Two-phase flows with granular stress

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Context

- Flow of weakly compressible grains (powder, sand, etc.) inside a compressible gas;
- Importance of the granular stress when the grains are packed;
- Averaged model (the solid phase is represented by an equivalent continuous media);
- Two-velocity, two-pressure mathematical model;
- Relaxation of the pressure equilibrium in order to gain stability;
- Stable and useful approximation for real applications.
Granular stress $R$

Gas phase = (G)
Solid phase = (S)

$p_G$
$p_S$

Dilute case: $p_S - p_G = 0$.

$p_G$
$p_S$

Packed case: $p_S - p_G = R > 0$. 

$R$
Averaging process

Averaging in a small volume $V$ around point $x$

- particle $i = 1 \cdots N$
- mass $M_i$
- volume $V_i$

$$\alpha_s(x) = \frac{\sum V_i}{V}, \quad \alpha_G = 1 - \alpha_s$$

$$\rho_s(x) = \frac{\sum M_i}{\sum V_i}.$$
Outlines

Two-phase granular flow models
  Unstable one-pressure model
  More stable two-pressure model
  Entropy and closure

Thermodynamically coherent granular stress
  Shape of the granular stress
  Entropy and granular stress

Hyperbolicity study
  Stability of the relaxed system
  Instability of the one-pressure model

Numerical approximation: splitting method
  Convection step
  Relaxation step

Numerical results
  Stability study
  Combustion chamber

Conclusion

Bibliography
Two-phase granular flow models
**Unstable one-pressure model**

A gas phase (G) \( k = 1 \), a solid phase (S) \( k = 2 \).

Seven unknowns: partial densities \( \rho_k(x, t) \), velocities \( u_k(x, t) \), internal energies \( e_k(x, t) \), gas volume fraction \( \alpha_1(x, t) \).

Pressure law: \( p_k = p_k(\rho_k, e_k) \).

Other definitions: \( m_k = \alpha_k \rho_k \), \( \alpha_2 = 1 - \alpha_1 \), \( E_k = e_k + \frac{u_k^2}{2} \).

The whole six-equation PDE system reads [3]

\[
\begin{align*}
    m_{k,t} + (m_k u_k)_x &= 0, \\
    (m_k u_k)_t + (m_k u_k^2 + \alpha_k p_k)_x - p_1 \alpha_k,x &= 0, \quad (1) \\
    (m_k E_k)_t + ((m_k E_k + \alpha_k p_k)u_k)_x + p_1 \alpha_k,t &= 0,
\end{align*}
\]

with the algebraic relation

\[
p_2 = p_1 + R.
\]
More stable two-pressure model

The previous system is generally not hyperbolic. Therefore, we relax the algebraic pressure relation. The seven-equation PDE system reads [1]

\[
\begin{align*}
    m_{k,t} + (m_k u_k)_x &= 0, \\
    (m_k u_k)_t + (m_k u_k^2 + \alpha_k p_k)_x - p_1 \alpha_{k,x} &= 0, \\
    (m_k E_k)_t + ((m_k E_k + \alpha_k p_k)u_k)_x + p_1 \alpha_{k,t} &= 0, \\
    \alpha_{1,t} + u_2 \alpha_{1,x} &= P.
\end{align*}
\]

(2)

And the source term \(P\) has to contain the granular modeling.
Entropy and closure

The gas entropy $s_1$ satisfies the standard relation ($T_k$ is the temperature of phase $k$)

$$T_1 ds_1 = de_1 - \frac{p_1}{\rho_1^2} d\rho_1.$$

For the entropy $s_2$ of the solid phase, we take into account the granular stress.

$$T_2 ds_2 = de_2 - \frac{p_2}{\rho_2^2} d\rho_2 - \frac{R}{m_2} d\alpha_2.$$

After some computations, we find the following entropy dissipation equation

$$\left( \sum_k m_k s_k \right)_t + \left( \sum_k m_k u_k s_k \right)_x = \frac{P}{T_2} (p_1 + R - p_2).$$
A natural choice that ensures positive dissipation is

\[
P = \frac{1}{\tau_p} \alpha_1 \alpha_2 (p_1 + R - p_2), \quad \tau_p \geq 0.
\]

The choice of the pressure relaxation parameter \( \tau_p \) is very important. We can also write

\[
p_1 + R - p_2 = \frac{\tau_p}{\alpha_1 \alpha_2} (\alpha_{1,t} + u_2 \alpha_{1,x}).
\]

- for \( \tau_p = t_{eq} = 0 \), we recover the instantaneous six-equation equilibrium model \( p_2 = p_1 + R \);
- \( \tau_p = t_{eq} p_{ref} \) where \( t_{eq} \) is the characteristic time of the pressure equilibrium and \( p_{ref} \) a reference pressure;
- for \( \tau_p > 0 \), the system should be more stable.
Thermodynamically coherent granular stress
Shape of the granular stress

