A stable, robust and high order accurate numerical method for Eulerian simulation of spray and particle transport on unstructured meshes

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1. Motivation and objectives

The general framework of the present contribution is the numerical simulation of physical phenomena where a discrete cloud of dense inclusions, liquid or solid, also called the dispersed phase, is transported within a continuous fluid phase. The large range of applications includes domains of multiphase combustion and alumina particles in rocket engines, as well as pollutant particle dispersion or cosmology.

This paper addresses the dynamics of the discrete particle phase. A common and widespread way of modeling this phase is to describe it at the level of each inclusion, considered as a point particle: the microscopic level. Each particle interacts with its local surrounding, and its state is then simply governed by a set of ordinary differential equations. This method, referred to as Lagrangian Discrete Particle Simulation, has quickly gained in popularity for its relative simplicity. It is however no longer suitable when a large number of particles has to be tracked to reach statistical convergence, as needed in most realistic applications. Furthermore, as the particle phase can become highly inhomogeneous, overcoming this issue by means of parallelization is complicated because of load balancing (Garcia 2009).

These drawbacks of the Lagrangian method explain why we are interested here in a mesoscopic approach, referred to as Eulerian. The particle distribution is represented by a Number Density Function (NDF), whose values depend on different parameters: space-time position, droplet size, velocity and temperature. The NDF variations are then governed by an evolutionary PDE in the parameter space, also called the phase space, which is known as the Williams-Boltzmann equation (Williams 1958). Because the phase space is high-dimensional, the direct resolution of the Williams-Boltzmann is hardly considered, and Eulerian methods instead solve for a finite set of moments, which are integrated quantities over the phase space. Because some information is lost during this last process, a closure model has to be given in order to compensate for the unknown information about higher order moments. To deal with the complex dynamics of particles in turbulent flows, several closures have been proposed in the literature (see Vié et al. 2012 and references therein). The main point is that, if the Stokes number based on the Kolmogorov time scale is close to one, high segregation effects occur, leading to the formation of depletion zones and stiff accumulations regions. Such effects can be reproduced using a monokinetic closure (Laurent & Massot 2001; de Chaisemartin 2009; Fréret et al. 2012), which leads to the well-known Pressureless Gas Dynamics system of equations (PGD). This system is weakly hyperbolic and is known to generate δ-shocks, i.e., strong accumulations, which often coexist with vacuum neighboring regions. Such mathematical singularities are difficult to handle, and particular care has to be given to
the numerical method. We are interested here in simulating this system because, while being predictive for low Stokes number, it is a challenging test case.

For sprays on structured grids, de Chaisemartin (2009) has proposed a second order kinetic scheme based on the work of Bouchut et al. (2003). It uses the underlying kinetic equation to obtain an exact evaluation in time of the fluxes at each interface, which leads to a minimal level of numerical dissipation. The final scheme has the important property of intrinsically preserving the natural properties at PDE level for the PGD system: the positivity of the number density and a discrete maximum principle on the velocity, which is not the case with classical linear high order finite volume schemes. This approach has been used for the simulation of turbulent particulate flows, and has also been adapted to more complex moment methods for polydisperse flows (Kah et al. 2012). For unstructured grids, a scheme has been proposed (Kah et al. 2012), but it is based on an approximate evaluation in time of the fluxes using a Runge-Kutta method, and hence no longer minimizes the dissipation; this imposes to reach higher order for the numerical scheme. Classical centered schemes, either finite element or finite volume, require artificial diffusion to stabilize the computation. This approach needs to optimize several parameters, and does not formally prevent the occurrence of negative number density, or high velocity oscillations.

In this paper, we present a Discontinuous Galerkin (DG) formulation for the simulation of PGD. Based on the work of Zhang & Shu (2010) and Zhang et al. (2012), this scheme is built to preserve the mean state within each element in a convex space of admissible states without destroying the overall arbitrarily high order accuracy of the scheme. The convex constraints on the mean states are essential for preserving the positivity of the number density and the maximum principle on the velocity. The content of the paper is the following: Section 2 gives a global overview of the modeling process, in order to understand the key features of PGD that our numerical scheme has to respect. In Section 3, we describe the numerical method in detail, first in one dimension of space, for the sake of legibility of our contribution, then extended to two dimensional triangular meshes. Once this has been done, the extension to any unstructured mesh is straightforward. Finally, numerical results and computation efficiency are discussed in Section 4.

