# A Bhatnagar-Gross-Krook-like Model Kinetic Equation for a Granular Gas of Inelastic *Rough* Hard Spheres

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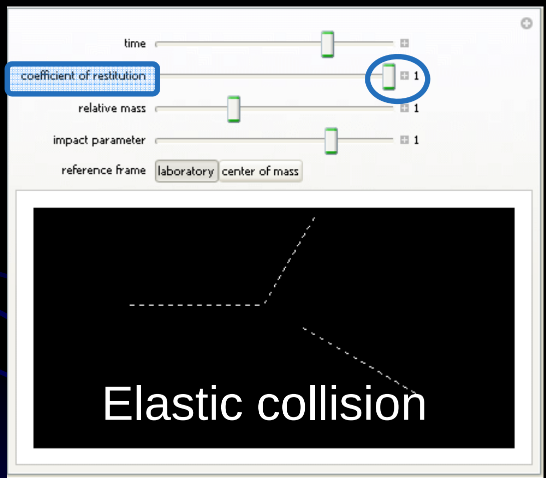
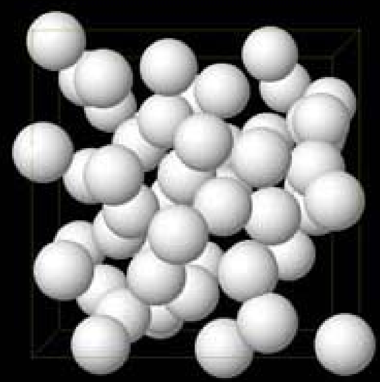
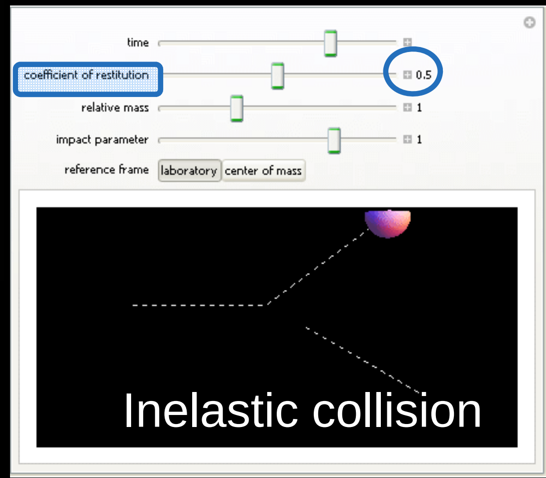
# Minimal model of a granular gas: A gas of *identical smooth inelastic* hard spheres



Elastic collision



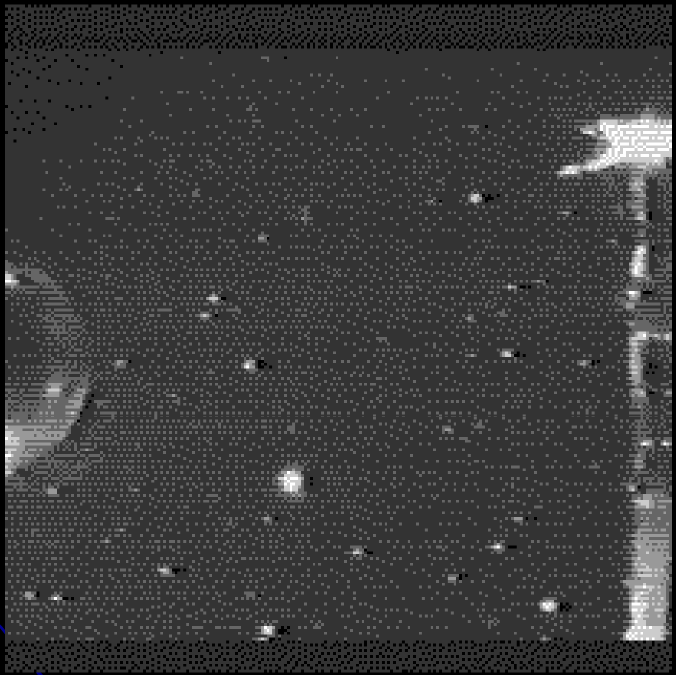


Inelastic collision

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

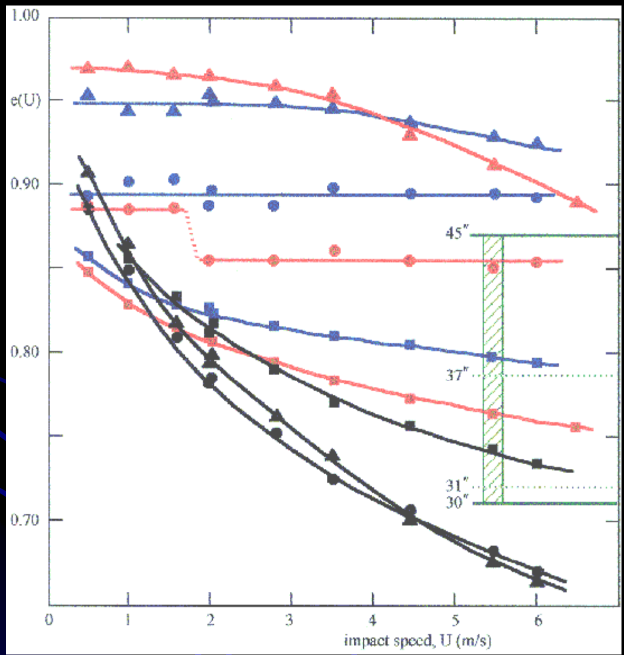
# This minimal model ignores …

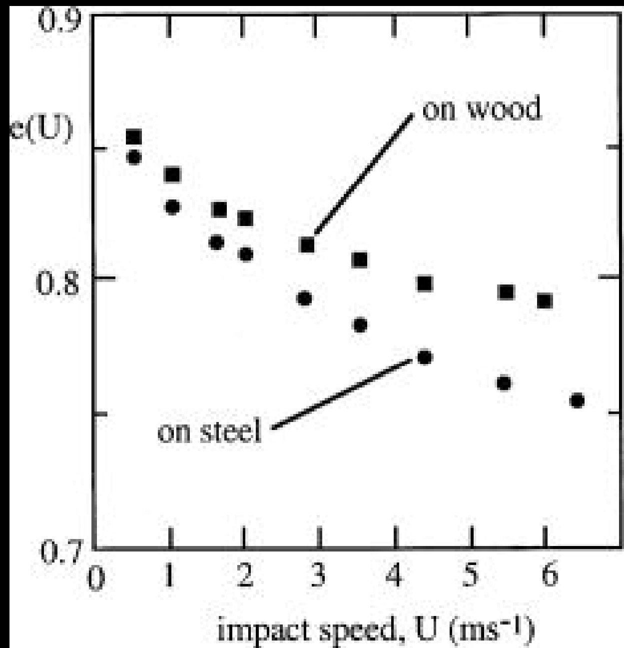
Interstitial fluid



Caltech Granular Flows Group (http://www.its.caltech.edu/~granflow/)

