High order numerical methods for moments models

Katia Ait Ameur (CMAP, École Polytechnique)

M. Essadki, S. Kokh, M. Massot, T. Pichard,

23-11-2022

Outline

Outline

Two-phase flows in combustions engines

Source: C. Dumouchel CORIA Rouen

Industrial applications

Liquid propulsion: aeronautic or automotive combustion chambers

- Combustion of polydisperse evaporating sprays
- Soots formation

Global objective: Predict, using simulations, the dynamic and evaporation of the spray stemming from the atomization of the liquid phase.

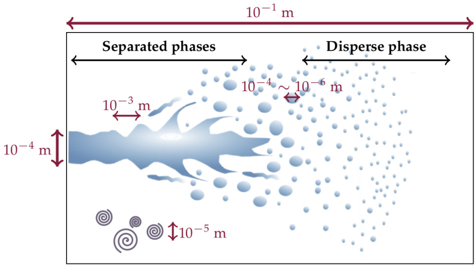
Multi-scales two-phase flow: seperated and disperse phases

Separated phases

DNS, Front tracking (Glimm et al, 2001), Interface capturing: Level Set (Osher, Sethian, 1988))

Disperse phases

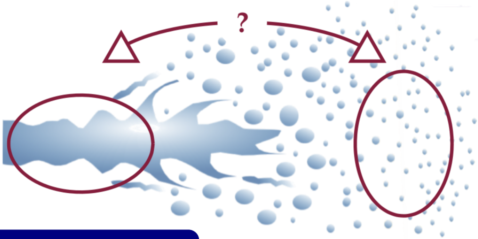
Kinetic model: Population Balance equation (Williams, 1958)



Reduced-order models

- Computational cost: $N_{cells} > 10^9, \quad N_{iter} > 10^6$
- Averaged two-fluid models (Baer, Nunziato, 1986): modeling sub-scale interface
- Eulerian moment method

Coupling strategies



Litterature review

- (Vallet et al, 2001), averaged two-fluid model + Lagrangian model
- (Herrmann, 2013), interface capturing method + Lagrangian approach
- (Le Touze, 2015), two-fluid model + kinetic based moment model
- (Drui, 2017), (Cordesse,2020), (Loison, 2023), averaged model enriched with small scales dynamics

Our strategy

- Use a unified set of variables to describe the interface topology
- Enriched averaged two-phase flows with geometrical variables
- Moment models to describe the disperse phase (Essadki, 2020)

Modeling of the disperse phase

Internal variables ξ: droplet size S, velocity c:

$$f(x,\xi,t) \quad \Omega = \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}_+$$

Population Balance Equation, Williams Boltzmann equation: (Williams, 1958)

$$\partial_t f + \partial_x (cf) = 0$$

Moments:

$$m_k(t,x) = \int_\Omega \xi^k f(x,\xi,t) d\xi$$

Equations for a finite number of moments:

$$\partial_t m_k + \partial_x \left(\int_\Omega \xi^k cfd\xi \right) = 0$$

Issues

- The equations needs to be closed
- Reconstruction of the NDF from the moments
- Design realizable numerical schemes

Kinetic modeling of the disperse phase

Number density function: $f(t,x,c,S)$

Williams-Boltzmann equation [Williams, F.,1958]:

$$\partial_t f + \partial_x(cf) = 0$$

Monokinetic closure law:

$$f(t,x,c,S) = n(t,x,S)\delta(c-u).$$

Eulerian moment method

- Velocity moments:

$$\mathcal{M}_m = \int c^m f(t,x,c,S)dc, \quad \begin{pmatrix} n \\ nu \end{pmatrix}$$

  Semi-kinetic equation:

$$\begin{cases} \partial_t n & + \quad \partial_x(nu) = 0, \\ \partial_t(nu) & + \quad \partial_x(nu^2) = 0 \end{cases}$$

- Fractionnal size moments:

$$m_{k/2} = \int S^{k/2} n(t,x,S)dS, \quad \begin{pmatrix} m_0 \\ m_{1/2} \\ m_1 \\ m_{3/2} \end{pmatrix}$$

Fractionnal high order moment model

$$\begin{cases} \partial_t m_0 + \partial_x(m_0 u) & = & 0 \\ \partial_t m_{1/2} + \partial_x(m_{1/2} u) & = & 0 \\ \partial_t m_1 + \partial_x(m_1 u) & = & 0 \\ \partial_t m_{3/2} + \partial_x(m_{3/2} u) & = & 0 \\ \partial_t (m_1 u) + \partial_x(m_1 u^2) & = & 0 \end{cases}$$

Link with separated phases two-phase flow: Baer-Nunziato type models enriched with geometrical variables of the interface, [Essadki, 2018]:

- $m_{3/2}$: volume fraction
- m_1: interfacial area density
- m_0: average Gauss curvature
- $m_{1/2}$: mean curvature

Other strategy based on pertubation analysis of non spherical droplets [Loison et al, in preparation].

