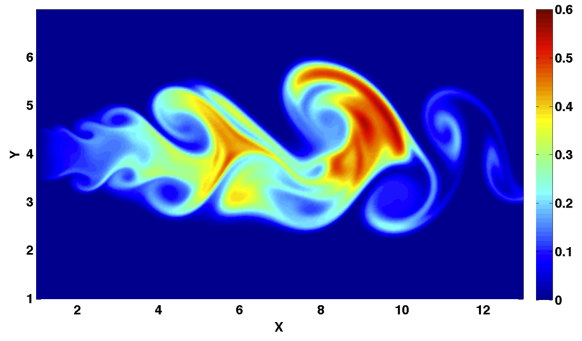
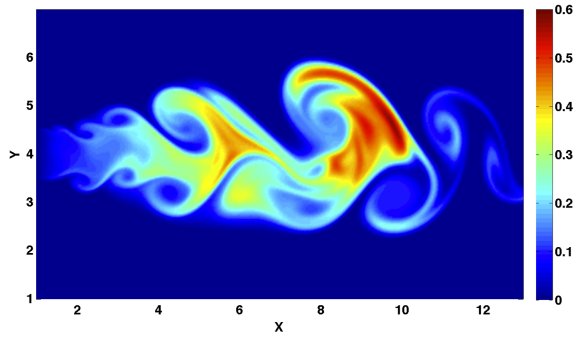
## Eulerian code MUSES3D [de Chaisemartin, 2009]

- Generic solver allowing implementation of new methods
- Fully parallelized (efficiency one on Certainty up to 512 cores)
- Coupling with a gaseous (Low Mach) + Lagrangian solver ASPHODELE from J. Reveillon, CORIA, Rouen
  $\Rightarrow$ possibility of Eulerian and Lagrangian computation on the same gaseous field

# Comparison with the Multi-fluid model

| | EMSM | Multi-Fluid with 10 sections |
|---|---|---|
| $m_{3/2}$ |  |  |
| $Y_F$ |  |  |

Excellent agreement $\Rightarrow$ validation of EMSM

EM reconstruction optimized up to the frontier of moment space adaptive (Kah et al JCP 2012 - Vié et al JCP 2013)

# Implementation in semi-industrial codes

## CEDRE code (ONERA)
(F. Doisneau, Collab. J. Dupays, A. Murrone)

- non-structured meshes (cell-center)
- DNS / LES
- Multi-fluid with two size moments

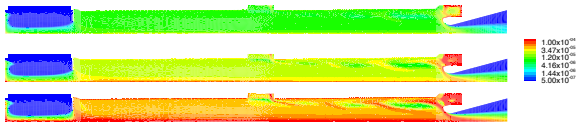
## Two PhDs: F. Doisneau, A. Sibra
Collab. J. Dupays

- first Multi-Fluid computations of a booster with coalescence
- improvement of the two-way coupling strategy - combustion of aluminium
  [Doisneau et al 2013, Doisneau et al 2014]

## IFP-C3D code (IFPEn)

- moving meshes (ALE)
- RANS

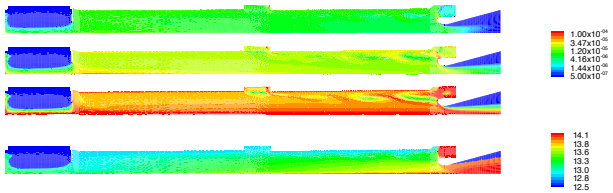
**polydisperse computation**: selective repartition of droplets



Volume fraction per section and $d_{30}$ mean diameter ($\mu$m) of section 3 for polydisperse particles

30% overestimation of pressure oscillation levels with monodisperse computation

**polydisperse computation with coalescence**: significative influence of the coalescence



Volume fraction per section and $d_{30}$ mean diameter ($\mu$m) of section 3 for liquid polydisperse particles

19% decreasing of pressure oscillation levels with the coalescence

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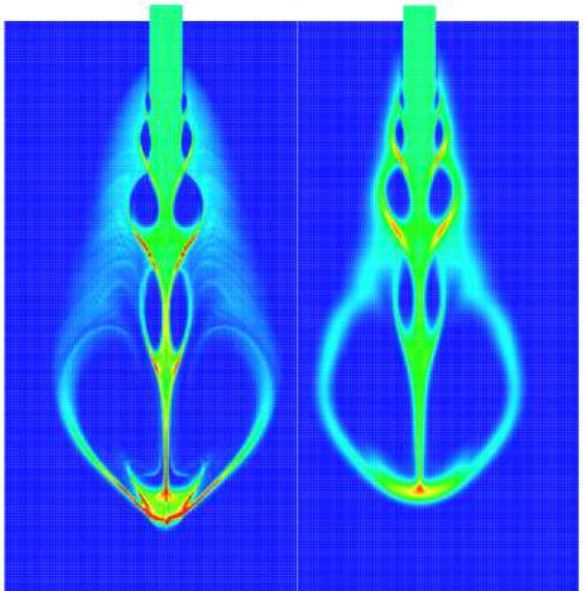
- EMSM with four size moments

## Two PhDs: D. Kah, O. Emre
Collab. S. Jay, S. de Chaisemartin, Q.-H Tran

- injection computations
- mesh movement with preservation of moment space [Kah et al 2014, Emre et al 2014, Emre et al 2015]

Lagrangian EMSM



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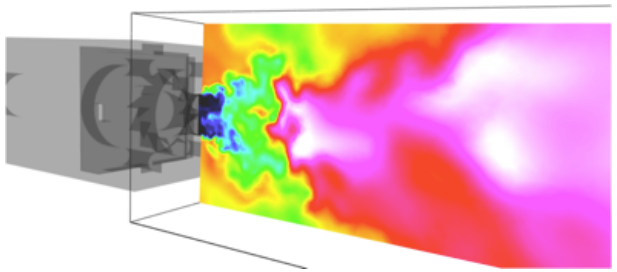
## AVBP code (CERFACS and IFPen)

- complex geometry
- non-structured meshes (cell vertex)
- LES (Vié et al 2013)

## A. Vié
Collab. B. Cuenot

- first LES computations (Multi-Fluid + MEF formalism)



# Outline

# Eulerian moment method

## Mesoscopic description: simplified **Williams-Boltzmann equation**

Monodisperse, constant size and temperature [Williams 1958]

$$\partial_t f + \partial_{\boldsymbol{x}} \cdot (\boldsymbol{u} f) + \partial_{\boldsymbol{u}} \cdot (\mathrm{F} f) = 0, \quad \mathrm{F} = \frac{\boldsymbol{U_g} - \boldsymbol{u}}{\tau_p} \tag{1}$$

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## Macroscopic description: **moment equations**

Integrating (1) over the velocity phase space:

$$\partial_t \mathcal{M}_k + \partial_{\boldsymbol{x}} \cdot \mathcal{M}_{k+1} = k \frac{\mathcal{M}_{k-1} \odot \boldsymbol{U_g} - \mathcal{M}_k}{\tau_p} \tag{2}$$

where $\mathcal{M}_k = \int_{\mathbb{R}^d} \left(\otimes^k \boldsymbol{u}\right) f(t, \boldsymbol{x}, \boldsymbol{u}) d\boldsymbol{u}$

Closure problem: the highest order flux is unknown

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# Kinetic-Based Moment Method

## Kinetic-Based Moment Method

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Closure: based on the choice of a presumed shape of the NDF ($f$)

- having as many parameters as the number of moments one needs to control

### Advantages

- Coupling with the gas
- Parallel computing
- Well posed systems
- Direct link with the kinetic level

### Challenges

- Numerical schemes
  - Realizability preservation

### Realizability

Every set of moments has to be associated with a positive $f$

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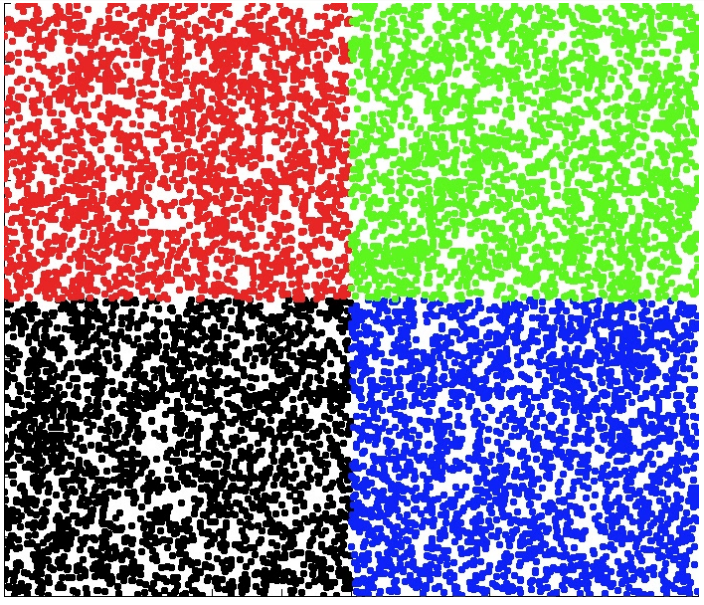
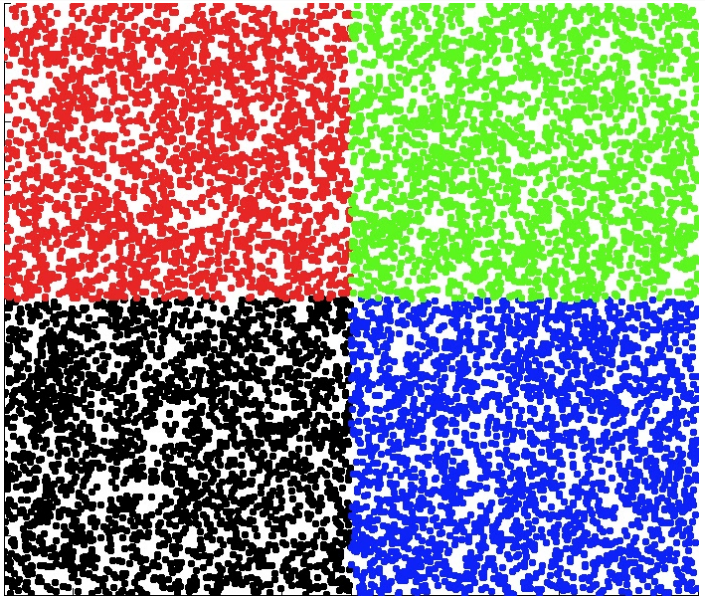
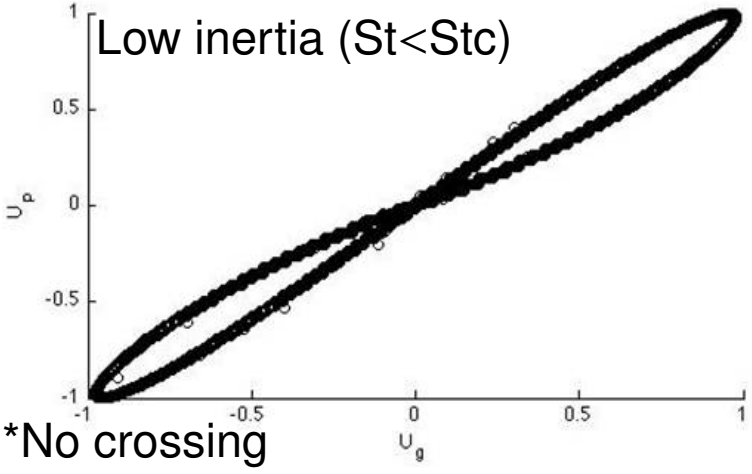
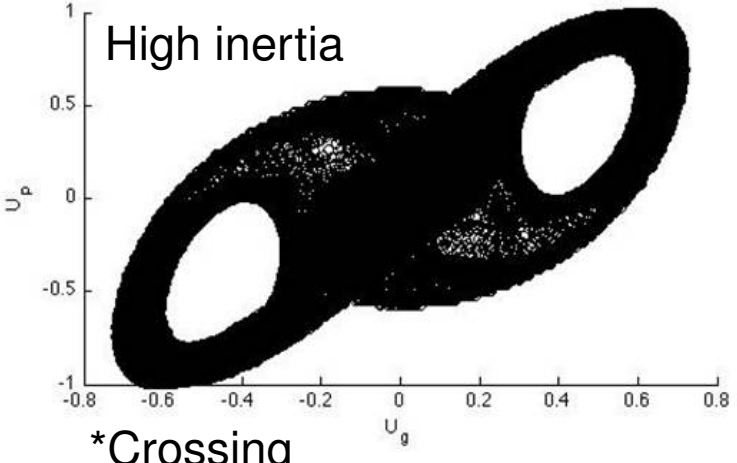







*No crossing
*High velocity correlation
*Monokinetic




*Crossing
*Complex correlation
*Polykinetic

# Kinetic-Based Moment Method

| | | | | |
|---|---|---|---|---|
| M00 | M10 | M20 | M30 | M40 |
| M01 | M11 | M21 | M31 | M41 |
| M02 | M12 | | | |
| M03 | M13 | | | |
| M04 | M14 | (Laurent et al. 2012) | | |

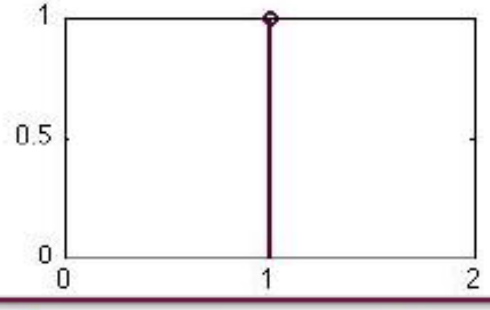
**StK=0** **StK=1** *Stokes number*

*Zeroth order*

- Equilibrium Eulerian (Ferry et al. 2003)

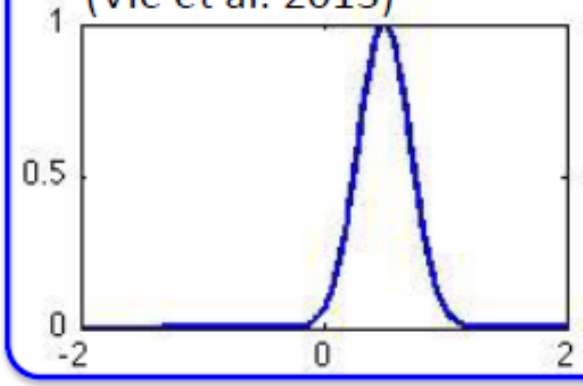
*First order*

- Monokinetic Assumption (Laurent & Massot 2001)



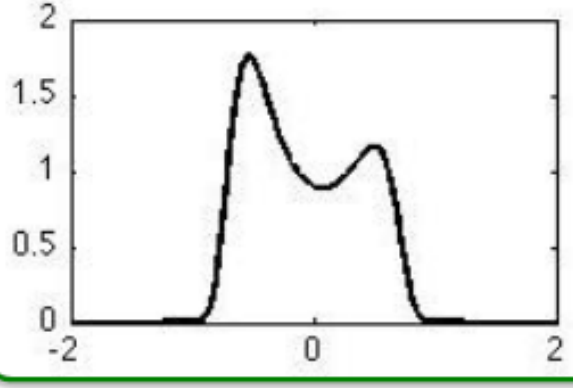

*Second order*

- 2-Phi-EASM (Masi & Simonin 2012)
- Anisotropic Gaussian (Vié et al. 2013)




*Third and fourth order moments*

- CQMOM (Yuan & Fox 2010)
- Multi-Gaussian (Chalons et al. 2010)




**1** *Number of moments* **3** **4** **6** **12** **17**

# Outline

1. High order moment methods in size, with realizable and accurate numerical methods

2. High order moment methods in velocity, with realizable and accurate numerical methods
   - Up to second order moment methods (statistical crossing)
   - Higher order moment methods (deterministic crossing)
   - Multi-Gaussian model

3. Dealing with model coupling and asymptotic limits
   - A Hybrid model and related relaxation scheme
   - An Asymptotic-Preserving Relaxation scheme

# Kinetic-Based Moment Method

## Mono-Kinetic

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

## Anisotropic Gaussian

$$f(t,\boldsymbol{x},\boldsymbol{u}) = \rho(t,\boldsymbol{x})\mathcal{N}(\boldsymbol{u}-\boldsymbol{u_d},\boldsymbol{\Sigma})$$

## Mono-Kinetic

$$\begin{cases} \partial_t\rho + \partial_{\boldsymbol{x}}\cdot(\rho\boldsymbol{u_d}) = 0 \\ \partial_t(\rho\boldsymbol{u_d}) + \partial_{\boldsymbol{x}}\cdot(\rho\boldsymbol{u_d}\otimes\boldsymbol{u_d}) = \dfrac{\rho(\boldsymbol{U_g}-\boldsymbol{u_d})}{\tau_p} \end{cases}$$

- PGD (P=0) : weakly hyperbolic
- can generate $\delta$-shocks and singularities: difficult to handle numerically
- reproduces the dynamics of low inertia particles with stiff accumulation and void regions

# Kinetic-Based Moment Method

## Mono-Kinetic

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

## Anisotropic Gaussian

$$f(t,\boldsymbol{x},\boldsymbol{u}) = \rho(t,\boldsymbol{x})\mathcal{N}(\boldsymbol{u}-\boldsymbol{u_d},\boldsymbol{\Sigma})$$

$$\mathcal{N} = \frac{\exp\left(-\frac{1}{2}(\boldsymbol{u}-\boldsymbol{u_d})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{u}-\boldsymbol{u_d})\right)}{\left((2\pi)^d|\boldsymbol{\Sigma}|\right)^{1/2}}$$

## Anisotropic-Gaussian

$$\begin{cases} \partial_t\rho + \partial_{\boldsymbol{x}}\cdot(\rho\boldsymbol{u_d}) = 0 \\ \partial_t(\rho\boldsymbol{u_d}) + \partial_{\boldsymbol{x}}\cdot(\rho\boldsymbol{u_d}\otimes\boldsymbol{u_d}+\mathbf{P}) = \dfrac{\rho(\boldsymbol{U_g}-\boldsymbol{u_d})}{\tau_p} \\ \partial_t(\rho\mathbf{E}) + \partial_{\boldsymbol{x}}\cdot((\rho\mathbf{E}+\mathbf{P})\odot\boldsymbol{u_d}) = \dfrac{\rho(\boldsymbol{U_g}\odot\boldsymbol{u_d}-2\mathbf{E})}{\tau_p} \end{cases}$$

where

- $\mathbf{E} = \frac{1}{2}\boldsymbol{u_d}\otimes\boldsymbol{u_d} + \frac{\mathbf{P}}{2\rho}$
- $\mathbf{P} = \rho\boldsymbol{\Sigma}$

- Entropy structure
- Hyperbolic

# Kinetic-Based Moment Method

## Mono-Kinetic

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- $\mathbf{P} = \rho\boldsymbol{\Sigma}$

- Entropy structure
- Hyperbolic

# Kinetic-Based Moment Method

## Isotropic Gaussian: Euler System

$$\begin{cases} \partial_t \rho + \partial_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u_d}) = 0 \\ \partial_t (\rho \boldsymbol{u_d}) + \partial_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u_d} \otimes \boldsymbol{u} + \mathbf{P}) = \dfrac{\rho(\boldsymbol{U_g} - \boldsymbol{u_d})}{\tau_p} \\ \partial_t (\rho \mathcal{E}) + \partial_{\boldsymbol{x}} \cdot ((\rho \mathcal{E} + \mathcal{P}) \cdot \boldsymbol{u_d}) = \dfrac{\rho(\boldsymbol{U_g} \cdot \boldsymbol{u_d} - 2\mathcal{E})}{\tau_p} \end{cases}$$

with $\mathcal{E} = tr(\mathbf{E}) = \frac{1}{2} |\boldsymbol{u_d}|^2 + \sigma$, and $\mathbf{P} = \mathcal{P}\mathbf{I} = \rho\sigma\mathbf{I}$

$$\begin{cases} \partial_t \rho + \partial_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u_d}) = 0 \\ \partial_t (\rho \boldsymbol{u_d}) + \partial_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u_d} \otimes \boldsymbol{u_d} + \mathbf{P}) = \dfrac{\rho(\boldsymbol{U_g} - \boldsymbol{u_d})}{\tau_p} \\ \partial_t (\rho \mathbf{E}) + \partial_{\boldsymbol{x}} \cdot ((\rho \mathbf{E} + \mathbf{P}) \odot \boldsymbol{u_d}) = \dfrac{\rho(\boldsymbol{U_g} \odot \boldsymbol{u_d} - 2\mathbf{E})}{\tau_p} \end{cases}$$

where

- $\mathbf{E} = \frac{1}{2} \boldsymbol{u_d} \otimes \boldsymbol{u_d} + \frac{\mathbf{P}}{2\rho}$
- $\mathbf{P} = \rho \boldsymbol{\Sigma}$

- Entropy structure
- Hyperbolic

# Numerical Scheme: FV MUSCL/HLL

## Free transport in the $x$-direction:

$$\partial_t \mathbf{M} + \partial_x \mathcal{F}(\mathbf{M}) = 0$$

## Structured Meshes

Directional Splitting

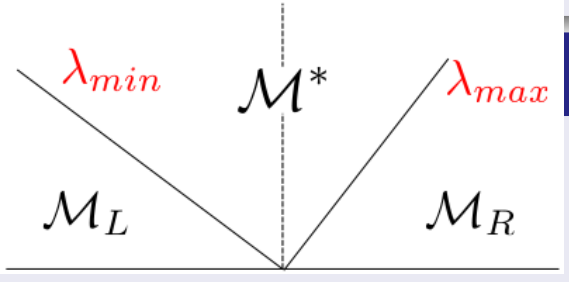
## Realizability Preserving Numerical Flux $\mathcal{F}^*$

$$\mathbf{M}_{i-1}^n, \mathbf{M}_i^n, \mathbf{M}_{i+1}^n \in \mathcal{S} \Rightarrow \quad \mathbf{M}_i^{n+1} \in \mathcal{S}$$

$$\mathbf{M}_i^{n+1} = \mathbf{M}_i^n - \frac{\Delta t}{|C_i|}\left(\mathcal{F}^*(\mathbf{M}_{i+1}^n, \mathbf{M}_i^n) - \mathcal{F}^*(\mathbf{M}_i^n, \mathbf{W}_{i-1}^n)\right)$$

## Flux evaluation

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




$$\mathcal{F}^{HLL} = \frac{1}{2}\left(\mathcal{F}(\mathbf{M}_L) + \mathcal{F}(\mathbf{M}_R)\right) - \frac{|\lambda_{min}|}{2}\left(\mathbf{M}^* - \mathbf{M}_L\right) - \frac{|\lambda_{max}|}{2}\left(\mathbf{M}_R - \mathbf{M}^*\right)$$

# Numerical Scheme: FV MUSCL/HLL

## Realizability (AG)

- $\rho > 0$,
- $p_{11} > 0, p_{22} > 0$,
- $p_{11}p_{22} - p_{12}^2 > 0$.