# Non-constant coefficient of restitution

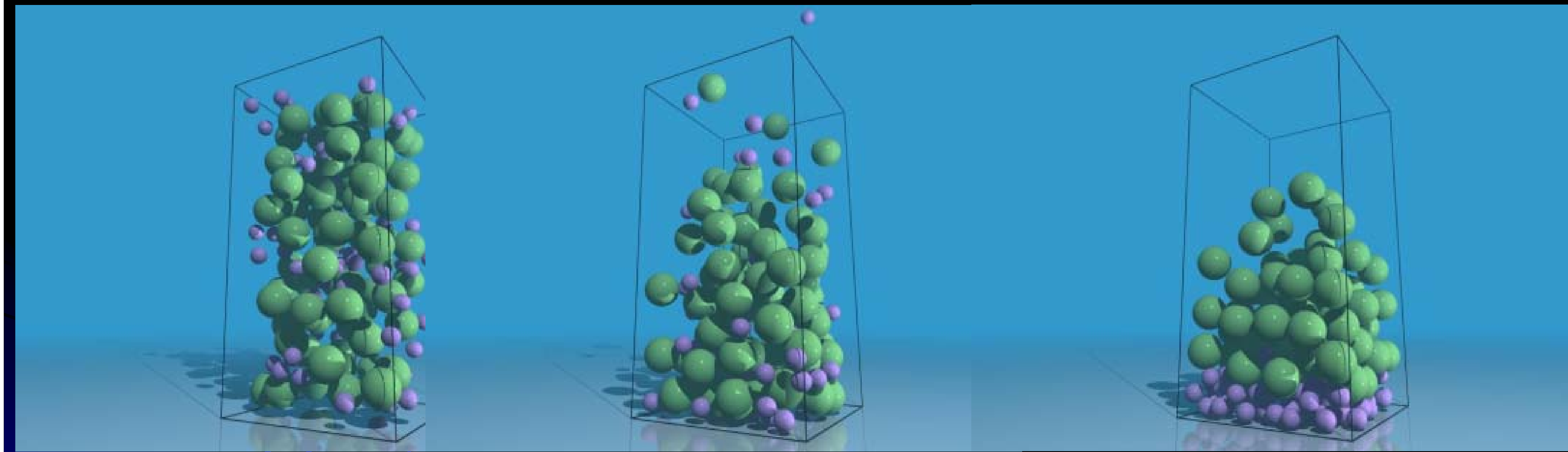



www.oxfordcroquet.com/tech/

## Non-spherical shape

## Polydispersity



http://www.cmt.york.ac.uk/~ajm143/nuts.html

# Roughness

# 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

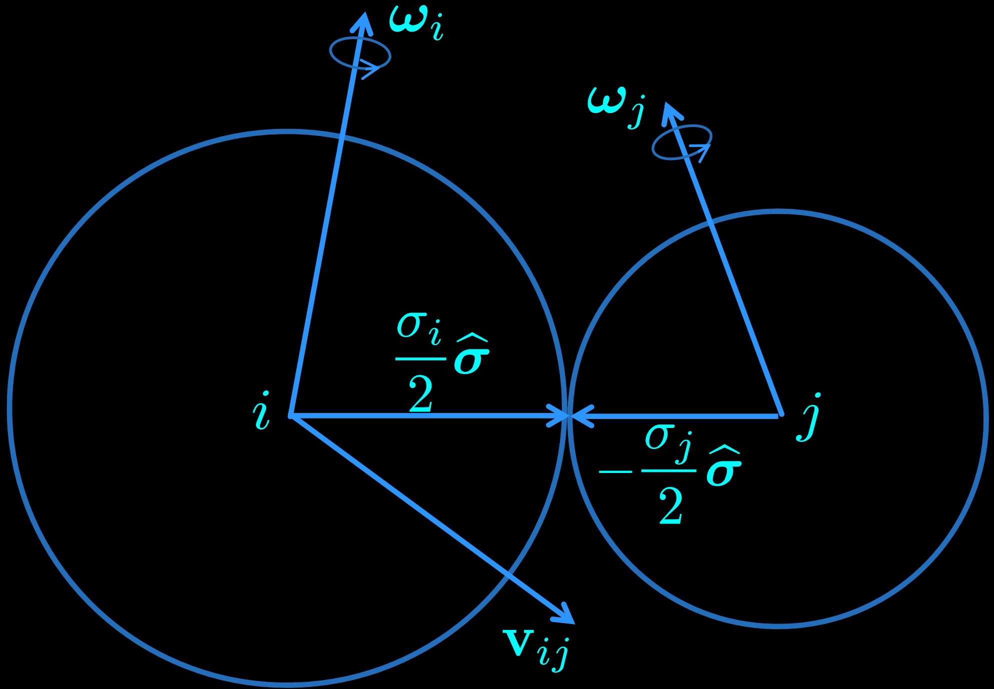
Several circles (Kandinsky, 1926)

Galatea of the Spheres (Dalí, 1952)

# Outline

- Energy production rates in a mixture of inelastic rough hard spheres.
- Simple kinetic model for monodisperse systems.
- Application to the simple shear flow.
- Conclusions and outlook.

# Collisions of inelastic rough hard spheres



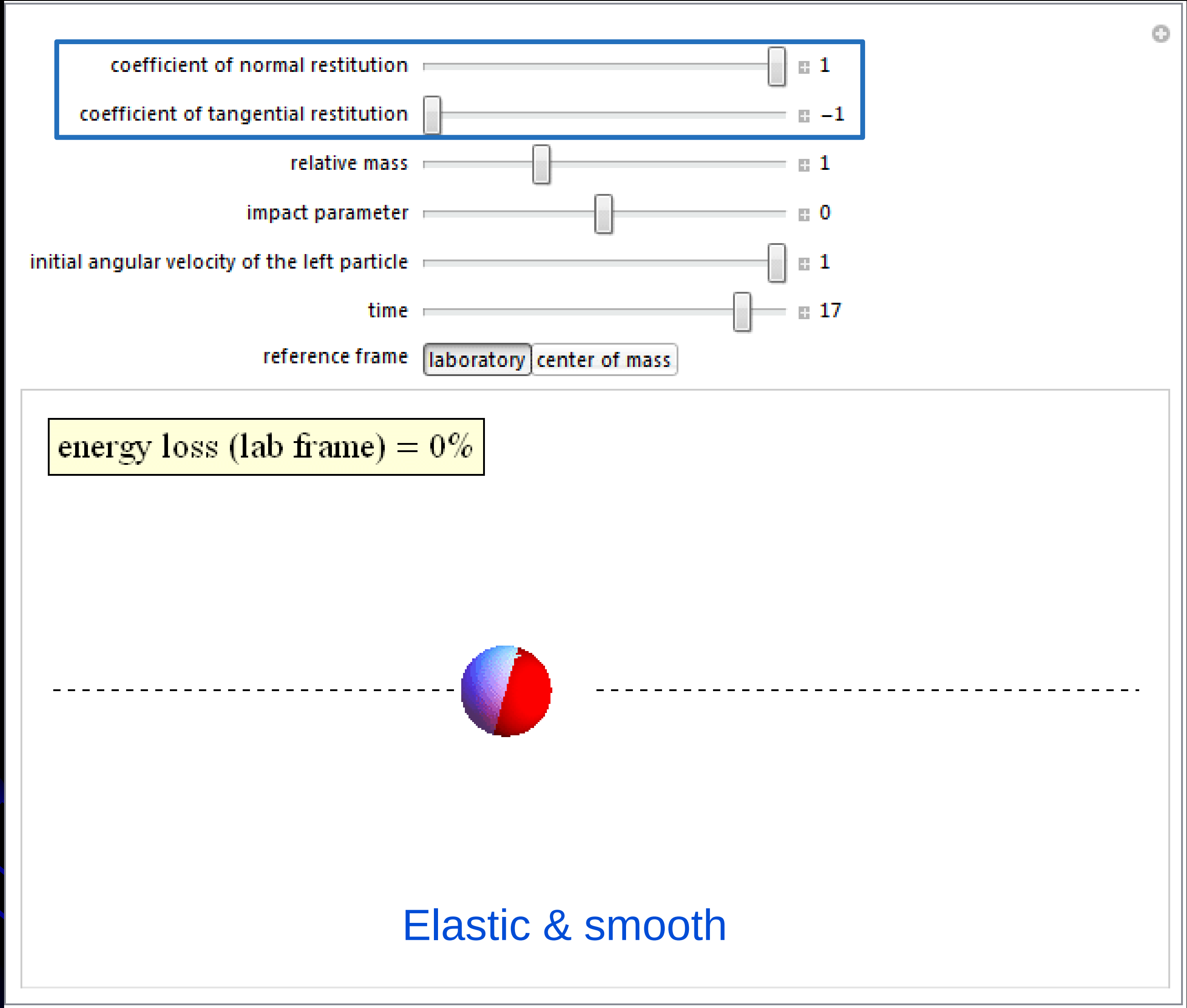

- Coefficients of normal restitution $\alpha_{ij}$
- Coefficients of tangential restitution $\beta_{ij}$
  - $\alpha_{ij}=1$ for perfectly elastic particles
  - $\beta_{ij}=-1$ for perfectly smooth particles
  - $\beta_{ij}=+1$ for perfectly rough particles

# Energy collisional loss

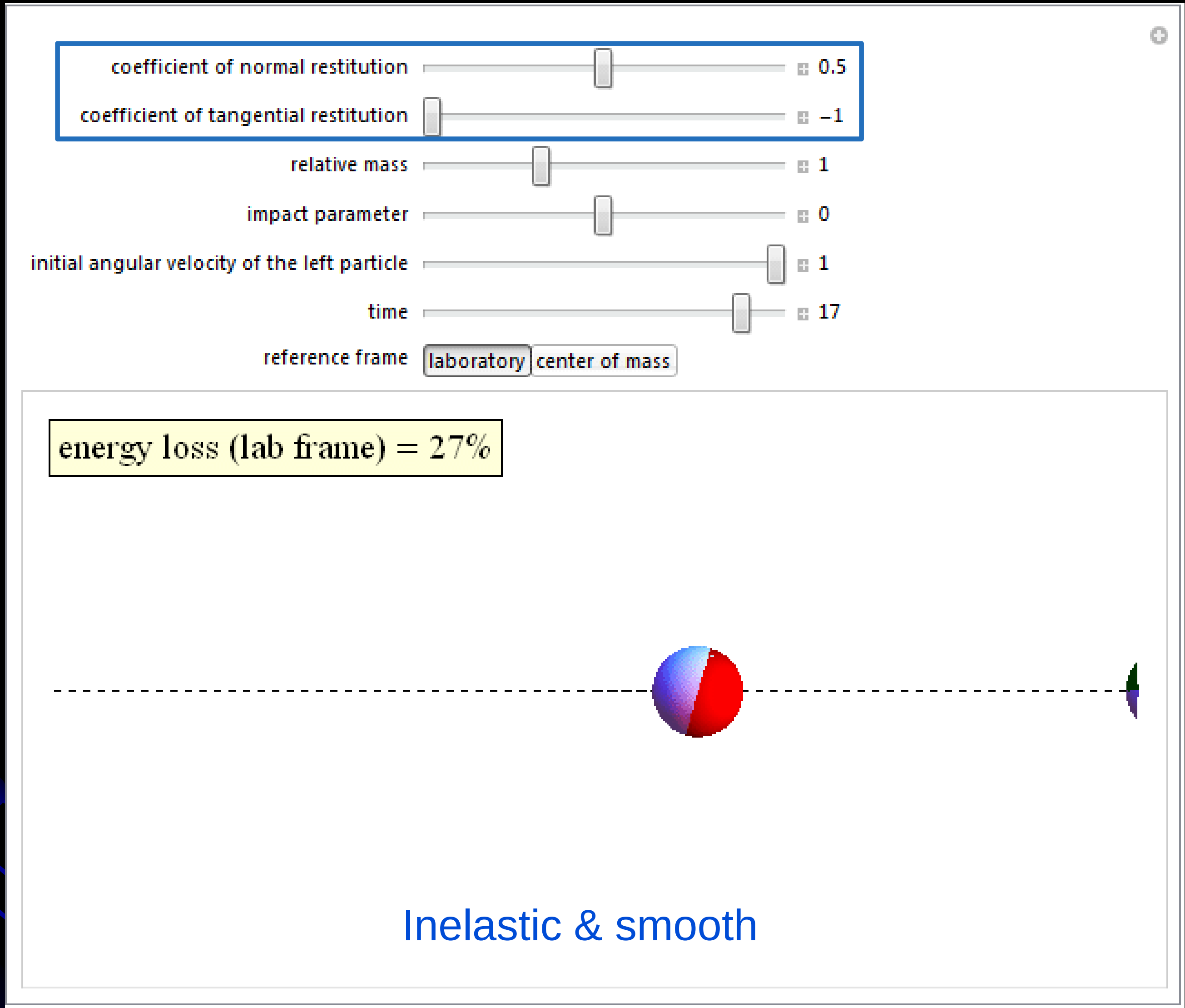
$$E_{ij} = \frac{1}{2}m_i v_i^2 + \frac{1}{2}m_j v_j^2 + \frac{1}{2}I_i \omega_i^2 + \frac{1}{2}I_j \omega_j^2$$