Numerical challenges

$$\begin{cases} \partial_t m_1 & + \quad \partial_x(m_1 u) = 0, \\ \partial_t(m_1 u) & + \quad \partial_x(m_1 u^2) = 0, \\ \partial_t \vec{M} & + \quad \partial_x(\vec{M}u) = 0, \qquad \vec{M} = (m_0, m_{1/2}, m_{3/2}) \end{cases}$$

- **Realizability** condition:

$$\forall (t,x), \quad (m_0, m_{1/2}, m_1, m_{3/2}) \in \mathbb{M}_3^{1/2}$$

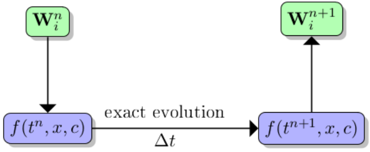
- **Maximum principle** on the velocity u
- Weakly hyperbolic, δ-shocks singularities.
- **Kinetic Finite Volume** schemes [Bouchut et al, 2003],[de Chaisemartin, 2009], [Kah et al, 2012]
- **MUSCL-Hancock** schemes [Vié, Laurent, Massot, 2013]
- **Runge Kutta Discontinuous Galerkin** schemes [Cockburn, Shu, 1989],[Zhang, Shu, 2012], [Larat et al, 2012], [Sabat, 2016]

Outline

Kinetic Finite Volume scheme

$$\partial_t f + c\partial_x f = 0 \Longleftrightarrow \begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2) = 0 \end{cases}$$

Exact solution: $f(t,x,c) = f(t_n, x - c(t-t_n), c)$.



Second order scheme Piecewise linear reconstruction:

$$\begin{cases} \rho(x) = \rho_i^n + D_{\rho_i}(x - x_i), \\ u(x) = \bar{u}_i^n + D_{u_i}(x - x_i) \end{cases}$$

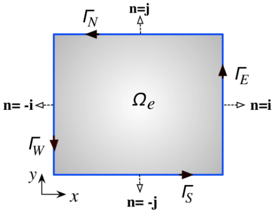
Minmod limiter [van Leer, 1974],[Toro, 2009]: realizability and stability.

DG discretization[1]

$$\partial_t W + \nabla \cdot F(W) = 0$$

(k+1)-th order method: ϕ_i, basis functions of polynomials of order k.

$$W_h(x,t) = \sum_{i=0}^{m} W_i(t)\phi_i(x)$$



From the variational formulation:

$$\int_{\Omega_e} \partial_t W_h \phi_h d\Omega - \int_{\Omega_e} F(W_h) \cdot \nabla \phi_h d\Omega + \int_{\Gamma_e} \hat{F} \cdot n \phi_h d\Gamma = 0$$

$$M_i \frac{d\hat{W}_i}{dt} = \int_{\Omega_e} F(W_i) \cdot \nabla \phi_j d\Omega - \sum_{e=1}^{4} \int_e \phi_j \hat{F}_{i,e} \cdot n_{i,e} d\Gamma, \quad i = 1, \cdots, N_e.$$

- Local mass and rigidity matrices.
- Numerical flux $\hat{F}$.
- High order scheme in space and time with SSP Runge Kutta time integrators

[1] [Cockburn, Shu, 1998],[Gottlieb, Ketcheson, Shu, 2009]

Outline

Limitation and realizability

Theorem [Zhang, Shu, 2010, 2012]

G, convex set of realizable states.
Assuming:

- $W_i(T^n) \in G$ and $\hat{F}$, realizable.
- Realizability at quadrature nodes x_q: $W_i^q \in G$
- CFL condition: $\dfrac{\Delta t \lambda_i}{\Delta x} \leq \min_q \omega_q$.

then the DG solution at T^{n+1} is realizable.

