KINETIC THEORY FOR GRANULAR MIXTURES AT MODERATE DENSITIES: SOME APPLICATIONS

Vicente Garzó

Departamento de Física and Instituto de Computación Científica Avanzada (ICCAEx), Universidad de Extremadura, Badajoz, Spain

STATISTICAL PHYSICS in EXTREMADURA

Instituto de Computación Científica Avanzada UEx

Rheology of disordered particles - suspensions, glassy and granular materials, June 2018, Kyoto

OUTLINE

1. Granular binary mixtures. *Smooth* inelastic hard spheres: Enskog kinetic equation for ***moderately dense*** systems

2. Homogeneous cooling state

3. Navier-Stokes hydrodynamics: transport coefficients

4. *Instabilities* in granular dense mixtures

5. Thermal diffusion *segregation*

6. Conclusions

INTRODUCTION

Granular systems are constituted by macroscopic grains that collide inelastically so that the total energy decreases with time

Behaviour of granular systems under many conditions exhibit a great similarity to ordinary fluids

Rapid flow conditions: hydrodynamic-like type equations. Good example of a system which is inherently in ***non-equilibrium***

Dominant transfer of momentum and energy is through ***binary inelastic*** collisions. Subtle modifications of the usual macroscopic balance equations

To isolate collisional dissipation: ***idealized*** microscopic model

Smooth hard spheres
with *inelastic* collisions

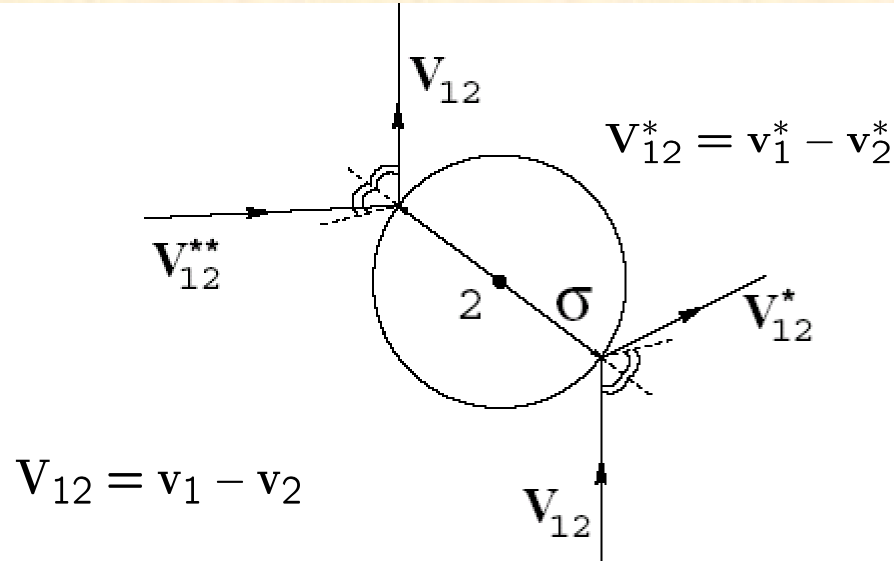


FIG. 1: Sketch of inelastic collisions (after T.P.C. van Noije & M.H. Ernst).

$$\boxed{\mathbf{V}^*_{12} \cdot \widehat{\boldsymbol{\sigma}} = -\alpha \mathbf{V}_{12} \cdot \widehat{\boldsymbol{\sigma}}}$$

Coefficient of restitution

$$\boxed{0 < \alpha \leq 1}$$

Direct collision

$$\mathbf{v}^*_1 = \mathbf{v}_1 - \frac{1}{2}(1+\alpha)\,(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}^*_2 = \mathbf{v}_2 + \frac{1}{2}(1+\alpha)\,(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{V}_{12})\widehat{\boldsymbol{\sigma}}$$

Momentum conservation

$$\mathbf{v}_1 + \mathbf{v}_2 = \mathbf{v}_1^* + \mathbf{v}_2^*$$

Collisional energy change

$$\Delta E = \frac{1}{2} m \left(v_1^{*2} + v_2^{*2} - v_1^2 - v_2^2 \right) = -\frac{m}{4}(1 - \alpha^2)(\mathbf{V}_{12} \cdot \hat{\boldsymbol{\sigma}})^2$$

Very **simple** model that *captures* many properties of granular flows, especially those associated with dissipation

Real granular systems characterized by some degrees of *polidispersity* in density and size: *Multicomponent* granular systems

Mechanical parameters: $\{m_i, \sigma_i, \alpha_{ij}\}, \quad i = 1, \cdots, s$

Direct collision:

$$\mathbf{v}_1' = \mathbf{v}_1 - \frac{m_j}{m_i + m_j}\left(1 + \alpha_{ij}\right)(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2' = \mathbf{v}_2 + \frac{m_i}{m_i + m_j}\left(1 + \alpha_{ij}\right)(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\boxed{\mathbf{V}_{12} \equiv \mathbf{g}_{12}}$$

$$(\Delta E)_{ij} = \frac{1}{2}\left(m_i v_1'^2 + m_j v_2'^2 - m_i v_1^2 - m_j v_2^2\right) = -\frac{1}{2}\frac{m_i m_j}{m_i + m_j}(1 - \alpha_{ij}^2)(\mathbf{g}_{12}\cdot\widehat{\boldsymbol{\sigma}})^2$$

REVISED ENSKOG KINETIC THEORY

S-multicomponent mixture of smooth hard spheres or disks of masses m_i, diameters σ_i, and coefficients of restitution α_{ij}

At a kinetic level: $f_i(\mathbf{r}_1,\mathbf{v}_1;t)$

$$\boxed{\left(\partial_t + \mathbf{v}_1\cdot\nabla_{\mathbf{r}_1} + m_i^{-1}\mathbf{F}_i\cdot\nabla_{\mathbf{v}_1}\right) f_i(\mathbf{r}_1,\mathbf{v}_1;t) = C_i(\mathbf{r}_1,\mathbf{v}_1;t)}$$

$$\begin{aligned} C_i(\mathbf{r}_1,\mathbf{v}_1;t) &= \sum_{j=1}^{s}\sigma_{ij}^{d-1}\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12}) \\ &\times\left(\alpha_{ij}^{-2} f_{ij}(\mathbf{r}_1,\mathbf{v}_1'',\mathbf{r}_1-\boldsymbol{\sigma}_{ij},\mathbf{v}_2'';t) - f_{ij}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_1+\boldsymbol{\sigma}_{ij},\mathbf{v}_2;t)\right) \end{aligned}$$

Two-particle distribution function

Collision rules:

$$\mathbf{v}_1'' = \mathbf{v}_1 - \mu_{ji}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{v}_2'' = \mathbf{v}_2 + \mu_{ij}\left(1+\alpha_{ij}^{-1}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\widehat{\boldsymbol{\sigma}}$$

where $\mu_{ij}=m_i/(m_i+m_j)$

Kinetic theory approach: ***velocity*** correlations are neglected (molecular chaos hypothesis !!)

$$f_{ij}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_2,\mathbf{v}_2;t) \to \chi_{ij}\left(\mathbf{r}_1,\mathbf{r}_2 \mid \{n_i\}\right) f_i(\mathbf{r}_1,\mathbf{v}_1;t) f_j(\mathbf{r}_2,\mathbf{v}_2;t)$$

Spatial correlations (volume exclusion effects)

Subtle point: How is defined the pair correlation function *out of equilibrium*?

Let us consider here a monocomponent ordinary gas
for the sake of simplicity

In 1922, Enkog assumed that the pair correlation is the *same function* of the number density as in a fluid at equilibrium with the density evaluated at the point of contact (**Standard** Enskog Theory, **SET**)

$$\chi^{\mathsf{SET}}(\mathbf{r},\mathbf{r}') = 1 + n\left(\frac{\mathbf{r}+\mathbf{r}'}{2}\right)\int V(\mathbf{r},\mathbf{r}'|\mathbf{r}'')\,\mathrm{d}\mathbf{r}'' + \frac{1}{2!}n^2\left(\frac{\mathbf{r}+\mathbf{r}'}{2}\right)\int\int V(\mathbf{r},\mathbf{r}'|\mathbf{r}''\mathbf{r}''')\,\mathrm{d}\mathbf{r}''\mathrm{d}\mathbf{r}''' + \cdots$$

Husimi V-functions of the virial expansion

Conceptual *drawback* of SET: its extension to mixtures leads to inconsistencies with Onsager's reciprocity relations

H. van Beijeren and M. Ernst (Physica A, (1973)) proposed the **Revised** Enskog Theory, RET

Pair correlation is the same ***functional*** of density as in a nonuniform equilibrium

$$\chi^{\mathsf{RET}}(\mathbf{r},\mathbf{r}') = 1 + \int n(\mathbf{r}')\, V(\mathbf{r},\mathbf{r}'|\mathbf{r}'')\, \mathrm{d}\mathbf{r}'' + \frac{1}{2!}\int\int n(\mathbf{r}')n(\mathbf{r}'')V(\mathbf{r},\mathbf{r}'|\mathbf{r}''\mathbf{r}''')\, \mathrm{d}\mathbf{r}''\mathrm{d}\mathbf{r}''' + \cdots$$

Monocomponent fluids: SET and RET yield the ***same***
Navier-Stokes transport coefficients. They differ at the Burnett hydrodynamic order

(López de Haro, VG, Physica A **197**, 98 (1993))

Multicomponent fluids. SET and RET give ***different*** expressions for the Navier-Stokes transport coefficients associated with mass and heat fluxes

(López de Haro, Cohen, Kincaid, J. Chem. Phys. **78**, 2746 (1983))

Good theory for granular mixtures is the extension of the RET to inelastic collisions

Bad news for the RET: 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 RET: 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);
Rericha et al., PRL (2002);…..)

RET is *still* a valuable theory for granular fluids for *densities* beyond the Boltzmann limit and *dissipation* beyond the quasielastic limit

MACROSCOPIC BALANCE EQUATIONS

Hydrodynamic fields

$$n_i(\mathbf{r},t)=\int d\mathbf{v} f_i(\mathbf{r},\mathbf{v},t)$$

$$\mathbf{U}(\mathbf{r},t)=\frac{1}{\rho(\mathbf{r},t)}\sum_i\int d\mathbf{v} m_i\mathbf{v} f_i(\mathbf{r},\mathbf{v},t)$$

$$T(\mathbf{r},t)=\frac{1}{n(\mathbf{r},t)}\sum_i\int d\mathbf{v}\frac{m_i}{d}(\mathbf{v}-\mathbf{U})^2 f_i(\mathbf{r},\mathbf{v},t)$$

Macroscopic equations are ***exact*** since they are obtained from the first hierarchy equation (without the Enskog approximation)

MACROSCOPIC BALANCE EQUATIONS

$$I_\psi = \sum_{i=1}^{s} \int \mathrm{d}\mathbf{v}_1 \psi(\mathbf{v}_1) C_i(\mathbf{r}_1, \mathbf{v}_1; t)$$

After some algebra…..

$$\boxed{\begin{aligned} I_\psi &= \frac{1}{2} \sum_{i,j=1}^{s} \sigma_{ij}^{d-1} \int \mathrm{d}\mathbf{v}_1 \int \mathrm{d}\mathbf{v}_2 \int \mathrm{d}\widehat{\boldsymbol{\sigma}} \Theta(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12}) \\ &\times \Big\{ \Big[\psi_i(\mathbf{v}_1') + \psi_j(\mathbf{v}_2') - \psi_i(\mathbf{v}_1) - \psi_j(\mathbf{v}_2) \Big] f_{ij}(\mathbf{r}_1, \mathbf{v}_1, \mathbf{r}_1 + \boldsymbol{\sigma}_{ij}, \mathbf{v}_2; t) \\ &+ \nabla_{\mathbf{r}_1} \cdot \boldsymbol{\sigma}_{ij} \left[\psi_i(\mathbf{v}_1') - \psi_i(\mathbf{v}_1) \right] \int_0^1 \mathrm{d}\lambda f_{ij} \left[\mathbf{r}_1 - \lambda \boldsymbol{\sigma}_{ij}, \mathbf{v}_1, \mathbf{r}_1 + (1-\lambda)\boldsymbol{\sigma}_{ij}, \mathbf{v}_2; t) \right] \Big\} \end{aligned}}$$