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

Energy is conserved *only* if the spheres are
- elastic ($\alpha_{ij}$=1) and
- either
  - perfectly smooth ($\beta_{ij}$=-1) or
  - perfectly rough ($\beta_{ij}$=+1)




http://demonstrations.wolfram.com/InelasticCollisionsOfTwoRoughSpheres/

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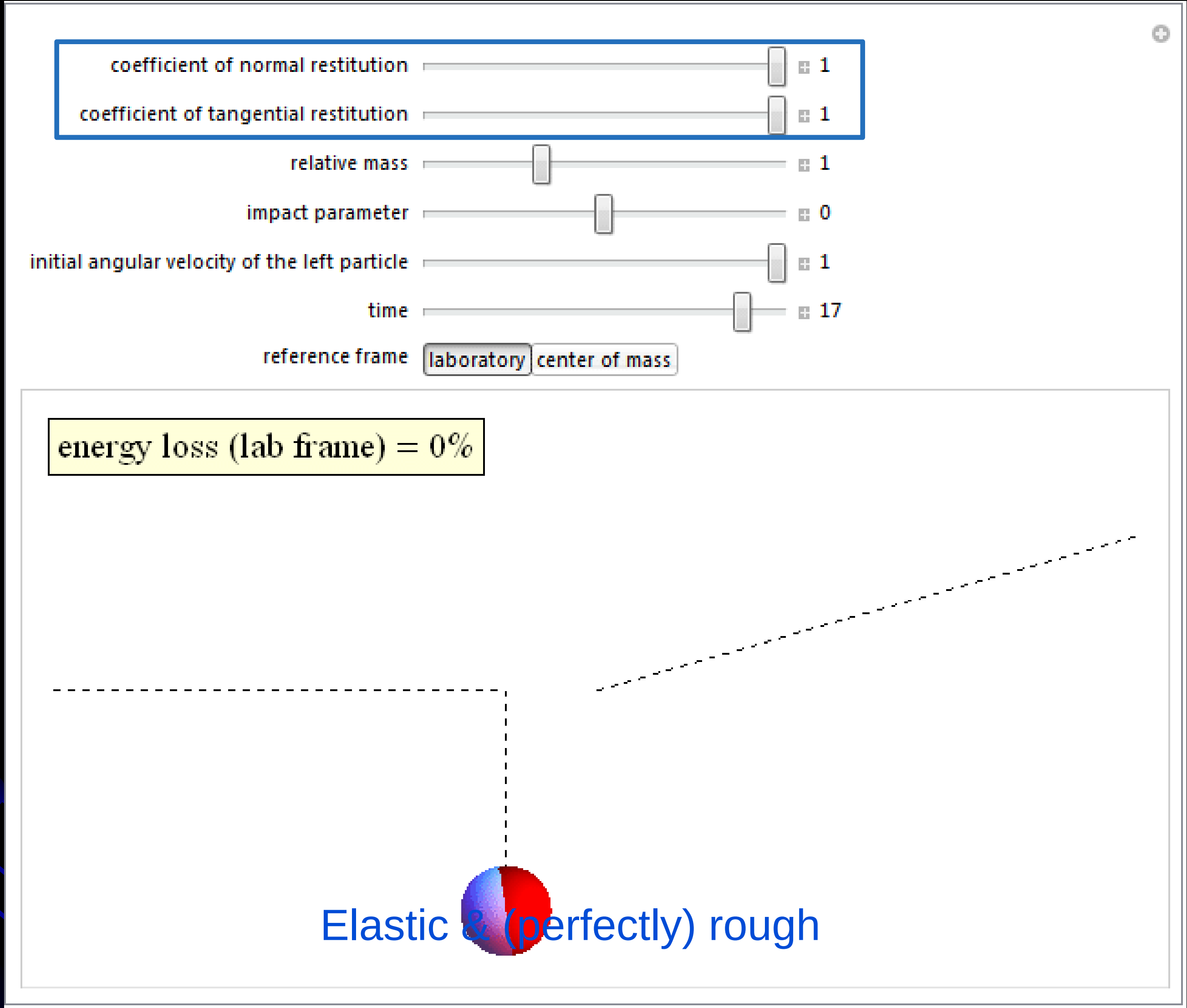


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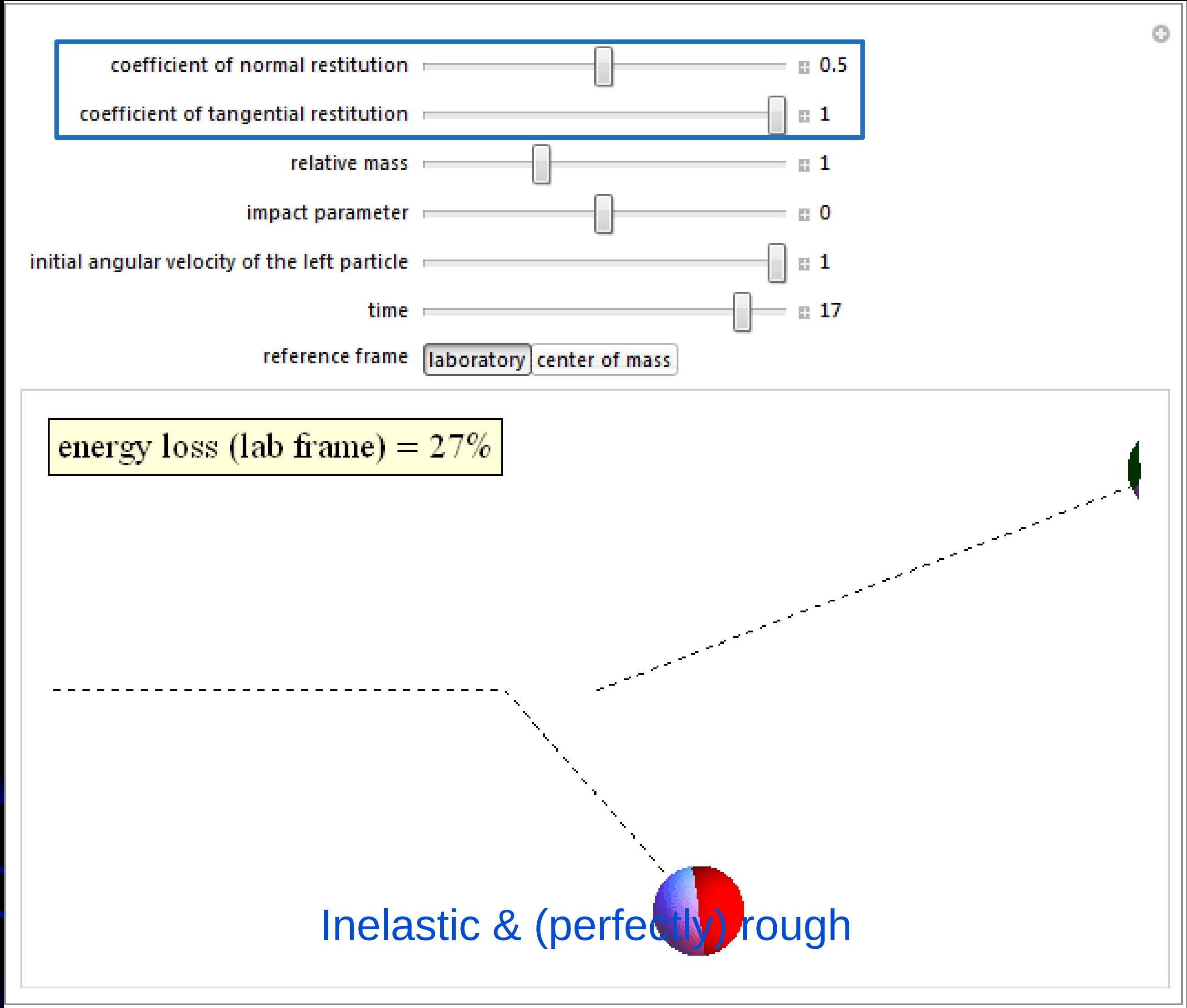
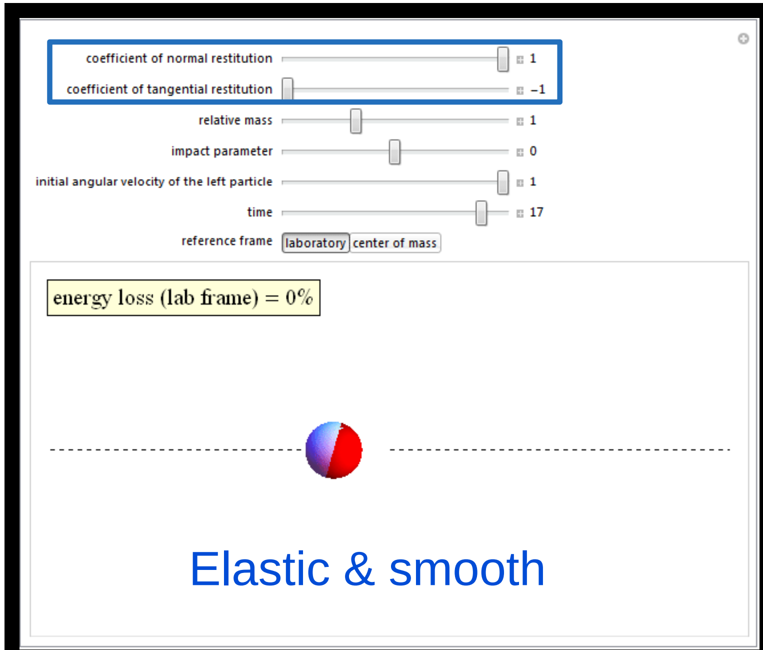
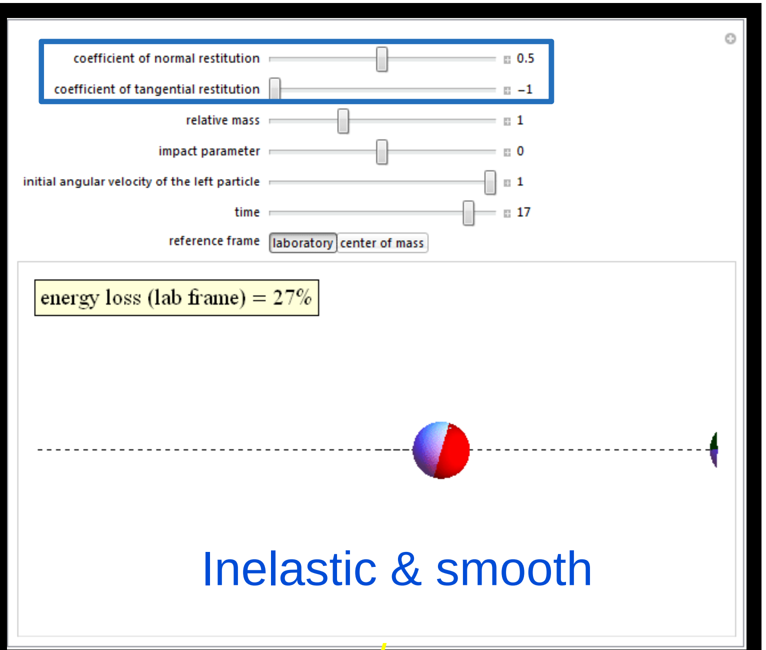



