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A Finite Volume Scheme to Compute Incompressible Gas-solid Two-Phase Flows

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Abstract

We present in this paper some new Finite Volume method to compute gas-solid two-phase flows on triangular meshes, when assuming that both phases have constant densities. The governing set of equations which is expected to describe the behaviour of the flow is a four-equation model, which accounts for mass balance and momentum balance within each phase. Granular pressure effects are accounted for so that one may compute either dilute flows or very dense flows up to the maximum compactness rate. Thanks to the latter, the maximum principle for the void fraction of particles is ensured at the continuous level, as shown in a previous work. Moreover, the fractional step method which is applied for herein enables to preserve both the lower bound and the upper bound in the discrete case, when using a Godunov scheme. The Rusanov scheme which is applied for herein also enables to ensure the same property on the lower bound of the void fraction, whatever the unstructured mesh is, and the upper bound provided that some condition on the time step holds. This renders the whole algorithm rather attractive, though Rusanov scheme is a bit less accurate than Godunov scheme, as confirmed by measurements of the rate of convergence in L1 norm in the purely single phase framework, when focusing on shock tube experiments. Standard second-order extensions with respect to time and space may obviously be derived using present formulation.

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Introduction

When computing two phase flows using the two fluid approach, a particular case arises when densities within both phases are constant. This occurs for instance when simulating gas-solid flows, assuming that the gas flow velocities are very small compared with the speed of sound waves in the gas phase. In this frame, the two governing equations for partial densities may be combined, in such a way that a divergence free constraint for a specific velocity (namely \( \alpha_1 \bar{U}_1 + \alpha_2 \bar{U}_2 \)) occurs, while the other equation simply represents the unsteady governing equation for the volumetric fraction of particles. As occurs when computing standard Navier Stokes equations for an incompressible fluid, the whole algorithm should take this specificity into account in order to build a stable numerical method. This is precisely the main objective of the present study.

The governing set of equations is recalled first, and closure laws are defined, including the specific form of the granular pressure which enables to preserve the maximum principle for the void fraction. The time scheme is detailed first, and space discretizations are given afterwards. The Finite Volume approach allows computations on unstructured triangular meshes. A prediction step first provides an initial guess for the mean momentum field within each phase, together with the mean particle void fraction. A second so-called correction step slightly modifies the momentum field, for given ‘frozen’ void fraction field, by solving the pressure field which ensures the divergence free constraint. Extensive validation of the prediction step, which involves the first order Runge-Kutta scheme ([32]) to approximate convective fluxes, is reported in [7]. This includes computation of particle shock waves but also strong double rarefaction waves where a vacuum of particles may appear. Numerical schemes to account for viscous fluxes are detailed in [6] and [12], based on the initial proposition and theoretical convergence results which can be found in [18] and [28]. We only provide in this paper an interesting two-dimensional test case which shows the ability of the scheme to deal with the maximum compactness rate, and meanwhile to cope with low gas velocity fields. This case is also documented in [15], [16] and [17], where the numerical approach assumes that the compressibility of the gas phase is non-vanishing.

Governing equations

Using standard averaging process, governing equations for the mean partial masses and the mean momentum in each phase may be written as:

\[
\frac{\partial}{\partial t} \left( \alpha_k \rho_k \right) + \nabla \cdot (\alpha_k \rho_k \bar{U}_k) + \Gamma_k = 0
\]

\[
\frac{\partial}{\partial t} \left( \alpha_k \rho_k \bar{U}_k \right) + \nabla \cdot (\alpha_k \rho_k \bar{U}_i \otimes \bar{U}_k)
+ \nabla \cdot (\alpha_k \rho_k \left( u'_{i,k} \otimes u'_{k,k} \right) ) + \alpha_k \nabla P_k \\
- \nabla \cdot \left( \alpha_k \bar{T}_k \right) + \bar{J}_k = \alpha_k \rho_k \bar{E}_k
\]

In the following, the gas phase is labelled with subscript 1, and the particle phase with index 2. Closure laws are the following, assuming of course that \( \alpha_1 + \alpha_2 = 1 \), and also that both \( \rho_1 \) and \( \rho_2 \) are constant.

