ENSKOG KINETIC THEORY FOR
MONODISPERSE GRANULAR GASES

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Rheology of disordered particles - suspensions, glassy and granular materials, June 2018, Kyoto
1. *The model*: gas of hard spheres with *inelastic* collisions

2. *Enskog* kinetic equation for granular fluids. Macroscopic balance equations

3. Homogeneous cooling state (*HCS*)

4. *Navier-Stokes* transport coefficients. Approximate methods

5. Comparison with *computer simulations*

6. Conclusions
Understanding the behavior of granular matter is a very relevant challenge, not only from a practical point of view but also from a more fundamental perspective.

Granular materials are ubiquitous both in nature and industry (second most used material after the water). They are also familiar to us in our daily lives (kitchen).

Behavior is extremely complex and sometimes unexpected.
Granular matter: conglomeration of macroscopic discrete particles (size around one micra) with **dissipative** interactions

*Complex* systems that are inherently **out** of equilibrium!!

Conventional methods of *equilibrium* statistical mechanics and thermodynamics fail

Two states: compact and activated
Compact: grains form a static packed configuration within the container due to the combined effect of gravity and inelasticity in collisions

Any initial motion is quickly dissipated. Sugar or rice left unshaken in a jar appears to be inactive, although they have some kinetic energy due to the room temperature. However, their gravitational energy is much larger than their energy of motion

Problem: Stresses within the system and distribution of forces on the container (mitigate possible explosions in granular storage silos)
Activated: External energy compensates for the energy dissipated by collisions and effects of gravity

Rapid flow conditions: motion of grains is similar to motion of molecules or atoms in a classical gas. They behave like a fluid and flow. Hydrodynamic-like description. Granular gas

Kinetic theory does not make any assumption on the conservative or dissipative character of collisions. Appropriate tool!!

Transfer of momentum and energy is through binary collisions

Simplest microscopic model: smooth inelastic hard spheres
“Smooth hard spheres with inelastic collisions”

$$V_{12}^* \cdot \hat{\sigma} = -\alpha V_{12} \cdot \hat{\sigma}$$

Coefficient of normal restitution

$$0 < \alpha \leq 1$$
Throughout the talk:

Direct collision: \((v_1, v_2) \rightarrow (v'_1, v'_2)\)

\[ g_{12} = v_1 - v_2 \]

\[ g'_{12} = v'_1 - v'_2 \]

Conservation of momentum: \(v_1 + v_2 = v'_1 + v'_2\)

\[ v'_1 = v_1 - \frac{1}{2}(1 + \alpha)(\hat{\sigma} \cdot g_{12})\hat{\sigma} \]

\[ v'_2 = v_2 + \frac{1}{2}(1 + \alpha)(\hat{\sigma} \cdot g_{12})\hat{\sigma} \]
Change in kinetic energy:

$$\Delta E \equiv E' - E = -\frac{m}{2}(\hat{\sigma} \cdot g_{12})^2(1 - \alpha^2) \leq 0$$

Energy is lost in each collision, never gained

*Restituting* collisions: \((v''_1, v''_2) \rightarrow (v'_1, v'_2)\)

\[
(\hat{\sigma} \cdot g''_{12}) = -\alpha^{-1}(\hat{\sigma} \cdot g_{12})
\]

\[
dv''_1 dv''_2 = \alpha^{-1} dv_1 dv_2 \quad dv'_1 dv'_2 = \alpha dv_1 dv_2
\]
One-particle velocity distribution function

\[ f(r, v, t) \, dr \, dv \rightarrow t \text{ located around } r \text{ and moving with } v \]

*Dilute* gas: fraction of the volume occupied by granular material is negligible compared to the total volume.

*Boltzmann* kinetic equation

- *Dilute gas* (binary collisions)
- *“Molecular chaos”*
Rate of change of $f$ with time:
\[
\frac{\partial f}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{\text{str}} + \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}
\]

Interactions are absent (Knudsen gas):
\[
\left(\frac{\partial f}{\partial t}\right)_{\text{str}} = -\mathbf{v} \cdot \nabla f - \frac{1}{m} \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{F} f)
\]

External force

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Collisional change of \( f(r, v_1, t)\, dr\, dv_1 \) during \((t, t + dt)\)

\[
\left( \frac{\partial f}{\partial t} \right)_{\text{coll}} \, dv_1 = (G - L)dv_1
\]

Gain term  
Loss term

Number of collisions per unit time into an element of solid angle between a beam of incident particles and a target particle

\[
\sigma^{d-1} |(\hat{\sigma} \cdot g_{12})| f(v_1) \, d\hat{\sigma} \, dv_1
\]

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Since there is not only one target particle, then

$$\sigma^{d-1}|(\hat{\sigma} \cdot \mathbf{g}_{12})| f(\mathbf{v}_1) f(\mathbf{v}_2) d\hat{\sigma} d\mathbf{v}_1 d\mathbf{v}_2 dt$$

Average total number of collisions suffering particles with velocity $\mathbf{v}_1$

$$Ld\mathbf{v}_1 = \sigma^{d-1} \int d\mathbf{v}_2 \int d\hat{\sigma} \Theta(\hat{\sigma} \cdot \mathbf{g}_{12})(\hat{\sigma} \cdot \mathbf{g}_{12}) f(\mathbf{v}_1) f(\mathbf{v}_2) d\mathbf{v}_1$$