2. Mesoscopic “kinetic” modeling of the dynamics of particles

We consider a disperse phase composed of particles, small enough to neglect their volume and allow a point-particle approximation. The statistics of such a disperse phase can be represented by a Number Density Function (NDF) \( f(t, x, \varphi) \) where \( t \) is the time, \( x \) the position and \( \varphi \) the phase space composed of as many dimensions as the number of parameters needed to describe the state of a particle. For example, \( \varphi = (\vec{c}, S, T) \) represents the space of admissible states in terms of velocity, size and temperature. In this phase space, the dynamics of \( f \) is governed by the Williams-Boltzmann equation (Williams 1958):

\[
\partial_t f + \vec{\partial}(\vec{\partial} f) + \vec{\partial}(\vec{F} f) + \partial_S (R_S f) + \partial_T (K f) = \Gamma + Q, \tag{2.1}
\]

where the first two terms represent the free transport of the spray, \( \vec{F} = d_\vec{c} \vec{c} \) is the acceleration due to the drag force coming from the underlying carrier fluid, \( R_S = -d_S \) the rate of change in the droplet size (evaporation), \( K = d_T \) the rate of change of the droplet temperature and \( \Gamma \) and \( Q \) are additional source terms to take collision and secondary break-up into account. By introducing a characteristic particle relaxation time
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τ, we can further model the drag force interaction as: \( \vec{F} = (\vec{u}_g - \vec{c})/\tau_p \), with \( \vec{u}_g \) being the carrying gas velocity.

Given the high number of dimensions of the phase space, the direct resolution of kinetic equation (2.1) is hardly considered. It is interesting to integrate this equation over whole directions of the phase space and to deduce the equations governing the evolution of the various moments of the NDF, \( f \). In order to focus on transport and drag force, we consider a unique size for all particles, and neglect collisions, secondary break-up, evaporation and heat transfer, thus canceling the four last terms of (2.1). In fact, modeling strategies have already been proposed for each term (de Chaisemartin 2009; Doisneau et al. 2012; Rimbert et al. 2012) and we envision taking them into account using a specific splitting strategy, see for example Doisneau et al. (2012).

If we consider a monokinetic assumption, we can now write the NDF as:

\[
f(t, \vec{x}, \vec{c}) = \rho(t, \vec{x}) \delta(\vec{c} - \vec{u}(\vec{x}, t))
\]

where \( \vec{u}(t, \vec{x}) \) is the mean velocity of the disperse phase. By integrating Eq. (2.1) over the velocity space, it yields in a straightforward manner to the PGD system of equations with source terms:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \vec{u}}{\partial x} &= 0, \\
\frac{\partial \rho \vec{u}}{\partial t} + \frac{\partial \left( \rho \vec{u} \otimes \vec{u} \right)}{\partial x} &= \frac{\rho(\vec{u}_g - \vec{u})}{\tau}.
\end{align*}
\]

If we consider the free transport part of this system, it has three main properties (see Bouchut 1994 for details): (1) it is weakly hyperbolic, in the sense that the Jacobian of the flux has in each direction a unique eigenvalue of multiplicity \( d \), the space dimension, but is non-diagonalizable. This implies the ability of the system to generate \( \delta \)-shocks, i.e., stiff accumulations of particles, that need to be handled by the numerical scheme; (2) \( \rho \geq 0 \) to ensure that the pair of moments \((\rho, \rho \vec{u})\) is always linked to \( f(t, \vec{x}, \vec{c}) \geq 0 \) (realizability condition); and (3) \( \vec{u} \) must satisfy a maximum principle. Such properties define a convex space of valid moment sets, called the realizable space. Therefore convex constraints have to be held on the numerical solution states to deal with singular solutions, such as \( \delta \)-shocks. Considering the treatment of the source terms, as the current study is focused on the free transport part, we evaluate the source terms using the mean value of the state inside each cell. A specific treatment adapted to DG can be envisaged, but is out the scope of the present work.