Usually, $R = R(\alpha_2)$ [4]
Entropy and granular stress

How to choose the granular stress $R$ for compressible solid phases? Exemple: for a stiffened gas equation of state

$$
p_2 = p_2(\rho_2, e_2) = (\gamma_2 - 1)\rho_2 e_2 - \gamma_2 \pi_2 \quad , \quad \gamma_2 > 1.
$$

We suppose that $R = R(\rho_2, \alpha_2)$. We express that the entropy is a closed differential form ($1/T_2$ is an integrating factor of the energy form)

$$
d s_2 = \frac{1}{T_2} \left( \frac{p_2}{\rho_2^2} d \rho_2 - \frac{R}{m_2} d \alpha_2 \right). 
$$

We find

$$
R(\rho_2, \alpha_2) = \rho_2^{\gamma_2} r(\alpha_2).
$$

Particular choice

$$
r(\alpha_2) = \lambda \alpha_2^{\gamma_2} \quad \Rightarrow \quad R = \lambda m_2^{\gamma_2}.
$$
Hyperbolicity study
Stability of the relaxed system \((\tau_p > 0)\)

Let

\[ Y = (\alpha_1, \rho_1, u_1, s_1, \rho_2, u_2, s_2)^T. \]

In this set of variables the system becomes

\[ Y_t + B(Y)Y_x = (P, 0, 0, 0, 0, 0, 0)^T \]

\[ B(Y) = \begin{bmatrix}
    u_2 & u_1 & \rho_1 & p_{1,s_1} & u_1 & \rho_1 & p_{1,s_1} \\
    \rho_1(u_1-u_2) & \rho_1 & \rho_1 & \rho_1 & \rho_1 & \rho_1 & \rho_1 \\
    \frac{u_1}{\alpha_1} & \frac{u_1}{\rho_1} & \frac{u_1}{\rho_1} & \frac{u_1}{\rho_1} & \frac{u_1}{\rho_1} & \frac{u_1}{\rho_1} & \frac{u_1}{\rho_1} \\
    \frac{p_1-p_2}{m_2} & \frac{p_1-p_2}{m_2} & \frac{p_1-p_2}{m_2} & \frac{p_1-p_2}{m_2} & \frac{p_1-p_2}{m_2} & \frac{p_1-p_2}{m_2} & \frac{p_1-p_2}{m_2} \\
    \frac{c_1^2}{\rho_1} & \frac{c_1^2}{\rho_1} & \frac{c_1^2}{\rho_1} & \frac{c_1^2}{\rho_1} & \frac{c_1^2}{\rho_1} & \frac{c_1^2}{\rho_1} & \frac{c_1^2}{\rho_1} \\
    \frac{c_2^2}{\rho_2} & \frac{c_2^2}{\rho_2} & \frac{c_2^2}{\rho_2} & \frac{c_2^2}{\rho_2} & \frac{c_2^2}{\rho_2} & \frac{c_2^2}{\rho_2} & \frac{c_2^2}{\rho_2} \\
    \frac{p_2,s_2}{\rho_2} & \frac{p_2,s_2}{\rho_2} & \frac{p_2,s_2}{\rho_2} & \frac{p_2,s_2}{\rho_2} & \frac{p_2,s_2}{\rho_2} & \frac{p_2,s_2}{\rho_2} & \frac{p_2,s_2}{\rho_2} \\
    \frac{u_2}{u_2} & \frac{u_2}{u_2} & \frac{u_2}{u_2} & \frac{u_2}{u_2} & \frac{u_2}{u_2} & \frac{u_2}{u_2} & \frac{u_2}{u_2}
\end{bmatrix}, \quad c_k = \sqrt{\frac{\gamma_k(p_k + \pi_k)}{\rho_k}}. \]

\[ \det(\lambda_1, \ldots, \lambda_7) = (u_2-\lambda)^2(u_1-\lambda)(u_1-c_1-\lambda)(u_1+c_1-\lambda)(u_2-c_2-\lambda)(u_2+c_2-\lambda). \]

The system is hyperbolic [6, 2].
Instability of the one-pressure model \((\tau_p = 0)\)

When \(\tau_p \to 0\), formally, we end up with a standard single pressure model

\[ p_2 = p_1 + R. \]

We can remove an equation (for example the volume fraction evolution) and we find a six-equation system

\[ Z = (\rho_1, u_1, s_1, \rho_2, u_2, s_2)^T. \]

\[ Z_t + C(Z)Z_x = 0. \]