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

Balance equation for the partial densities

$$\boxed{D_t n_i + n_i \nabla \cdot \mathbf{U} + m_i^{-1} \nabla \cdot \mathbf{j}_i = 0}$$

Balance equation for the flow velocity

$$\boxed{\rho D_t U_\beta + \nabla_\gamma P_{\gamma\beta} = \sum_{i=1}^{s} n_i (\mathbf{r}, t)\, F_{i\beta} (\mathbf{r})}$$

Balance equation for the granular temperature

$$\boxed{\frac{d}{2} n \left(D_t + \zeta \right) T + P_{\gamma\beta} \nabla_\gamma U_\beta + \nabla \cdot \mathbf{q} - \frac{d}{2} T \sum_{i=1}^{s} \frac{\nabla \cdot \mathbf{j}_i}{m_i} = \sum_{i=1}^{s} \frac{\mathbf{F}_i \cdot \mathbf{j}_i}{m_i}}$$

Cooling rate

$$D_t \equiv \partial_t + \mathbf{v} \cdot \nabla$$

Mass flux

$$\mathbf{j}_i(\mathbf{r}_1, t) = m_i \int d\mathbf{v}_1 \mathbf{V}_1 f_i(\mathbf{r}_1, \mathbf{v}_1; t)$$

V=v-U

Pressure tensor

$$P_{\gamma\beta}(\mathbf{r}_1, t) = P^k_{\gamma\beta}(\mathbf{r}_1, t) + P^c_{\gamma\beta}(\mathbf{r}_1, t)$$

Kinetic contribution **Collisional contribution**

$$P^k_{\gamma\beta}(\mathbf{r}_1, t) = \sum_{i=1}^{s} \int d\mathbf{v}_1 m_i V_{1\beta} V_{1\gamma} f_i(\mathbf{r}_1, \mathbf{v}_1; t)$$

$$\begin{aligned} P^c_{\gamma\beta}(\mathbf{r}_1, t) &= \frac{1}{2} \sum_{i,j=1}^{s} m_j \mu_{ij} \left(1 + \alpha_{ij}\right) \sigma^d_{ij} \int d\mathbf{v}_1 \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}} \cdot \mathbf{g}_{12})^2 \\ &\quad \times \widehat{\sigma}_\beta \widehat{\sigma}_\gamma \int_0^1 dx\, f_{ij}(\mathbf{r}_1 - x\boldsymbol{\sigma}_{ij}, \mathbf{v}_1, \mathbf{r}_1 + (1-x)\boldsymbol{\sigma}_{ij}, \mathbf{v}_2; t). \end{aligned}$$

Heat flux $\mathbf{q}\left(\mathbf{r}_1,t\right)=\mathbf{q}^k\left(\mathbf{r}_1,t\right)+\mathbf{q}^c\left(\mathbf{r}_1,t\right)$

$$\mathbf{q}^k\left(\mathbf{r}_1,t\right)=\sum_{i=1}^s\int d\mathbf{v}_1\frac{1}{2}m_iV_1^2\mathbf{V}_1f_i(\mathbf{r}_1,\mathbf{v}_1;t)$$

$$\begin{aligned}\mathbf{q}^c\left(\mathbf{r}_1,t\right) &= \sum_{i,j=1}^s\frac{1}{8}\left(1+\alpha_{ij}\right)m_j\mu_{ij}\sigma_{ij}^d\int d\mathbf{v}_1\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}\,\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})\\ &\times(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})^2\left[\left(1-\alpha_{ij}\right)\left(\mu_{ji}-\mu_{ij}\right)(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})+4\widehat{\boldsymbol{\sigma}}\cdot\mathbf{G}_{ij}\right)\\ &\times\widehat{\boldsymbol{\sigma}}\int_0^1 dx\,f_{ij}(\mathbf{r}_1-x\boldsymbol{\sigma}_{ij},\mathbf{v}_1,\mathbf{r}_1+(1-x)\,\boldsymbol{\sigma}_{ij},\mathbf{v}_2;t),\end{aligned}$$

$\mathbf{G}_{ij}=\mu_{ij}\mathbf{V}_1+\mu_{ji}\mathbf{V}_2$ is the center-of-mass velocity

Cooling rate

$$\zeta = \frac{1}{2dnT}\sum_{i,j=1}^{s}\left(1-\alpha_{ij}^{2}\right)m_i\mu_{ji}\sigma_{ij}^{d-1}\int d\mathbf{v}_1\int d\mathbf{v}_2\int d\widehat{\boldsymbol{\sigma}}$$
$$\times\Theta(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})(\widehat{\boldsymbol{\sigma}}\cdot\mathbf{g}_{12})^{3}f_{ij}(\mathbf{r}_1,\mathbf{v}_1,\mathbf{r}_1+\boldsymbol{\sigma}_{ij},\mathbf{v}_2;t)$$

Balance equations become a closed set of hydrodynamic equations for (n_i,**U**,T) once the *fluxes* and the *cooling rate* are expressed as ***functionals*** of (n_i,**U**,T) ("constitutive relations")

CHAPMAN-ENSKOG NORMAL SOLUTION

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

$$\boxed{f_i(\mathbf{r},\mathbf{v};t) = f_i(\mathbf{v}|\{n_i(\mathbf{r},t)\},\mathbf{U}(\mathbf{r},t),T(\mathbf{r},t)\})}$$

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

$$f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \cdots$$

Some *controversy* about the possibility of going from kinetic theory to hydrodynamics by using the Chapman-Enskog 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** (ζ^{-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

HOMOGENEOUS COOLING STATE
(zeroth-order approximation)

Spatially *homogeneous* isotropic states

$$\partial_t f_i(v,t) = \sum_j J_{ij}[v|f_i(t), f_j(t)]$$

Partial temperatures $\longrightarrow$ $n_i T_i = \frac{m_i}{d}\int d\mathbf{v}\; v^2 f_i(\mathbf{v})$

Granular temperature $\longrightarrow$ $T = \sum_i x_i T_i, \quad x_i = n_i/n$

Cooling rates for T_i $\longrightarrow$ $\zeta_i = -\partial_t \ln T_i, \quad \zeta = T^{-1}\sum_i x_i T_i \zeta_i$

Assumption

Hydrodynamic or ***normal*** state: all the *time* dependence of vdf occurs only through the temperature T(t)

$$f_i(v,t) = n_i v_0^{-d}(t)\Phi_i(c), \qquad c \equiv \frac{v}{v_0(t)}$$

$$v_0(t)^2 \propto T(t)$$

Consequence: ***temperature ratios*** must be ***constant*** (independent of time)

Binary mixture: $\gamma = T_1/T_2$

HCS condition: $\partial_t \ln \gamma = \zeta_2 - \zeta_1 \longrightarrow \zeta_1 = \zeta_2$

Elastic collisions: $\zeta_1 = \zeta_2 = 0, \quad T_1 = T_2 = T$

$\downarrow$

Equipartition theorem for classical statistical mechanics

What happens if the collisions are **inelastic** ? $\boxed{\gamma \neq 1}$

VG&J. W. Dufty PRE **60,** 5706 (1999)

Time evolution of temperature ratio γ. Comparison with Monte Carlo simulations

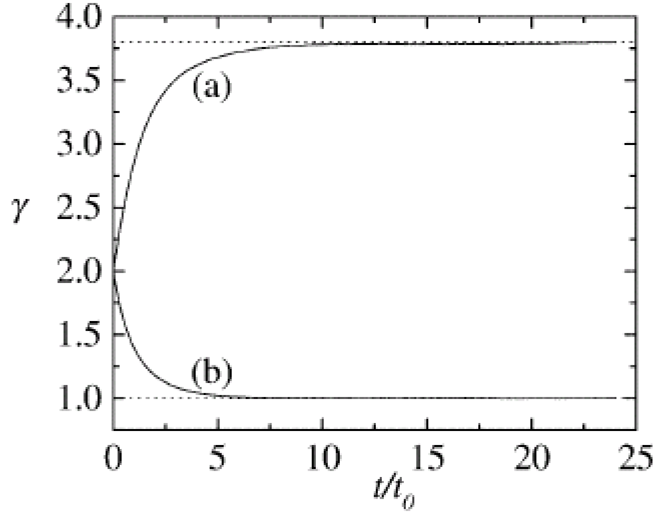


Fig. 1. Time evolution of $\gamma(t) = T_1(t)/T_2(t)$ for $n^* = 0$, $\delta = 2$, $w = 1$, $\mu = 10$, and $\alpha = 0.5$ (a) and $\alpha = 1$ (b). The dotted lines refer to the theoretical predictions. Time is measured in units of $t_0 \equiv \lambda_{11}/v_{01}(0)$

Montanero&VG, Granular Matter **4**, 17 (2002)

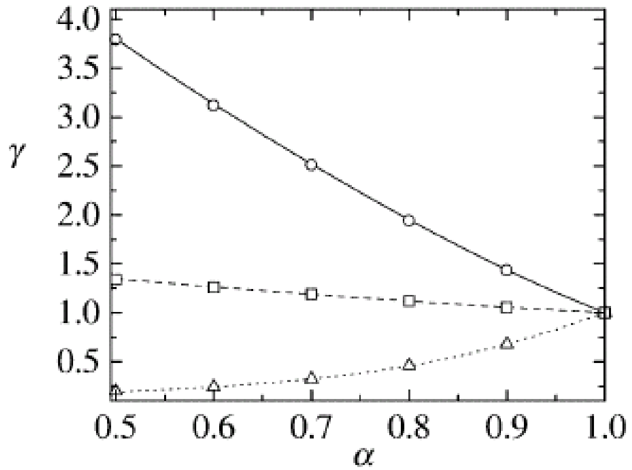


Fig. 4. Plot of the temperature ratio γ versus the restitution coefficient α for $n^* = 0$, $\delta = 2$, $w = 1$ and three different values of the mass ratio: $\mu = 1/10$ (dotted line and triangles), $\mu = 2$ (dashed line and squares) and $\mu = 10$ (solid line and circles). The lines are the theoretical predictions and the symbols correspond to the simulation results

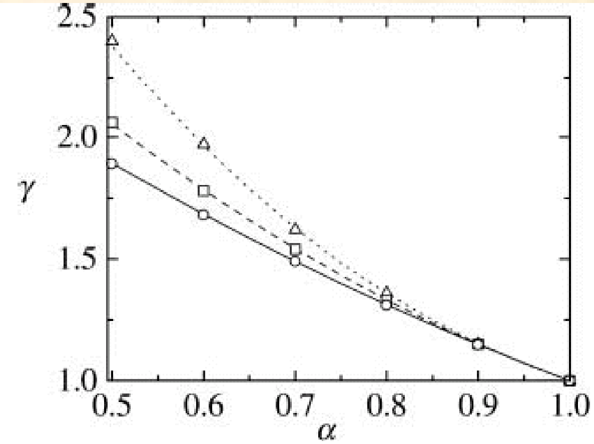


Fig. 5. Plot of the temperature ratio versus the restitution coefficient α for $n^* = 0$, $w = 1$, $\mu = 4$ and three different values of the concentration ratio: $\delta = 1/4$ (dotted line and triangles), $\delta = 1$ (dashed line and squares) and $\delta = 4$ (solid line and circles). The lines are the theoretical predictions and the symbols correspond to the simulation results

Comparison with *molecular dynamics* (MD) simulations

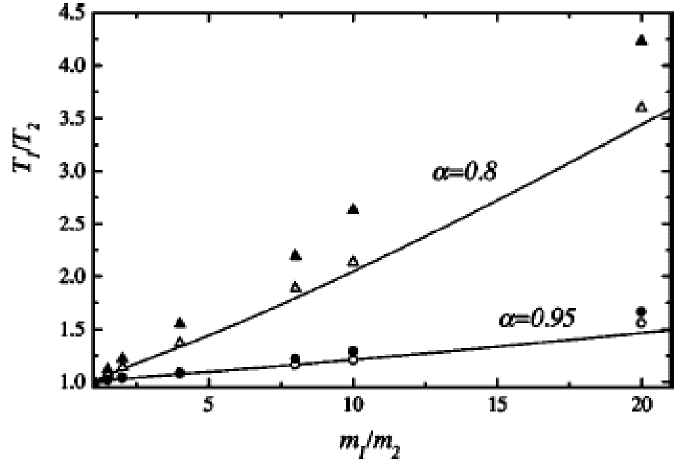


FIG. 2. Plot of the temperature ratio T_1/T_2 as a function of the mass ratio m_1/m_2 for $\sigma_1/\sigma_2=\phi_1/\phi_2=1$, and two different values of α: $\alpha=0.95$ (solid line and circles) and $\alpha=0.8$ (solid line and triangles). The lines are the Enskog predictions and the symbols refer to the MD simulation results. The open (solid) symbols correspond to $\phi=0.1$ ($\phi=0.2$).