3. A high order realizable space preserving numerical scheme on unstructured grids

This section summarizes the main ideas of Zhang & Shu (2010) and Zhang et al. (2012), and extends their framework to the particular case of the weakly hyperbolic Pressureless Gas Dynamic system.

3.1. One dimensional analysis

In one dimension of space, the system of conservation laws can be written:

\[
\frac{\partial W}{\partial t} + \frac{\partial \mathcal{F}(W)}{\partial x} = 0, \quad x \in [0, 1], \ t \in [0, T],
\]

where \( W(x, t) \) is the unknown state and \( \mathcal{F}(W) \) the conservative flux. In the case of the PGD system, one has \( W = (\rho, \rho \vec{u}) \) and \( \mathcal{F}(W) = (\rho \vec{u}, \rho \vec{u}^2) \). A problem with initial condition \( W_0 \) and periodic boundary condition is considered:

\[
W(0, t) = W(1, t), \ \forall 0 < t < T, \quad W(x, 0) = W_0(x), \ \forall x \in [0, 1].
\]
Without loss of generality, \([0, 1]\) is discretized into \(N\) regular sub-intervals. Let

\[
x_{i - 1/2} = \frac{i - 1}{N}, \quad x_i = \frac{i}{N}, \quad x_{i + 1/2} = \frac{i + 1}{N}, \quad i = 1, ..., N,
\]

and \(C_i\) be the interval \([x_{i - 1/2}, x_{i + 1/2}]\).

### 3.1.1. Classical DG Formulation

If \(k \in \mathbb{N}^+\) is the desired order of the method, let \(\varphi_j(x), j = 1, ..., k + 1\) be \(k + 1\) basis functions of polynomials of order \(k\) within \(C_i\). Without further explanation (see Cockburn \\& Shu 1998), the Discontinuous Galerkin approximation of equation (3.1) is the piecewise polynomial solution

\[
W_h(x, t) = \sum_{i,j} W_i^j(t)\varphi_i(x)\chi_{C_i}(x),
\]

where subscript \(h\) stands for a mesh characteristic size and \(\chi_{C_i}\) is \(C_i\) indicator function, of the following differential system:

\[
|C_i| (M)_h dW_i^k + \left(\mathcal{F}^+_{i + 1/2} \varphi_i^j(x_{i + 1/2}) - \mathcal{F}^-_{i - 1/2} \varphi_i^j(x_{i - 1/2})\right),
\]

\[
= \int_{C_i} \mathcal{F}(W_h(x))\partial_x \varphi_i dx, \quad \forall i = 1, ..., N, \quad \forall j = 1, ..., k,
\]

where \(M\) is the discrete problem mass matrix given by \((M)_h = \int_{C_i} \varphi_i(x)\varphi_i(x) dx\) and \(\mathcal{F}^+_{i + 1/2}\) and \(\mathcal{F}^-_{i - 1/2}\) are the numerical fluxes at \(x_{i + 1/2}\) and \(x_{i - 1/2}\), respectively. This numerical scheme in space has a truncation error of order \(h^{k+1}\) for regular enough solutions. Furthermore, when a \((k + 1)\)th-order accurate scheme in time is used to integrate each equation of system (3.2), the scheme is globally \((k + 1)\)th-order in space and time. This is always going to be the case when using a \(k + 1\)-step Runge-Kutta (RK) method.

### 3.1.2. Realizability preserving high order scheme

In the rest of this section, we consider a forward Euler approximation in time, which is also a 1-step Strong Stability Preserving (SSP) RK method. This restriction is only for the sake of simplicity and all the results generalize to any SSP time integrator. In the following, we explain how to generate a realizability preserving high order numerical scheme that satisfies the realizability conditions defined in Section 2 for the PGD system.