## Realizable AND Conservative reconstruction

- Primitive Variables: $\mathbf{U} = (\rho, \boldsymbol{u_d}, \mathbf{P})$
- Realizable reconst.: $\mathbf{U}_j(x) = \overline{\mathbf{U}_j} + \mathbf{D}_{\mathbf{U}}(x - x_j)$
- Conservative correction: $\int_{C_j} \mathbf{M}\left(\mathbf{U}_j(x)\right) = \overline{\mathbf{M}_j}$ imposed by the conservation of the cell value for each moment in order to ensure that the fluxes will not affect the realizability (Vié et al. 2015)

# Time integration

## SSP-RK2 Time Integration (Gottlieb et al. 2001)

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

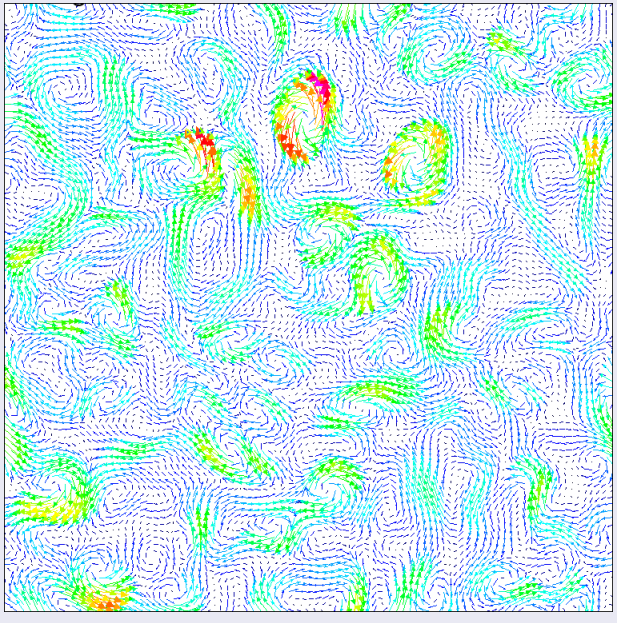
$$\mathbf{M}_i^{n+1} = \frac{\mathbf{M}_i^n}{2} + \frac{1}{2}\left[\mathbf{M}_i^{(1)} - \frac{\Delta t}{\Delta x}\left(\mathcal{F}_{i+1/2}^{(1)} - \mathcal{F}_{i-1/2}^{(1)}\right)\right]$$

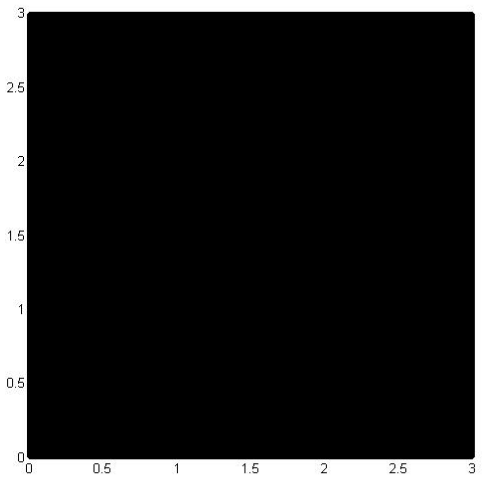
- $2^{\text{nd}}$-order in space and time and realizable scheme, under CFL 0.5
  - $\mathbf{M}^n \in \mathcal{S} \Rightarrow \mathbf{M}^{n+1} \in \mathcal{S}$

# 2D DNS results

## Test case

- Frozen HIT velocity field
- Homogeneous spray at t=0
- 2 Stokes numbers: 1 and 5





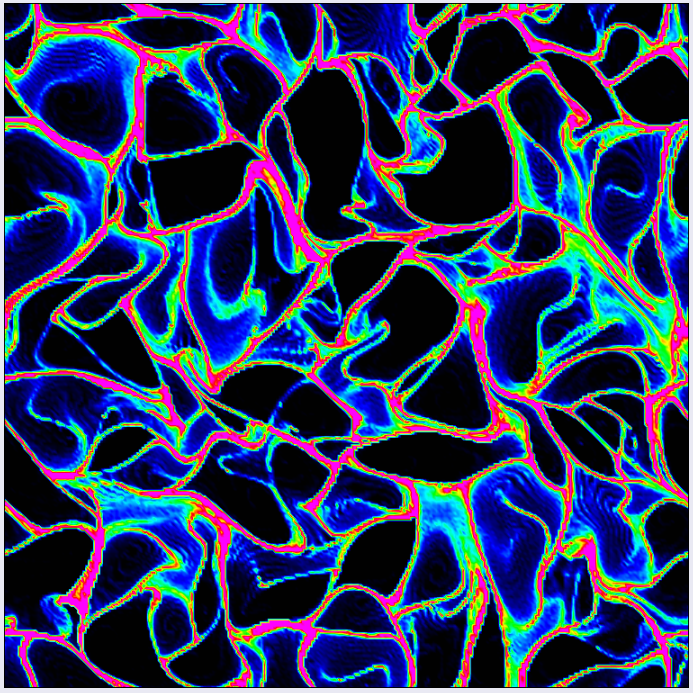

## Results

- Snapshots of the number density
- Segregation vs. time for different models
- Segregation and MCE vs. St

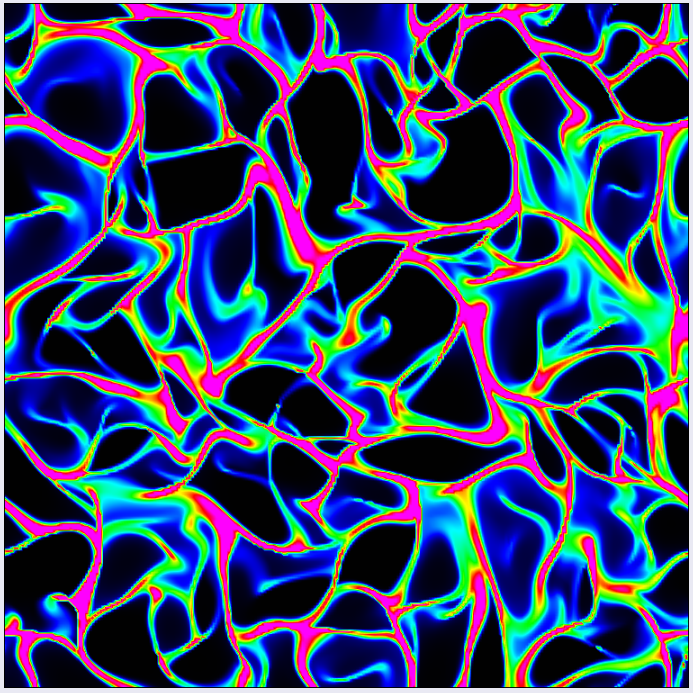
Segregation: spatial correlation of the number density field at a given cell size length

# Number density Mesh $256^2$ St=1

## Lagrangian



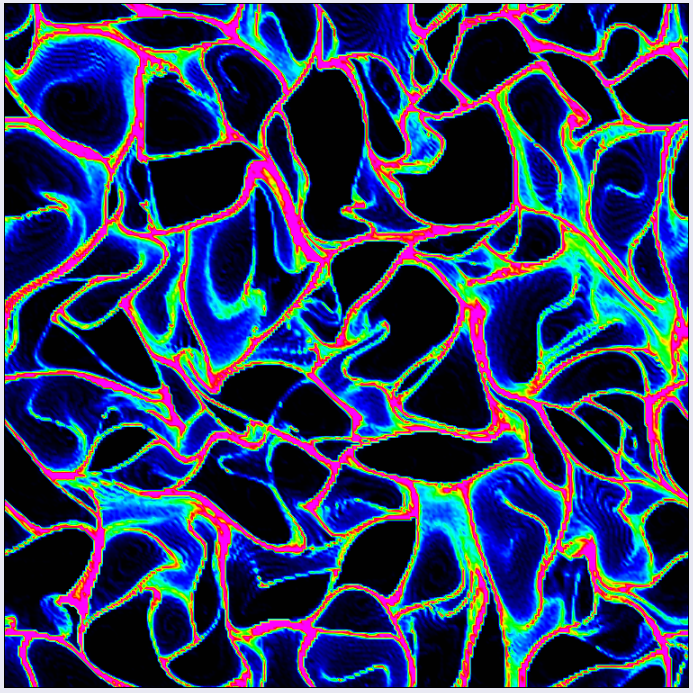
## Mono-Kinetic



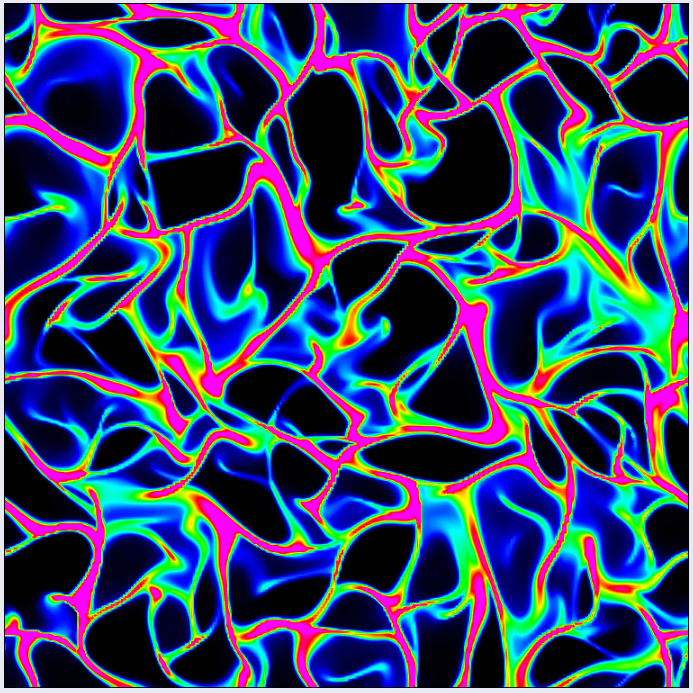
AG qualitatively match the Lagrangian results, no unphysical accumulations

# Number density Mesh $256^2$ St=1

## Lagrangian



## Isotropic Gaussian



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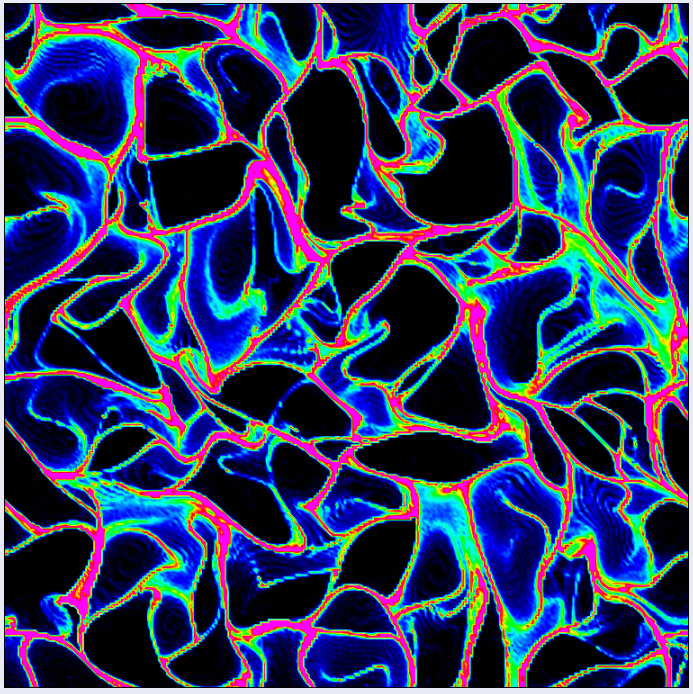
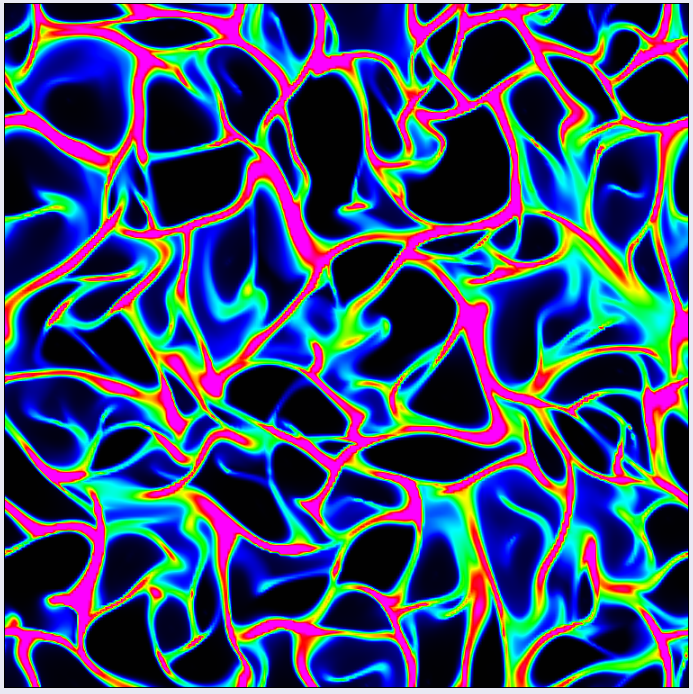


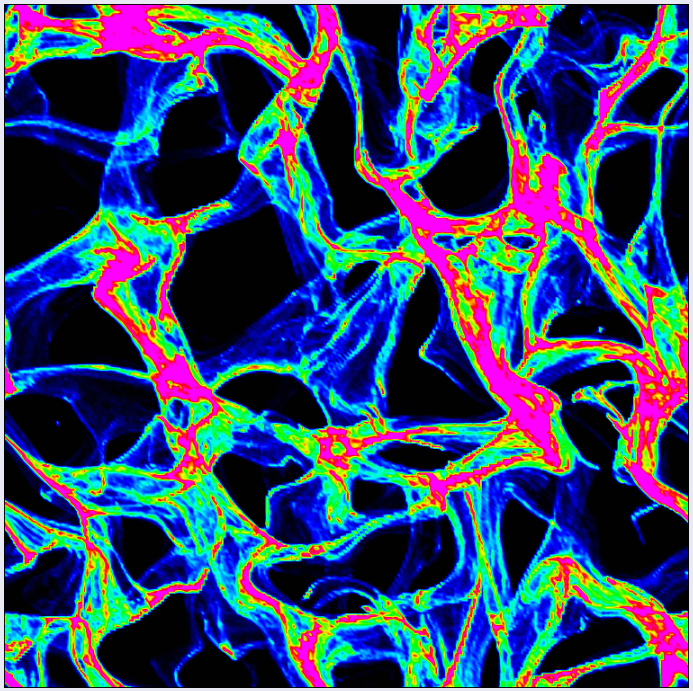
## Anisotropic Gaussian



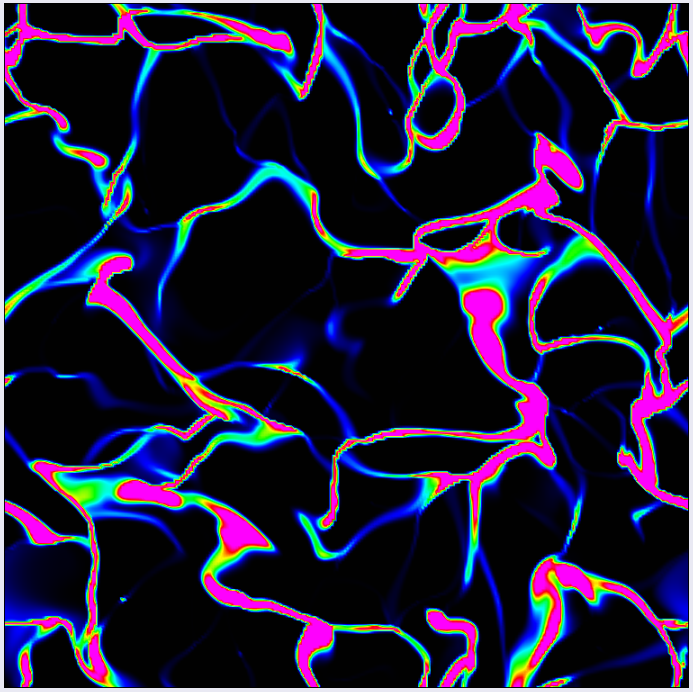
AG qualitatively match the Lagrangian results, no unphysical accumulations

# Number density Mesh $256^2$ St=5

## Lagrangian



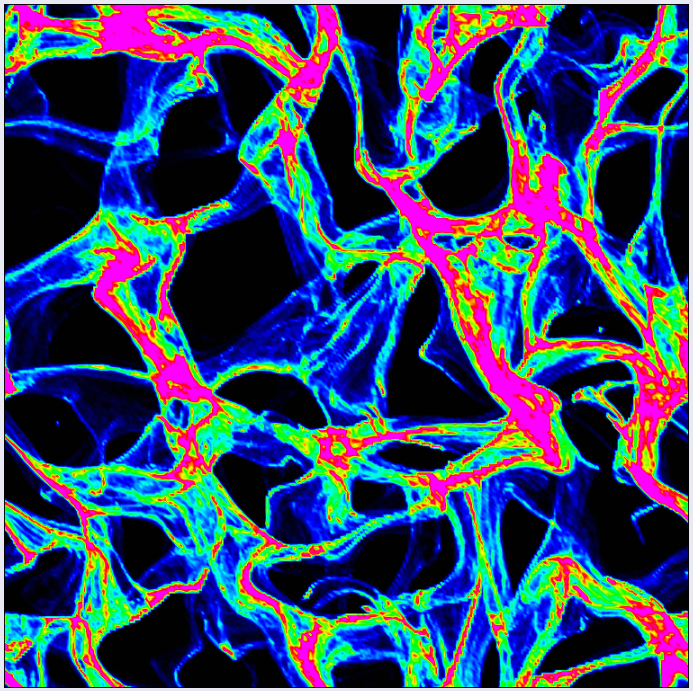
## Mono-Kinetic



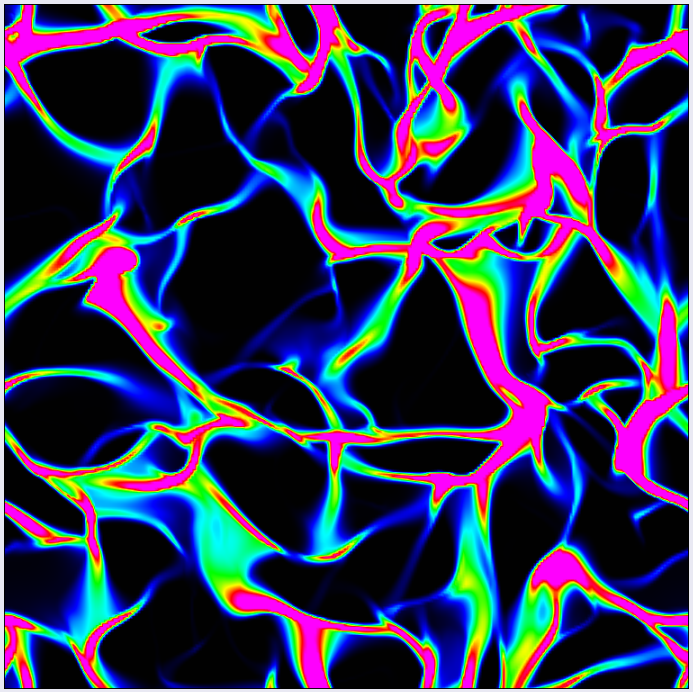
AG qualitatively match the Lagrangian results, no unphysical accumulations

# Number density Mesh $256^2$ St=5

## Lagrangian



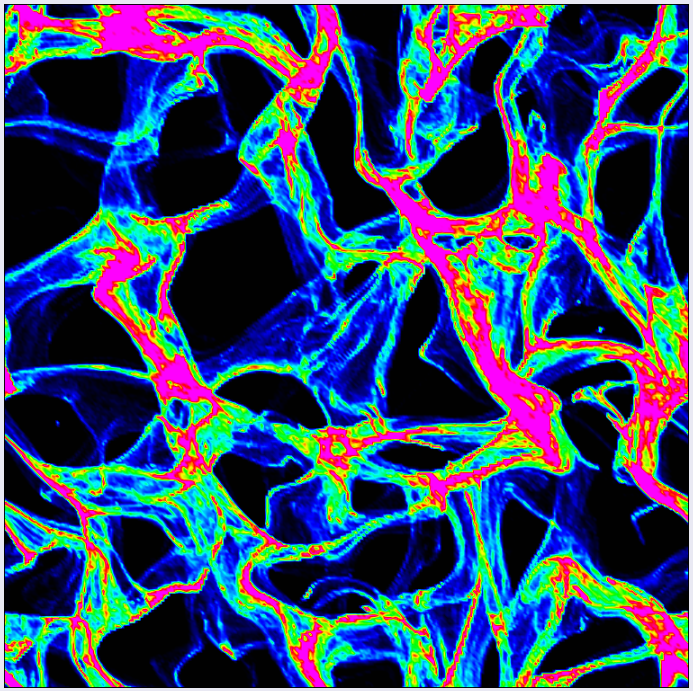
## Isotropic Gaussian



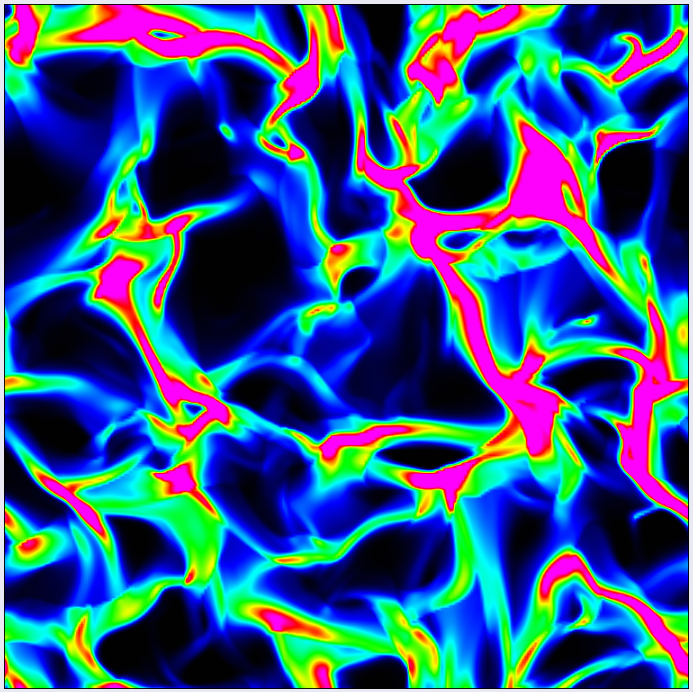
AG qualitatively match the Lagrangian results, no unphysical accumulations

# Number density Mesh $256^2$ St=5

## Lagrangian

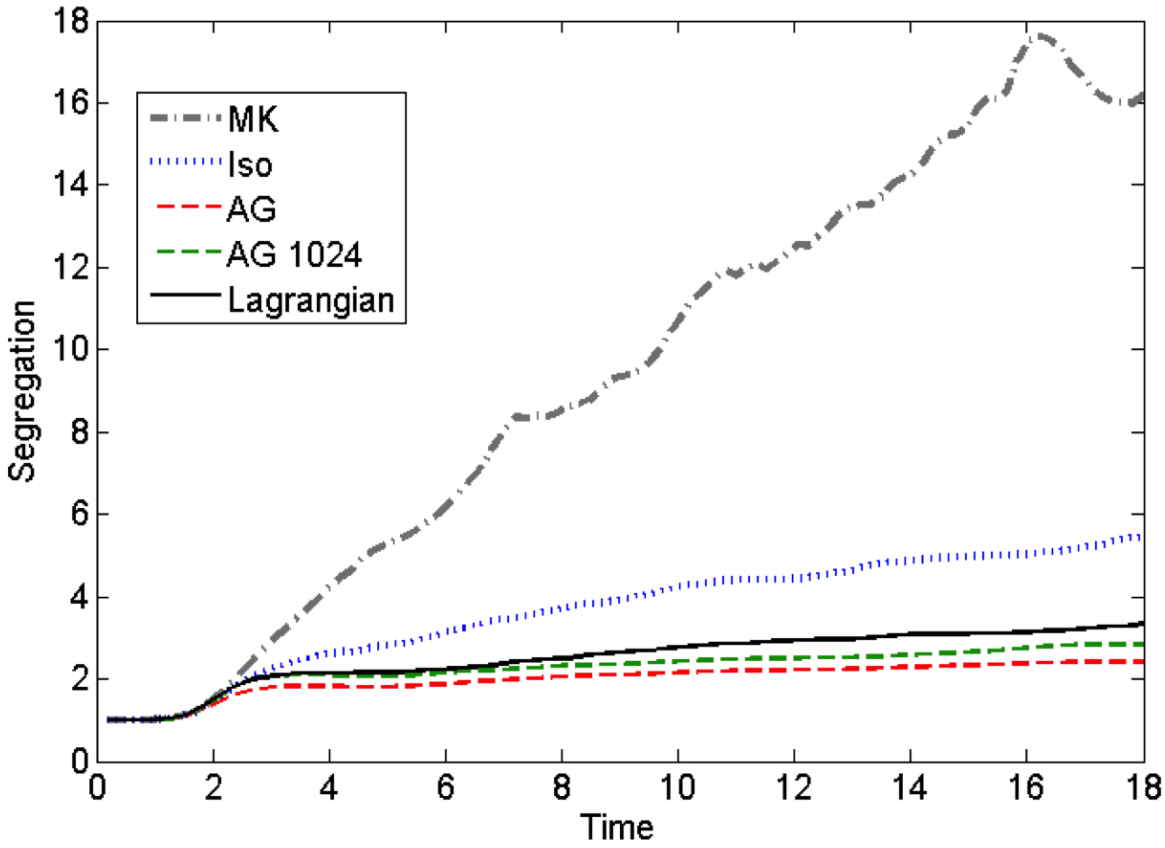


## Anisotropic Gaussian



AG qualitatively match the Lagrangian results, no unphysical accumulations

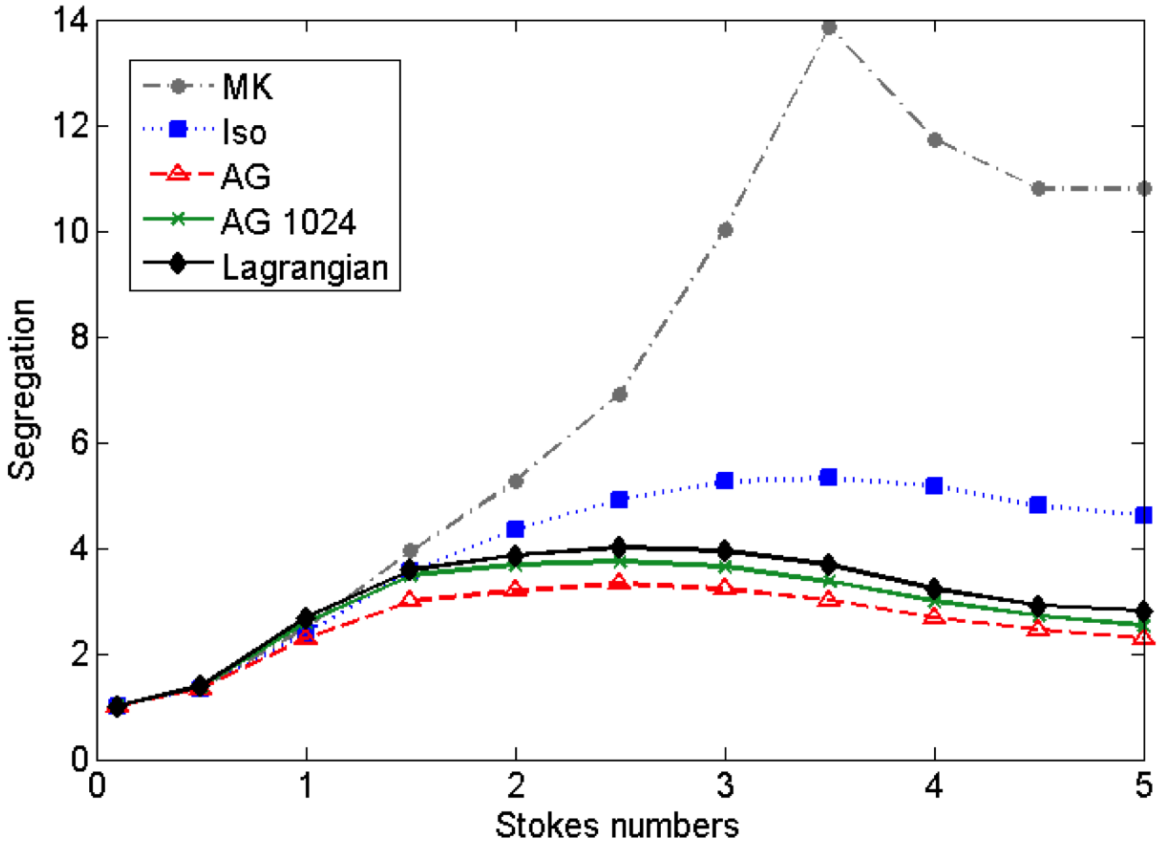
# Segregation vs. time (St=5)