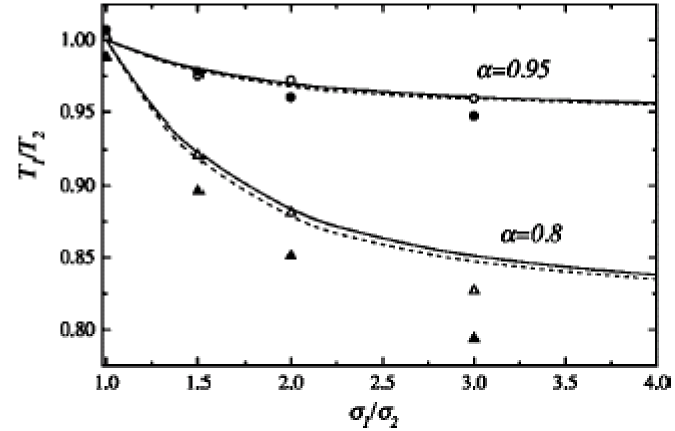


FIG. 3. Plot of the temperature ratio T_1/T_2 as a function of the size ratio σ_1/σ_2 for $m_1/m_2=\phi_1/\phi_2=1$, and two different values of α: $\alpha=0.95$ (lines and circles) and $\alpha=0.8$ (lines and triangles). The lines are the Enskog predictions and the symbols refer to the MD simulation results. The solid (dashed) lines correspond to $\phi=0.1$ ($\phi=0.2$), while the open (solid) symbols correspond to $\phi=0.1$ ($\phi=0.2$).

Dahl, Hrenya,VG& Dufty, PRE **66**, 041301 (2002)

Breakdown of energy equipartition

Computer simulation studies: Barrat&Trizac GM **4**, 57 (2002); Krouskop&Talbot, PRE **68**, 021304 (2003); Wang *et al*. PRE **68**, 031301 (2003); Brey et al. PRE **73**, 031301 (2006); Schroter *et al*. PRE **74**, 011307 (2006);…….

Real experiments: Wildman&Parker, PRL **88**, 064301 (2002); Feitosa&Menon, PRL **88**, 198301 (2002).

All these results ***confirm*** this new feature in granular mixtures !!

NAVIER-STOKES HYDRODYNAMIC EQUATIONS

Previous studies: Jenkins et al. JAM 1987; PF 1989; Zamankhan, PRE 1995;
Arnarson et al. PF 1998; PF 1999; PF 2004;
Serero et al. JFM 2006

Limited to the quasielastic limit. They are based on the energy equipartition assumption

Our **motivation**: Determination of the transport coefficients by using a kinetic theory which takes into account the effect of temperature differences on them. **NO limitation** to the degree of dissipation

The distribution functions are given by

$$
\begin{aligned}
f_i^{(1)}(\mathbf{V}) \;=\;& \mathcal{A}_i(\mathbf{V})\cdot\nabla\ln T+\sum_{j=1}^{s}\mathcal{B}_i^j(\mathbf{V})\cdot\nabla\ln n_j \\
&+\mathcal{C}_{i,\gamma\eta}(\mathbf{V})\frac{1}{2}\left(\partial_\gamma U_\eta+\partial_\eta U_\gamma-\frac{2}{d}\delta_{\gamma\eta}\nabla\cdot\mathbf{U}\right) \\
&+\mathcal{D}_i(\mathbf{V})\nabla\cdot\mathbf{U}
\end{aligned}
$$

After some efforts….

$$\left(\left(\mathcal{L}-\frac{1}{2}\zeta^{(0)}\right)\boldsymbol{\mathcal{A}}\right)_i=\mathbf{A}_i$$

$$\left(\mathcal{L}\boldsymbol{\mathcal{B}}^j\right)_i-n_j\frac{\partial\zeta^{(0)}}{\partial n_j}\boldsymbol{\mathcal{A}}_i=\mathbf{B}_i^j$$

$$\left(\left(\mathcal{L}+\frac{1}{2}\zeta^{(0)}\right)\mathcal{C}_{\gamma\eta}\right)_i=C_{i,\gamma\eta}$$

$$\left(\left(\mathcal{L}+\frac{1}{2}\zeta^{(0)}\right)\mathcal{D}\right)_i=D_i$$

$$(\mathcal{L}X)_i=-\sum_{j=1}^{N}\left(J_{\mathrm{E},ij}^{(0)}[X_i,f_j^{(0)}]+J_{\mathrm{E},ij}^{(0)}[f_i^{(0)},X_j]\right)$$

Inhomogeneous terms are defined in terms of $f_i^{(0)}$

CONSTITUTIVE EQUATIONS

A. Cooling rate

$$\zeta \to \zeta^{(0)} + \zeta_U \nabla \cdot \mathbf{U}$$

$$\zeta^{(0)} = \frac{B_3}{2dnT} \sum_{i,j=1}^{s} \left(1-\alpha_{ij}^2\right) \frac{m_i m_j}{m_i+m_j} \chi_{ij} \sigma_{ij}^{d-1} \int d\mathbf{v}_1 \int d\mathbf{v}_2 f_i^{(0)}(V_1) f_j^{(0)}(V_2)\, g_{12}^3$$

$$\begin{aligned} \zeta_U &= -\frac{d+2}{dnT} B_4 \sum_{i,j=1}^{s} \left(1-\alpha_{ij}^2\right) \mu_{ji} \chi_{ij} \sigma_{ij}^{d} n_i n_j T_i \\ &\quad + \frac{B_3}{dnT} \sum_{i,j=1}^{s} \left(1-\alpha_{ij}^2\right) \frac{m_i m_j}{m_i+m_j} \chi_{ij} \sigma_{ij}^{d-1} \int d\mathbf{v}_1 \int d\mathbf{v}_2\, g_{12}^3 f_i^{(0)}(\mathbf{V}_1) \mathcal{D}_j(\mathbf{V}_2) \end{aligned}$$

B. Mass fluxes

$$\mathbf{j}_i = -\sum_{j=1}^{s} m_i m_j \frac{n_j}{\rho} D_{ij} \nabla \ln n_j - \rho D_i^T \nabla \ln T$$

Transport coefficients :

$$\boxed{\begin{aligned} D_i^T &= -\frac{m_i}{\rho d}\int d\mathbf{v}\mathbf{V}\cdot\mathcal{A}_i(\mathbf{V}) \\ D_{ij} &= -\frac{\rho}{m_j n_j d}\int d\mathbf{v}\mathbf{V}\cdot\mathcal{B}_i^j(\mathbf{V}) \end{aligned}}$$

B. Pressure tensor

$$P_{\gamma\beta} = p\delta_{\gamma\beta} - \eta\left(\nabla_\gamma U_\beta + \nabla_\beta U_\gamma - \frac{2}{d}\nabla\cdot\mathbf{U}\right) - \kappa\nabla\cdot\mathbf{U}$$

Equation of state

$$\boxed{p = nT + B_2\sum_{i,j=1}^{s}\mu_{ji}\left(1+\alpha_{ij}\right)\sigma_{ij}^{d}\chi_{ij}n_i n_j T_i}$$

Shear viscosity

$$\eta = \eta^k + \eta^c$$

$$\eta^k = \sum_{i=1}^{s}\eta_i^k = -\frac{1}{(d+2)(d-1)}\sum_{i=1}^{s}\int d\mathbf{v}\, m_i V_\lambda V_\gamma \mathcal{C}_{i,\lambda\gamma}(\mathbf{V})$$

$$\eta^c = \frac{2B_2}{(d+2)}\sum_{i,j=1}^{s}\mu_{ij}\left(1+\alpha_{ij}\right)\chi_{ij}n_i\sigma_{ij}^{d}\eta_j^k + \frac{d}{d+2}\kappa^c$$

Bulk viscosity

$$\kappa = \kappa^k + \kappa^c \qquad \boxed{\kappa^k = 0}$$

$$\boxed{\begin{aligned}\kappa^c &= \frac{B_3\,(d+1)}{2d^2}\sum_{i,j=1}^{s} m_j\mu_{ij}\left(1+\alpha_{ij}\right)\chi_{ij}\sigma_{ij}^{d+1} \\ &\quad\times\int d\mathbf{v}_1\int d\mathbf{v}_2 f_i^{(0)}(\mathbf{V}_1)f_j^{(0)}(\mathbf{V}_2)g_{12}\end{aligned}}$$

$$B_k = \pi^{(d-1)/2}\frac{\Gamma\left(\frac{d+1}{2}\right)}{\Gamma\left(\frac{k+d}{2}\right)}, \qquad k \geq 0$$

C. Energy flux

$$\mathbf{q} = -\lambda \nabla T - T^2 \sum_{i,j=1}^{s} D_{q,ij} \nabla \ln n_j$$

Transport coefficients $\lambda = \lambda^k + \lambda^c$

$$\boxed{\lambda^k = \sum_{i=1}^{s} \lambda_i^k = -\frac{1}{dT} \sum_{i=1}^{s} \int d\mathbf{v} \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{A}_i(\mathbf{V})}$$

$$\boxed{D_{q,ij}^k = -\frac{1}{dT^2} \int d\mathbf{v} \frac{1}{2} m_i V^2 \mathbf{V} \cdot \mathcal{B}_i^j(\mathbf{V})}$$

$$\lambda^c = \sum_{i,j=1}^{s} \frac{1}{8}\left(1+\alpha_{ij}\right) m_j \mu_{ij} \sigma_{ij}^d \chi_{ij} \left\{ 2B_4 \left(1-\alpha_{ij}\right)\left(\mu_{ij}-\mu_{ji}\right) n_i \left[\frac{2}{m_j}\lambda_j^k + (d+2)\frac{T_i}{m_i m_j T}\rho D_j^T\right] + \frac{8B_2}{2+d} n_i \left[\frac{2\mu_{ij}}{m_j}\lambda_j^k - (d+2)\frac{T_i}{m_i m_j T}\left(2\mu_{ij}-\mu_{ji}\right)\rho D_j^T\right] - T^{-1} C_{ij}^T \right\}$$

$$D_{q,ij}^c = \sum_{p=1}^{s} \frac{1}{8}\left(1+\alpha_{ip}\right) m_p \mu_{ip} \sigma_{ip}^d \chi_{ip} \left\{ 2B_4 \left(1-\alpha_{ip}\right)\left(\mu_{ip}-\mu_{pi}\right) \times n_i \left[\frac{2}{m_p} D_{q,pj}^k + (d+2)\frac{T_i}{T^2}\frac{m_j n_j}{\rho m_i} D_{pj}\right] + \frac{8B_2}{d+2} n_i \left[\frac{2\mu_{pi}}{m_p} D_{q,pj}^k - (d+2)\left(2\mu_{ip}-\mu_{pi}\right)\frac{T_i}{T^2}\frac{n_j m_j}{m_i \rho} D_{pj}\right] - T^{-2} C_{ipj}^T \right\}$$