Gain term $\rightarrow (\mathbf{v}'', \mathbf{v}') \rightarrow (\mathbf{v}_1, \mathbf{v}_2)$

$$Gd\mathbf{v}_1 = \sigma^{d-1} \int d\mathbf{v}_2'' \int d\hat{\sigma} \Theta(\hat{\sigma} \cdot \mathbf{g}_{12}'')(\hat{\sigma} \cdot \mathbf{g}_{12}'') f(\mathbf{v}_1'') f(\mathbf{v}_2'') d\mathbf{v}_1''$$

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\[
\partial_t f + \mathbf{v} \cdot \nabla f + \frac{\partial}{\partial \mathbf{v}} \cdot \left( \frac{\mathbf{F}}{m} f \right) = J [\mathbf{v} | f(t), f(t)]
\]

\[
J [\mathbf{v}_1 | f, f] = \sigma^{d-1} \int d\mathbf{v}_2 \int d\mathbf{\hat{\sigma}} \Theta(\mathbf{\hat{\sigma}} \cdot \mathbf{g}_{12})(\mathbf{\hat{\sigma}} \cdot \mathbf{g}_{12}) \\
\times \left[ \alpha^{-2} f(\mathbf{r}, \mathbf{v}'_1; t) f(\mathbf{r}, \mathbf{v}'_2; t) - f(\mathbf{r}, \mathbf{v}_1; t) f(\mathbf{r}, \mathbf{v}_2; t) \right]
\]

Collision rules:

\[
\mathbf{v}'_1 = \mathbf{v}_1 - \frac{1}{2} (1 + \alpha^{-1}) (\mathbf{\hat{\sigma}} \cdot \mathbf{g}_{12}) \mathbf{\hat{\sigma}}
\]

\[
\mathbf{v}''_2 = \mathbf{v}_2 + \frac{1}{2} (1 + \alpha^{-1}) (\mathbf{\hat{\sigma}} \cdot \mathbf{g}_{12}) \mathbf{\hat{\sigma}}
\]

Differences with elastic BE: Presence of $\alpha^{-2}$ in gain term and collision rules.
ENSKOG KINETIC EQUATION

Extension of the BE to moderate densities. Mean free path is NOT much smaller than diameters of spheres.

New ingredients

- Volume accessible per particle is smaller than that of a dilute gas. Probability of finding a particle at a given point is influenced by the presence of the remaining particles of the gas. Non-equilibrium pair correlation function

- The one- particle velocity distribution functions must be evaluated at

$$r, r \pm \sigma$$
Limitation: Velocity correlations are still neglected (molecular chaos hypothesis)!!

\[
\partial_t f + \mathbf{v} \cdot \nabla f + \frac{\partial}{\partial \mathbf{v}} \cdot \left( \frac{\mathbf{F}}{m} f \right) = J_E [\mathbf{r}, \mathbf{v} | f(t), f(t)]
\]

\[
J_E(\mathbf{r}_1, \mathbf{v}_1; t) = \sigma^{d-1} \int d\mathbf{v}_2 \int \, d\hat{\sigma} \Theta(\hat{\sigma} \cdot \mathbf{g}_{12})(\hat{\sigma} \cdot \mathbf{g}_{12}) \times (\alpha^{-2} f_2(\mathbf{r}_1, \mathbf{v}_1'', \mathbf{r}_1 - \sigma, \mathbf{v}_2''; t) - f_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1 + \sigma, \mathbf{v}_2; t))
\]

\[
f_2(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_2, \mathbf{v}_2; t) = \chi(\mathbf{r}_1, \mathbf{r}_2) f(\mathbf{r}_1, \mathbf{v}_1; t) f(\mathbf{r}_2, \mathbf{v}_2; t)
\]

Pair correlation function

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Bad news for the Enskog equation (EE): Several MD simulations have shown that velocity correlations become important as density increases (McNamara & Luding, PRE (1998); Soto & Mareschal, PRE (2001); Pagonabarraga et al., PRE (2002))

Good news for the EE: Good agreement at the level of macroscopic properties for moderate densities and finite dissipation (Simulations: Brey et al., PF (2000); Lutsko, PRE (2001); Dahl et al., PRE (2002); Lois et al., PRE (2007); Bannerman et al., PRE (2009); Mitrano et al., PF (2011), PRE (2014) Experiments: Yang et al., PRL (2002); PRE (2004))

I still think that the EE is still a valuable theory for granular fluids for densities beyond the Boltzmann limit and dissipation beyond the quasielastic limit.

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Hydrodynamic fields

Number density

\[ n(r, t) = \int d\mathbf{v} f(r, \mathbf{v}; t) \]

Flow velocity

\[ U(r, t) = \frac{1}{n(r, t)} \int d\mathbf{v} \mathbf{v} f(r, \mathbf{v}; t) \]

Granular temperature

\[ T(r, t) = \frac{m}{dn(r, t)} \int d\mathbf{v} [\mathbf{v} - U(r, t)]^2 f(r, \mathbf{v}; t) \]
MACROSCOPIC BALANCE EQUATIONS

\[ I_\psi = \int d\mathbf{v}_1 \psi(\mathbf{v}_1) J_E(\mathbf{r}, \mathbf{v}_1 | f, f) \]

After some algebra…..

