High order numerical methods for moments models

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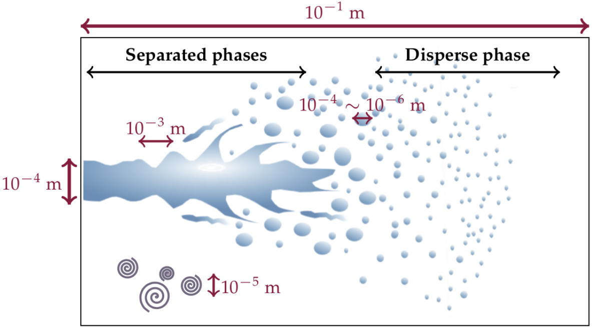
Outline

Outline

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



Separated phases

- large zones of pure fluids
- interface seperating the two-phases
- primary atomization

Disperse phases

- one carrier fluid
- cloud of polydisperse droplets
- droplets breakup, coalescence and evaporation

Kinetic modeling of the disperse phase

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

Williams-Boltzmann equation [Williams, F.,1958], free transport term only:

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

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:

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

- 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].

Toy problem

Pressureless Gas Dynamics system [Bouchut, F.,1994], [Laurent, Massot, 2001]:

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

- Weakly hyperbolic, δ-shocks singularities.
- **Realizability condition:** Every pair of moments $(\rho, \rho u)$ satisfies:

$$G = \left\{ \begin{pmatrix} \rho \\ \rho u \end{pmatrix} : \rho > 0, \quad m \leq u \leq M \right\}$$

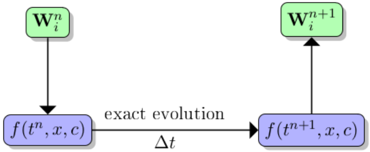
- **Kinetic Finite Volume** schemes [Bouchut et al, 2003],[de Chaisemartin, 2009], [Kah et al, 2012]
- **MUSCL-Hancock** schemes [Vié, Laurent, Massot, 2013]
- **Runge Kutta Discontinuous Galerkin** schemes [Cockburn, Shu, 1989],[Zhang, Shu, 2012], [Larat et al, 2012], [Sabat, 2016]

Outline

Kinetic Finite Volume scheme

$$\partial_t f + c\partial_x f = 0 \Longleftrightarrow \left\{ \begin{array}{lll} \partial_t \rho & + & \partial_x(\rho u) = 0 \\ \partial_t(\rho u) & + & \partial_x(\rho u^2) = 0 \end{array} \right. , \quad f(t,x,c) = \rho(t,x)\delta(c - u(t,x))$$

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



Second order scheme Piecewise linear reconstruction:

$$\left\{ \begin{array}{lll} \rho(x) & = & \rho_i^n + D_{\rho_i}(x - x_i), \\ u(x) & = & \bar{u}_i^n + D_{u_i}(x - x_i) \end{array} \right.$$

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

DG discretization[2]

$$\partial_t W + \partial_x F(W) = 0$$

(k+1)-th order method: $\phi_{i,j}$, basis functions of polynomials of order k.

$$W_i(x,t) = \sum_{j=0}^{m} W_{i,j}(t)\phi_{i,j}(x)$$

From the variational formulation:

$$M_i \frac{d\hat{W}_i}{dt} + \left(F^\star_{i+1/2}\phi_{i,j}(x_{i+1/2}) - F^\star_{i-1/2}\phi_{i,j}(x_{i-1/2})\right) = S_i \hat{F}_i, \quad i = 1, \cdots, N, \quad j = 1, \cdots, k.$$

- Local matrices M_i and S_i.
- Numerical flux $F^\star_{i+1/2}$.
- Arbitrarily high order scheme in space and time with SSP Runge Kutta[1] time integrators

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

[2] [Cockburn, Shu, 1998]

Limitation and realizability

Theorem [Zhang, Shu, 2010, 2012]

G, convex set of realizable states.
Assuming:

- $W_i(T^n) \in G$ and $F^\star$, 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.

Properties

- Conservative
- Accuracy preserved for smooth solutions.

