Kinetic theory of mixtures of inelastic rough hard spheres

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Outline

- What is a granular fluid?
- Mixture of inelastic rough hard spheres. The Boltzmann equation.
- Collisional thermal rates.
- Application to the homogeneous cooling state. Non-equipartition of energy.
- Conclusions and outlook.
What is a granular material?

- It is a conglomeration of discrete solid, macroscopic particles characterized by a loss of energy whenever the grains collide.
- The constituents must be large enough such that they are not subject to thermal motion fluctuations. Thus, the lower size limit for grains is about 1 µm.
What is a granular material?

- Examples of granular materials would include nuts, coal, sand, rice, coffee, corn flakes, fertilizer, and ball bearings.
What is a granular fluid?

- When the granular matter is driven and energy is fed into the system (e.g., by shaking) such that the grains are not in constant contact with each other, the granular material is said to **fluidize**.
Granular fluids (or gases) exhibit many interesting phenomena:

Granular eruptions (from University of Twente’s group)
Wave patterns in a vibrated container
(from A. Kudrolli’s group)

(Simulations by D. C. Rapaport)
Segregation in sheared flow
(Simulations by D. C. Rapaport)

Segregation in a rotating cylinder
(Simulations by D. C. Rapaport)

Flow(ers) and Jam(mers), Lisbon, 17-19th June 2009
Granular jet hitting a plane

Particles falling on an inclined heated plane

http://trevinca.ei.uvigo.es/~formella/
Minimal model of a granular gas: A gas of identical smooth inelastic hard spheres

http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/
But … real grains

Have a non-constant coefficient of restitution

www.oxfordcroquet.com/tech/

Flow(ers) and Jam(mers), Lisbon, 17-19th June 2009
But … real grains

Are non-spherical
But … real grains

Are polydisperse

http://www.cmt.york.ac.uk/~ajm143/nuts.html
But … real grains

Are rough
Model of a granular gas:
A mixture of inelastic rough hard spheres

This model unveils an inherent breakdown of energy equipartition in granular fluids, even in homogeneous and isotropic states.

Several circles
(Kandinsky, 1926)
Mechanical parameters:

- $X$ components ($i=1, \ldots, X$)
- Masses $m_i$
- Diameters $\sigma_i$
- Moments of inertia $I_i$
- Coefficients of normal restitution $\alpha_{ij}$
- Coefficients of tangential restitution $\beta_{ij}$

- $\alpha_{ij} = 1$ for elastic particles
- $\beta_{ij} = -1$ for smooth particles
- $\beta_{ij} = +1$ for totally rough particles
Collision rules:

Translational velocities: \( v'_i = v_i - \frac{1}{m_i} Q_{ij}, \quad v'_j = v_j + \frac{1}{m_j} Q_{ij} \)

Angular velocities: \( \omega'_i = \omega_i + \frac{\sigma_i}{2I_i} \hat{\sigma} \times Q_{ij}, \quad \omega'_j = \omega_j + \frac{\sigma_j}{2I_j} \hat{\sigma} \times Q_{ij} \)

Impulse exerted by \( i \) on \( j \):
\[
Q_{ij} = \overline{\beta}_{ij} \left[ g_{ij} - (g_{ij} \cdot \hat{\sigma})\hat{\sigma} + \frac{1}{2} \hat{\sigma} \times (\sigma_i \omega_i + \sigma_j \omega_j) \right] + \alpha_{ij} (g_{ij} \cdot \hat{\sigma})\hat{\sigma}
\]

\( g_{ij} \equiv v_i - v_j, \quad \alpha_{ij} \equiv m_{ij} (1 + \alpha_{ij}), \quad \overline{\beta}_{ij} \equiv \frac{m_{ij} \kappa_{ij}}{1 + \kappa_{ij}} (1 + \beta_{ij}) \)

\( m_{ij} \equiv \frac{m_i m_j}{m_i + m_j}, \quad \kappa_{ij} \equiv \kappa_i \kappa_j \frac{m_i + m_j}{\kappa_i m_i + m_j \kappa_j}, \quad \kappa_i \equiv \frac{I_i}{m_i (\sigma_i/2)^2} \)
Energy collisional loss

\[ E_{ij} = \frac{1}{2} m_i v_i^2 + \frac{1}{2} m_j v_j^2 + \frac{1}{2} I_i \omega_i^2 + \frac{1}{2} I_j \omega_j^2 \]

\[ E'_{ij} - E_{ij} = -(1 - \alpha_{ij}^2) \times \cdots \]
\[ -(1 - \beta_{ij}^2) \times \cdots \]

Energy is conserved *only* if the spheres are

* elastic \((\alpha_{ij}=1)\) and

* either
  * smooth \((\beta_{ij}=-1)\) or
  * totally rough \((\beta_{ij}=+1)\)
Partial (granular) temperatures