\[
I_\psi = \frac{1}{2} \sigma^{d-1} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\sigma \Theta(\hat{\sigma} \cdot g_{12}) (\hat{\sigma} \cdot g_{12}) \\
\times \left\{ \left[ \psi(\mathbf{v}_1') + \psi(\mathbf{v}_2') - \psi(\mathbf{v}_1) - \psi(\mathbf{v}_2) \right] f_2(\mathbf{r}, \mathbf{v}_1, \mathbf{r} + \sigma, \mathbf{v}_2; t) \\
+ \nabla \cdot \sigma \left[ \psi(\mathbf{v}_1') - \psi(\mathbf{v}_1) \right] \int_0^1 d\lambda f_2 \left[ \mathbf{r} - \lambda \sigma, \mathbf{v}_1, \mathbf{r} + (1 - \lambda) \sigma, \mathbf{v}_2; t \right] \right\}
\]

Two contributions: (i) collisional effect due to scattering with a change in velocities; (ii) pure collisional effect due to the spatial difference of the colliding pair

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\[ D_t n + n \nabla \cdot U = 0 \]
\[ D_t U + \rho^{-1} \nabla \cdot P = \sigma_U \]
\[ \frac{d}{2} n D_t T + \nabla \cdot q + P : \nabla U = -\frac{d}{2} n T \zeta + \sigma_T \]

\[ D_t \equiv \partial_t + U \cdot \nabla \]

Production of momentum due to external force

\[ \sigma_U = \int dv \ F \ f(v) \]

Production of energy due to external force

\[ \sigma_T = \int dv \ V \cdot F \ f(v) \quad V = v - U \]
Pressure tensor

Kinetic plus collisional contributions \( P = P^k + P^c \)

\[
P^k = \int \, dv \, mvvf(v)
\]

\[
P^c = \frac{1 + \alpha}{4} m \sigma^d \int dv_1 \int dv_2 \int d\hat{\sigma} \Theta(\hat{\sigma} \cdot g_{12})(\hat{\sigma} \cdot g_{12})^2 \hat{\sigma} \hat{\sigma}
\]

\[
\times \int_0^1 d\lambda \, \chi[r - \lambda \sigma, r + (1 - \lambda)\sigma]f(r - \lambda \sigma, v_1; t)f[r + (1 - \lambda)\sigma, v_2; t]
\]
Heat flux

\[ q = q^k + q^c \]

\[ q^k = \int dv \frac{m}{2} V^2 V f(v) \]

\[ q^c = \frac{1 + \alpha}{4} m \sigma^d \int dv_1 \int dv_2 \int d\hat{\sigma} \Theta(\hat{\sigma} \cdot g_{12})(\hat{\sigma} \cdot g_{12})^2 \hat{\sigma}(\hat{\sigma} \cdot G_{12}) \]

\[ \times \int_0^1 d\lambda \chi[r - \lambda \sigma, r + (1 - \lambda)\sigma] f(r - \lambda \sigma, v_1, t) f[r + (1 - \lambda)\sigma, v_2, t] \]

\[ G_{12} = \frac{V_1 + V_2}{2} \]

Collisional transfer contributions to fluxes vanish in the low-density limit but dominates at high density.
Cooling rate

It provides the energy loss rate due to inelastic collisions.
It vanishes for elastic collisions

\[ \zeta = (1 - \alpha^2) \frac{m \sigma^{d-1}}{4dnT} \int dv_1 \int dv_2 \int d\hat{\sigma} \Theta(\hat{\sigma} \cdot g_{12})(\hat{\sigma} \cdot g_{12})^3 \times \chi(r, r + \sigma)f(r, v_1; t)f(r + \sigma, v_2; t) \]

Macroscopic equations are exact within the Enskog equation
DILUTE GAS

\[ \chi \to 1, \quad f(r \pm \sigma, v; t) \approx f(r, v; t) \]

\[ P \to P^k \quad q \to q^k \]

\[ \zeta = (1 - \alpha^2) \frac{m\sigma^{d-1}}{4dnT} \int dv_1 \int dv_2 \int d\hat{\sigma} \Theta(\hat{\sigma} \cdot g_{12})(\hat{\sigma} \cdot g_{12})^3 f(r, v_1; t)f(r, v_2; t) \]
Spatially homogeneous isotropic time-dependent state

\[ \frac{\partial}{\partial t} f(v; t) = \chi J_B [v | f, f] \]

Energy equation

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

Dimensional analysis shows that \( \zeta(t) \propto \sqrt{T(t)} \)

\[ T(t) = \frac{T(0)}{\left(1 + \frac{1}{2}\zeta(0)t\right)^2} \]

Haff’s cooling law (JFM 1983)
Since $T(t)$, the solution is not the local equilibrium distribution. Its explicit form is not known.

However, for times longer than the mean free time it is expected that

$$f(v; t) = n v_{\text{th}}^{-d} \varphi \left( \frac{v}{v_{\text{th}}} \right), \quad v_{\text{th}}(t) = \sqrt{2T(t)/m}$$

In reduced units, the scaled distribution obeys the Boltzmann-Enskog equation

$$\frac{1}{2 \zeta^*} \frac{\partial}{\partial c} \cdot (c \varphi) = J_B^*[\varphi, \varphi]$$

$$\zeta^* = \zeta / (\chi \nu), \quad c = v / v_{\text{th}}$$

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Deviation of the scaled distribution with respect to its Gaussian form. Kurtosis

\[ a_2 = \frac{\langle c^4 \rangle}{\langle c^4 \rangle_M} - 1 \]

To get kurtosis one considers the leading term of the expansion of the scaled distribution in Sonine or Laguerre polynomials

\[ \varphi(c) \to \pi^{-d/2} e^{-c^2} \left[ 1 + \frac{a_2}{2} \left( c^4 - (d + 2)c^2 + \frac{d(d + 2)}{4} \right) \right] \]

Analytic expressions of kurtosis can be obtained by neglecting nonlinear terms

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Best accuracy:

\[ a_2 = \frac{16(1 - \alpha)(1 - 2\alpha^2)}{25 + 24d - \alpha(57 - 8d) - 2(1 - \alpha)\alpha^2} \]

Santos, Montanero GM 11, 157 (2009)

Brilliantov, Pöschel, EPL 74, 424 (2006)
Assumption: For long times (much longer than the mean free time) and far away from boundaries (bulk region) the system reaches a hydrodynamic regime.