Inelastic & (perfectly) rough

http://demonstrations.wolfram.com/InelasticCollisionsOfTwoRoughSpheres/

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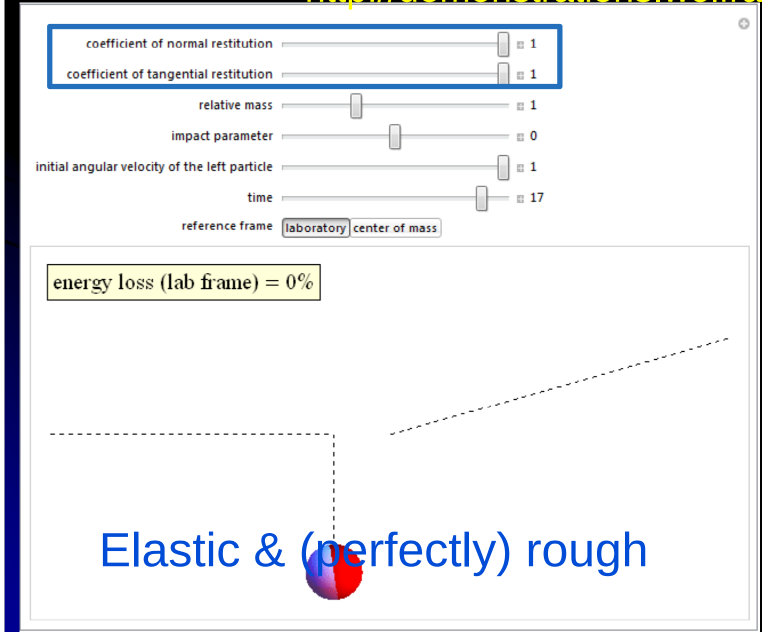
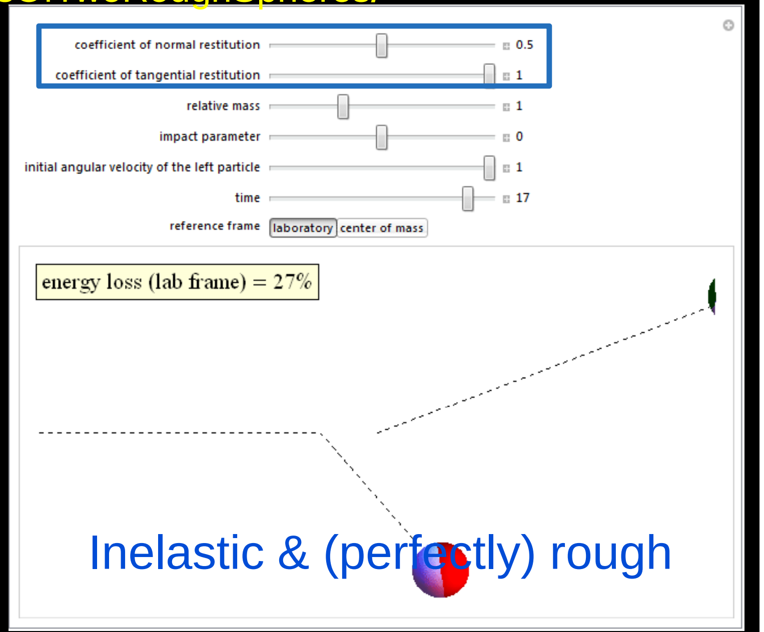


# Partial (granular) temperatures

Translational temperatures: $T_i^{\mathrm{tr}} = \frac{m_i}{3}\langle(\mathbf{v}_i - \mathbf{u})^2\rangle$

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

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

*Energy production* rates:

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

Binary collisions

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

Net *cooling* rate:

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

# Energy production rates. Kinetic-theory estimates

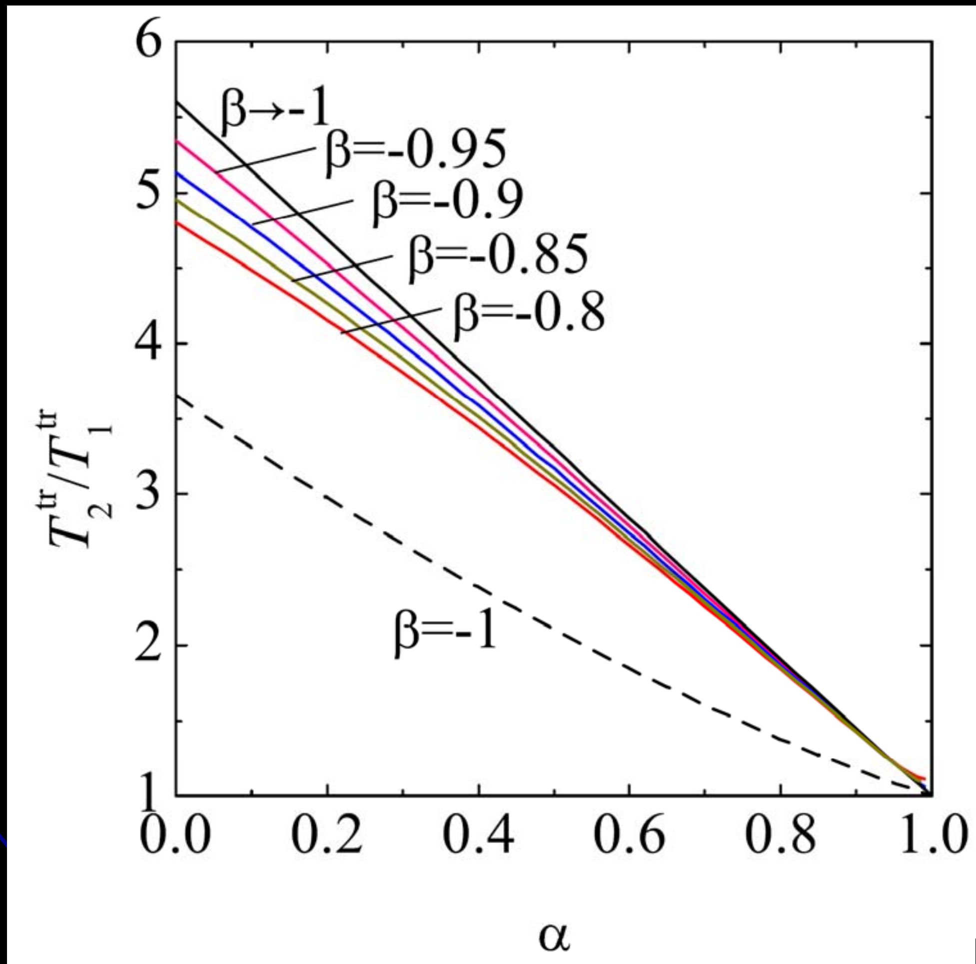
(A.S., G.M. Kremer, V. Garzó, 2010)

Two-body velocity distribution function:

$$f_{ij}(\mathbf{v}_i, \boldsymbol{\omega}_i; \mathbf{v}_j, \boldsymbol{\omega}_j) \;\to\; n_i n_j \left( \frac{m_i m_j}{4\pi^2 T_i^{\rm tr} T_j^{\rm tr}} \right)^{3/2} e^{-m_i \frac{(\mathbf{v}_i - \mathbf{u})^2}{2T_i^{\rm tr}} - m_j \frac{(\mathbf{v}_j - \mathbf{u})^2}{2T_j^{\rm tr}}} \times f_i^{\rm rot}(\boldsymbol{\omega}_i) f_j^{\rm rot}(\boldsymbol{\omega}_j)$$