MK and Iso: greatly overestimate the segregation

AG: converge to Lagrangian

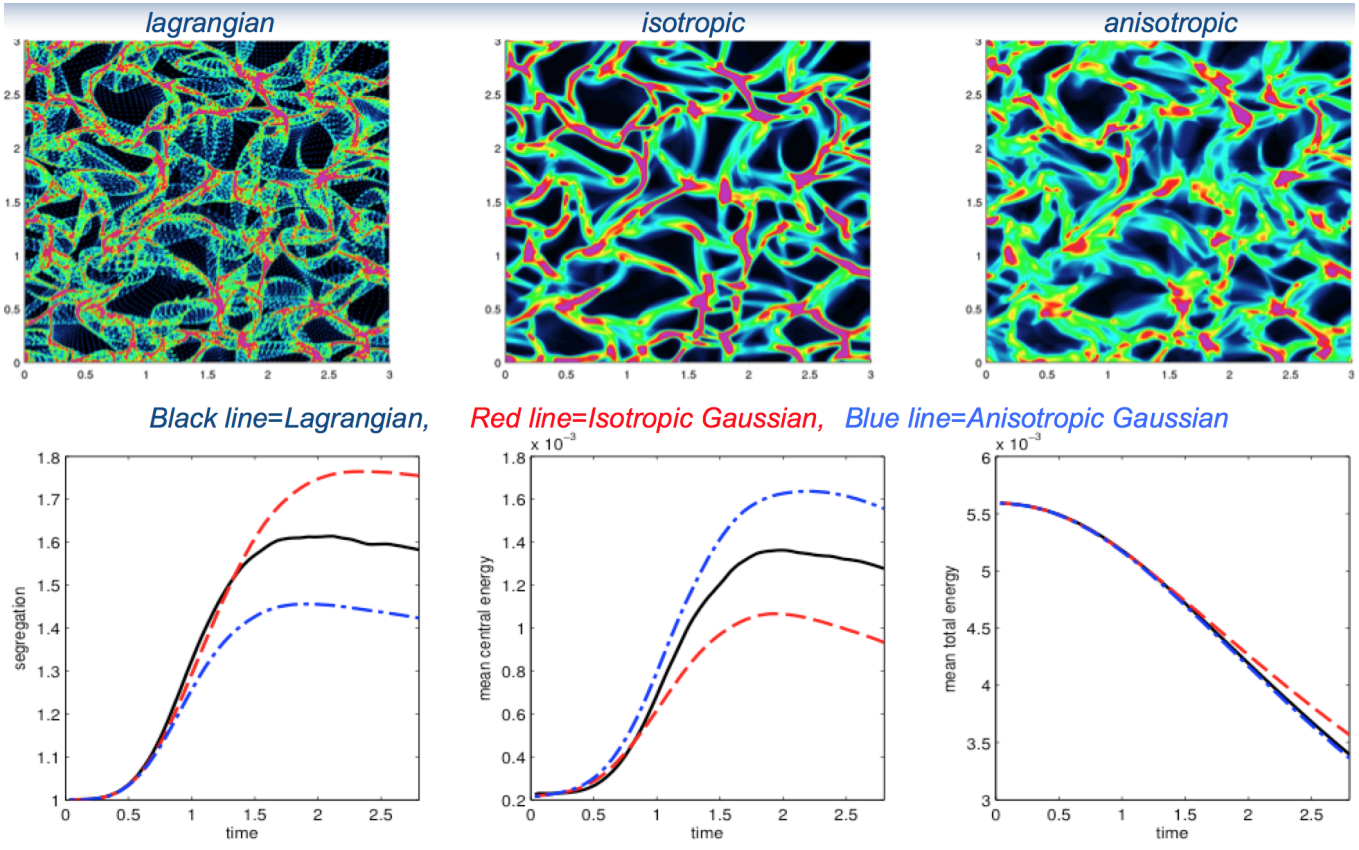
# Segregation vs. St




AG: right behavior for the range of Stokes number studied

# Taking into account statistical PTC

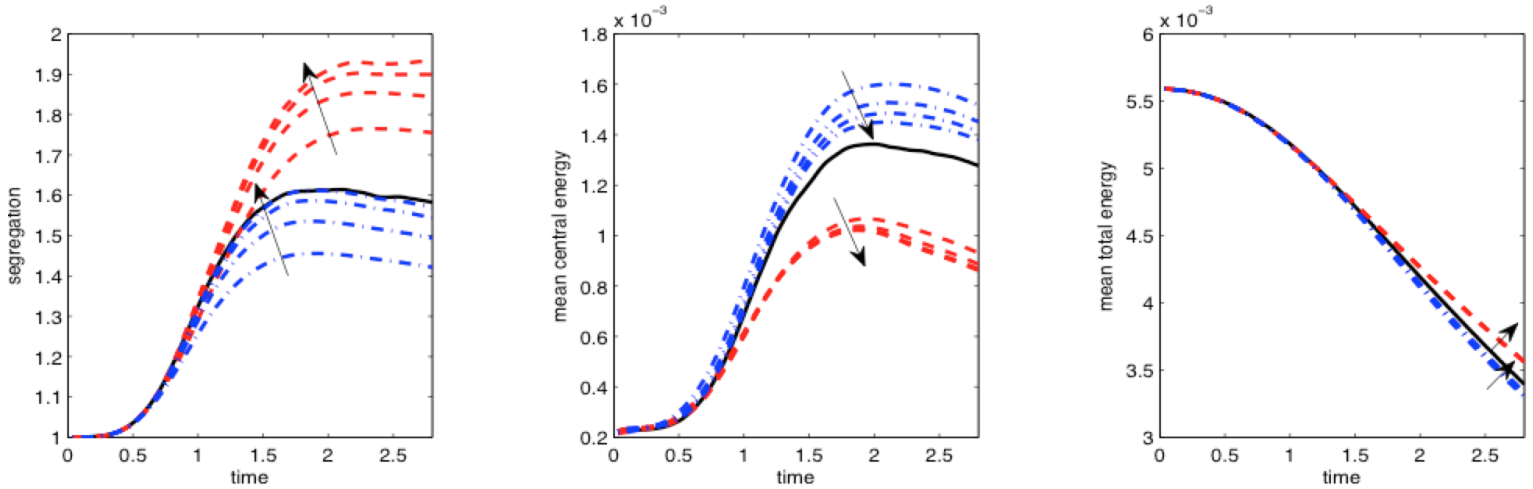
Lagrangian ref. solution - Isotropic Kinetic Closure - Gaussian Kinetic Closure




Stokes = 10 - Homogeneous Isotropic turbulence - density of particles
Vié, Doisneau, Massot, CICP 2015 - HLL realizable 2nd order in space and time.

# Taking into account statistical PTC

Mesh refinement indicated the proper choice in terms of modeling




*Black line=Lagrangian, Red line=Isotropic Gaussian, Blue line=Anisotropic Gaussian*

Stokes = 10 - Homogeneous Isotropic turbulence - density of particles
Vié, Doisneau, Massot, CICP 2015 - HLL realizable 2nd order in space and time.

# Taking into account statistical PTC

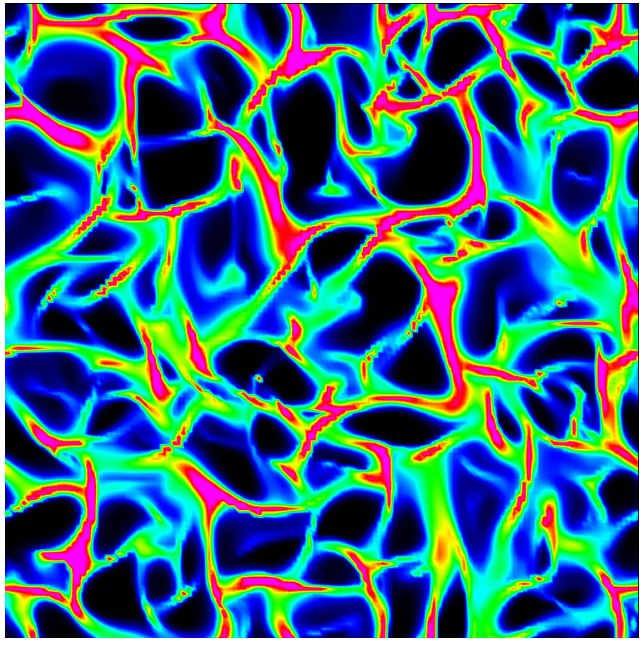
Lagrangian ref. solution - Gaussian Kinetic Closure - Algebraic Closure

Stokes = 5 - Shear layer + Homogeneous Isotropic turbulence - density of particles
Vié, Masi, Simonin, Massot (Summer Program 2012 - Stanford University - CTR).

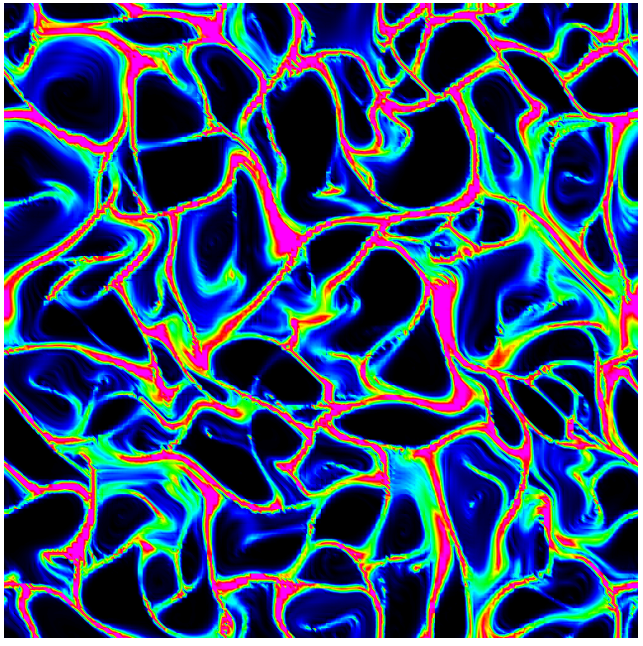
DNS (and LES) : Need to couple PGD and higher order moment methods

# High order numerical schemes and unstructured meshes

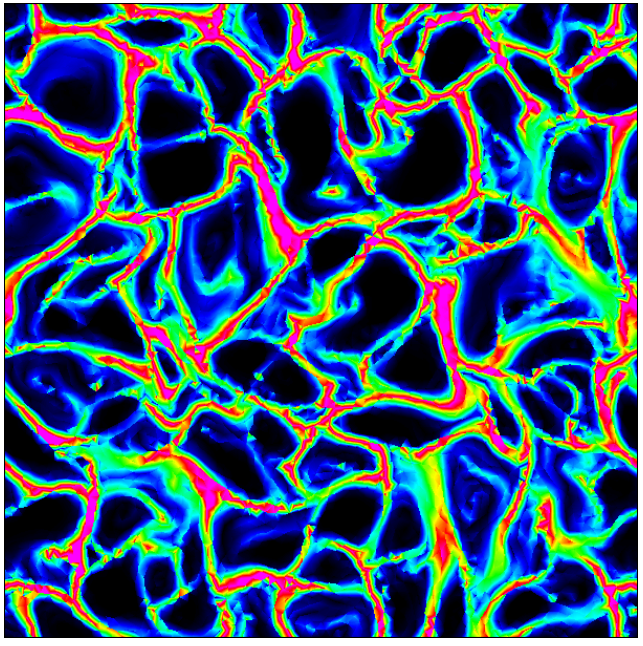
- 1D comparison of different numerical schemes (Larat el al. 2012, Sabat et al. 2015)
- Unstructured realizability preserving DG method (Larat el al. 2012, Sabat et al. 2014)



FV structured $128^2$



DG structured $128^2$



DG unstructured $64^2$

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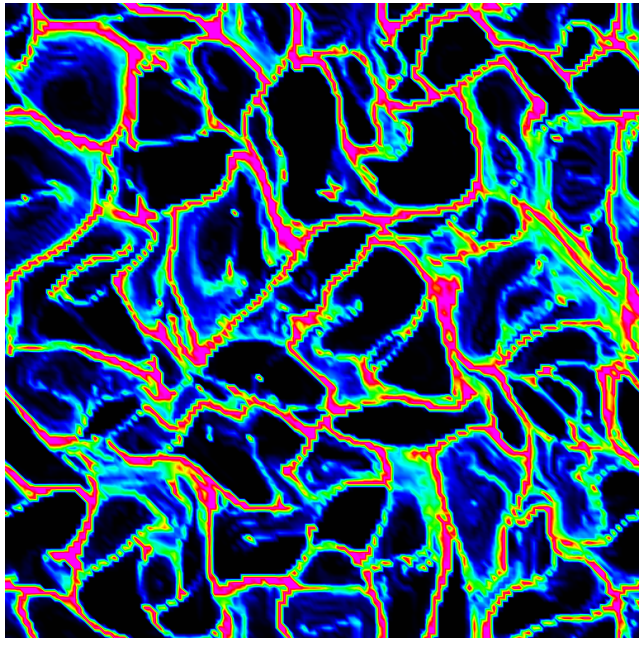
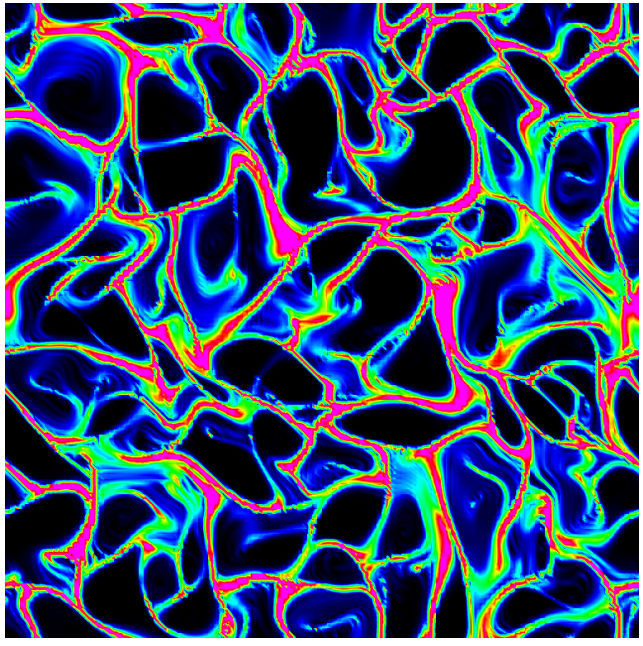


Lagrangian



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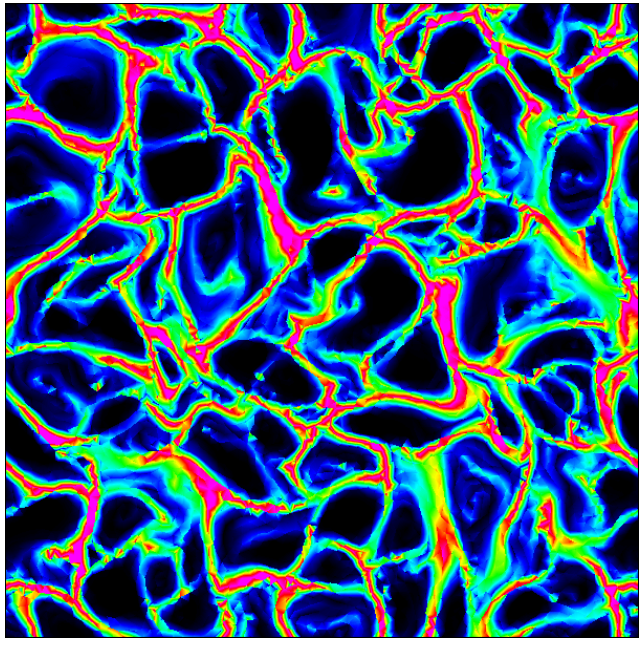

DG unstructured $64^2$

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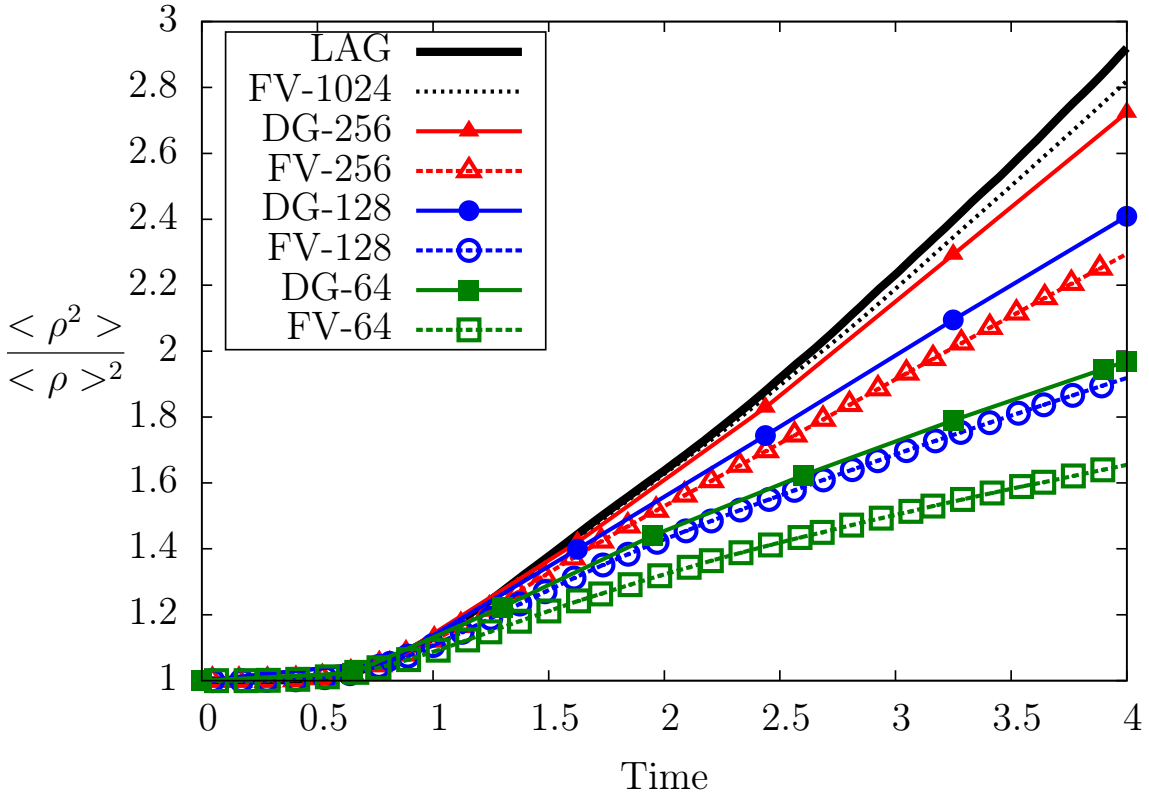

# Outline

# Moment method in velocity

## Simplified and dimensionless kinetic model

$f(\boldsymbol{x}, \boldsymbol{u}; t)$ : number density function (NDF)

Williams - Boltzmann transport equation

$$\partial_t f + \partial_{\boldsymbol{x}} \cdot (\boldsymbol{u} f) + \partial_{\boldsymbol{u}} \left( \frac{\boldsymbol{U_g} - \boldsymbol{u}}{\mathrm{St}} f \right) = 0$$

## Eulerian description

- Moments of the NDF:
  $M^{\boldsymbol{j}} = \int \boldsymbol{u}^{\boldsymbol{j}} f(\boldsymbol{x}, \boldsymbol{u}; t) \mathrm{d}\boldsymbol{u} = \int u_1^{j_1} \dots u_d^{j_d} f(\boldsymbol{x}, \boldsymbol{u}; t) \mathrm{d}u_1 \dots \mathrm{d}u_d$
- moment vector: $\mathcal{M} = (M^{\boldsymbol{j}})_{\boldsymbol{j} \in \mathcal{S}}$, $\quad \mathcal{S}$ finite subset of $\mathbb{N}^d$
- equations on $\mathcal{M}$

example in 1D:

$$\partial_t M^j + \partial_x M^{j+1} = \frac{U_g M^{j-1} - M^j}{\mathrm{St}}$$

$\rightarrow$ need a closure for $M^{N+1}$

# Closure

## Objective

Express higher order moments as a function of the moment vector $\mathcal{M}$

**1D case**

## Finite Hamburger moment problem for the moment vector $\mathcal{M}$:

for $\mathcal{M} = (M^0, M^1, \ldots, M^N)^t$, find a non-negative real function $f_{\mathcal{M}}$ defined on $\mathbb{R}$ such that

$$\forall j \in \{0, 1, \ldots, N\} \qquad M^j = \int u^j f_{\mathcal{M}}(x, u; t) \mathrm{d}u$$

**Hankel determinants:**

$$H_m = \begin{vmatrix} M^0 & \ldots & M^{m-1} \\ \vdots & & \vdots \\ M^{m-1} & \ldots & M^{2m-2} \end{vmatrix}$$

the problem has a solution (an infinity in fact) if $H_m > 0$ for $m = 1, \ldots, N+1$.

**2D/3D case**

## Problem:

for $\mathcal{M} = (M^i)$ find a non-negative real function $f_{\mathcal{M}}$ defined on $\mathbb{R}$ such that

# Closure

## Objective

Express higher order moments as a function of the moment vector $\mathcal{M}$

**1D case**

## Finite Hamburger moment problem for the moment vector $\mathcal{M}$:

for $\mathcal{M} = (M^0, M^1, \ldots, M^N)^t$, find a non-negative real function $f_{\mathcal{M}}$ defined on $\mathbb{R}$ such that

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**2D/3D case**

## Problem:

for $\mathcal{M} = (M^j)_{j \in \mathcal{S}}$, find a non-negative real function $f_{\mathcal{M}}$ defined on $\mathbb{R}$ such that

$$\forall \boldsymbol{j} \in \mathcal{S} \qquad M^{\boldsymbol{j}} = \int \boldsymbol{u}^{\boldsymbol{j}} f_{\mathcal{M}}(\boldsymbol{x}, \boldsymbol{u}; t) \mathrm{d}\boldsymbol{u}$$

**Theoretical difficulties:**

$\rightarrow$ choice $\mathcal{S}$
$\rightarrow$ existence of solutions

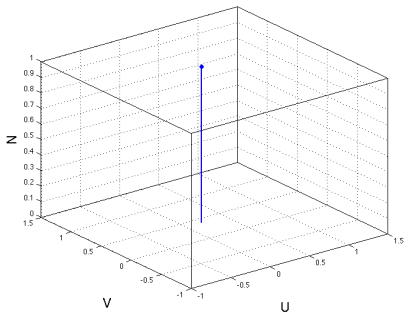
# Closure examples

0 — 1 — 10 — St

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

## Monokinetic assumption

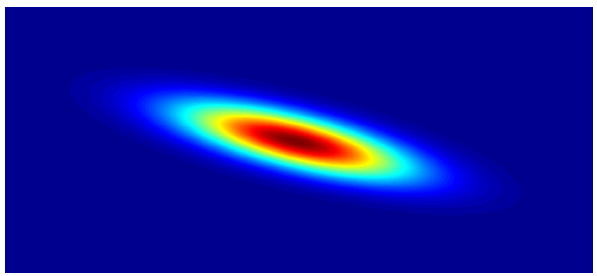
[de Chaisemartin, 2009]




## Algebraic-Closure-Based

[Simonin et al., 2002, Masi and Simonin, 2012]

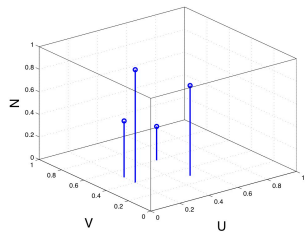
## Anisotropic Gaussian closure [Vié et al 2015]



## Quadrature closure

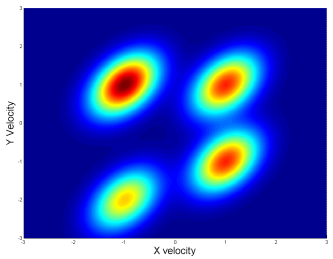
[Fox et al., 2008, de Chaisemartin et al., 2009,

Yuan et al 2011, Chalons et al., 2012]




## Multi-Gaussian closure

[Chalons et al., 2013]



# Outline

# Multi-gaussian closure - 1D case

## model for advection: $\partial_t f + \partial_x(uf) = 0$

$$\partial_t \mathcal{M} + \partial_x \mathcal{F}(\mathcal{M}) = 0$$

Moment vector: $\mathcal{M} = (M^0, M^1, M^2, M^3, M^4)^t$

Flux $\mathcal{F}(\mathcal{M}) = (M^1, M^2, M^3, M^4, \overline{M}^5)^t$

## Centered norm. moments on $M^1/M^0$

$$e = \frac{M^0 M^2 - (M^1)^2}{(M^0)^2},$$

$$q = \frac{(M^3(M^0)^2 - (M^1)^3) - 3M^1(M^0 M^2 - (M^1)^2)}{(M^0)^3}$$

$$\eta = \frac{-3(M^1)^4 + M^4(M^0)^3 - 4(M^0)^2 M^1 M^3 + 6M^0(M^1)^2 M^2}{(M^0)^4}.$$

## Closure

$$f^G(u) = \sum_{\alpha=1}^{2} \frac{\rho_\alpha}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(u-u_\alpha)^2}{2\sigma^2}\right)$$

with $\rho_1$, $\rho_2$, $u_1$, $u_2$ and $\sigma$ such that

$$\forall j \in \{0,1,2,3,4\} \qquad \int_{\mathbb{R}} u^j f^G(u)\mathrm{d}u = M^j$$

and

$$\overline{M}^5 = \int_{\mathbb{R}} u^5 f^G(u)\mathrm{d}u$$

## Proposition

*Be* $\Omega = \left\{\mathcal{M},\ M^0 > 0,\ e > 0,\ \eta > e^2 + \frac{q^2}{e},\ \text{and } \eta \leq 3e^2 \text{ if } q = 0\right\}$.

*Setting* $\mathbf{U} = (\rho_1, \rho_2, \rho_1 u_1, \rho_2 u_2, \sigma)^t$, *the function* $\mathbf{U} = \mathbf{U}(\mathcal{M})$ *is one-to-one and onto when* $u_1 \neq u_2$, *provided that we set* $\rho_1 = \rho_2$ *in the case* $u_1 = u_2$. *Moreover,* $\sigma^2$ *the unique real root of the polynomial* $\mathcal{P} = 2(X-e)^3 + (\eta - 3e^2)(X-e) + q^2$.

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with $\rho_1$, $\rho_2$, $u_1$, $u_2$ and $\sigma$ such that

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## Proposition

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*Setting* $\mathbf{U} = (\rho_1, \rho_2, \rho_1 u_1, \rho_2 u_2, \sigma)^t$, *the function* $\mathbf{U} = \mathbf{U}(\mathcal{M})$ *is one-to-one and onto when* $u_1 \neq u_2$, *provided that we set* $\rho_1 = \rho_2$ *in the case* $u_1 = u_2$. *Moreover,* $\sigma^2$ *the unique real root of the polynomial* $\mathcal{P} = 2(X-e)^3 + (\eta - 3e^2)(X-e) + q^2$.