Normal solution \( f(r, v; t) = f(v|\{n(r, t)\}, U(r, t), T(r, t)) \)

In some situations, gradients are controlled by boundary or initial conditions. Small spatial gradients:

\[ f = f^{(0)} + \epsilon f^{(1)} + \ldots \]
The expansion generates a similar expansion for the fluxes and the cooling rate. In addition, the Enskog operator and the time derivatives are given by

\[ J_E = J_E^{(0)} + \varepsilon J_E^{(1)} + \cdots, \quad \partial_t = \partial_t^{(0)} + \varepsilon \partial_t^{(1)} + \cdots \]

Time dependence is only through the hydrodynamic fields

\[ \partial_t^{(k)} = (\partial_t^{(k)} n) \partial n + (\partial_t^{(k)} U_i) \partial U_i + (\partial_t^{(k)} T) \partial T \]

From the balance equations

\[ \partial_t^{(0)} n = \partial_t^{(0)} U_i = 0, \quad \partial_t^{(0)} T = -T \zeta^{(0)} \]

\[ D_t^{(1)} n = -n \nabla \cdot U, \quad D_t^{(1)} U = -\rho^{-1} \nabla p + g, \quad D_t^{(1)} T = -\frac{2}{d} T \nabla \cdot U - T \zeta^{(1)} \]

\[ D_t^{(1)} = \partial_t^{(1)} + U \cdot \nabla \]
Some *controversy* about the possibility of going from kinetic theory to hydrodynamics by using the CE method

The **time scale** for $T$ is set by the (inverse) **cooling rate** instead of spatial gradients. This new time scale, $T$ is *much faster* than in the usual hydrodynamic scale. Some hydrodynamic excitations decay much slower than $T$

For **large inelasticity** ($\zeta^{-1}$ small), *perhaps* there were **NO** time scale separation between hydrodynamic and kinetic excitations: **NO AGING** to hydrodynamics!!

We assume the validity of a hydrodynamic description and compare with computer simulations.
Several first previous attempts to determine the Navier-Stokes transport coefficients

- J. Jenkins, M. W. Richman, PF 28, 3485 (1985)

**Limitation:** Nearly elastic spheres. Reference state is the Maxwell-Boltzmann distribution function. Solution to zeroth-order must not be chosen *a priori* and must be consistently obtained!!

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**ZERO-ORDER SOLUTION**

\[
\partial_t^{(0)} f^{(0)} = \chi J_B[f^{(0)}, f^{(0)}]
\]

This equation has the same form as the EE for the HCS, but now the zeroth-order solution is a *local* HCS distribution

\[
f^{(0)}(\mathbf{r}, \mathbf{v}; t) = n(\mathbf{r}, t) v_{th}(\mathbf{r}, t)^{-d} \varphi(c)
\]

Normal solution: \[
\partial_t^{(0)} f^{(0)} = \partial_T f^{(0)} \partial_t^{(0)} T = -\zeta^{(0)} T \partial_T f^{(0)}
\]

\[
\frac{1}{2} \zeta^{(0)} \frac{\partial}{\partial \mathbf{V}} \cdot (\mathbf{V} f^{(0)}) = \chi J_B[f^{(0)}, f^{(0)}]
\]

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The zeroth-order distribution is isotropic in velocity

\[ q^{(0)} = 0 \]

\[ P_{ij}^{(0)} = p \delta_{ij}, \quad p = nT \left[ 1 + 2^{d-2}(1 + \alpha)\phi\chi \right] \]

\[ \zeta^{(0)} = \frac{\pi^{(d-1)/2}}{4d\Gamma\left(\frac{d+3}{2}\right)} \left(1 - \alpha^2\right) \frac{m\sigma^{d-1}}{nT} \chi \int dv_1 \int dv_2 g_{12}^3 f^{(0)}(v_1)f^{(0)}(v_2) \]

Solid volume fraction \( \phi = \frac{\pi^{d/2}}{2^{d-1}d\Gamma\left(\frac{d}{2}\right)}n\sigma^d \)
FIRST-ORDER SOLUTION

Motivation: determine the transport coefficients \textit{without} limitation to the degree of dissipation

After some efforts….

\[
\left( \partial_t^{(0)} + \mathcal{L} \right) f^{(1)} = A(V) \cdot \nabla \ln T + B(V) \cdot \nabla \ln n \\
+ C_{ij}(V) \frac{1}{2} \left( \frac{\partial U_i}{\partial r_j} + \frac{\partial U_j}{\partial r_i} - 2 \delta_{ij} \nabla \cdot U \right) + D(V) \nabla \cdot U
\]

Boltzmann-Enskog linearized operator

\[
\mathcal{L}X = -\chi \left( J_B[f^{(0)}, X] + J_B[X, f^{(0)}] \right)
\]

