Non-equipartition of energy in homogeneous granular gases

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STATISTICAL PHYSICS in EXTREMADURA

*In collaboration with Gilberto M. Kremer and Vicente Garzó


航空工学教室
DEPARTMENT OF
AERONAUTICAL ENGINEERING

NONLINEAR TRANSPORT

IN THE COUETTE FLOW

OF A DILUTE GAS

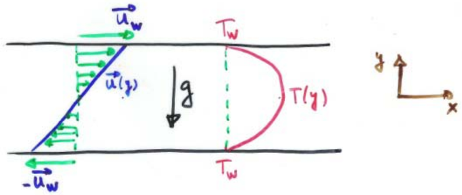
UNDER A GRAVITY FIELD

André's Santos

(University of Extremadura, Spain)

Kyoto, March 23 (1999)

PLANAR COUETTE FLOW



Assumptions:

* Rarefied gas
* Non-Newtonian regime

- Usually, one ignores the effect of gravity on the properties of the gas (at most, g is introduced in the momentum balance equations)

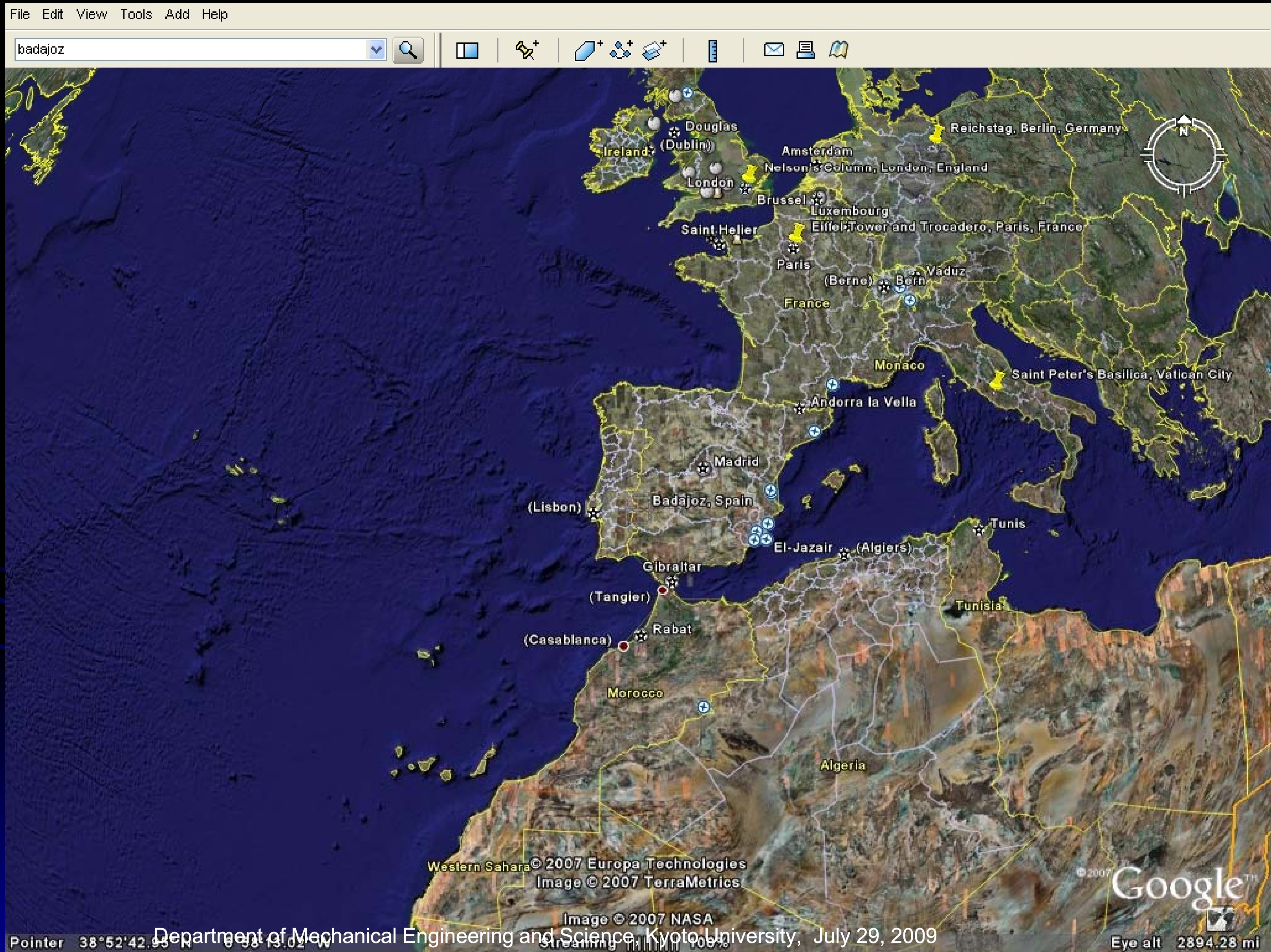
This is because, under ordinary conditions,

$$h \equiv \frac{2k_BT/m}{g} \gg \lambda$$

h: characteristic length associated with gravity; λ: mean free path

Air at room pressure and temperature: $\lambda/h \sim 10^{-11}$

- However, what if gravity and/or rarefaction are large enough as to make, say $\lambda/h \sim 10^{-3}$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badajoz
Douglas
(Dublin)
Ireland
London
Amsterdam
Reichstag, Berlin, Germany
Nelson's Column, London, England
Brussel
Luxembourg
Saint Helier
Eiffel Tower and Trocadero, Paris, France
Paris
Vaduz
(Berne)
Bern
France
Monaco
Saint Peter's Basilica, Vatican City
Andorra la Vella
Madrid
Badajoz, Spain
(Lisbon)
Tunis
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Outline

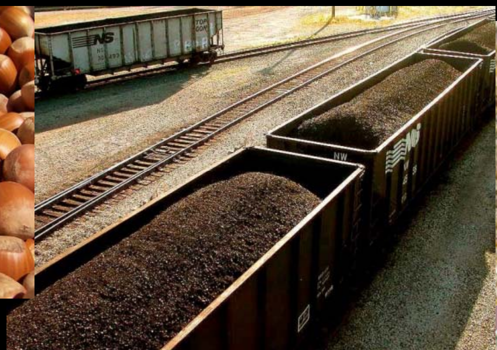
- What is a granular material?
- Mixture of inelastic rough hard spheres. The Boltzmann equation.
- Collisional thermal rates. Equilibration and cooling rates.
- Application to the homogeneous cooling state. Non-equipartition of energy.
- Simple kinetic model for monodisperse systems. Application to the uniform shear flow.
- 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.

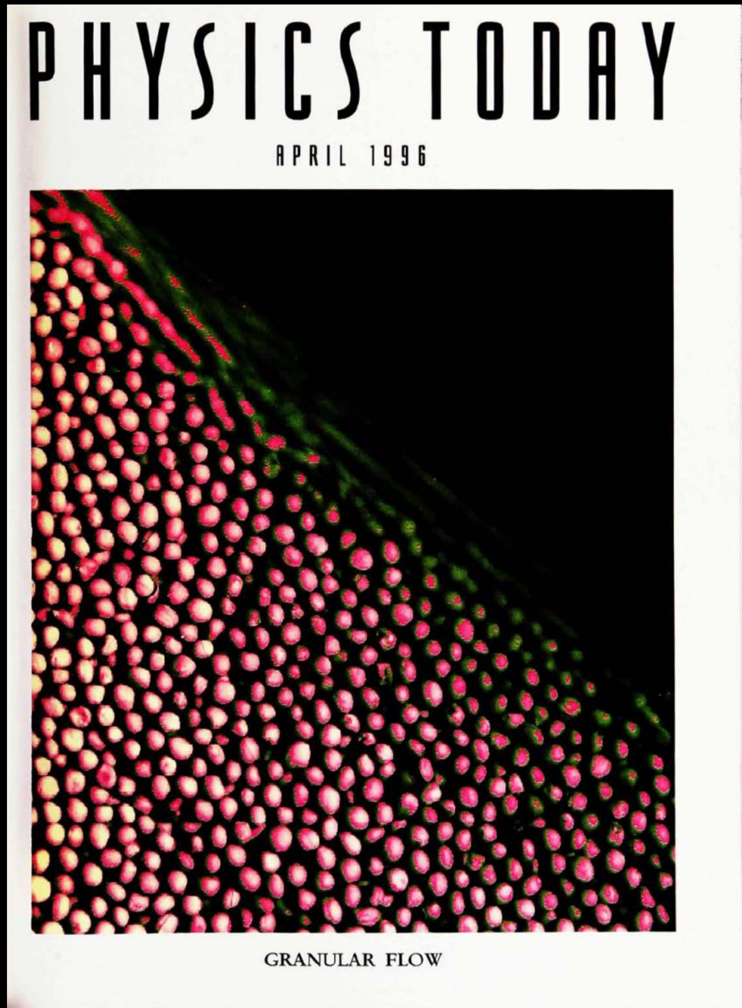



What is a granular material?

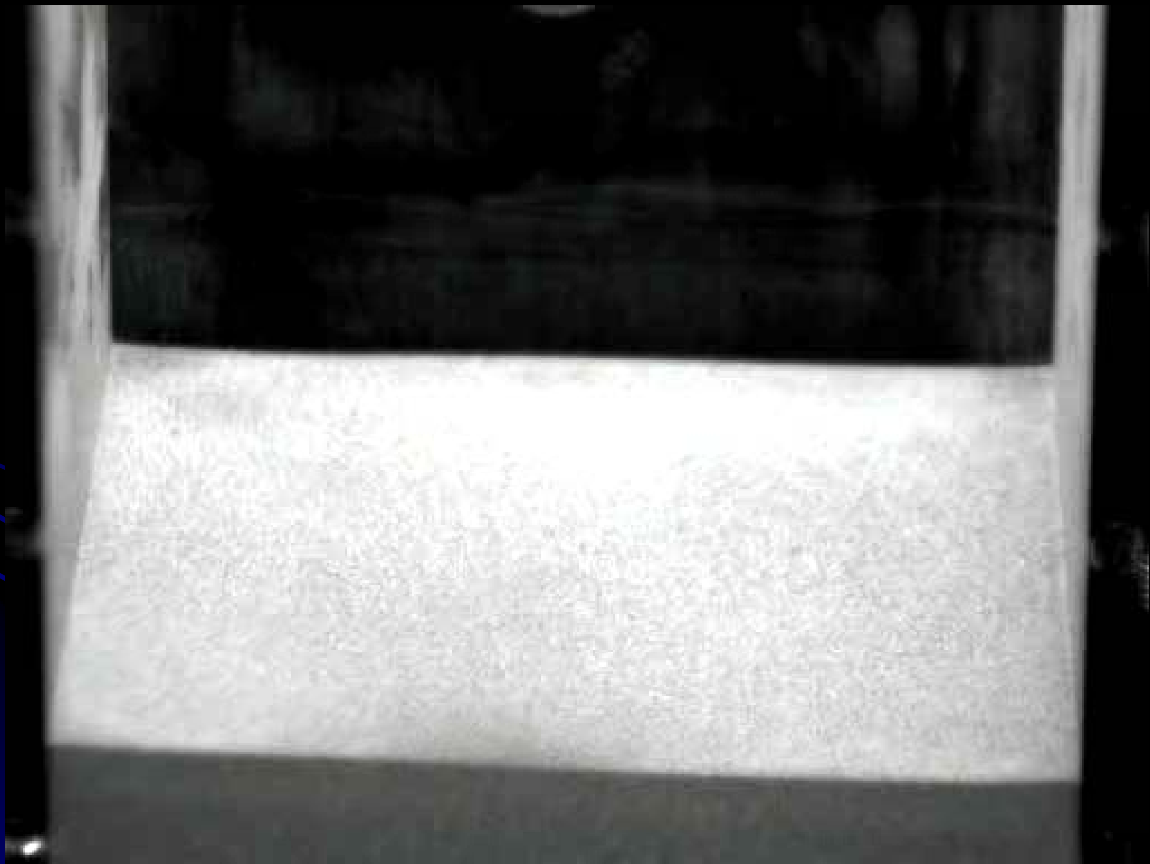
- Granular materials are commercially important in applications as diverse as pharmaceutical industry, agriculture, and energy production.
- They are ubiquitous in nature and are the second-most manipulated material in industry (the first one is water).

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*.