Translational temperatures: \( T_{i}^{\text{tr}} = \frac{m_i}{3} \langle v_i^2 \rangle \)

Rotational temperatures: \( T_{i}^{\text{rot}} = \frac{I_i}{3} \langle \omega_i^2 \rangle = \frac{m_i \kappa_i}{12} \sigma_i^2 \langle \omega_i^2 \rangle \)

Total temperature: \( T = \sum_i \frac{n_i}{2n} (T_{i}^{\text{tr}} + T_{i}^{\text{rot}}) \)
Collisional rates of change for temperatures

Thermal rates:

\[ \xi_{tr}^i = - \frac{1}{T_{tr}^i} \left( \frac{\partial T_{tr}^i}{\partial t} \right)_{\text{coll}}, \quad \xi_{tr}^i = \sum_j \xi_{tr}^{ij} \]

\[ \xi_{rot}^i = - \frac{1}{T_{rot}^i} \left( \frac{\partial T_{rot}^i}{\partial t} \right)_{\text{coll}}, \quad \xi_{rot}^i = \sum_j \xi_{rot}^{ij} \]

Net cooling rate:

\[ \zeta = - \frac{1}{T} \left( \frac{\partial T}{\partial t} \right)_{\text{coll}}, \quad \zeta = \sum_i \frac{n_i}{2nT} \left( \xi_{tr} T_{tr}^i + \xi_{rot} T_{rot}^i \right) \]
Our main goal

To obtain the binary thermal rates $\xi_{ij}^{\text{tr}}$ and $\xi_{ij}^{\text{rot}}$
in terms of
$T_{i}^{\text{tr}}, T_{j}^{\text{tr}}, T_{i}^{\text{rot}}, T_{j}^{\text{rot}}, n_{i}, n_{j}$
and the mechanical parameters
$m_{i}, m_{j}, \sigma_{i}, \sigma_{j}, \kappa_{i}, \kappa_{j}, \alpha_{ij}, \beta_{ij}$
Boltzmann equation:

\[ \partial_t f_i(r, v_i, \omega_i, t) + v_i \cdot \nabla f_i(r, v_i, \omega_i, t) = \sum_j J_{ij}[r, v_i, \omega_i, t | f_i, f_j] \]

Binary collisions

Flow(ers) and Jam(mers), Lisbon, 17-19th June 2009
Additional assumptions

1. No convection, no chirality:
   \[ \langle \mathbf{v}_i \rangle = \langle \mathbf{v}_j \rangle, \quad \langle \omega_i \rangle = \langle \omega_j \rangle = 0 \]

2. Translational and rotational degrees of freedom uncorrelated:
   \[ f_i(\mathbf{v}_i, \omega_i) = f_i^{\text{tr}}(\mathbf{v}_i) f_i^{\text{rot}}(\omega_i) \]

3. Maxwellian form:
   \[ f_i^{\text{tr}}(\mathbf{v}_i) = n_i \left( \frac{m_i}{2 \pi T_i^{\text{tr}}} \right)^{3/2} \exp \left( - \frac{m_i v_i^2}{2 T_i^{\text{tr}}} \right) \]
Results

\[ \xi_{ij}^{tr} = \frac{\nu_{ij}}{m_i T_i^{tr}} \left[ 2 \left( \bar{\alpha}_{ij} + \bar{\beta}_{ij} \right) T_i^{tr} - \left( \bar{\alpha}_{ij}^2 + \bar{\beta}_{ij}^2 \right) \left( \frac{T_i^{tr}}{m_i} + \frac{T_j^{tr}}{m_j} \right) \right. \\
\left. - \bar{\beta}_{ij} \left( \frac{T_i^{rot}}{m_i \kappa_i} + \frac{T_j^{rot}}{m_j \kappa_j} \right) \right] \]

\[ \xi_{ij}^{rot} = \frac{\nu_{ij}}{m_i \kappa_i T_i^{rot}} \bar{\beta}_{ij} \left[ 2 T_i^{rot} - \bar{\beta}_{ij} \left( \frac{T_i^{tr}}{m_i} + \frac{T_j^{tr}}{m_j} + \frac{T_i^{rot}}{m_i \kappa_i} + \frac{T_j^{rot}}{m_j \kappa_j} \right) \right] \]

\[ \nu_{ij} \equiv \frac{4 \sqrt{2\pi}}{3} n_j \sigma_{ij}^2 \sqrt{\frac{T_i^{tr}}{m_i}} + \frac{T_j^{tr}}{m_j} \]
Decomposition

Thermal rates = Equilibration rates + Cooling rates

Net cooling rate = \( \sum \) Cooling rates

(After Stefan Luding’s scratch on a paper tablecloth, yesterday)
Simple application:
The Homogeneous Cooling State (HCS)