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\[ A(V|n, U, T) = \frac{1}{2} V \frac{\partial}{\partial V} \cdot (V f^{(0)}) - \frac{p}{\rho} \frac{\partial f^{(0)}}{\partial V} + \frac{1}{2} \mathcal{K} \left[ \frac{\partial}{\partial V} \cdot (V f^{(0)}) \right] \]

\[ B(V|n, U, T) = -V f^{(0)} - \frac{p}{\rho} \left( 1 + \phi \frac{\partial \ln \phi^*}{\partial \phi} \right) \frac{\partial f^{(0)}}{\partial V} - \left( 1 + \frac{1}{2} \phi \frac{\partial \ln \chi}{\partial \phi} \right) \mathcal{K} \left[ f^{(0)} \right] \]

\[ C_{ij}(V|n, U, T) = V_i \frac{\partial f^{(0)}}{\partial V_j} + \mathcal{K}_i \left[ \frac{\partial f^{(0)}}{\partial V_j} \right] \]

\[ D(V|n, U, T) = \frac{1 - p^*}{d} \frac{\partial}{\partial V} \cdot (V f^{(0)}) + \frac{1}{d} \mathcal{K}_i \left[ \frac{\partial f^{(0)}}{\partial V_i} \right] - \frac{1}{2} \zeta U \frac{\partial}{\partial V} \cdot (V f^{(0)}) \]

where \( p^* \equiv p/(nT), \quad \zeta^{(1)} = \zeta U \nabla \cdot U \)

\[ \mathcal{K}[X] = \sigma^d \chi \int dV_2 \int d\hat{\sigma} \Theta(\hat{\sigma} \cdot g_{12})(\hat{\sigma} \cdot g_{12}) \hat{\sigma} \left[ \alpha^{-2} f^{(0)}(v''_1)X(v''_2) + f^{(0)}(v''_1)X(v''_2) \right] \]
The first-order solution has the form

\[ f^{(1)} = \mathcal{A}(\mathbf{V}) \cdot \nabla \ln T + \mathcal{B}(\mathbf{V}) \cdot \nabla \ln n + C_{ij}(\mathbf{V}) \frac{1}{2} \left( \frac{\partial U_i}{\partial r_j} + \frac{\partial U_j}{\partial r_i} - \frac{2}{d} \delta_{ij} \nabla \cdot \mathbf{U} \right) + \mathcal{D}(\mathbf{V}) \nabla \cdot \mathbf{U} \]

To obtain the integral equations verifying the unknowns, one has to take into account

\[ \partial_t^{(0)} \begin{pmatrix} \mathcal{A} \\ \mathcal{B} \end{pmatrix} = (\partial_t^{(0)} T) \partial_T \begin{pmatrix} \mathcal{A} \\ \mathcal{B} \end{pmatrix} = \frac{1}{2} \zeta^{(0)} \frac{\partial}{\partial \mathbf{V}} \left( \begin{pmatrix} \mathbf{V} \mathcal{A} \\ \mathbf{V} \mathcal{B} \end{pmatrix} \right) \]

\[ \partial_t^{(0)} \begin{pmatrix} C_{ij} \\ \mathcal{D} \end{pmatrix} = (\partial_t^{(0)} T) \partial_T \begin{pmatrix} C_{ij} \\ \mathcal{D} \end{pmatrix} = \frac{1}{2} \zeta^{(0)} \begin{pmatrix} C_{ij} \\ \mathcal{D} \end{pmatrix} + \frac{1}{2} \zeta^{(0)} \frac{\partial}{\partial \mathbf{V}} \left( \begin{pmatrix} \mathbf{V} C_{ij} \\ \mathbf{V} \mathcal{D} \end{pmatrix} \right) \]

\[ \partial_t^{(0)} \nabla \ln T = \nabla \left( T^{-1} \partial_t^{(0)} T \right) = -\zeta^{(0)} \left( 1 + \phi \frac{\partial \ln \chi}{\partial \phi} \right) \nabla \ln n - \frac{1}{2} \zeta^{(0)} \nabla \ln T \]
Since the hydrodynamic gradients are *all* independent, then

\[
\frac{1}{2} \zeta^{(0)} \frac{\partial}{\partial \mathbf{V}} \cdot (\mathbf{V} \mathbf{A}) - \frac{1}{2} \zeta^{(0)} \mathbf{A} + \mathcal{L} \mathbf{A} = \mathbf{A}
\]

\[
\frac{1}{2} \zeta^{(0)} \frac{\partial}{\partial \mathbf{V}} \cdot (\mathbf{V} \mathbf{B}) + \mathcal{L} \mathbf{B} = \mathbf{B} + \zeta^{(0)} \left(1 + \phi \frac{\partial \ln \chi}{\partial \phi}\right) \mathbf{A}
\]

\[
\frac{1}{2} \zeta^{(0)} \frac{\partial}{\partial \mathbf{V}} \cdot (\mathbf{V} C_{ij}) + \frac{1}{2} \zeta^{(0)} C_{ij} + \mathcal{L} C_{ij} = C_{ij}
\]

\[
\frac{1}{2} \zeta^{(0)} \frac{\partial}{\partial \mathbf{V}} \cdot (\mathbf{V} D) + \frac{1}{2} \zeta^{(0)} D + \mathcal{L} D = D
\]
\[ P_{ij}^{(1)} = -\eta \left( \partial_j U_i + \partial_i U_j - \frac{2}{d} \delta_{ij} \nabla \cdot \mathbf{U} \right) - \delta_{ij} \eta_b \nabla \cdot \mathbf{U} \]

Shear viscosity

Bulk viscosity

\[ q^{(1)} = -\kappa \nabla T - \mu \nabla n \]