# Computation algorithm

## Step 1: computation of $\sigma$

Finding the unique real root of

$$\mathcal{P} = 2(X-e)^3 + (\eta - 3e^2)(X-e) + q^2$$

$\rightarrow$ A limiter is added to control the maximal value of the eigenvalues

## Step 2: computation of $\rho_1$, $\rho_2$, $u_1$, $u_2$

One solves:

$$\begin{aligned} M^0 &= \rho_1 + \rho_2, \\ M^1 &= \rho_1 u_1 + \rho_2 u_2, \\ M^2 - \sigma^2 M^0 &= \rho_1 u_1^2 + \rho_2 u_2^2, \\ M^3 - 3\sigma^2 M^1 &= \rho_1 u_1^3 + \rho_2 u_2^3, \end{aligned}$$

$\rightarrow$ Quadrature algorithm for computation of abscissas and weights (or analytical formula).

# System property

## Model

$$\partial_t \mathcal{M} + \partial_x \mathcal{F}(\mathcal{M}) = 0 \tag{4}$$

Moment vector: $\mathcal{M} = (M^0, M^1, M^2, M^3, M^4)^t$

Flux $\mathcal{F}(\mathcal{M}) = (M^1, M^2, M^3, M^4, \overline{M}^5)^t$

## Closure

$$f^G_{\mathcal{M}}(u) = \sum_{\alpha=1}^{2} \frac{\rho_\alpha}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(u-u_\alpha)^2}{2\sigma^2}\right)$$

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## Théorème

*Assuming that $\mathcal{M} = (M_0, M_1, M_2, M_3, M_4)^t$ lives in $\Omega$, then the system (4) is hyperbolic.*

# Numerical scheme

## Kinetic Flux-Splitting scheme

- Finite volumes:

$$\mathcal{M}_c^n = \frac{1}{\Delta x} \int_{x_{c-1/2}}^{x_{c+1/2}} \mathcal{M}(t^n, x) \mathrm{d}x$$

- Conservative

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

- Upwind scheme at the kinetic level
- Flux splitting:

$$\mathcal{F}_{c+1/2} = \mathcal{F}^+_{c+1/2} + \mathcal{F}^-_{c+1/2}$$

$$\left( \mathcal{F}^+_{c+1/2} \right)^i = \int_0^\infty f^G_{\mathcal{M}_c^n}(u) u^{i+1} \mathrm{d}u,$$

$$\left( \mathcal{F}^-_{c+1/2} \right)^i = \int_{-\infty}^0 f^G_{\mathcal{M}_{c+1}^n}(u) u^{i+1} \mathrm{d}u.$$

→ Realizability

# Results - Riemann problem

## 1D Riemann problem

Two homogeneous sprays, initially at equilibrium, which are crossing.

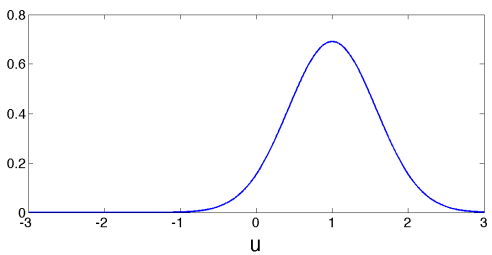
Initial conditions

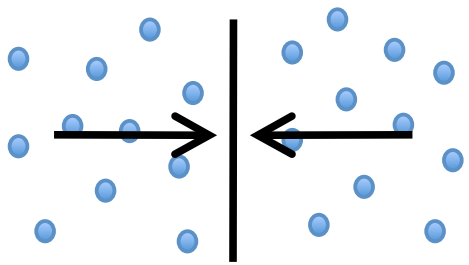
$$M^0 = 1 \qquad e = \frac{1}{3} \qquad q = 0 \qquad \eta = \frac{1}{3}$$

and

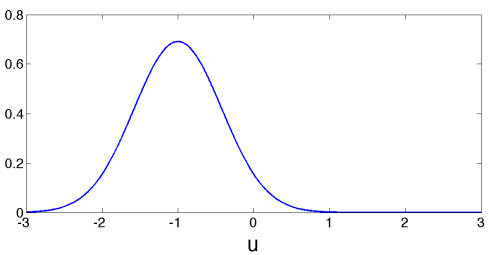
$$U_m = \frac{M_1}{M_0} = \begin{cases} 1 & \text{if } x < 0, \\ -1 & \text{otherwise.} \end{cases}$$

$t = 0$:



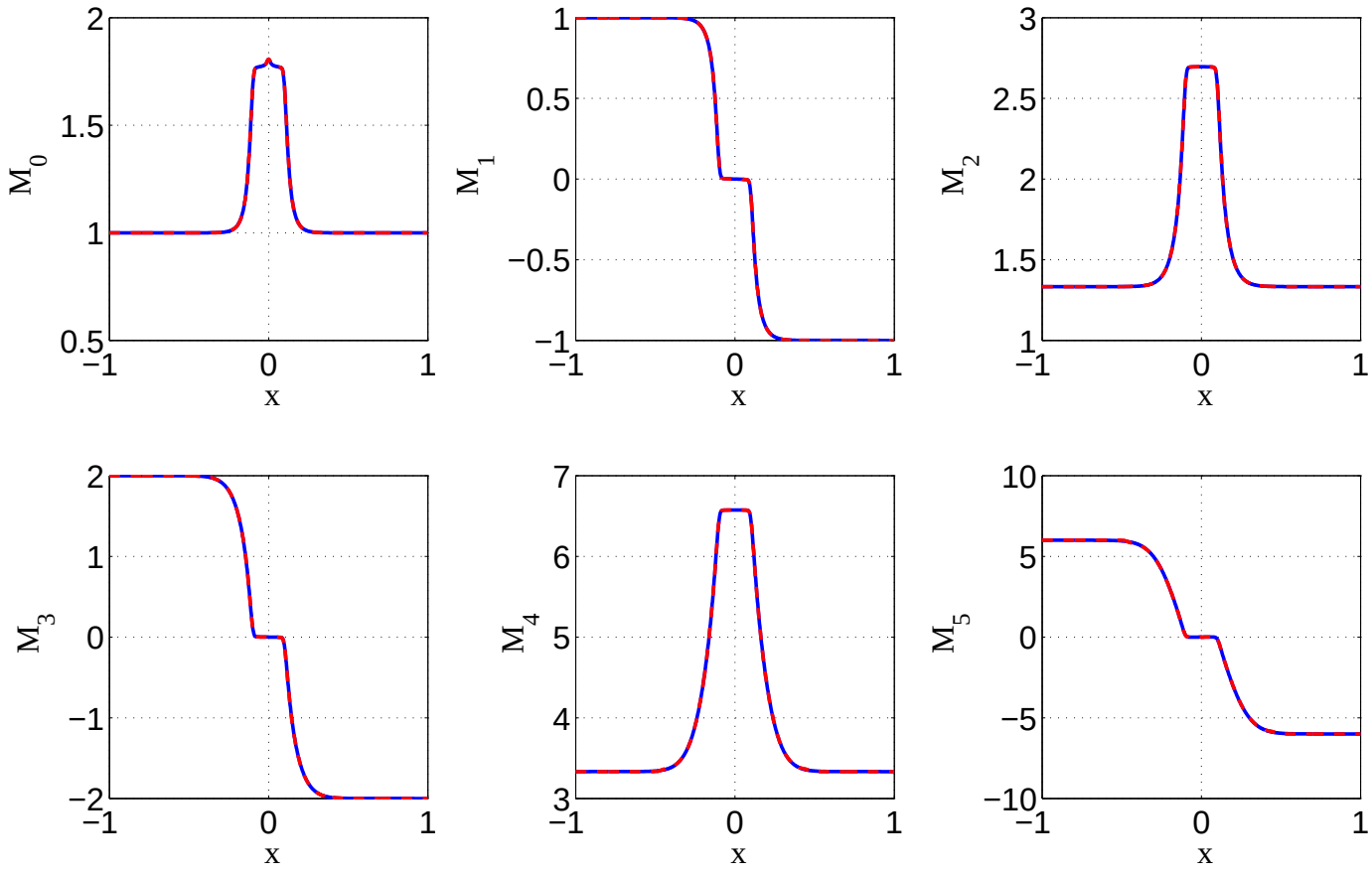



X=0



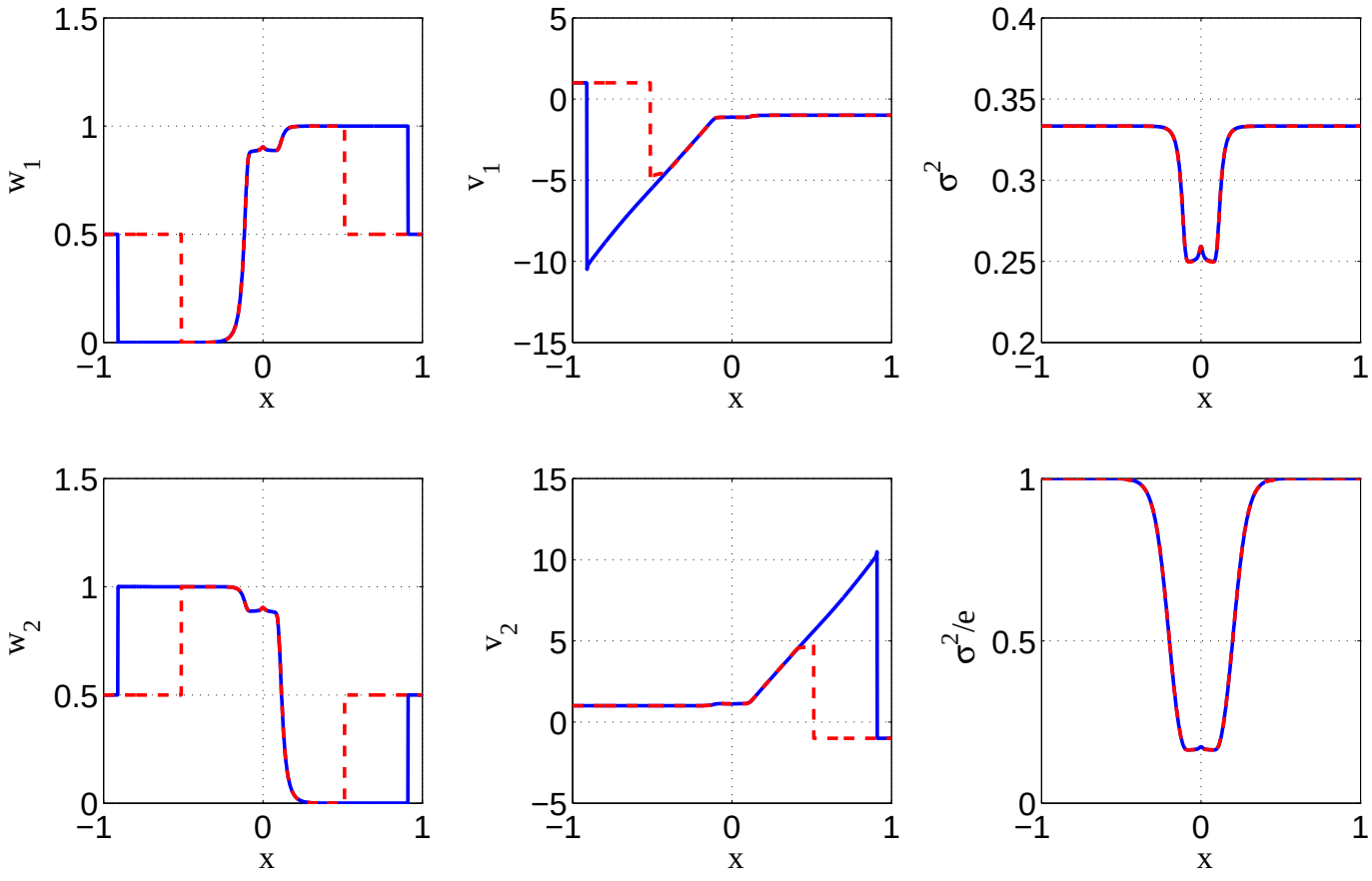
# Results - Riemann problem

$t = 0.5$ : computed and reconstructed moments



# Results - Riemann problem

$t = 0.5$ : abscissas, weights, $\sigma^2$




Limiter on $\sigma^2$ : abscissas are bounded with a neglectable effect on moments

# Multi-gaussien model - 2D case

Ingredients:

- dimensionnal splitting
- conditionnal quadrature [Yuan et al 2011] $M^{i,j} = \int v^j f(v|u) \int u^i f(u) du dv$

## Equations in the $x$ direction

$$\partial_t M^{i,j} + \partial_x M^{i+1,j} = 0$$

## Set of moments

$$\begin{bmatrix} \mathbf{M}^{0,0} & \mathbf{M}^{0,1} & \mathbf{M}^{0,2} & \mathbf{M}^{0,3} & \mathbf{M}^{0,4} \\ \mathbf{M}^{1,0} & \mathbf{M}^{1,1} & \mathbf{M}^{1,2} & \mathbf{M}^{1,3} & \mathbf{M}^{1,4} \\ \mathbf{M}^{2,0} & M^{2,1} & & & \\ \mathbf{M}^{3,0} & M^{3,1} & & & \\ \mathbf{M}^{4,0} & M^{4,1} & & & \end{bmatrix}.$$

$\rightarrow$ Hyperbolic system

## Kinetic description

$$f_{12}(t,x,u,v) = \sum_{\alpha=1}^{2} \sum_{\beta=1}^{2} \rho_\alpha \rho_{\alpha\beta} g(u; u_\alpha, \sigma_1) g(v; v_{\alpha\beta}, \sigma_{2\alpha}),$$

with the Gaussian function: $g(u;\mu,\sigma) = \dfrac{1}{\sigma\sqrt{2\pi}} \exp\left(-\dfrac{(u-\mu)^2}{2\sigma^2}\right)$.

$\rightarrow$ computation of three 1D multi-gaussian closures

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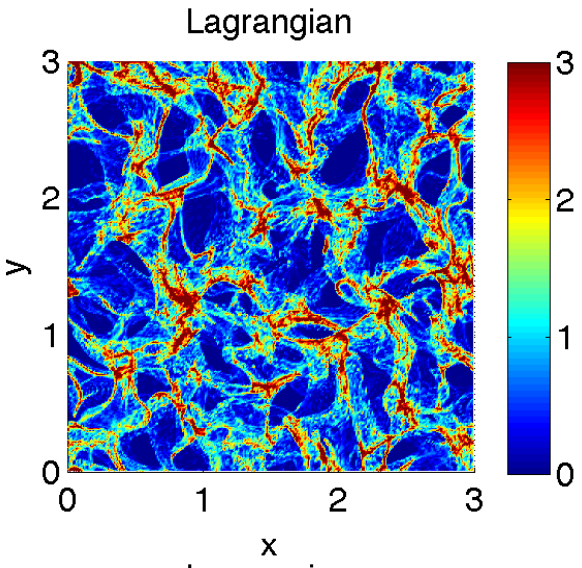
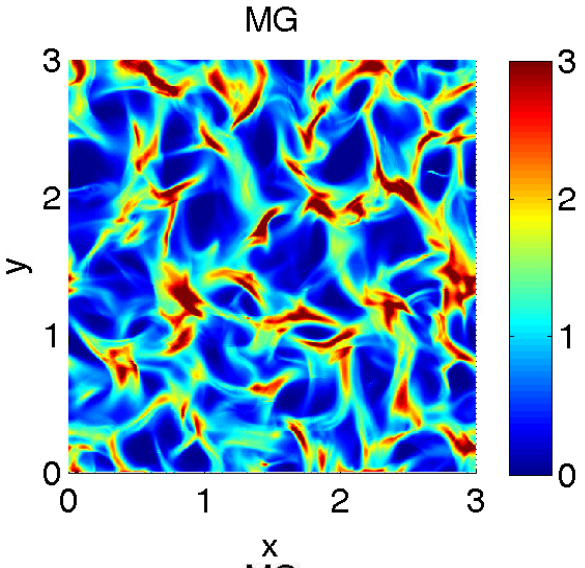
$\rightarrow$ computation of three 1D multi-gaussian closures

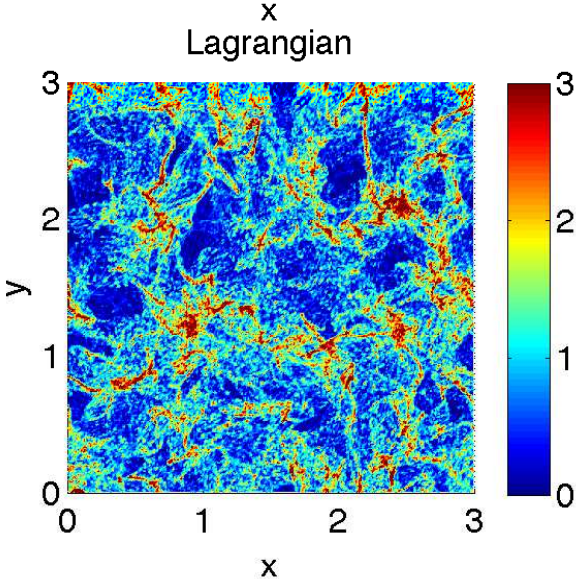
# Results - numerical comparisons on a 2D HIT

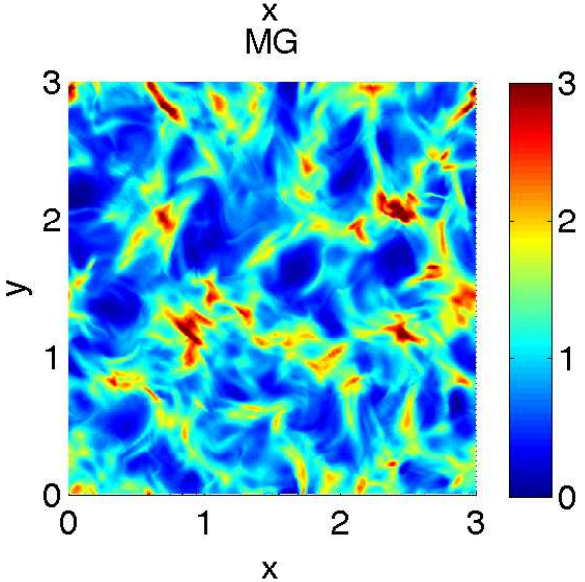
$\mathrm{St} = 5$




$\mathrm{St} = 10$




Good agreement

# Outline

# Main goal

## Eulerian Large Eddy Simulation of turbulent polydisperse two-phase flows

### Turbulence DNS and LES

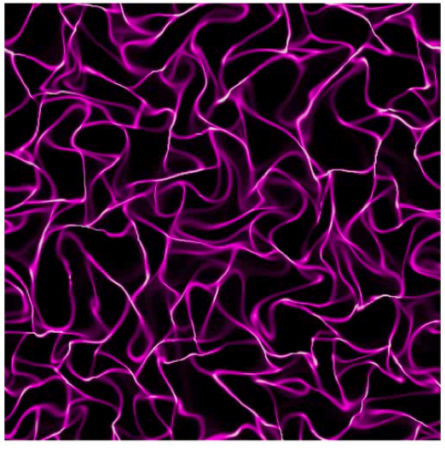
- Trajectory crossings
- Subgrid scale motion

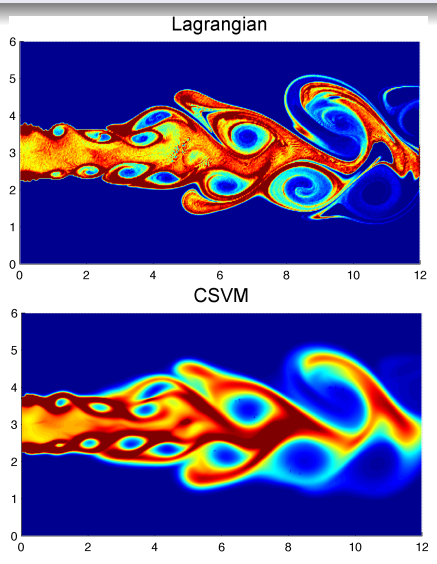
### Polydispersion

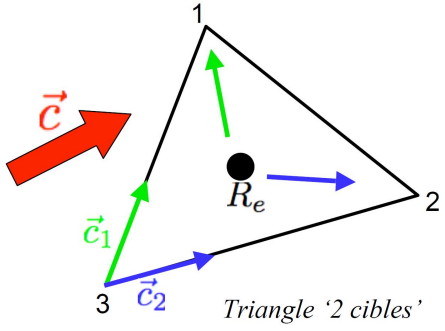
- Evaporation
- Coalescence, break-up
- Drag force
- Transport

### Numerical methods

- Realizable
- Robust
- Arbitrary elements
- High order

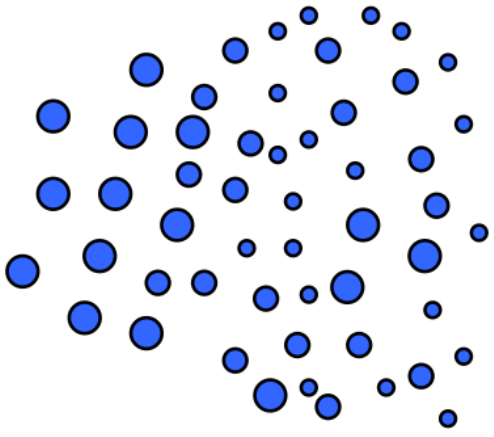





*Triangle '2 cibles'*

# Two-phase flow modeling



**Williams-Boltzmann equation for the Number Density Function (NDF)**

$$\frac{\partial f}{\partial t} + v_m \frac{\partial f}{\partial x_m} + \frac{\partial}{\partial v_m}\left(\frac{u_{g,m} - v_m}{St} f\right) = 0$$

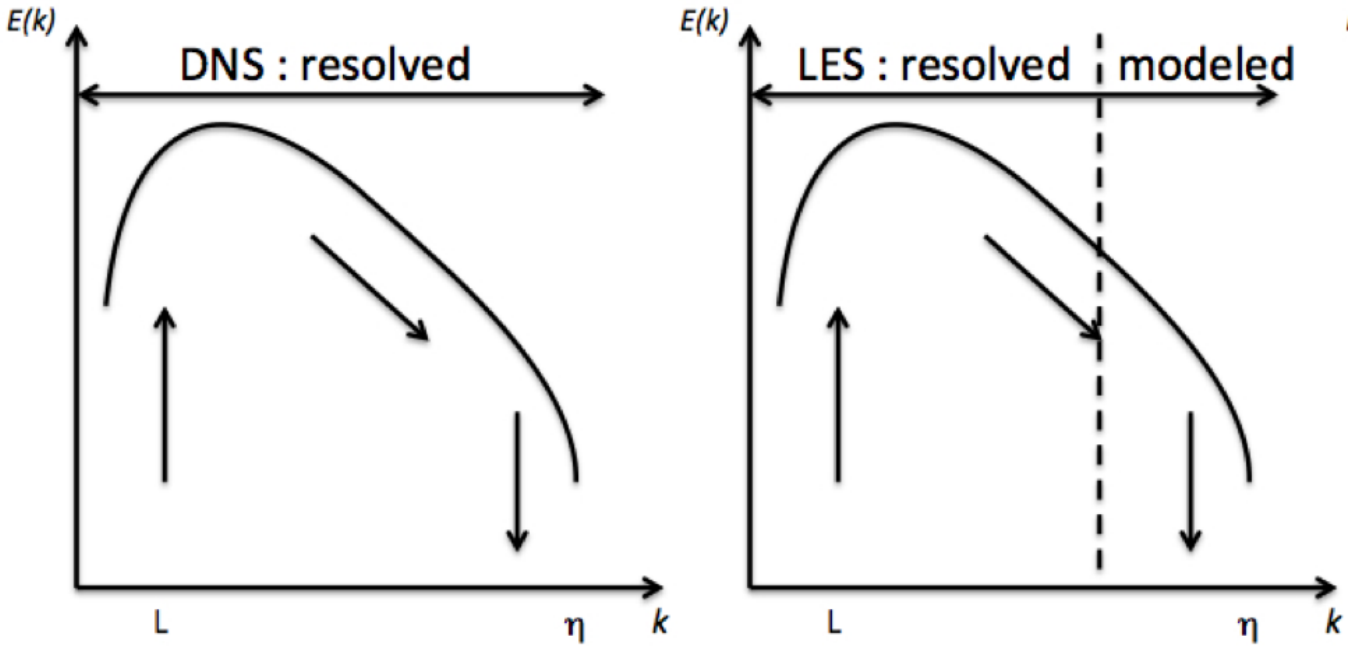
## Eulerian description

- Moments of the NDF $M_{ijk} = \int u^i v^j w^k f(t, \mathbf{x}, \mathbf{v}) \mathrm{d}\mathbf{v}$
- System of conservation equations on moments

# Large Eddy Simulation

## Why Large Eddy Simulation?

Because in industrial applications, Direct Numerical Simulations are unreachable, due to the large spectrum of size and time scales in the flow.



# Large Eddy Simulation of disperse phase flows

## The classical way: filtering at the moment level (Moreau et al. 2010)

- Integration of the WBE in velocity to obtain the moment equations (ME)
- Filtering of the moment equations

$$\textbf{WBE} \quad \frac{\partial f}{\partial t} + v_m \frac{\partial f}{\partial x_m} + \frac{\partial}{\partial v_m}\left(\frac{u_{g,m} - v_m}{St} f\right) = 0$$

$$\textbf{ME} \quad \frac{\partial M^i}{\partial t} + \frac{\partial}{\partial x}\left(M^{i+1}\right) = -\frac{i}{St}\left(M^i - u_g M^{i-1}\right)$$

$$\textbf{filtered ME} \quad \frac{\partial \overline{M}^i}{\partial t} + \frac{\partial}{\partial x}\left(\overline{M}^{i+1}\right) = -\frac{i}{St}\left(\overline{M}^i - \overline{u_g M}^{i-1}\right)$$

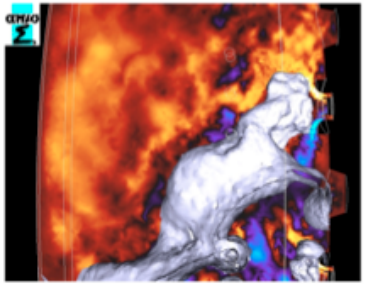
## Problem

Designing realizable numerical methods is difficult, as the structure of the resulting system of equations is difficult to determine.