At first order, the general Lax-Friedrichs scheme writes:

\[
\mathcal{F}^+_{i + 1/2} = \frac{\mathcal{F}(\bar{W}_{i + 1}) + \mathcal{F}(\bar{W}_i)}{2} - \frac{\alpha_{i + 1}^r}{2}(\bar{W}_{i + 1} - \bar{W}_i),
\]

where \(\alpha_{i + 1}^r\) is greater than the eigenvalues (velocities) of the Jacobian of \(\mathcal{F}\) at \(\bar{W}_{i + 1}\), \(\bar{W}_i\).

The state in \(C_i\) is updated by:

\[
\bar{W}_i^{r+1} = \bar{W}_i^r - \frac{\Delta t}{|C_i|} \left(\mathcal{F}^+_{i + 1/2} - \mathcal{F}^-_{i - 1/2}\right)
\]

\[
= \left(1 - \beta_i^{r+1} - \beta_i^{r-1}\right)\bar{W}_i + \beta_i^{r+1}\left(\bar{W}_{i + 1}^r - \frac{\mathcal{F}(\bar{W}_{i + 1}^r)}{\alpha_{i + 1}^r}\right) + \beta_i^{r-1}\left(\bar{W}_{i - 1}^r + \frac{\mathcal{F}(\bar{W}_{i - 1}^r)}{\alpha_{i - 1}^r}\right),
\]

with \(\beta_i^r\) defined by

\[
\beta_i^r = \frac{\Delta t\alpha_i^r}{2|C_i|}.
\]
In the case of PGD, we can define the following abstract state
\[ W^{\ast, \pm}_j = W_j \pm \frac{\mathcal{F}(W_j)}{a_j} = \left( 1 \pm \frac{u_j}{a_j} \right) \rho_j, \quad (1 \pm \frac{u_j}{a_j})(\rho a_j) \right), \quad j = i \pm 1, \]
so that if the density of \( W_j \) is strictly positive, the resulting state \( W^{\ast, \pm}_j \) also has a strictly positive density and the same velocity as \( W_j \). Therefore, when the following CFL condition holds:
\[ \frac{\Delta t (a^{i+1}_q + a^{-1}_{q-1})}{2|C|} \geq 1, \]
\( W^{\ast, 1}_{i+1} \) has a strictly positive density and its velocity is a convex combination of those of \( W_{i-1}, W_i \) and \( W_{i+1} \), hence satisfying the maximum principle.

Let us now go to higher order. Using an appropriate Gauss-Lobatto formula, the following statement is exact, provided \( 2m - 3 \geq k \):
\[ W_i = \int_{C_i} W_h(x) dx = \sum_{q=1}^{m} \omega_q W_h(x_q), \quad (3.5) \]
where \( x_q, q = 1, \ldots, m \) are the coordinates of the Gauss-Lobatto quadrature points within \( C_i \) and \( \omega_q \) their associated strictly positive weights. For later purposes, we extend these quadrature points to \( q = 0, \ldots, m+1 \), setting \( x_0 \) (resp. \( x_{m+1} \)) as the coordinate of the right (resp. left) quadrature point in the left (resp. right) neighboring cell. Then by summing Eq. (3.2) over all the degrees of freedom \( j \) of one cell \( C_i \), assuming the time derivative terms have been approximated by a forward Euler scheme, we obtain:
\[ W^{\ast, 1}_{i+1} = W^m_i - \frac{\Delta t}{|C|} \left( \mathcal{F}^{\ast}_{i+\frac{1}{2}} - \mathcal{F}^{\ast}_{i-\frac{1}{2}} \right), \quad (3.6) \]
where the numerical fluxes \( \mathcal{F}^{\ast}_{i+\frac{1}{2}} \) and \( \mathcal{F}^{\ast}_{i-\frac{1}{2}} \) depend on the reconstructed states on each side of the cell boundary and one can write:
\[ \mathcal{F}^{\ast}_{i+\frac{1}{2}} - \mathcal{F}^{\ast}_{i-\frac{1}{2}} = \mathcal{F}^{\ast}(x_{i+\frac{1}{2}}) - \mathcal{F}^{\ast}(x_{i-\frac{1}{2}}) = \sum_{q=1}^{m} \mathcal{F}^{\ast}(x_{q+1}) - \mathcal{F}^{\ast}(x_{q}). \quad (3.7) \]
Combining (3.6), (3.5) and (3.7), we finally get
\[ W^{\ast, 1}_{i+1} = \sum_{q=0}^{m} \omega_q \left( W_h(x_q) - \frac{\Delta t}{\omega_q |C|} \left( \mathcal{F}^{\ast}(x_{q+1}) - \mathcal{F}^{\ast}(x_{q}) \right) \right). \quad (3.8) \]
All quadrature weights being strictly positive, this is a convex combination of first order abstract updates at quadrature points. Thus, \( W^{\ast, 1}_{i+1} \) has a strictly positive density and its velocity is a convex combination of the velocities at quadrature points, if the density is strictly positive at all the quadrature points and the stronger CFL constraint
\[ \frac{\Delta t a^{q+1}_q}{|C|} \leq \min_q \omega_q, \quad (3.9) \]
holds everywhere. Even though the last restriction on the time step could appear as very strong, it is in fact close enough to the CFL constraints of the current, widely used, RK-DG methods (see Zhang et al. 2012 for more detail).
3.1.3. Mean value and accuracy preserving realizability space projection