Thermal conductivity

Diffusive heat conductivity
Bulk viscosity has only \textit{collisional} contributions

\[ \eta_b = \frac{\pi^{(d-1)/2}}{\Gamma \left( \frac{d+3}{2} \right)} \frac{d + 1}{4d^2} m \sigma^{d+1} \chi (1 + \alpha) n^2 v_{th} I_\eta \]

\[ I_\eta = \frac{1}{n^2 v_{th}} \int dv_1 \int dv_2 f^{(0)}(V_1) f^{(0)}(V_2) g_{12} \]

Shear viscosity \[ \eta = \eta_k + \eta_c \]

\[ \eta_c = \frac{2^{d-1}}{d + 2} \phi \chi (1 + \alpha) \eta_k + \frac{d}{d + 2} \eta_b \]

\[ \eta_k = \frac{\eta_0}{\nu \eta - \frac{1}{2} \zeta} \left[ 1 - \frac{2^{d-2}}{d + 2} (1 + \alpha) (1 - 3\alpha) \phi \chi \right] \]
Shear viscosity of a low-density \textit{elastic} gas of hard spheres

\[ \eta_0 = \frac{(d + 2)}{8} \frac{\Gamma \left( \frac{d}{2} \right)}{\pi^{(d-1)/2}} \sigma^{1-d} \sqrt{mT} \]

Solid volume fraction \[ \phi = \frac{\pi^{d/2}}{2^{d-1} d \Gamma \left( \frac{d}{2} \right)} n \sigma^d \]

\[ \tilde{\zeta}_0^* \equiv \frac{\zeta^{(0)}}{\nu_0}, \quad \nu_\eta^* \equiv \frac{\nu_\eta}{\nu_0} \quad \nu_0 = nT/\eta_0 \]

Effective collision frequency associated with momentum transport

\[ \nu_\eta = \frac{\int dv \; R_{ij}(V) \mathcal{L} C_{ij}(V)}{\int dv \; R_{ij}(V) C_{ij}(V)} \]

\[ R_{ij}(V) = m \left( V_i V_j - \frac{1}{d} \delta_{ij} V^2 \right) \]
Thermal conductivity \[ \kappa = \kappa_k + \kappa_c \]

\[ \kappa_c = 3 \frac{2^{d-2}}{d + 2} \phi \chi (1 + \alpha) \kappa_k + \frac{\pi^{(d-1)/2}}{8d \Gamma \left( \frac{d+3}{2} \right)} m \sigma^{d+1} \chi (1 + \alpha) n^2 \nu_{th}^3 I_K \]

\[ I_K = \frac{1}{n^2 \nu_{th}^3} \int d\mathbf{v}_1 \int d\mathbf{v}_2 f^{(0)}(\mathbf{V}_1) f^{(0)}(\mathbf{V}_2) \left[ g_{12}^{-1} (g_{12} \cdot G_{12})^2 + g_{12} G_{12}^2 + \frac{3}{2} g_{12} (g_{12} \cdot G_{12}) + \frac{1}{4} g_{12}^3 \right] \]

\[ \kappa_k = \kappa_0 \frac{d-1}{d} \left( v_{\kappa}^* - 2 \zeta_0^* \right)^{-1} \left\{ 1 + 2a_2 + \frac{2^{d-3}}{d+2} \phi \chi (1 + \alpha)^2 [2\alpha - 1 + a_2 (1 + \alpha)] \right\} \]
Thermal conductivity of a low-density elastic gas of elastic hard spheres

\[ \kappa_0 = \frac{d(d + 2) \eta_0}{2(d - 1) m} \]

Effective collision frequency associated with energy transport

\[ \nu_\kappa = \frac{\int d\mathbf{v} S(\mathbf{V}) \cdot \mathcal{L} \mathcal{A}(\mathbf{V})}{\int d\mathbf{v} S(\mathbf{V}) \cdot \mathcal{A}(\mathbf{V})} \]

\[ S(\mathbf{V}) = \left( \frac{1}{2} m V^2 - \frac{d + 2}{2} T \right) V \]

Rheology of disordered particles - suspensions, glassy and granular materials, June 2018, Kyoto
Heat diffusivity coefficient  \( \mu = \mu_k + \mu_c \)

\[
\mu_c = 3 \frac{2^{d-2}}{d + 2} \phi \chi (1 + \alpha) \mu_k
\]

\[
\mu_k = 2 \frac{\kappa_0 T}{n} \left( 2 \nu^*_\mu - 3 \zeta_0^* \right)^{-1} \left\{ \zeta_0^* \kappa_k^* \left( 1 + \phi \frac{\partial \ln \chi}{\partial \phi} \right) + \frac{d - 1}{d} \alpha_2 \\
-3 \frac{2^{d-2}(d-1)}{d(d+2)} \phi \chi (1 + \alpha) \left( 1 + \frac{1}{2} \frac{\partial \ln \chi}{\partial \phi} \right) \left[ \alpha (1 - \alpha) \\
- \frac{\alpha_2}{6} (10 + 2d - 3\alpha + 3\alpha^2) \right] \right\}
\]

\[
\nu_\mu = \frac{\int d\nu S(\mathbf{V}) \cdot \mathcal{L}_B(\mathbf{V})}{\int d\nu S(\mathbf{V}) \cdot \mathcal{B}(\mathbf{V})}
\]

\[
\kappa_k^* \equiv \frac{\kappa_k}{\kappa_0}
\]
First-order contribution to the cooling rate