Some *limiting* cases

✓ Mechanically equivalent particles [Garzó&Dufty PRE **59**, 5895 (1999)+Lutsko, PRE **72** 021306 (2005)]

✓ Binary mixtures at low-density [Garzó&Dufty, PF **14**, 1476 (2002)+Garzó&Montanero, JSP **129**, 27(2007)]

✓ Elastic hard spheres [López de Haro, Cohen&Kincaid, JCP **78**, 2746 (1983)]

Self-consistency of our results

Constitutive equations (binary mixture)

$$\mathbf{j}_1 = -\frac{m_1^2 n}{\rho} D_{11} \nabla \ln n_1 - \frac{m_1 m_2 n_2}{\rho} D_{12} \nabla \ln n_2 - \rho D_T \nabla \ln T$$

$$P_{\gamma\beta} = p\delta_{\gamma\beta} - \eta \left(\nabla_\gamma U_\beta + \nabla_\beta U_\gamma - \frac{2}{d} \nabla \cdot \mathbf{U} \right) - \kappa \nabla \cdot \mathbf{U}$$

$$\mathbf{q} = -T^2 D_{q,1} \nabla \ln n_1 - T^2 D_{q,2} \nabla \ln n_2 - \lambda \nabla T$$

Eight transport coefficients: $\left\{ D_{11}, D_{12}, D_T, \eta, \kappa, D_{q,1}, D_{q,2}, \lambda \right\}$

Parameter space: $\{ m_1/m_2, \sigma_1/\sigma_2, x_1, \phi, \alpha_{11}, \alpha_{22}, \alpha_{12} \}$

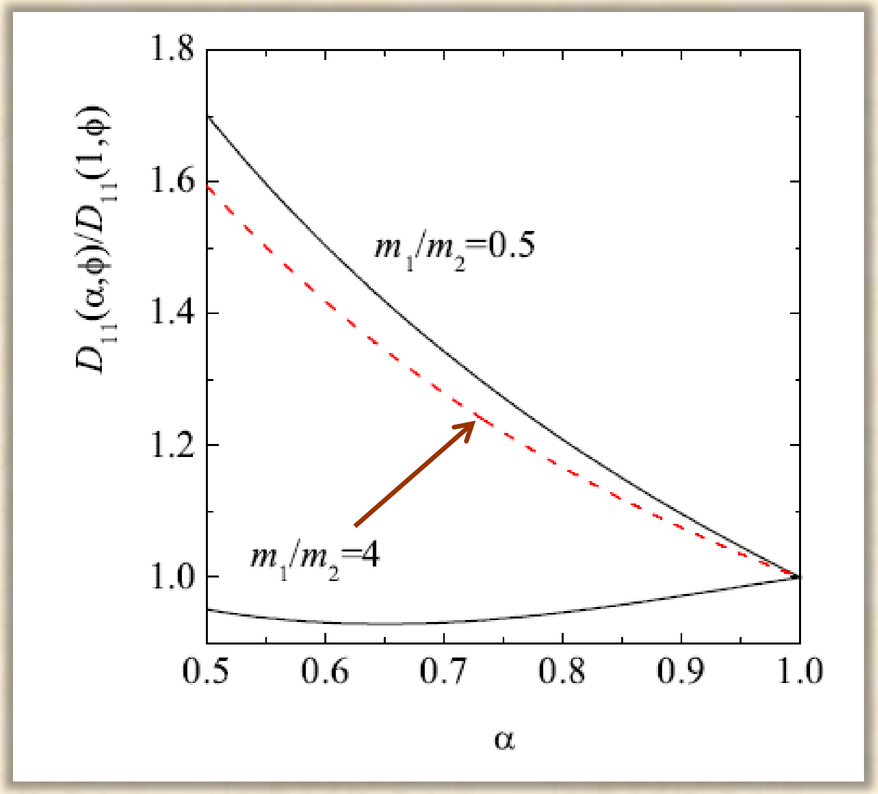
Transport coefficients given in terms of solutions of coupled linear integral equations. Complex mathematical problem

Sonine polynomial approximation. Only leading terms are usually considered

To test the accuracy of the Sonine solution: comparison with numerical solutions of the RET (DSMC)

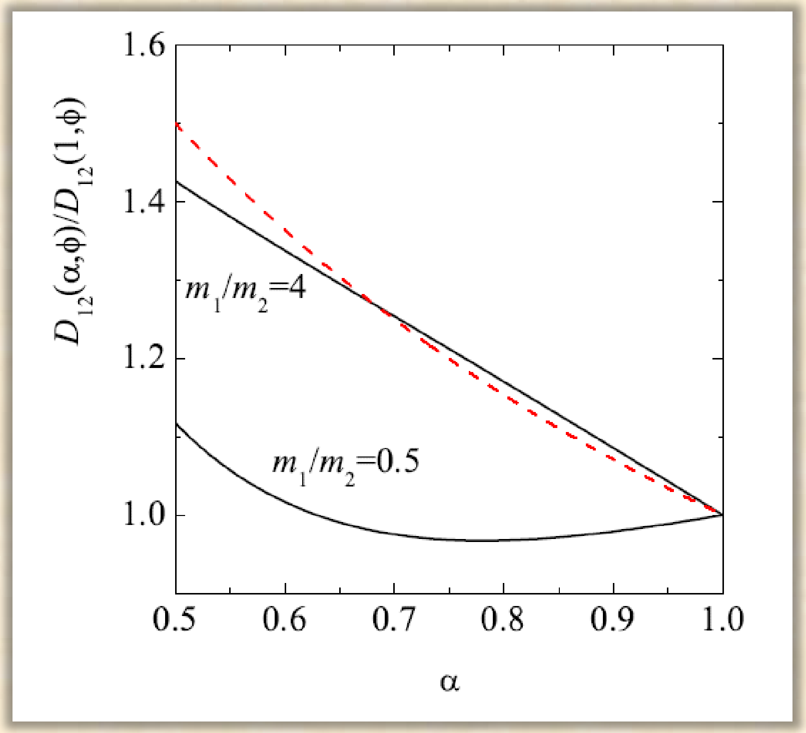
VG, J. Dufty, C. Hrenya, PRE **76**, 031303 (2007); 031304 **76**(2007);
J.A. Murray, VG, C. Hrenya, Powder Tech. **220**, 24 (2012)

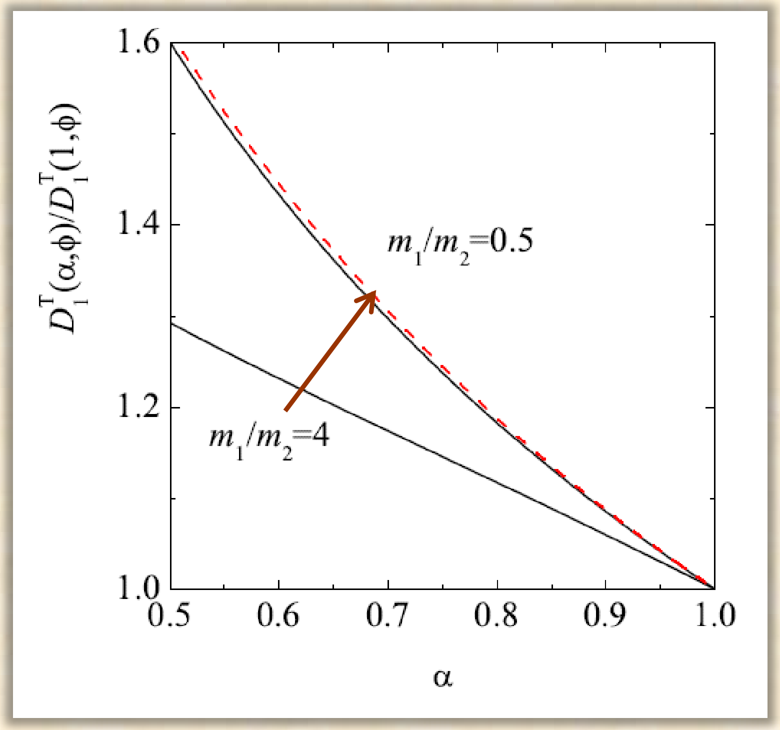
Influence of energy equipartition on transport

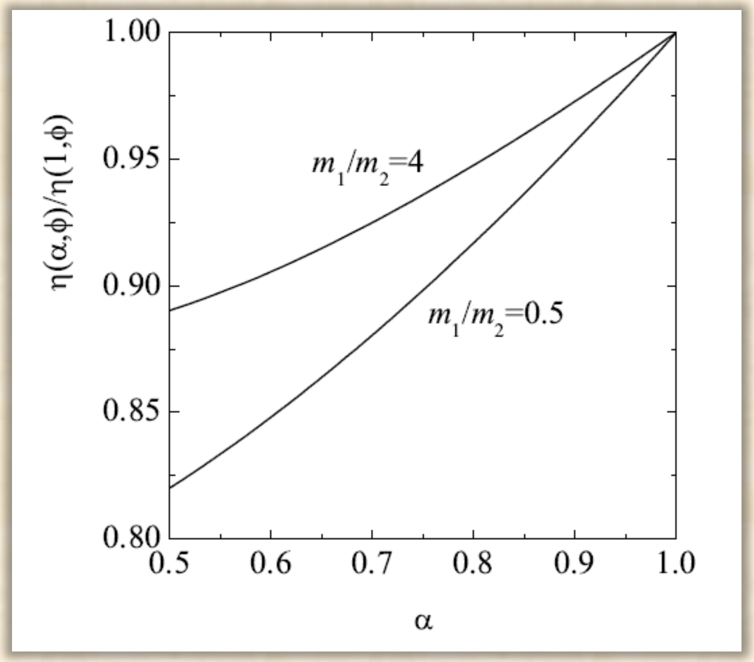


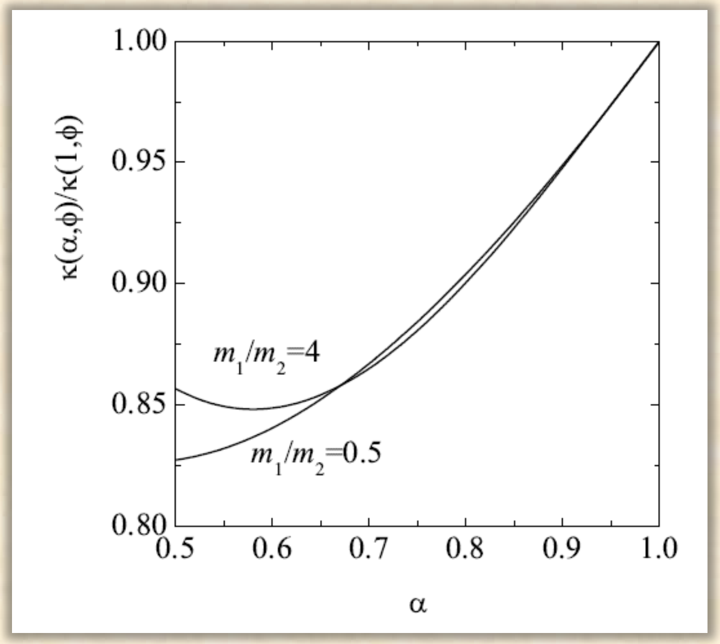
Energy equipartition assumed (dashed line)

$$x_1 = \frac{1}{2}, \sigma_1 = \sigma_2, \phi = 0.2$$


1.6
1.4
1.2
1.0
0.5
0.6
0.7
0.8
0.9
1.0
α
$D_{12}(\alpha,\phi)/D_{12}(1,\phi)$
m_1/m_2=4
m_1/m_2=0.5


1.6
1.4
1.2
1.0
0.5
0.6
0.7
0.8
0.9
1.0
α
$D_1^T(\alpha,\phi)/D_1^T(1,\phi)$
m_1/m_2=0.5
m_1/m_2=4