Molecular chaos+Maxwellian approx. for translational distribution

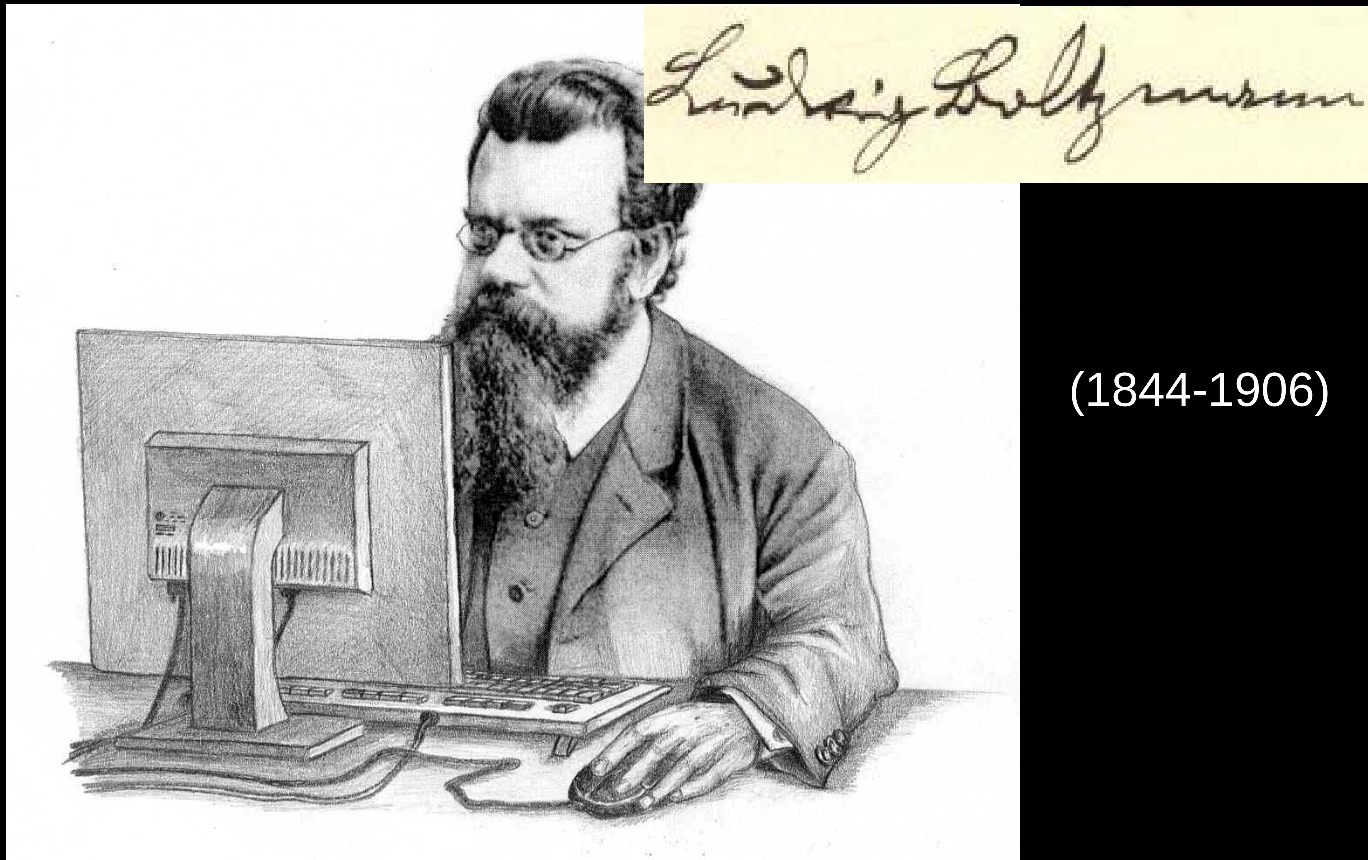
# Paradoxical "ghost'' effect in the Homogeneous Free Cooling State




(see poster 203 this evening)

# A simple kinetic model for *monodisperse* inelastic *rough* hard spheres

(Cartoon by Bernhard Reischl, University of Vienna)



(1844-1906)

## Boltzmann equation:

$$\partial_t f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) + \mathbf{v}\cdot\nabla f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) = \underbrace{J[\mathbf{v},\boldsymbol{\omega}|f,f]}_{\text{Inelastic+Rough collisions}}$$

Inelastic+Rough collisions

# Antecedents for *smooth* particles

Boltzmann eq.: $\partial_t f(\mathbf{r},\mathbf{v},t) + \mathbf{v}\cdot\nabla f(\mathbf{r},\mathbf{v},t) = J[\mathbf{v}|f,f]$

Elastic collisions:
[Bhatnagar-Gross-Krook (BGK) & Welander, 1954]

$$J[\mathbf{v}|f,f] \to -\nu\,(f - f_0)\,, \quad f_0 = n\left(\frac{m}{2\pi T}\right)^{3/2}\exp\left[-\frac{m(\mathbf{v}-\mathbf{u})^2}{2T}\right]$$

Inelastic collisions:
[Brey, Dufty, Santos, 1999]

$$J[\mathbf{v}|f,f] \to -\lambda(\alpha)\nu\,(f - f_0) + \frac{\zeta(\alpha)}{2}\frac{\partial}{\partial \mathbf{v}}\cdot[(\mathbf{v}-\mathbf{u})f]$$

# Simple kinetic model for *monodisperse* inelastic rough hard spheres

Four key ingredients we want to keep:

"de-spinning" rate

1. $(\partial_t \mathbf{\Omega})_{\text{coll}} = -\zeta_\Omega \mathbf{\Omega}, \quad \mathbf{\Omega} \equiv \langle \boldsymbol{\omega} \rangle$

2. $(\partial_t T^{\text{tr}})_{\text{coll}} = -\xi^{\text{tr}} T^{\text{tr}}, \quad T^{\text{tr}} \equiv \frac{m}{3}\langle (\mathbf{v}-\mathbf{u})^2 \rangle$

Energy production rates

3. $(\partial_t T^{\text{rot}})_{\text{coll}} = -\xi^{\text{rot}} T^{\text{rot}}, \quad T^{\text{rot}} \equiv \frac{I}{3}\langle \omega^2 \rangle$

4. $\int d\mathbf{v}_1 \int d\boldsymbol{\omega}_1 \, \mathbf{v}_1 J_{12}[\mathbf{v}_1, \boldsymbol{\omega}_1 | f_1, f_2] \approx \lambda \int d\mathbf{v}_1 \int d\boldsymbol{\omega}_1 \, \mathbf{v}_1 J_{12}[\mathbf{v}_1, \boldsymbol{\omega}_1 | f_1, f_2] \Big|_{\substack{\alpha = 1 \\ \beta = -1}}$

Elastic smooth spheres

$$\lambda(\alpha, \beta) \equiv \frac{1+\alpha}{2} + \frac{\kappa}{1+\kappa}\frac{1+\beta}{2}, \quad \kappa \equiv \frac{4I}{m\sigma^2}$$

# Collisional rates of change

$$\zeta_\Omega = \frac{5}{6}\frac{1+\beta}{1+\kappa}\nu$$

$$\xi^{\mathrm{tr}} = \frac{5}{12}\left[1-\alpha^2+\frac{\kappa}{1+\kappa}\left(1-\beta^2\right)+\frac{\kappa}{(1+\kappa)^2}\left(1+\beta\right)^2\left(1-\frac{T^{\mathrm{rot}}(1+X)}{T^{\mathrm{tr}}}\right)\right]\nu$$

$$\xi^{\mathrm{rot}} = \frac{5}{12}\frac{1+\beta}{1+\kappa}\frac{T^{\mathrm{tr}}}{T^{\mathrm{rot}}}\left[(1-\beta)\frac{T^{\mathrm{rot}}(1+X)}{T^{\mathrm{tr}}}-\frac{\kappa}{1+\kappa}(1+\beta)\left(1-\frac{T^{\mathrm{rot}}(1+X)}{T^{\mathrm{tr}}}\right)\right]\nu$$

$$X \equiv \frac{\kappa m\sigma^2\Omega^2}{12T^{\mathrm{rot}}}, \quad \nu \equiv \frac{16}{5}\sigma^2 n\sqrt{\pi T^{\mathrm{tr}}/m}$$

# The kinetic model. Joint distribution

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

$$\begin{aligned} J[f,f] \;\to\; & -\lambda\nu\,(f - f_0) \\ & + \tfrac{1}{2}\xi^{\mathrm{tr}}\tfrac{\partial}{\partial \mathbf{v}}\cdot[(\mathbf{v}-\mathbf{u})f] + \tfrac{1}{2}\tfrac{\partial}{\partial \boldsymbol{\omega}}\cdot\left\{\left[2\zeta_\Omega\boldsymbol{\Omega} + \overline{\xi}^{\mathrm{rot}}(\boldsymbol{\omega}-\boldsymbol{\Omega})\right]f\right\} \end{aligned}$$

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

$$\overline{T}^{\mathrm{rot}} \equiv \frac{I}{3}\langle(\boldsymbol{\omega}-\boldsymbol{\Omega})^2\rangle = T^{\mathrm{rot}}(1-X), \quad \overline{\xi}^{\mathrm{rot}} = \frac{\xi^{\mathrm{rot}} - 2\zeta_\Omega X}{1-X}$$

# A simpler version. Marginal distributions

$$f^{\mathrm{tr}}(\mathbf{r},\mathbf{v},t)=\int d\boldsymbol{\omega}\, f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t), \quad f^{\mathrm{rot}}(\mathbf{r},\boldsymbol{\omega},t)=\frac{1}{n}\int d\mathbf{v}\, f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)$$

$$\boxed{\partial_t f^{\mathrm{tr}}+\mathbf{v}\cdot\nabla f^{\mathrm{tr}}=-\lambda\nu\left(f^{\mathrm{tr}}-f_0^{\mathrm{tr}}\right)+\frac{1}{2}\xi^{\mathrm{tr}}\frac{\partial}{\partial\mathbf{v}}\cdot\left[(\mathbf{v}-\mathbf{u})f^{\mathrm{tr}}\right]}$$

$$\left(\frac{1}{n}\int d\mathbf{v}\,\mathbf{v}f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)\to\mathbf{u}f^{\mathrm{rot}}(\mathbf{r},\boldsymbol{\omega},t)\right)$$

$$\begin{aligned}\partial_t f^{\mathrm{rot}}+\mathbf{u}\cdot\nabla f^{\mathrm{rot}} &= -\lambda\nu_0\left(f^{\mathrm{rot}}-f_0^{\mathrm{rot}}\right)\\ &+\frac{1}{2}\frac{\partial}{\partial\boldsymbol{\omega}}\cdot\left\{\left[2\zeta_\Omega\boldsymbol{\Omega}+\overline{\xi}^{\mathrm{rot}}(\boldsymbol{\omega}-\boldsymbol{\Omega})\right]f^{\mathrm{rot}}\right\}\end{aligned}$$

