Kinetic theory of mixtures of inelastic rough hard spheres

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Outline

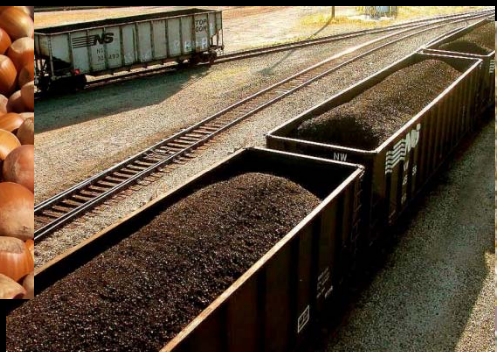
- What is a granular fluid?
- Mixture of inelastic rough hard spheres. The Boltzmann equation.
- Collisional thermal rates.
- Application to the homogeneous cooling state. Non-equipartition of energy.
- Conclusions and outlook.

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?

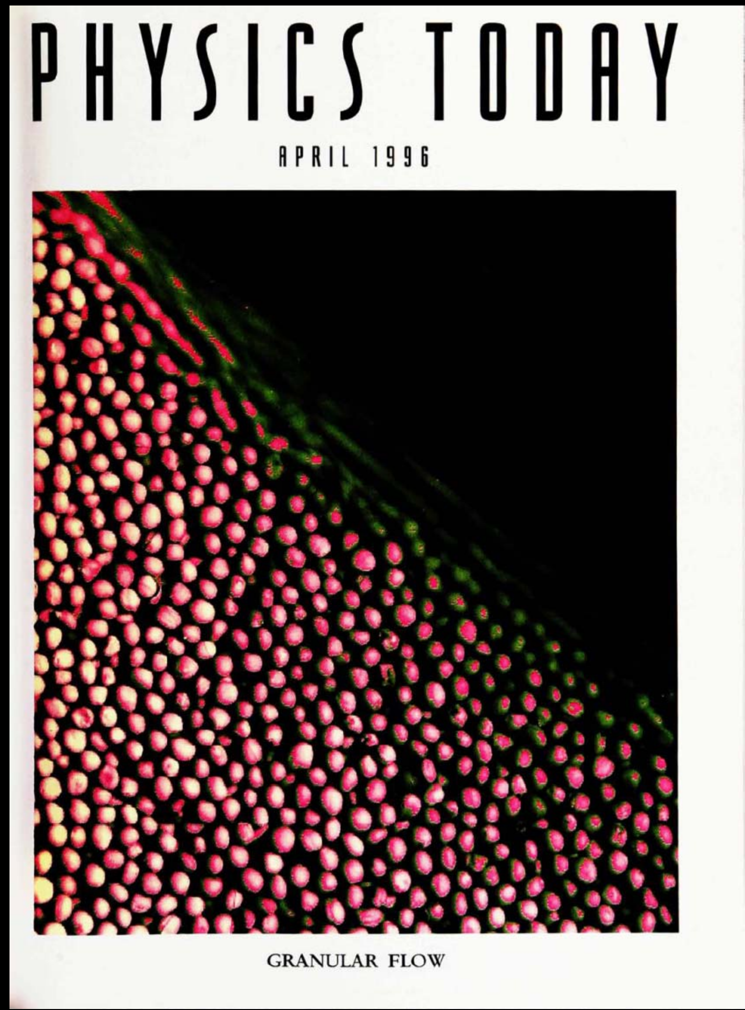
- Examples of granular materials would include nuts, coal, sand, rice, coffee, corn flakes, fertilizer, and ball bearings.

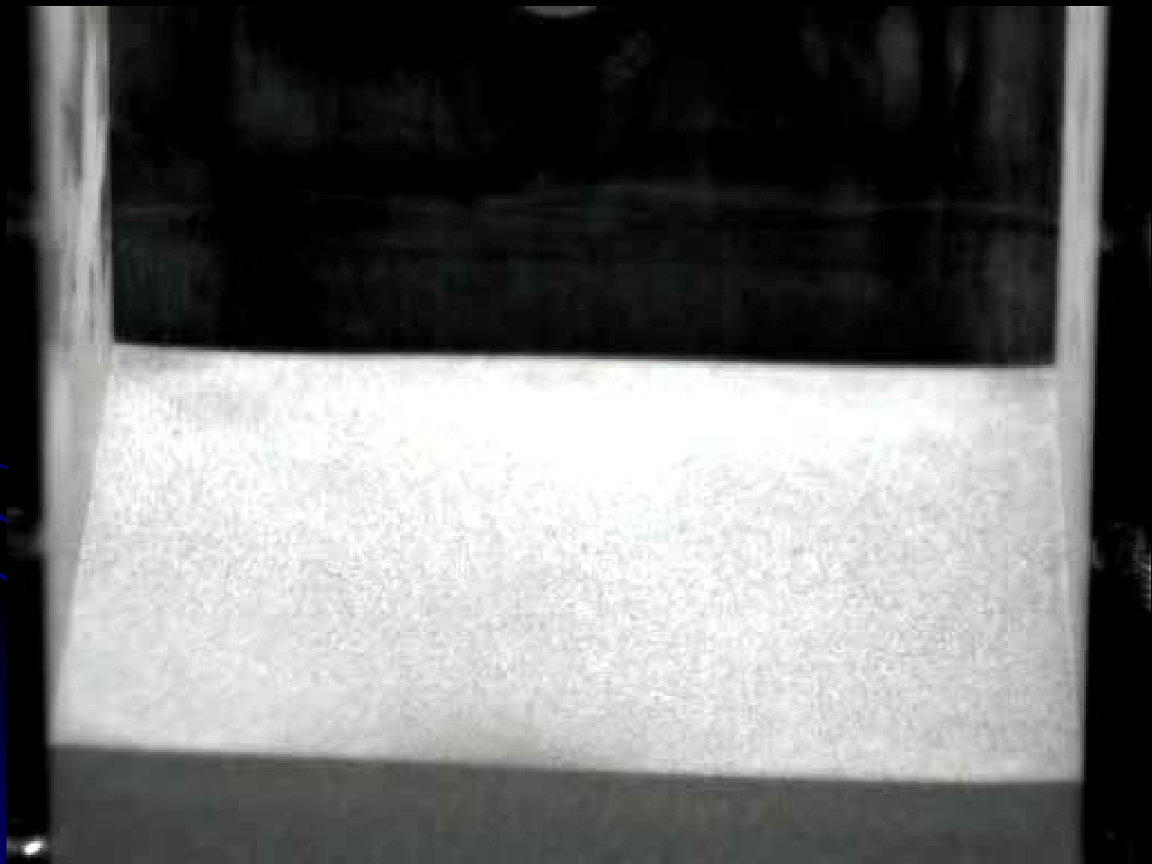



What is a granular *fluid*?

- 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*.