Challenges

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

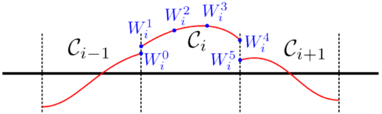
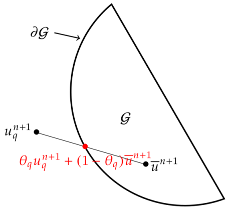


Figure 2. Quadrature points on the cell C_i



Outline

Numerical procedure

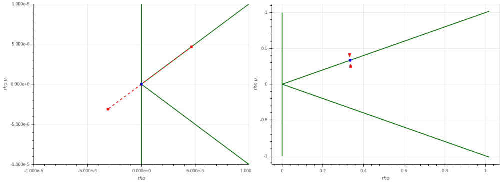
For each quadrature point q:

- If $\rho_q < \epsilon$, $\epsilon = 10^{-12}$:

$$\tilde{\rho}_q = \bar{\rho} + \theta_q^1 \left[\rho_q - \bar{\rho}\right], \quad \theta_q^1 \in [0,1], \text{ such that: } \tilde{\rho}_q = \epsilon.$$

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

$$(\tilde{\rho u})_q = (\bar{\rho u}) + \theta_q^2 \left[(\rho u)_q - (\bar{\rho u})\right], \quad \theta_q^2 \in [0,1], \text{ such that: } (\tilde{\rho u})_q = \rho_q u_{\max}.$$



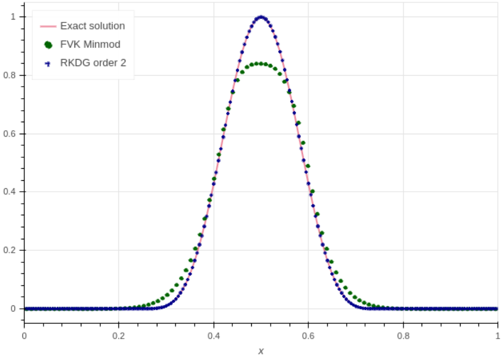
For each cell:

$$\begin{pmatrix} \tilde{\rho}_q \\ (\tilde{\rho u})_q \end{pmatrix} = \begin{pmatrix} \bar{\rho} \\ (\bar{\rho u}) \end{pmatrix} + \theta \left[\begin{pmatrix} \tilde{\rho}_q \\ (\tilde{\rho u})_q \end{pmatrix} - \begin{pmatrix} \bar{\rho} \\ (\bar{\rho u}) \end{pmatrix} \right], \quad \theta = \min_q(\theta_q^1, \theta_q^2)$$

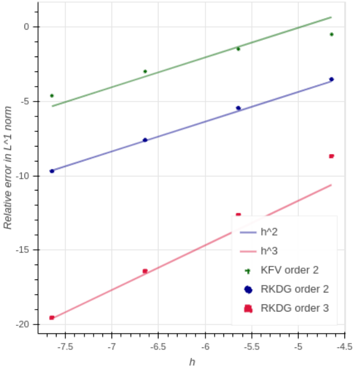
Advection

Gaussian initial condition:

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

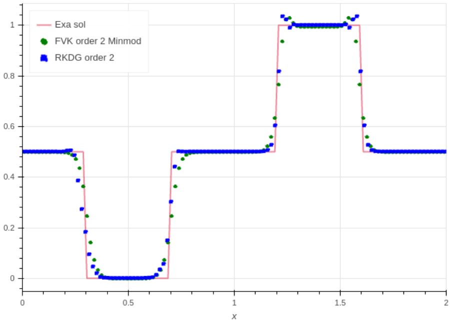


Density.

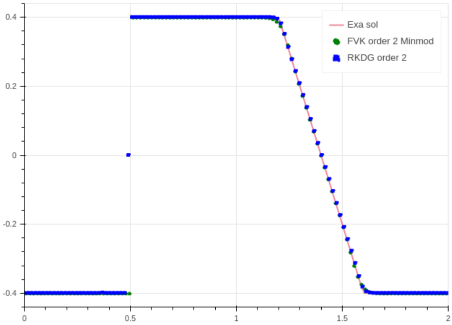


Vacuum test case

Initial condition: $\rho(x,0) = 0.5, u(x,0) = \begin{cases} -0.4 & \text{if} \quad 0.5 < x \text{ or } x > 1.8, \\ 0.4 & \text{if} \quad 0.5 < x < 1, \\ 1.4 - x & \text{if} \quad 1 < x < 1.8, \end{cases}$



