Influence of particle roughness on some properties of granular gases

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In collaboration with
Gilberto M. Kremer and Vicente Garzó

El fluido de esferas penetrables. Teoría y simulación

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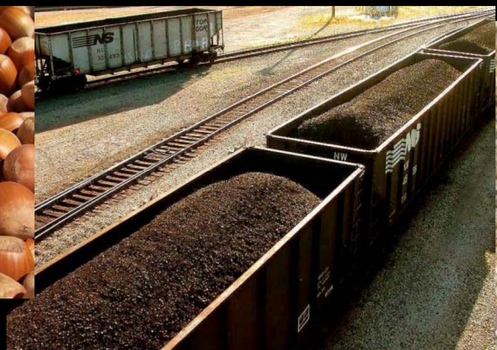
SPhinX
STATISTICAL PHYSICS in EXTREMADURA

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?

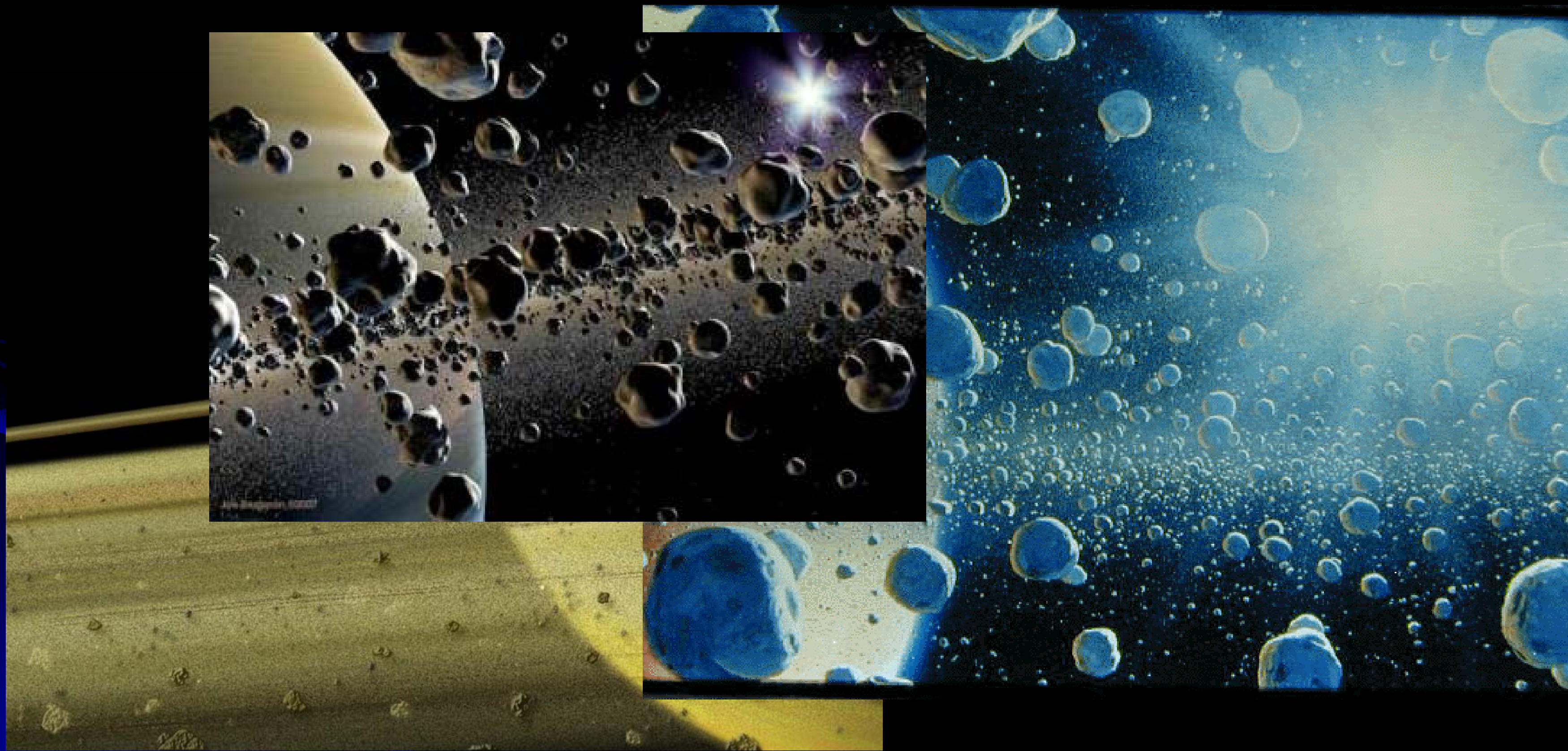
- Examples of granular materials would include nuts, coal, sand, rice, coffee, corn flakes, fertilizer, ball bearings, …




What is a granular material?

- … and even Saturn’s rings

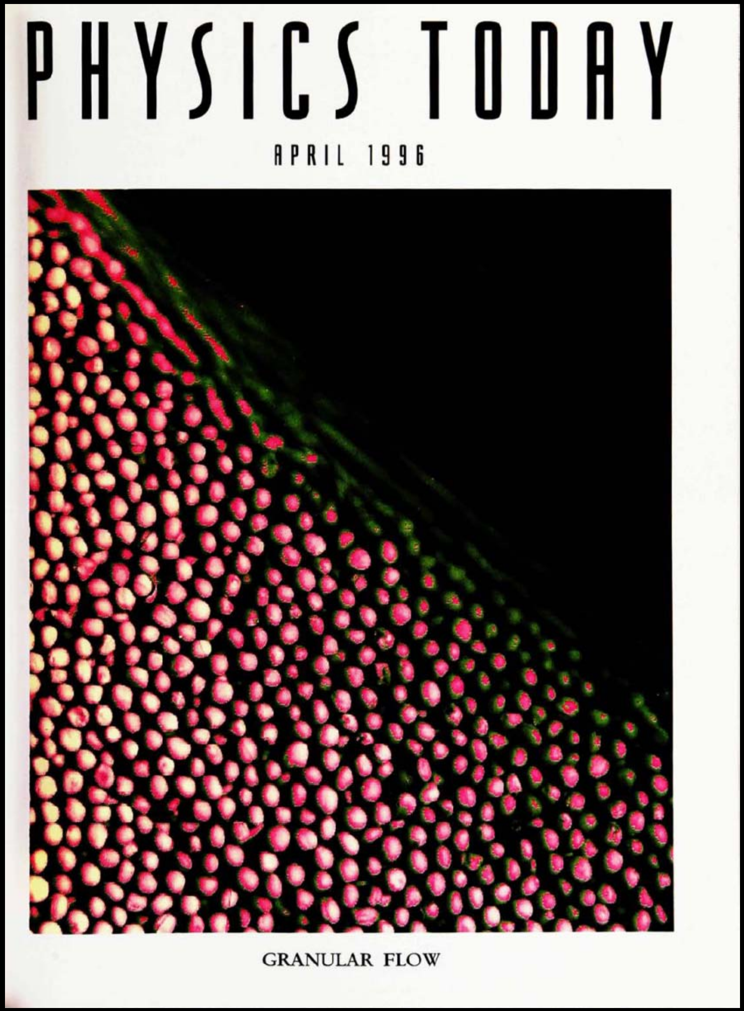


What is a granular material?