# Large Eddy Simulation of disperse phase flows

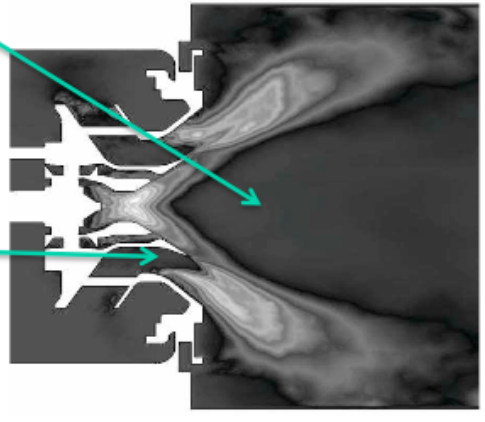
## Février, Simonin *et al.* 2002, 2005

- 1rst and trace of the 2nd order velocity moments of the NDF => moderate Stokes numbers, can handle first uncorrelated motion at the DNS level and then LES subgrid scale after filtering
- Monodisperse : $f(t, \mathbf{x}, \mathbf{u}, \cancel{\mathcal{S}}) \rightarrow f(t, \mathbf{x}, \mathbf{u})$
  (see **Vié *et al.* ICMF 2010, FTC 2012** for extension to polydisperse)
- Extended to LES of spray combustion
- Implemented in the LES solver AVBP: massively parallel computing of industrial applications (See **Boileau *et al.* 2008**)



*Spray ignition - Cerfacs*

*Kinetic energy in a multi-point gas turbine injector Jeagle 09*



- For low Stokes numbers, or very weak turbulent energy, the model does not degenerate to PGD
- Resulting shocks and δ-shocks are very delicate to handle with the standard centered schemes used for LES
- Vacuum regions cannot be treated exactly

# Large Eddy Simulation of disperse phase flows

## An other way: filtering at the kinetic level (Reeks 1991, Zaichik et al. 2009)

- Filtering of the kinetic equation
- Integration of the filtering WBE in velocity to obtain the moment equations

**WBE** $$\frac{\partial f}{\partial t} + v_m \frac{\partial f}{\partial x_m} + \frac{\partial}{\partial v_m}\left(\frac{u_{g,m} - v_m}{St} f\right) = 0$$

**filtered WBE** $$\frac{\partial \bar{f}}{\partial t} + c_p \frac{\partial \bar{f}}{\partial x} + \frac{\partial}{\partial c_p}\left[\frac{\bar{u}_g - c_p}{St} f\right] = \frac{\partial}{\partial c_p}\left[\lambda \frac{\partial \bar{f}}{\partial x} + \mu \frac{\partial \bar{f}}{\partial c_p}\right]$$

**filtered ME** $$\frac{\partial \overline{M}^i}{\partial t} + \frac{\partial}{\partial x}\left(\overline{M}^{i+1} + i\lambda \overline{M}^{i-1}\right) = -\frac{i}{St}\left(\overline{M}^i - \bar{u}_g \overline{M}^{i-1} - (i-1) St \mu \overline{M}^{i-2}\right)$$

## Good news

This method leads to an hyperbolic system of equations with source terms, with a well-defined underlying kinetic equation, really helpful to design realizable methods. PhD Macole Sabat 2015, Sabat et al 2015

# Gaussian closure and 3-equation system

$$\frac{\partial \overline{M}^i}{\partial t} + \frac{\partial}{\partial x}\left(\overline{M}^{i+1} + i\lambda \overline{M}^{i-1}\right) = -\frac{i}{St}\left(\overline{M}^i - \overline{u}_g \overline{M}^{i-1} - (i-1)St\mu \overline{M}^{i-2}\right)$$

## Closure problem

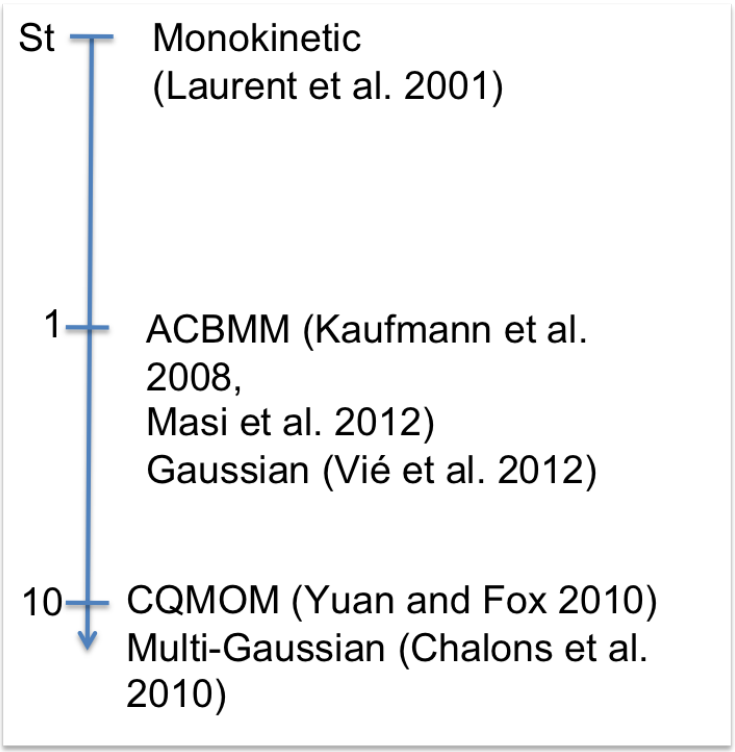
For a given set of moments $M^{0,\dots,N}$, the moment $M^{N+1}$ is needed.
Here we propose to use a Gaussian closure:

$$f(t,x,c_p) = \frac{\rho(t,x)}{\sqrt{4\pi\varepsilon(t,x)}} \exp\left(-\frac{(c_p - u(t,x))^2}{4\varepsilon(t,x)}\right)$$

for which 3 parameters are needed: $\rho$, $u$ and $\epsilon$.

## Interest of the Gaussian closure for two-phase flows

Capture primary aspects trajectory crossings that occurs in turbulent flows
Enable to simulate turbulent flows at Stokes numbers close to 1



# Gaussian closure and 3-equation system

## Euler-like system of equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$
$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + P}{\partial x} = -\frac{\rho(u - \overline{u}_g)}{St}$$
$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u E + P}{\partial x} = -\frac{\rho u(u - \overline{u}_g)}{St} - \frac{\rho(2\varepsilon - St\mu)}{St}$$

where:

$$\rho = M^0, \quad \rho u = M^1, \quad \rho E = \frac{1}{2}M^2, \quad \rho\varepsilon = M^2 - M^0 u^2, \quad P = 2\rho\varepsilon + \rho\lambda$$

**The subgrid scale influence is seen on the source terms as well as on the pressure law**

# Asymptotic behavior

Considering the expression of $\lambda$ and $\mu$:

$$\lambda = \frac{\tau_g}{St(1+St)}, \qquad \mu = \frac{\tau_g}{St(1+St)}$$

where $\tau_g$ is the subgrid scale energy of the gas phase.

## Sound speed

The sound speed tends to infinity when $St$ tends to 0:

$$c = \sqrt{6\varepsilon + 3\lambda} \underset{St \to 0}{\longrightarrow} \infty$$

**One may want to treat the acoustic part implicitly**

## Asymptotic equation on the density

For low Stokes number, we obtain a diffusion equation on the number density

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \bar{u}_g}{\partial x} = \frac{\partial}{\partial x}\left(St\lambda \frac{\partial \rho}{\partial x}\right)$$

The velocity and the internal energy are then written:

$$u = u_g - \frac{St\lambda}{\rho}\frac{\partial \rho}{\partial x}, \quad \varepsilon = \frac{St}{2}\left(\mu - \lambda \frac{\partial u}{\partial x}\right)$$

**One may want to recover the asymptotic behavior - not natural for classical schemes**

# Asymptotic behavior / model coupling

In the zones of the flow where $\tau_g = 0$ and thus $\lambda = \mu = 0$, when no particle trajectory crossing is present, we should solve for

## PGD system of equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$
$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} = -\frac{\rho(u - \bar{u}_g)}{St}$$

# Outline

# A relaxation scheme for PGD

Without the drag, the PGD system can be seen as the limit as $\eta \to +\infty$ of the system:

## Relaxed Euler system of equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$
$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + P}{\partial x} = -\frac{\rho(u - \overline{u}_g)}{St}$$
$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho E u + P u}{\partial x} = -\frac{\rho u(u - \overline{u}_g)}{St} - \eta \rho \varepsilon$$

and we solve the convective part of the pressure relaxation model taking $\eta = 0$

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + \Pi) = 0, \\ \partial_t(\rho E) + \partial_x(\rho E u + \Pi u) = 0, \\ \partial_t(\rho \Pi) + \partial_x(\rho \Pi u + a^2 u) = 0, \end{cases}$$

$$\partial_t \mathcal{V} + \partial_x \mathcal{G}(\mathcal{V}) = 0. \tag{5}$$

# A relaxation scheme for PGD

We then solve

$$\begin{cases} \partial_t \rho = 0, \\ \partial_t (\rho u) = 0, \\ \partial_t (\rho E) = 0, \\ \partial_t (\rho \Pi) = \eta \rho (p - \Pi), \end{cases}$$

in the asymptotic regime $\eta \to \infty$. The conservative variables $\rho$, $\rho u$ and $\rho E$ are thus constant, while $\Pi$ is set to be equal to $p$ in this step.

# A relaxation scheme for PGD

We now give the Riemann solution. We propose to take $a$ nonconstant in the Riemann solution and we choose to solve

$$\partial_t a + u\,\partial_x a = 0. \tag{6}$$

The diagonal form is given by

$$\begin{cases} \partial_t(\Pi + au) + (u + a\tau)\partial_x(\Pi + au) = 0, \\ \partial_t(\Pi - au) + (u - a\tau)\partial_x(\Pi - au) = 0, \\ \partial_t(\Pi + a^2\tau) + u\,\partial_x(\Pi + a^2\tau) = 0, \\ \partial_t(\varepsilon - \frac{\Pi^2}{2a^2}) + u\,\partial_x(\varepsilon - \frac{\Pi^2}{2a^2}) = 0, \\ \partial_t a + u\,\partial_x a = 0. \end{cases}$$

The quantities $(\Pi \pm au)$, respectively $(\Pi + a^2\tau)$, $(\varepsilon - \frac{\Pi^2}{2a^2})$ and $a$, are (strong) Riemann invariants for the eigenvalues $u \pm a\tau$, resp. $u$.

# A relaxation scheme for PGD

The self-similar Riemann solution $(x,t) \mapsto \mathcal{V}(x/t; \mathcal{V}_L, \mathcal{V}_R; a_L, a_R)$ and initial data

$$\mathcal{V}(x, t=0) = \begin{cases} \mathcal{V}_L & \text{if} \quad x < 0, \\ \mathcal{V}_R & \text{if} \quad x > 0, \end{cases}$$

is made of four constant states $\mathcal{V}_L, \mathcal{V}_L^*, \mathcal{V}_R^*$ and $\mathcal{V}_R$, separated by three contact discontinuities associated with $\lambda_k = \lambda_k(\mathcal{V})$, $k = 1, 2, 3$ and propagating with speeds denoted by $\lambda(\mathcal{V}_L, \mathcal{V}_L^*)$, $\lambda(\mathcal{V}_L^*, \mathcal{V}_R^*)$ and $\lambda(\mathcal{V}_R^*, \mathcal{V}_R)$. More precisely, we have

$$\mathcal{V}(\frac{x}{t}; \mathcal{V}_L, \mathcal{V}_R) = \begin{cases} \mathcal{V}_L & \text{if} \quad \frac{x}{t} < \lambda(\mathcal{V}_L, \mathcal{V}_L^*), \\ \mathcal{V}_L^* & \text{if} \quad \lambda(\mathcal{V}_L, \mathcal{V}_L^*) < \frac{x}{t} < \lambda(\mathcal{V}_L^*, \mathcal{V}_R^*), \\ \mathcal{V}_R^* & \text{if} \quad \lambda(\mathcal{V}_L^*, \mathcal{V}_R^*) < \frac{x}{t} < \lambda(\mathcal{V}_R^*, \mathcal{V}_R), \\ \mathcal{V}_R & \text{if} \quad \lambda(\mathcal{V}_R^*, \mathcal{V}_R) < \frac{x}{t}. \end{cases}$$

# A relaxation scheme for PGD

The intermediate states $\mathcal{V}_L^*, \mathcal{V}_R^*$, as well as the speeds of propagation, are determined and yield: $\lambda(\mathcal{V}_L, \mathcal{V}_L^*) = \lambda_1(\mathcal{V}_L) = u_L - a_L\tau_L$, $\lambda(\mathcal{V}_L^*, \mathcal{V}_R^*) = u^*$, $\lambda(\mathcal{V}_R^*, \mathcal{V}_R) = \lambda_3(\mathcal{V}_R) = u_R + a_R\tau_R$ and

$$u_L^* = u_R^* = u^* = \frac{a_L u_L + a_R u_R + \Pi_L - \Pi_R}{a_L + a_R},$$

$$\Pi_L^* = \Pi_R^* = \frac{a_R\Pi_L + a_L\Pi_R - a_L a_R(u_R - u_L)}{a_L + a_R},$$

$$\frac{1}{\rho_L^*} = \frac{1}{\rho_L} + \frac{a_R(u_R - u_L) + \Pi_L - \Pi_R}{a_L(a_L + a_R)}, \quad \frac{1}{\rho_R^*} = \frac{1}{\rho_R} + \frac{a_L(u_R - u_L) + \Pi_R - \Pi_L}{a_R(a_L + a_R)},$$

$$\varepsilon_L^* = \varepsilon_L - \frac{\Pi_L^2}{2a_L^2} + \frac{\Pi^{*2}}{2a_L^2}, \quad \varepsilon_R^* = \varepsilon_R - \frac{\Pi_R^2}{2a_R^2} + \frac{\Pi^{*2}}{2a_R^2}.$$

At this stage, the initial states $\mathcal{V}_L$ and $\mathcal{V}_R$ and more precisely the free parameters $a_L$ and $a_R$ are implicitly assumed to be such that the waves in the Riemann solutions are ordered as they should, namely

$$\lambda_1(\mathcal{V}_L) = u_L - \frac{a_L}{\rho_L} < u^\star < \lambda_3(\mathcal{V}_R) = u_R + \frac{a_R}{\rho_R}. \tag{7}$$

# A relaxation scheme for PGD

Following Bouchut (2004), we define $a_L = a_L(\mathcal{V}_L)$ and $a_R = a_R(\mathcal{V}_R)$ as follows:
if $p_R \geq p_L$

$$\frac{a_L}{\rho_L} = \max(c_L, c_{min}) + \alpha\left(\frac{p_R - p_L}{\rho_R c_R} + u_L - u_R\right)_+,$$

$$\frac{a_R}{\rho_R} = \max(c_R, c_{min}) + \alpha\left(\frac{p_L - p_R}{a_L} + u_L - u_R\right)_+,$$

if $p_R \leq p_L$

$$\frac{a_R}{\rho_R} = \max(c_R, c_{min}) + \alpha\left(\frac{p_L - p_R}{\rho_L c_L} + u_L - u_R\right)_+,$$

$$\frac{a_L}{\rho_L} = \max(c_L, c_{min}) + \alpha\left(\frac{p_R - p_L}{a_R} + u_L - u_R\right)_+,$$

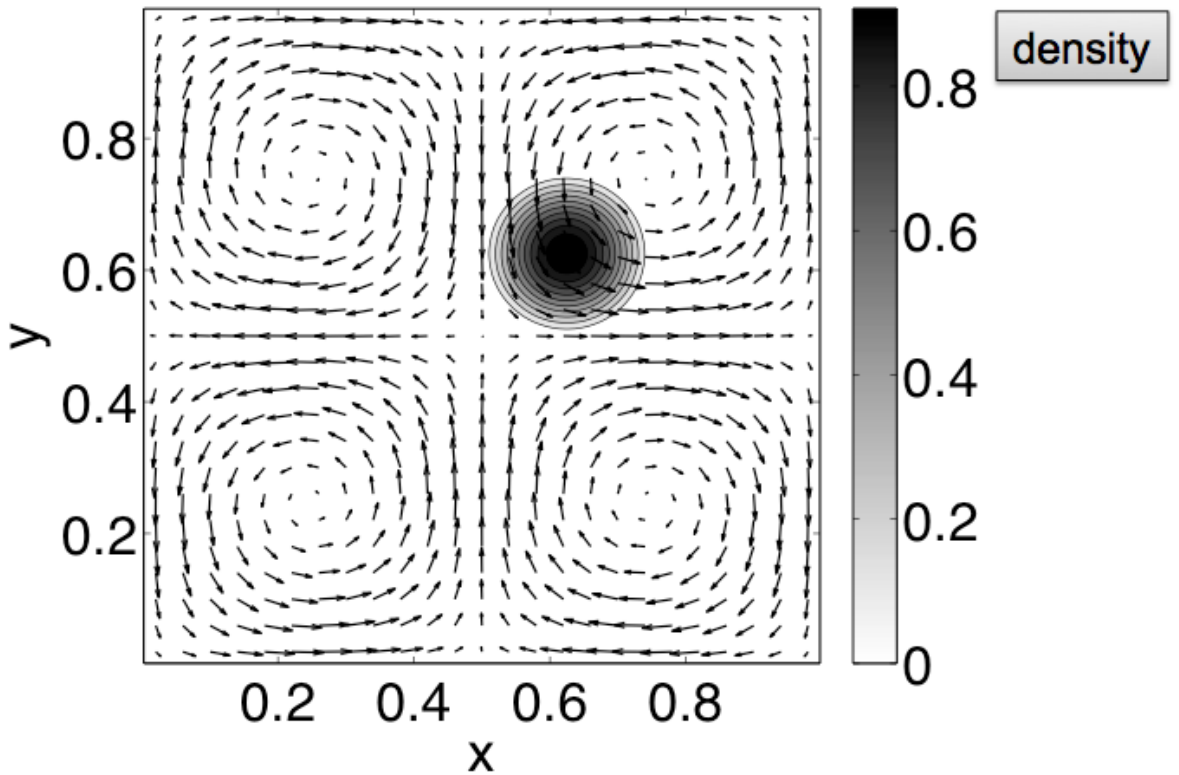
with $\alpha = (\gamma + 1)/2$, $c_{min} > 0$ and where $p_{L,R} = p_{L,R}(\mathcal{U}_{L,R})$, $c_{L,R} = c_{L,R}(\mathcal{U}_{L,R})$.

First, it is shown to fullfil (7) and to give the positivy of the intermediate densities $\rho_L^*$ and $\rho_R^*$. Then, it complies with the sub-characteristic condition $a > \rho c$. At last, it guarantees the nonlinear stability of the underlying relaxation scheme that will be described in the following, and the possibility of handling vacuum in the sense that the speeds of propagation $\lambda_1(\mathcal{V}_L)$ and $\lambda_3(\mathcal{V}_R)$ remain finite. Discrete entropy inequalities as well as maximum principles can be proved.

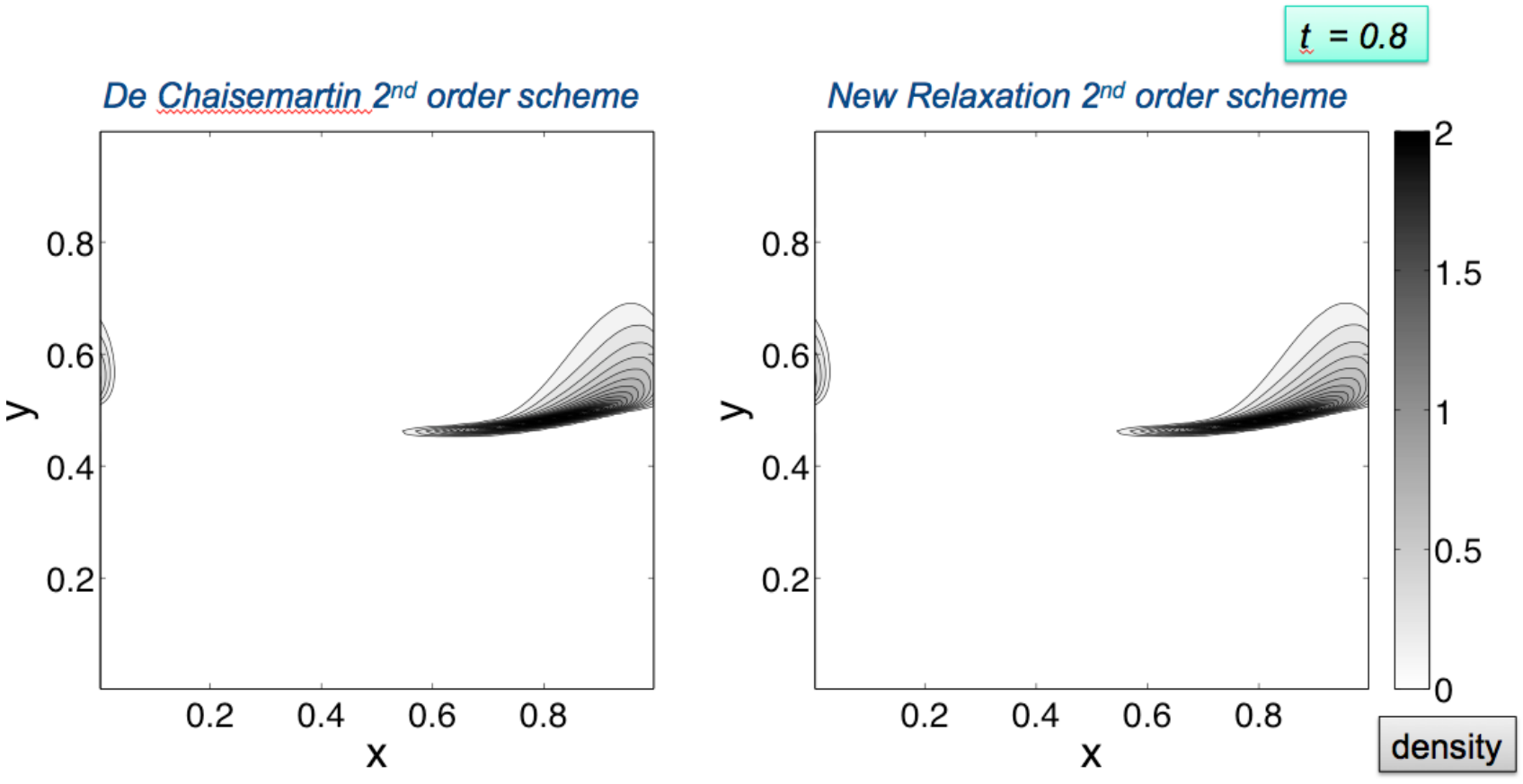
# A relaxation scheme for PGD : Results

$t = 0$

*Taylor-Green vortices of the gaseous flow and initial droplet distribution*



# A relaxation scheme for PGD : Results



# A Hybrid model and related relaxation scheme

It is important to notice that the same formalism will be used for both systems. Just note that in the pressureless case, $E$ must be understood as a function of the unknowns $\rho$ and $\rho u$, namely

$$E = \frac{(\rho u)^2}{2\rho},$$

but not as an unknown with evolution given by the passive transport equation

$$\partial_t \rho E + \partial_x (\rho E u) = 0.$$

We use a Godunov scheme for the first step before projection:

$$\mathcal{V}_j^{n+1-} = \mathcal{V}_j^n - \frac{\Delta t}{\Delta x}(g(\mathcal{V}_j^n, \mathcal{V}_{j+1}^n) - g(\mathcal{V}_{j-1}^n, \mathcal{V}_j^n)),$$

$$j \in \mathbb{Z}, \quad n \geq 0,$$

where the numerical flux function writes for all $j \in \mathbb{Z}$

$$g(\mathcal{V}_j^n, \mathcal{V}_{j+1}^n) = \mathcal{G}\Big(\mathcal{V}\big(0; \mathcal{V}_j^n, \mathcal{V}_{j+1}^n; a_L(\mathcal{V}_j^n), a_R(\mathcal{V}_{j+1}^n)\big)\Big). \tag{8}$$

Let us recall that the numerical flux (8) is here explicitly known.

# A Hybrid model and related relaxation scheme

We set for all $j \in \mathbb{Z}$

$$\mathcal{V}_j^{n+1} = \begin{pmatrix} \mathcal{U}_j^{n+1} \\ (\rho\Pi)_j^{n+1} \end{pmatrix} \tag{9}$$

with

$$\mathcal{U}_j^{n+1} = \mathcal{U}_j^{n+1-} \quad \text{and} \quad (\rho\Pi)_j^{n+1} = p(\mathcal{U}_j^{n+1})$$

in the case of the gas dynamics equations, and

$$\mathcal{U}_j^{n+1} = (\rho, \rho u, \frac{(\rho u)^2}{2\rho})_j^{n+1-} \quad \text{and} \quad (\rho\Pi)_j^{n+1} = 0$$

in the pressureless case. This is equivalent to solve in the asymptotic regime $\eta = +\infty$

$$\begin{cases} \partial_t \rho = 0, \\ \partial_t(\rho u) = 0, \\ \partial_t(\rho E) = 0, \\ \partial_t(\rho\Pi) = -\eta\rho(p - \Pi), \end{cases} \tag{10}$$

in the case of the gas dynamics equations, and for PGD:

$$\begin{cases} \partial_t \rho = 0, \\ \partial_t(\rho u) = 0, \\ \partial_t(\rho E) = -\eta\rho\varepsilon, \\ \partial_t(\rho\Pi) = -\eta\rho(p - \Pi), \end{cases} \tag{11}$$

# A Hybrid model and related relaxation scheme

Recall that the conservative unknowns are $\rho$, $\rho u$ and $\rho E$ for the gas dynamics and $\rho$ and $\rho u$ for the PGD. The main difference then clearly lies in the treatment of the energy equation.