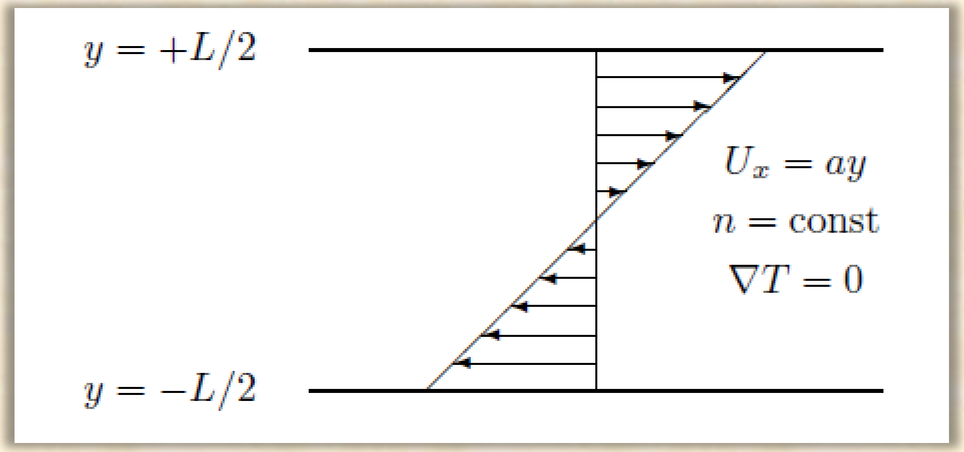

1.00
0.95
0.90
0.85
0.80
0.5
0.6
0.7
0.8
0.9
1.0
η(α,ϕ)/η(1,ϕ)
α
m1/m2=4
m1/m2=0.5


1.00
0.95
0.90
0.85
0.80
0.5
0.6
0.7
0.8
0.9
1.0
κ(α,ϕ)/κ(1,ϕ)
α
m1/m2=4
m1/m2=0.5

Shear viscosity coefficient of a **heated** binary mixture

From a computational point of view, it is difficult to measure this coefficient. **Strategy**: (Driven) simple shear flow

$$n_i=\text{const.},\ \nabla T=0,\ U_{i,x}=ay$$



Ordinary fluid (elastic collisions): T(t) increases with time due to *viscous heating*.

$$\frac{\partial T}{\partial t} = -\frac{2}{dn} P_{xy} a > 0$$

Average collision frequency $\nu(t) \propto T(t)^{1/2}$ (hard spheres). Thus, $a^* = a/\nu(t) \to 0$ and so, one can *measure* the N-S shear viscosity in the long time limit [Naitoh&Ono, JCP (1979); Montanero&Santos PRE (1996)]

$$\boxed{\frac{\nu}{nT}\eta = -\lim_{t\to\infty} \frac{P_{xy}^*}{a^*}, \qquad P_{xy}^* = P_{xy}/nT}$$

Granular fluid (inelastic collisions): Energy sink in the temperature balance equation

$$\boxed{\partial_t T = -\frac{2}{dn} a P_{xy} + (-\zeta T)}$$

Is it possible to ***frustrate*** the cooling effects so that the viscous heating is still able to heat the system as in the elastic case? One can identify the (heated) shear viscosity when $a^* \to 0$

Granular fluid is excited by an external energy source that exactly compensates for the collisional cooling (Gaussian thermostat)

$$\mathbf{F}_i^{\text{exc}}(\mathbf{V}) = \frac{1}{2} m_i \zeta \mathbf{V}$$

Kinetic theory: First Sonine approximation to get η of a heated granular binary mixture:

$$\mathcal{C}_{i,\gamma\beta}(\mathbf{V}) \to -f_{i,M}(\mathbf{V}) \frac{\eta_i^k}{n_i T_i^2} m_i \left(V_\gamma V_\beta - \frac{1}{d} V^2 \delta_{\gamma\beta} \right)$$

The expression of η slightly differs from the one obtained in the free cooling case

Shear viscosity coefficient of a (heated) granular fluid

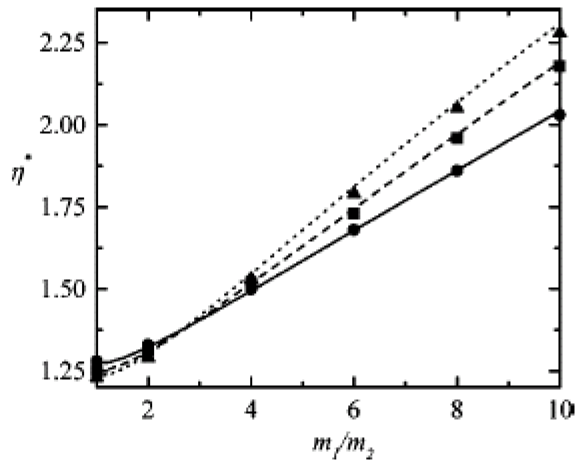


FIG. 6. Plot of the reduced shear viscosity η^* as a function of the mass ratio m_1/m_2, for $\phi=0.2$, $\sigma_1/\sigma_2=1$, $x_1=1/2$ and three different values of the restitution coefficient α: $\alpha=0.9$ (solid line and circles), $\alpha=0.8$ (dashed line and squares), and $\alpha=0.7$ (dotted line and triangles). The lines are the theoretical predictions and the symbols refer to the results obtained from Monte Carlo simulations.

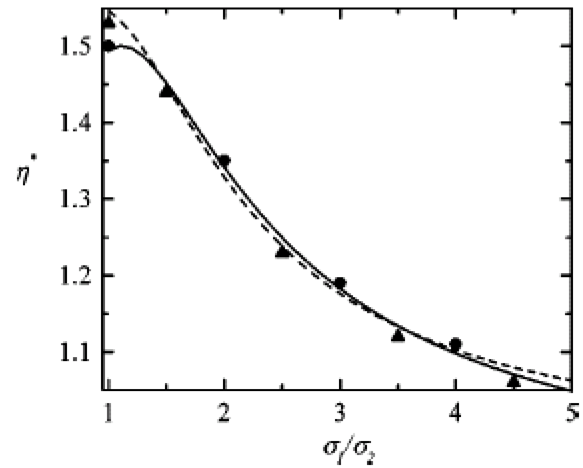


FIG. 7. Plot of the reduced shear viscosity η^* as a function of the size ratio σ_1/σ_2 for $\phi=0.2$, $m_1/m_2=4$, $x_1=1/2$ and two different values of the restitution coefficient α: $\alpha=0.9$ (solid line and circles) and $\alpha=0.7$ (dashed line and triangles). The lines are the theoretical predictions and the symbols refer to the results obtained from Monte Carlo simulations.

VG&J.M. Montanero, PRE **68,** 041302 (2003)

Tracer diffusion coefficient: Diffusion of impurities in granular gas under HCS

When the excess gas is in HCS, the diffusion equation is

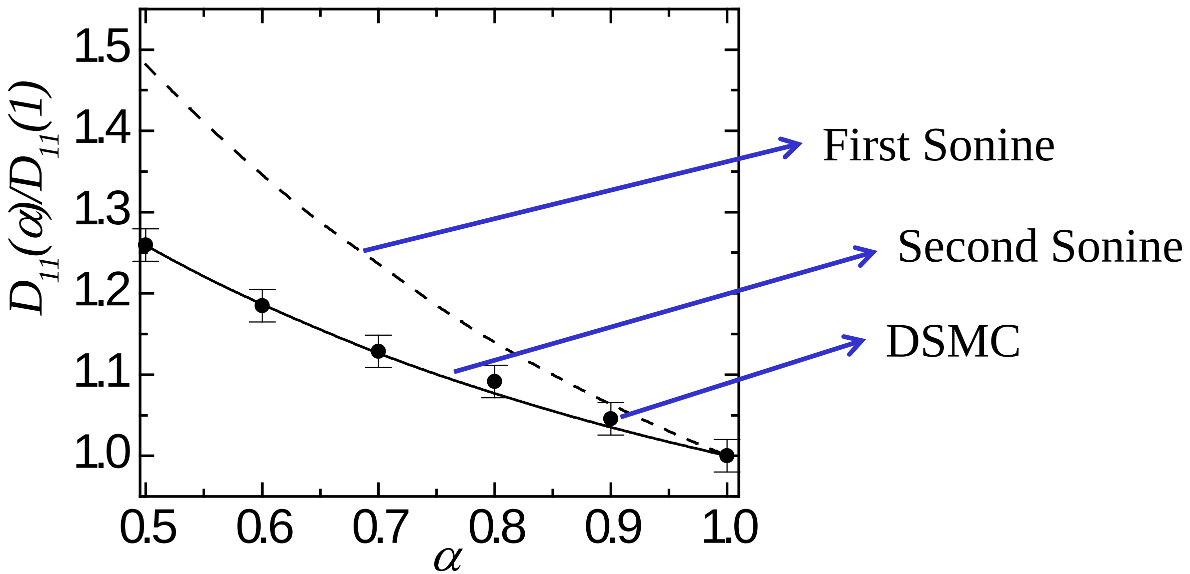
$$\boxed{\partial_t x_1(\mathbf{r},t) = D_{11}(t)\nabla^2 x_1, \qquad D_{11}(t) \propto \sqrt{T(t)}}$$

Mean square position of impurity after a time interval t

$$\boxed{\frac{\partial}{\partial t}\langle|\mathbf{r}(t)-\mathbf{r}(0)|^2\rangle = \frac{2dD_{11}(t)}{n_2}}$$

Einstein form is used to measure D_{11} in DSMC simulations [Brey *et al.* PF **12**, 876 (2000)]

First two Sonine approximations are considered !!



$$m_1/m_2 = 1/4; \sigma_1/\sigma_2 = 1/2; \phi = 0.2$$

$$\alpha_{22} = \alpha_{12} \equiv \alpha, x_1 \to 0$$

VG&Montanero, PRE **68**, 021301 (2004)

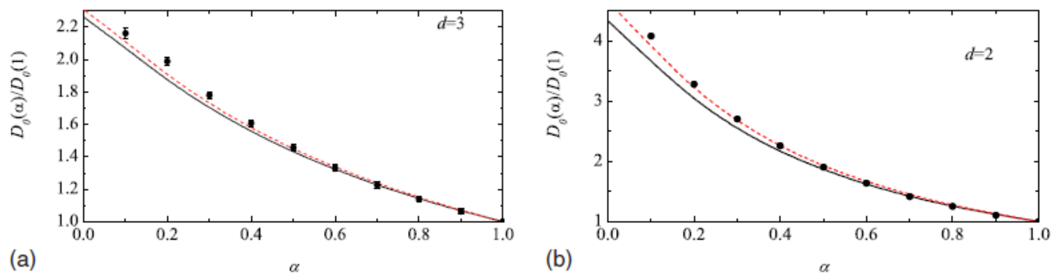


FIG. 6. (Color online) Reduced kinetic diffusion coefficient $D_0(\alpha)/D_0(1)$ as a function of the (common) coefficient of restitution $\alpha=\alpha_0$ for $m_0/m=2$, $\sigma_0/\sigma=2$, and $\phi=0.2$. The left panel is for hard spheres ($d=3$) while the right panel is for hard disks ($d=2$). The solid lines correspond to the second Sonine approximation and the dashed lines refer to the first Sonine approximation. The symbols are the results obtained from Monte Carlo simulations. Here, $D_0(1)$ is the elastic value of the thermal diffusion coefficient consistently obtained in each approximation.