The last thing is now to ensure that the numerical solution $\mathbf{W}_h$ respects the constraints at the quadrature points. To achieve this, we need a smart projection at each time step that ensures the last property, without changing the cell mean value and without destroying the solution accuracy. The idea is that for any quadrature state $\mathbf{W}_i^q$ lying outside the space of constraints, there exist a unique $\theta \in [0, 1]$ such that $\mathbf{W}_i^q = \theta \mathbf{W}_i + (1 - \theta) \mathbf{W}_i$ is at the boundary of the constraint space. Within each cell $C_i$, we can now redefine the numerical solution as

$$\mathbf{W}_h(x) = \theta_i (\mathbf{W}_h(x) - \mathbf{W}_i) + \mathbf{W}_i, \quad \theta_i = \min_{q=1,...,m} \theta_q.$$  

First, the mean value of the updated numerical solution is obviously $\mathbf{W}_i$. Next, if the continuous solution is smooth enough, $\|\mathbf{W}_h - \mathbf{W}_i\| = O(h)$ and $\|\mathbf{W}_h - \mathbf{W}_i\| = O(h^{k+1})$ if $\theta_i - 1 = O(h^k)$. This last property is thoroughly demonstrated in Zhang (2011), which ends the proof that $\mathbf{W}_h$ is a $k+1$th-order approximation of $\mathbf{W}_h$, respecting the convex constraints at all the quadrature points of the mesh.

3.2. Realizability preserving DG method in two dimensions

What mostly prevents the straightforward generalization of the previous reasoning to two dimensional triangular meshes is how to define an exact quadrature with positive weights on the triangles such that an equivalent form of Eq. (3.7) can be written. We first recall the DG variational formulation of a 2D conservation law. Let $\mathbf{F}(\mathbf{W}) = (f(\mathbf{W}), g(\mathbf{W}))$ be a conservative flux and $\mathbf{F}^+(\mathbf{W}_i, \mathbf{W}_j, \mathbf{n}_j)$ an associated numerical flux across an edge with normal $\mathbf{n}_j$, separating two states $\mathbf{W}_i$ and $\mathbf{W}_j$. $\mathbf{F}^+$ is chosen to be realizability preserving, like the general Lax-Friedrichs flux in (3.4). If $T$ is a triangle of the mesh and $j$ a degree of freedom of this triangle with $\varphi_j^T(x)$ its associated $k$th-order basis function, the scheme reads:

$$\int_T (\mathcal{M})_j d_t \mathbf{W}_j^T + \int_{\partial T} \mathbf{F}^+ (\mathbf{W}_{ext}(s), \mathbf{W}_{int}(s), \mathbf{n}(s)) \varphi_j^T(s) \, ds = \int_T \mathbf{F}(\mathbf{W}(x)).\mathbf{n} \varphi_j^T \, dx.$$  