- Interfacial mass transfer term:
  \( \Gamma_k = 0 \)
- Pressure balance:
  \( P_1 = P_2 = P \)
- The turbulence within gas phase may be neglected:
  \( \langle u'_{i} \otimes u'_{i} \rangle_1 = 0 \)
- The viscous strain tensor within the gas phase is given by:
  \( \tau = \mu_1 \left( \nabla u_1 + \nabla u_1^T - \frac{2}{3} (\nabla \cdot u_1) I_d \right) \)
• The whole strain for the particle phase, including granular pressure effects, may be written:

\[
\rho_2 (\mathbf{u}_2' \otimes \mathbf{u}_2') - \tau_2 = \rho_2 \Theta (\alpha_2) \mathbf{L}
\]

\[-\mu_2 (\nabla \mathbf{u}_2 + \nabla \mathbf{u}_2^T) \nabla \mathbf{u}_2 - \frac{2}{3} (\nabla \cdot \mathbf{u}_2) \mathbf{I} \mathbf{L} \]

where:

\[
\alpha_2 \Theta (\alpha_2) = \alpha_2 - \frac{\alpha_2 \alpha_{max}}{\alpha_2 - \alpha_{max}} + 2 (\alpha_2)_{max} \ln \left( \frac{\alpha_{max}}{\alpha_2} \right)
\]

The specific form of the granular pressure law \( \Theta (\alpha_2) \) enables computing either dilute flows or dense flows (since \( \Theta (\alpha_2) \) grows up to infinite as \( \alpha_2 \) tends towards \( \alpha_{max} \)). The square of the celerity of particle waves is:

\[
c_2^2 = \left( \alpha_2 \Theta (\alpha_2) \right)^2 = \left( \frac{\alpha_2}{\alpha_{max} - \alpha_2} \right)^2
\]

• The interfacial momentum transfer term only accounts for drag effects:

\[
\mathbf{L}_I = -\mathbf{L}_T = -\alpha_1 \alpha_2 K_T (\mathbf{U}_2 - \mathbf{U}_1)
\]

Other detailed forms of the granular pressure can be found in [2], [4], [17], [23], [25], [27], [30]. The drag coefficient assumes that Ergun’s law is valid in the dense limit.

We may also introduce the total energy for the two-phase model which is:

\[
E = \sum_{k=1,2} \frac{\alpha_k \rho_k U_k U_k}{2} + \rho_2 \eta (\alpha_2)
\]

\[
E = \sum_{k=1,2} \left( \frac{\alpha_k \rho_k U_k}{2} \right) U_k + P \left( \sum_{k=1,2} \alpha_k U_k \right) + \rho_2 \mu (\alpha_2) \mathbf{L}_2
\]

Functions above are in agreement with:

\[
\mu (\alpha_2) = \eta (\alpha_2) + \alpha_2 \Theta (\alpha_2)
\]

\[
\eta (\alpha_2) = \int_0^{\alpha_2} \left( \frac{\alpha_2 \Theta (\alpha_2)}{\alpha_2} \right)' d\alpha_2
\]

Thus one may easily derive the following governing equation for the total energy:

\[
\frac{\partial}{\partial t} (E) + \nabla \cdot (E) - \nabla \cdot \left( \sum_{k=1,2} \frac{\Sigma_k U_k}{\mu (\alpha_2)} \right) = S
\]