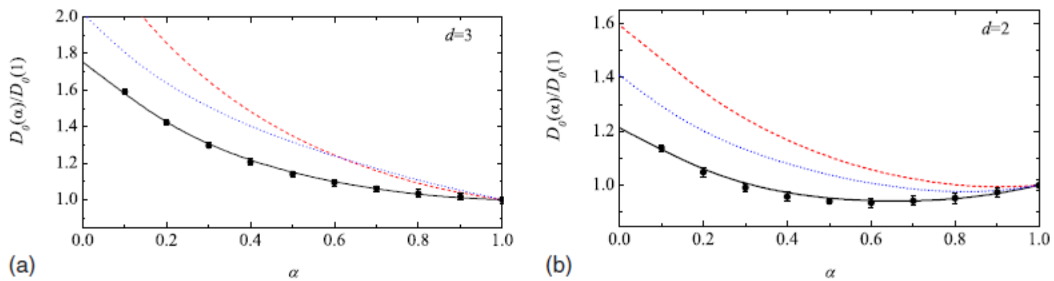


FIG. 5. (Color online) Reduced kinetic diffusion coefficient $D_0(\alpha)/D_0(1)$ as a function of the (common) coefficient of restitution $\alpha=\alpha_0$ for $m_0/m=1/5$, $\sigma_0/\sigma=1/2$, and $\phi=0.2$. The left panel is for hard spheres ($d=3$) while the right panel is for hard disks ($d=2$). The solid lines correspond to the second Sonine approximation, the dashed lines refer to the first Sonine approximation, and the dotted lines are the modified Sonine approximation. The symbols are the results obtained from Monte Carlo simulations. Here, $D_0(1)$ is the elastic value of the thermal diffusion coefficient consistently obtained in each approximation.

VG&F.Vega Reyes, PRE **79**, 041303 (2009); JFM **623**, 387 (2009)

INSTABILITIES IN FREELY COOLING *DENSE* GRANULAR BINARY MIXTURES

In contrast to ordinary fluids, *instabilities* (such as dynamic particle clusters) occur in freely cooling (HCS) granular gases. Pionnering work of Goldhirsch&Zanetti (PRL **70**, 1619 (1993)); McNamara (PF A **5**, 3056 (1993))

(Peter Mitrano, CU)

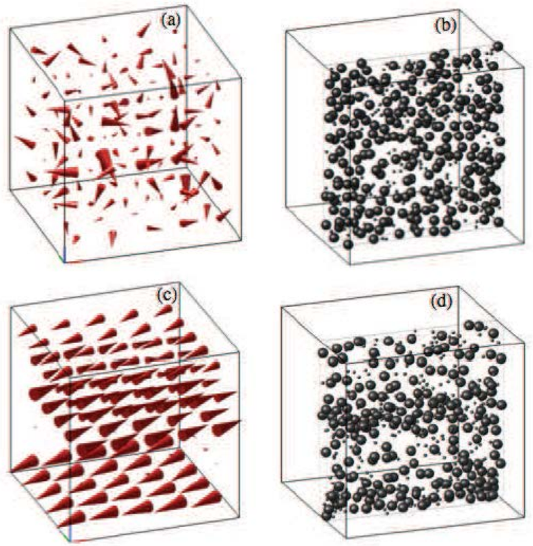


Fig. 6.11 Visualizations from an MD simulation of an equimolar mixture ($x_1 = 0.5$) with $m_1/m_2 = 2$, $\sigma_1/\sigma_2 = 3$, $\phi = 0.2$, and $\alpha = 0.7$ of (a) stable, coarse-grained velocity field at five collisions per particle (or "cpp"), (b) stable particle positions at five cpp, (c) unstable, coarse-grained velocity field at 400 cpp, and (d) cluster systems at 400 cpp. Figure reproduced with permission from the American Physical Society.

General trends: (i) instabilities are more likely in larger domains; and (ii) velocity vortices manifest more readily than particle clusters

This is also a very good problem to assess Navier-Stokes hydrodynamics derived from Kinetic Theory

For given values of the mechanical parameters of the system, there exists a **critical** system lenght demarcates (stable) homogeneous flow from one with *velocity-vortex* instabilities or one exhibiting the *clustering* instability

LINEAR STABILITY ANALYSIS

HCS is *unstable* with respect to long enough wavelength perturbations.
Stability analysis of the nonlinear hydrodynamic equations with respect to HCS for small initial excitations

HCS solution

$$\nabla x_{1H} = \nabla n_H = \nabla T_H = 0, \mathbf{U}_H = \mathbf{0},$$

$$\partial_t \ln T_H = -\zeta_{0H}$$

This basic solution is unstable to linear perturbations

We linearize the Navier-Stokes equations
with respect to the HCS solution. Deviations of the hydrodynamic
fields from their values in HCS are *small*

$$\boxed{\begin{gathered} x_1(\mathbf{r},t) = x_{1H} + \delta x_1(\mathbf{r},t), n(\mathbf{r},t) = n_H + \delta n(\mathbf{r},t), \\ \mathbf{U}(\mathbf{r},t) = \delta\mathbf{U}(\mathbf{r},t), T(\mathbf{r},t) = T_H + \delta T(\mathbf{r},t) \end{gathered}}$$

Equation for the velocity field :

$$\boxed{\rho_H \partial_t \delta\mathbf{U} + \nabla_\ell p_H = \eta_H \nabla^2 \delta\mathbf{U} + \left(\frac{d-2}{d}\eta_H - \frac{2}{d}\kappa_H\right) \nabla(\nabla \cdot \delta\mathbf{U})}$$

Linearization about HCS yields a set of partial differential eqs. with coefficients that are independent of space **BUT** depend on time. Time dependence can be eliminated by

$$\tau = \int_0^t dt' \nu_H(t'), \ell = \frac{\nu_H(t)}{v_H(t)} \mathbf{r}$$

$$\nu_H \propto n_H \sigma_{12}^{d-1} v_H, v_H = \sqrt{2T_H/(m_1 + m_2)}$$

Set of coupled linear differential equations with *constant* coefficients

Set of Fourier transformed dimensionless variables:

$$\rho_{1,\mathbf{k}}(\tau) = \frac{\delta x_{1\mathbf{k}}(\tau)}{x_{1H}}, \qquad \rho_{\mathbf{k}}(\tau) = \frac{\delta n_{\mathbf{k}}(\tau)}{n_H}$$

$$\mathbf{w}_{\mathbf{k}}(\tau) = \frac{\delta \mathbf{U}_{\mathbf{k}}(\tau)}{v_H(\tau)}, \qquad \theta_{\mathbf{k}}(\tau) = \frac{\delta T_{\mathbf{k}}(\tau)}{T_H(\tau)}$$

$$\delta y_{\mathbf{k}\beta}(\tau) = \int d\boldsymbol{\ell} e^{-i\mathbf{k}\cdot\boldsymbol{\ell}} \delta y_\beta(\boldsymbol{\ell}, \tau)$$

$$\delta y_{\mathbf{k}\beta} \equiv \left\{ \rho_{1,\mathbf{k}}, \rho_{\mathbf{k}}, \mathbf{w}_{\mathbf{k}}, \theta_{\mathbf{k}} \right\}$$

Transversal component of the velocity field is *decoupled* from the other modes. This identifies “d-1” shear (transversal) modes

$$\left(\frac{\partial}{\partial\tau} - \zeta_{0H}^* + \frac{1}{2}\eta_H^* k^2\right)\mathbf{w}_{\mathbf{k}\perp} = 0$$

$$\mathbf{w}_{\mathbf{k}\perp}(\tau) = \mathbf{w}_{\mathbf{k}\perp}(0)e^{s_\perp\tau},\ s_\perp(k) = \zeta_{0H}^* - \frac{1}{2}\eta_H^* k^2$$

There exists a critical wave number:

$$k_\perp^c = \sqrt{\frac{2\zeta_{0H}^*}{\eta_H^*}}$$

$k < k_\perp^c$ $\longrightarrow$ Shear modes grow exponentially!!

The remaining 4 longitudinal modes are *coupled* and are the eigenvalues of a 4X4 matrix

There exists two critical wave numbers:

$$\boxed{k_\perp^c = \sqrt{\frac{2\zeta_{0H}^*}{\eta_H^*}}, \qquad k_\parallel^c}$$

Solution of a quartic equation

For wave numbers smaller than these critical values, the system becomes unstable

Periodic boundary conditions, the smallest k is $2\pi/L$

If the system length L>Lc, then the system becomes unstable

$$\boxed{\frac{2\pi}{L_c^*} = \max\left\{k_\perp^c, k_\parallel^c\right\}}$$

In most of the studied cases, the linear stability analysis predicts that the HCS is unstable to velocity vortices and linearly stable to particle clusters.

$$\boxed{k_\perp^c > k_\parallel^c}$$

Stringent ***assessment*** of kinetic theory calculations!!!

MONOCOMPONENT GRANULAR FLUIDS

VG, PRE 72, 021106 (2005)

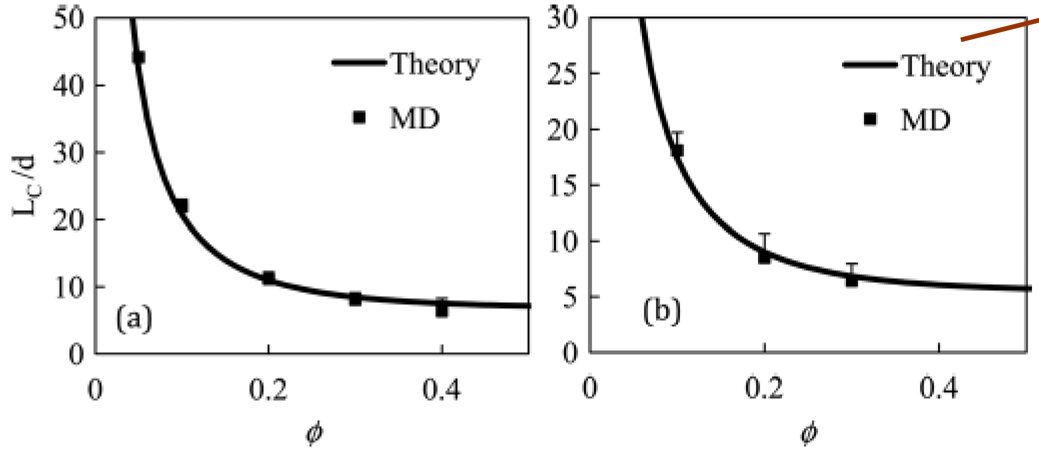


FIG. 8. Comparison of the critical length scale (L_C/d) for (a) $e = 0.8$ and (b) $e = 0.7$. The "error bars" correspond to the transition length scale range obtained from MD simulations (see Sec. IV A and Figure 5). Theoretical predictions are obtained from the linear stability analysis of Garzó (Ref. 23).

P. Mitrano *et al*. PF **23**, 093303 (2011)

Standard Sonine approximation

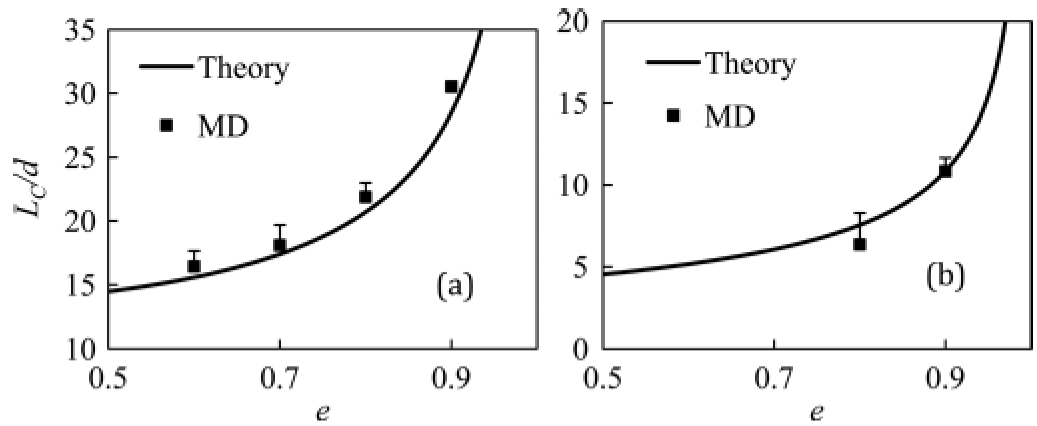


FIG. 9. Comparison of the critical length scale for (a) $\phi = 0.1$ and (b) $\phi = 0.4$. The "error bars" correspond to the transition length scale range obtained from MD simulations (see Sec. IV A and Figure 5). Theoretical predictions are obtained from a linear stability analysis of Garzó (Ref. 23).