In the simple case where \(R = \lambda m_2^{\gamma_2}\), let

\[ \Delta = \alpha_1 \alpha_2 + \delta (\alpha_1 \rho_2 a_2^2 + \alpha_2 \rho_1 c_1^2), \]

and

\[ \tilde{\delta} = \frac{\alpha_2}{\lambda \gamma_2 \rho_2^{\gamma_2}}. \]
Then we find

\[ C(\mathbb{Z}) = \begin{bmatrix}
    u_i + \frac{\rho_i \rho_c \alpha_i^2 \delta^i_{-i}}{\Delta} & \frac{\alpha_i \rho_i (\alpha_i + \rho_i \alpha_i^2 \delta)}{\Delta} & \frac{\rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} \\
    \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} \\
    \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} \\
    \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} \\
    \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} \\
    \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta} & \frac{\alpha_i \rho_i \alpha_i^2 \delta (u_i-u_i)}{\Delta}
\end{bmatrix} \]

- The eigenvalues can be computed only numerically.
- We observe that when \( R \to 0 \), the system is generally not hyperbolic.
- We observe also that when \( R \to \infty \), we recover hyperbolicity;
- When \( R = 0 \), the convection matrix has to be computed in another way.
Numerical approximation: splitting method

- The two-pressure model is hyperbolic and more stable.
- The one-pressure model is commonly used in applications on coarse meshes (high damping of the numerical viscosity).
- We can approximate the one-pressure model by the more general two-pressure model.
- A time step is made of a convection stage and a relaxation stage. In the relaxation stage, we apply the exact or relaxed pressure equilibrium.
Convection step

Let

$$w = (\alpha_1, m_1, m_1 u_1, m_1 E_1, m_2, m_2 u_2, m_2 E_2)^T,$$

The system can be written

$$w_t + f(w)_x + G(w)w_x = (P, 0, 0, 0, 0, 0, 0)^T$$

In the first half step the source term is omitted. We use a standard Rusanov scheme

$$\frac{w_i^* - w_i^n}{\Delta t} + \frac{f_{i+1/2}^n - f_{i-1/2}^n}{\Delta x} + G(w_i^n) \frac{w_{i+1}^n - w_{i-1}^n}{2\Delta x} = 0,$$

$$f_{i+1/2}^n = f(w_i^n, w_{i+1}^n) \text{ numerical conservative flux,}$$

$$f(a, b) = \frac{f(a) + f(b)}{2} - \frac{\lambda}{2}(b - a).$$

For \(\lambda\) large enough, the scheme is entropy dissipative. Typically, we take

$$\lambda = \max [\rho \left( f'(a) + G(a) \right), \rho \left( f'(b) + G(b) \right)].$$
Relaxation step

In the second half step, we have formally to solve

\[ \alpha_{1,t} = P, \]
\[ m_{k,t} = u_{k,t} = 0, \]
\[ (m_k e_k)_t + p_1 \alpha_{k,t} = 0. \]

Because of mass and momentum conservation we have \( m_k = m_k^* \) and \( u_k = u_k^* \). In each cell we have to compute \((\alpha_1, p_1, p_2)\) from the previous state \( w^* \)

\[ p_2 = p_1 + \lambda m_2 \gamma^2 + \tau_p \frac{\alpha_2 - \alpha_2^*}{\alpha_1 \alpha_2 \Delta t}, \]
\[ m_1 e_1 + m_2 e_2 = m_1^* e_1^* + m_2^* e_2^*, \]
\[ (m_1 e_1 - m_1^* e_1^*) + p_1 (\alpha_1 - \alpha_1^*) = 0. \]
After some manipulations, we have to solve

\[ H(\alpha_2) = (\pi_2 - \pi_1)(\alpha_1 + (\gamma_1 - 1)(\alpha_1 - \alpha_1^*)) (\alpha_2 + (\gamma_2 - 1)(\alpha_2 - \alpha_2^*)) \\
+ (\alpha_2^{2-\gamma^2} m_2^{\gamma^2} \theta(\alpha_2) + \frac{\tau_p}{(1 - \alpha_2)} \frac{\alpha_2 - \alpha_2^*}{\Delta t} - A_2)(\alpha_1 + (\gamma_1 - 1)(\alpha_1 - \alpha_1^*)) \\
+ A_1(\alpha_2 + (\gamma_2 - 1)(\alpha_2 - \alpha_2^*)) = 0, \]

with

\[ A_k = \alpha_k^* (p_k^* + \pi_k) > 0. \]

**Theorem:** for stiffened gas laws and the simple granular law, \( H \) is concave, \( H(0) < 0 \) and \( H(\beta_2) > 0 \) with

\[ 0 < \beta_2 = \frac{(1 - \alpha_2^*) + \alpha_2^* \gamma_1}{\gamma_1} < 1. \]

There is a unique \( \alpha_2 \) in \([0, \beta_2[ \subset ]0, 1[\) such that \( H(\alpha_2) = 0. \)
Numerical application
Stability study