Up to first order in spatial gradients

\[ \zeta = \zeta^{(0)} + \zeta_U \nabla \cdot \mathbf{U} \]

\[ \zeta_U = -\frac{3}{4d} 2^d \phi \chi (1 - \alpha^2) + \frac{\pi (d-1)/2}{2d \Gamma \left( \frac{d+3}{2} \right)} (1 - \alpha^2) \frac{m \sigma^{d-1}}{nT} \int dv_1 \int dv_2 f^{(0)} (V_1) D(V_2) g_{12}^3 \]

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Dilute gas expressions:  \( \phi \rightarrow 0, \quad \chi \rightarrow 1 \)

\[
\eta = \frac{\eta_0}{\nu^*_\eta - \frac{1}{2} \zeta^*_0}
\]

\[
\kappa = \frac{d - 1}{d} \frac{\kappa_0}{\nu^*_\kappa - 2 \zeta^*_0} (1 + 2a_2)
\]

\[
\mu = 2 \frac{T \zeta^*_0 \kappa + \frac{d-1}{d} \kappa_0 a_2}{n \left(2 \nu^*_\mu - 3 \zeta^*_0\right)}
\]

Brey, Dufty, Kim, Santos PRE 58, 4638 (1998)
So far, all the results are formally **exact!!**

However, transport coefficients given in terms of

\[
\{ \zeta^*, a_2, I_\eta, I_\kappa, \nu_\eta^*, \nu_\kappa^*, \nu_\mu^* \}
\]

……..whose forms are not exactly known !!!
In the case of the zeroth-order distribution, one takes the leading term in a Sonine polynomial expansion. In this case,

\[ \zeta^*_0 = \frac{d + 2}{4d} \chi(1 - \alpha^2) \left(1 + \frac{3}{16} a_2\right) \]

\[ a_2 = \frac{16(1 - \alpha)(1 - 2\alpha^2)}{25 + 24d - \alpha(57 - 8d) - 2(1 - \alpha)\alpha^2} \]

\[ I_\eta = \sqrt{2} \frac{\Gamma \left( \frac{d+1}{2} \right)}{\Gamma \left( \frac{d}{2} \right)} \left(1 - \frac{a_2}{16}\right), \quad I_\kappa = \sqrt{2} \frac{\Gamma \left( \frac{d+3}{2} \right)}{\Gamma \left( \frac{d}{2} \right)} \left(1 + \frac{7}{16} a_2\right) \]
The knowledge of the effective collision frequencies requires to solve linear integral equations. To get explicit results, one has to resort to some approximations.

**Standard first Sonine approximation**

Method used in ordinary gases: truncate the Sonine polynomial expansion of the unknowns after the first term

\[
\begin{pmatrix}
\mathcal{A}(V) \\
\mathcal{B}(V) \\
C_{ij}(V)
\end{pmatrix} \rightarrow -f_M(V)
\]

\[
\begin{pmatrix}
\frac{2}{d+2} \frac{m}{nT^2} \kappa_k S(V) \\
\frac{2}{d+2} \frac{m}{nT^2} \mu_k S(V) \\
\frac{\eta_k}{nT^2} R_{ij}(V)
\end{pmatrix}
\]

Maxwellian distribution
Non-Gaussian properties of the zeroth-order distribution might be relevant for strong dissipation. Possible source of discrepancy between theory and simulations. Alternative route to the standard method: replace Maxwellian distribution by the HCS distribution

\[
\begin{pmatrix}
A(V) \\
B(V) \\
C_{ij}(V)
\end{pmatrix} 
\rightarrow -f^{(0)}(V) 
\begin{pmatrix}
\frac{2}{d+2} \frac{m}{nT^2} \frac{\kappa_k}{1 + \frac{d+8}{2} a_2} \\
\frac{2}{d+2} \frac{m}{nT^2} \frac{\mu_k}{1 + \frac{d+8}{2} a_2} \\
\frac{1}{1 + a_2 nT^2} R_{ij}
\end{pmatrix}
\]

HCS distribution
Table 3.1 Explicit expressions of the Navier–Stokes transport coefficients

\[
\begin{align*}
\eta &= \eta_k \left[ 1 + \frac{2^{d-1}}{d+2} \phi \chi (1 + \alpha) \right] + \frac{d}{d+2} \eta_b, \\
\eta_k &= \left( \nu_{\eta}^* - \frac{1}{2} \xi_{0}^* \right)^{-1} \left[ 1 - \frac{2^{d-2}}{d+2} \phi \chi (1 + \alpha)(1 - 3\alpha)\phi \chi \right] \eta_0, \\
\eta_b &= \frac{2^{2d+1}}{\pi(d+2)} \phi^2 \chi (1 + \alpha) \left( 1 - \frac{a_2}{16} \right) \eta_0, \\
\kappa &= \kappa_k \left[ 1 + 3 \frac{2^{d-2}}{d+2} \phi \chi (1 + \alpha) \right] + \frac{2^{2d+1}(d-1)}{(d+2)^2 \pi} \phi^2 \chi (1 + \alpha) \left( 1 + \frac{7}{16} a_2 \right) \kappa_0, \\
\kappa_k &= \frac{d-1}{d} \left( \nu_{k}^* - 2 \xi_{0}^* \right)^{-1} \left\{ 1 + 2a_2 + 3 \frac{2^{d-3}}{d+2} \phi \chi (1 + \alpha)^2 \left[ 2\alpha - 1 + a_2(1 + \alpha) \right] \right\} \kappa_0, \\
\mu &= \mu_k \left[ 1 + 3 \frac{2^{d-2}}{d+2} \phi \chi (1 + \alpha) \right], \\
\mu_k &= \frac{2T}{n} \left( 2\nu_{\mu}^* - 3\xi_{0}^* \right)^{-1} \left\{ \xi_{k}^* \kappa_k \left[ 1 + \phi \frac{\partial \ln \chi}{\partial \phi} \right] + \frac{d-1}{d} \phi \chi (1 + \alpha) \left[ \alpha(1 - \alpha) - \frac{a_2}{6} (10 + 2d - 3\alpha + 3\alpha^2) \right] \right\} \kappa_0.
\end{align*}
\]