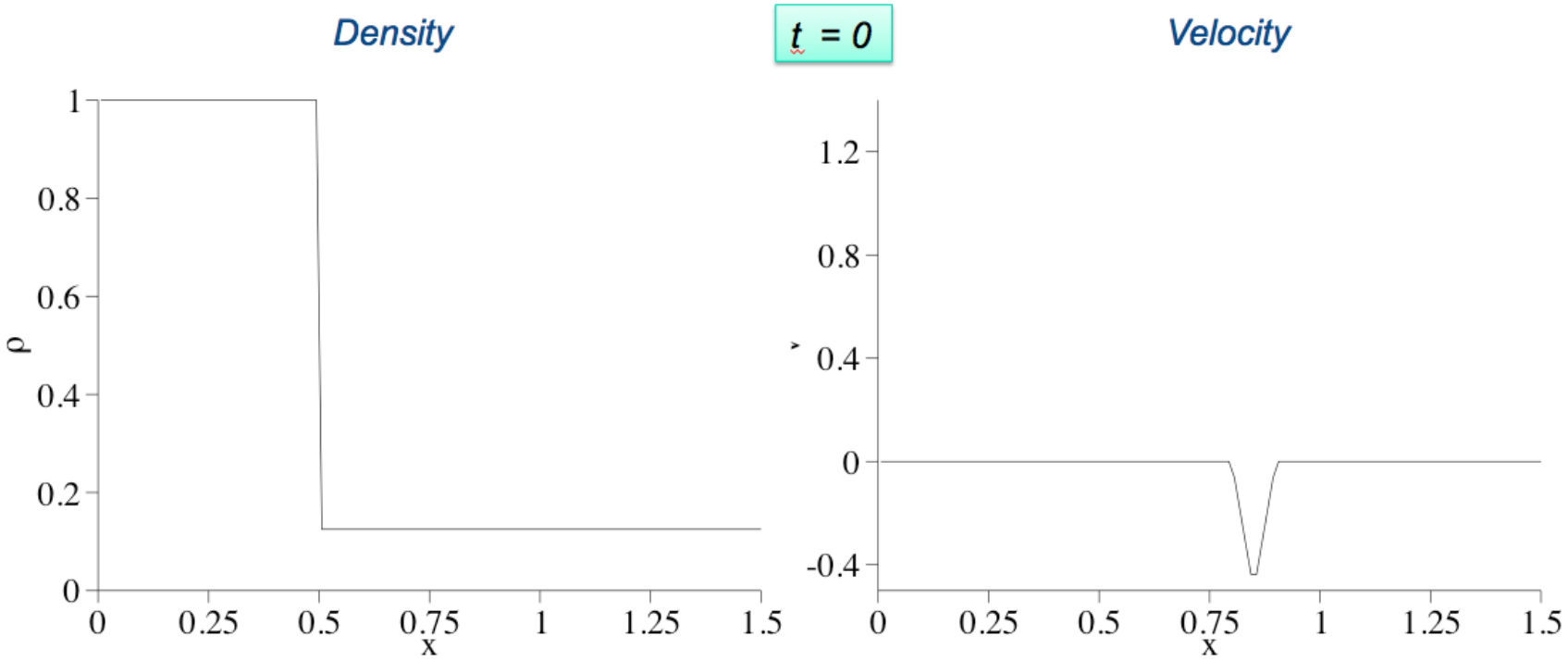
For the sake of clarity, we begin by introducing a color function $Y$ such that $Y = 1$ for gas dynamics and $Y = 0$ for PGD. From a numerical point of view, a given cell $C_j^n$ is said to be *pressureless*, $Y_j^n = 0$, if the internal energy $\varepsilon_j^n = (\rho E - \frac{(\rho u)^2}{2\rho})_j^n$ is less than a given threshold $\varepsilon_{min}$, and *with pressure*, $Y_j^n = 1$, otherwise.

In agreement with the threshold $c_{min}$ already introduced for the sound speed in the definition of $a_L$ and $a_R$, we set

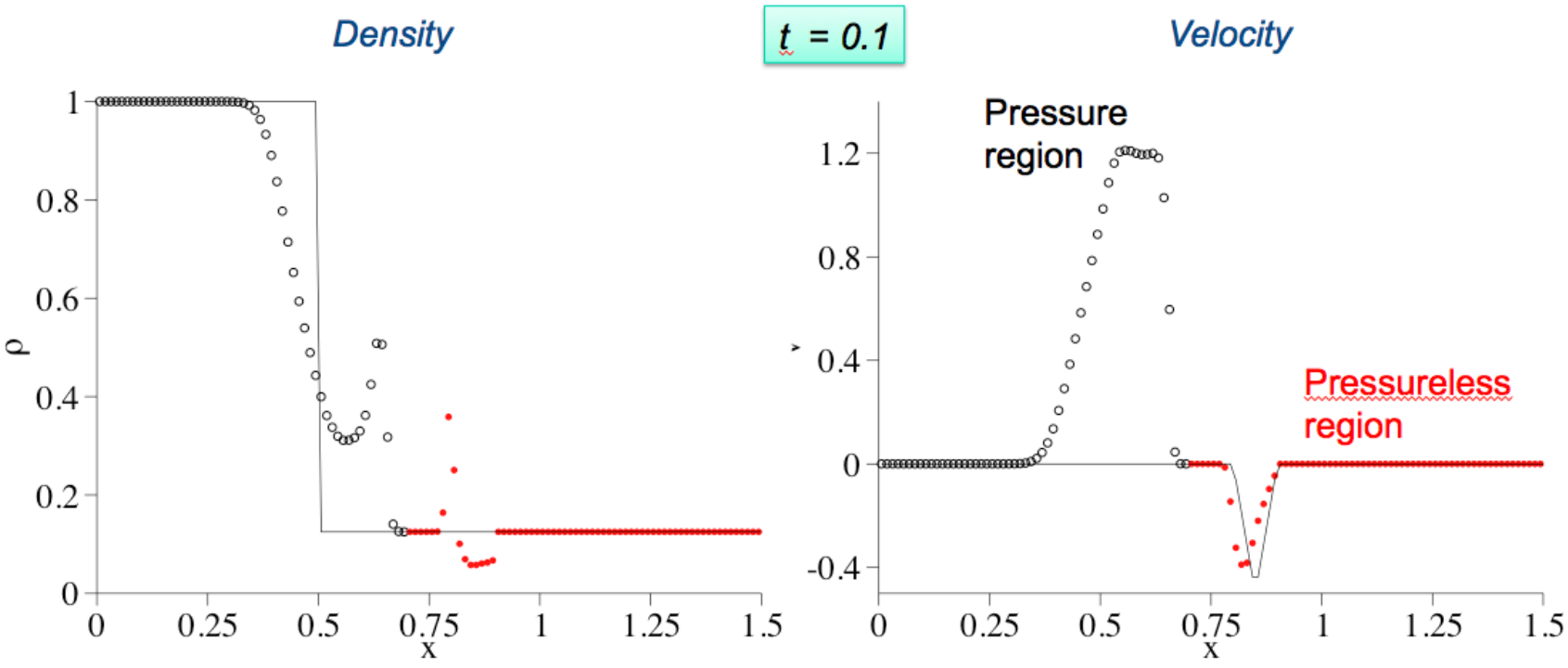
$$\varepsilon_{min} = \frac{c_{min}^2}{\gamma(\gamma - 1)}. \tag{12}$$

We thus distinguish between zones with PGD where the internal energy is exactly zero and zones where the energy level is above the defined small threshold, a property which is preserved by the pure convective part of the evolution.

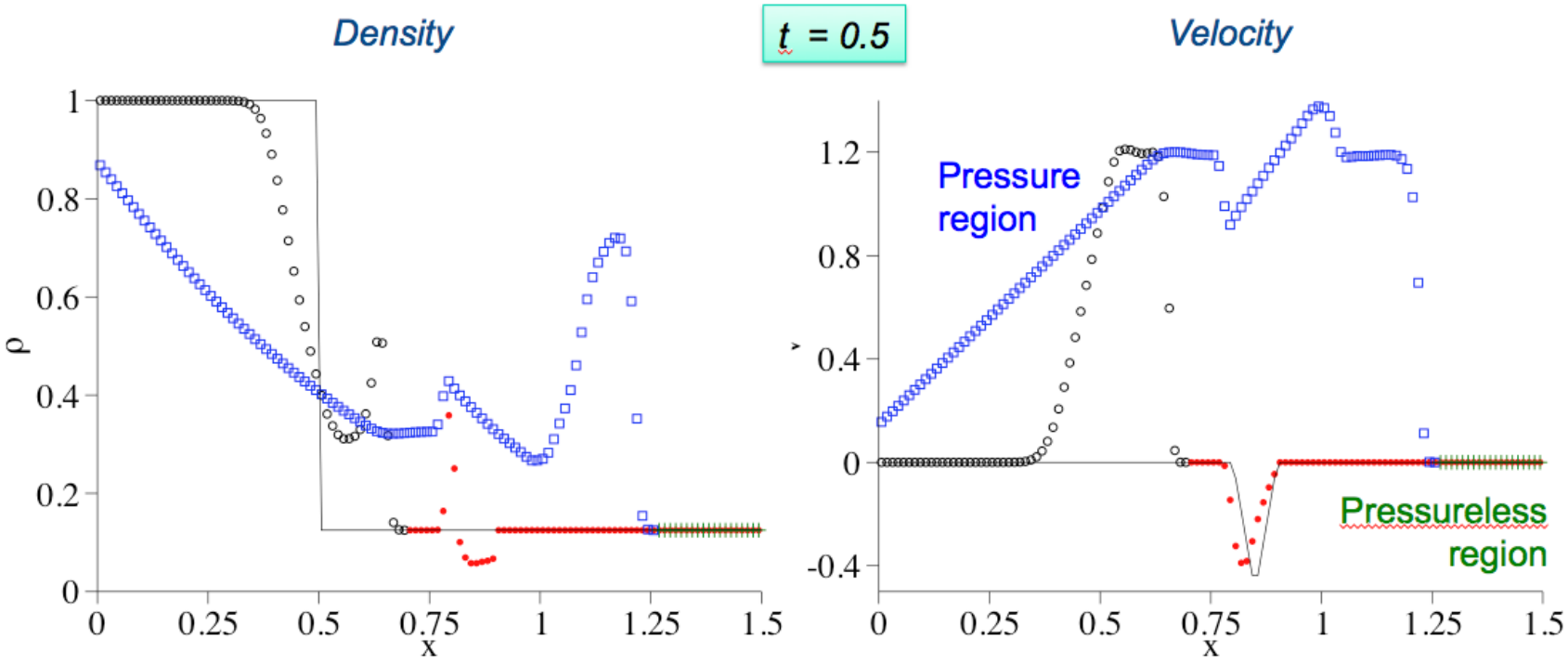
# A Hybrid model and related relaxation scheme : Results



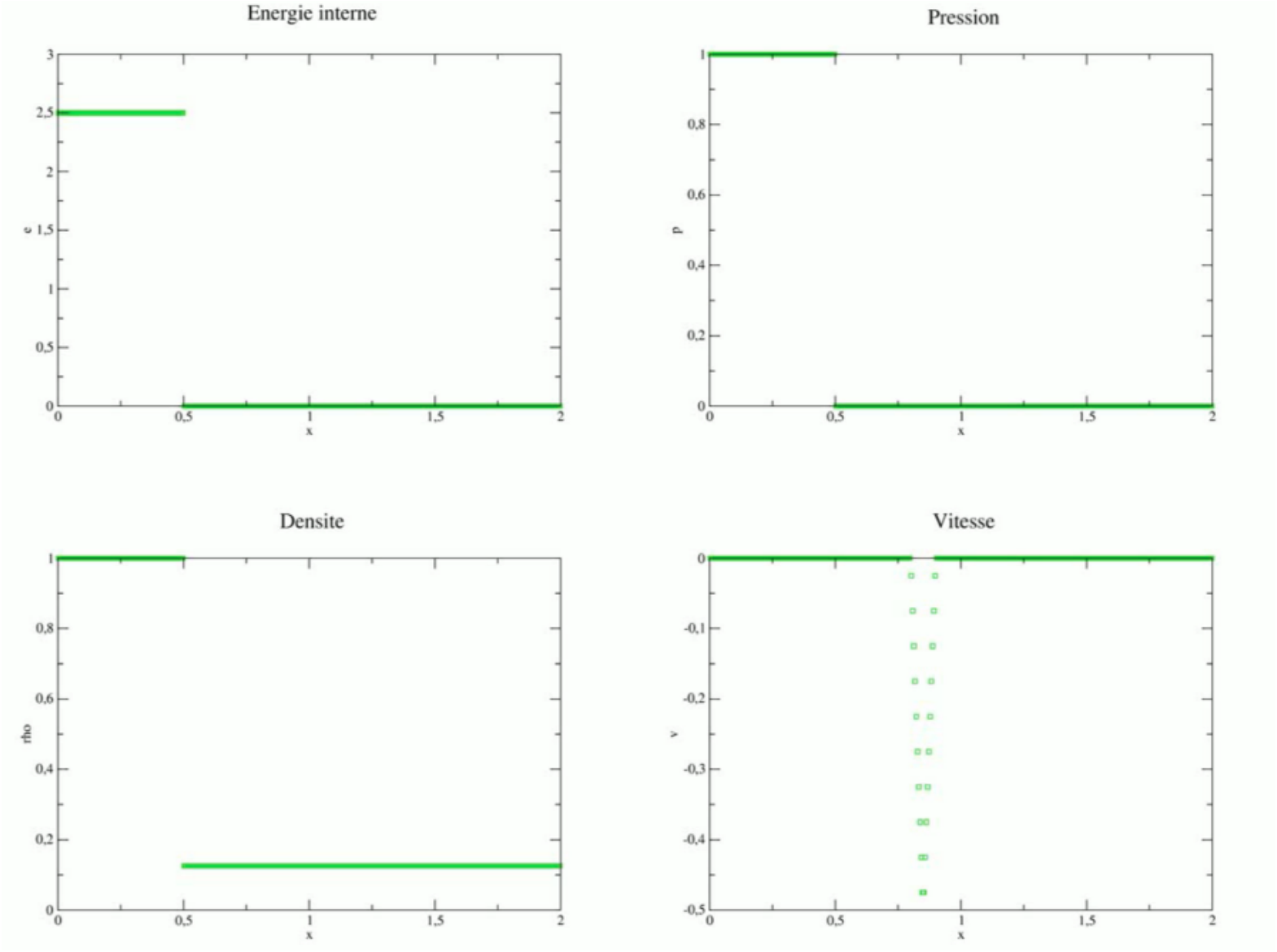
# A Hybrid model and related relaxation scheme : Results



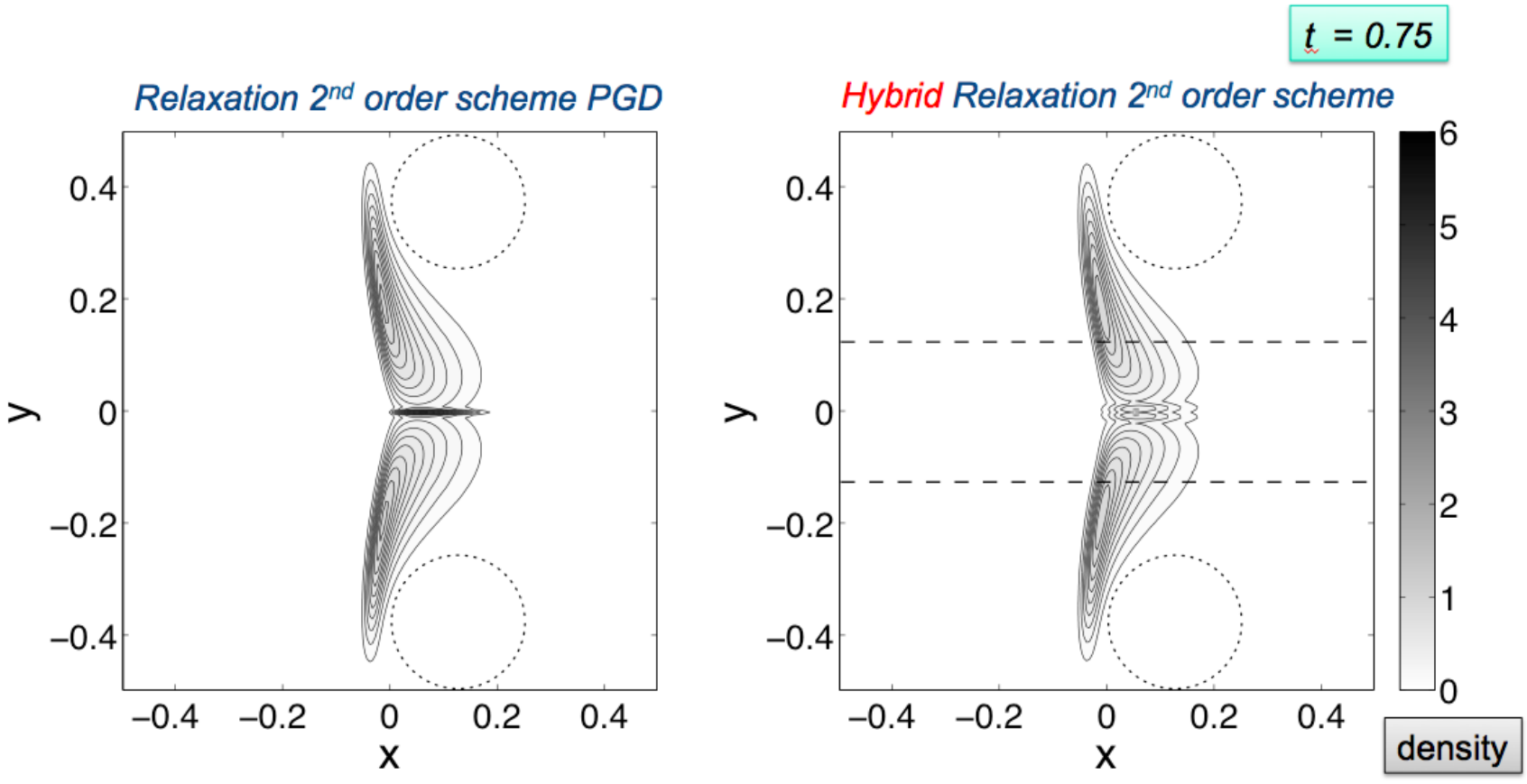
# A Hybrid model and related relaxation scheme : Results



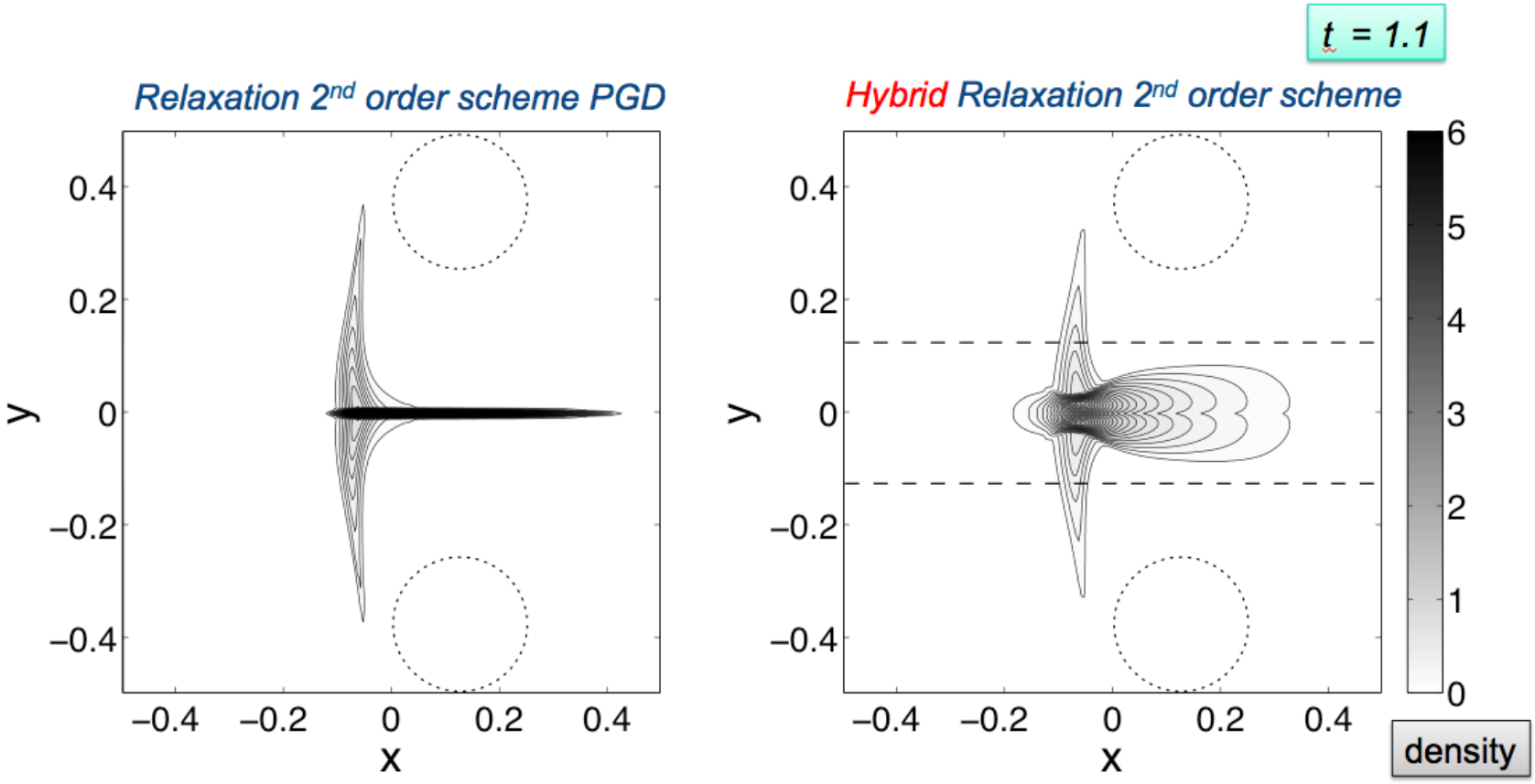
# A Hybrid model and related relaxation scheme : Results



# A Hybrid model and related relaxation scheme : Results

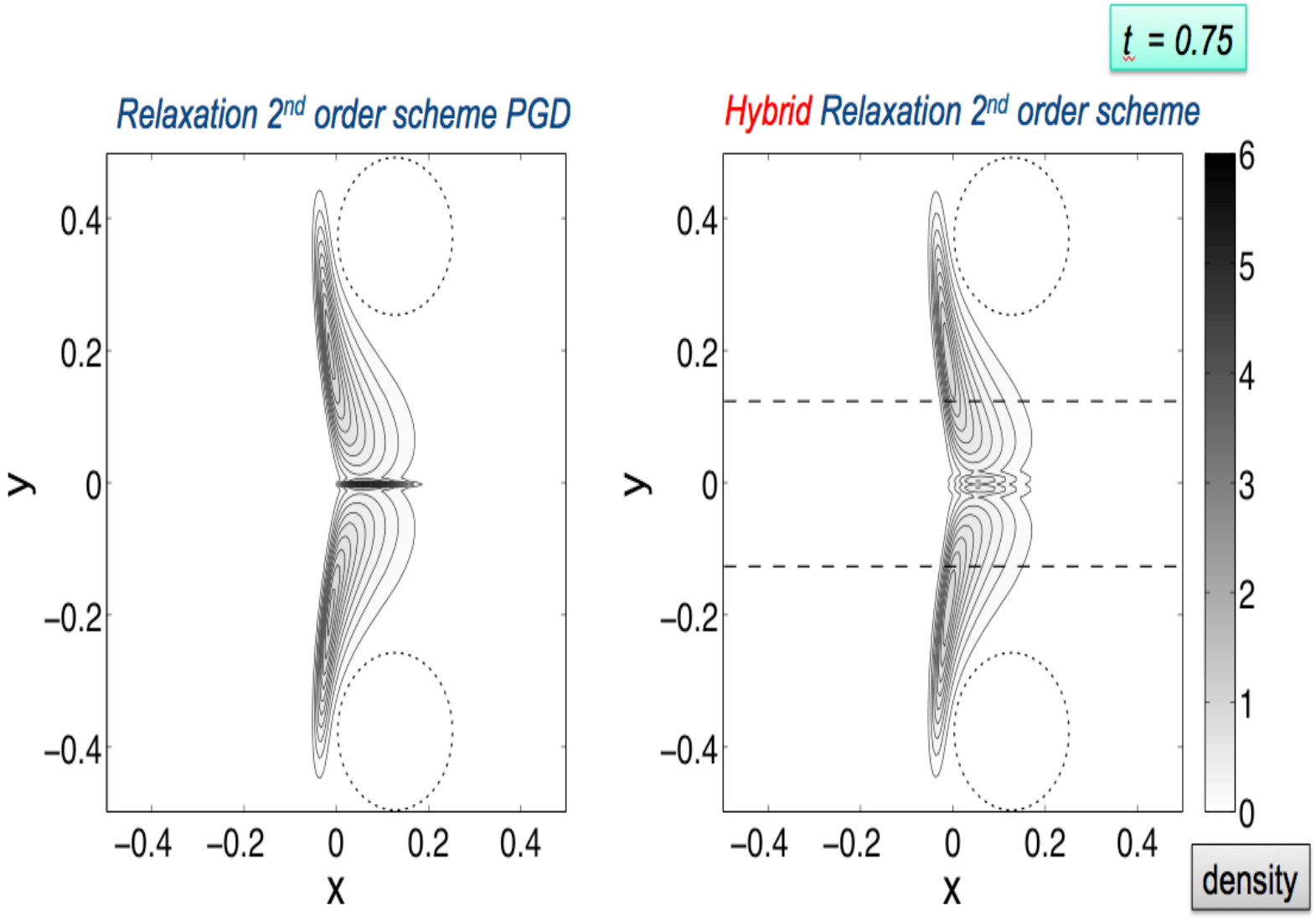


# A Hybrid model and related relaxation scheme : Results



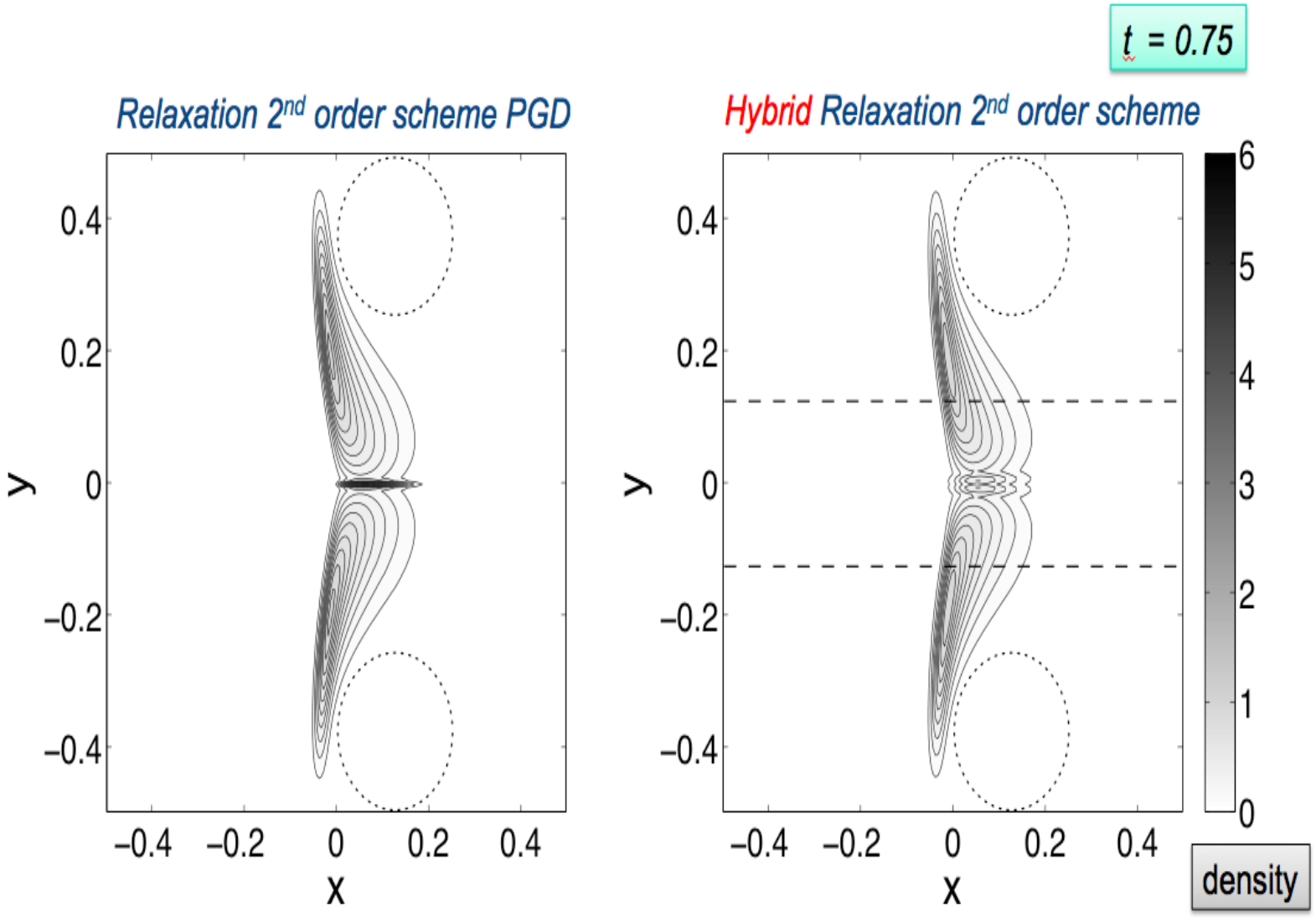
# A Hybrid model and related relaxation scheme : Results