Convex moments set $\mathcal{G}$:

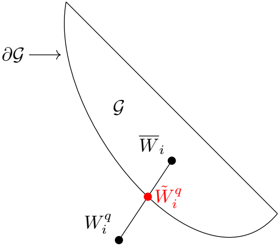
$$\tilde{W}_i^q = \theta_q W_i^q + (1-\theta_q)\bar{W}_i$$

$$\tilde{W}_i = \theta_i \left(W_i - \bar{W}_i^{n+1} \right) + \bar{W}_i^{n+1}, \quad \theta_i = \min_q \theta_q$$

$\longrightarrow$ Properties: conservative, accuracy

Challenges

- High order moment models
- Projection method
- Stability near the boundary of the moments set



Projection method

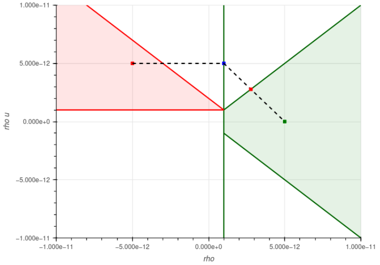
Step-by-step projection

- Realizability constraint:

$$\tilde{\rho}^1 = \theta^1 \rho + (1-\theta^1)\overline{\rho}$$

- Maximum principle on the velocity:

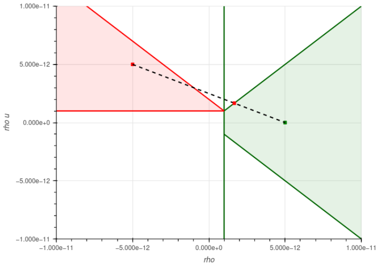
$$\begin{pmatrix} \tilde{\rho} \\ \tilde{\rho}\tilde{u} \end{pmatrix} = \theta^2 \begin{pmatrix} \tilde{\rho}^1 \\ \rho u \end{pmatrix} + (1-\theta^2) \begin{pmatrix} \overline{\rho} \\ \overline{\rho u} \end{pmatrix}$$



Straight projection

Realizability constraint and maximum principle on the velocity:

$$\begin{pmatrix} \tilde{\rho} \\ \tilde{\rho}\tilde{u} \end{pmatrix} = \theta \begin{pmatrix} \rho \\ \rho u \end{pmatrix} + (1-\theta) \begin{pmatrix} \overline{\rho} \\ \overline{\rho u} \end{pmatrix}$$



$\longrightarrow$ Do they preserve the order accuracy of the DG method?

Order accuracy

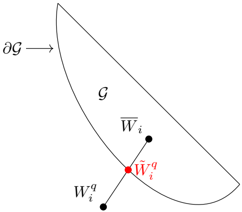
Conditionnal preservation of the order

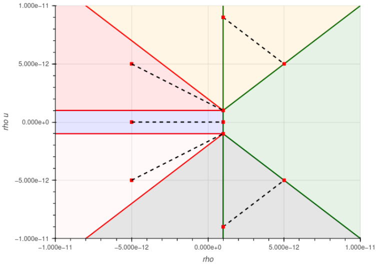
$$||\tilde{W}_i^q - W_{ex}|| = (1-\theta)||\bar{W}_i - W_{ex}|| + \theta||W_i^q - W_{ex}||$$
$$\leq (1-\theta)\mathcal{O}(\Delta x) + \theta\mathcal{O}(\Delta x^{k+1})$$

- **Hypothesis:** $d(W_{ex}, \partial\mathcal{G}) \geq M.$
- $1-\theta = \dfrac{||\tilde{W}_i^q - W_i^q||}{||W_i^q - \bar{W}_i||} \leq \mathcal{O}(\Delta x^{k+1})$

Unconditionnal preservation of the order

- $\mathcal{P}_{\min} W_i^q = argmin_{V\in\mathcal{G}}||W_i^q - V||$
- Does not provide conservative projection method





Comparisons of projections

Admissible set:

$$G = \{\rho > \epsilon, \quad \rho u_{\min} \leq \rho u \leq \rho u_{\max}\}$$

- Orangeregion:

$$\mathcal{P}_{Straight} = \mathcal{P}_{Zhang} \text{ and } \mathcal{P}_{\min} = \mathcal{P}^{\perp}_{\rho u = \rho u_{\max}}$$

- Red region:

$$\mathcal{P}_{Straight} \neq \mathcal{P}_{Zhang} \text{ and } \mathcal{P}_{\min} = (\epsilon, \epsilon u_{\max})$$

- Blue region:

$$\mathcal{P}_{Straight} \neq \mathcal{P}_{Zhang} = \mathcal{P}_{\min} = \mathcal{P}^{\perp}_{\rho = \epsilon}$$

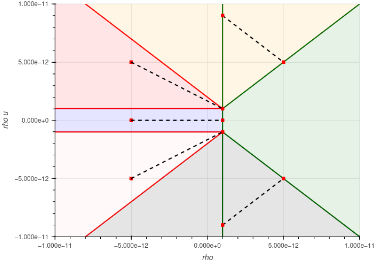
- Pink region:

$$\mathcal{P}_{Straight} \neq \mathcal{P}_{Zhang} \text{ and } \mathcal{P}_{\min} = (\epsilon, \epsilon u_{\min})$$