# An even simpler version. Translational distribution

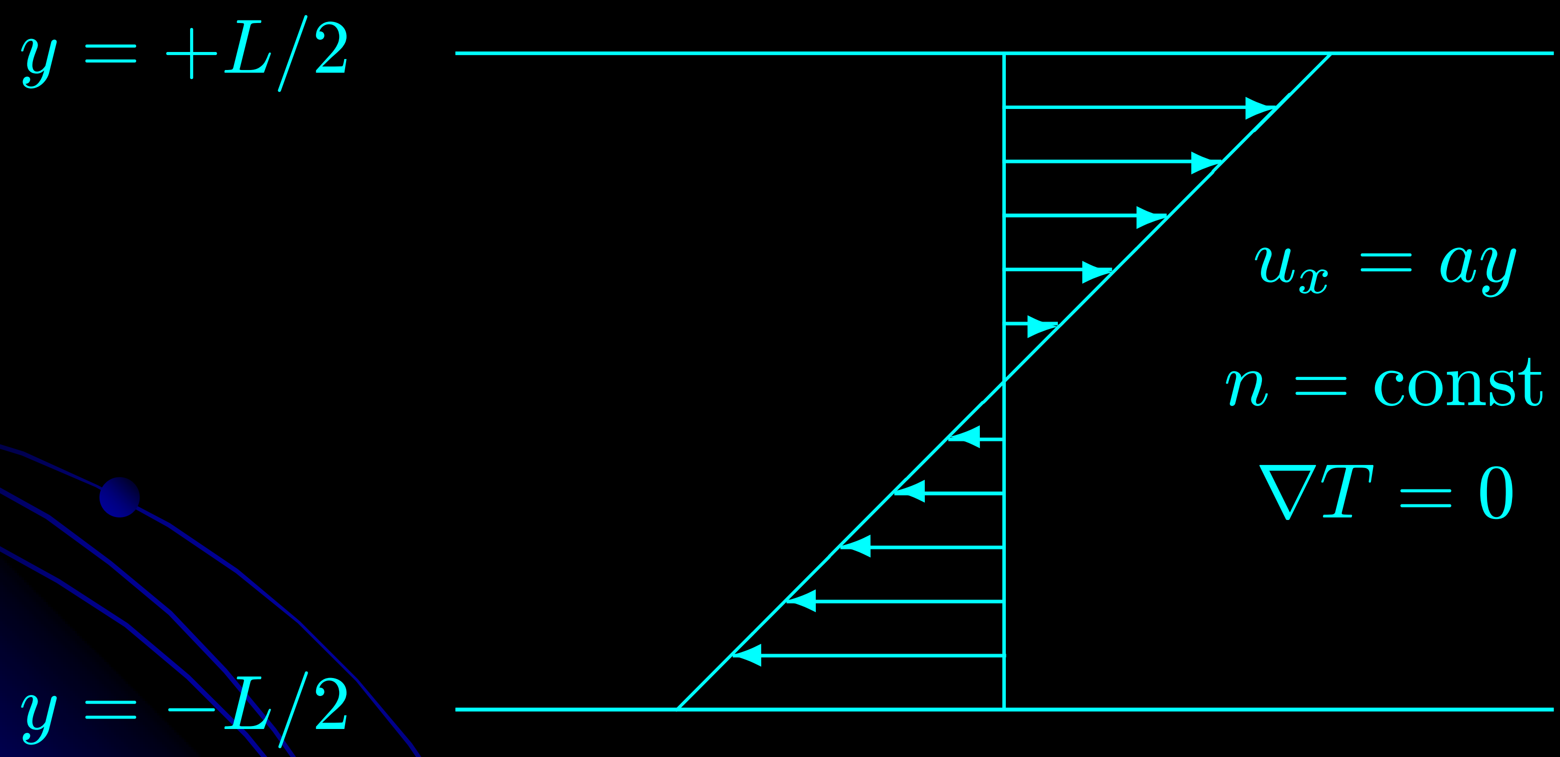
$$f^{\mathrm{tr}} = \int d\boldsymbol{\omega}\, f, \quad \boldsymbol{\Omega} = \frac{1}{n}\int d\mathbf{v}\int d\boldsymbol{\omega}\,\boldsymbol{\omega} f, \quad T^{\mathrm{rot}} = \frac{I}{3n}\int d\mathbf{v}\int d\boldsymbol{\omega}\,\omega^2 f$$

$$\partial_t f^{\mathrm{tr}} + \mathbf{v}\cdot\nabla f^{\mathrm{tr}} = -\lambda\nu_0\left(f^{\mathrm{tr}} - f_0^{\mathrm{tr}}\right) + \frac{1}{2}\xi^{\mathrm{tr}}\frac{\partial}{\partial\mathbf{v}}\cdot\left[(\mathbf{v}-\mathbf{u})f^{\mathrm{tr}}\right]$$

$$\left(\int d\mathbf{v}\int d\boldsymbol{\omega}\,\mathbf{v}\boldsymbol{\omega} f \to n\mathbf{u}\boldsymbol{\Omega}, \quad \frac{I}{3}\int d\mathbf{v}\int d\boldsymbol{\omega}\,\mathbf{v}\omega^2 f \to n\mathbf{u}T^{\mathrm{rot}}\right)$$

$$\partial_t\boldsymbol{\Omega} + \mathbf{u}\cdot\nabla\boldsymbol{\Omega} = -\zeta_\Omega\boldsymbol{\Omega}, \quad \partial_t T^{\mathrm{rot}} + \mathbf{u}\cdot\nabla T^{\mathrm{rot}} = -\xi^{\mathrm{rot}}T^{\mathrm{rot}}$$

# Application to simple shear flow (steady state)




$$u_x = ay$$

$$n = \text{const}$$

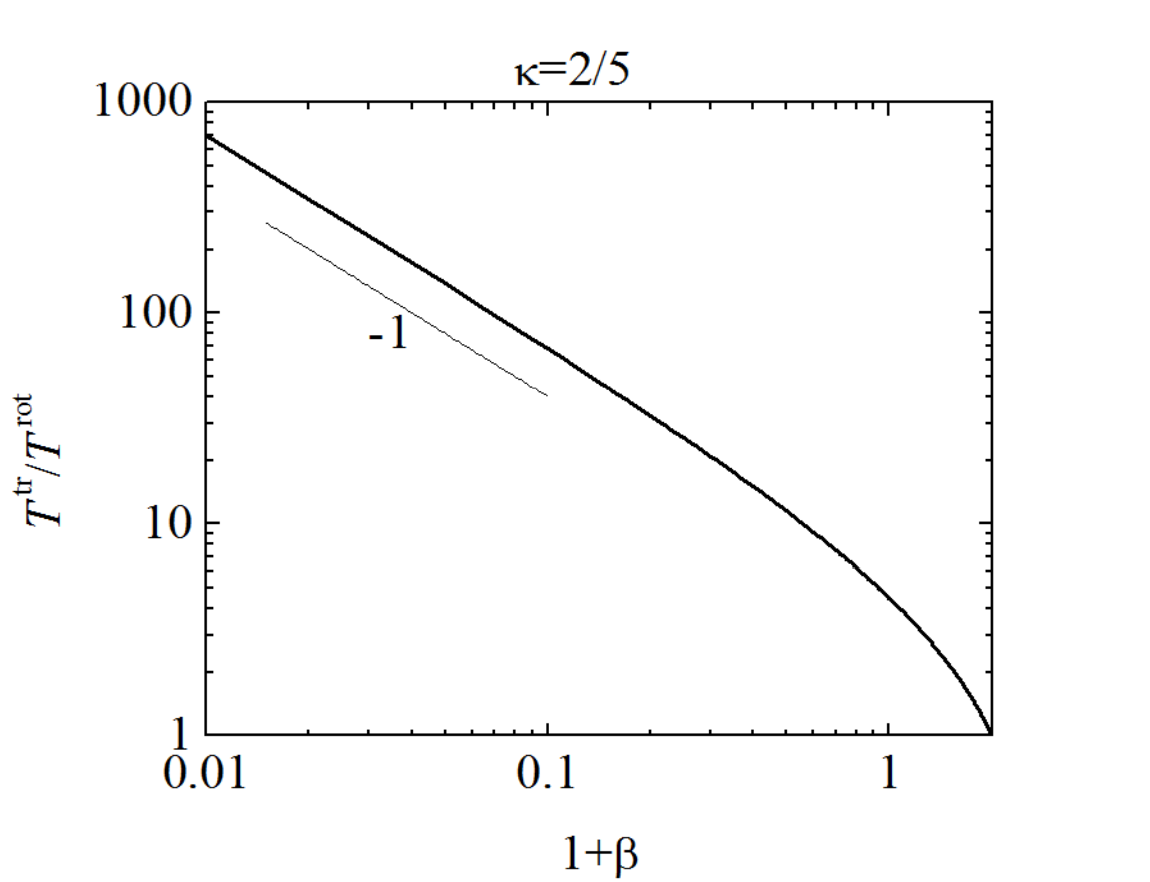
$$\nabla T = 0$$

# Application to simple shear flow

## Translational/Rotational temperature ratio

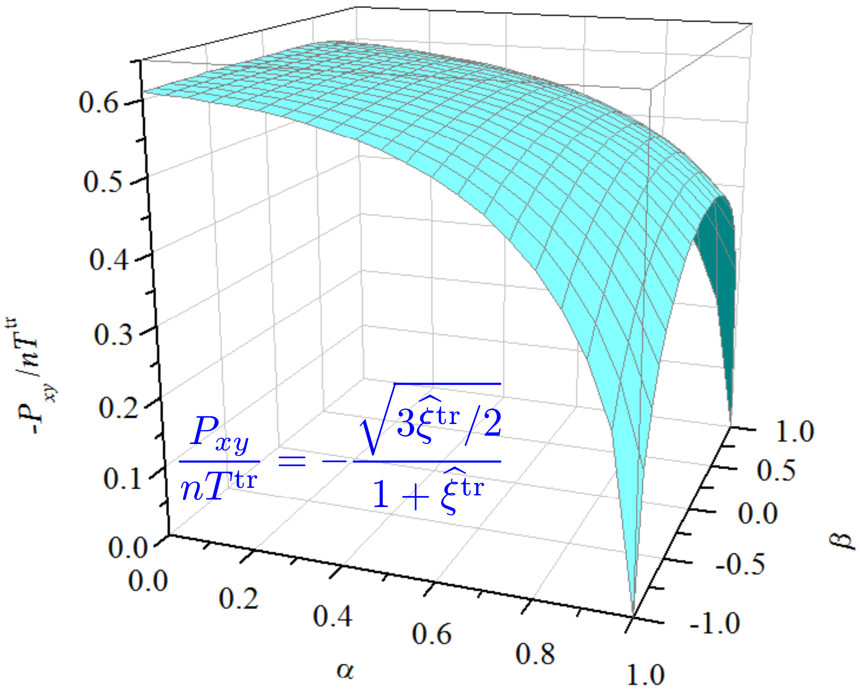
$$\xi^{\mathrm{rot}} = 0 \Rightarrow \boxed{\frac{T^{\mathrm{tr}}}{T^{\mathrm{rot}}} = \frac{2\kappa + 1 - \beta}{\kappa(1+\beta)}}$$