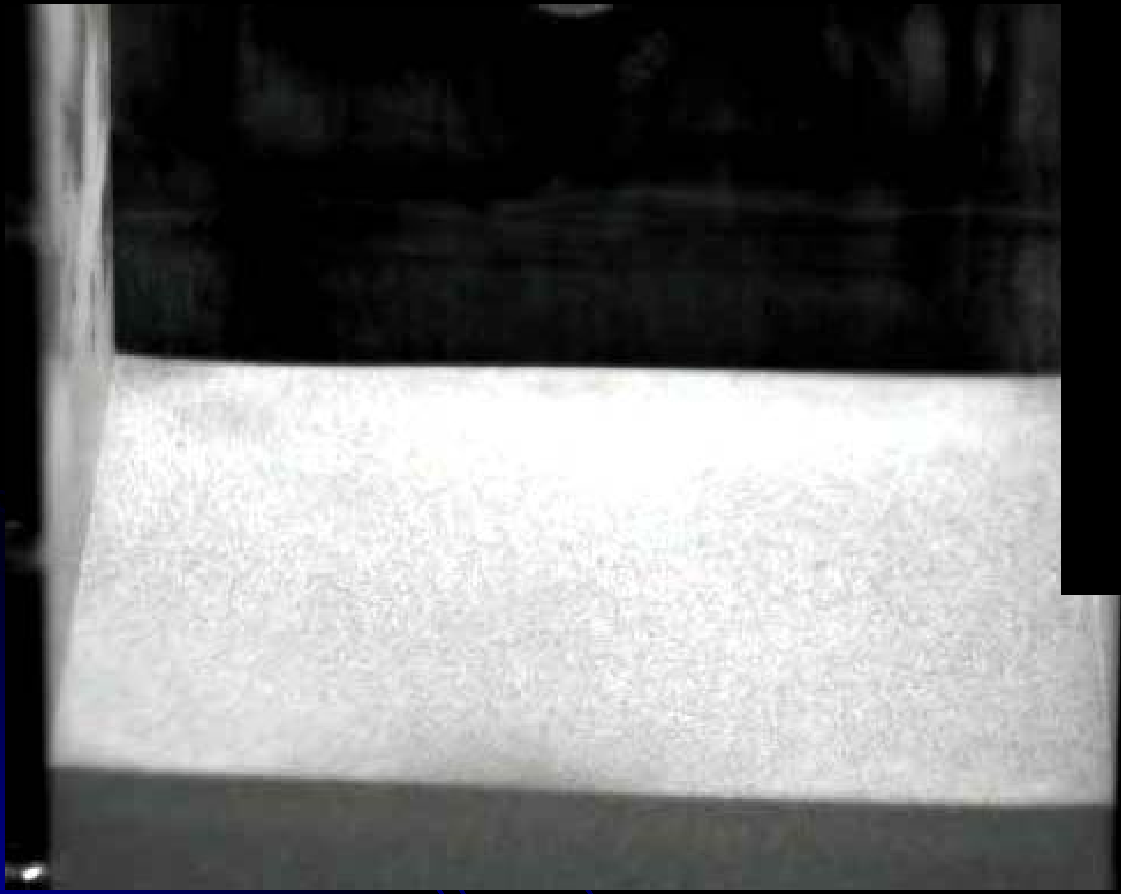
- Granular materials are commercially important in applications as diverse as pharmaceutical industry, agriculture, and energy production.
- They are ubiquitous in nature and are the second-most manipulated material in industry (the first one is water).

What is a granular *fluid*?

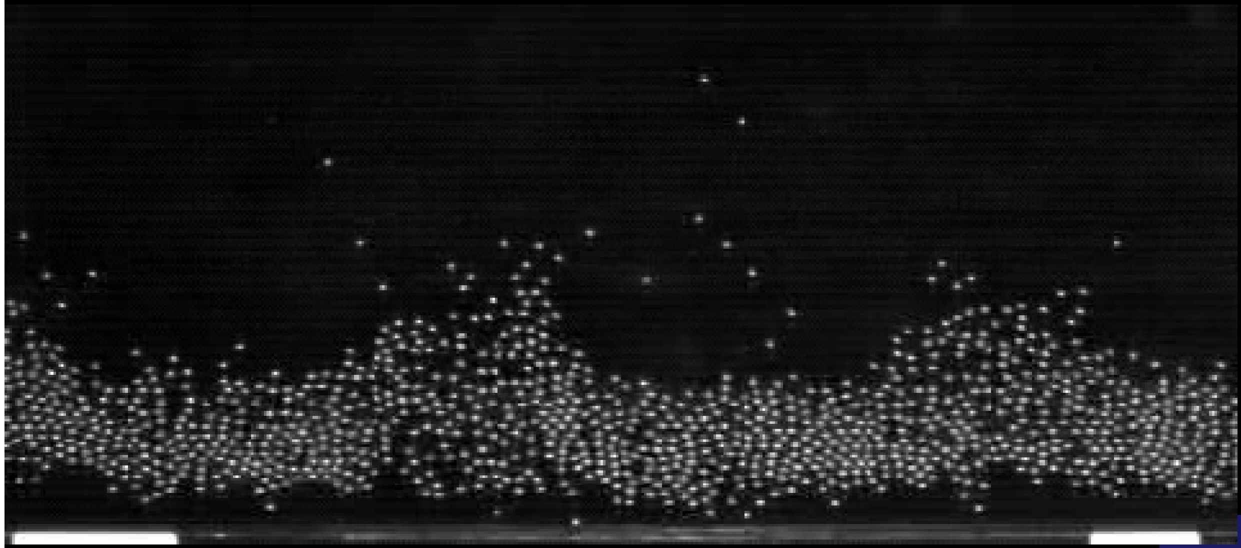
- When the granular matter is driven and energy is fed into the system (e.g., by shaking) such that the grains are not in constant contact with each other, the granular material is said to *fluidize*.



Granular fluids (or gases) exhibit many interesting phenomena:

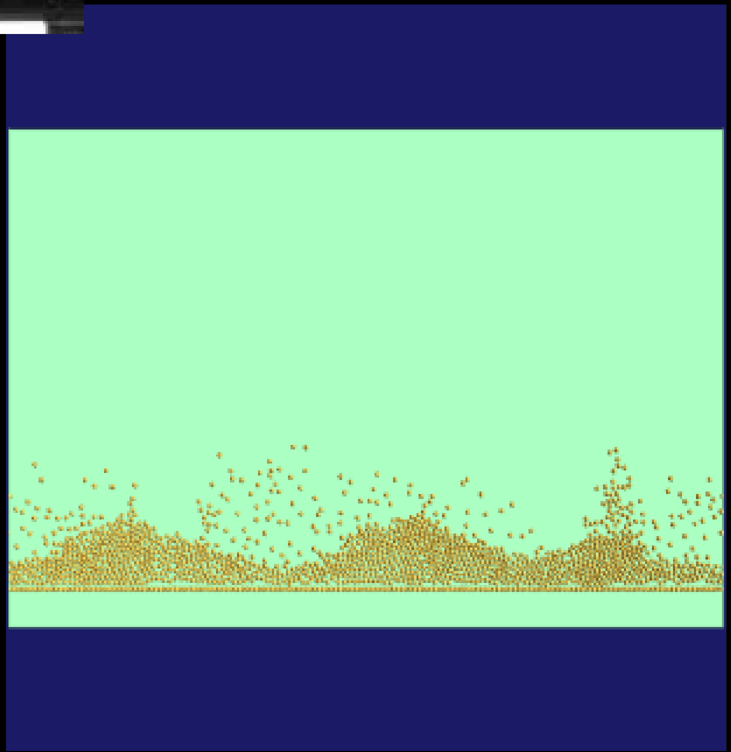


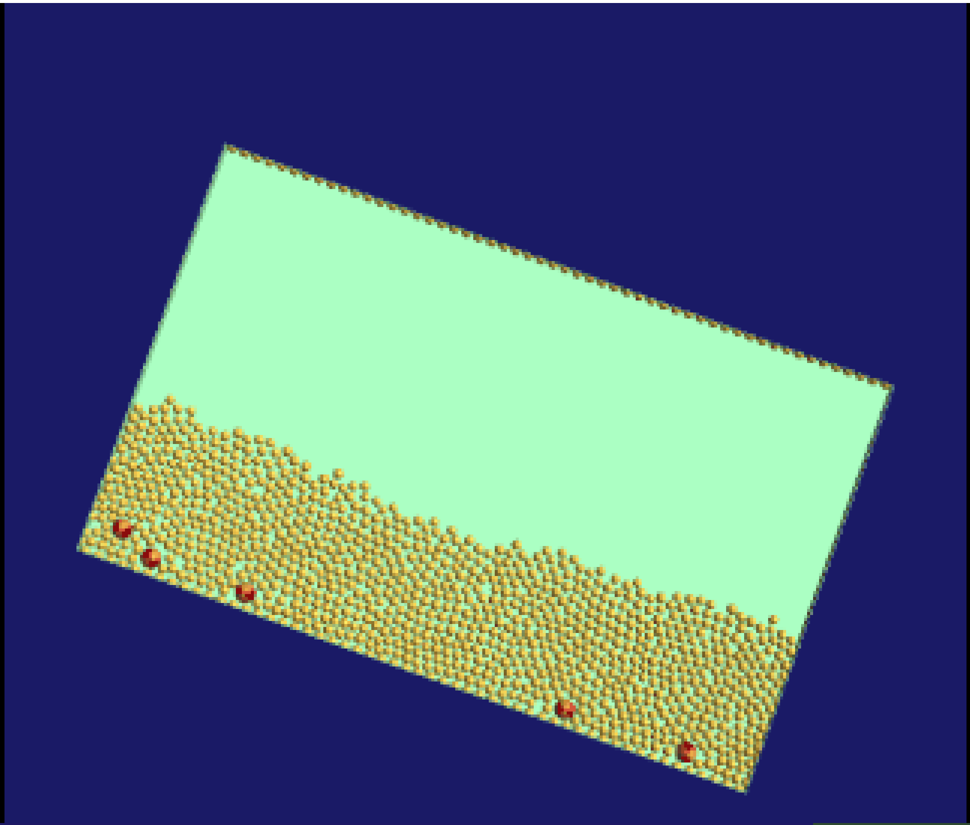
Granular eruptions (from University of Twente's group)



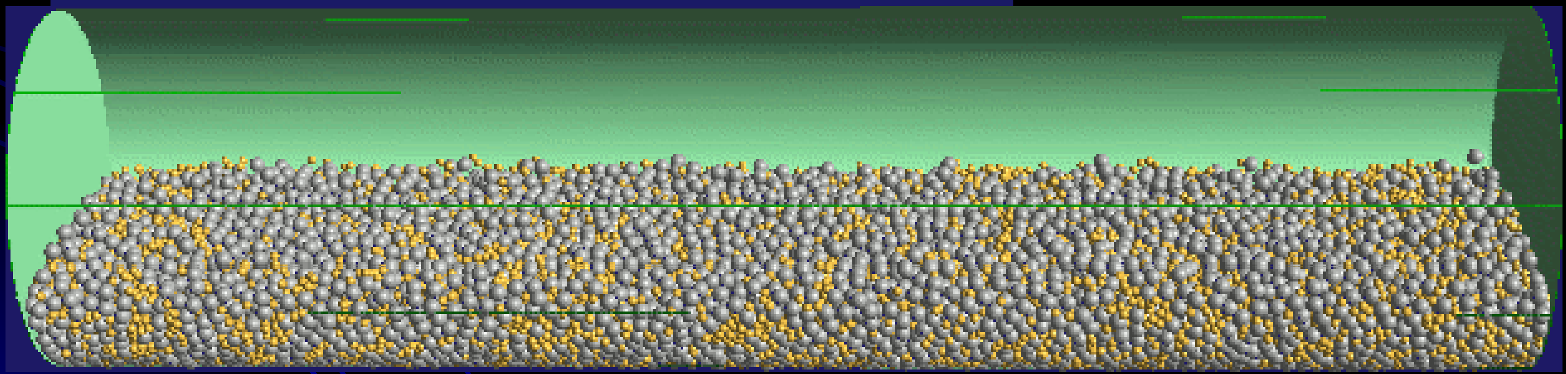
Wave patterns in a vibrated container
(from A. Kudrolli's group)

(Simulations by D. C. Rapaport)



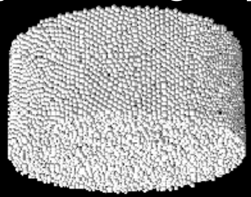


Segregation in sheared flow
(Simulations by D. C. Rapaport)

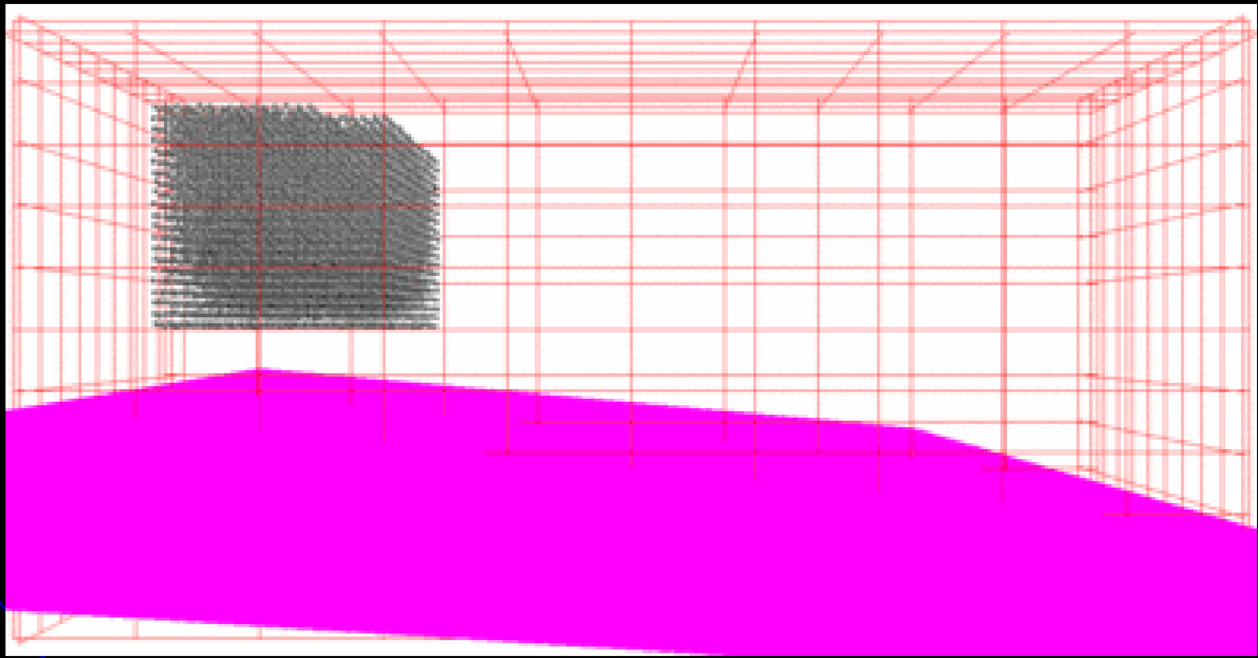


Segregation in a rotating cylinder
(Simulations by D. C. Rapaport)