(3.10)

As in the previous subsection, we now sum over all the degrees of freedom $j$ of $T$ and get the equation governing the evolution of the mean value in $T$:

$$d_t \mathbf{W}_T + \int_{\partial T} \mathbf{F}^+ (\mathbf{W}_{ext}(s), \mathbf{W}_{int}(s), \mathbf{n}(s)) \, ds = 0.$$  

(3.11)

The contour integral in the previous equation can be estimated at the accuracy of the scheme using the appropriate Gauss quadrature. Let then $N_q^{\partial T}$ denote the number of Gauss quadrature points used per edge and $N_q^T$ the number of quadrature points used to compute the right hand side of (3.10) on the whole element. If we want to generalize formula (3.8) to two dimensions in order to propagate the convex constraint from one time step to another, we need to find an element quadrature formula with the following properties:

- it is exact for polynomial of order $k$;
- all its quadrature weights are strictly positive;
- its restriction to the edges of the element are the Gauss quadrature points used to integrate the numerical flux on $\partial T$.

A general procedure to achieve such a quadrature is given in Zhang et al. (2012). The main idea is that such a quadrature naturally exists on quadrangles by the tensorial
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product of 1D Gauss quadrature points in one direction and 1D Gauss-Lobatto quadra-
ture points in the other direction. Such a 2D quadrature can then be carried on triangles
using the three non one-to-one $Q^1$ transformations of the plan which send the top edge of
the reference quadrangle onto each of the three vertices of the triangle respectively and
the remaining three edges of the quadrangle on the three edges of the triangle. Zhang
et al. (2012) describe thoroughly the transformations, the three resulting set of quadra-
ture points and the quadrature weights of the new quadrature: the superposition of the
three obtained quadrature. It is then shown that the new quadrature fulfills the three
above requirements.

Finally, when a SSP scheme in time is used to approximate the time derivative in Eq.
(3.11), e.g., forward Euler, when the 2D new quadrature is used to replace the mean state
in $T$ at time step $n$ ($\bar{W}^n_T$), and all these terms are smartly rearranged, the mean state in
$T$ at time step $n + 1$ ($\bar{W}^{n+1}_T$) can be expressed as a convex combination of the states in the
interior of $T$ and convex constraints preserving fluxes between the states at the Gauss
quadrature points on the edges of $T$ and its neighbors (see Zhang et al. 2012 for more
details). Thus, if the states at all the quadrature points lie in the space of constraints,
$\bar{W}^{n+1}_T$ automatically does in too. The final process is then to ensure that the constraints
are verified at each quadrature point of each triangle of the mesh and this is done using
the same algorithm as the one described at the end of the 1D subsection.

4. Numerical results

This section now presents results on PGD test cases in one and two dimensions of
space. However, in order to assess the accuracy of the method, a simple linear advection
problem with a relatively smooth initial condition is first considered.

4.1. 1D test cases

In order to validate our understanding and the performance of the general scheme, we
have first applied it on one dimensional test cases. The first one is a linear scalar advection
of a regularized hat function. The goal is to show that the scheme behaves well in the
presence of pseudo-discontinuities, that no oscillations occur and that we still keep the
desired order of accuracy. Next, we proceed to a more complex case in the Pressureless
Gas Dynamic (PGD) framework. We study the collision of two symmetric one dimensional
droplet clouds. The solution is known to produce a Dirac singularity in finite time on the
density component, what is called a $\delta$-shock.