HIGHLY DISSIPATIVE GRANULAR FLUIDS

Modified Sonine approximation (VG *et al.*, Physica A **376** 94 (2007))

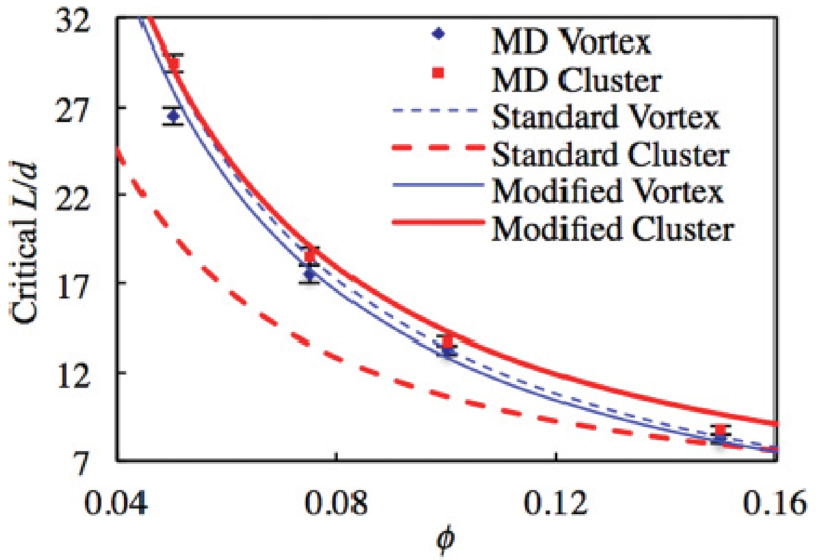
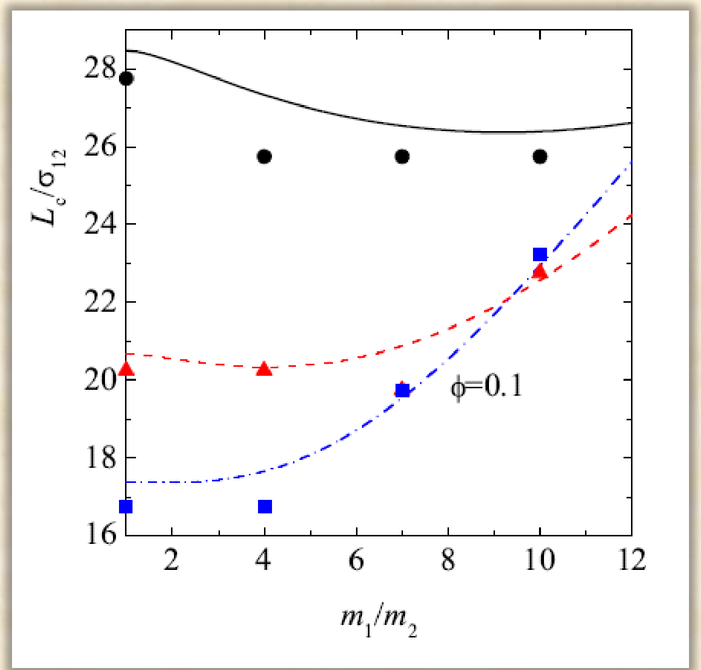
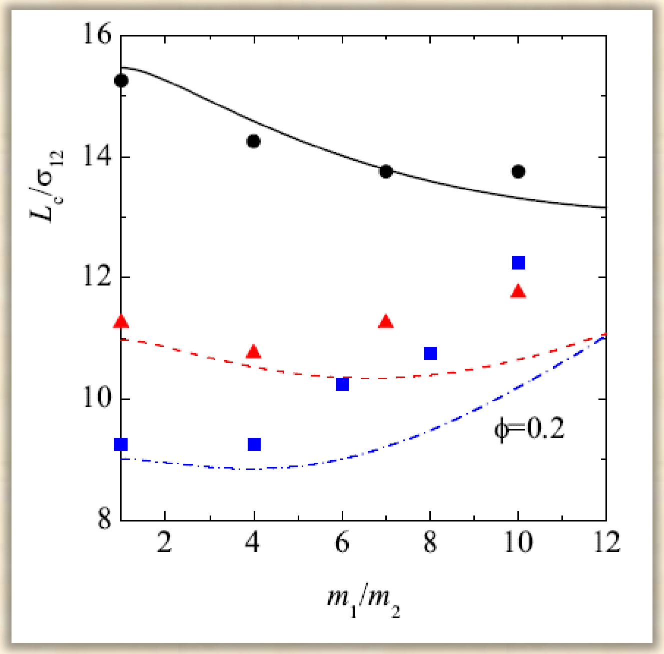


FIG. 4. (Color online) Critical length scale for vortex and cluster instabilities (i.e., L_{Vortex}/d and L_{Cluster}/d, respectively) plotted as a function of solids fraction for $e = 0.25$. The solid and dashed lines correspond to the modified and standard theories, respectively.

Mitrano, VG, Hilger, Ewasko, Hrenya, PRE **85**, 041303 (2012)

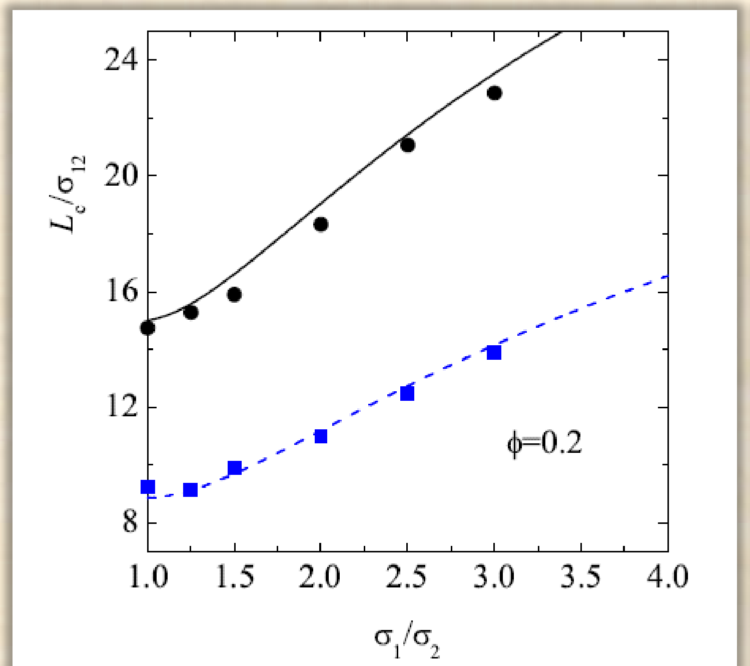
BINARY GRANULAR DENSE MIXTURES

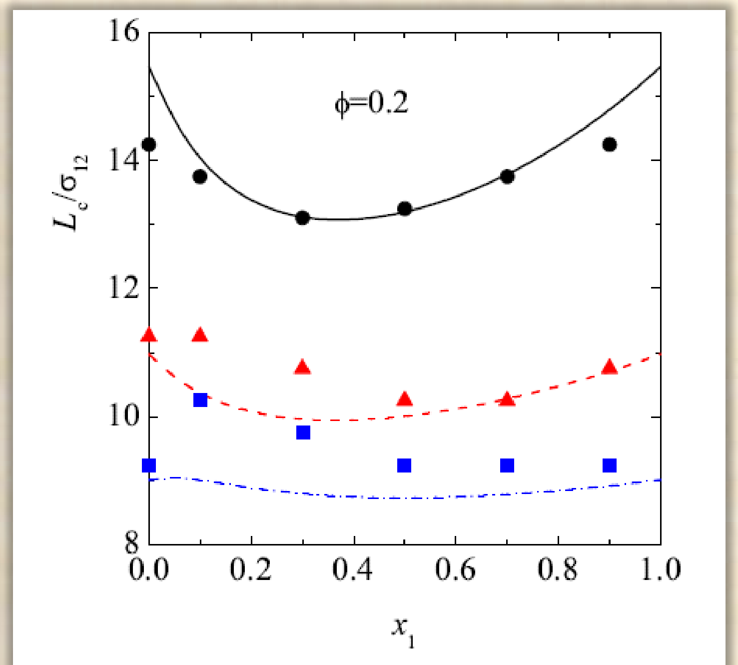




$$x_1 = 0.1, \quad \sigma_1/\sigma_2 = 1$$

P. Mitrano, VG and C.M. Hrenya, PRE **89**, 020201(R) 2013



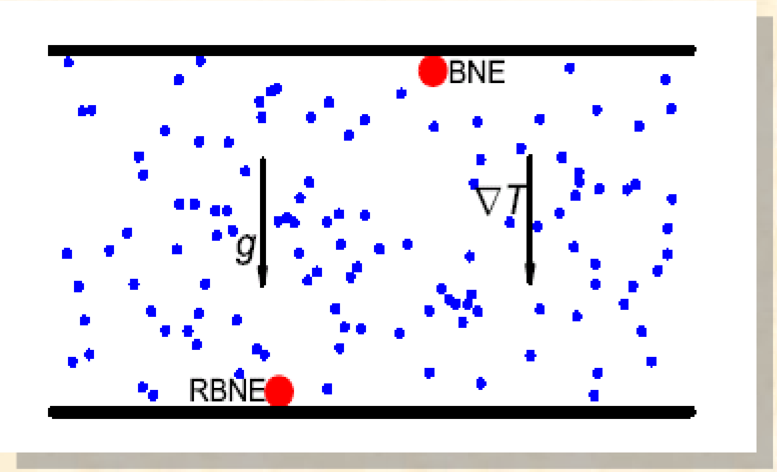


$x_1 = 0.5, \quad m_1/m_2 = 2 \qquad \sigma_1/\sigma_2 = 1, \quad m_1/m_2 = 6$

Even in the extreme case of small concentration (mole fraction 0.1) and large dissipation the discrepancies are smaller than 10%

THERMAL DIFFUSION SEGREGATION

Objective: Segregation problem driven by the presence of a thermal gradient and the gravitational field in a *moderately* dense ganular fluid



Model system: dense *granular* fluid (species 2)+**intruder (species 1)**

(granular binary mixture in the **tracer** limit)

Mechanical parameters of the system

$$\{m_2, m_1, \sigma_2, \sigma_1, \alpha_{22}, \alpha_{12}\}$$

Experimental conditions: *inhomogeneous* steady state without convection (*zero* mass flux) and gradients along the z direction

$$\boxed{-\Lambda \partial_z \ln T = \partial_z \ln(n_1/n)}$$

$\Lambda > 0 \longrightarrow$ Intruder rises with respect fluid (**BNE**)

$\Lambda < 0 \longrightarrow$ Intruder falls with respect fluid (**RBNE**)

Hydrodynamic description to evaluate thermal diffusion Λ

a) *Momentum* balance equation:

$$\boxed{\frac{\partial p}{\partial z} = \frac{\partial p}{\partial T}\partial_z T + \frac{\partial p}{\partial n}\partial_z n = -\rho g}$$

b) *Constitutive* equation for the mass flux of intruder:

$$\boxed{j_{1z} = -\frac{m_1^2}{\rho} D_{11}\partial_z n_1 - \frac{m_1 m_2}{\rho} D_{12}\partial_z n - \frac{\rho}{T} D_1^T \partial_z T}$$

Non-convecting steady state $\longrightarrow$ $j_{1z} = 0$

Density gradients in terms of gravity and thermal gradient

$$\boxed{\Lambda = \frac{\beta D_1^{T*} - (p^* + g^*)(D_{11}^* + D_{12}^*)}{\beta D_{11}^*}}$$

$$p^* = p/nT, g^* = \rho g/n\partial_z T < 0$$

$$\beta = p^* + \phi\partial_\phi p^*, \phi = [\pi^{d/2}/2^{d-1}d\Gamma(d/2)]n\sigma^d$$