- Grey region:

$$\mathcal{P}_{Straight} = \mathcal{P}_{Zhang} \text{ and } \mathcal{P}_{\min} = \mathcal{P}^{\perp}_{\rho u = \rho u_{\min}}$$

$$\mathcal{P}_{\min}(U) = argmin_{V \in \mathcal{G}} ||U - V||$$



$\longrightarrow$ Behavior at the vacuum limit for $\mathcal{P}_{Zhang}$ and $\mathcal{P}_{Straight}$:

$$\begin{pmatrix} \overline{\rho} \\ \rho u \end{pmatrix} \longrightarrow \begin{pmatrix} \epsilon \\ \epsilon u \end{pmatrix}, \; u_{\min} \leq u \leq u_{\max}$$

Behavior at the vacuum limit

- Zhang and Shu projection method:

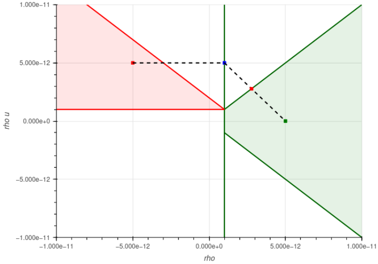
$$\begin{cases} (i) & \rho \longrightarrow \epsilon \\ (ii) & (\epsilon, \rho u) \longrightarrow (\tilde{\rho}, \tilde{\rho u}) \\ & \begin{pmatrix} \tilde{\rho} \\ \tilde{\rho u} \end{pmatrix} = \theta_{\rho u} \begin{pmatrix} \epsilon \\ \rho u \end{pmatrix} + (1 - \theta_{\rho u}) \begin{pmatrix} \overline{\rho} \\ \overline{\rho u} \end{pmatrix} \end{cases}$$

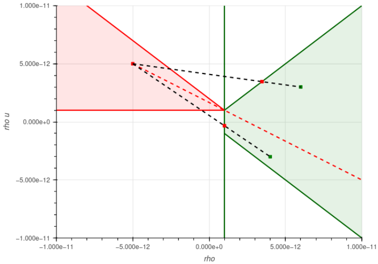
- Straight projection:

$$\begin{cases} (\rho, \rho u) \longrightarrow (\tilde{\rho}, \tilde{\rho u}) \\ \begin{pmatrix} \tilde{\rho} \\ \tilde{\rho u} \end{pmatrix} = \theta \begin{pmatrix} \rho \\ \rho u \end{pmatrix} + (1 - \theta) \begin{pmatrix} \overline{\rho} \\ \overline{\rho u} \end{pmatrix}, \\ \theta = \max(\theta_\rho, \theta_{\rho u}) \end{cases}$$

Choice of projection method

Straight projection preserves all the properties.





High order moment model

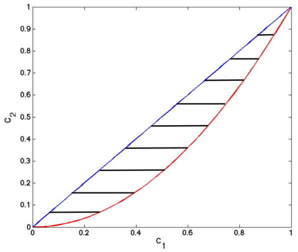
$$\partial_t W + \partial_x F(W) = 0, \quad W = \left(m_0, m_{1/2}, m_1, m_{3/2}, m_1 u\right) \in \mathbb{M}_3^{1/2}$$

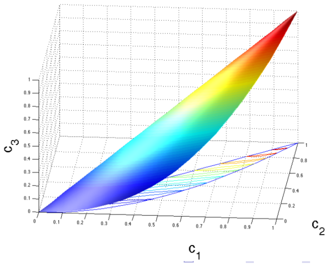
Caracterisation of moments set with Hankel determinants [Dette and Studden, 1997]

$$\vec{m}_{N/2} = \left(m_0, m_{1/2}, \cdots, m_{N/2}\right) \in \mathbb{M}_N^{1/2} \Leftrightarrow \underline{H}_i \text{ and } \bar{H}_i \text{ are non negative for } i = 0, \cdots, N.$$

First constraints: $m_0 > 0$ and for $c_{k/2} = \dfrac{m_{k/2}}{m_0}$:

$$c_{1/2} > 0, \quad c_{1/2}^2 < c_1 < c_{1/2}, \quad \frac{c_1^2}{c_{1/2}} < c_{3/2} < \frac{c_1^2}{c_{1/2}} + \frac{(c_1 - c_{1/2}^2)(c_{1/2} - c_1)}{c_{1/2}(1 - c_{1/2})}$$