4.1.1. The regularized hat linear advection

Let us consider the simple one dimensional linear advection equation

$$\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0, \quad (x,t) \in [0,1] \times [0,\frac{1}{a}], \quad (4.1)$$

where $u$ is a scalar unknown and $a$ is the constant advection speed ($a = 1$ without loss
of generality). The periodic boundary condition is ensured by $u(0,t) = u(1,t), \forall t$. Finally,
the initial condition is given in the form of a regularized hat-shaped function. Given a
thickness parameter $0 < \varepsilon < 0.25$, we prescribe for all $x \in [0,1]$: \[
    u(x,0) = u_0(x) = \begin{cases}
        0.5 \left( 1 + \tanh \left( \frac{\varepsilon}{0.25-x} + \frac{\varepsilon}{0.25+\varepsilon} \right) \right), & 0.25 \leq x \leq 0.25 + \varepsilon, \\
        1, & 0.25 + \varepsilon \leq x \leq 0.75 - \varepsilon, \\
        0.5 \left( 1 + \tanh \left( -\frac{\varepsilon}{0.75-x} - \frac{\varepsilon}{0.75+\varepsilon} \right) \right), & 0.75 - \varepsilon \leq x \leq 0.75, \\
        0, & \text{otherwise}.
    \end{cases}
\] (4.2)

Because the initial condition $u_0$ takes its value between 0 and 1, we want $u_t(x,t)$ to stay between these two bounds. This is here our constraint. We then perform a series of simulations with different values of $h = \Delta x = 1/N$ and $0 < \varepsilon < 0.2$, and compare the solution at time $t = 1$ (after it has completed a full rotation around [0,1]), with the initial condition. Results are presented in Figure 1. On the top left image, we can appreciate the good behavior of the numerical solution even when the exact solution is stiff: $\varepsilon = 0.05$. No slope limiter has been used here and the CFL constraint is 0.9 times the theoretical stability constraint. This means (see 3.9) $\Delta t < 0.9h$ at first order, $\Delta t < 0.45h$ at second order and $\Delta t < 0.15h$ at third order. We did not use 1.0 because we wanted to avoid the exact solution obtained at first order. The variation of the mean values of the cells is perfectly monotonic. Moreover, when looking at the convergence curves, the order of accuracy is very satisfying. The convergence slope at third order in space and time meets the theoretical order of accuracy, even for small values of $\varepsilon$. We observe two distinct behaviors: when $\Delta x = 1/N < \varepsilon/10$ the scheme converges at lower order, but it recovers its theoretical order as soon as enough points lie in the stiff region. The convergence on coarser meshes is however much better than the expected first order when the numerical scheme sees a shock and it fully recovers the higher order when the representation of the exact solution is smooth enough.

**4.1.2. The PGD Dirac singularity**

We now present a more complex problem. We consider the one dimensional Pressureless Gas Dynamic system, with $\rho$ the density and $\rho u$ the first order velocity momentum:

\[
\begin{align*}
    \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} &= 0, \\
    \frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} &= 0.
\end{align*}
\] (4.3a) (4.3b)
We are still interested in the unity domain \([0, 1]\) with periodic boundary conditions. The first equation is a transport equation at advection speed \(u\). Next, when \(\rho\) and \(u\) are both regular enough, partial derivatives of Eq. (4.3b) can be expanded and by subtracting the first relation we get the Burgers equation on \(u\). Initial condition

\[
\rho(x, 0) = \rho_0(x) = \begin{cases} 
a & x \leq 0.5 \\
-a & x > 0.5 
\end{cases},
\]

is known to be a steady solution of the Burgers equation. We set \(a = 1\) and initialize \(\rho\) with a function which is very regular on \([0, 1]\) and symmetric with respect to 0.5, let us say

\[
\rho(x, 0) = \rho_0(x) = \sin^4(2\pi x).
\]

The symmetric perturbations in \(\rho\) are then propagating toward each other and the density is irreversibly concentrating at \(x = 0.5\). The solution of system (4.3) with initial condition (4.4)-(4.5) (which is \(C^1\) when considering the conserved state \(W = (\rho, \rho u)\)) becomes singular and steady at time \(t = 0.5\) with

\[
\rho = m \, \delta_{0.5} \quad , \quad u = \begin{cases} 
1 & \text{if } x < 0.5 \\
0 & \text{if } x = 0.5 \\
-1 & \text{if } x > 0.5 
\end{cases},
\]