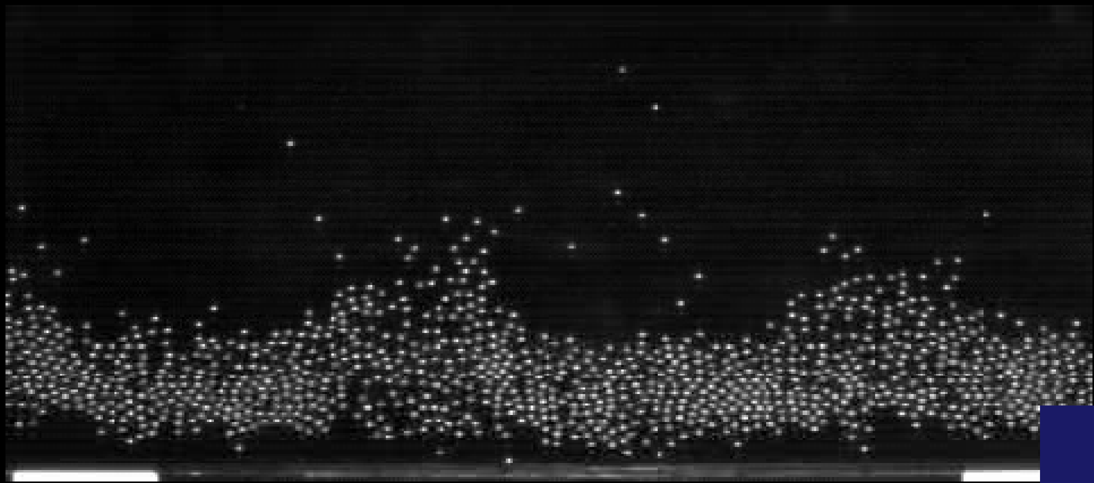


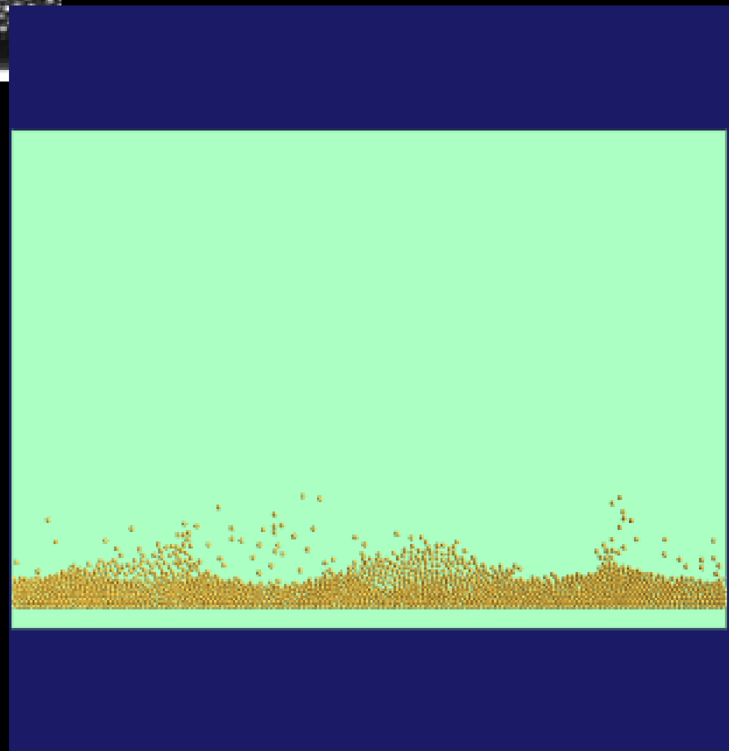
Granular fluids (or gases) exhibit many interesting phenomena:



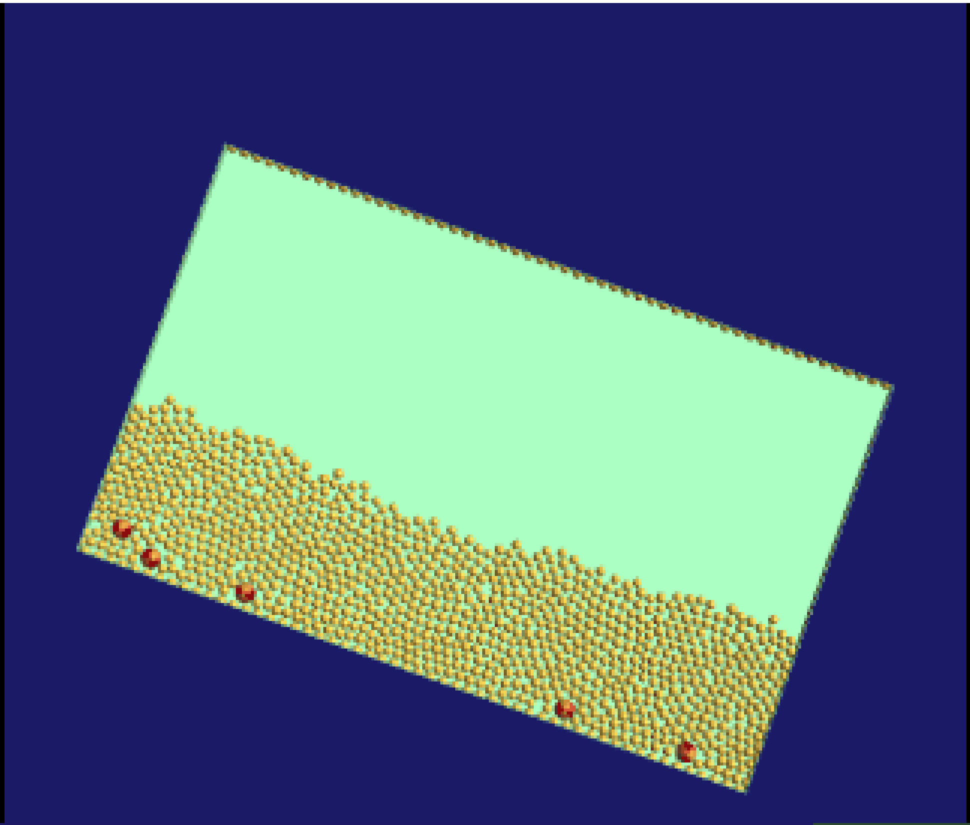
Granular eruptions (from University of Twente's group)

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

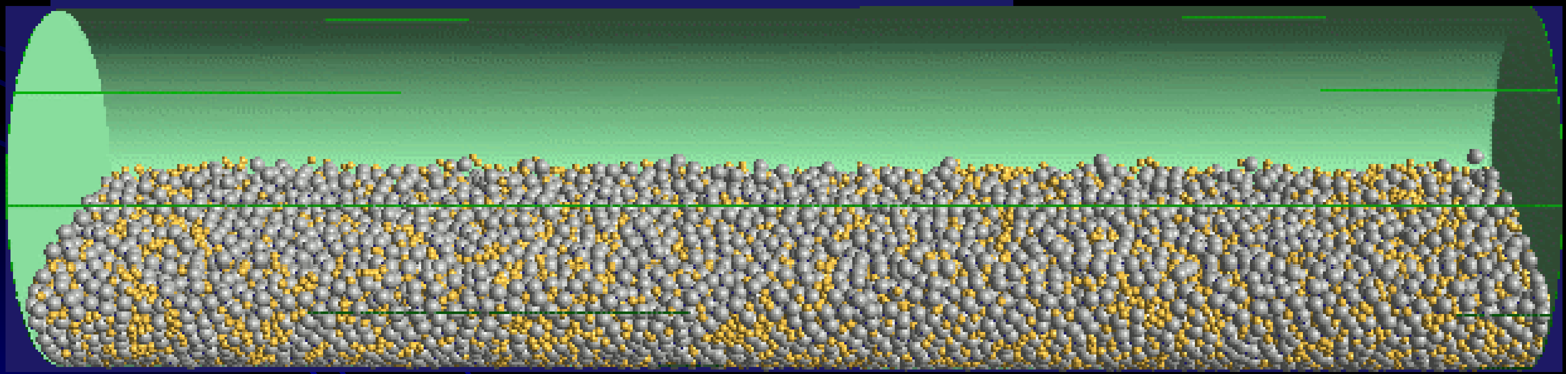




(Simulations by D. C. Rapaport)

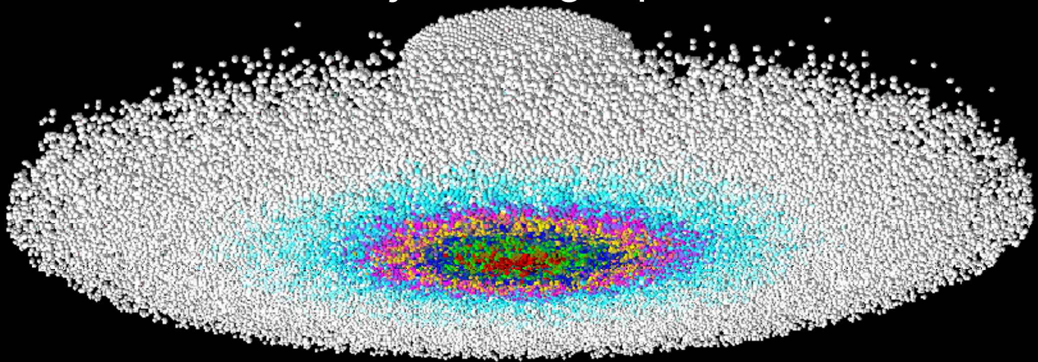


Segregation in sheared flow
(Simulations by D. C. Rapaport)

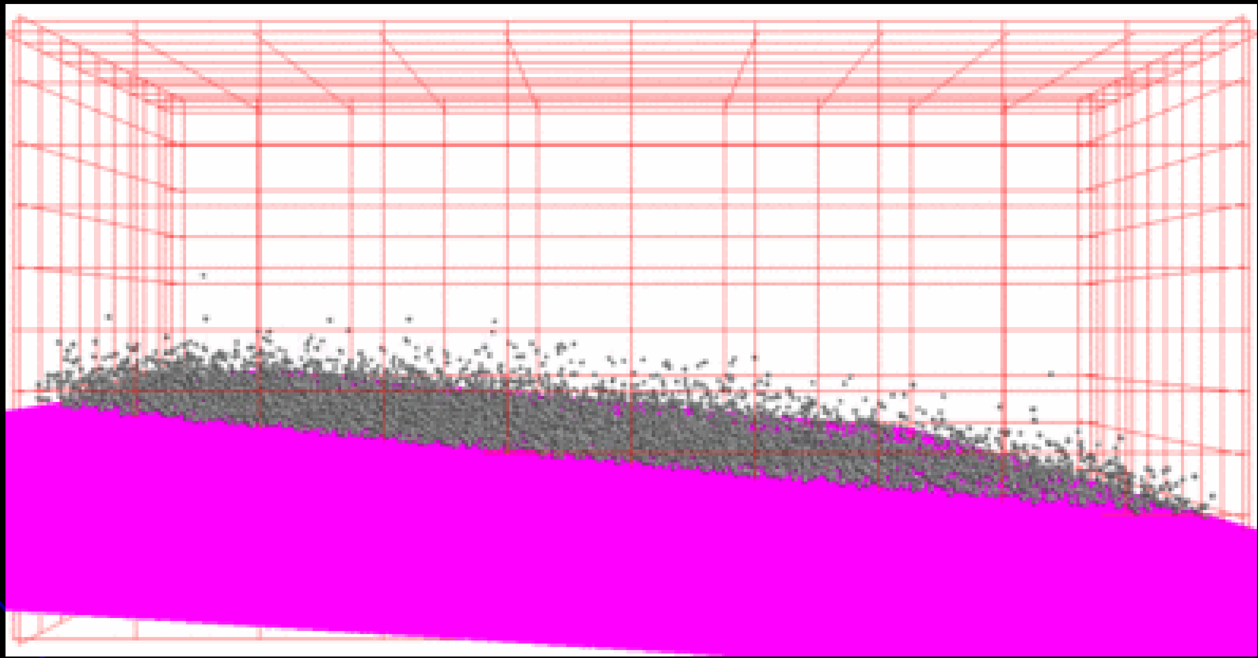


Segregation in a rotating cylinder
(Simulations by D. C. Rapaport)

Granular jet hitting a plane

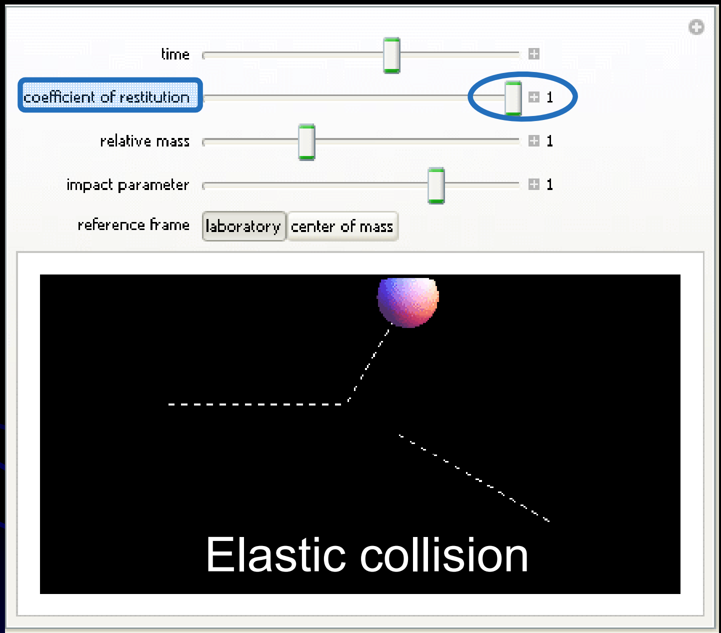


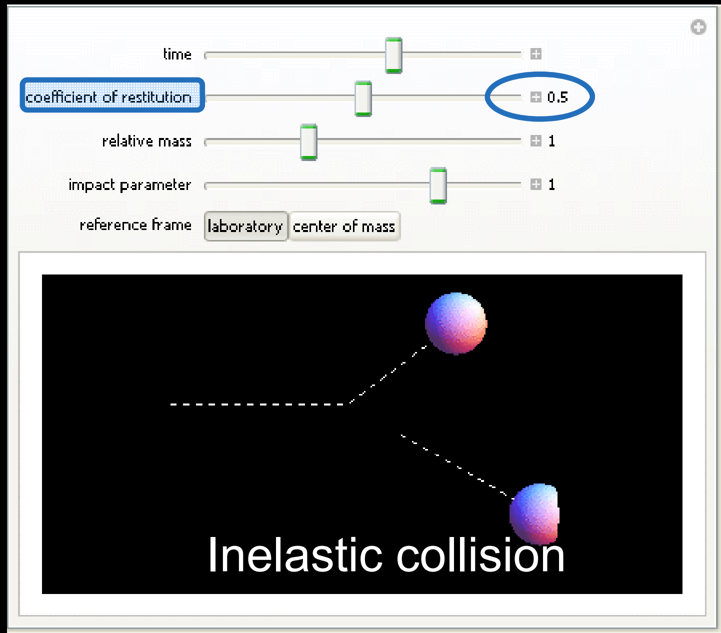
Particles falling on an inclined heated plane