Early theoretical attempts:

Dense gases: *Homogeneous* temperature

•*Elastic* systems: Jenkins and Yoon PRL 2002

•*Quasielastic* particles: Trujillo, Alam & Herrmann EPL 2003

Dilute gases: *Inhomogeneous* temperature

•*Weak* dissipation: Serero *et al*. JFM 2006

•*Arbitrary* degree of dissipation:

Brey *et al*. PRL 2005; Garzó EPL 2006

Our theory
(i) goes beyond weak dissipation limit, (ii) combined effect of gravity and thermal gradient,
(iii) applies for moderate densities

It covers some of the aspects *not* previously accounted for in previous theories, but it also assumes a **Navier-Stokes** description (first order in spatial gradients)

VG, PRE **78**, 020301 (R) (2008); EPJE **29**, 261 (2009); New J. Phys. **13**, 055020 (2013)

COMPARISON WITH SIMULATIONS

Simple case: *dilute* granular gas in the absence of gravity

Thermal diffusion segregation in driven steady states characterized by a **uniform** heat flux

$$\boxed{\frac{\partial q_z}{\partial z} = -\frac{d}{2} nT\left(\zeta - \sigma_T\right) - P_{xz}\frac{\partial U_x}{\partial z} = 0}$$

Collisional cooling

External forcing term

Viscous heating term

Two types of uniform-heat-flux steady flows:

Case I: No shear with a stochastic external forcing

$$\boxed{U_x(z) = 0, \quad \sigma_T = \zeta}$$

This is the case closer to the Navier-Stokes description

Case II: No volume driving and boundary shear; i.e, both walls are in relative motion (sheared granular gas)

$$\boxed{\frac{d}{2} n T \zeta = -P_{xz} \frac{\partial U_x}{\partial z}}$$

Case I: Monte Carlo simulations (DSMC method)

Case II. Molecular dynamics simulations

Parameter space

$$d = 3, \quad \alpha_{22} = \alpha_{12} \equiv \alpha$$

$$\mu \equiv m_1/m_2, \quad \omega \equiv \sigma_1/\sigma_2$$

F. Vega Reyes, VG, N. Khalil, PRE **89**, 052206 (2014)

Temperature ratio $\chi \equiv T_1/T_2$

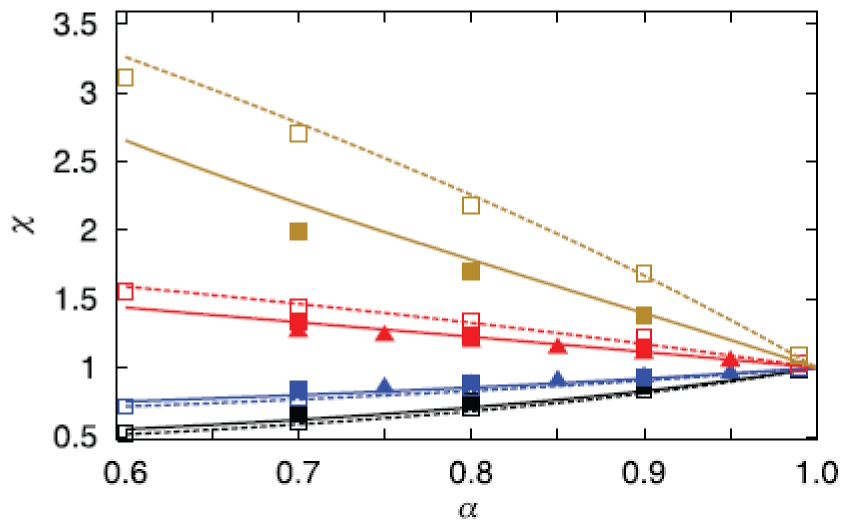


FIG. 2. (Color online) Temperature ratio vs (common) coefficient of restitution $\alpha = \alpha_0$ for $\omega = 1$ and several values of relative mass μ: $\mu = 1/4$ (black), $\mu = 1/2$ (blue), $\mu = 2$ (red), and $\mu = 4$ (brown). Dashed and solid lines refer to the theoretical values obtained for case I (no shear) [28] and case II (shear) [40], respectively. Open symbols represent case I simulations; filled symbols, case II simulations (triangles, MD; squares, DSMC). All figures in this work represent spheres ($d = 3$).

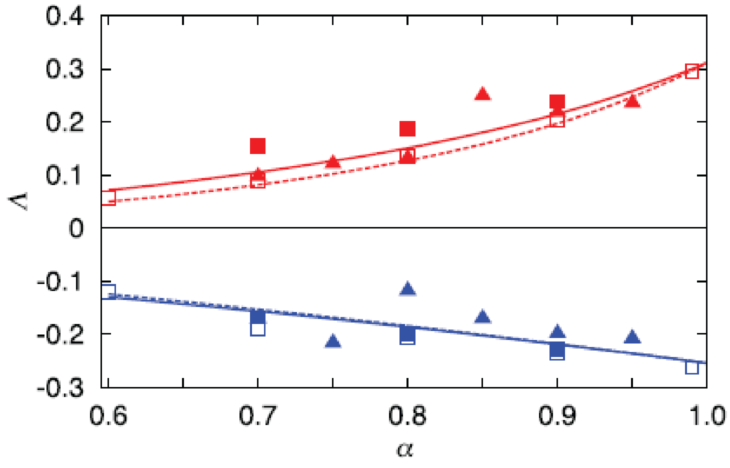


FIG. 3. (Color online) Thermal diffusion factor Λ vs (common) coefficient of restitution $\alpha = \alpha_0$ for $\omega = 1$. Two relative mass cases are represented: $\mu = 1/2$ (blue) and $\mu = 2$ (red). Dashed and solid lines correspond to theoretical predictions obtained for case I and case II, respectively. Both cases show rather similar curves. Open symbols, case I simulation data; filled symbols, case II simulation data (triangles, MD; squares, DSMC).

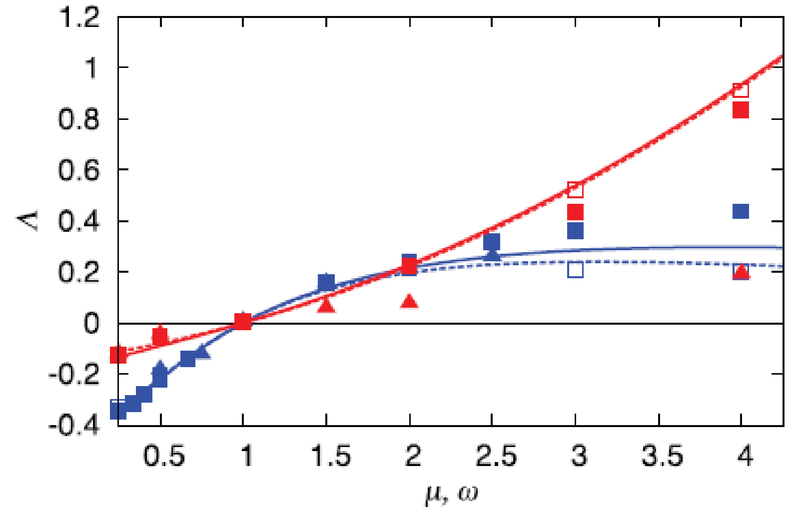


FIG. 4. (Color online) Thermal diffusion factor Λ vs relative mass μ and diameter ω. The case $\alpha = \alpha_0 = 0.9$: for relative size $\omega = 1$ and variable relative mass μ (blue) and for $\mu = 1$ and variable relative size ω (red). The meaning of the lines and the symbols is the same as in Fig. 3.

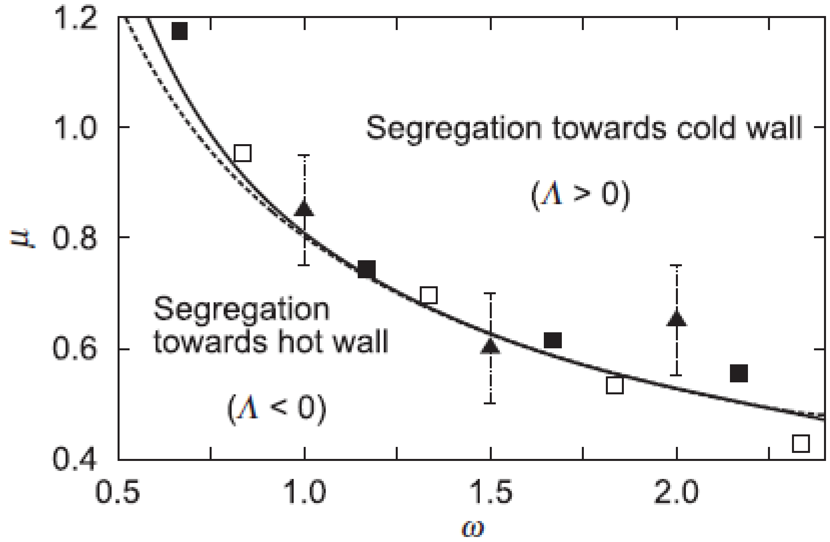


FIG. 5. Plot of the marginal segregation curve ($\Lambda = 0$) for a system with $\alpha = 0.9$ and $\alpha_0 = 0.7$. Dashed and solid lines represent theoretical predictions derived for cases I and II, respectively. Open symbols, case I simulations; filled symbols, case II simulations (triangles, MD; squares, DSMC). Error bars were estimated by using the difference between the values obtained in the bulk region (which are plotted) and those obtained in the whole system.

CONCLUSIONS

✓Hydrodynamic description (derived from kinetic theory) appears to be a powerful tool for analysis and predictions of rapid flow gas dynamics of granular mixtures at ***moderate*** densities.

✓New and interesting result: partial temperatures (which measure the mean kinetic energy of each species) are different (***breakdown*** of energy equipartition theorem). Energy nonequipartition has important and new quantitative effects on transport coefficients

✓A ***normal*** solution is obtained by applying the Chapman-Enskog method for states close to the HCS. ***Exact*** expressions for the equation of state, the cooling rate and transport coefficients have been obtained to first-order in spatial gradients (Navier-Stokes hydrodynamic order)

CONCLUSIONS

✓Explicit forms for the kinetic and collisional contributions to the cooling rate and transport coefficients are obtained by considering the leading terms in a Sonine polynomial expansion

✓Analytical results for the tracer diffusion and shear viscosity coefficients are compared against DSMC simulations. Good agreement is found over a wide range of values of parameters of the system

✓***Instability*** of HCS: Good agreement of kinetic theory with extensive MD simulations for finite dissipation and moderate densities. Stringent test of kinetic theory

CONCLUSIONS

✓A ***segregation*** criterion has been derived from the Enskog kineti theory. It covers some of the aspects not preoperly accounted for in previous theoretical attempts. Goor agreement with DSMC and MD simulations for dilute binary granular mixtres

SOME OPEN PROBLEMS

Extension to inelastic **rough** spheres

Influence of **interstitial** fluid on grains (suspensions)
Previous results for monodisperse gas-solid flows
(VG, Tenneti, Subramaniam, Hrenya, JFM **712**, 129 (2012)) and dilute binary mixtures (Khalil, VG, PRE **58**, 052201 (2013))

Granular hydrodynamics for **far from equilibrium** steady states

UEx (Spain)

- José María Montanero
- Francisco Vega Reyes
- Nagi Khalil

External collaborations

- James W. Dufty (University of Florida, USA)
- Christine Hrenya, Peter Mitrano (University of Colorado, USA)

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

Ministerio de Economía y Competitividad (Spain)
Grant no. FIS2016-76359-P, Junta de Extremadura Grant no. GR18079,
both partially financed by FEDER funds

JUNTA DE EXTREMADURA

Fondo Europeo de Desarrollo Regional
"Una manera de hacer Europa"

Unión Europea