Independent of $\alpha$

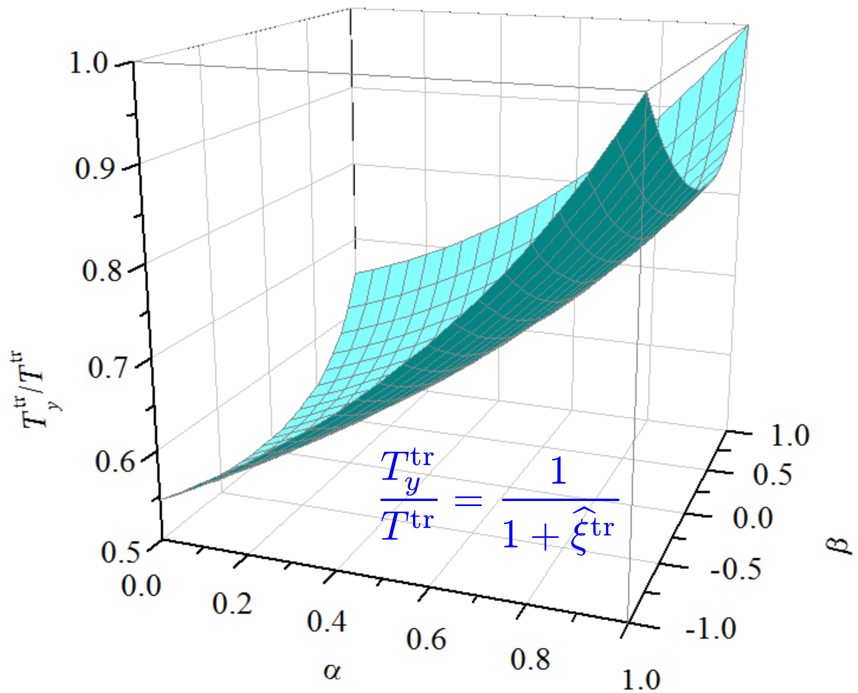


# Application to simple shear flow

Shear stress




Anisotropic translational temperature



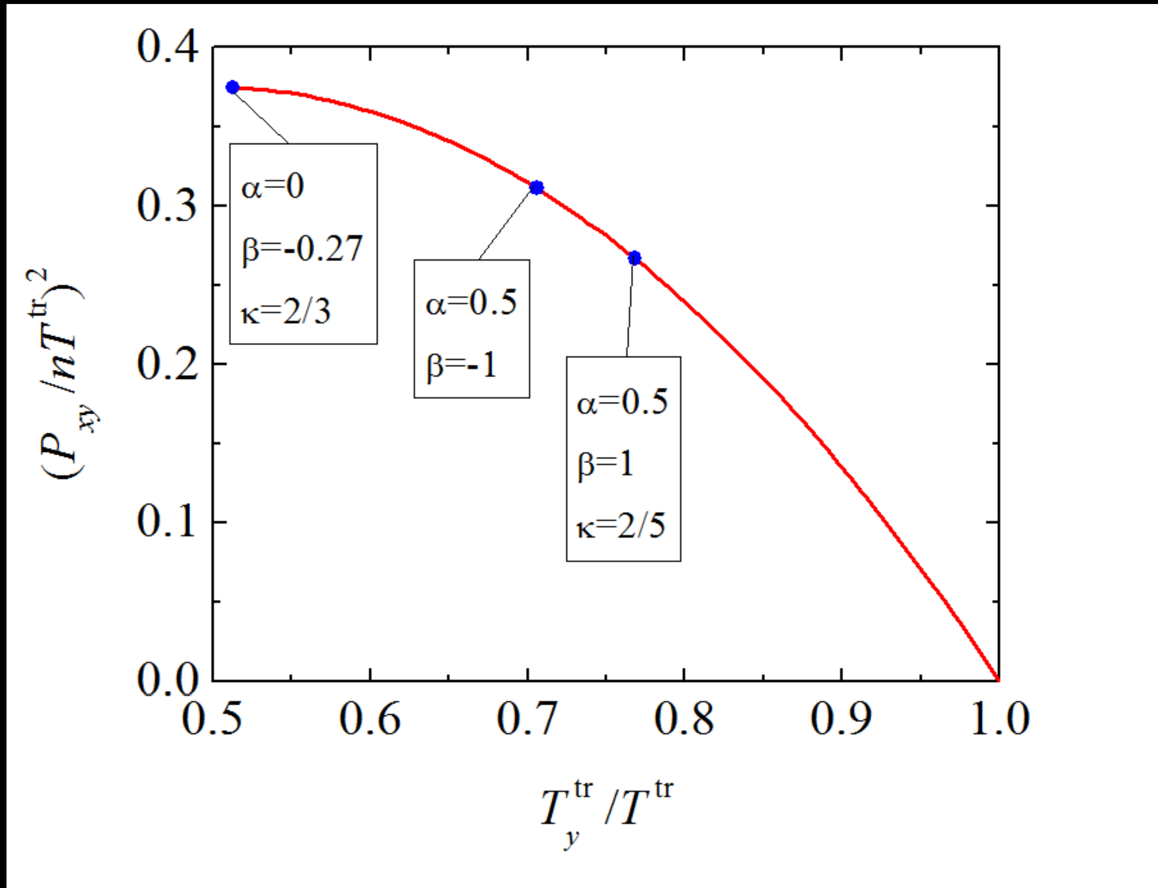

Scaled energy production rate

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

# Application to simple shear flow

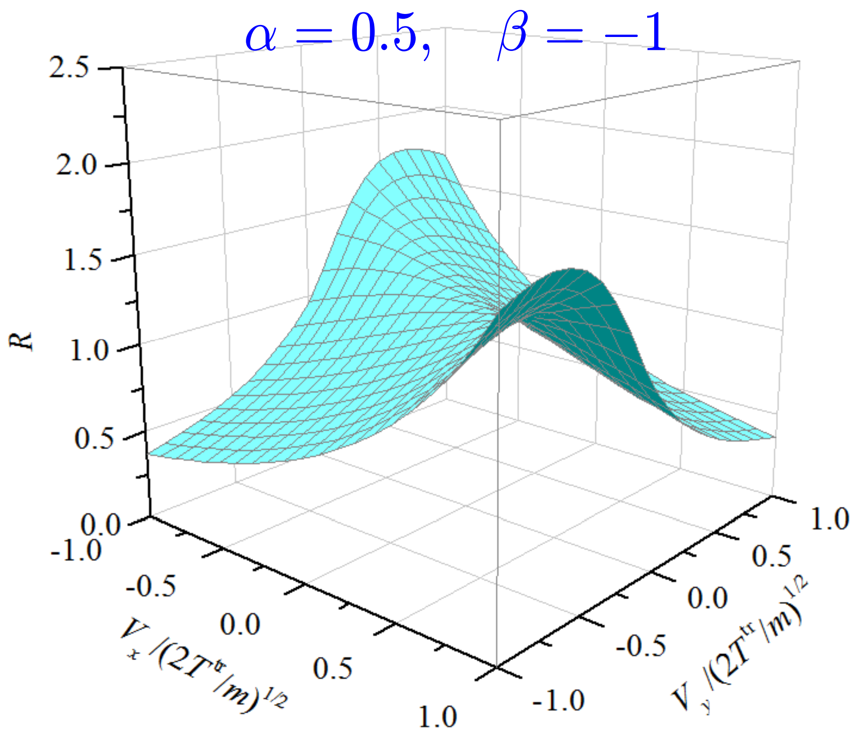
## "Universal" relationship

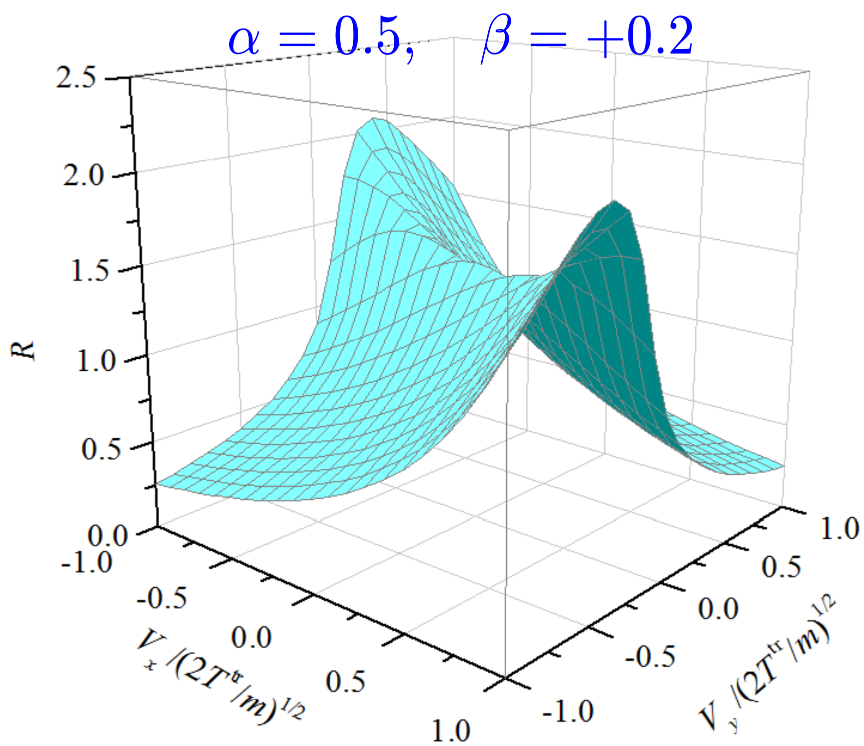
$$\left(\frac{P_{xy}}{nT^{\rm tr}}\right)^2 = \frac{3}{2}\frac{T_y^{\rm tr}}{T^{\rm tr}}\left(1-\frac{T_y^{\rm tr}}{T^{\rm tr}}\right)$$