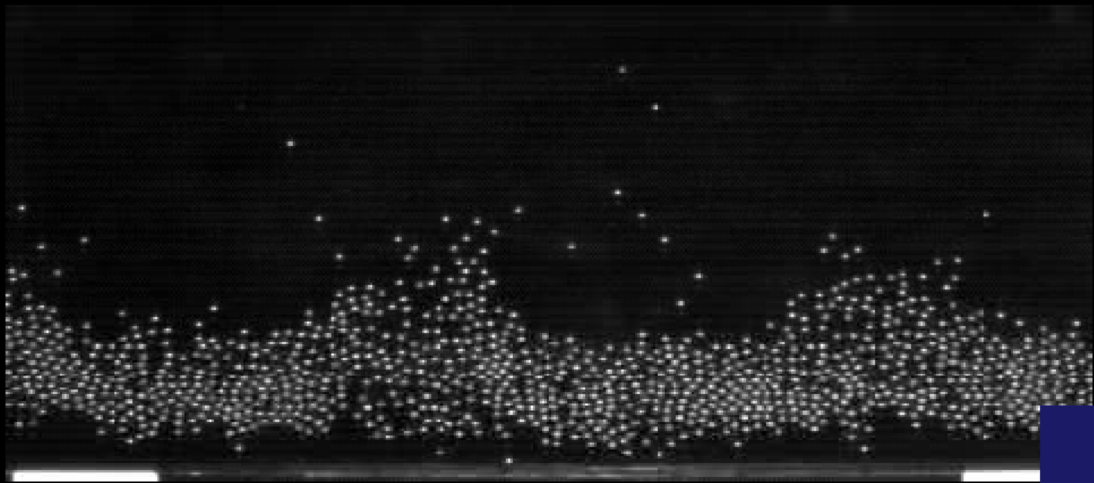


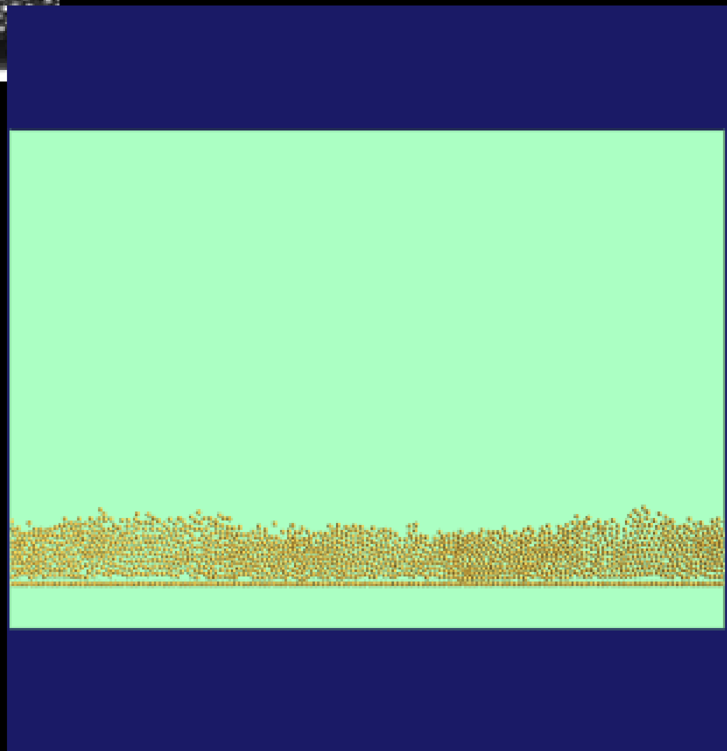
Granular fluids (or gases) exhibit many interesting phenomena:



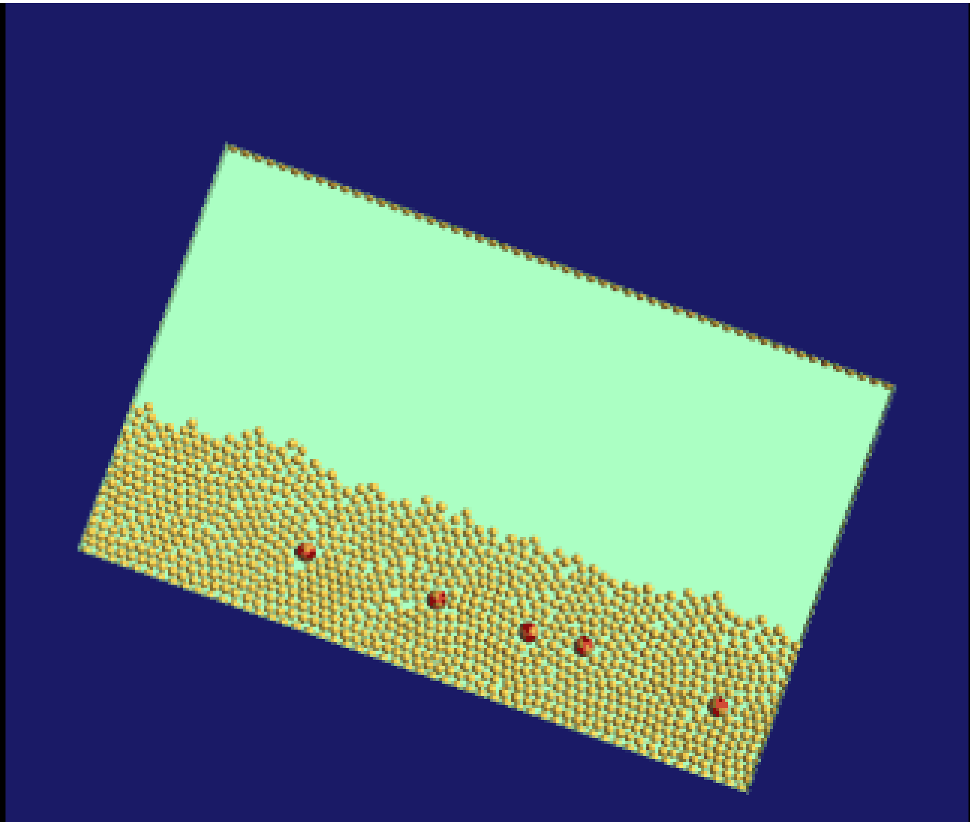
Granular eruptions
(from University of
Twente's group)

Wave patterns in a vibrated container
(from A. Kudrolli's group)

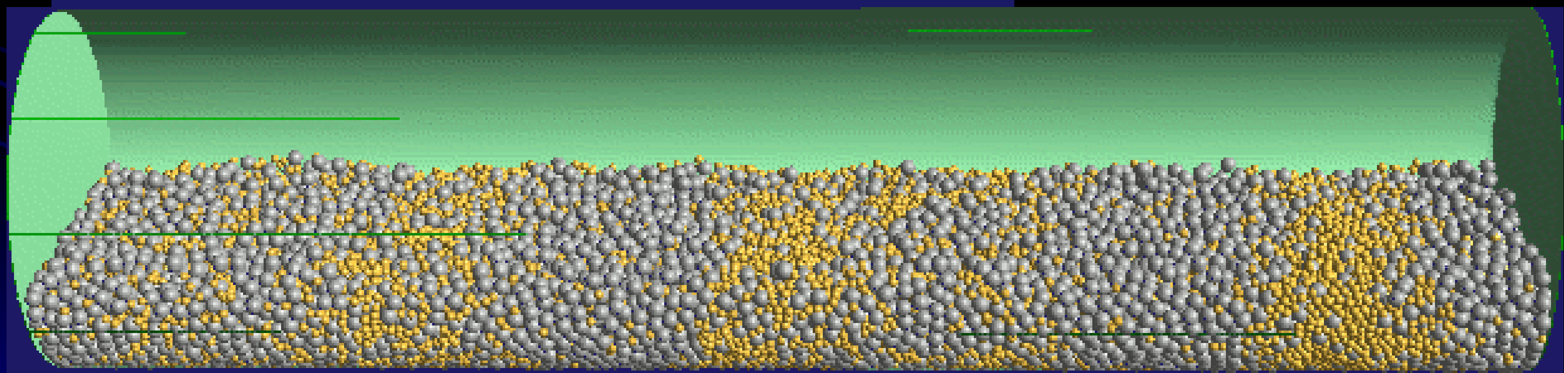




(Simulations by D. C. Rapaport)

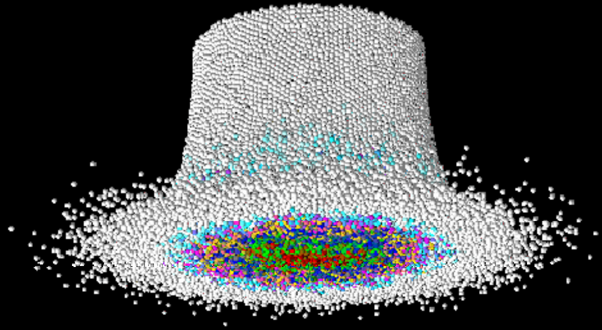


Segregation in sheared flow
(Simulations by D. C. Rapaport)