where \(m\) denotes the conserved total mass, and \(\delta_{\epsilon}\) the Dirac distribution. These figures show the evolution of the particle density. The constraint space is preserved all along the simulation. At time \(t = 0.5\), all the matter is concentrated in a sharp needle at \(x = 0.5\) and \(\rho\) is positive everywhere. The \(\delta\)-shock is contained within 2 cells on each side of the singularity and this stays true when refining the mesh. Detail of the velocity shows that the condition \(-1 < u < 1\) still applies, and \(u\) varies monotonically. Furthermore, vacuum has been created outside of the interval \([0.42, 0.58]\), where \(u = \frac{\rho_u}{\rho}\) is undefined. This proves the low level of numerical diffusion close to transition to vacuum zones.

### 4.2. 2D test case: a homogeneous spray over a frozen HIT

In this subsection, we are interested in testing the robustness of the algorithm on two dimensional cases where singularities such as \(\delta\)-shocks occur. The goal is to be able to capture these singularities accurately (possibly within one mesh cell), while maintaining the positivity of the density and ensuring a maximum principle on the advection velocity.

This last test case is a one way interaction between a monokinetic spray which is homogeneous at \(t = 0\) and a steady homogeneously turbulent velocity field. As explained
in Section 2, under the monokinetic assumption the Williams-Boltzmann equation is equivalent to the PGD with source term system (2.2), with a zero pressure-like tensor. Let us underline that a refined integration of the spatially varying source term, even in the case of a non-linear source, could be integrated without much difficulties in the present framework, providing a higher order spatial coupling between the gaseous field and the droplet repartition. However, we use here a simple integration of the source term for the sake of comparison with the FV method proposed in this contribution. The right hand side is taken into account with a second order Strang splitting method. The underlying gas velocity field being given, steady and constant per element, the ODE given by the splitting can be analytically integrated, which greatly simplifies the implementation. The simulation begins with a constant droplet density throughout the domain, after which the computation is allowed to converge toward steady state. We compare the result given by the new unstructured second order method with the one given by a structured second order TVD finite volume method (de Chaisemartin 2009). This is shown in Figure 3. Top-right is the “reference” structured solution. The structured mesh has first been cut into triangles and second order DG method has been run on the obtained mesh. The DG result provides much finer structures and droplet clusters than the FV result. This is
due to smaller numerical dissipation. On the other hand, the DG computation requires a much higher CPU time, about 5 more time per degree of freedom. We have then been running the same case on a coarser mesh. As one can see in Figure 3, the result obtained with DG on a $h = 1/64$ unstructured mesh is qualitatively comparable to the $256^2$ structured FV reference result. In terms of computational time, the FV computation took 142.36s, when the unstructured DG on the coarser unstructured mesh took 123.08s. Of course, this study is only qualitative and further tools need to be developed to assess the competitiveness of our DG method, but it still is a very promising comparison between FV and DG approaches.

5. Final words

In this paper, we have presented a very promising numerical method for the Eulerian direct simulation of particle and spray dynamics in turbulent flows. These dynamics are described in a Eulerian point of view, through hyperbolic or weakly hyperbolic systems of conservation laws for the evolution of the moments of the NDF. A realizability preserving arbitrary high order Discontinuous Galerkin method has been designed in order to solve the singularity and vacuum generating Pressureless Gas Dynamics system coupled to Stokes drag force for monodisperse inclusions. Through the different test cases considered, we have appreciated the robustness and accuracy of the DG method, even when considering isotropic unstructured grids and singular solution. Furthermore, for an equivalent quality of the results, the computational time of DG, even if designed for unstructured grids, is comparable to the FV scheme with optimal numerical dissipation on structured grids. In the ultimate objective of designing an accurate, robust and efficient scheme for unstructured meshes, the present DG scheme appears to be an interesting first step, as it fulfills all the realizability and robustness properties, which are of primary interested for applications to realistic configurations in complex geometries.

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REFERENCES


DOISNEAU, F., LAURENT, F., MURRONE, A., DUPAYS, J. & MASSOT, M. 2012 Eulerian