Restricting to the frame of closed geometry with no slip conditions on the whole boundary, enables to write the following inequality:

\[
\frac{\partial}{\partial t} (\int \Omega E \ d\Omega) \leq \text{RHS}
\]

with:

\[
\text{RHS} = - \int \Omega \left( \sum_{k=1,2} (\alpha k \rho_k U_k) \right) \eta (\alpha_2) \ d\Omega
\]

due to the form of the interfacial momentum transfer term \( \mathbf{L}_I \) and since:

\[
\Sigma_k = \alpha_k \mu_k \left( \nabla \mathbf{u}_k + \nabla \mathbf{u}_k^T \right) \nabla \mathbf{u}_k - \frac{2}{3} (\nabla \cdot \mathbf{u}_k) \mathbf{I}
\]

This shows that one may control the total energy of the whole system with respect to time.

**Numerical method**

The basic underlying ideas are the following, and rely on a recent proposal to solve Navier-Stokes equations ([5], [6], [13], [8]), and on previous experience within the frame of compressible gas-solid two-phase flows ([17]). It is first assumed that, in order to derive a sufficiently stable scheme, one needs to build some scheme which enables non viscous computations; hence, only convective effects, buoyancy forces, drag forces and mean pressure gradient are accounted for herein.

The whole scheme is split into two parts:

• a predictive step provides some approximation of the void fraction field and the mean momentum within each phase;

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a corrective step enables to ensure the divergence free constraint \( \nabla \cdot (\alpha_1 \mathbf{U}_1 + \alpha_2 \mathbf{U}_2) = 0 \).

\[
W^n + \Delta t (\alpha_1 \alpha_2 K_T) \left( \begin{array}{c}
\frac{V - V_i}{U^2 - U_i} \\
\frac{U^2 - U_i}{\rho_i}
\end{array} \right) = W^n
\]

In the following, the state variable lies in \( \mathbb{R}^5 \):

\[
W = \begin{bmatrix}
\alpha_2 \\
\alpha_2 U_2 \\
\alpha_2 U_3 \\
\alpha_1 U_1 \\
\alpha_1 U_1^c
\end{bmatrix}
\]

Suitable schemes to compute viscous effects are recalled in [22], [18], [28], [12], [3]. These allow preserving the maximum principle for elliptic equations on triangular meshes which agree with Delaunay’s condition, and are indeed very cheap schemes which provide second order accuracy, even when the former condition is violated (on the basis of numerical observed convergence, since no theoretical proof can be given in that case).

In the predictor step, Rusanov’s scheme has been chosen since it ensures that the positivity requirement on cell averages is fulfilled. A proof can be found in [7], whenever one deals with the explicit or the non linear implicit version of the scheme. Drag terms are very simply computed using an implicit centered scheme. The mean gas pressure gradient is integrated over the cell, using Green’s formula, and a centered scheme.

If \( V(i) \) represents the patch of neighboring cells of cell \( i \), the volume of which is noted \( \Omega_i \), and denoting by \( k_{ij} \) the measure of the interface connecting cells \( i \) and \( j \), and \( n_{ij} \) the outwards unit normal vector of interface \( ij \) oriented from cell \( i \) to cell \( j \), then straightforward integration provides:

\[
W^n_i + \Delta t (\alpha_1 \alpha_2 K_T) i \left( \begin{array}{c}
\frac{V - V_i}{U^2 - U_i} \\
\frac{U^2 - U_i}{\rho_i}
\end{array} \right) = W^n_i
\]

\[
- \frac{\Delta t}{\Omega_i} \sum_{j \in V(i)} k_{ij} F^{Rus} (W^n_i, W^n_j, \mathbf{u}_{ij})
\]

\[
- \frac{\Delta t}{\Omega_i} \sum_{j \in V(i)} k_{ij} \left( \begin{array}{c}
\frac{a_2 + P_i n_{ij}}{a_1 + P_i n_{ij}}
\end{array} \right)^n - \Delta t \left( \begin{array}{c}
\frac{a_2 \mathbf{g}}{a_1 \mathbf{g}}
\end{array} \right)^n
\]