Pressureless gas dynamics: no subgrid energy source



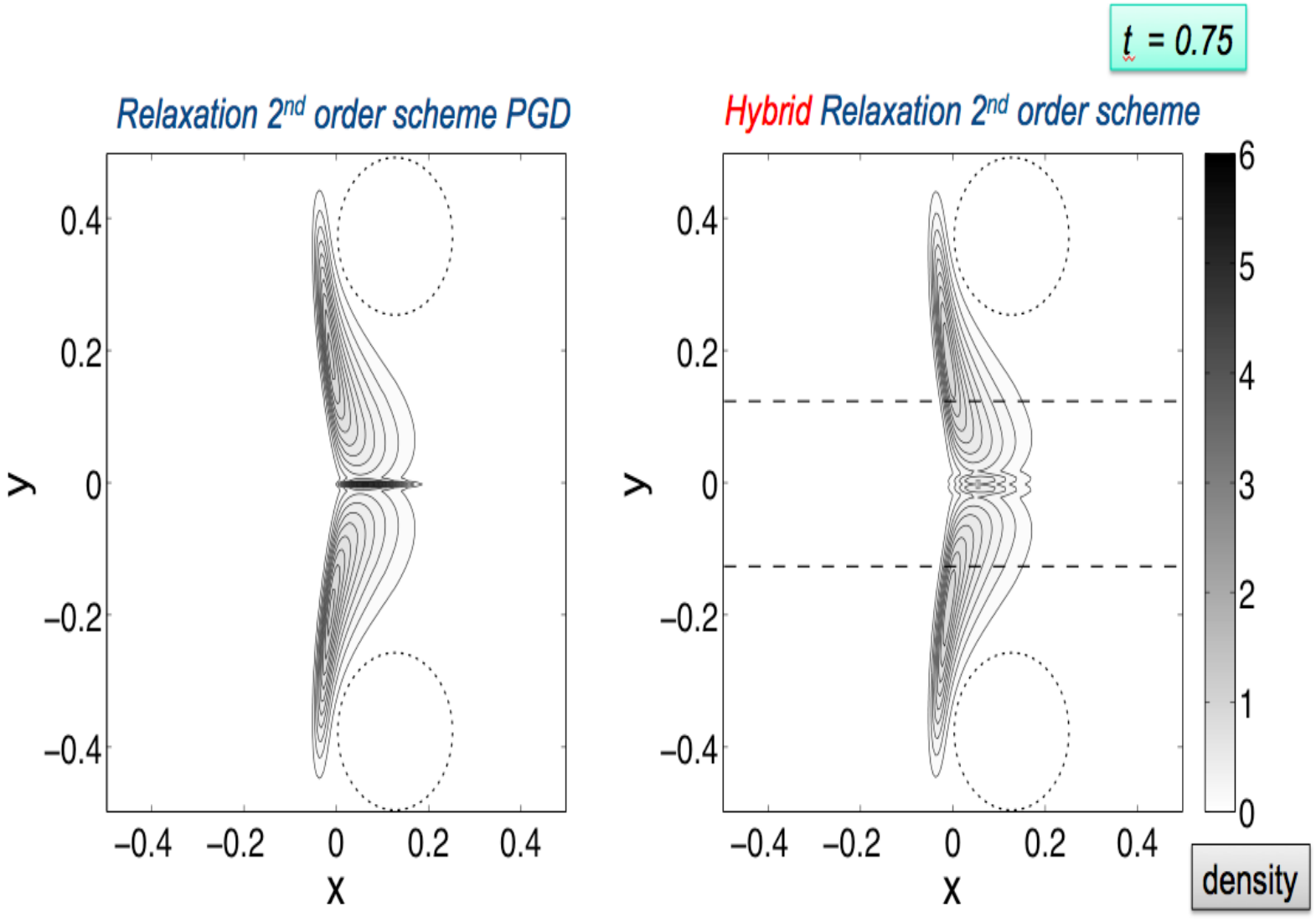
# A Hybrid model and related relaxation scheme : Results

Hybrid scheme: subgrid energy source in the center layer



# A Hybrid model and related relaxation scheme : Results

Hybrid scheme: subgrid energy source in the center layer

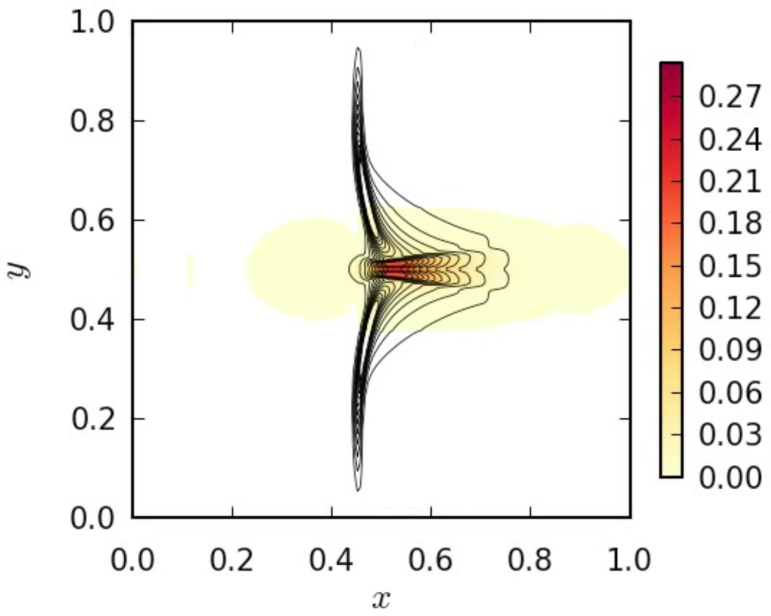


# A Hybrid model and related relaxation scheme

Hybrid scheme: original way of coupling pressureless and gas dynamics

(or high order KBMM - AG)

with accurate transport of number density and velocity




Boileau, Chalons, Massot, SIAM SISC, 2015 - HAL

# Outline

# Gaussian closure and 3-equation system

## Euler-like system of equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0$$
$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2 + P}{\partial x} = -\frac{\rho(u - \overline{u}_g)}{St}$$
$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u E + P}{\partial x} = -\frac{\rho u(u - \overline{u}_g)}{St} - \frac{\rho(2\varepsilon - St\,\mu(St))}{St}$$

where:

$$\rho = M^0, \quad \rho u = M^1, \quad \rho E = \frac{1}{2}M^2, \quad \rho\varepsilon = M^2 - M^0 u^2, \quad P = 2\rho\varepsilon + \rho\lambda(St)$$

**The subgrid scale influence is seen on the source terms as well as on the pressure law**

# Asymptotic behavior

Considering the expression of $\lambda$ and $\mu$:

$$\lambda = \frac{\tau_g}{St(1+St)}, \qquad \mu = \frac{\tau_g}{St(1+St)}$$

where $\tau_g$ is the subgrid scale energy of the gas phase.

## Sound speed

The sound speed tends to infinity when $St$ tends to 0:

$$c = \sqrt{6\varepsilon + 3\lambda} \underset{St \to 0}{\longrightarrow} \infty$$

**One may want to treat the acoustic part implicitly**

## Asymptotic equation on the density

For low Stokes number, we obtain a diffusion equation on the number density

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \bar{u}_g}{\partial x} = \frac{\partial}{\partial x}\left(St\lambda \frac{\partial \rho}{\partial x}\right)$$

The velocity and the internal energy are then written:

$$u = u_g - \frac{St\lambda}{\rho}\frac{\partial \rho}{\partial x}, \quad \varepsilon = \frac{St}{2}\left(\mu - \lambda \frac{\partial u}{\partial x}\right)$$

**One may want to recover the asymptotic behavior - not natural for classical schemes**

# An Asymptotic-Preserving Relaxation scheme

## Main ingredients of the numerical scheme

Chalons, Girardin and Kokh, 2014 SISC

- Lagrange-Projection Coquel and al., 2010
- Relaxation strategy Chalons and Coquel, 2005
- HLLC scheme with source terms Gallice 2003, Chalons et al. 2010

# Lagrange-Projection

## Principles

Idea: Separate the acoustic waves from the transport velocity
Design principle: Splitting of the fluxes

Lagrangian step: implicit or explicit step

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial u}{\partial x} = 0$$
$$\frac{\partial \rho u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \frac{\partial P}{\partial x} = -\frac{\rho(u - \bar{u}_g)}{St}$$
$$\frac{\partial \rho E}{\partial t} + \rho E \frac{\partial u}{\partial x} + \frac{\partial P u}{\partial x} = -\frac{\rho u(u - \bar{u}_g)}{St} - \frac{\rho(2\varepsilon - St\mu)}{St}$$

Transport step: explicit step

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} = 0$$
$$\frac{\partial \rho u}{\partial t} + u \frac{\partial \rho u}{\partial x} = 0$$
$$\frac{\partial \rho E}{\partial t} + u \frac{\partial \rho E}{\partial x} = 0$$

The lagrangian step is written in lagrangian coordinates $\tau = 1/\rho$ and $\tau \partial_x = \partial_m$

$$\frac{\partial \tau}{\partial t} - \frac{\partial u}{\partial m} = 0$$
$$\frac{\partial u}{\partial t} + \frac{\partial P}{\partial m} = -\frac{(u - \bar{u}_g)}{St}$$
$$\frac{\partial E}{\partial t} + \frac{\partial P u}{\partial m} = -\frac{u(u - \bar{u}_g)}{St} - \frac{(2\varepsilon - St\mu)}{St}$$

# Relaxation strategy

## Principles

Idea: Deal with a larger system but with a simpler structure, avoiding non-linearities

Design principle: Consider P as a new unknown of the system that we denote $\Pi$

At the beginning of each time step, we impose that $\Pi = p$:

$$\frac{\partial \tau}{\partial t} - \frac{\partial u}{\partial m} = 0$$
$$\frac{\partial u}{\partial t} + \frac{\partial \Pi}{\partial m} = -\frac{(u - \overline{u}_g)}{St}$$
$$\frac{\partial E}{\partial t} + \frac{\partial \Pi u}{\partial m} = -\frac{u(u - \overline{u}_g)}{St} - \frac{(2\varepsilon - St\mu)}{St}$$
$$\frac{\partial \Pi}{\partial t} + a^2 \frac{\partial \Pi}{\partial m} = 0$$

where $a > \rho c$.

Adding the change of variable $w^{\pm} = \Pi \pm au$:

$$\frac{\partial \tau}{\partial t} - \frac{\partial u}{\partial m} = 0$$
$$\frac{\partial w^+}{\partial t} + a \frac{\partial w^+}{\partial m} = -\frac{(u - \overline{u}_g)}{St}$$
$$\frac{\partial w^-}{\partial t} - a \frac{\partial w^-}{\partial m} = \frac{(u - \overline{u}_g)}{St}$$
$$\frac{\partial E}{\partial t} + \frac{\partial \Pi u}{\partial m} = -\frac{u(u - \overline{u}_g)}{St} - \frac{(2\varepsilon - St\mu)}{St}$$

# HLLC with source terms

## Principles

Idea: Tacking into account the source terms in the intermediate state of the HLLC scheme

Design principle: the source term is evaluated at the interfaces, instead of the cell centers

$$\partial_t \mathbf{U} + \partial_x \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U})$$

where:

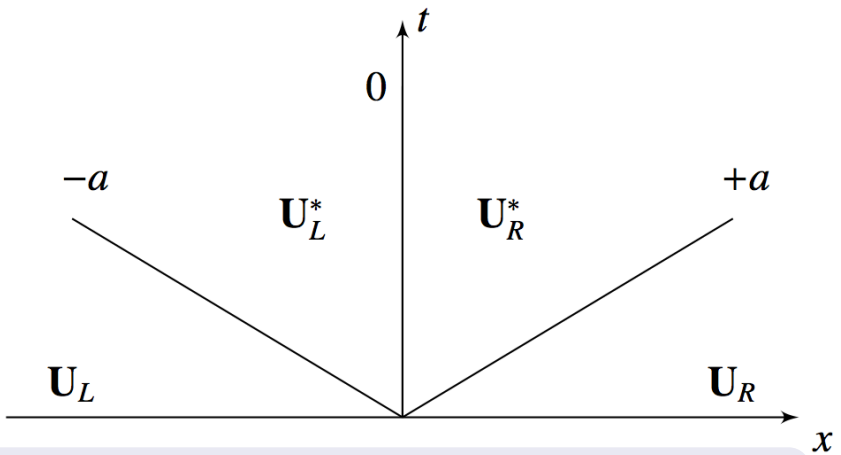
$$\mathbf{U} = \left(\tau, \overrightarrow{w}, \overleftarrow{w}, E\right)^T, \qquad \mathbf{F}(\mathbf{U}) = \left(u, a\overrightarrow{w}, -a\overleftarrow{w}, \Pi u\right)^T,$$

$$\mathbf{S}(\mathbf{U}) = \left(0, -\frac{u-\overline{u}_g}{\mathrm{St}}, \frac{u-\overline{u}_g}{\mathrm{St}}, -u\frac{u-\overline{u}_g}{\mathrm{St}} - \frac{2\epsilon - \mathrm{St}\mu}{\mathrm{St}}\right)^T$$

# HLLC scheme with source terms

## Four-state approximation

$$\mathbf{W}(\frac{m}{t};\mathbf{U}_L,\mathbf{U}_R) = \begin{cases} \mathbf{U}_L, & \frac{m}{t} < -a \\ \mathbf{U}_L^*, & -a < \frac{m}{t} < 0 \\ \mathbf{U}_R^*, & 0 < \frac{m}{t} < a \\ \mathbf{U}_R, & \frac{m}{t} > a \end{cases}$$




## Consistency in the integral sense with source terms

$$\int_{-\Delta x/2}^{\Delta x/2} \mathbf{W}(x;\mathbf{U}_L,\mathbf{U}_R)dx = \frac{\Delta x}{2}(\mathbf{U}_L+\mathbf{U}_R) - \Delta t(\mathbf{F}_L+\mathbf{F}_R) + \Delta t\Delta x\tilde{\mathbf{S}}(\mathbf{U}_L,\mathbf{U}_R)$$

where:

$$\lim_{\substack{\mathbf{U}_L,\mathbf{U}_R \to \mathbf{U} \\ \Delta t,\Delta x \to 0}} \tilde{\mathbf{S}}(\Delta x,\Delta t;\mathbf{U}_L,\mathbf{U}_R) = \mathbf{S}(\mathbf{U})$$

## Using Rankine-Hugoniot relationships, all the states are defined

# Final scheme

$$\mathbf{U}_j^{n+1} = \mathbf{U}_j^n - \frac{\Delta t}{\Delta m_j}\left(\mathbf{F}_{j+1/2}^n - \mathbf{F}_{j-1/2}^n\right) + \frac{\Delta t}{2}\left(\frac{\Delta m_{j+1/2}}{\Delta m_j}\mathbf{S}_{j+1/2}^n + \frac{\Delta m_{j-1/2}}{\Delta m_j}\mathbf{S}_{j-1/2}^n\right) + \Delta t \mathbf{S}_j^{E-n}$$

where:

$$\mathbf{F}_{j+1/2}^n = \begin{pmatrix} u_{j+1/2}^* \\ a w_{j+1/2}^{+,*} \\ -a w_{j+1/2}^{-,*} \\ p_{j+1/2}^* u_{j+1/2}^* \end{pmatrix}, \quad \mathbf{S}_{j+1/2}^n = \begin{pmatrix} 0 \\ -\frac{a}{\mathrm{St}}\left(u_{j+1/2}^* - \overline{u}_g\right) \\ \frac{a}{\mathrm{St}}\left(u_{j+1/2}^* - \overline{u}_g\right) \\ \frac{-u_{j+1/2}^*}{\mathrm{St}}\left(u_{j+1/2}^* - \overline{u}_g\right) \end{pmatrix}, \quad \mathbf{S}_j^{E-n} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{1}{\mathrm{St}}\left(2\epsilon_j^n - \mathrm{St}\mu\right) \end{pmatrix}$$

$$u_{j+1/2}^* = \frac{1}{2a + \frac{\Delta m_{j+1/2}}{\mathrm{St}}}\left(a\left(u_{j+1}^n + u_j^n\right) - \left(\Pi_{j+1}^n - \Pi_j^n\right) + \frac{\Delta m_{j+1/2}}{\mathrm{St}}\overline{u}_g\right)$$

$$p_{j+1/2}^* = \frac{\Pi_{j+1} + \Pi_j}{2} - \frac{a\left(u_{j+1}^n - u_j^n\right)}{2}$$

# Projection step

The last step of the scheme is the projection step, which corresponds to the evolution to to material waves. This step is done in an explicit manner to keep accuracy. Considering $\mathbf{X} = (\rho, \rho u, \rho E)^T$, the projection step is:

$$\mathbf{X}_j^{n+1} = \mathbf{X}_j^n + \frac{\Delta t}{\Delta x}\left[u_{j-1/2}^{*,+}\mathbf{X}_{j-1}^n + \left[u_{j+1/2}^{*,-} - u_{j-1/2}^{*,+}\right]\mathbf{X}_j^n - u_{j+1/2}^{*,-}\mathbf{X}_{j+1}^n\right]$$

where $\alpha^{\pm} = (\alpha \pm |\alpha|)/2$.

# Finally

## We have

- A Lagrange-Projection scheme that allows to separate acoustic and material waves, and to apply an implicit treatment on acoustic waves and an explicit treatment on material waves (to keep a good precision)
- A relaxation scheme that simplify the structure of the hyperbolic system resulting from the Lagrange-Projection
- A HLLC scheme that account for source terms at the interfaces

**It leads to an optimal scheme that takes the better of existing strategies to overcome the problem raised by the asymptotic limits of our modeling approach**

## Theorem

Under the CFL condition and with sufficiently large $a$, the implicit-explicit in time numerical scheme is well defied and satisfies the stability properties :

- It is a conservative scheme for the density, as well as for velocity and energy when the source terms are omitted;
- the density is positive for all times provided that the initial density is positive;
- the scheme is asymptotic preserving.

# The test case

## Dispersion of a droplet cloud in a turbulent gas field

Test case proposed in Hyland et al. 1999

- Exact analytical solutions of the dispersion of a Dirac $\delta$-function in the phase space (both in space and velocity)
- 1D and 2D cases
- time-evolving coefficients

Here:

- 1D cases
- equilibrium coefficients (constant in time)

## Physics of the test case

- The initial droplet cloud is spread by the subgrid-scale of the gas phase
- the density gradients generate droplet fluxes through $\lambda$, due to the correlations imposed by the turbulence
- $\mu$ tends to relax the particle energy towards the gas subgrid energy

# The test case

## Initial and Boundary conditions

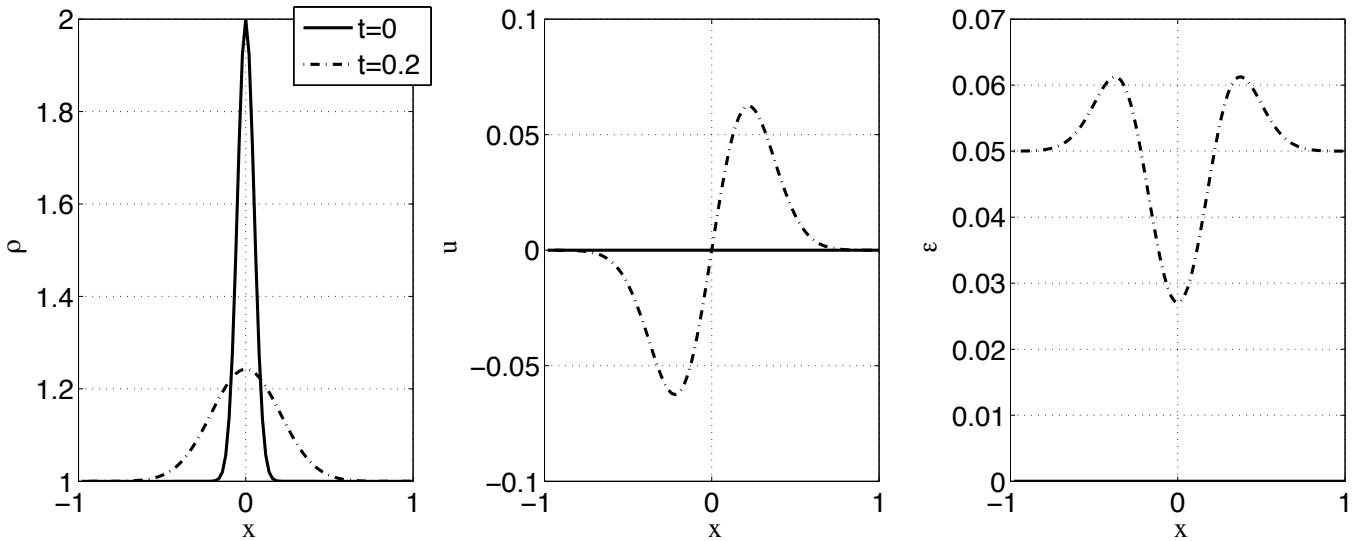
- Gaussian spatial distribution:
  $\rho_0(x) = 1 + \exp\left(-\frac{x^2}{2(\sigma_x^0)^2}\right)$ where $\sigma_x^0 = 0.05$
- Zero initial velocity or internal energy for the disperse phase: $u_0 = 0$ and $\varepsilon_0 = 0$
- No mean gas velocity but non-zero subgrid energy: $\overline{u}_g = 0$, $\tau_g = 0.1$
- Dirichlet Boundary condition:
  $\mathbf{U}(t, x = -2) = \mathbf{U}(t = 0, x = -2)$,
  $\mathbf{U}(t, x = 2) = \mathbf{U}(t = 0, x = 2)$

## Numerical parameters

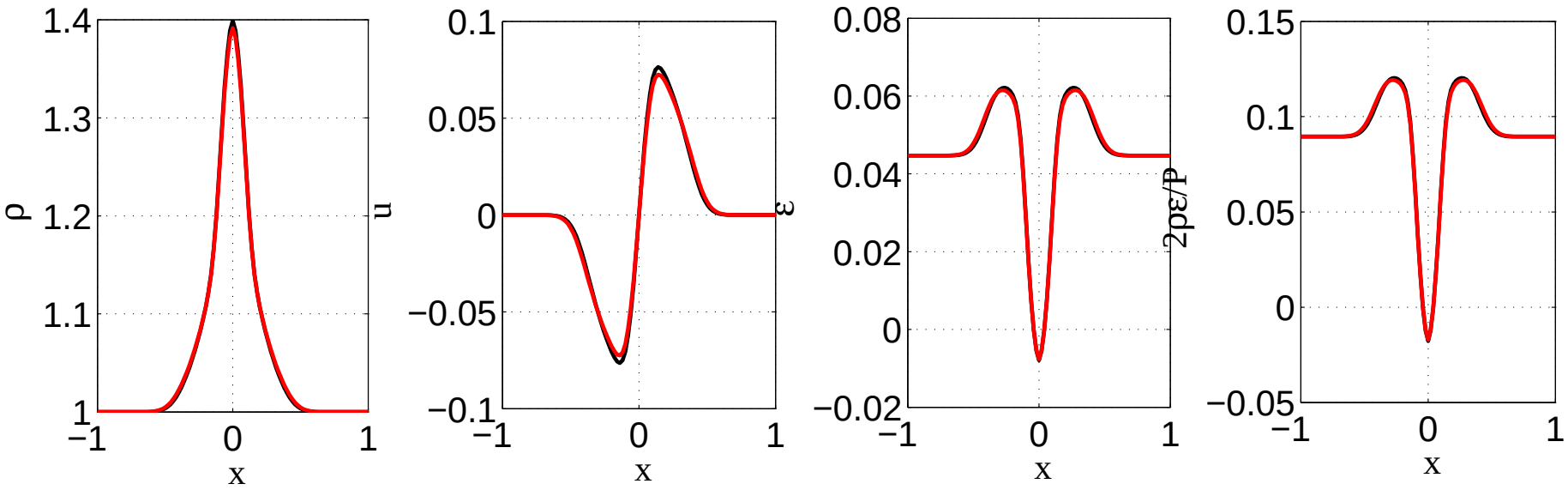
$CFL = 0.5$, $\Delta t = \min(\Delta t_{conv}, \mathrm{St}/2)$