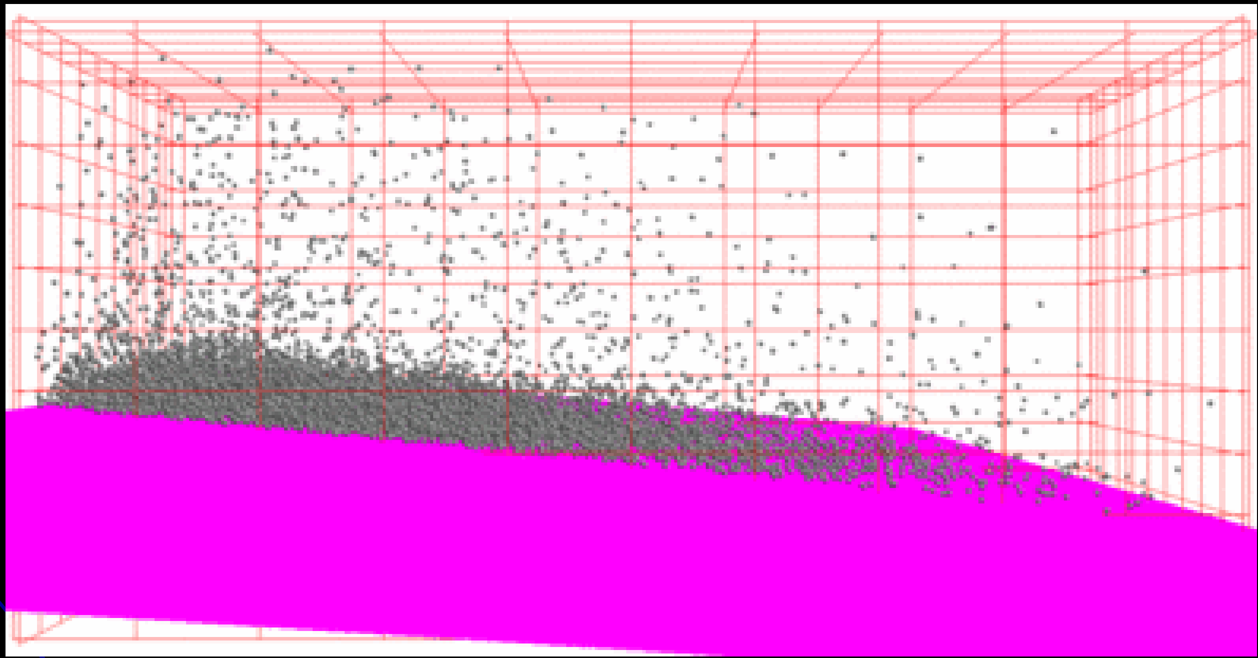


Segregation in a rotating cylinder
(Simulations by D. C. Rapaport)

Granular jet hitting a plane

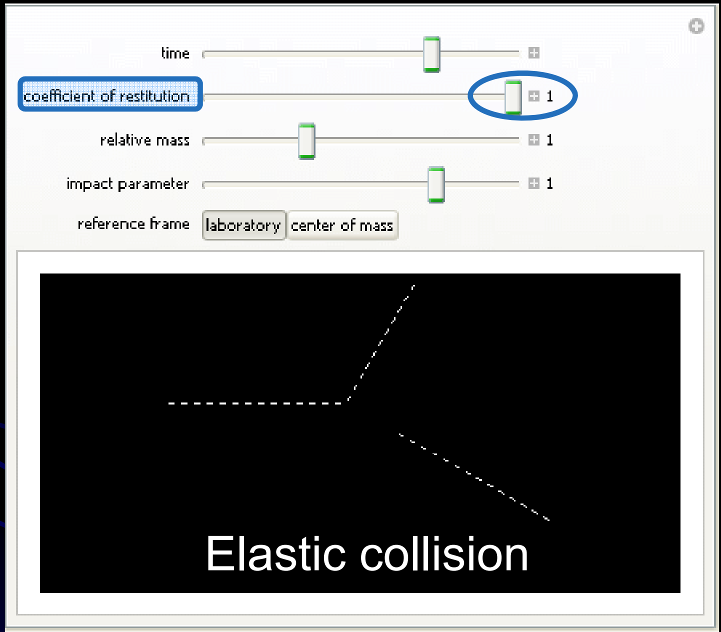


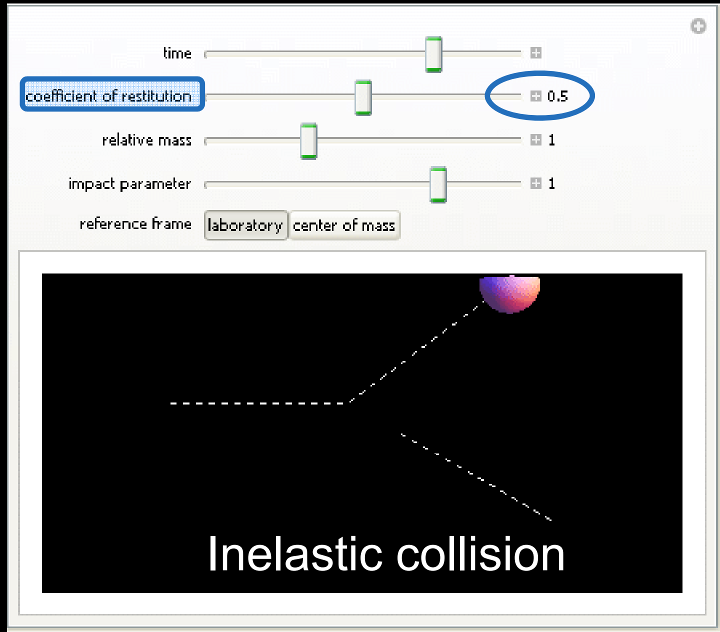
Particles falling on an inclined heated plane



http://trevinca.ei.uvigo.es/~formella/

Minimal model of a granular gas: A gas of *identical smooth inelastic* hard spheres