The scheme is thus the following, assuming that \( \Delta t \) represents some prescribed time step:

\[
F^{Rus} (W^n_i, W^n_j, \mathbf{u}_{ij}) =
\]

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\[ \begin{align*}
\frac{1}{2} \left\{ \begin{array}{l}
\alpha_1^n \mathbf{U}_k^n \cdot \mathbf{n}_{ij} + \alpha_2^n \mathbf{U}_j^n \cdot \mathbf{n}_{ij} \\
- (\rho_{Rusanov})_{ij}^n \left( \alpha_2^n - \alpha_1^n \right)
\end{array} \right. \\
\left. \begin{array}{l}
\left( \alpha_1^n \mathbf{U}_k^n \cdot \mathbf{n}_{ij} \right) \mathbf{U}_{n}^n + \left( \alpha_2^n \mathbf{U}_j^n \cdot \mathbf{n}_{ij} \right) \mathbf{U}_{n}^n \\
+ \left( \alpha_1^n \Theta \left( \alpha_2^n \right) + \alpha_2^n \Theta \left( \alpha_1^n \right) \right) \mathbf{n}_{ij} \\
- (\rho_{Rusanov})_{ij}^n \left( \alpha_2^n \mathbf{U}_j^n - \alpha_1^n \mathbf{U}_k^n \right)
\end{array} \right. \\
\left. \begin{array}{l}
\left( \alpha_1^n \mathbf{U}_k^n \cdot \mathbf{n}_{ij} \right) \mathbf{U}_{n}^n + \left( \alpha_1^n \mathbf{U}_j^n \cdot \mathbf{n}_{ij} \right) \mathbf{U}_{n}^n \\
- (\rho_{Rusanov})_{ij}^n \left( \alpha_1^n \mathbf{U}_j^n - \alpha_2^n \mathbf{U}_k^n \right)
\end{array} \right. \\
\end{align*} \]

where the spectral radius \((\rho_{Rusanov})_{ij}^n\) equals:

\[
(\rho_{Rusanov})_{ij}^n = \max_{k=1,j} \left\{ \left| \mathbf{U}_{n}^n \cdot \mathbf{n}_{ij} \right| + c_{s,k}^n \right\}
\]

- the mean interface value of pressure is:

\[
P_{ij}^n = t_{ij} P_{i}^n + \left( 1 - t_{ij} \right) P_{j}^n
\]

where

\[
t_{ij} = \frac{(x_{ij} - x_i) \cdot (x_j - x_i)}{(x_j - x_i)^2},
\]

if \(x_i\) stands for the intersection of normal bisectors of edges of triangular cell \(i\), \(x_j\) its counterpart for cell \(j\), \(x_{ij}\) the mid-point of edge connecting cells \(i\) and \(j\).

The CFL number which is used in computations is based on the following definition:

\[
CFL = \frac{\Delta t \sum_{j \in V(i)} (\rho_{Rusanov})_{ij}^n l_{ij}}{2 \Omega_i}
\]

It enables preserving the positivity of void fraction \(\alpha_2\) when applying for Rusanov’s scheme (provided CFL <1, see [1] and [7]). Wall boundary conditions are treated in such a way that the approximate granular pressure is greater than its neighbouring value in cell close to the wall, when:

\[
\mathbf{U}_{n_{i}} \cdot \mathbf{n}_{i} \geq 0
\]

and weaker in the case of a local double rarefaction wave, namely when \(\mathbf{U}_{n_{i}} \cdot \mathbf{n}_{i} \leq 0\). Thus the scheme is in agreement with both the one dimensional Riemann problem solution, and hence with that of Godunov scheme [24], whereas Roe’s scheme ([29]) may provide unphysical approximations (see [9] or [17]).