Density



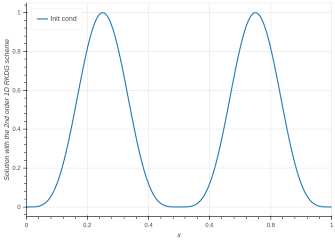
Velocity

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

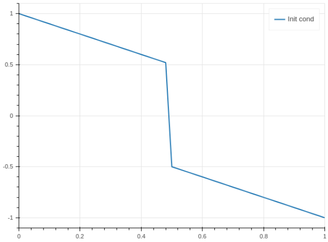
PGD system - δ-shock

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



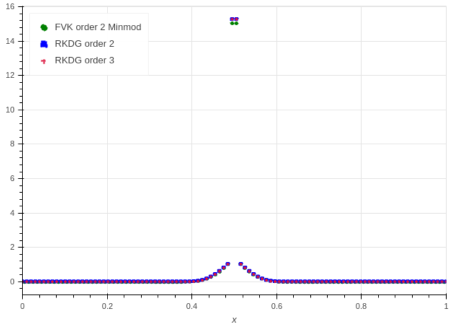
Velocity

Realizability domain:

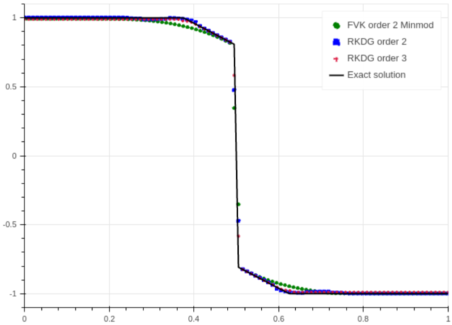
$$G := \left\{ \begin{pmatrix} \rho_i \\ \rho_i u_i \end{pmatrix}, \rho_i > 0, \quad m_i \leq u_i \leq M_i \right\}, m_i = \min(u_{i-1}, u_i, u_{i+1}), M_i = \max(u_{i-1}, u_i, u_{i+1})$$

δ-shock

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



Density



Velocity

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

Outline

Moments space

Transport part of the high order moment model [Essadki et al, 2018]:

$$\partial_t U + \partial_x F(U) = 0, \quad U = \begin{pmatrix} m_0 \\ m_{1/2} \\ m_1 \\ m_{3/2} \\ m_1 u \end{pmatrix} \in \mathbb{M}_N^{1/2}$$

Caracterisation of moments space with Hankel determinants $\underline{H}_i$, $\bar{H}_i$

Theorem [Dette and Studden, 1997]

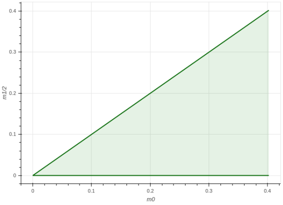
$$\vec{m}_N = \begin{pmatrix} m_0 \\ m_1 \\ \vdots \\ m_N \end{pmatrix} \in \mathbb{M}_N \Leftrightarrow \underline{H}_i \text{ and } \bar{H}_i \text{ are non negative for } i = 0, \cdots, N.$$

Realizability conditions

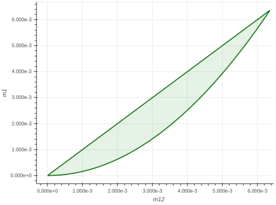
- $\underline{H}_0 = \bar{H}_0 = m_0 \geq 0.$
- $\underline{H}_1 \geq 0, \quad \bar{H}_1 \geq 0: \quad 0 \leq m_1 \leq m_0.$
- $\underline{H}_2 \geq 0, \quad \bar{H}_2 \geq 0: \quad \dfrac{m_1^2}{m_0} \leq m_2 \leq m_1.$
- $\underline{H}_3 \geq 0, \quad \bar{H}_3 \geq 0: \quad \dfrac{m_2^2}{m_1} \leq m_3 \leq m_2 - \dfrac{(m_1 - m_2)^2}{m_0 - m_1}.$

Maximum principle:

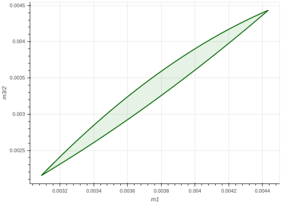
$$m_1 u_{\min} \leq m_1 u \leq m_1 u_{\max}.$$



(m_0, m_1) plane



(m_1, m_2) plane



(m_2, m_3) plane

Numerical procedure

For each quadrature point q:

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

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

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

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

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

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

For each cell:

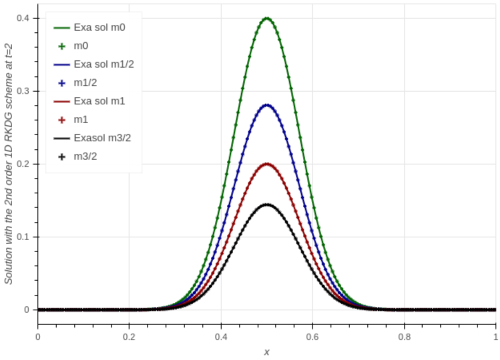
$$\begin{pmatrix} (\tilde{m}_0)_q \\ (\tilde{m}_{1/2})_q \\ (\tilde{m}_1)_q \\ (\tilde{m}_{3/2})_q \\ (\tilde{m_1 u})_q \end{pmatrix} = \begin{pmatrix} \bar{m}_0 \\ \bar{m}_{1/2} \\ \bar{m}_1 \\ \bar{m}_{3/2} \\ (\bar{m_1 u}) \end{pmatrix} + \theta \left[\begin{pmatrix} (\tilde{m}_0)_q \\ (\tilde{m}_{1/2})_q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

Advection

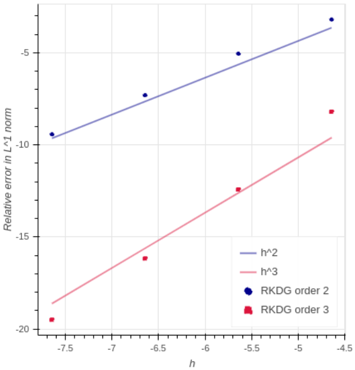
Initial moments:

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

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

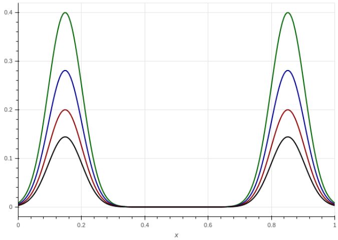


Fractionnal moments

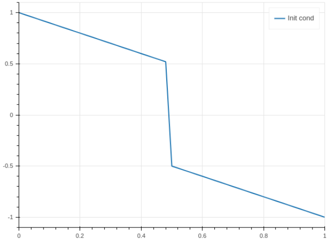


δ-shock test case

Initial condition:



Fractionnal moments

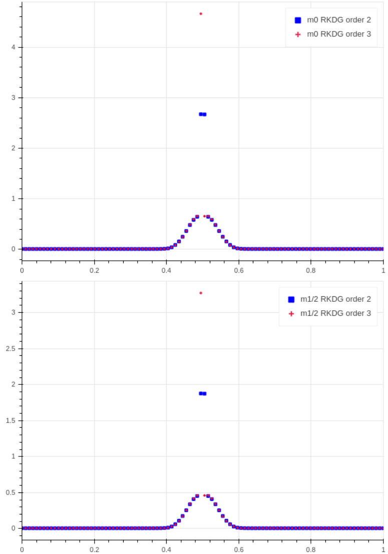


Velocity

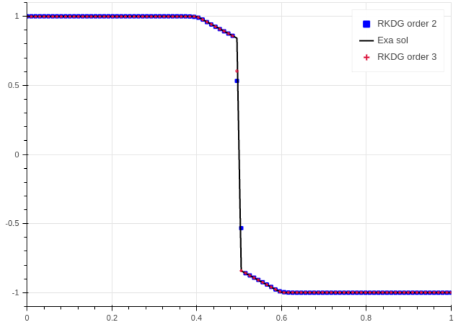
Realizability domain:

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

δ-shocks



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

Summary

- RKDG and the KFV are robust and accurate for the capture of singularities in moments models.
- Slope limiters for KFV scheme smear out discontinuities.
- Realizable RKDG schemes: projection in the convex set of moments [Ait Ameur et al, in preparation]

Outlook

- Extension to velocity moments models with Gaussian closures and to multidimensionnal problems.
- Link with separated phase models enriched by subscale flow modelling, [Loison et al, in preparation]
- Numerical methods for the unified modeling of two phase flows with separated and dispersed phases: Lagrange projection like methods, adaptive multiresolution SAMURAI library [Gouarin et al, 2021]

Thank you for your attention.