Granular jet hitting a plane

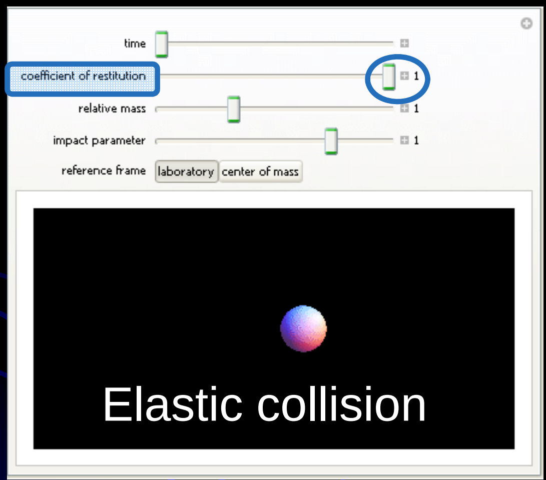


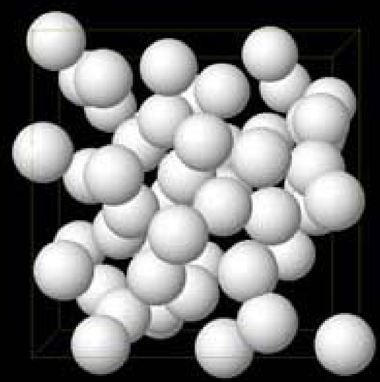
Particles falling on an inclined heated plane