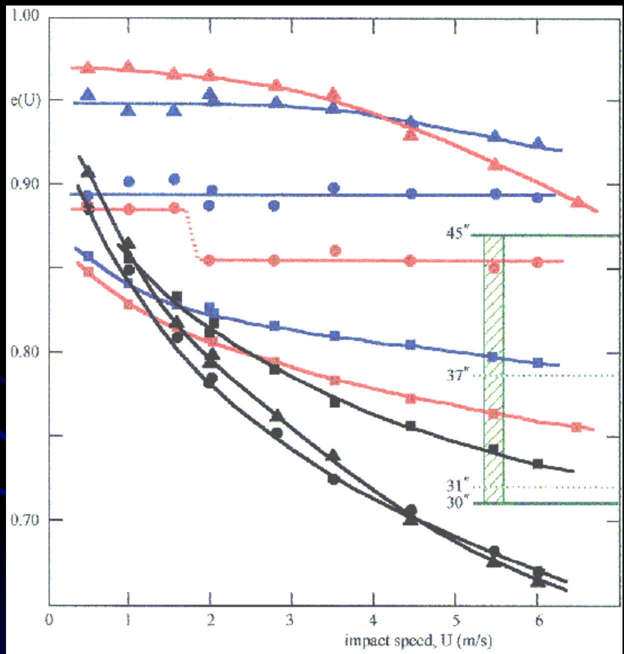


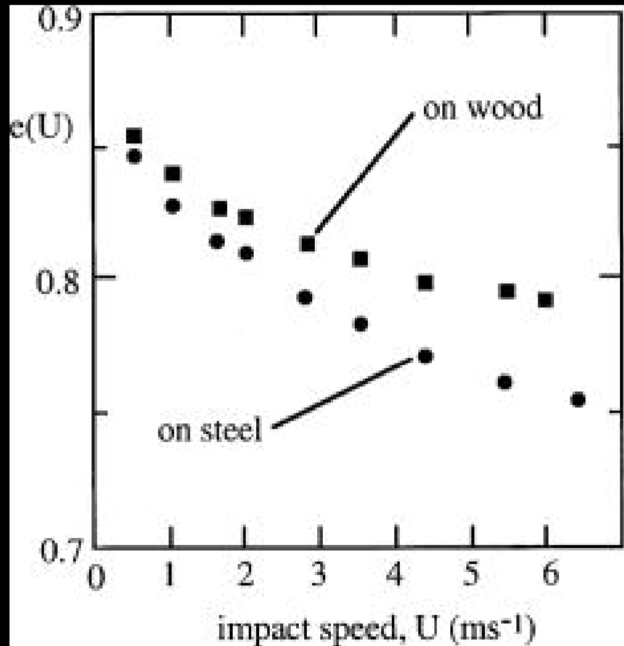


http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/

But … real grains

Have a non-constant coefficient of restitution





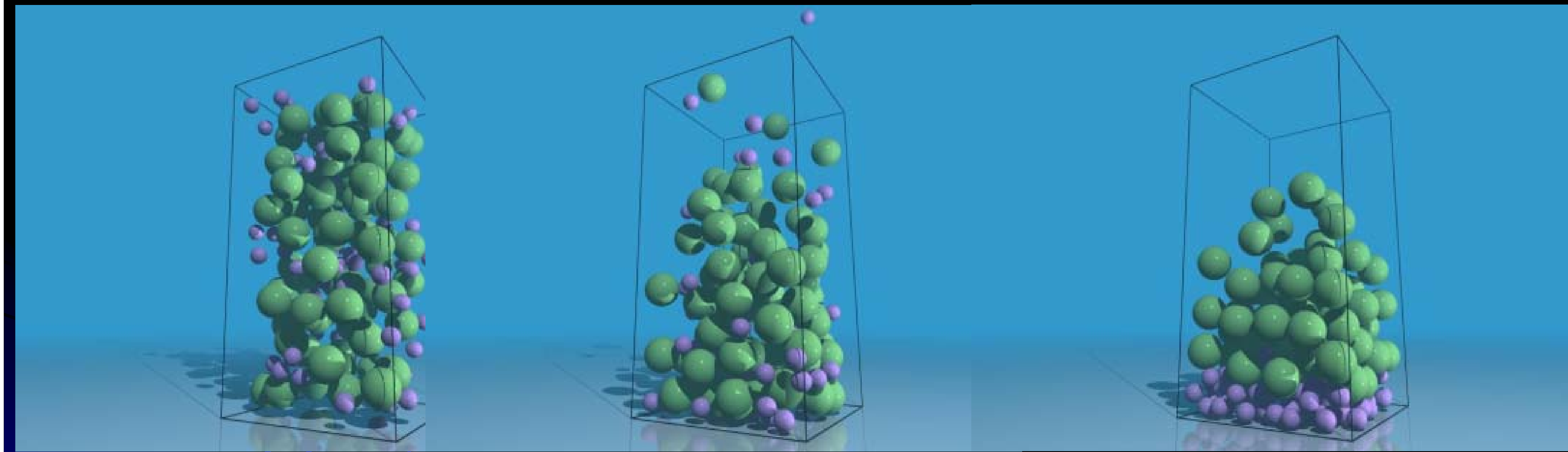
www.oxfordcroquet.com/tech/

But … real grains

Are non-spherical

But … real grains

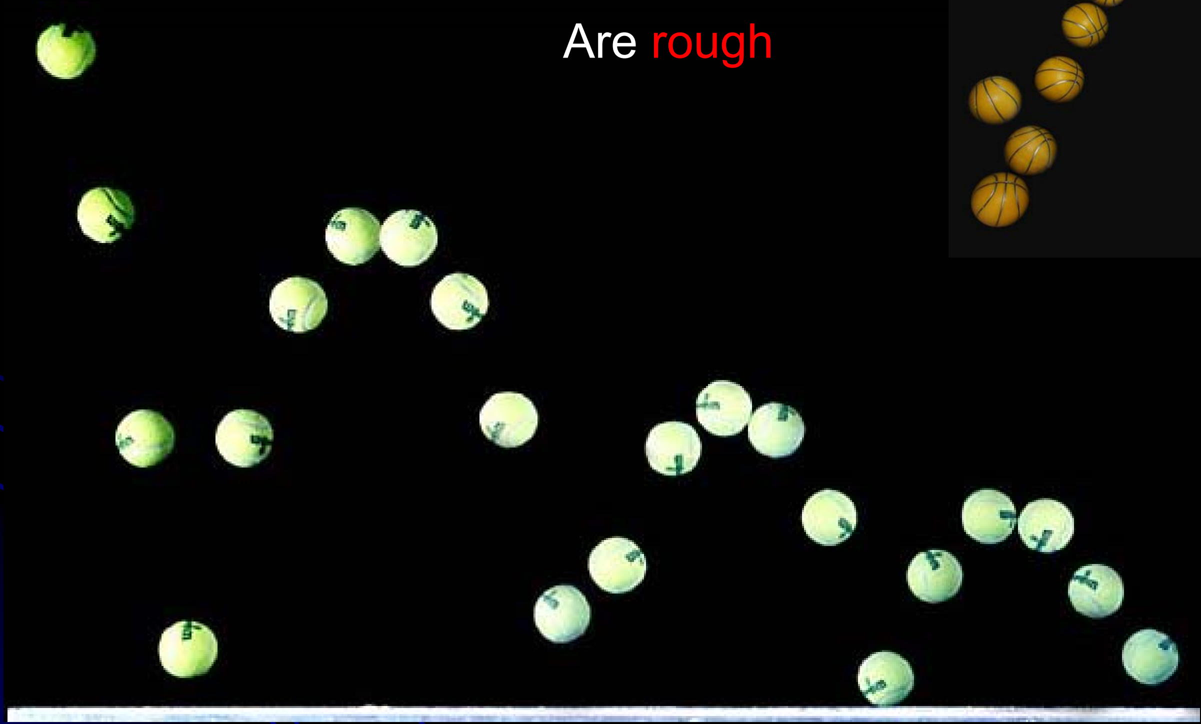
Are polydisperse



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, …, X)
- Masses m_i
- Diameters σ_i
- Moments of inertia I_i
- Coefficients of normal restitution α_{ij}
- Coefficients of tangential restitution β_{ij}
- $\alpha_{ij}=1$ for elastic particles
- $\beta_{ij}=-1$ for smooth particles
- $\beta_{ij}=+1$ for totally rough particles

Collision rules:

Translational velocities: $\mathbf{v}'_i = \mathbf{v}_i - \frac{1}{m_i}\mathbf{Q}_{ij}, \quad \mathbf{v}'_j = \mathbf{v}_j + \frac{1}{m_j}\mathbf{Q}_{ij}$

Angular velocities: $\boldsymbol{\omega}'_i = \boldsymbol{\omega}_i + \frac{\sigma_i}{2I_i}\widehat{\boldsymbol{\sigma}} \times \mathbf{Q}_{ij}, \quad \boldsymbol{\omega}'_j = \boldsymbol{\omega}_j + \frac{\sigma_j}{2I_j}\widehat{\boldsymbol{\sigma}} \times \mathbf{Q}_{ij}$

Smooth spheres

Impulse exerted by i on j:

$$\mathbf{Q}_{ij} = \overline{\beta}_{ij}\left[\mathbf{g}_{ij} - (\mathbf{g}_{ij}\cdot\widehat{\boldsymbol{\sigma}})\widehat{\boldsymbol{\sigma}} + \frac{1}{2}\widehat{\boldsymbol{\sigma}} \times (\sigma_i\boldsymbol{\omega}_i + \sigma_j\boldsymbol{\omega}_j)\right] + \overline{\alpha}_{ij}(\mathbf{g}_{ij}\cdot\widehat{\boldsymbol{\sigma}})\widehat{\boldsymbol{\sigma}}$$

$$\mathbf{g}_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j, \quad \overline{\alpha}_{ij} \equiv m_{ij}\left(1+\alpha_{ij}\right), \quad \overline{\beta}_{ij} \equiv \frac{m_{ij}\kappa_{ij}}{1+\kappa_{ij}}\left(1+\beta_{ij}\right)$$