Straight projection for moment models

For each quadrature point q:

- If $\underline{H}_i < 0$, or $\bar{H}_i < 0$:

$$(\widetilde{m_{i/2}})_q = (\overline{m_{i/2}}) + \theta_q^i \left[(m_{i/2})_q - \overline{m_{i/2}}\right], \quad \theta_q^i \in [0,1],$$

  such that: $\underline{H}_i = 0, \quad \bar{H}_i = 0, \quad i = 0, \cdots, 3.$

- If $(m_1 u)_q > (m_1)_q u_{\max}$:

$$(\widetilde{m_1 u})_q = (\overline{m_1 u}) + \theta_q^4 \left[(m_1 u)_q - (\overline{m_1 u})\right], \quad \theta_q^4 \in [0,1],$$

  such that: $(\widetilde{m_1 u})_q = (m_1)_q u_{\max}$.

For each cell:

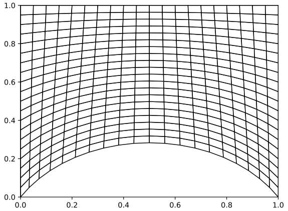
$$\begin{pmatrix} (\tilde{m}_0)_q \\ (\widetilde{m_{1/2}})_q \\ (\tilde{m}_1)_q \\ (\widetilde{m_{3/2}})_q \\ (\widetilde{m_1 u})_q \end{pmatrix} = \begin{pmatrix} \bar{m}_0 \\ \overline{m_{1/2}} \\ \bar{m}_1 \\ \overline{m_{3/2}} \\ (\overline{m_1 u}) \end{pmatrix} + \theta \left[\begin{pmatrix} (\tilde{m}_0)_q \\ (\widetilde{m_{1/2}})_q \\ (\tilde{m}_1)_q \\ (\widetilde{m_{3/2}})_q \\ (\widetilde{m_1 u})_q \end{pmatrix} - \begin{pmatrix} \bar{m}_0 \\ \overline{m_{1/2}} \\ \bar{m}_1 \\ \overline{m_{3/2}} \\ (\overline{m_1 u}) \end{pmatrix} \right], \quad \theta = \min_q(\theta_q^0, \theta_q^1, \theta_q^2, \theta_q^3, \theta_q^4)$$

Outline

Josiepy, a PDE solver written in Python

$$\frac{\partial q}{\partial t} + \nabla \cdot F(q) + B(q) \cdot \nabla q - \nabla \cdot (K(q) \cdot \nabla q) + s(q) = 0$$

- Euler solver (including an exact RP solver for generic EOS)
- Baer-Nunziato solver
- Compressible Navier Stokes
- Heat Equation
- Baer Nunziato model enriched with geometrical variables.
- Ode solvers, arbitrary RK methods
- Composite BC
- Runge Kutta Discontinuous Galerkin schemes

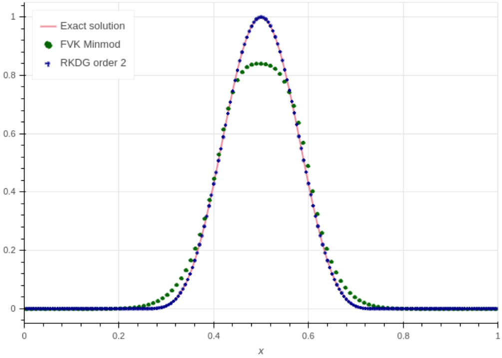


https://gitlab.com/rubendibattista/josiepy

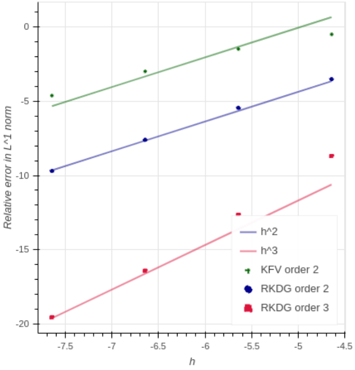
Advection

Gaussian initial condition:

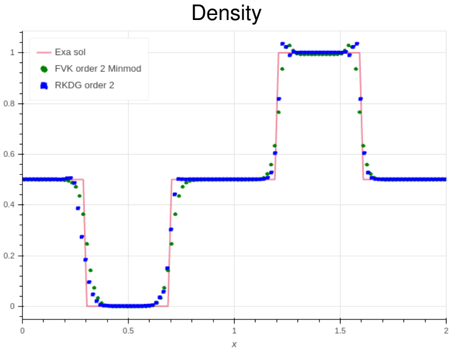
$$u(x) = 1, \rho(x,0) = \begin{cases} (\cos(\pi(2x-1)))^4 & \text{if} \quad 0.25 < x < 0.75, \\ 0 & , \text{otherwise} \end{cases}$$