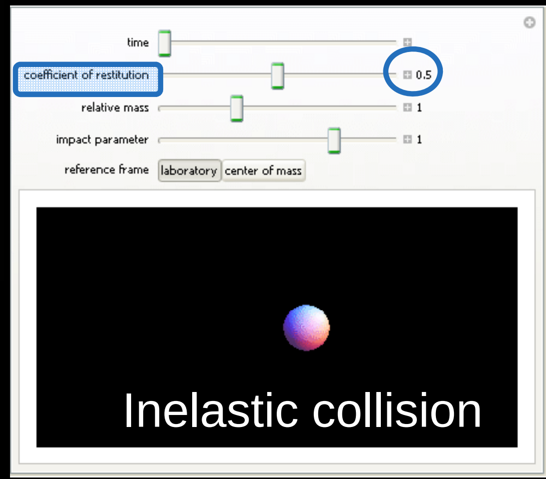


http://trevinca.ei.uvigo.es/~formella/

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



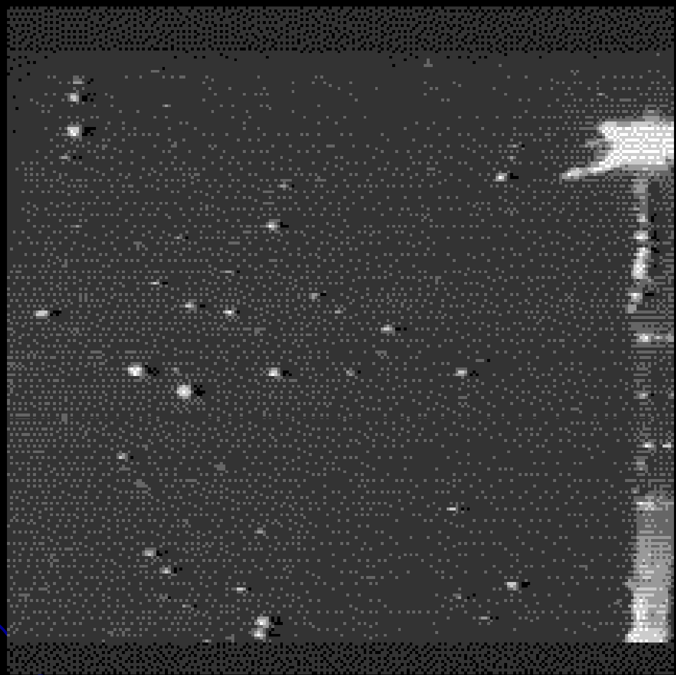




http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/

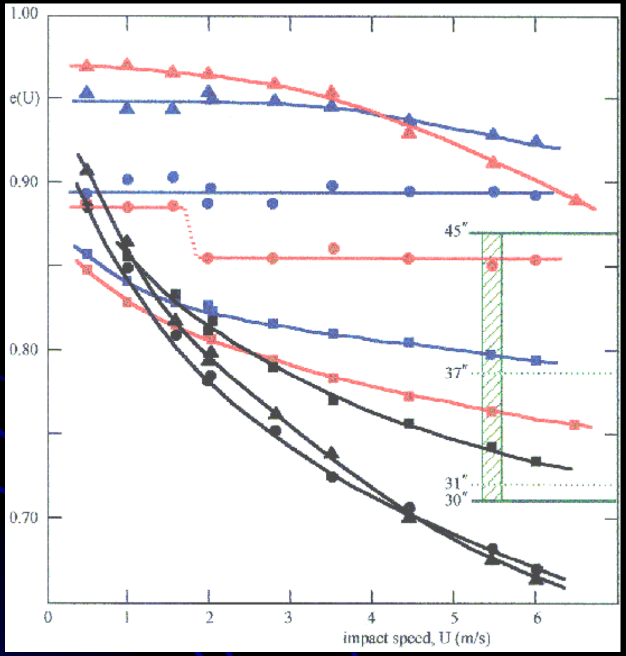
This minimal model ignores …

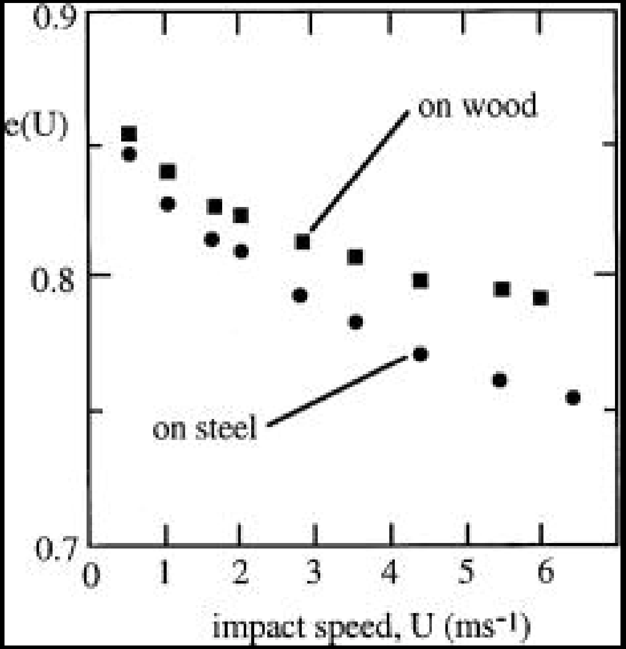
Interstitial fluid



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

Non-constant coefficient of restitution

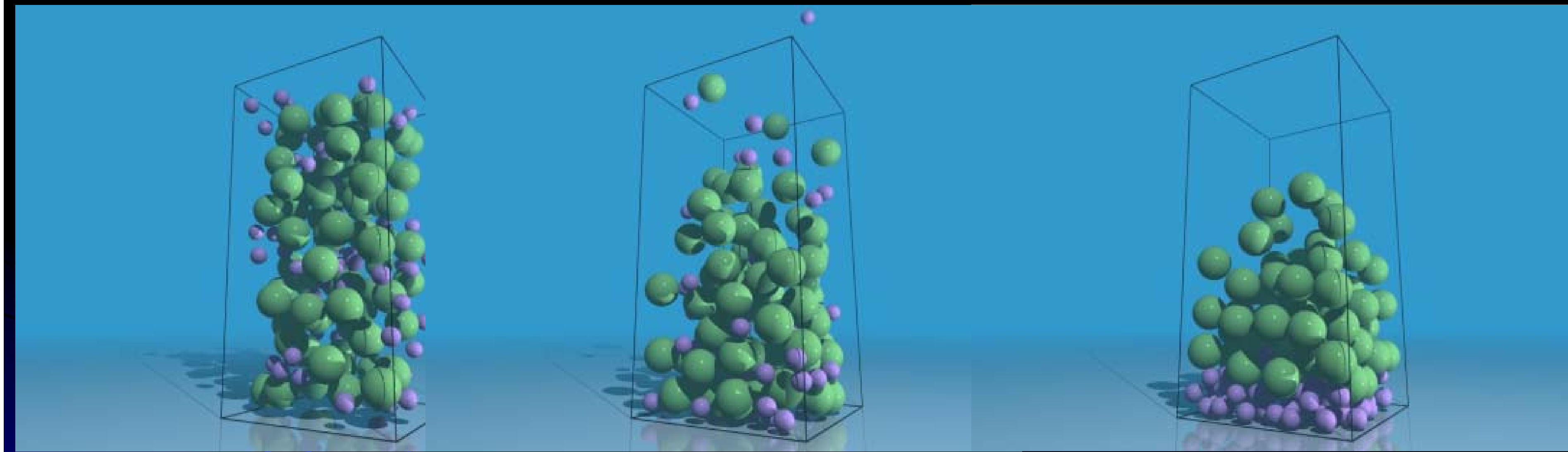




www.oxfordcroquet.com/tech/

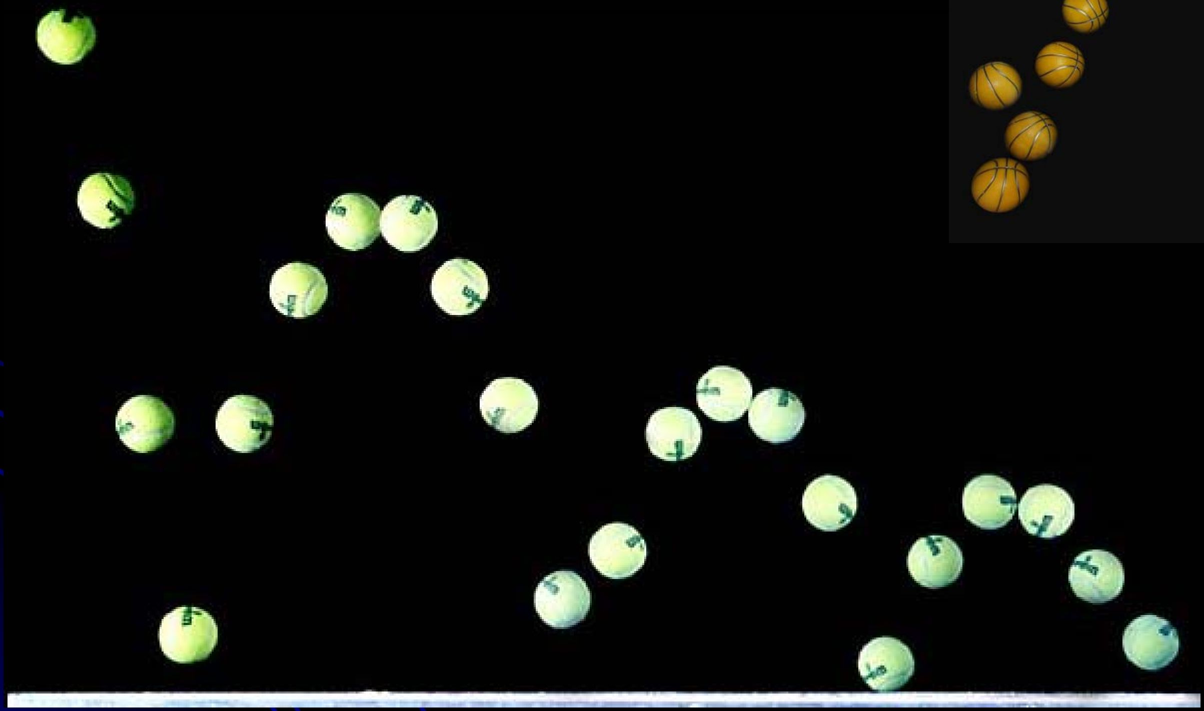
Non-spherical shape

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

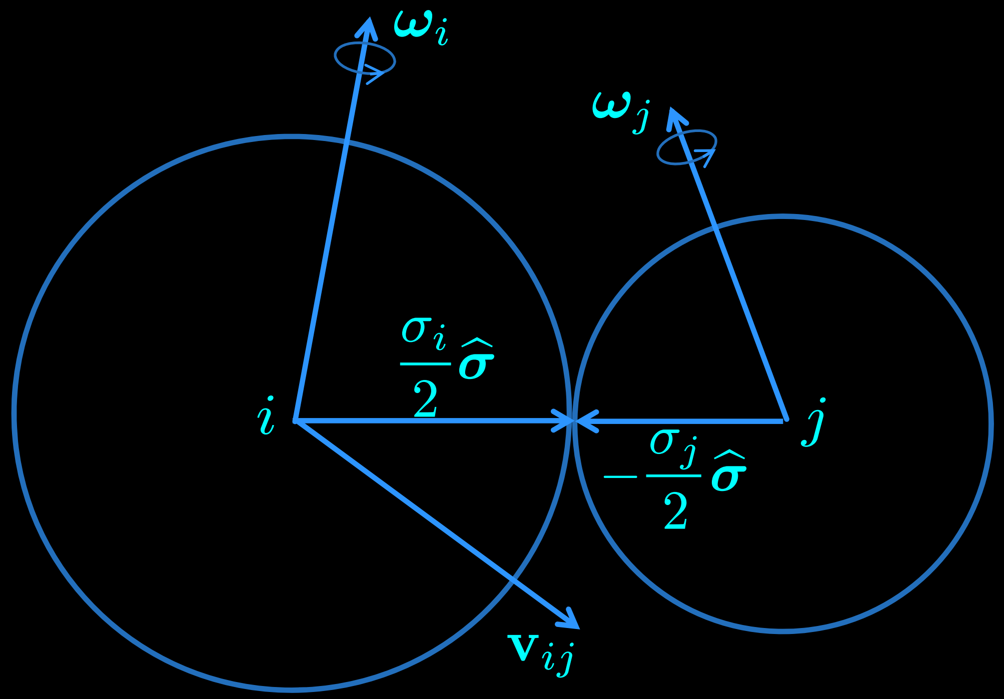
- (Collisional) energy production rates in a mixture of inelastic rough hard spheres.
- Application to the homogeneous free cooling state.
- Simple kinetic model for monodisperse systems.
- Application to the simple shear flow.
- Conclusions and outlook.