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

Energy collisional loss

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

$$\begin{aligned} E'_{ij} - E_{ij} &= -(1-\alpha_{ij}^2) \times \cdots \\ &\quad -(1-\beta_{ij}^2) \times \cdots \end{aligned}$$

Energy is conserved *only* if the spheres are
- elastic (α_{ij}=1) and
- either
  - smooth (β_{ij}=-1) or
  - totally rough (β_{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: $T = \sum_i \frac{n_i}{2n} \left(T_i^{\text{tr}} + T_i^{\text{rot}} \right)$

Collisional rates of change for temperatures

Thermal rates:

$$\xi_i^{\text{tr}} = -\frac{1}{T_i^{\text{tr}}}\left(\frac{\partial T_i^{\text{tr}}}{\partial t}\right)_{\text{coll}}, \quad \xi_i^{\text{tr}} = \sum_j \xi_{ij}^{\text{tr}}$$

$$\xi_i^{\text{rot}} = -\frac{1}{T_i^{\text{rot}}}\left(\frac{\partial T_i^{\text{rot}}}{\partial t}\right)_{\text{coll}}, \quad \xi_i^{\text{rot}} = \sum_j \xi_{ij}^{\text{rot}}$$

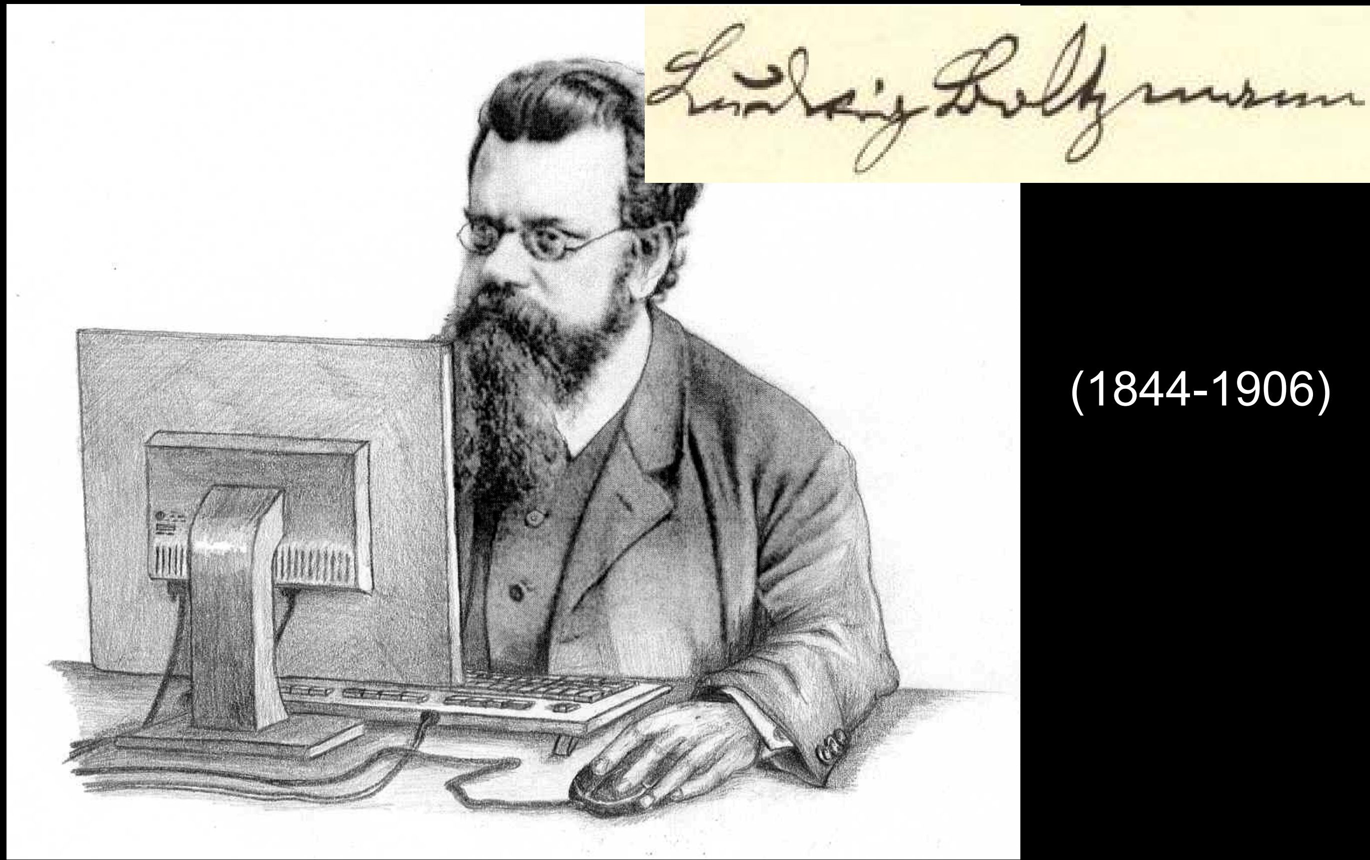
Net cooling rate:

$$\zeta = -\frac{1}{T}\left(\frac{\partial T}{\partial t}\right)_{\text{coll}}, \quad \zeta = \sum_i \frac{n_i}{2nT}\left(\xi_i^{\text{tr}} T_i^{\text{tr}} + \xi_i^{\text{rot}} T_i^{\text{rot}}\right)$$

Our main goal

To obtain the binary thermal rates
$\xi_{ij}^{\rm tr}$ and $\xi_{ij}^{\rm rot}$
in terms of
$T_i^{\rm tr}$, $T_j^{\rm tr}$, $T_i^{\rm rot}$, $T_j^{\rm rot}$, n_i, n_j
and the mechanical parameters
m_i, m_j, σ_i, σ_j, κ_i, κ_j, α_{ij}, β_{ij}

(Cartoon by Bernhard Reischl, University of Vienna)



(1844-1906)

Boltzmann equation:

$$\partial_t f_i(\mathbf{r}, \mathbf{v}_i, \boldsymbol{\omega}_i, t) + \mathbf{v}_i \cdot \nabla f_i(\mathbf{r}, \mathbf{v}_i, \boldsymbol{\omega}_i, t) = \sum_j \underbrace{J_{ij}[\mathbf{r}, \mathbf{v}_i, \boldsymbol{\omega}_i, t | f_i, f_j]}_{\text{Binary collisions}}$$

Additional assumptions

1. No convection, no chirality:

$$\langle \mathbf{v}_i \rangle = \langle \mathbf{v}_j \rangle, \quad \langle \boldsymbol{\omega}_i \rangle = \langle \boldsymbol{\omega}_j \rangle = \mathbf{0}$$

2. Translational and rotational degrees of freedom uncorrelated:

$$f_i(\mathbf{v}_i, \boldsymbol{\omega}_i) = f_i^{\mathrm{tr}}(\mathbf{v}_i) f_i^{\mathrm{rot}}(\boldsymbol{\omega}_i)$$

3. Maxwellian form:

$$f_i^{\mathrm{tr}}(\mathbf{v}_i) = n_i \left(\frac{m_i}{2\pi T_i^{\mathrm{tr}}} \right)^{3/2} \exp\left(-\frac{m_i v_i^2}{2T_i^{\mathrm{tr}}} \right)$$

Results

$$\xi_{ij}^{\mathrm{tr}} = \frac{\nu_{ij}}{m_i T_i^{\mathrm{tr}}}\Bigg[2\left(\overline{\alpha}_{ij}+\overline{\beta}_{ij}\right)T_i^{\mathrm{tr}} - \left(\overline{\alpha}_{ij}^2+\overline{\beta}_{ij}^2\right)\left(\frac{T_i^{\mathrm{tr}}}{m_i}+\frac{T_j^{\mathrm{tr}}}{m_j}\right)$$

$$-\overline{\beta}_{ij}^2\left(\frac{T_i^{\mathrm{rot}}}{m_i\kappa_i}+\frac{T_j^{\mathrm{rot}}}{m_j\kappa_j}\right)\Bigg]$$