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

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

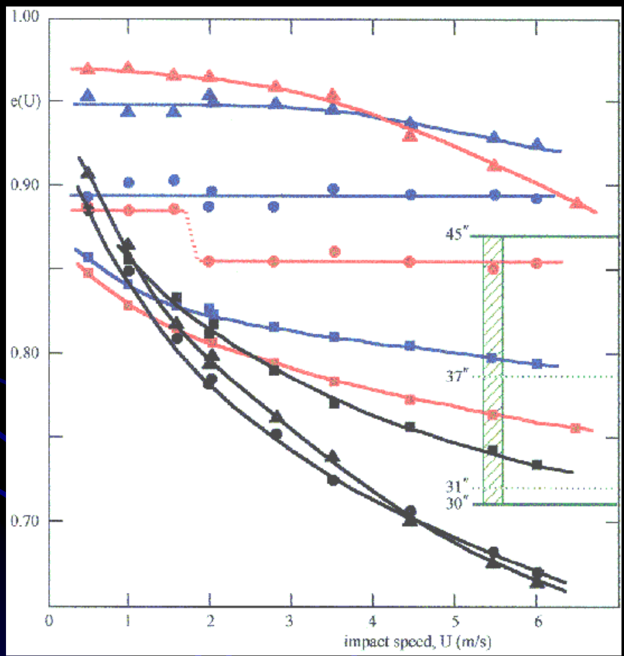


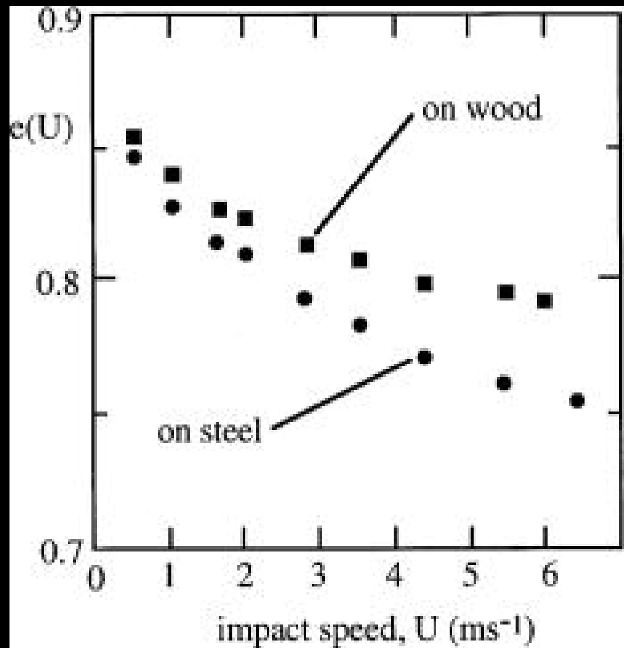


http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/

But … real grains

Have a non-constant coefficient of restitution





www.oxfordcroquet.com/tech/

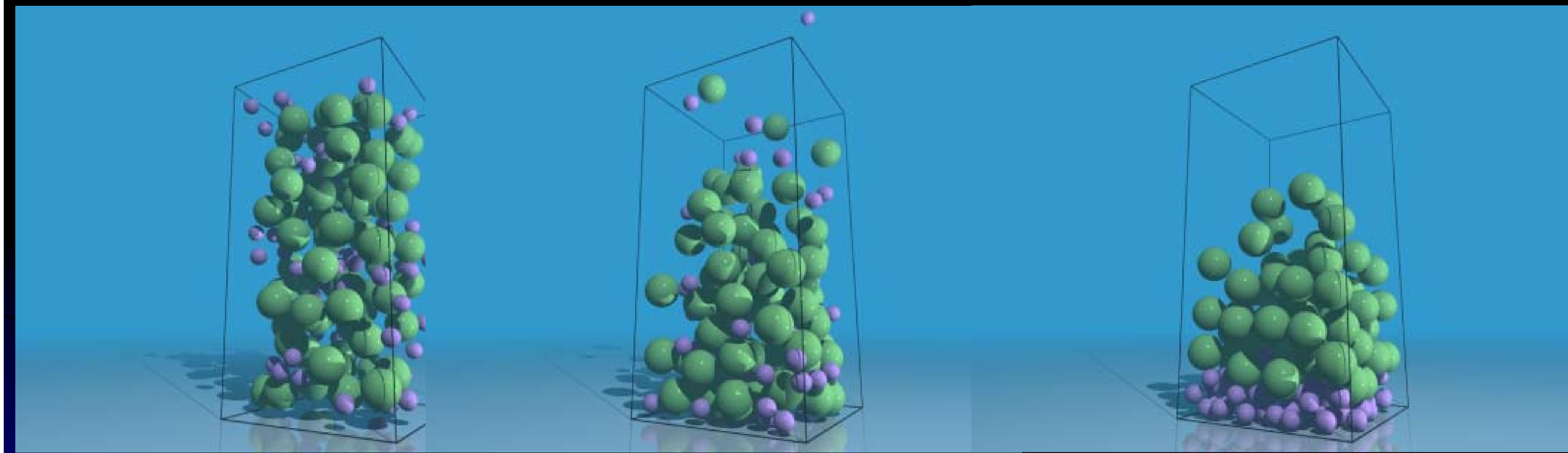
But … real grains

Are non-spherical




But … real grains

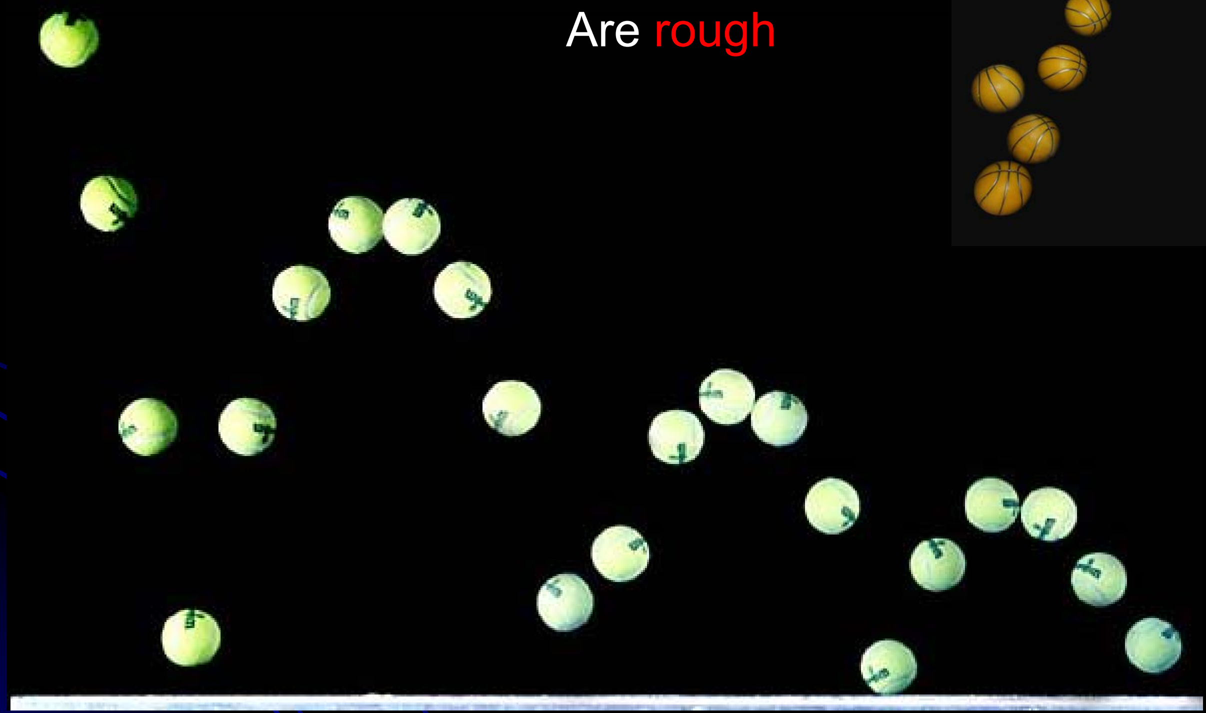
Are polydisperse



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

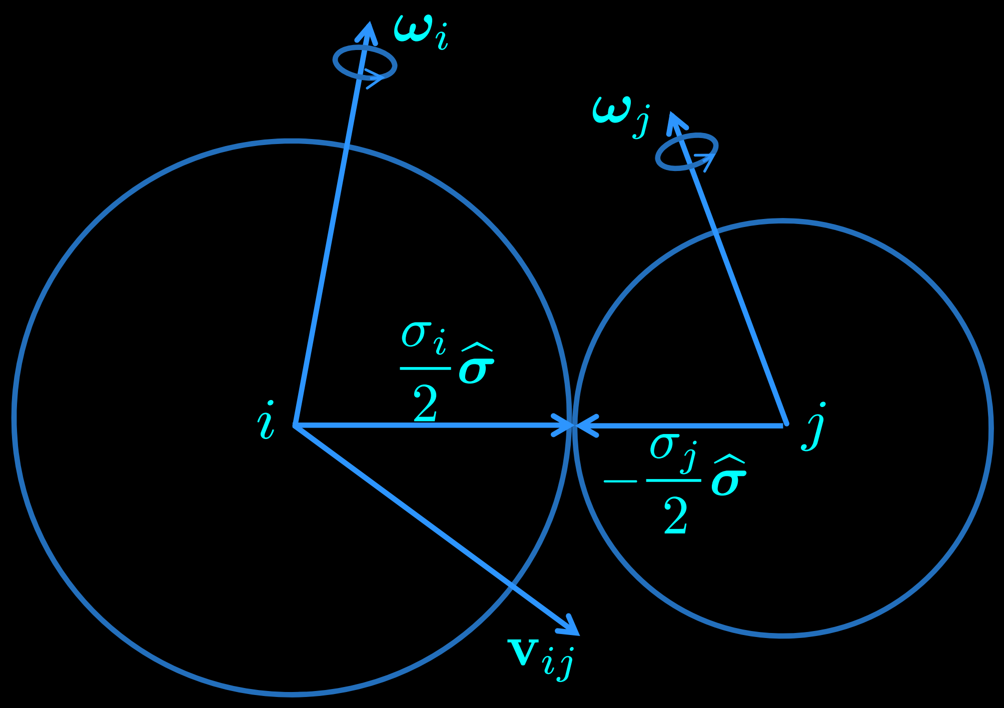
This model unveils an inherent breakdown of energy equipartition in granular fluids, even in homogeneous and isotropic states

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

Pre-collisional quantities



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:

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

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

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

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
  - perfectly smooth (β_{ij}=-1) or
  - perfectly rough (β_{ij}=+1)

Partial (granular) temperatures

Translational temperatures: $T_i^{\mathrm{tr}} = \frac{m_i}{3}\langle v_i^2 \rangle$

Rotational temperatures: $T_i^{\mathrm{rot}} = \frac{I_i}{3}\langle \omega_i^2 \rangle = \frac{m_i \kappa_i}{12}\sigma_i^2 \langle \omega_i^2 \rangle$

Total temperature: $T = \sum_i \frac{n_i}{2n}\left(T_i^{\mathrm{tr}} + T_i^{\mathrm{rot}}\right)$

Collisional rates of change for temperatures

Thermal rates:

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

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

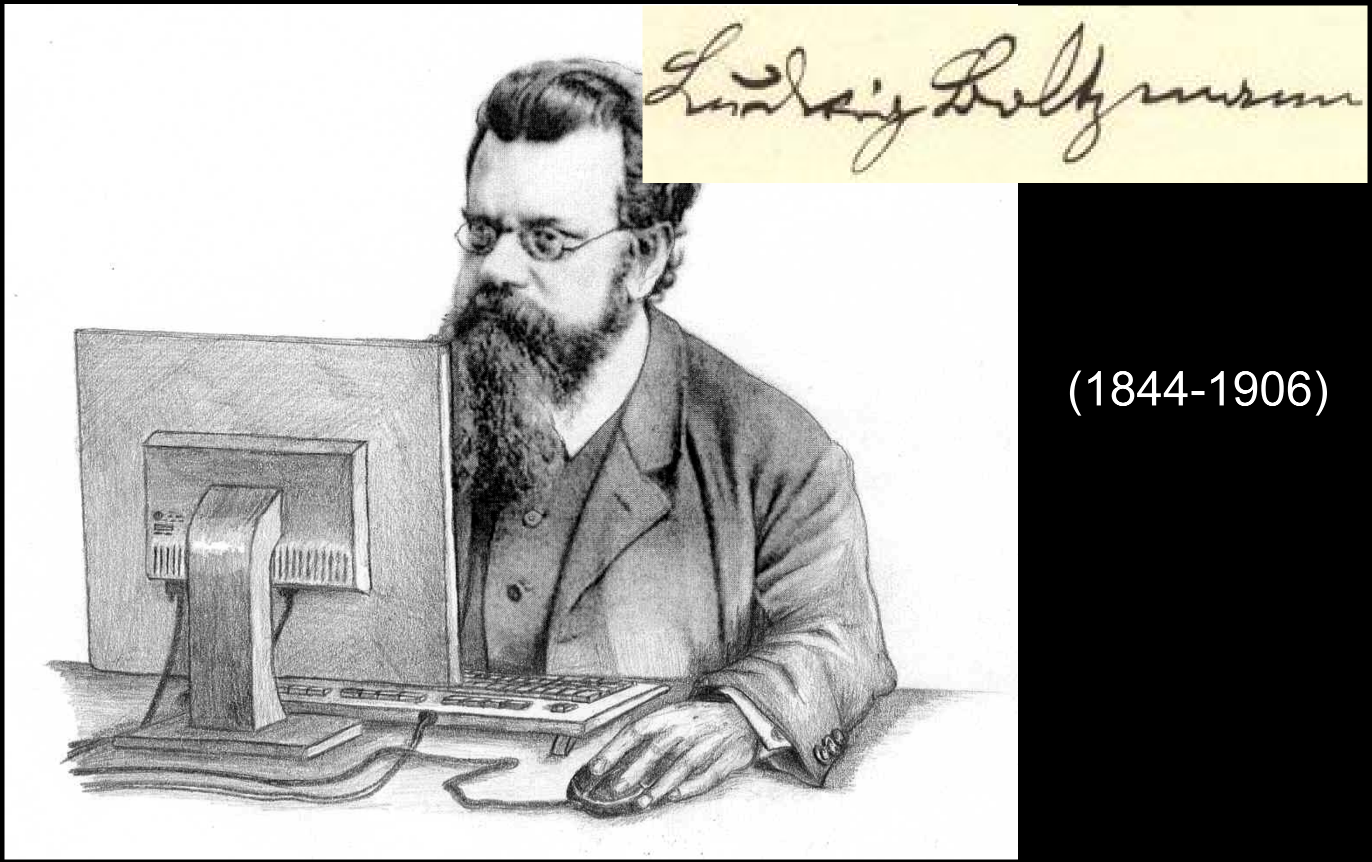
Net *cooling* rate:

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

Our main goal

To obtain the binary thermal rates
ξ_{ij}^{tr} and ξ_{ij}^{rot}
in terms of
$T_i^{\mathrm{tr}},\ T_j^{\mathrm{tr}},\ T_i^{\mathrm{rot}},\ T_j^{\mathrm{rot}},\ n_i,\ n_j$
and the mechanical parameters
$m_i,\ m_j,\ \sigma_i,\ \sigma_j,\ \kappa_i,\ \kappa_j,\ \alpha_{ij},\ \beta_{ij}$

(Cartoon by Bernhard Reischl, University of Vienna)



(1844-1906)

Boltzmann equation:

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

“Exact” results

$$\xi_{ij}^{\mathrm{tr}} = \frac{n_j\sigma_{ij}^2\pi}{3T_i^{\mathrm{tr}}}\Bigg[\left(\overline{\alpha}_{ij}+\overline{\beta}_{ij}\right)\langle v_{ij}\mathbf{v}_i\cdot\mathbf{v}_{ij}\rangle + \frac{2\overline{\beta}_{ij}}{3}\langle(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j)\cdot(\mathbf{v}_i\times\mathbf{v}_j)\rangle$$
$$-\frac{\overline{\alpha}_{ij}^2+\overline{\beta}_{ij}^2}{2m_i}\langle v_{ij}^3\rangle - \frac{\overline{\beta}_{ij}^2}{16m_i}\langle v_{ij}^{-1}\left[\mathbf{v}_{ij}\cdot(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j)\right]^2\rangle - \frac{3\overline{\beta}_{ij}^2}{16m_i}\langle v_{ij}\left(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j\right)^2\rangle\Bigg]$$

$$\xi_{ij}^{\mathrm{rot}} = \frac{n_j\sigma_{ij}^2\pi}{24T_i^{\mathrm{rot}}}\overline{\beta}_{ij}\Bigg\{3\sigma_i\langle v_{ij}\left[\boldsymbol{\omega}_i\cdot(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j)\right]\rangle - \sigma_i\langle v_{ij}^{-1}\left[\mathbf{v}_{ij}\cdot(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j)\right](\mathbf{v}_{ij}\cdot\boldsymbol{\omega}_i)\rangle$$
$$-\frac{\overline{\beta}_{ij}}{m_i\kappa_i}\left[4\langle v_{ij}^3\rangle + \frac{3}{2}\langle v_{ij}\left(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j\right)^2\rangle - \frac{1}{2}\langle v_{ij}^{-1}\left[\mathbf{v}_{ij}\cdot(\sigma_i\boldsymbol{\omega}_i+\sigma_j\boldsymbol{\omega}_j)\right]^2\rangle\right]\Bigg\}$$

Additional assumptions

1. No mutual diffusion, 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

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

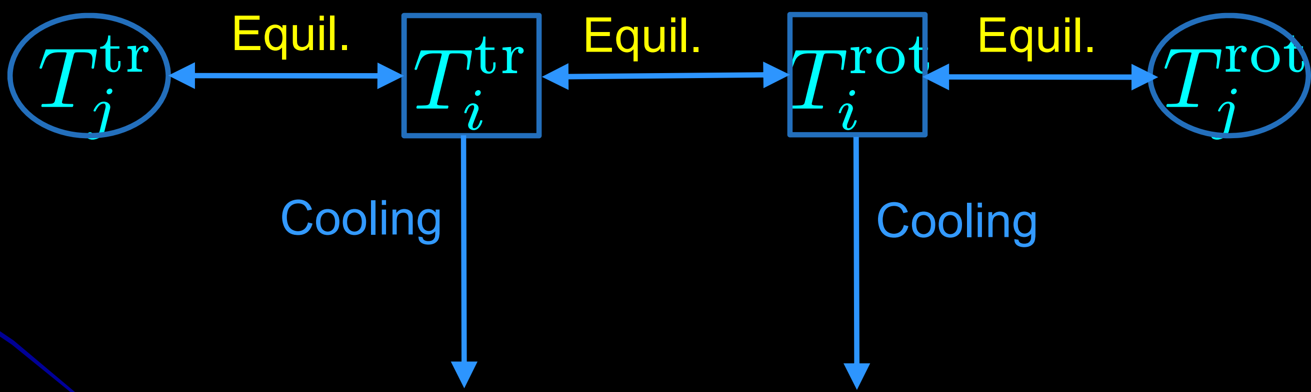
$$\xi_{ij}^{\mathrm{rot}} = \frac{\nu_{ij}}{m_i \kappa_i T_i^{\mathrm{rot}}} \overline{\beta}_{ij} \left[2T_i^{\mathrm{rot}} - \overline{\beta}_{ij}\left(\frac{T_i^{\mathrm{tr}}}{m_i} + \frac{T_j^{\mathrm{tr}}}{m_j} + \frac{T_i^{\mathrm{rot}}}{m_i \kappa_i} + \frac{T_j^{\mathrm{rot}}}{m_j \kappa_j}\right)\right]$$

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

Decomposition

Thermal rates = Equilibration rates + Cooling rates

Net cooling rate = Σ Cooling rates



Decomposition

$$\xi_{ij}^{\mathrm{tr}} = \xi_{ij}^{\mathrm{tr},\alpha} + \xi_{ij}^{\mathrm{tr},\beta} + \zeta_{ij}^{\mathrm{tr}} + \kappa_i \frac{T_i^{\mathrm{rot}}}{T_i^{\mathrm{tr}}} \xi_{ij}^{\mathrm{rot}}$$

$$\xi_{ij}^{\mathrm{rot}} = \xi_{ij}^{\mathrm{rot},\beta} + \zeta_{ij}^{\mathrm{rot}}$$

Thermal rates

$$\xi_{ij}^{\mathrm{tr},\alpha} \propto (1+\alpha_{ij})(T_i^{\mathrm{tr}} - T_j^{\mathrm{tr}})$$

$$\xi_{ij}^{\mathrm{tr},\beta} \propto (1+\beta_{ij})(T_i^{\mathrm{tr}} - T_i^{\mathrm{rot}})$$

$$\xi_{ij}^{\mathrm{rot},\beta} \propto (1+\beta_{ij}) \left\{ T_i^{\mathrm{rot}} - T_j^{\mathrm{rot}}, T_i^{\mathrm{tr}} - T_j^{\mathrm{tr}}, T_i^{\mathrm{tr}} - T_i^{\mathrm{rot}} \right\}$$

Equilibration rates

$$\zeta_{ij}^{\mathrm{tr}} \propto (1-\alpha_{ij}^2)$$

$$\zeta_{ij}^{\mathrm{rot}} \propto (1-\beta_{ij}^2)$$

Cooling rates

Net cooling rate

$$\zeta = \sum_i \frac{n_i}{2nT}\left(\xi_i^{\mathrm{tr}} T_i^{\mathrm{tr}} + \xi_i^{\mathrm{rot}} T_i^{\mathrm{rot}}\right)$$

$$\zeta = \sum_{ij} \frac{n_i \nu_{ij}}{4nT} \frac{m_i m_j}{m_i + m_j} \left[(1 - \alpha_{ij}^2) \left(\frac{T_i^{\mathrm{tr}}}{m_i} + \frac{T_j^{\mathrm{tr}}}{m_j} \right) + \frac{\kappa_{ij}}{1+\kappa_{ij}} (1 - \beta_{ij}^2) \left(\frac{T_i^{\mathrm{tr}}}{m_i} + \frac{T_j^{\mathrm{tr}}}{m_j} + \frac{T_i^{\mathrm{rot}}}{m_i \kappa_i} + \frac{T_j^{\mathrm{rot}}}{m_j \kappa_j} \right) \right]$$

Simple application: The Homogeneous Cooling State (HCS)

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

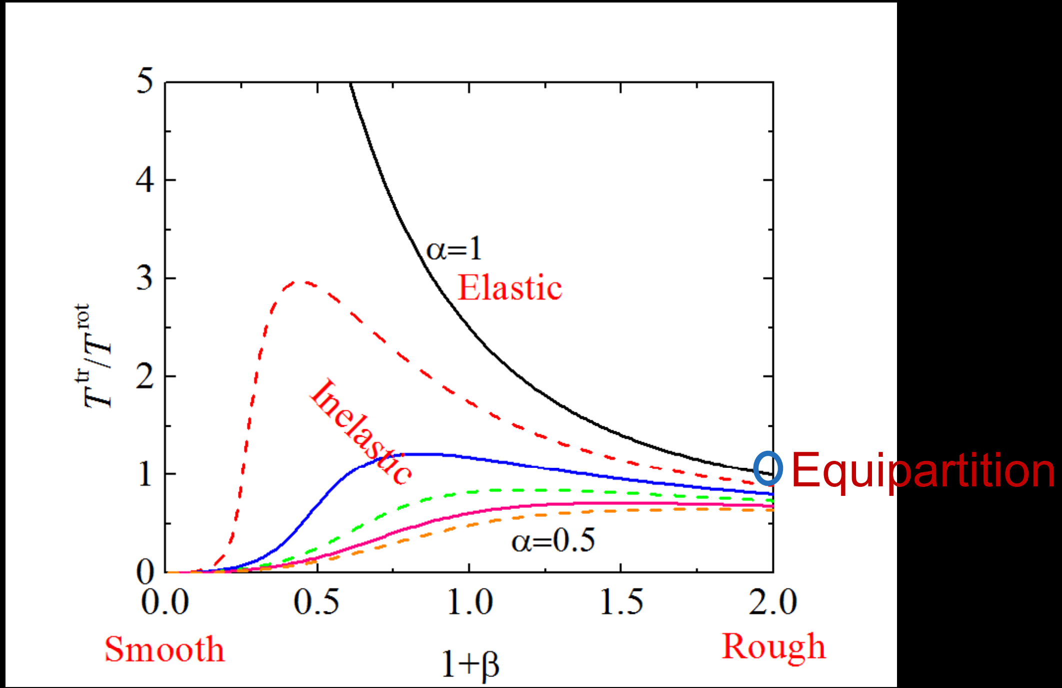
$$\partial_t f_i(\mathbf{v}_i, \boldsymbol{\omega}_i, t) = \sum_j J_{ij}[\mathbf{v}_i, \boldsymbol{\omega}_i, t | f_i, f_j]$$

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

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

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

Single-component case (κ=2/5)



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

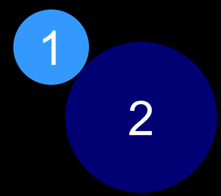
$$\left.\begin{array}{l}\alpha = 1 \\ \beta \to -1\end{array}\right\} \Rightarrow \left\{\begin{array}{l}\xi^{tr} \sim \kappa(1+\beta) \Rightarrow \partial_t T^{tr} < 0 \\ \xi^{rot} \sim (1+\beta) \Rightarrow \partial_t T^{rot} < 0\end{array}\right\} \Rightarrow \xi^{tr} < \xi^{rot} \Rightarrow \boxed{\frac{T^{tr}}{T^{rot}}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