We have constructed an entropy dissipative approximation of a non-hyperbolic system!
What happens numerically?
Consider a simple Riemann problem in the interval \([-1/2, 1/2]\).
\(\gamma_1 = 1.0924\) and \(\gamma_2 = 1.0182\). We compute the solution at time \(t = 0.00075\). The CFL number is 0.9.
Data:

<table>
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<th>((R))</th>
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<td>(\rho_1)</td>
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<td>57.34072568</td>
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<tr>
<td>(u_1)</td>
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<td>0</td>
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<tr>
<td>(p_1)</td>
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<td>(150 \times 10^5)</td>
</tr>
<tr>
<td>(\rho_2)</td>
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<td>358.8982226</td>
</tr>
<tr>
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<td>0</td>
</tr>
<tr>
<td>(p_2)</td>
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<td>(150 \times 10^5)</td>
</tr>
<tr>
<td>(\alpha_1)</td>
<td>0.25</td>
<td>0.25</td>
</tr>
</tbody>
</table>
\( \tau_p = 0, \ R = 0 \)

**Figure:** Void fraction, 50 cells, \( \tau_p = 0, \ R = 0 \).
\( \tau_p = 0, \ R = 0 \)

**Figure:** Void fraction, 1,000 cells, \( \tau_p = 0, \ R = 0 \).
\( \tau_p = 0, \ R = 0 \)

Figure: Void fraction, 10,000 cells, \( \tau_p = 0, \ R = 0 \).
\( \tau_p = 0, \ R = 0 \)

Figure: Void fraction, 100,000 cells, \( \tau_p = 0, \ R = 0 \).

Linearly unstable but non-linearly stable...
\( \tau_p > 0, \ R = 0 \)

**Figure:** Pressure, 50,000 cells, \( \tau_p = 0, 2, 10, \ R = 0 \).

The relaxation clearly stabilizes the results...
\( \tau_p = 0, \ R > 0 \)

Figure: Pressures \( p_1 \) and \( p_2 \), 10,000 cells, \( \tau_p = 0, \ R = 500m_2^{\gamma/2} \).
\[ \tau_p = 0, \ R > 0 \]

**Figure:** Eigenvalues: imaginary part \( I = \sqrt{\sum_{i=1}^{6} \text{Im}(\lambda_i)^2} \), 1,000 cells, \( R = 0 \) or \( R = 500 m_2^{\gamma_2} \).

The granular stress slightly improves the stability...
Combustion chamber

We consider now a simplified gun [3, 5]. The right boundary of the computational domain is moving. We activate the granular stress and other source terms (chemical reaction and drag), which are all entropy dissipative. The instabilities would occur on much finer grids...

Other source terms are added.

\[
\begin{align*}
m_{k,t} + (m_k u_k)_x &= \pm M, \\
(m_k u_k)_t + (m_k u_k^2 + \alpha_k p_k)_x - p_1 \alpha_k, x &= \pm Q, \\
(m_k E_k)_t + ((m_k E_k + \alpha_k p_k) u_k)_x + p_1 \alpha_k, t &= S_k, \\
\alpha_k, t + v_2 \alpha_k, x &= \pm P.
\end{align*}
\]
The mass transfer term is defined by the simplified relations

\[ M = \alpha_2 \rho_2 \frac{3 \dot{r}}{r} \]

\[ \dot{r} = 5 \times 10^{-3} \text{ m/s (combustion velocity of the grains)} \] (3)

\[ r = 10^{-3} \text{ m (radius of the grains)} \]

The momentum source term is given by

\[ Q = M u_2 - D \]

\[ D = C \alpha_1 \alpha_2 \rho_2 (u_1 - u_2) |u_1 - u_2| \text{ (drag force)} \] (4)

\[ C = \frac{3}{4r} \text{ (simplified shape factor)} \]

The energy source terms are

\[ S_1 = -u_2 D + MQ_{ex} \]

\[ S_2 = u_2 D \]

\[ Q_{ex} = 37.3839 \times 10^6 \text{ J/kg (chemical combustion energy)} \] (5)
Figure: Pressure evolution at the breech and the shot base during time. Comparison between the Gough and the relaxation model.
Figure: Porosity at the final time. Relaxation model with granular stress.
Figure: Velocities at the final time. Relaxation model with granular stress.
Figure: Pressures at the final time. Relaxation model with granular stress.
Figure: Density of the solid phase at the final time. Relaxation model with granular stress.
Conclusion

- Good generalization of the one pressure models;
- Extension of the relaxation approach to flows with granular stress;
- Rigorous entropy dissipation and maximum principle on the volume fraction;
- Stability for a finite relaxation time;
- The instability is (fortunately) preserved by the scheme for fast pressure equilibrium;
- The model can be used in practical configurations (the solid phase remains almost incompressible).
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