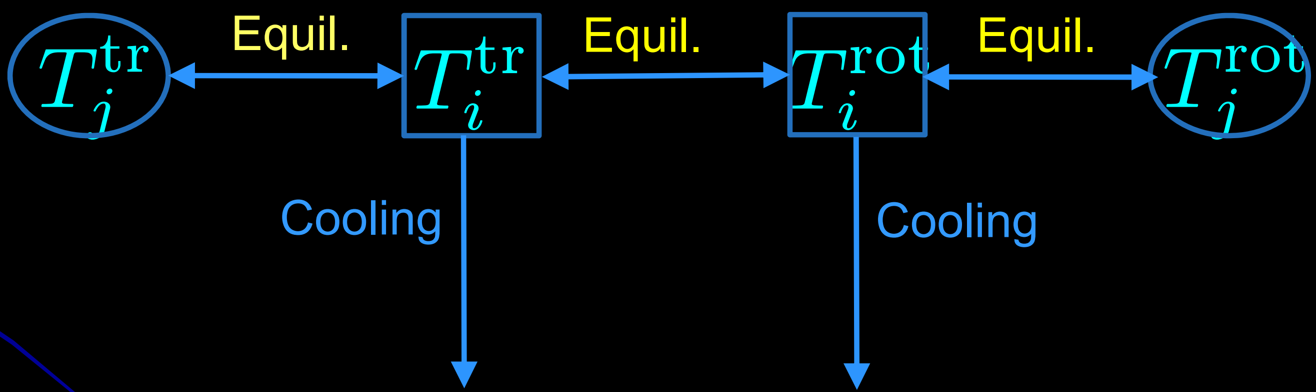
$$\xi_{ij}^{\mathrm{rot}} = \frac{\nu_{ij}}{m_i\kappa_i T_i^{\mathrm{rot}}}\overline{\beta}_{ij}\left[2T_i^{\mathrm{rot}} - \overline{\beta}_{ij}\left(\frac{T_i^{\mathrm{tr}}}{m_i}+\frac{T_j^{\mathrm{tr}}}{m_j}+\frac{T_i^{\mathrm{rot}}}{m_i\kappa_i}+\frac{T_j^{\mathrm{rot}}}{m_j\kappa_j}\right)\right]$$

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

Decomposition

Thermal rates = Equilibration rates + Cooling rates

Net cooling rate = Σ 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

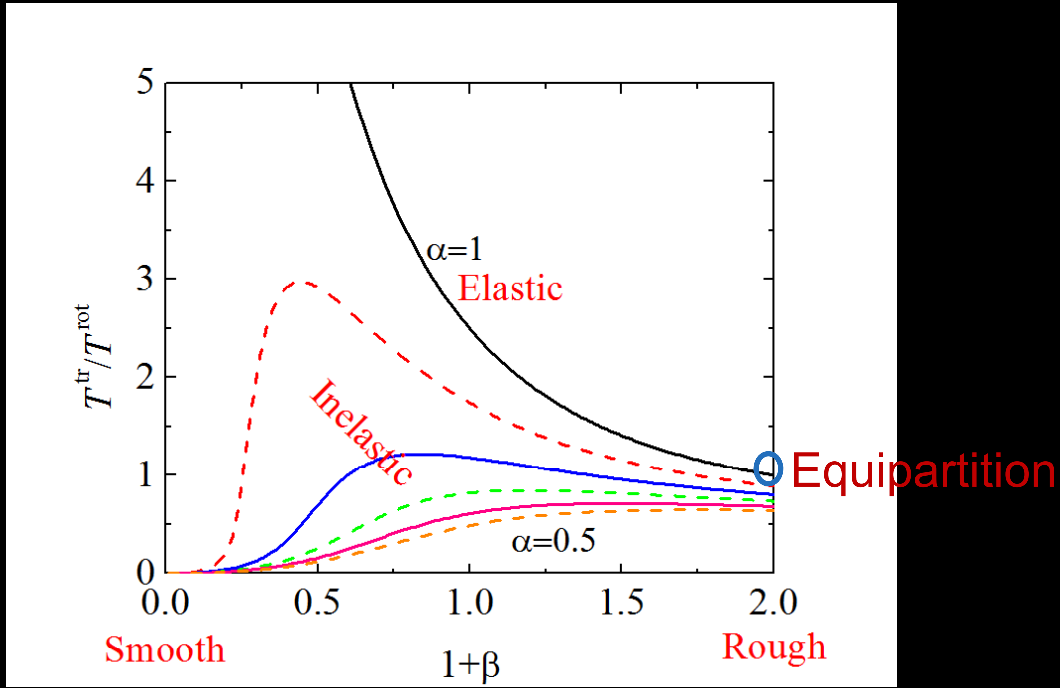
$$\partial_t f_i(\mathbf{r}, \mathbf{v}_i, \boldsymbol{\omega}_i, t) = \sum_j J_{ij}[\mathbf{r}, \mathbf{v}_i, \boldsymbol{\omega}_i, t | f_i, f_j]$$

$$\frac{\partial T}{\partial t} = -\zeta T$$

$$\frac{\partial}{\partial t}\frac{T_i^{\mathrm{tr}}}{T} = -\left(\xi_i^{\mathrm{tr}} - \zeta\right)\frac{T_i^{\mathrm{tr}}}{T}, \quad \frac{\partial}{\partial t}\frac{T_i^{\mathrm{rot}}}{T} = -\left(\xi_i^{\mathrm{rot}} - \zeta\right)\frac{T_i^{\mathrm{rot}}}{T}$$

$$t \to \infty \Rightarrow \xi_1^{\mathrm{tr}} = \xi_2^{\mathrm{tr}} = \cdots = \xi_1^{\mathrm{rot}} = \xi_2^{\mathrm{rot}} = \cdots$$

Single-component case (κ=2/5)



$$\left.\begin{array}{l}\alpha<1\\ \beta\to -1\end{array}\right\}\Rightarrow\left\{\begin{array}{l}\xi^{\rm tr}\sim(1-\alpha^2)\Rightarrow\partial_t T^{\rm tr}<0\\ \xi^{\rm rot}\to 0\Rightarrow T^{\rm rot}\to\text{const}\end{array}\right\}\Rightarrow\boxed{\frac{T^{\rm tr}}{T^{\rm rot}}\to 0}$$

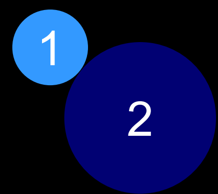
$$\left.\begin{array}{l}\alpha=1\\ \beta\to -1\end{array}\right\}\Rightarrow\left\{\begin{array}{l}\xi^{\rm tr}\sim\kappa(1+\beta)\Rightarrow\partial_t T^{\rm tr}<0\\ \xi^{\rm rot}\sim(1+\beta)\Rightarrow\partial_t T^{\rm rot}<0\end{array}\right\}\Rightarrow\xi^{\rm tr}<\xi^{\rm rot}\Rightarrow\boxed{\frac{T^{\rm tr}}{T^{\rm rot}}\to\infty}$$