The latter approximate value \(\overline{W}_i^n\) is used as an initial condition for the corrective step. Governing continuous equations are thus:

\[
\nabla \cdot \mathbf{V} = 0
\]

\[
\frac{\partial}{\partial t} (\alpha_1 \mathbf{U}_1) + \frac{\alpha_1}{\rho_1} \nabla \phi = 0
\]

\[
\frac{\partial}{\partial t} (\alpha_2 \mathbf{U}_2) + \frac{\alpha_2}{\rho_2} \nabla \phi = 0
\]

\[
\frac{\partial \alpha_2}{\partial t} = 0
\]

noting \(\mathbf{V} = \alpha_1 \mathbf{U}_1 + \alpha_2 \mathbf{U}_2\), and if \(\phi\) some mean gas pressure perturbation. The latter system requires no initial condition for \(\phi\) variable.

Equations 4, 5 and 6 may be combined to give:

\[
\frac{\partial \mathbf{V}}{\partial t} + K \nabla \phi = 0
\]

\[
\frac{\partial}{\partial t} (\rho_1 \mathbf{U}_1 - \rho_2 \mathbf{U}_2) = 0
\]

introducing : \(K = \left( \frac{\alpha_1}{\rho_1} + \frac{\alpha_2}{\rho_2} \right)\).

Time discretization is then as follows:

\[
\nabla \mathbf{V}^{n+1} = 0
\]

\[
\mathbf{V}^{n+1} - \overline{W}^* \Delta t \nabla \phi^{n+1} = 0
\]

\[
\rho_1 \mathbf{U}_1^{n+1} - \rho_2 \mathbf{U}_2^{n+1} = \rho_1 \mathbf{U}_1^* - \rho_2 \mathbf{U}_2^*
\]

where : \(\phi^{n+1} = P^{n+1} - P^n\)
Taking the divergence of (10), and using stationary constraint (9), one gets some elliptic equation to update the mean velocity and gas pressure fields:

\[ \nabla \cdot \bar{V}^{n+1} = -\nabla \cdot \bar{V}^n + \Delta t \nabla \cdot (K^* \nabla \bar{\phi}^{n+1}) = 0 \]

Integrating over cell \( i \), one gets:

\[
\sum_{j \in V(i)} l_{ij} (\bar{V}^{n+1} \cdot \bar{n})_{ij} =
-\sum_{j \in V(i)} l_{ij} (\bar{V}^n \cdot \bar{n})_{ij}
+ \Delta t \sum_{j \in V(i)} l_{ij} (K^* \nabla \bar{\phi}^{n+1} \cdot \bar{n})_{ij}
= 0
\]

Variables \((\alpha_1 U_{1i})^{n+1}\) and \((\alpha_2 U_{2i})^{n+1}\) are hence obtained using definition of mean velocity \( \bar{V} \) together with equation (11):

\[
\left( \begin{array}{c}
\alpha_1^{n+1} \\
\alpha_2^{n+1} \\
\rho_1 \\
-\rho_2
\end{array} \right) \left( \begin{array}{c}
U_{1i}^{n+1} \\
U_{2i}^{n+1}
\end{array} \right)
= \left( \begin{array}{c}
\bar{V}^{n+1} \\
\rho_1 U_{1i}^{n} - \rho_2 U_{2i}^{n}
\end{array} \right)
\]

Note of course that this local problem is always well posed since the determinant always remains strictly positive:

\[ (\alpha_1 \rho_2 + \alpha_2 \rho_1) > \min(\rho_1, \rho_2) \]