Binary mixture

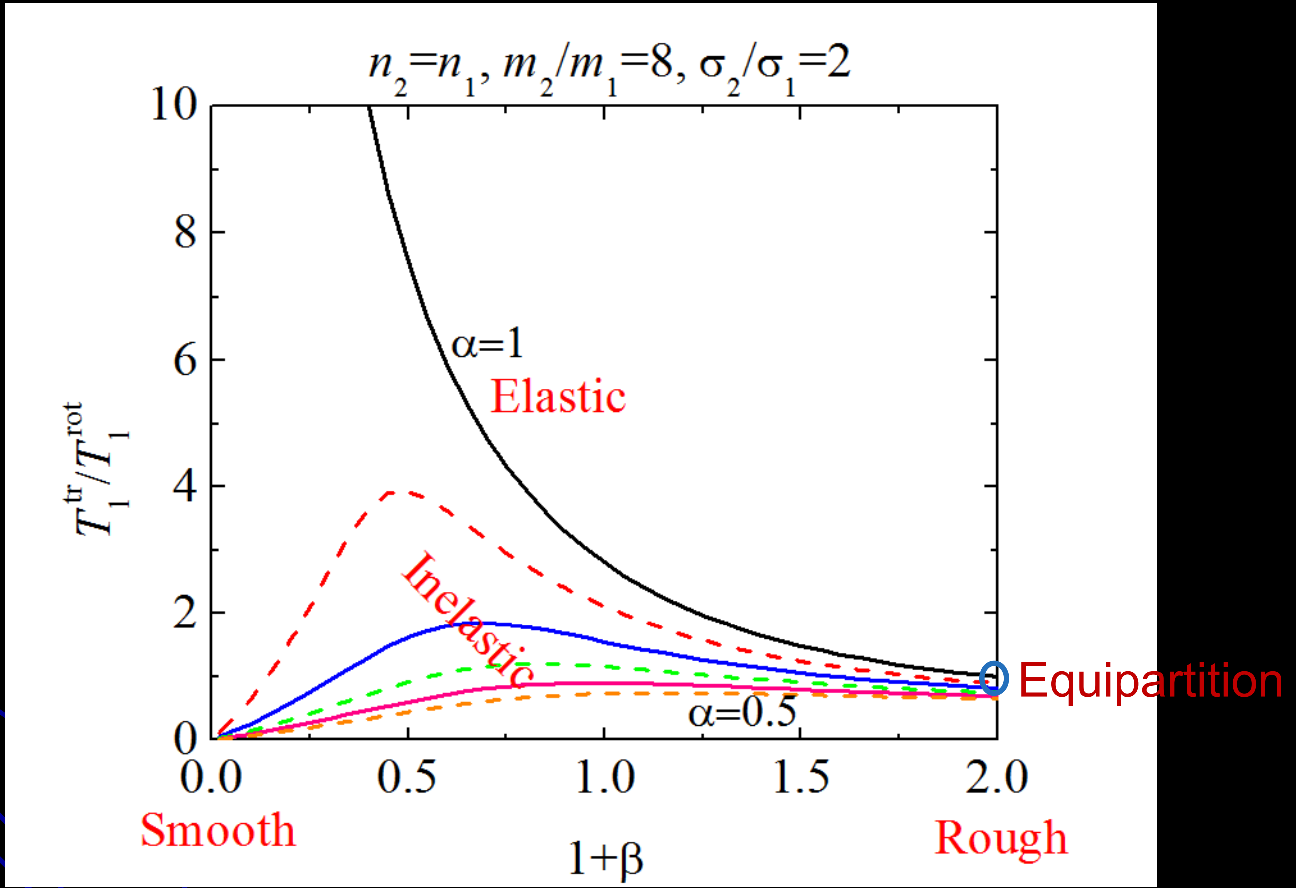
Three independent temperature ratios: $\frac{T_1^{\mathrm{tr}}}{T_1^{\mathrm{rot}}}, \frac{T_2^{\mathrm{tr}}}{T_1^{\mathrm{tr}}}, \frac{T_2^{\mathrm{rot}}}{T_1^{\mathrm{rot}}}$

Eleven parameters:

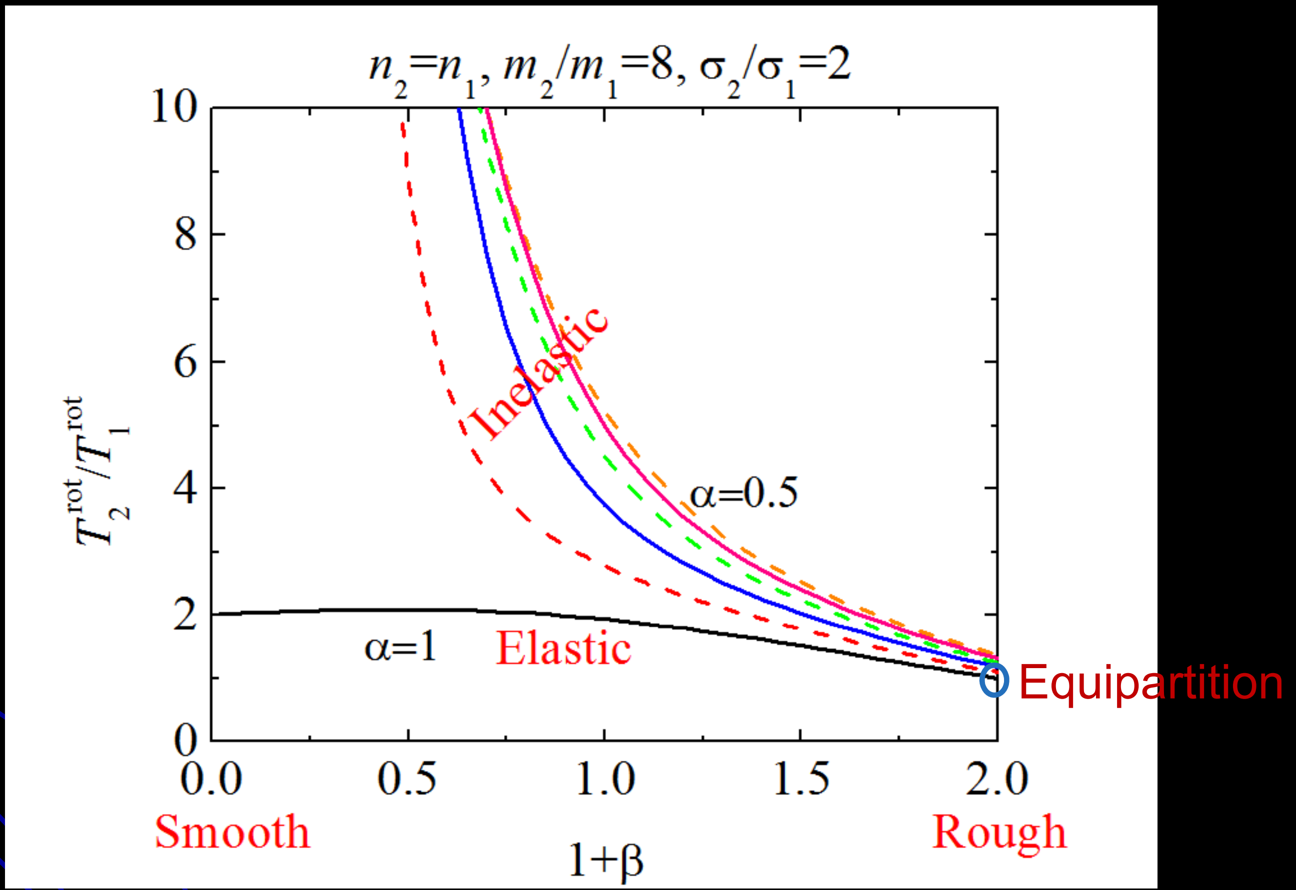
- Coefficients of normal restitution $\alpha_{11}=\alpha_{12}=\alpha_{22}=\alpha$
- Coefficients of tangential restitution $\beta_{11}=\beta_{12}=\beta_{22}=\beta$
- Inertia-moment parameters $\kappa_1=\kappa_2=\frac{2}{5}$
- Size ratio $\sigma_2/\sigma_1=2$
- Mass ratio $m_2/m_1=8$
- Mole fraction $n_1/(n_1+n_2)=\frac{1}{2}$



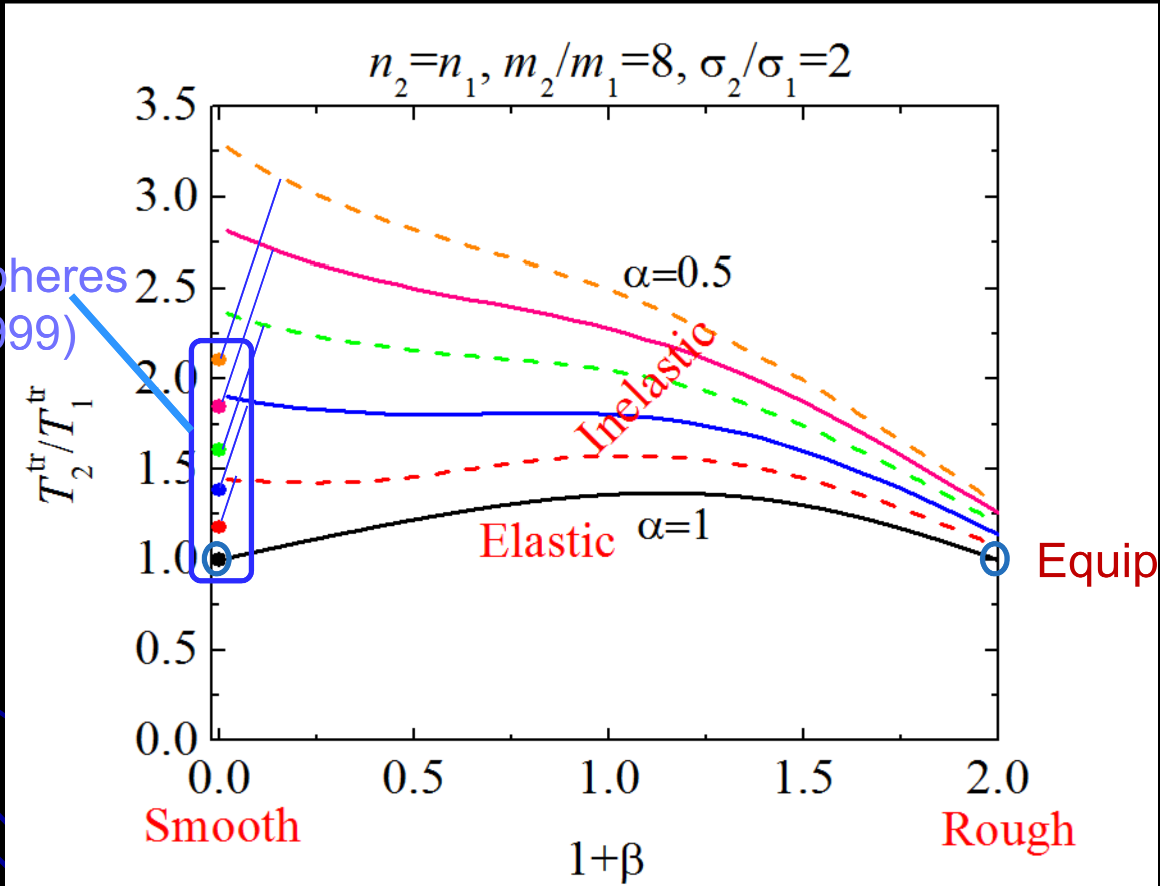
Translational/Rotational



Rotational/Rotational



Translational/Translational



“Pure” smooth spheres (Garzó&Dufty, 1999)