\textbf{Standard first Sonine approximation}

\[
\begin{align*}
\nu_{\eta}^* &= \frac{3}{4d} \chi \left( 1 - \alpha + \frac{2}{3} d \right) (1 + \alpha) \left( 1 - \frac{a_2}{32} \right), \\
\nu_{k}^* &= \nu_{\mu}^* = \frac{1 + \alpha}{d} \chi \left[ \frac{d-1}{2} + \frac{3}{16} (d+8)(1 - \alpha) + \frac{4 + 5d - 3(4 - d)\alpha}{512} \right] a_2.
\end{align*}
\]

\textbf{Modified first Sonine approximation}

\[
\begin{align*}
\nu_{\eta}^* &= \frac{3}{4d} \chi \left( 1 - \alpha + \frac{2}{3} d \right) (1 + \alpha) \left( 1 + \frac{7}{16} \alpha_2 \right), \\
\nu_{k}^* &= \nu_{\mu}^* = \frac{1 + \alpha}{d} \chi \left[ \frac{d-1}{2} + \frac{3}{16} (d+8)(1 - \alpha) + \frac{296 + 217d - 3(160 + 11d)\alpha}{256} \right] a_2.
\end{align*}
\]
Modern symbolic manipulators can be employed to obtain accurate estimates of the transport coefficients. Restricted to *dilute* gases.

Unknowns are expanded in powers of Sonine polynomials but using a *wrong* temperature. It avoids possible divergence of the Sonine expansion.

Limitation: one has to numerically solve a system of algebraic equations.
COMPARISON WITH COMPUTER SIMULATIONS

Shear viscosity of a moderate dense granular gas

Simple or uniform shear flow (USF)

Rheology of disordered particles - suspensions, glassy and granular materials, June 2018, Kyoto
The USF state is quite different in ordinary and granular fluids. For elastic collisions, temperature increases in time due to viscous heating term. This effect can be controlled by the introduction of a thermostat. However, in the absence of thermostat, the reduced shear rate tends to zero for long times

\[ a^*(t) = \lim_{t \to \infty} \frac{a}{\nu(t)} \to 0, \quad \nu(t) \propto \sqrt{T(t)} \]

Thus, viscous heating effect can be employed to measure the NS shear viscosity of hard spheres (Naito and Ono, J. Chem. Phys. 70, 4515 (1979))

One is tempted to do the same for granular fluids but……unfortunately viscous heating is compensated by collisional cooling and a steady state is achieved.

Rheology of disordered particles - suspensions, glassy and granular materials, June 2018, Kyoto
Strategy for measuring shear viscosity of a granular fluid. We consider the USF state modified by the introduction of two different terms:

- A deterministic external "friction" (drag) force with negative friction coefficient to compensate for collisional dissipation.
- A stochastic process to mimic the conditions appearing in the Chapman-Enskog solution.

DSMC method (Monte Carlo simulations)

\[ \eta^*(\alpha, \phi) \equiv \frac{\eta(\alpha, \phi)}{\eta(1, \phi)} \]

Rheology of disordered particles - suspensions, glassy and granular materials, June 2018, Kyoto
**Dilute** gases: three alternative methods


- Application of external force to USF. Montanero et al. (2005) (circles)
Heat flux transport coefficients

\[ \kappa^*(\alpha, 0) \equiv \frac{\kappa(\alpha, 0)}{\kappa(1, 0)} \quad \mu^*(\alpha, 0) \equiv \frac{n\mu(\alpha, 0)}{T\kappa_0} \]

Rheology of disordered particles - suspensions, glassy and granular materials, June 2018, Kyoto
DSMC simulations:
(1) Green-Kubo relations, Brey et. al, 2004 (triangles);
(2) External force, Montanero, Santos, Garzó Physica A 376, 75 (2007) (circles)
CONCLUSIONS

✓ Hydrodynamic equations have been exactly derived from Enskog kinetic theory. They appear to be a powerful tool for analysis and predictions of rapid flow gas dynamics at moderate densities.

✓ A normal solution to the Enskog equation has been then obtained for states close to the HCS. Navier-Stokes transport coefficients and cooling rate have been exactly given in terms of solutions of a set of coupled linear integral equations.

✓ Approximate forms for the transport coefficients have been obtained by three different methods: (i) standard first-Sonine solution, (ii) modified first-Sonine solution, and (iii) computer-aided method.
CONCLUSIONS

✓ Theoretical results have been compared against **two** types of simulations: DSMC (to confirm approximations to the kinetic equation) and MD (to confirm results beyond kinetic theory limitations).

✓ In general, the agreement between theory and simulations is very good, even for moderately dense systems and strong collisional dissipation.

✓ The above good agreement encourages the use of kinetic theory as a reliable and accurate tool to reproduce the trends observed in granular flows, specially those related to collisional dissipation.
External collaborations
• James W. Dufty (University of Florida, USA)

http://www.eweb.unex.es/eweb/fisteor/vicente/

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