I. Collisional energy production rates in a mixture of inelastic rough hard spheres

Material parameters:

- 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 perfectly elastic particles
- $\beta_{ij} = -1$ for perfectly smooth particles
- $\beta_{ij} = +1$ for perfectly rough particles

Collision rules



Notation: $\widetilde{\alpha}_{ij} \equiv m_{ij}\left(1+\alpha_{ij}\right), \quad \widetilde{\beta}_{ij} \equiv \frac{m_{ij}\kappa_{ij}}{1+\kappa_{ij}}\left(1+\beta_{ij}\right)$

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

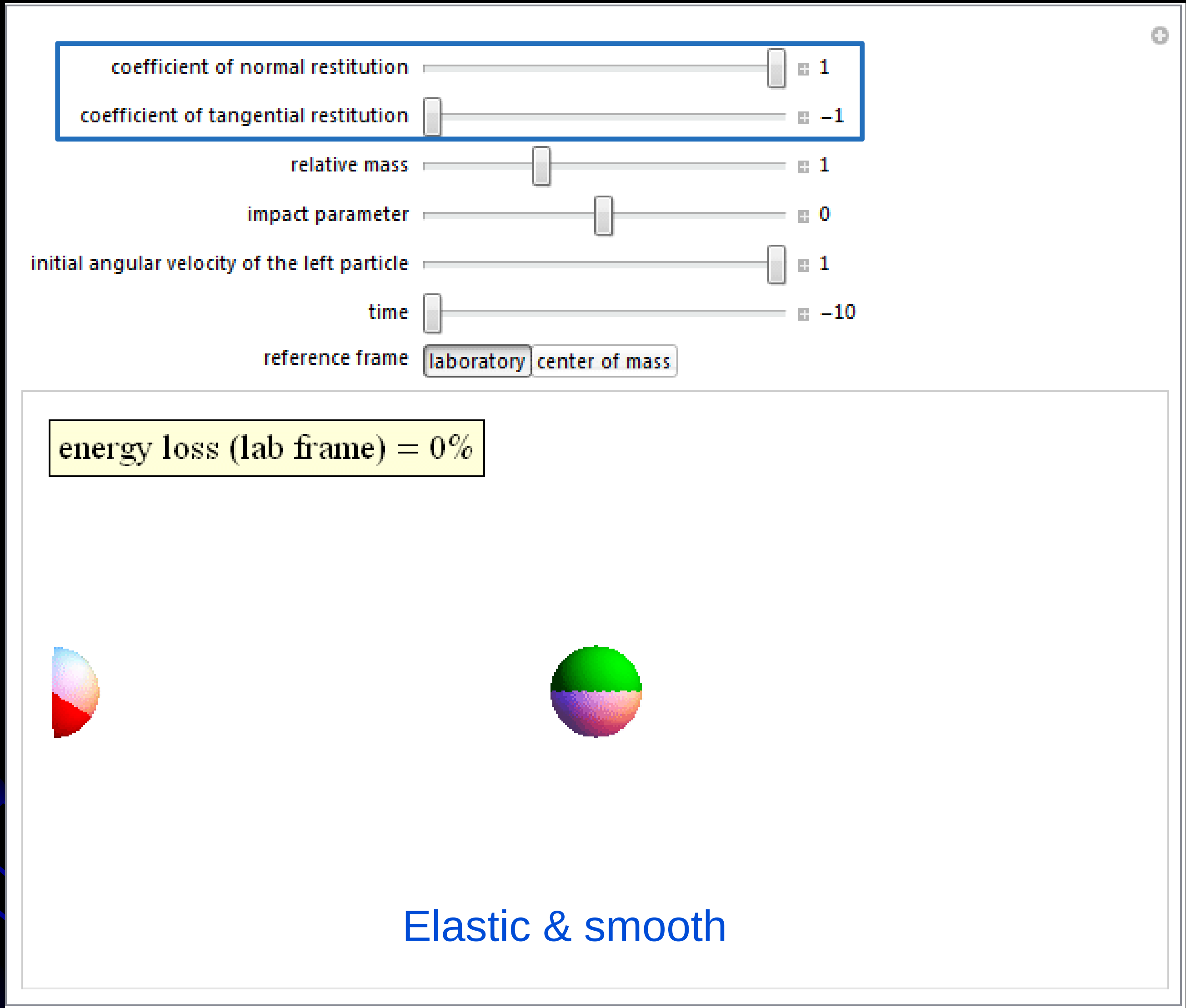
Energy collisional loss

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

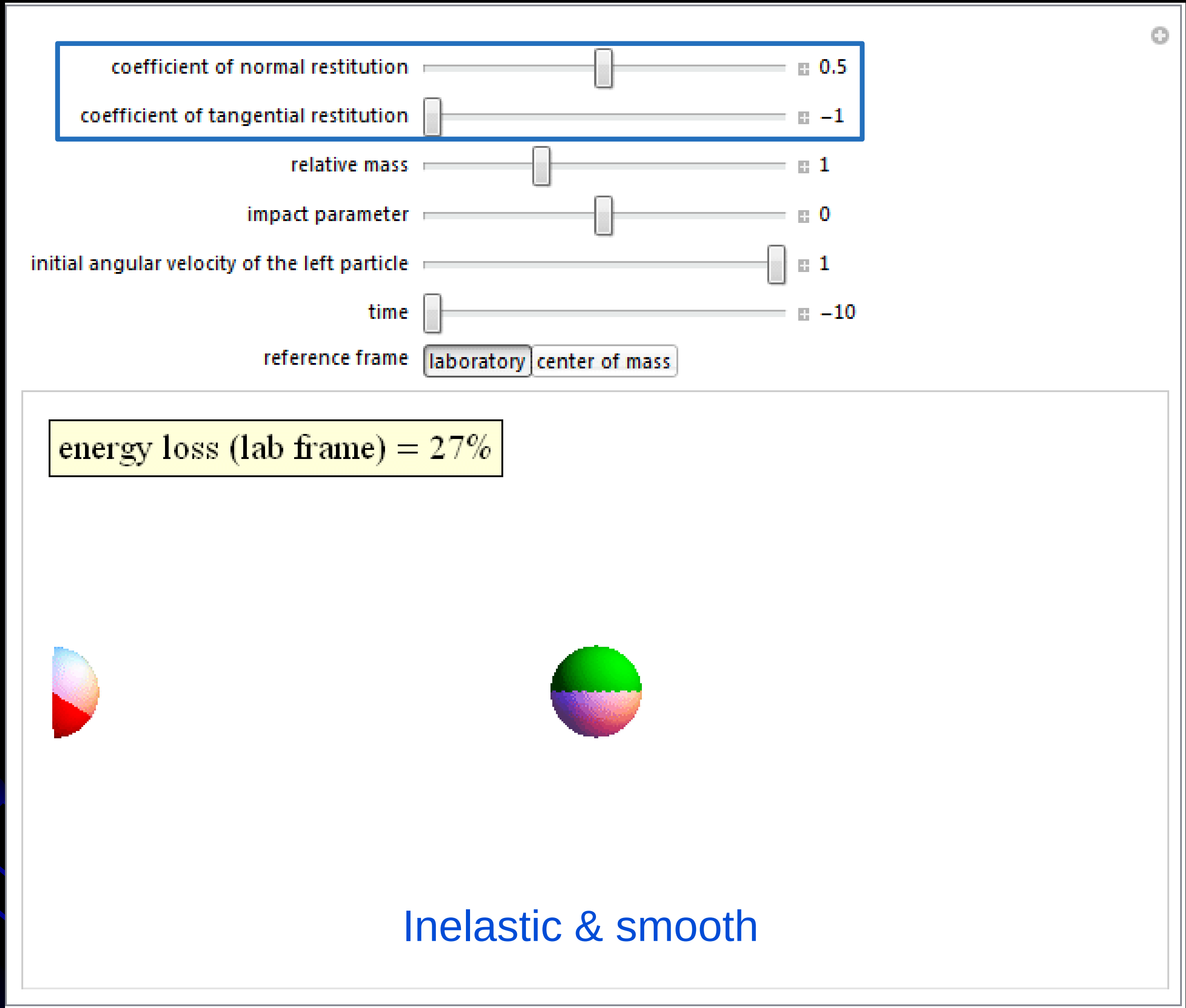
$$\begin{aligned} E'_{ij} - E_{ij} &= -(1-\alpha_{ij}^2)\times\cdots \\ &\quad -(1-\beta_{ij}^2)\times\cdots \end{aligned}$$