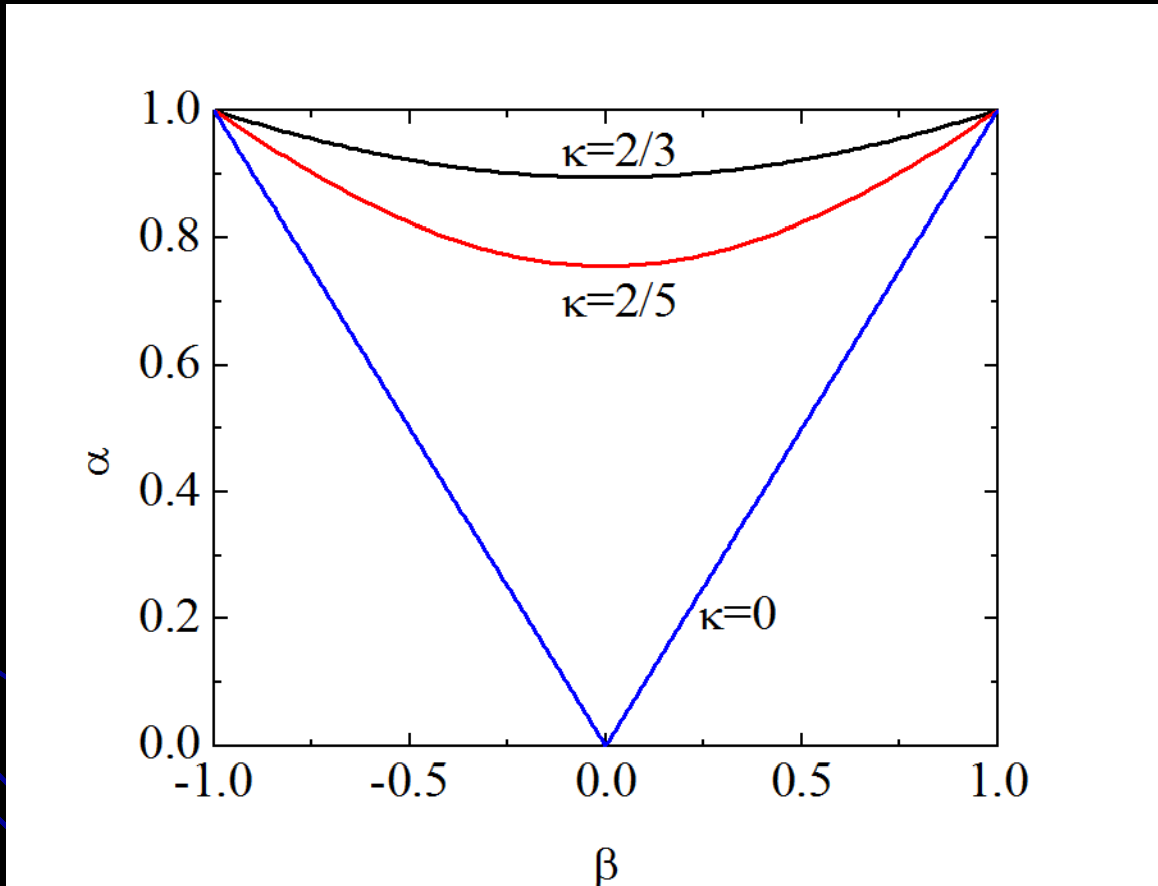
Equipartition

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

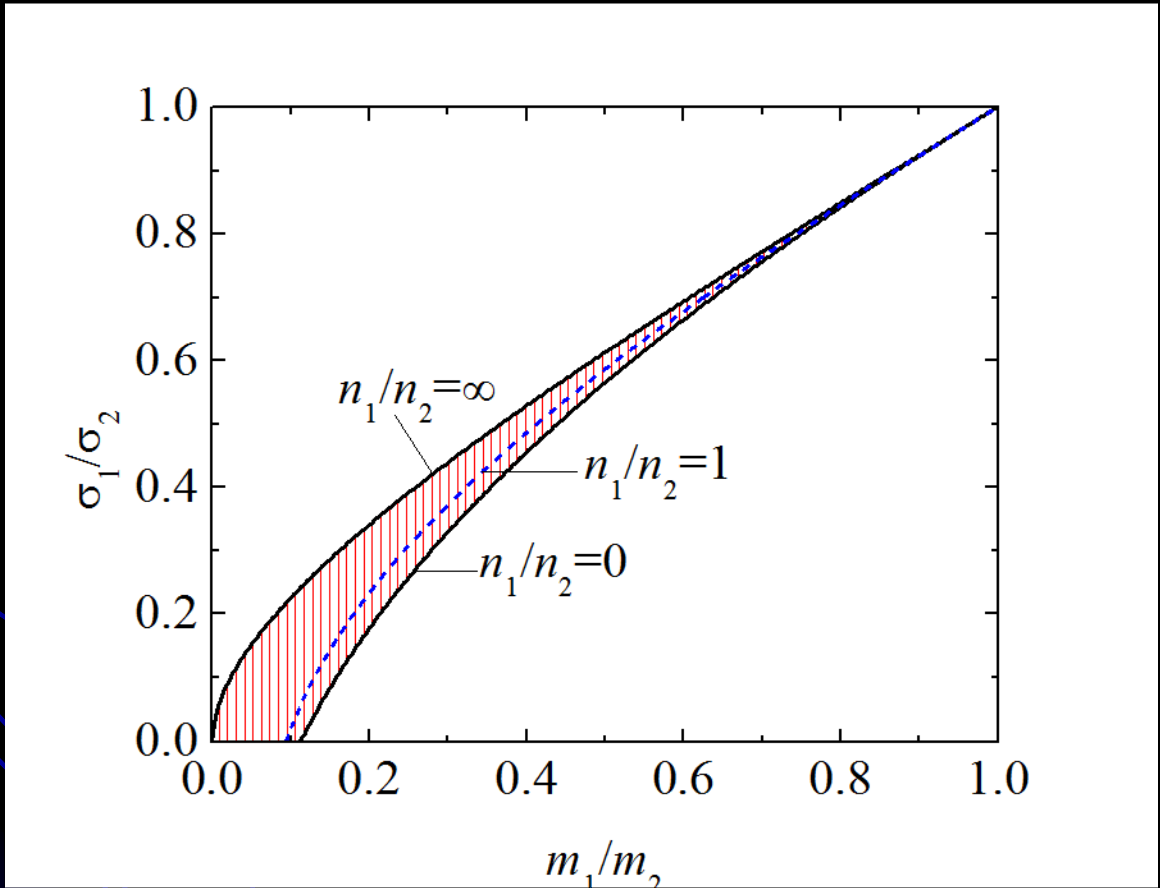
Locus of equipartition: Under which conditions does equipartition hold?

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

First condition: $1-\alpha^2 = \frac{1-\kappa}{1+\kappa}(1-\beta^2)$



Second condition: $$\frac{n_1}{n_2} = \frac{\sigma_{12}^2\sqrt{\frac{m_2}{m_1}} - \sigma_2^2\sqrt{\frac{m_1+m_2}{2m_2}}}{\sigma_{12}^2\sqrt{\frac{m_1}{m_2}} - \sigma_1^2\sqrt{\frac{m_1+m_2}{2m_1}}}$$



Simple kinetic model for *monodisperse* inelastic rough hard spheres

Three key ingredients we want to keep:

1. $(\partial_t T^{\rm tr})_{\rm coll} = -\xi^{\rm tr} T^{\rm tr}$
2. $(\partial_t T^{\rm rot})_{\rm coll} = -\xi^{\rm rot} T^{\rm rot}$

3. $$\int d\mathbf{v}_i \int d\boldsymbol{\omega}_i\, \mathbf{v}_i J_{ij}[\mathbf{v}_i, \boldsymbol{\omega}_i | f_i, f_j] = \frac{1+\alpha_{ij}+\beta_{ij}\kappa_{ij}/(1+\kappa_{ij})}{2} \times \int d\mathbf{v}_i \int d\boldsymbol{\omega}_i\, \mathbf{v}_i J_{ij}[\mathbf{v}_i, \boldsymbol{\omega}_i | f_i, f_j]\Big|_{\substack{\alpha_{ij}=1\\ \beta_{ij}=-1}}$$

Elastic smooth spheres

$$\partial_t f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) + \mathbf{v}\cdot\nabla f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) = J[\mathbf{r},\mathbf{v},\boldsymbol{\omega},t|f,f]$$

$$\begin{aligned} J[f,f] \;\rightarrow\; & -\lambda\nu_0\,(f - f_0) \\ & +\frac{\xi^{\mathrm{tr}}}{2}\frac{\partial}{\partial\mathbf{v}}\cdot[(\mathbf{v}-\mathbf{u})f] + \frac{\xi^{\mathrm{rot}}}{2}\frac{\partial}{\partial\boldsymbol{\omega}}\cdot(\boldsymbol{\omega} f) \end{aligned}$$

$$\lambda \equiv \frac{1+\alpha}{2} + \frac{\kappa}{1+\kappa}\frac{1+\beta}{2}, \quad \nu_0 = \frac{16\sqrt{\pi}}{5} n\sigma^2\sqrt{T^{\mathrm{tr}}/m}$$

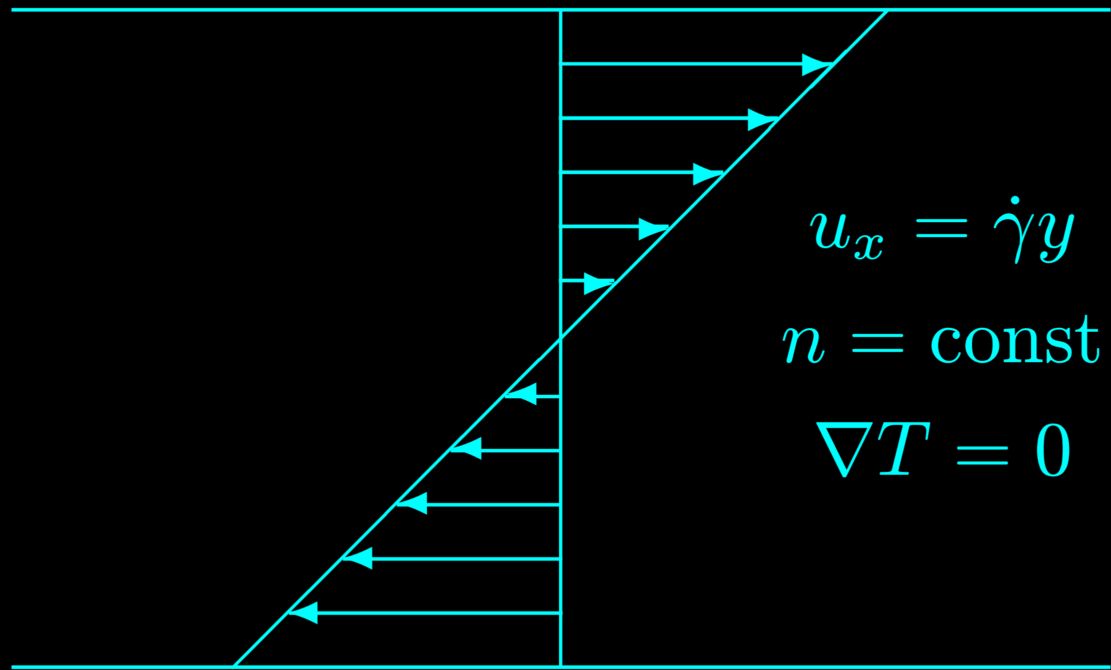
$$f_0 = n\left(\frac{mI}{4\pi^2 T^{\mathrm{tr}} T^{\mathrm{rot}}}\right)^{3/2} \exp\left[-\frac{m(\mathbf{v}-\mathbf{u})^2}{2T^{\mathrm{tr}}} - \frac{I\omega^2}{2T^{\mathrm{rot}}}\right]$$

An even simpler version …

$$
\left\{
\begin{aligned}
\partial_t f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t) + \mathbf{v}\cdot\nabla f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t) \;&=\; -\lambda\nu_0\left[f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t) - f_0^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t)\right] \\
&\quad + \frac{\xi^{\mathrm{tr}}}{2}\frac{\partial}{\partial \mathbf{v}}\cdot\left[(\mathbf{v}-\mathbf{u})f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t)\right] \\
\partial_t T^{\mathrm{rot}} + \nabla\cdot\left(\mathbf{u}\,T^{\mathrm{rot}}\right) &= -\xi^{\mathrm{rot}} T^{\mathrm{rot}}
\end{aligned}
\right.
$$

Application to simple shear flow

$y = +L/2$



$$u_x = \dot{\gamma} y$$

$$n = \text{const}$$

$$\nabla T = 0$$

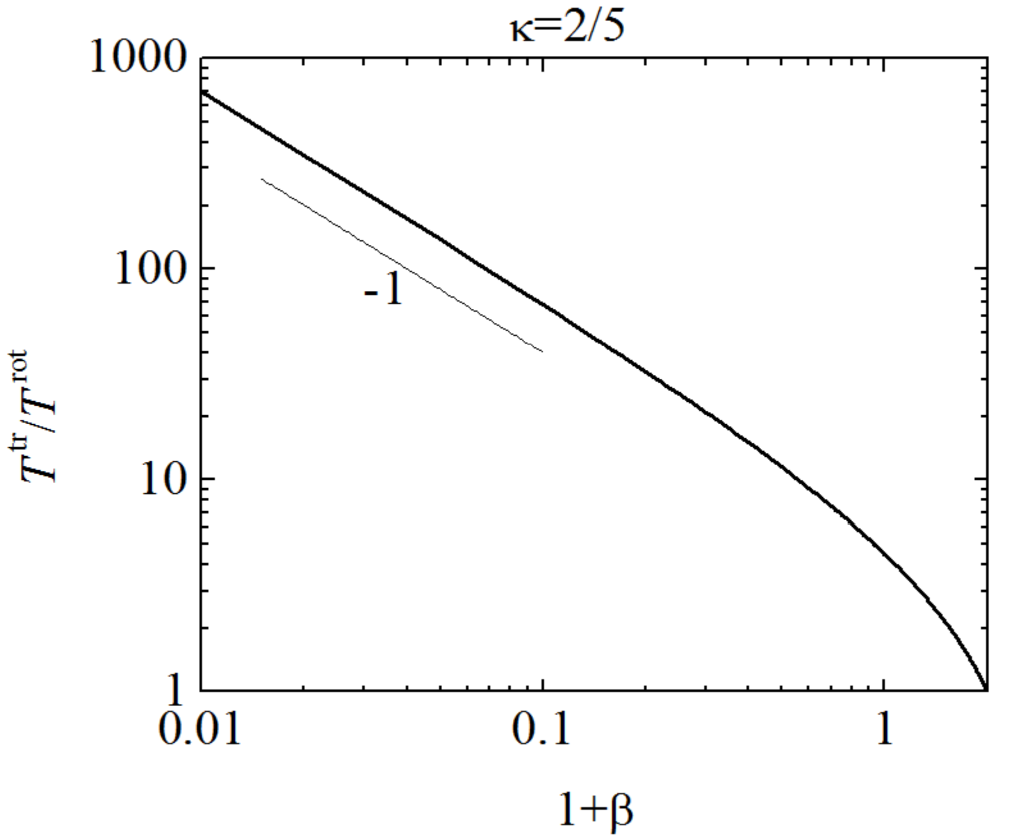
$y = -L/2$

Application to simple shear flow

Translational/Rotational temperature ratio

$$\xi^{\rm rot} = 0 \Rightarrow \boxed{\frac{T^{\rm rot}}{T^{\rm tr}} = \frac{\kappa(1+\beta)}{2\kappa+1-\beta}}$$