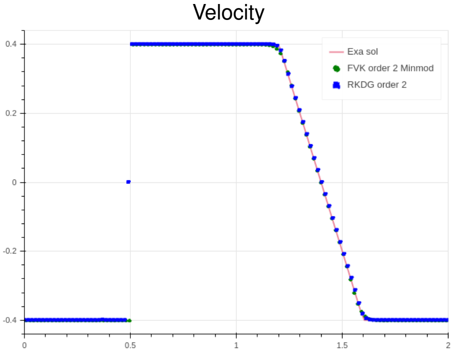


Density.



Vacuum test case





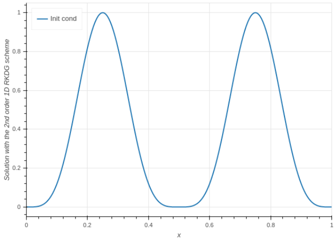
Mesh size	Order 2	
	Zhang & Shu	Straight
$N = 25$	10^{-6}	10^{-8}
$N = 50$	10^{-6}	10^{-12}
$N = 100$	10^{-9}	10^{-12}
$N = 200$	10^{-12}	10^{-12}

$\longrightarrow$ Robustness for accumulation zones and vaccum states.

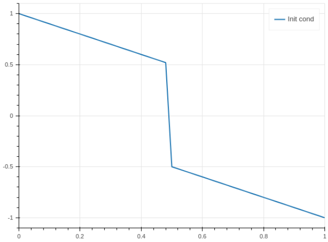
PGD system - δ-shock

Initial condition generating δ-shocks:

$$\rho(x,0) = (\sin(2\pi x))^4 \,, u(x,0) = \begin{cases} -x & \text{if} \quad x > 0.5, \\ -x+1 & , \text{otherwise} \end{cases}$$



Density



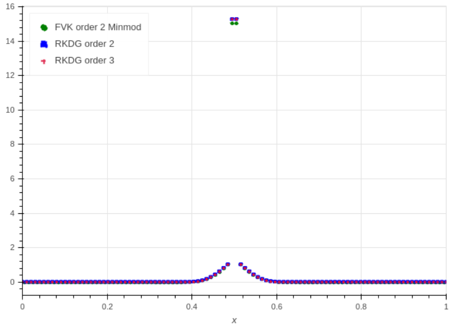
Velocity

Realizability domain:

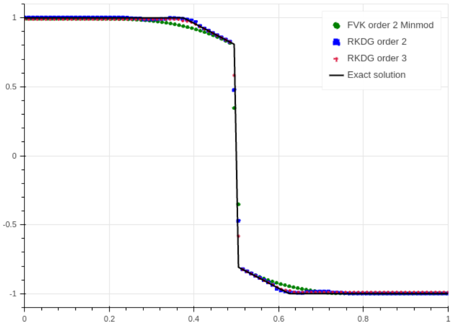
$$G := \left\{ \begin{pmatrix} \rho_i \\ \rho_i u_i \end{pmatrix}, \rho_i > 0, \quad m_i \leq u_i \leq M_i \right\}, m_i = \min(u_{i-1}, u_i, u_{i+1}), M_i = \max(u_{i-1}, u_i, u_{i+1})$$

δ-shock

Initial condition: $\rho(x,0) = (\sin(2\pi x))^4$, $u(x,0) = \begin{cases} -x & \text{if} \quad x > 0.5, \\ -x+1 & , \text{otherwise} \end{cases}$



Density



Velocity

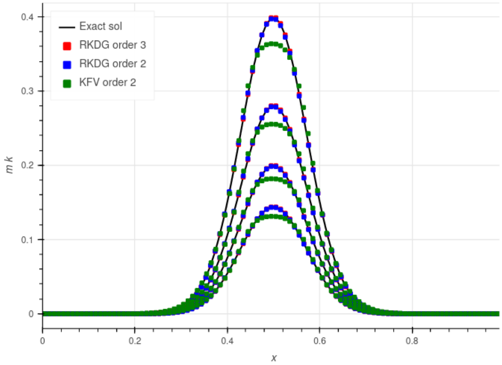
$\longrightarrow$ Robustness for δ-shock singularities and numerical diffusion of the velocity profile.