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)



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



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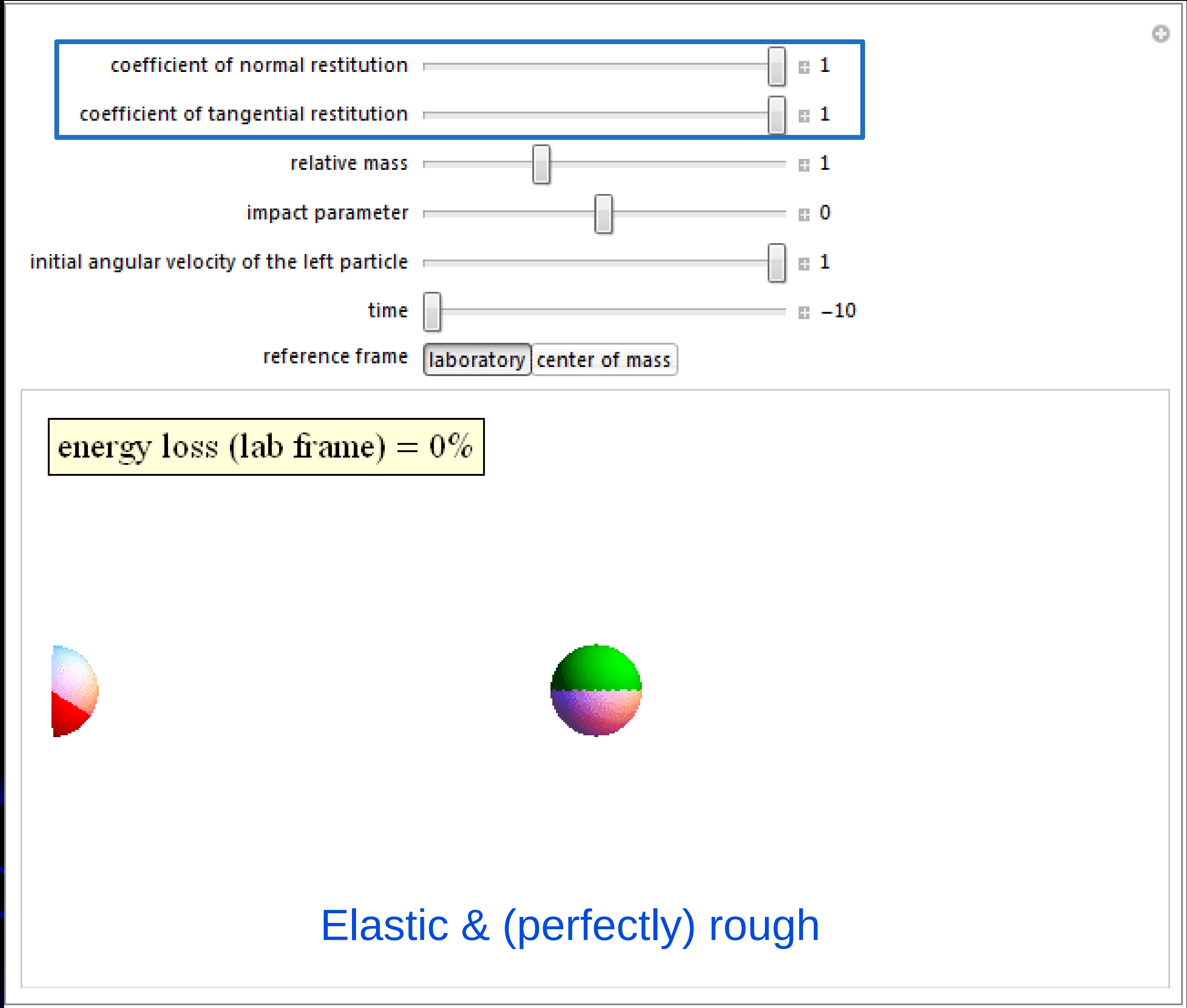