Independent of α



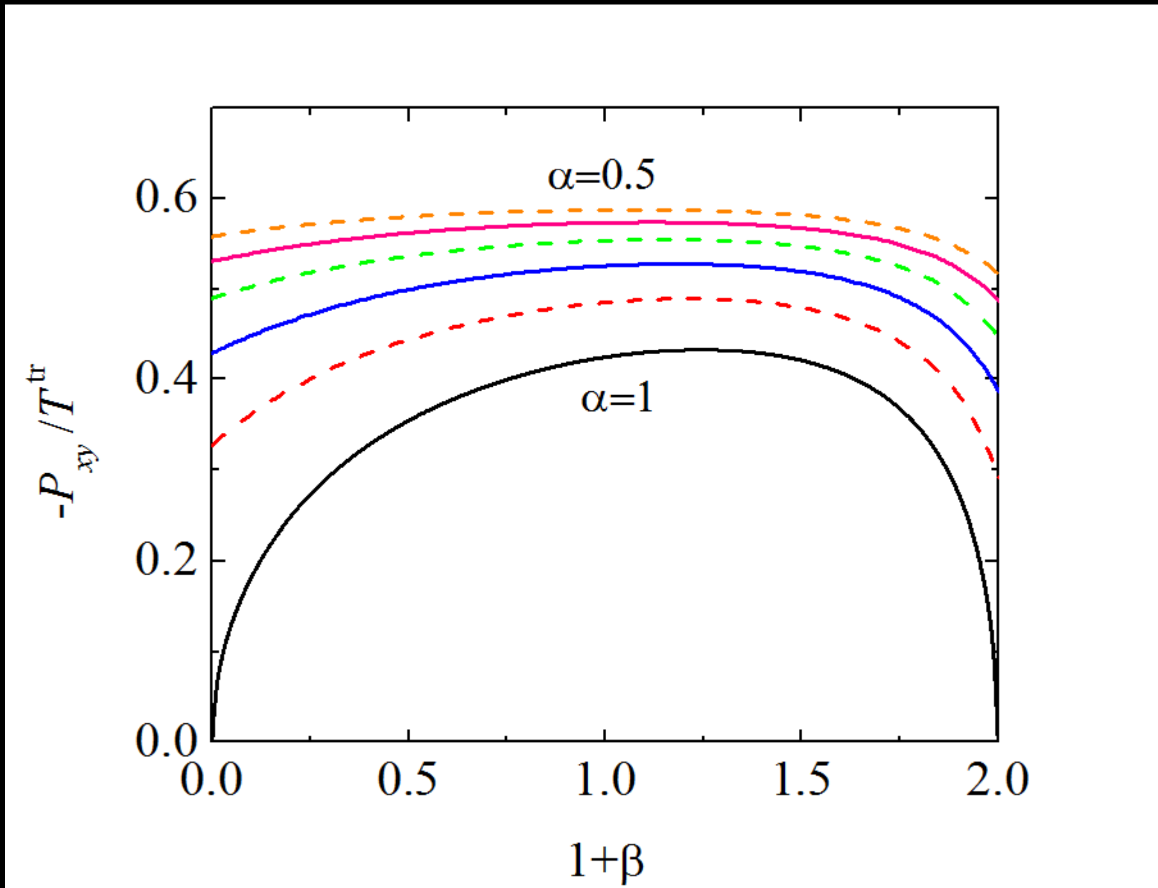
Application to simple shear flow

Shear stress

$$\frac{P_{xy}}{nT^{\rm tr}} = -\frac{\sqrt{3\widehat{\xi}^{\rm tr}/2}}{1+\widehat{\xi}^{\rm tr}}$$

$$\widehat{\xi}^{\rm tr} = \frac{5}{6}\frac{1-\alpha^2+2\kappa(1-\beta^2)/(2\kappa+1-\beta)}{1+\alpha+\kappa(1+\beta)/(1+\kappa)}$$

Scaled thermal rate

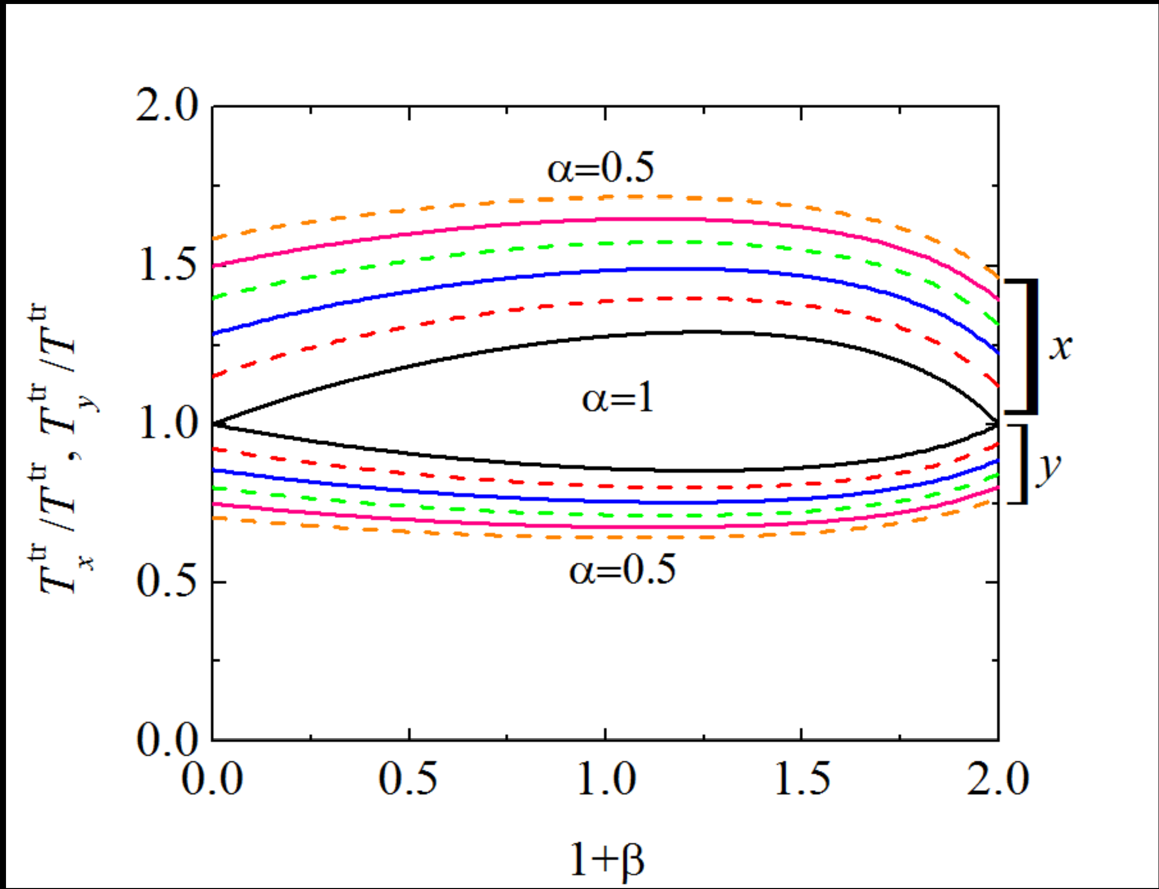


Application to simple shear flow

Anisotropic translational temperatures

$$\frac{T_x^{\mathrm{tr}}}{T^{\mathrm{tr}}} = \frac{1+3\widehat{\xi}^{\mathrm{tr}}}{1+\widehat{\xi}^{\mathrm{tr}}}$$

$$\frac{T_y^{\mathrm{tr}}}{T^{\mathrm{tr}}} = \frac{T_z^{\mathrm{tr}}}{T^{\mathrm{tr}}} = \frac{1}{1+\widehat{\xi}^{\mathrm{tr}}}$$



Conclusions and outlook

- Collisional thermal rates obtained for mixtures of inelastic rough hard spheres.
- Interesting non-equipartition phenomena in the HCS (“ghost” effect).
- 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. Simulations planned.
- Derivation of the Navier-Stokes constitutive equations.

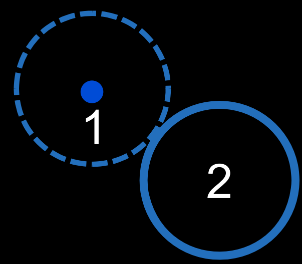
Thanks for your attention!

Binary mixture

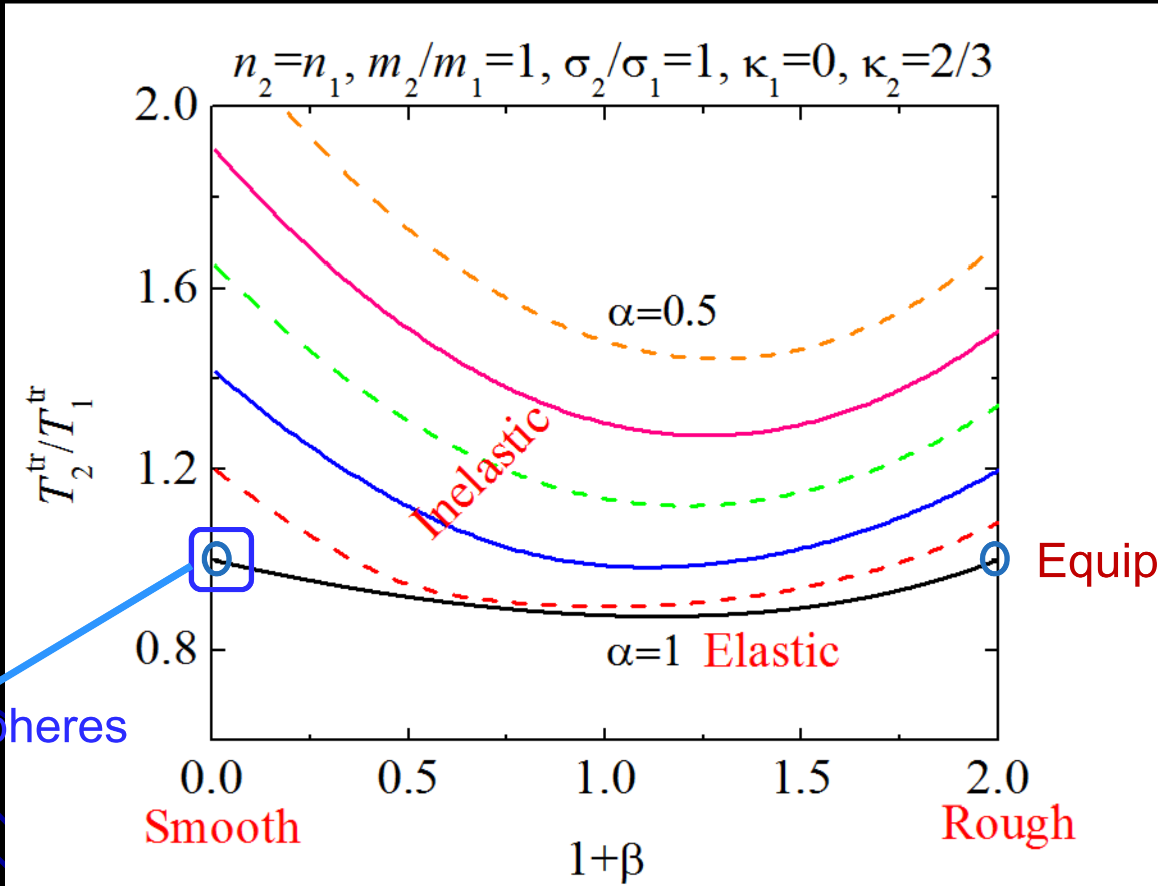
Three independent temperature ratios: $\dfrac{T_1^{\mathrm{tr}}}{T_1^{\mathrm{rot}}}, \dfrac{T_2^{\mathrm{tr}}}{T_1^{\mathrm{tr}}}, \dfrac{T_2^{\mathrm{rot}}}{T_1^{\mathrm{rot}}}$

Eleven parameters:

- Coefficients of normal restitution $\alpha_{11}, \alpha_{12}, \alpha_{22}$ $\alpha_{11} = \alpha_{12} = \alpha_{22} = \alpha$
- Coefficients of tangential restitution $\beta_{11}, \beta_{12}, \beta_{22}$ $\beta_{11} = \beta_{12} = \beta_{22} = \beta$
- Inertia-moment parameters κ_1, κ_2 $\kappa_1 = 0$, $\kappa_2 = \frac{2}{3}$
- 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