Binary mixture

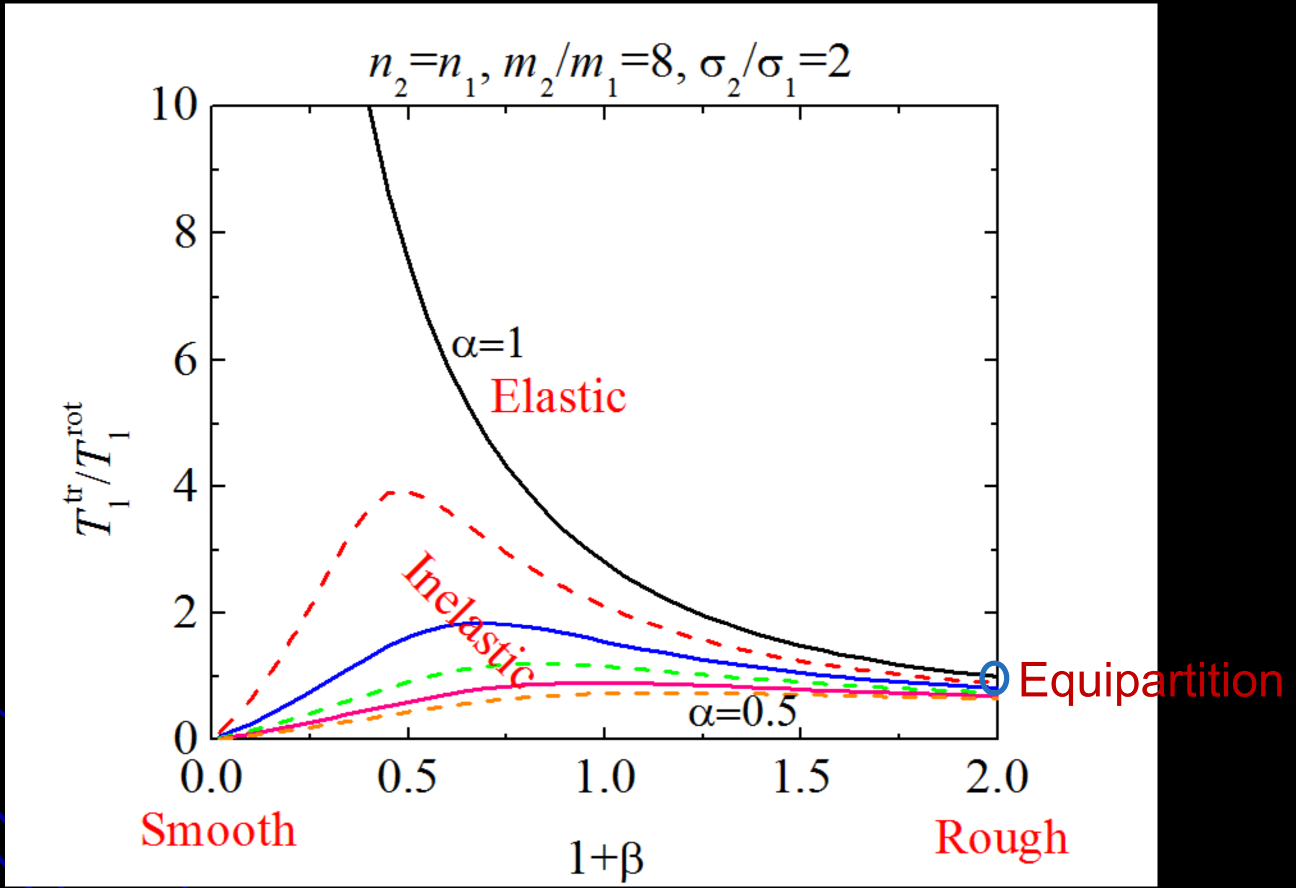
Three independent temperature ratios: $\frac{T_1^{\rm tr}}{T_1^{\rm rot}}, \frac{T_2^{\rm tr}}{T_1^{\rm tr}}, \frac{T_2^{\rm rot}}{T_1^{\rm rot}}$

Eleven parameters:

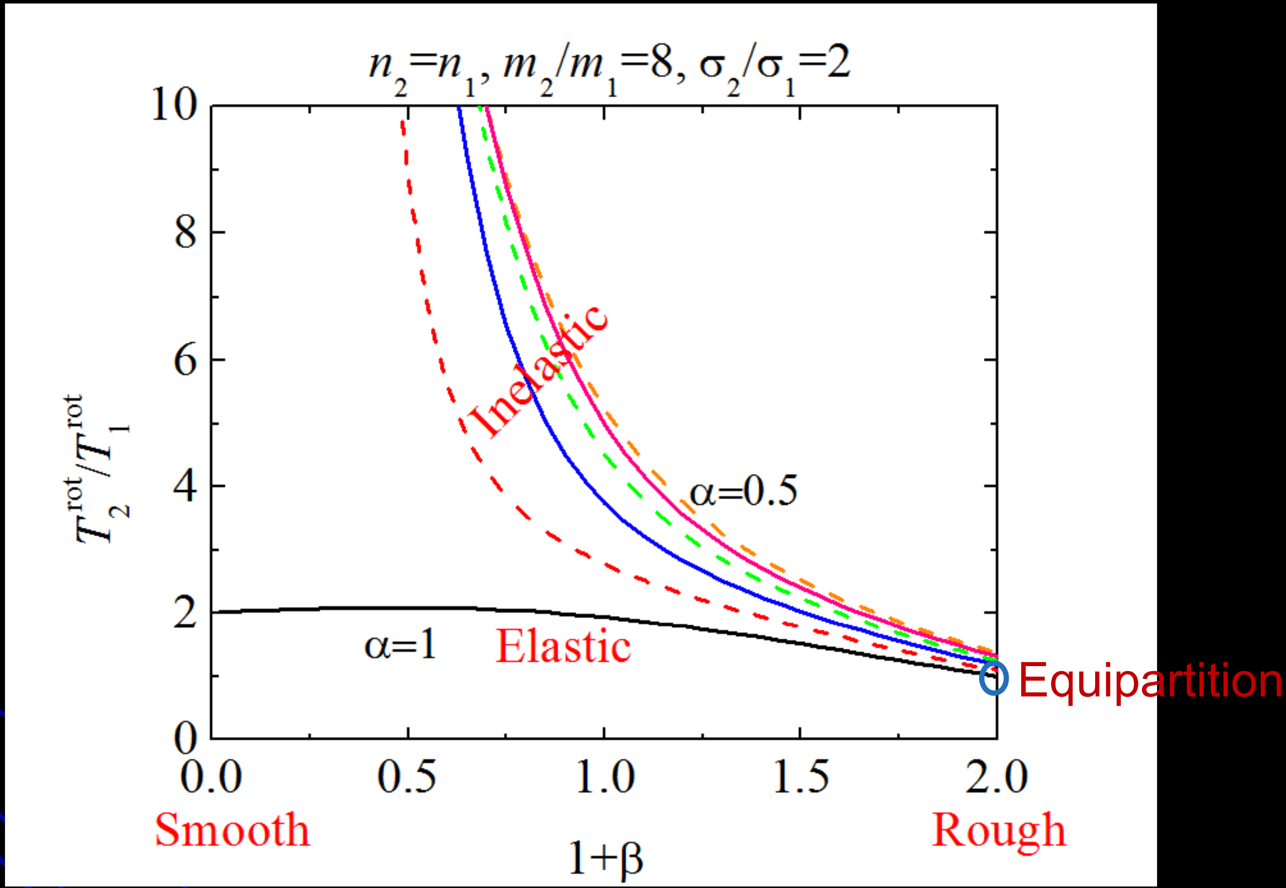
- Coefficients of normal restitution $\alpha_{11}=\alpha_{12}=\alpha_{22}=\alpha$
- Coefficients of tangential restitution $\beta_{11}=\beta_{12}=\beta_{22}=\beta$
- Inertia-moment parameters $\kappa_1=\kappa_2=\frac{2}{5}$
- Size ratio $\sigma_2/\sigma_1=2$
- Mass ratio $m_2/m_1=8$
- Mole fraction $n_1/(n_1+n_2)=\frac{1}{2}$