Advection

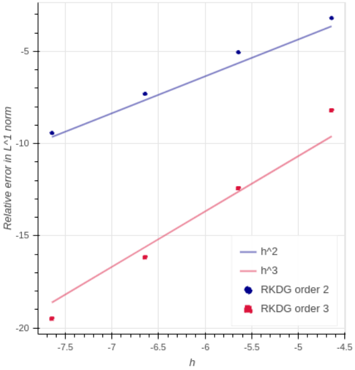
Initial moments:

$$m_{k/2}(x,0) = \frac{2}{k+2}\left(S_{\max}^{(k+2)/2} - S_{\min}^{(k+2)/2}\right)\exp\left(-\frac{(x-x_c)^2}{\sigma_x^2}\right), \quad u(x) = -1,$$

$$(S_{\min}, S_{\max}) = (0.3, 0.7), \quad x_c = 0.5, \quad \sigma_x = 0.1.$$



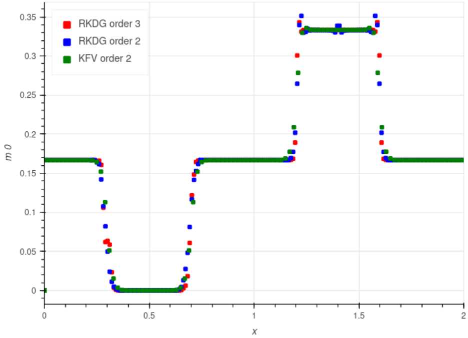
Fractionnal moments



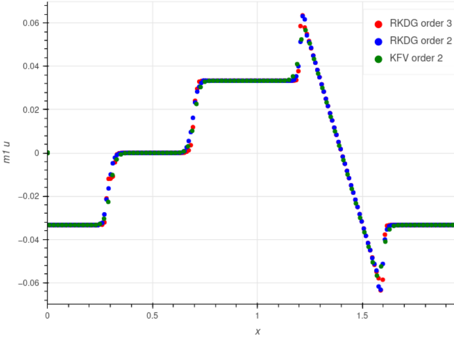
Vacuum test case

Initial condition:

$$m_k(x,0) = (2+k)^{-1} - (3+k)^{-1}, u(x,0) = \begin{cases} -0.4 & \text{if} \quad 0.5 < x \text{ or } x > 1.8, \\ 0.4 & \text{if} \quad 0.5 < x < 1, \\ 1.4 - x & \text{if} \quad 1 < x < 1.8, \end{cases}$$



First moment m_0

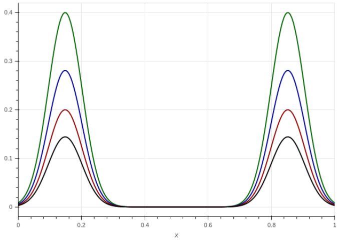


$m_1 u$

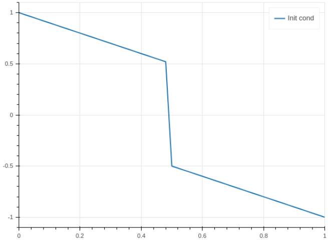
$\longrightarrow$ Robustness for accumulation zones and vaccum states.

δ-shock test case

Initial condition:



Fractionnal moments

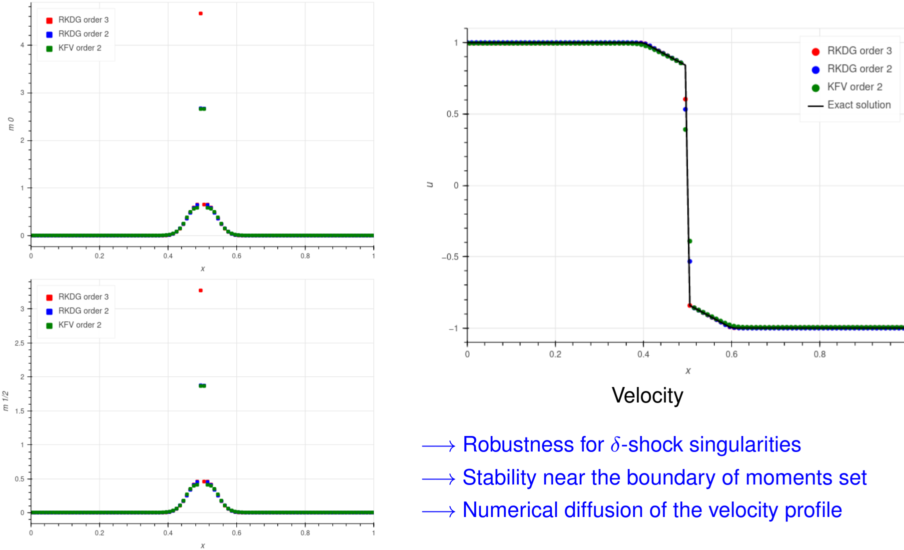


Velocity

Realizability domain:

$$G := \left\{ \begin{pmatrix} (m_0)_i \\ (m_{1/2})_i \\ (m_1)_i \\ (m_{3/2})_i \\ (m_1)_i u_i \end{pmatrix}, \underline{H}_i(m_0, \cdots, m_i) \geq 0, \bar{H}_i(m_0, \cdots, m_i) \geq 0, \quad \min_{C_i, C_{i\pm 1}} u \leq u_i \leq \max_{C_i, C_{i\pm 1}} u \right\}$$

δ-shock



First fractionnal moments: m_0, $m_{1/2}$.

Velocity

$\longrightarrow$ Robustness for δ-shock singularities

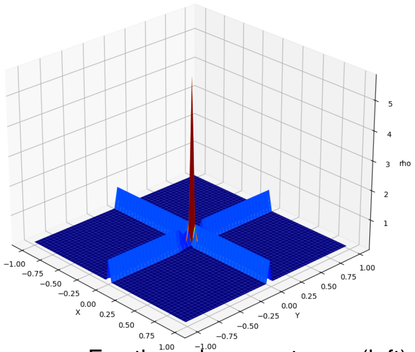
$\longrightarrow$ Stability near the boundary of moments set

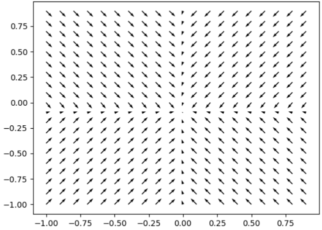
$\longrightarrow$ Numerical diffusion of the velocity profile

2D δ-shock test case

Initial condition:

$$m_k(x,y,0) = (2+k)^{-1} - (3+k)^{-1}, \quad (u,v)(x,y,0) = \begin{cases} (-0.25,-0.25) & x>0, y>0, \\ (0.25,-0.25) & x<0, y>0, \\ (0.25,0.25) & x<0, y<0, \\ (-0.25,0.25) & x>0, y<0 \end{cases}$$



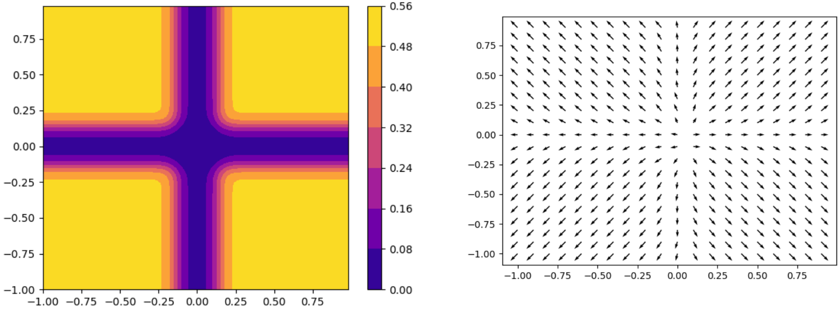


Fractionnal moment $m_{1/2}$ (left) and velocity field (right) at $t=0.5$.

2D Vacuum test case

Initial condition:

$$m_k(x,y,0) = (2+k)^{-1} - (3+k)^{-1}, \quad (u,v)(x,y,0) = \begin{cases} (0.4, 0.4) & x > 0, y > 0, \\ (-0.4, 0.4) & x < 0, y > 0, \\ (-0.4, -0.4) & x < 0, y < 0, \\ (0.4, -0.4) & x > 0, y < 0 \end{cases}$$



Fractionnal moment $m_{1/2}$ (left) and velocity field (right) at $t = 0.4$.

Summary

- RKDG and the KFV are robust and accurate for the capture of singularities in moments models.
- Straight projection method: conservative, order accuracy and stability near the boundary of moments set.
- Slope limiters for KFV scheme smear out discontinuities.
- Realizable and maximum principle satisfying RKDG schemes [Ait Ameur et al, in preparation]

Outlook

- Extension to more complex moment models for the disperse phase:
  - Accounting for the oscillations of the droplets in the spray: $\Xi = (S, \cdots)$
  - Treat additionnal phenomena: evaporation, drag force.
- Link with separated phase models enriched by subscale flow modelling, [Loison et al, in preparation]
- Numerical method for Baer Nunziato type models: Lagrange projection splitting method [Ait Ameur et al, in preparation]
- HPC: adaptive multiresolution SAMURAI library [Gouarin et al, 2021]

Thank you for your attention.