Equipartition

"Pure" smooth spheres

"Ghost" effect: A tiny amount of roughness has dramatic effects on the temperature ratio

Simple application: White-noise heating (steady state)

$$-\frac{\chi_0^2}{2}\left(\frac{\partial}{\partial \mathbf{v}_i}\right)^2 f_i(\mathbf{v}_i, \boldsymbol{\omega}_i) = \sum_j J_{ij}[\mathbf{v}_i, \boldsymbol{\omega}_i, t | f_i, f_j]$$

$$T_1^{\mathrm{tr}} \xi_1^{\mathrm{tr}} = T_2^{\mathrm{tr}} \xi_2^{\mathrm{tr}} = \cdots$$

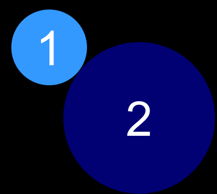
$$\xi_1^{\mathrm{rot}} = \xi_2^{\mathrm{rot}} = \cdots = 0$$

Binary mixture

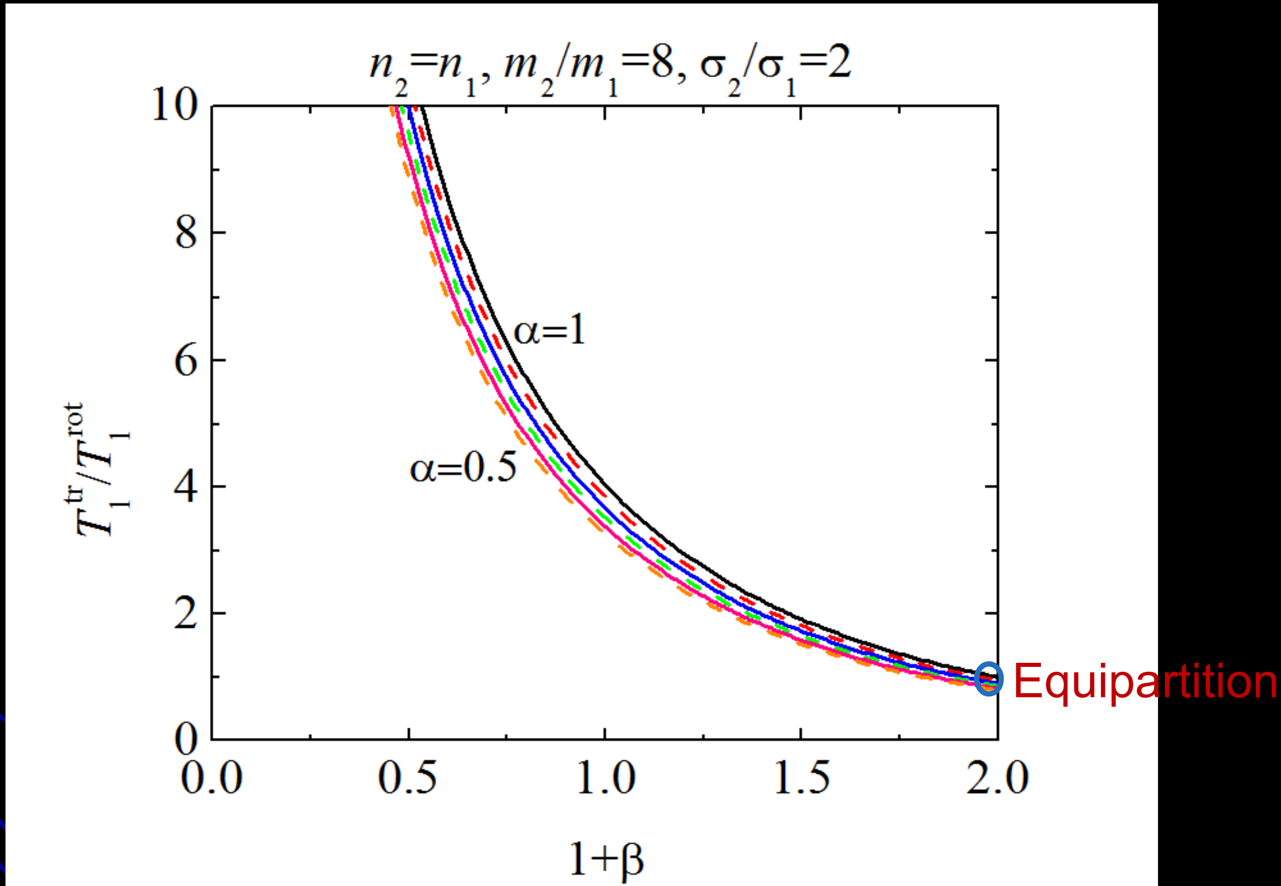
Three independent temperature ratios: $\frac{T_1^{\mathrm{tr}}}{T_1^{\mathrm{rot}}}, \frac{T_2^{\mathrm{tr}}}{T_1^{\mathrm{tr}}}, \frac{T_2^{\mathrm{rot}}}{T_1^{\mathrm{rot}}}$

Eleven parameters:

- Coefficients of normal restitution $\alpha_{11}, \alpha_{12}, \alpha_{22}$ $\alpha_{11} = \alpha_{12} = \alpha_{22} = \alpha$
- Coefficients of tangential restitution $\beta_{11}, \beta_{12}, \beta_{22}$ $\beta_{11} = \beta_{12} = \beta_{22} = \beta$
- Inertia-moment parameters κ_1, κ_2 $\kappa_1 = \kappa_2 = \frac{2}{5}$
- Size ratio $\sigma_2/\sigma_1 = 2$
- Mass ratio $m_2/m_1 = 8$
- Mole fraction $n_1/(n_1 + n_2) = \frac{1}{2}$

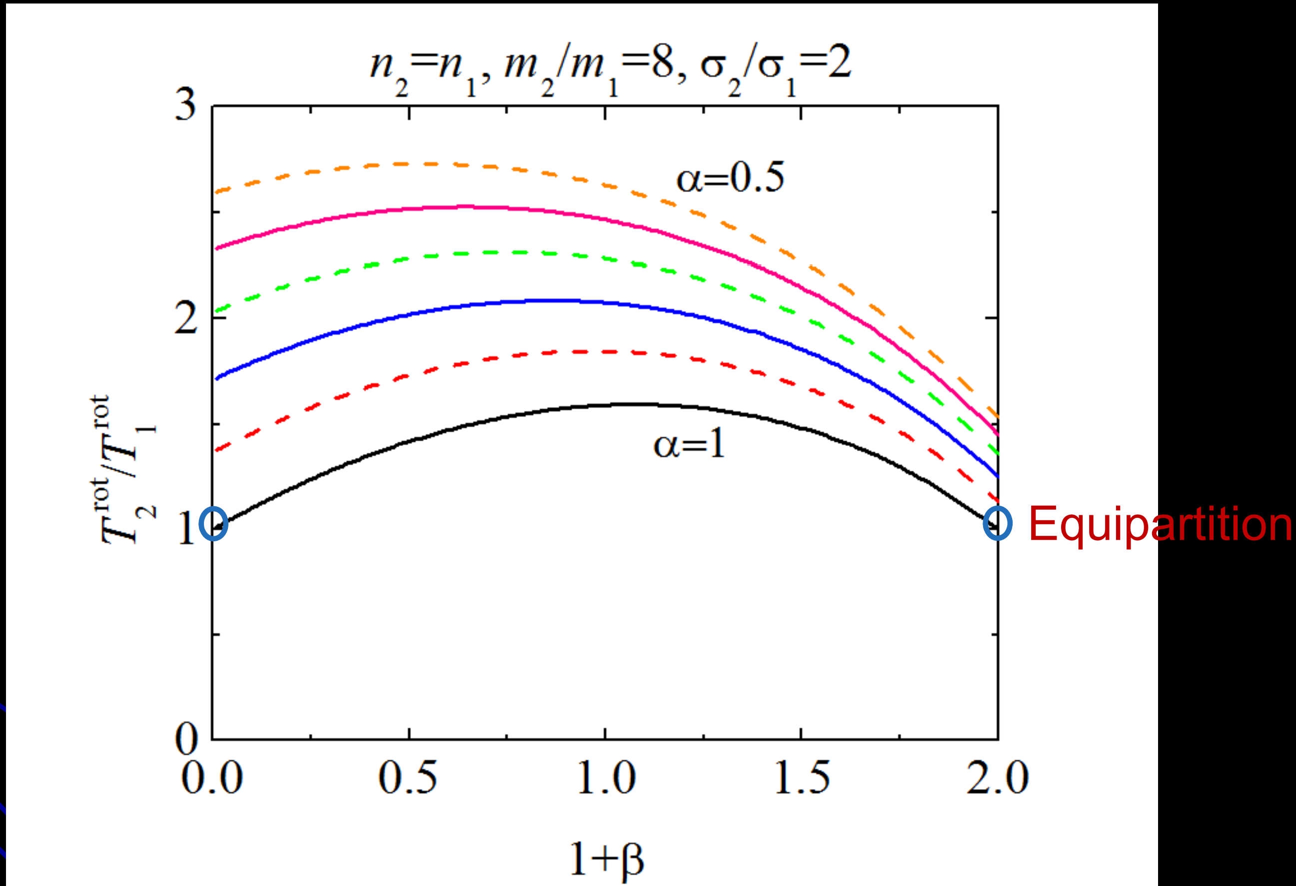


Translational/Rotational



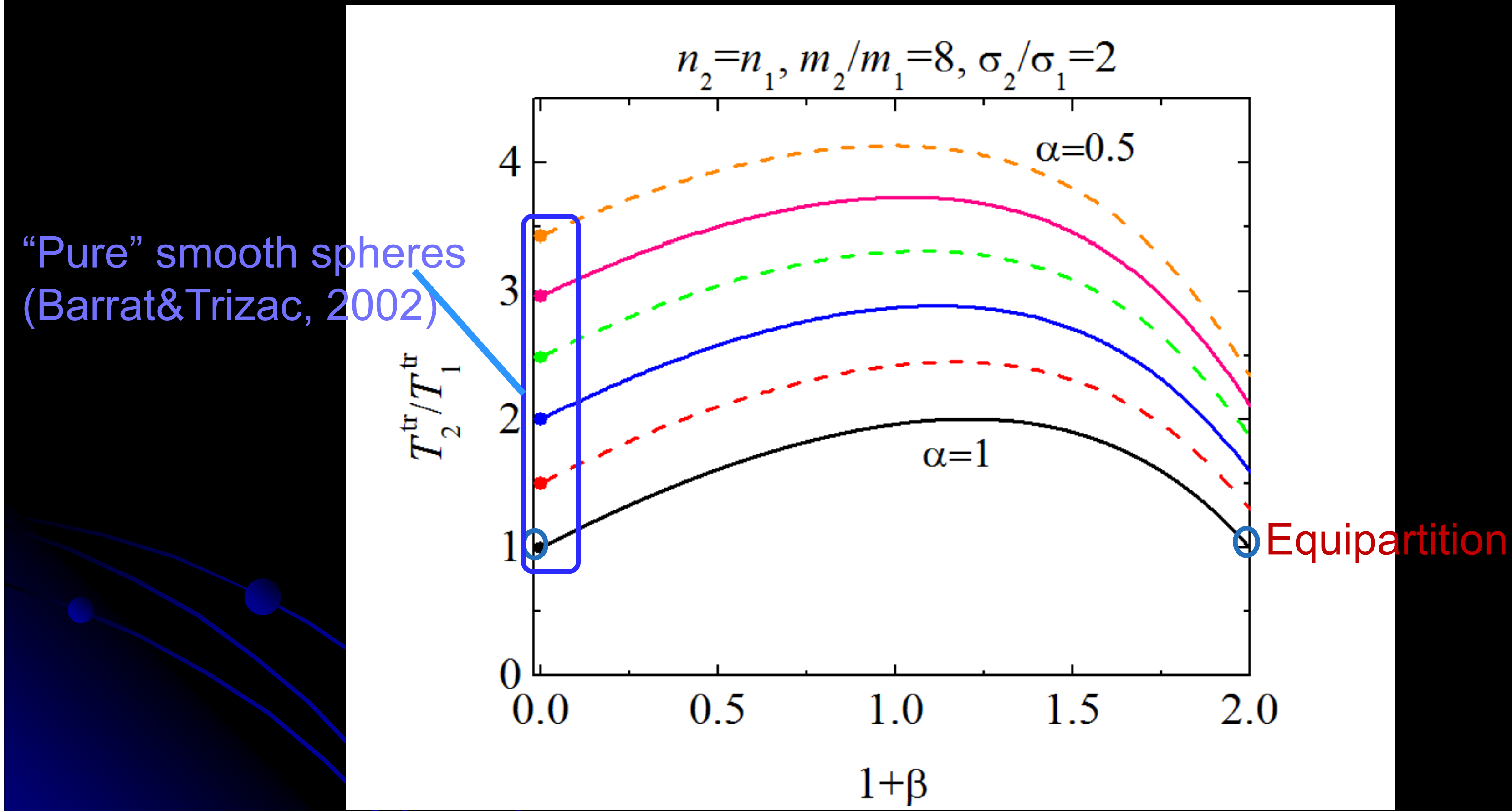
Weak influence of inelasticity

Rotational/Rotational



Same qualitative behavior for different inelasticities

Translational/Translational



No "ghost" effect! (steady state)