**Numerical results**

Some basic computations of isentropic Euler equations using granular pressure law instead of the standard polytropic law have been performed first to calibrate the convergence rate of Rusanov scheme, focusing on shock tube experiments in a single gas phase. This enables to check that the speed of convergence is exactly the same than the one associated with Roe’s
scheme or some approximate Godunov schemes such as VFRoe’s scheme with non conservative variables ([9], [10], [21]). We recall here that when shocks are present in the solution, the L1 error norm for the velocity component \( U \), namely \( e(U; h) \), varies as \( h^2 \) where \( \alpha \) is approximately 0.85 when using so-called first order scheme, and around 1 when using “second order” extension obtained with MUSCL reconstruction and RK2 time integration for instance. However, using Rusanov scheme instead of the latter requires using a mesh size of \( h/3 \) (instead of \( h \)) when making such a choice, if one aims at reaching the same accuracy. This renders Rusanov scheme rather attractive, since it ensures the positivity constraint on the discrete density, unlike other schemes on unstructured meshes. These results are reported in [7]. More details pertaining to the rate of convergence of above mentioned schemes may be found in [10], [11], [15] or [9] for instance. The inclusion of source terms such as drag terms does not modify the overall behaviour of the whole algorithm (see [7] for details).

We focus now on some very simple two phase flow which however requires robust schemes in order not to violate the maximum principle for the void fraction, which seems quite obvious when focusing on the flow conditions. The computational rectangular box has two vertical walls on the left and right hand sides. The bottom edge is open and a grid is located on the lower part, thus preventing solid particles to go out downwards. At the beginning of the computation, one drops a homogeneous cloud of particles (particle void fraction in the layer is assumed to be equal to 0.2) in quiet air. The boundary conditions on the top face are supposed to be the following :

\[
W_{haut} = \begin{cases} 
\alpha_{2haut} = 10^{-6} \\
U_{2haut} = 0 \\
U_{1haut} = 0 
\end{cases}
\]

The diameter of particles is : \( d_2 = 5 \text{ mm} \). Initial conditions are : 

\[
y \leq 1 \\
y > 1
\]

\[
\begin{align*}
\alpha_2 &= 0, 2 \\
U_2 &= 0, 0 \\
U_1 &= 0, 0
\end{align*}
\]

The CFL number (as defined above) is chosen to be 0.8 during the whole computation. The unstructured mesh contains 4004 triangles. One can easily see a very dense region on figure 1. The line where the particle Mach number (defined as the ratio of \( U_2 \) over \( c_2 \), which is defined above) is equal to one, corresponds to the upper face of the dense fluidized bed. The gas pressure is almost constant within the bed, and decreases to zero on the top boundary, where the gas pressure reference was set to 0. The maximum compactness rate obtained in this computation, which is around 0.57, is rather far from 0.64, due to the choice of the constant \( (q_2^2) \) which is rather high in this computation. This kind of dense fluidized bed computation is also examined in reference [14] where authors consider a three-equation model to compute the whole. An excellent analysis of the influence of particle diameter, turbulent effects, and of mesh size refinement is provided in reference [4]. Actually, expected converged solutions may only be found considering very fine meshes, due to the presence of the granular pressure terms in the whole set of equations, which result in stiff behaviour of solutions when the maximum compactness rate is approached somewhere in the computational domain. Up to the authors, models and methods introduced in [34] and [33] have not been used yet to compute this kind of flows.

**Conclusion**

We have presented herein a new Finite Volume scheme which enables computing low gas Mach number flows loaded with particles, even when the void fraction grows up to the maximum compactness rate. The method requires using a triangulation of the computational domain. The numerical approximation of the void fraction remains positive, provided that one agrees with a standard limitation of the
time step, which essentially depends on the celerity of void fraction waves in the dense limit, and only depends on the gas and particle velocity in the dilute regimes. A specific trick even enables to preserve the maximum principle on the void fraction (see [26]) ; in that case anyway, the time step becomes much smaller. The scheme is currently used to predict the behaviour of dense fluidized beds, when the incoming gas velocity below the bottom grid is non zero. Results may be compared with those obtained by Boelle and coauthors in [4], but also with those detailed in [17], and in [1].

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Figure 1: Mean void fraction (at the beginning - up/left, and at the end of computation - up/right), and mean vertical (down/right) and horizontal (down/left) velocity of particles