## Analytical solution of the diffusion equation

$$\rho(t,x) = 1 + \frac{\sigma_x^0}{\sigma_x(t)} \exp\left(-\frac{x^2}{2\sigma_x(t)^2}\right)$$
$$\sigma_x(t) = \sigma_x^0 + \sqrt{2\tau_g t}$$
$$u(t,x) = u_g - \frac{St\lambda}{\rho}\frac{\partial \rho(t,x)}{\partial x}$$
$$\varepsilon(t,x) = \frac{St}{2}\left(\mu - \lambda \frac{\partial u(t,x)}{\partial x}\right)$$

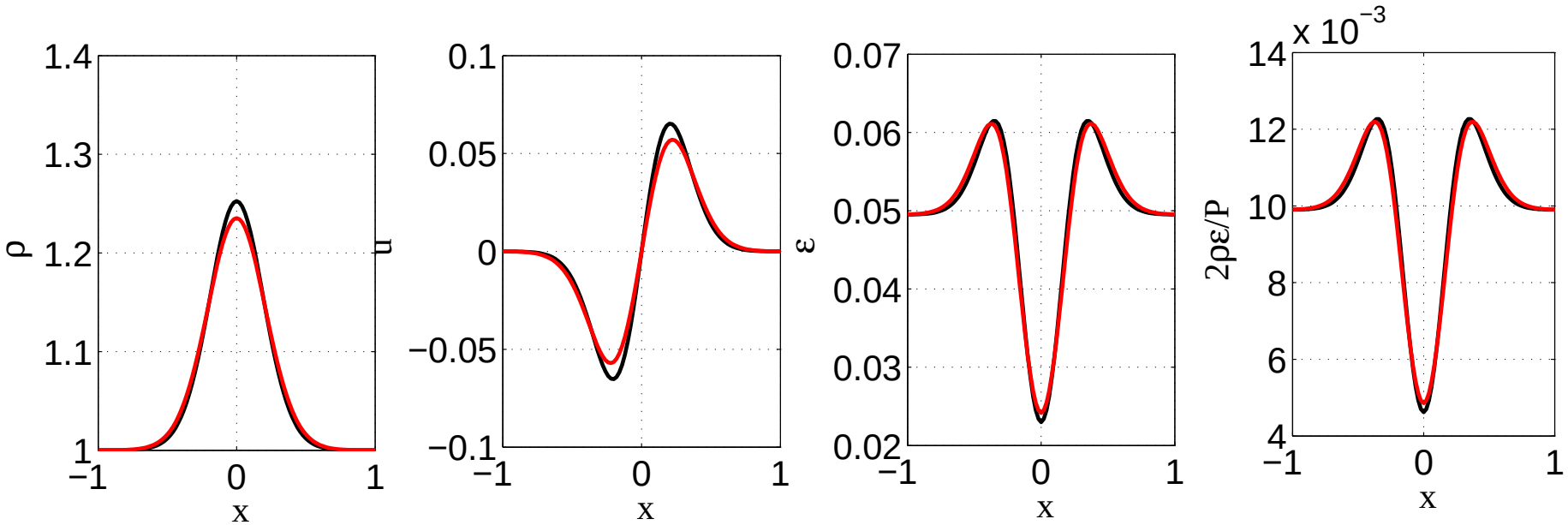


# Effect of Stokes number: $N_{cell} = 100$, Stokes number=$10^{-1}$



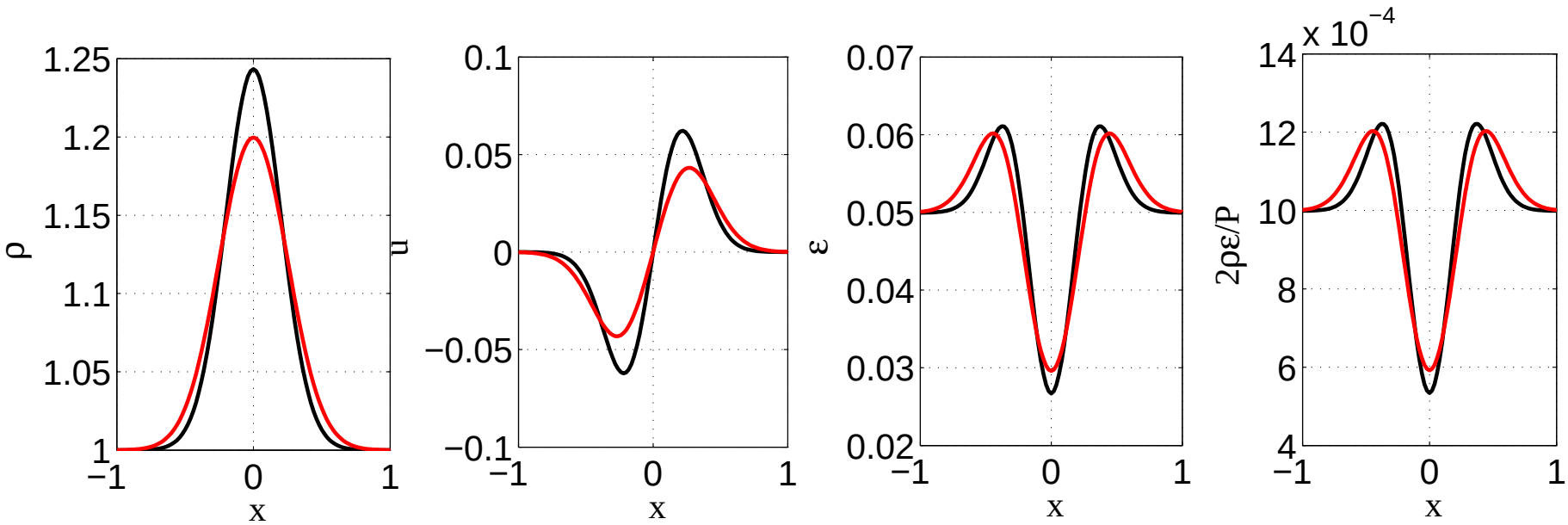

black - AP scheme red - non AP scheme

# Effect of Stokes number: $N_{cell} = 100$, Stokes number=$10^{-2}$



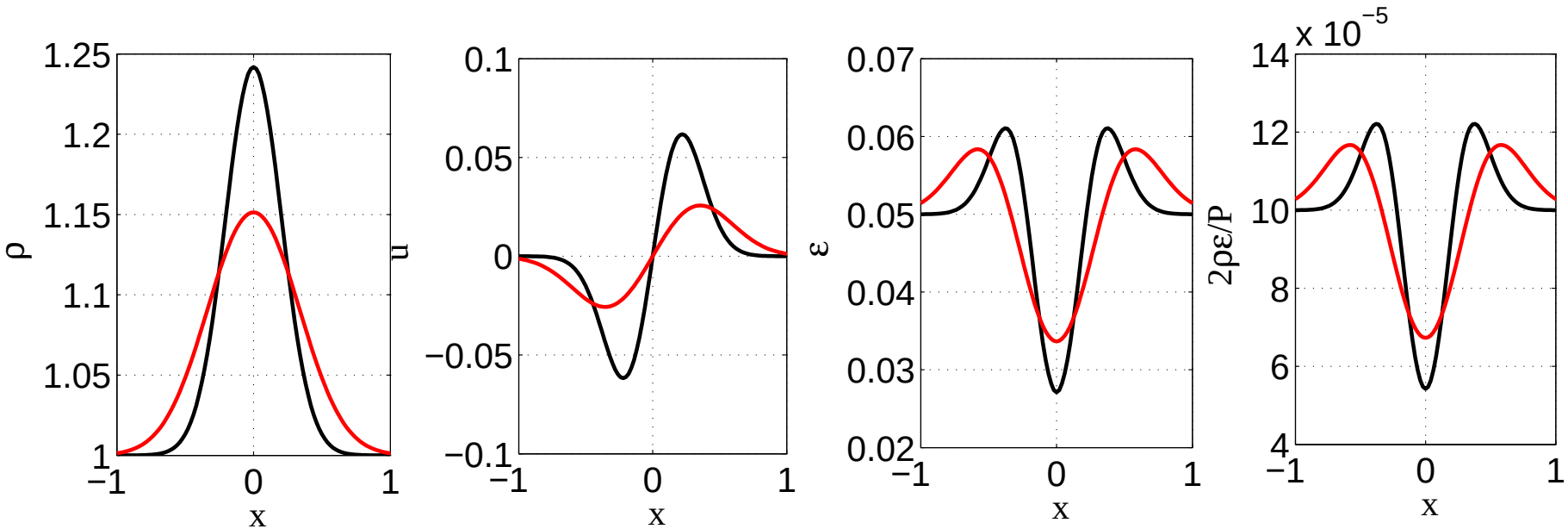

black - AP scheme red - non AP scheme

# Effect of Stokes number: $N_{cell} = 100$, Stokes number=$10^{-3}$



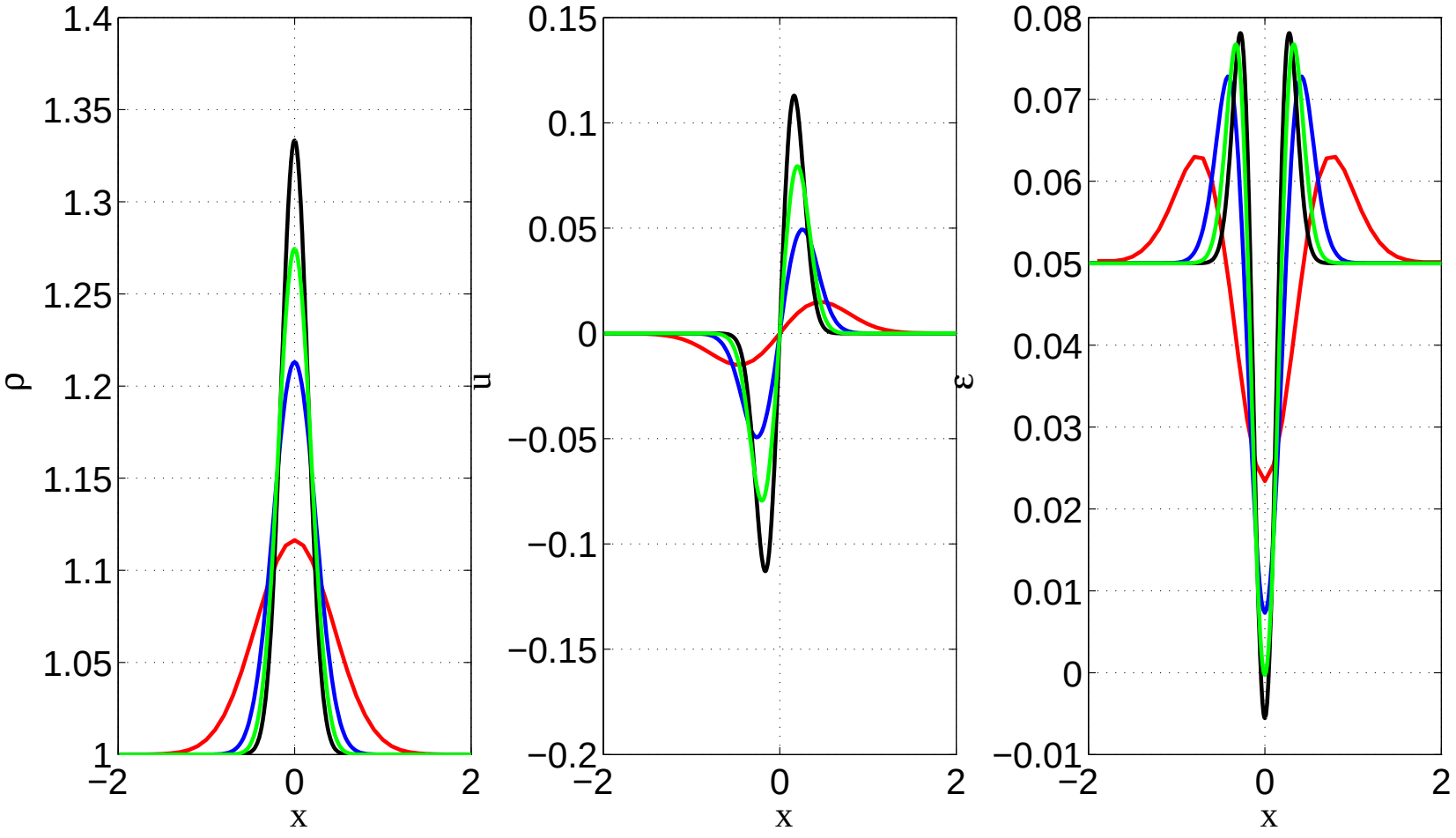

black - AP scheme red - non AP scheme

# Effect of Stokes number: $N_{cell} = 100$, Stokes number=$10^{-4}$



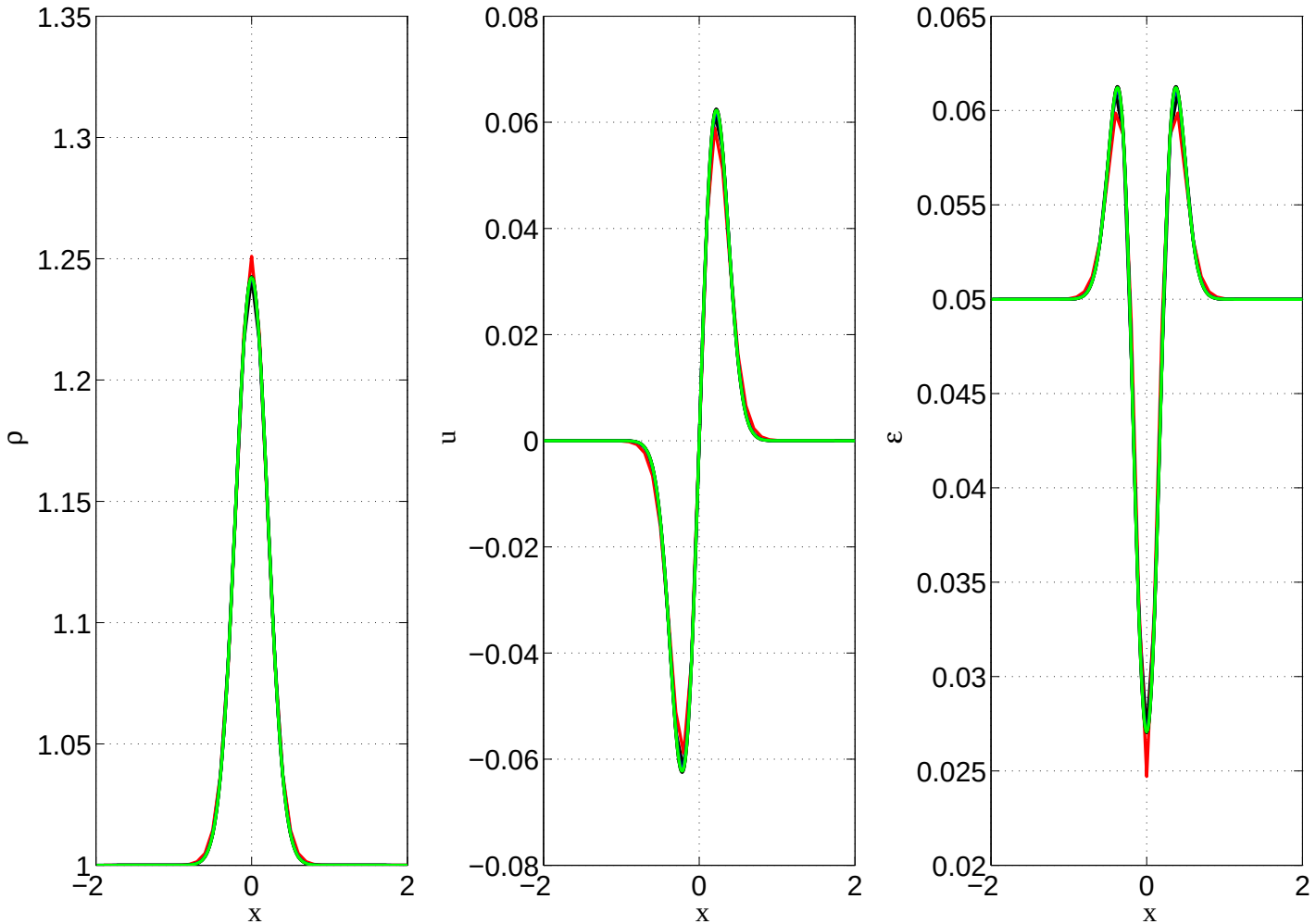

black - AP scheme red - non AP scheme

# Effect of discretization: Stokes number=$10^{-4}$, non AP scheme



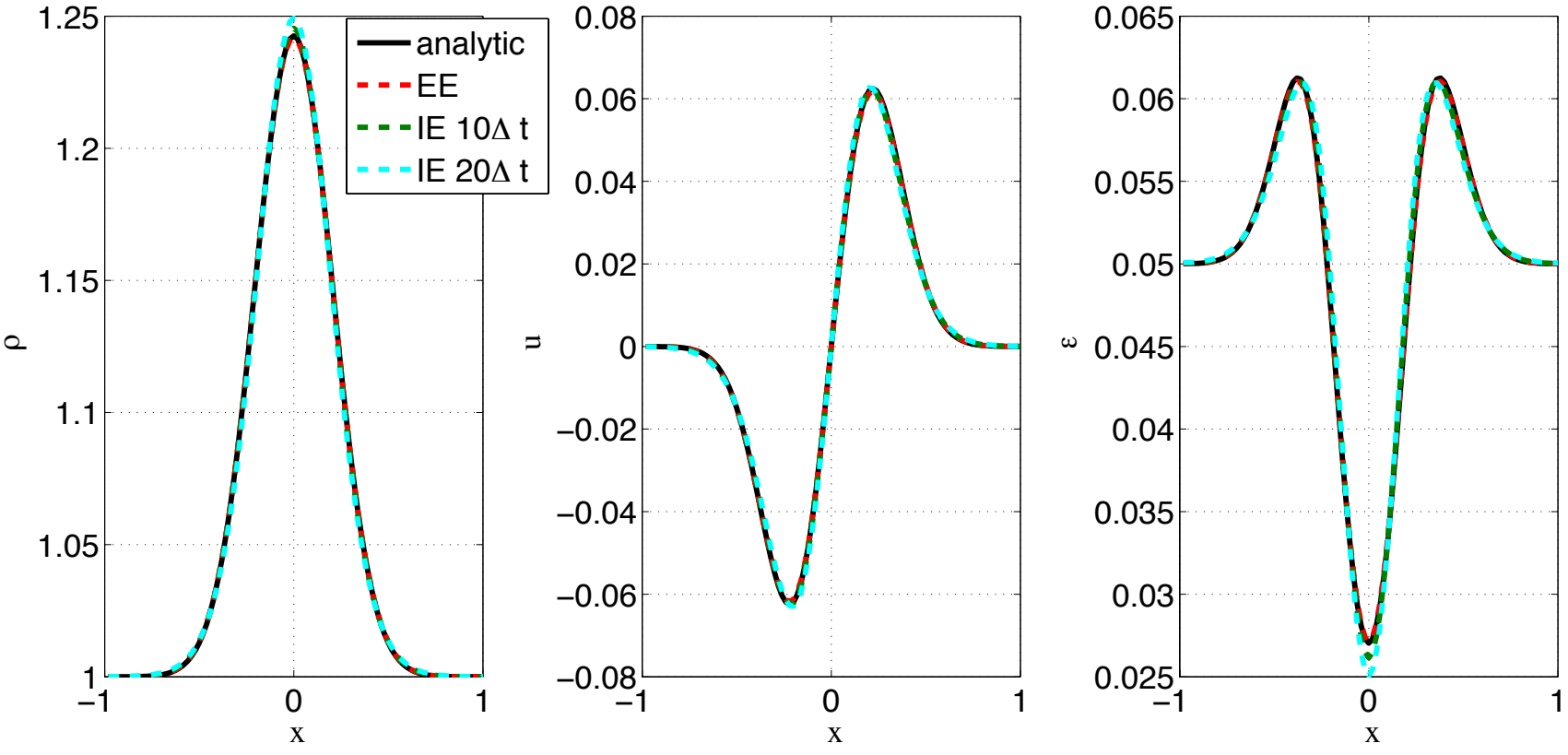

black - analytical red - 40 cells blue - 200 cells green 600 cells

# Effect of discretization: Stokes number=$10^{-4}$, AP scheme

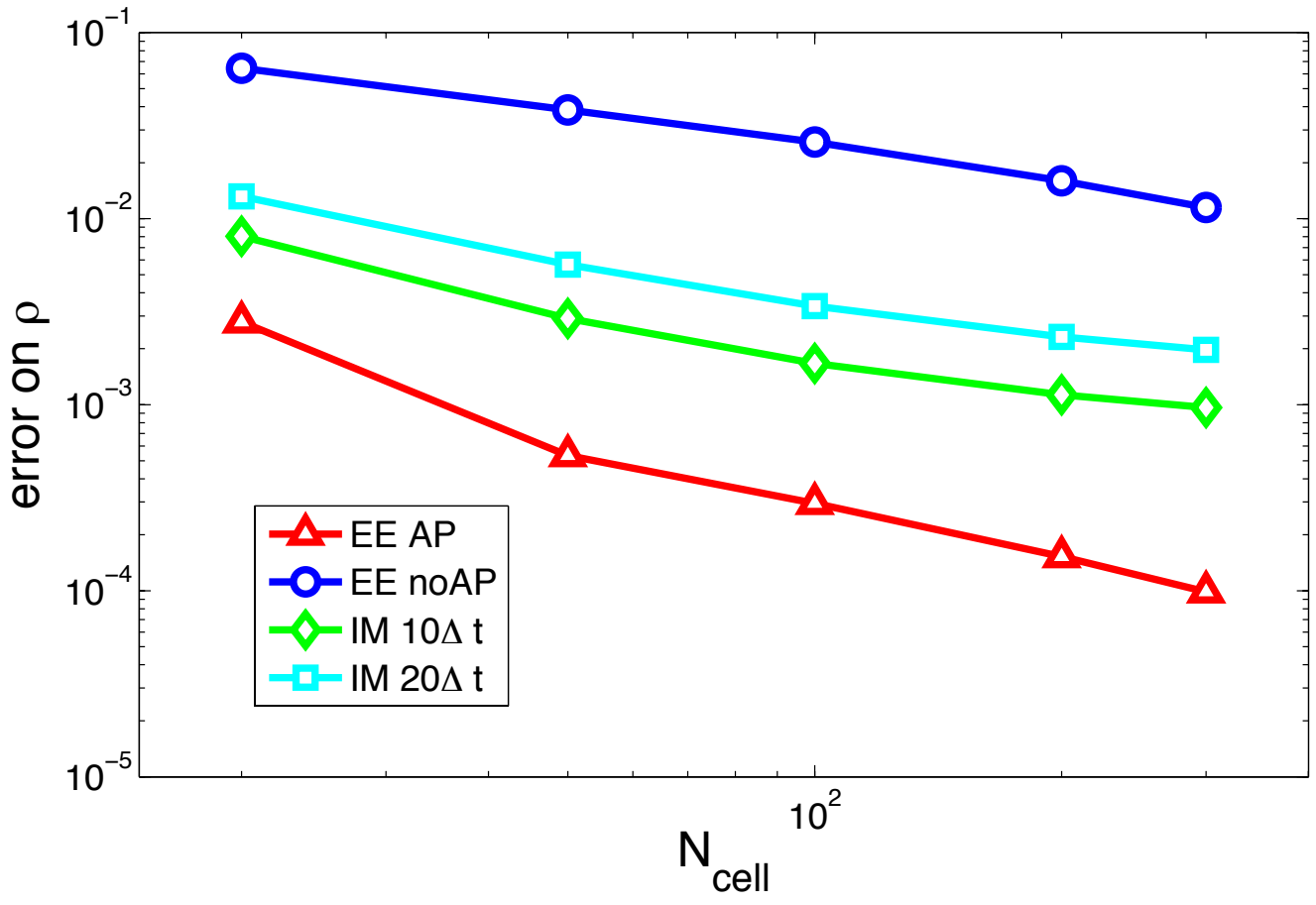



black - analytical red - 40 cells blue - 200 cells green 600 cells

# Implicit-Explicit formulation



# Error on the density




While using a bigger time step, the Implicit-Explicit scheme gives really accurate results, where the non AP scheme needs a fine mesh to reach accurate results (Chalons, Massot, Vié - SIAM MMS 2015).

# Conclusions

## Conclusions - Coupling PGD/Euler

- A hybrid relaxation scheme has been derived, which can handle automatically the interface between the two models
- Second order in time and space can be achieved and PGD with accurate resolution can be used in zones where neither crossing nor subgrid agitation is to be found
- Can handle energy created by crossing

## Conclusions - AP

- The AP Relaxation scheme of Chalons et al. have been extended to LES of disperse phase flows using the gaussian closure
- The results show the necessity of AP schemes, to keep a reasonable error regarding the asymptotic limit of the equations
- Moreover, the Implicit-Explicit formulation notably reduces the computational time, keeping the error an order of magnitude lower than a non AP scheme

# Perspectives

## Coupling of PGD with higher order velocity moment methods

- Anisotropic Gaussian (Cordier et al. 2014)

## Extension of the AP scheme to systems adapted to higher Stokes number

- Higher order kinetic-based moment methods - Anisotropic Gaussian (Vié et al. 2015)
- Quadrature-based moment methods (Yuan and Fox, 2010, Kah et al 2010, Chalons et al 2012), Multi-Gaussian (Chalons et al. 2010, Vié et al 2014)

## Extension to unstructured grids

- Convex-State-Preserving Discontinuous Galerkin methods applied to PGD and Euler-like equations (Larat et al. 2012, Sabat et al. 2014)
- How such an Asymptotic-Preserving strategy can be applied on unstructured grids?

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