The HCS is
• Spatially homogeneous
• Isotropic
• Undriven
• Freely cooling

\[ \partial_t f_i(r, v_i, \omega_i, t) = \sum_j J_{ij}(r, v_i, \omega_i, t| f_i, f_j) \]

\[ \frac{\partial T}{\partial t} = -\zeta T \]

\[ \frac{\partial T_{tr}^i}{\partial t} = - (\xi_{tr}^i - \zeta) \frac{T_{tr}^i}{T}, \quad \frac{\partial T_{rot}^i}{\partial t} = - (\xi_{rot}^i - \zeta) \frac{T_{rot}^i}{T} \]

\[ t \to \infty \Rightarrow \xi_{tr}^1 = \xi_{tr}^2 = \ldots = \xi_{rot}^1 = \xi_{rot}^2 = \ldots \]
Single-component case ($\kappa=2/5$)

\[ \alpha < 1 \quad \beta \to -1 \quad \Rightarrow \quad \{ \xi_{\text{tr}} \sim (1 - \alpha^2) \Rightarrow \partial_t T_{\text{tr}} < 0 \quad \xi_{\text{rot}} \to 0 \Rightarrow T_{\text{rot}} \to \text{const} \} \quad \Rightarrow \quad \frac{T_{\text{tr}}}{T_{\text{rot}}} \to 0 \]

\[ \alpha = 1 \quad \beta \to -1 \quad \Rightarrow \quad \{ \xi_{\text{tr}} \sim \kappa (1 + \beta) \Rightarrow \partial_t T_{\text{tr}} < 0 \quad \xi_{\text{rot}} \sim (1 + \beta) \Rightarrow \partial_t T_{\text{rot}} < 0 \} \quad \Rightarrow \quad \xi_{\text{tr}} < \xi_{\text{rot}} \Rightarrow \quad \frac{T_{\text{tr}}}{T_{\text{rot}}} \to \infty \]
Binary mixture

Three independent temperature ratios: \( \frac{T_{1}^{tr}}{T_{1}^{rot}}, \frac{T_{2}^{tr}}{T_{1}^{tr}}, \frac{T_{2}^{rot}}{T_{1}^{rot}} \)

Eleven parameters:

- Coefficients of normal restitution \( \alpha_{11}, \alpha_{12}, \alpha_{22} = \alpha \)
- Coefficients of tangential restitution \( \beta_{11}, \beta_{12}, \beta_{22} = \beta \)
- Inertia-moment parameters \( \kappa_{1}, \kappa_{2} = \frac{2}{5} \)
- Size ratio \( \sigma_{2}/\sigma_{1} = 2 \)
- Mass ratio \( m_{2}/m_{1} = 8 \)
- Mole fraction \( n_{1}/(n_{1} + n_{2}) = \frac{1}{2} \)
Translational/Rotational

\[ \frac{T_{1,\text{tr}}}{T_{1,\text{rot}}} \]

\( n_2 = n_1, m_2/m_1 = 8, \sigma_2/\sigma_1 = 2 \)

\( \alpha = 1 \)

Elastic

Inelastic

\( \alpha = 0.5 \)

Equipartition

Smooth

Rough
Rotational/Rotational

\[ n_2 = n_1, \frac{m_2}{m_1} = 8, \frac{\sigma_2}{\sigma_1} = 2 \]

- Inelastic
- Elastic
- Equipartition

Smooth
Rough

Flow(ers) and Jam(mers), Lisbon, 17-19th June 2009
“Pure” smooth spheres (Garzó & Dufty, 1999)

“Ghost” effect: A tiny amount of roughness has dramatic effects on the temperature ratio (enhancement of non-equipartition)
Binary mixture

Three independent temperature ratios: \( \frac{T_{1 \text{tr}}}{T_{1 \text{rot}}}, \frac{T_{2 \text{tr}}}{T_{1 \text{tr}}}, \frac{T_{2 \text{rot}}}{T_{1 \text{rot}}} \)

Eleven parameters:

- Coefficients of normal restitution \( \alpha_{11}, \alpha_{12}, \alpha_{22} = \alpha \)
- Coefficients of tangential restitution \( \beta_{11}, \beta_{12}, \beta_{22} = \beta \)
- Inertia-moment parameters \( \kappa_1, \kappa_2, \kappa_2 = \frac{2}{3} \)
- Size ratio \( \sigma_2/\sigma_1 = 1 \)
- Mass ratio \( m_2/m_1 = 1 \)
- Mole fraction \( n_1/(n_1 + n_2) = \frac{1}{2} \)
“Ghost” effect: A tiny amount of roughness has dramatic effects on the temperature ratio.
Conclusions and outlook

- Collisional thermal rates obtained for mixtures of inelastic rough hard spheres.
- Interesting non-equipartition phenomena in the HCS.
- Simulations planned to test the theoretical predictions.
- Proposal of a simple model kinetic equation for the single-component case.
- Solution of the above model in the uniform shear flow and derivation of the Navier-Stokes constitutive equations.
Thanks for your attention!