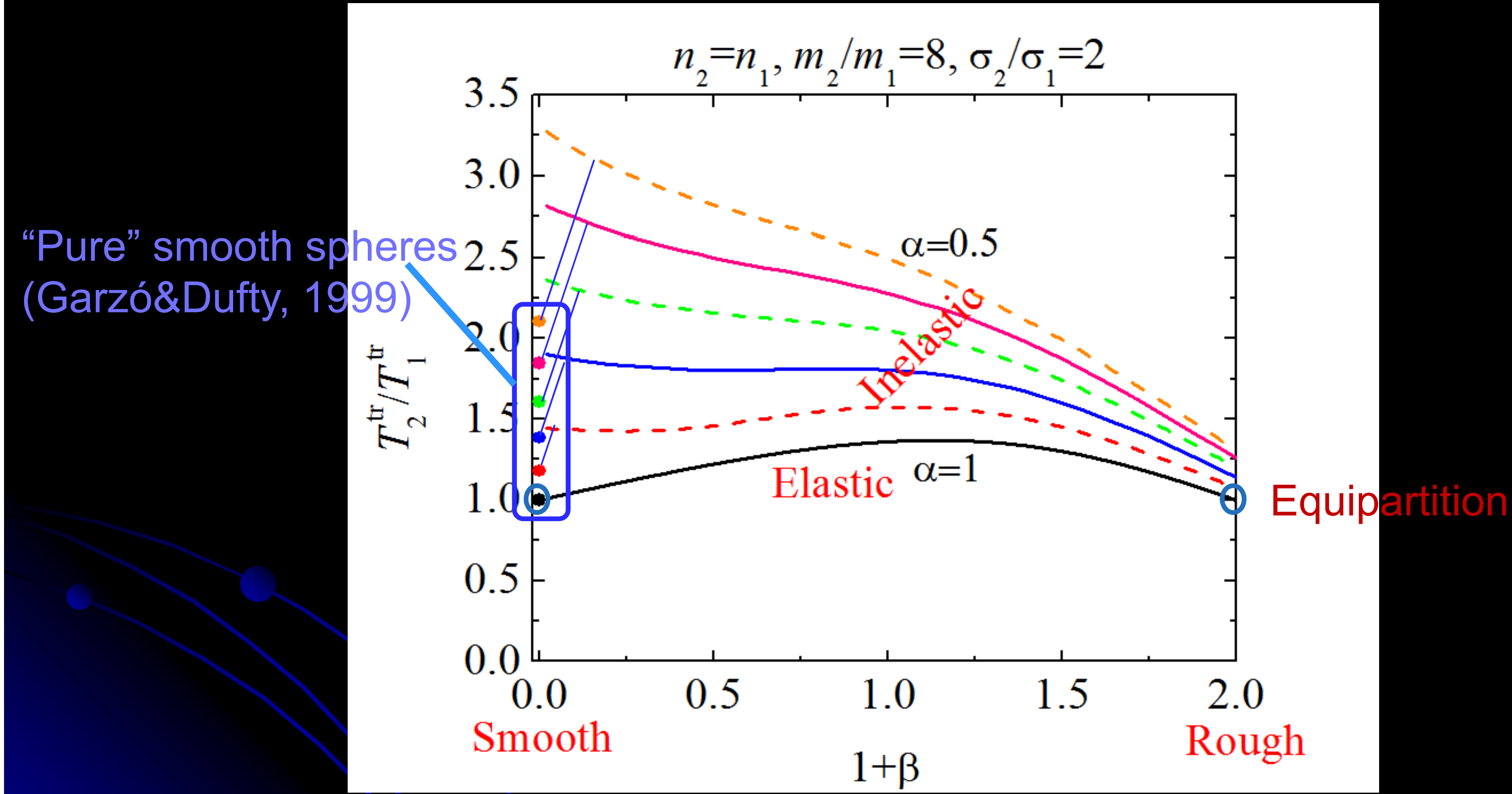
Translational/Rotational



Rotational/Rotational



Translational/Translational



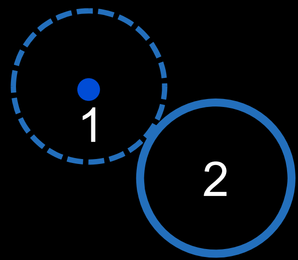
“Ghost” effect: A tiny amount of roughness has dramatic effects on the temperature ratio (enhancement of non-equipartition)

Binary mixture

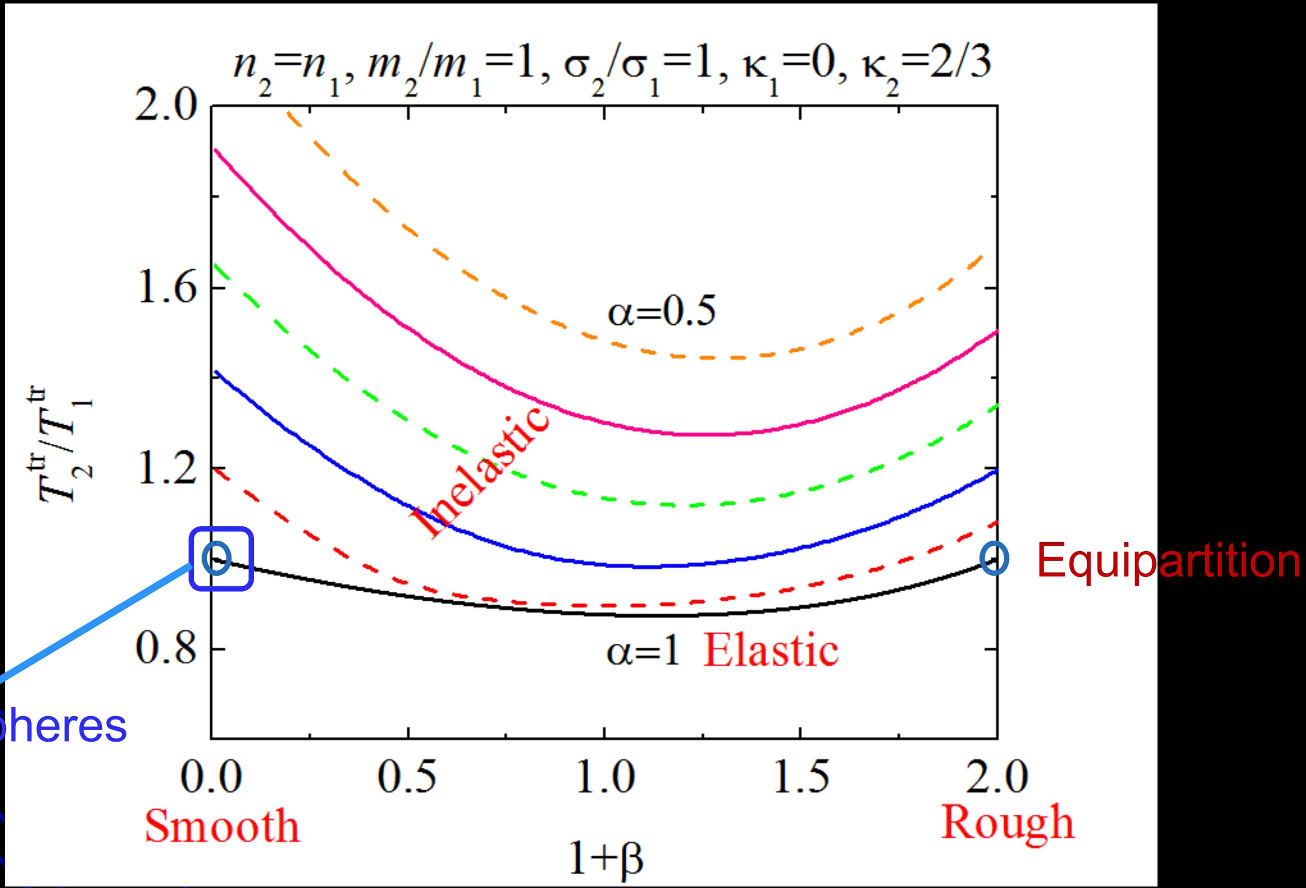
Three independent temperature ratios: $\frac{T_1^{\rm tr}}{T_1^{\rm rot}}, \frac{T_2^{\rm tr}}{T_1^{\rm tr}}, \frac{T_2^{\rm rot}}{T_1^{\rm rot}}$

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 $\kappa_1 = 0$, $\kappa_2 = \frac{2}{3}$
- Size ratio $\sigma_2/\sigma_1 = 1$
- Mass ratio $m_2/m_1 = 1$
- Mole fraction $n_1/(n_1+n_2) = \frac{1}{2}$



Translational/Translational



"Pure" smooth spheres

"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!