# Application to simple shear flow

## Velocity distribution function



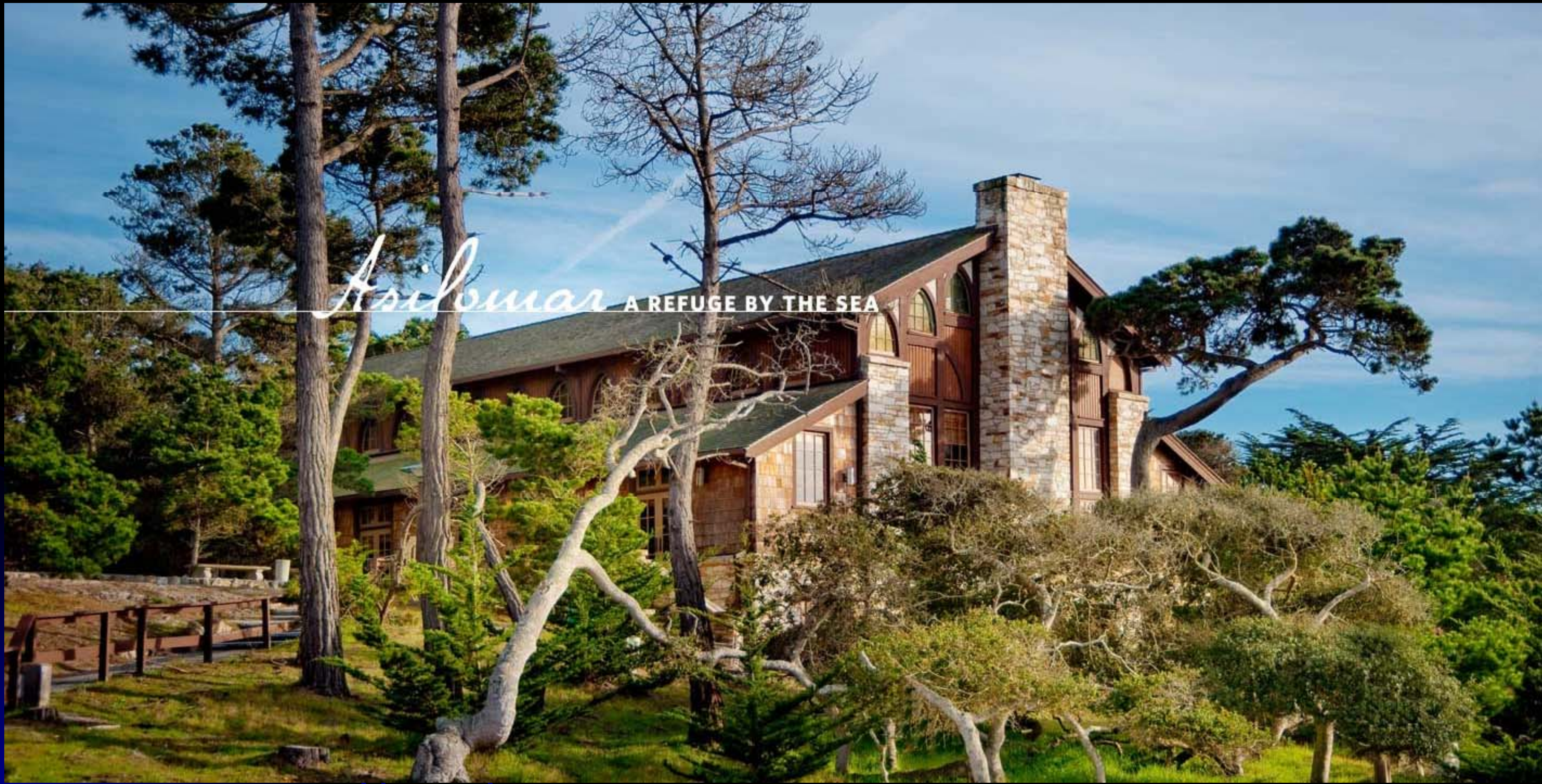




$$R(V_x, V_y) \equiv \frac{\int_{-\infty}^{\infty} dV_z\, f^{\rm tr}(\mathbf{V})}{\int_{-\infty}^{\infty} dV_z\, f_0^{\rm tr}(\mathbf{V})}$$

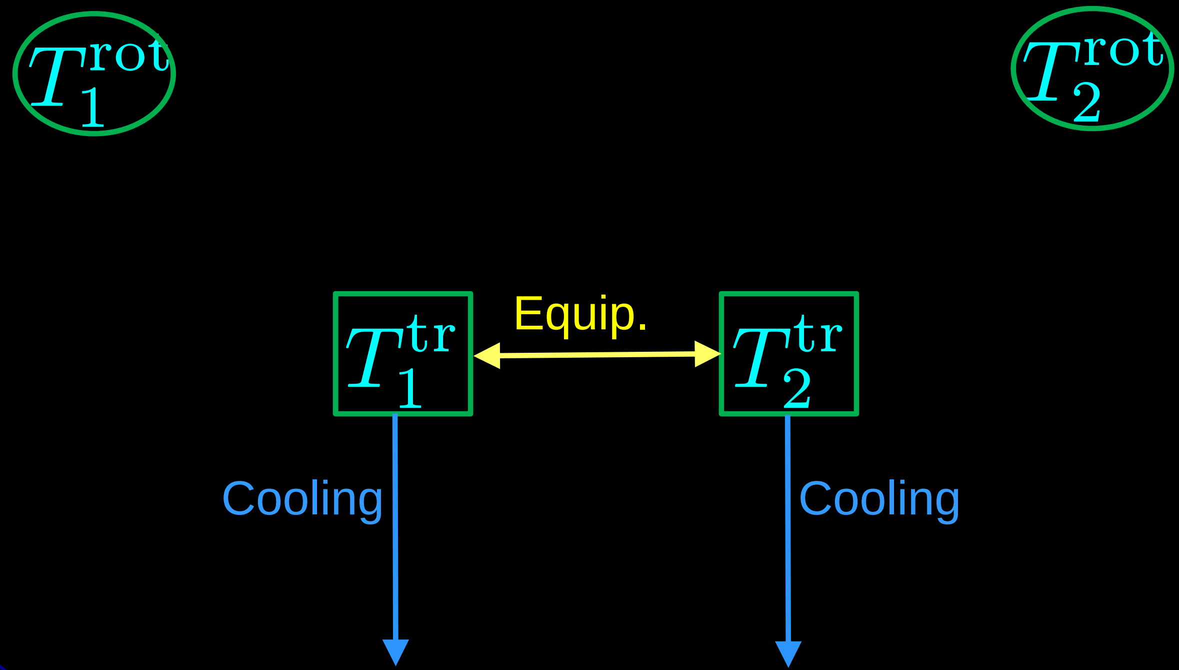
# Conclusions and outlook

- Collisional energy production rates obtained for mixtures of inelastic rough hard spheres.
- Homogeneous cooling state: Paradoxical effect in the quasi-smooth limit.
- 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 simple shear flow. Simulations planned.
- Application of the model to other states (Couette flow, force-driven Poiseuille flow, uniform longitudinal flow, …)
- Derivation of the Navier-Stokes constitutive equations.

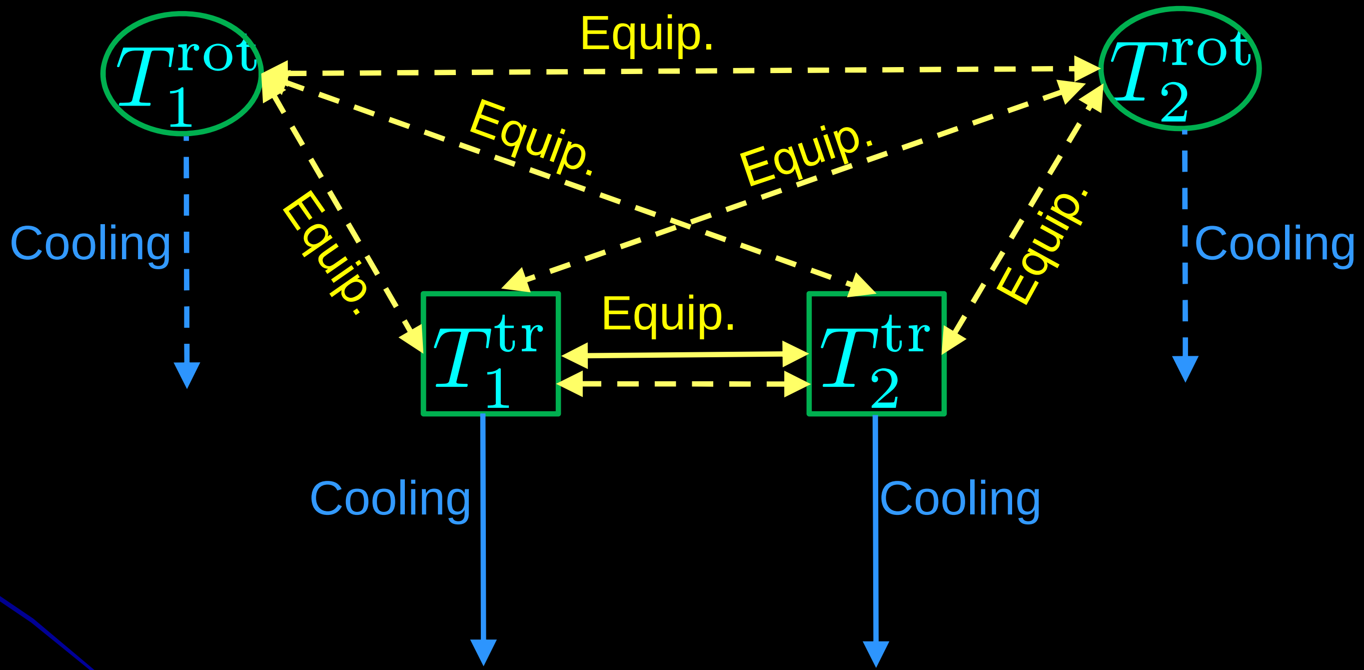
# Thanks for your attention!



# Homogeneous Free Cooling State. Smooth spheres ($\beta$=-1)



# Homogeneous Free Cooling State. Quasi-smooth spheres ($\beta \gtrsim$-1)



# “Ghost” effect in the limit $\beta \to -1$ Time evolution