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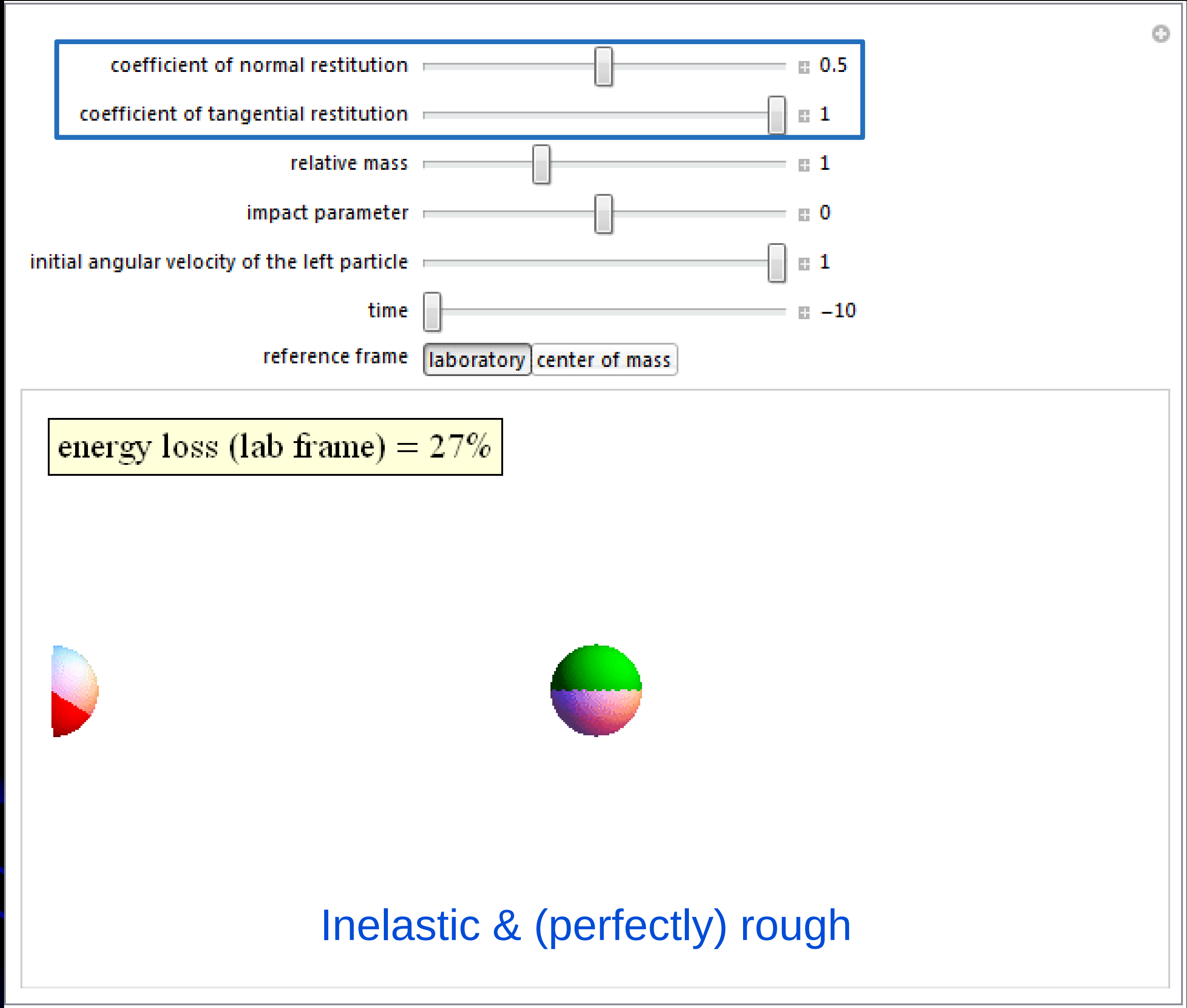

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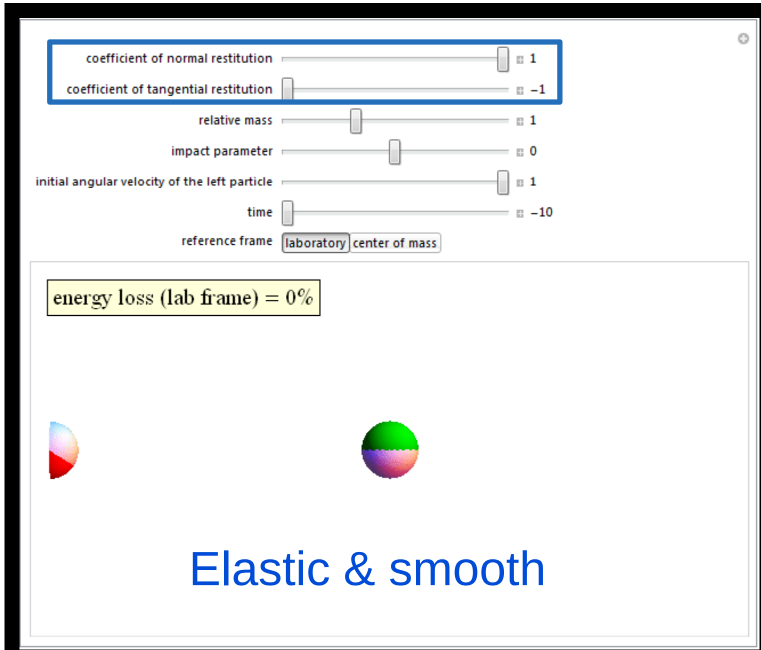
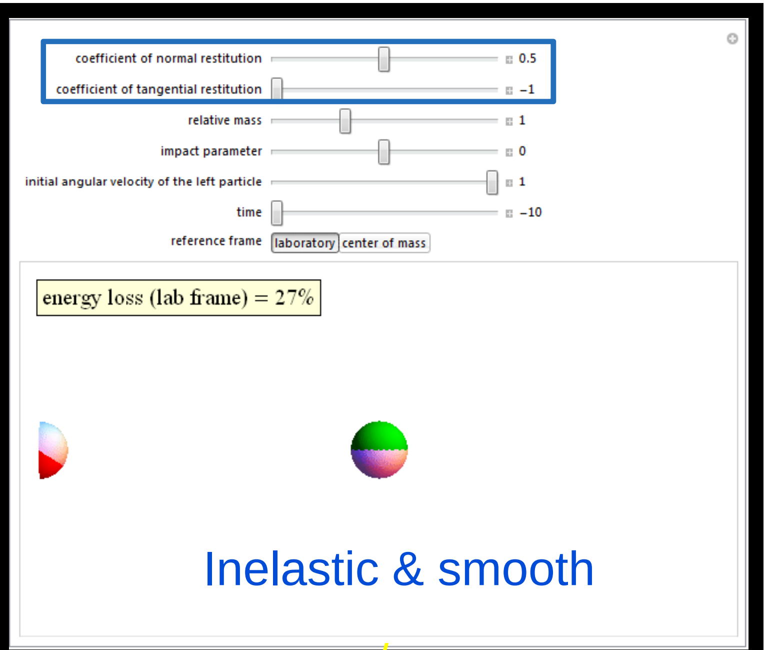
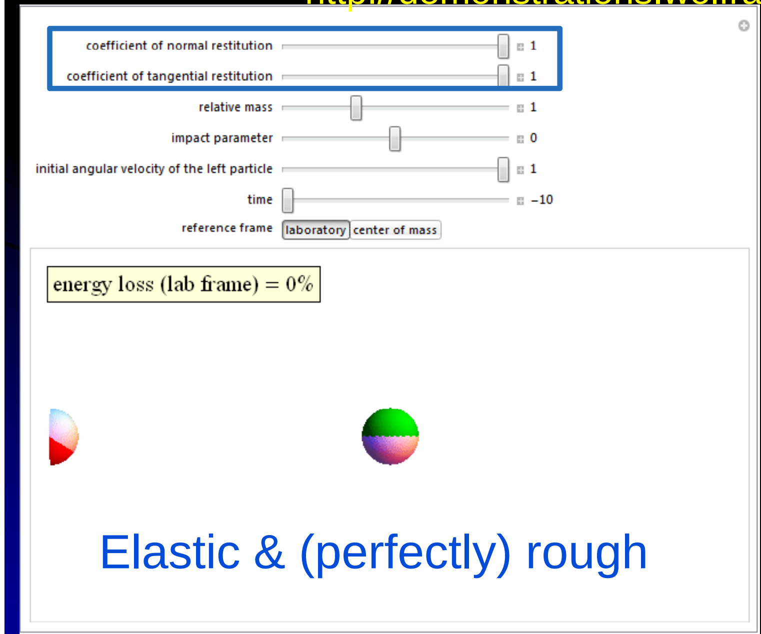


Elastic & smooth

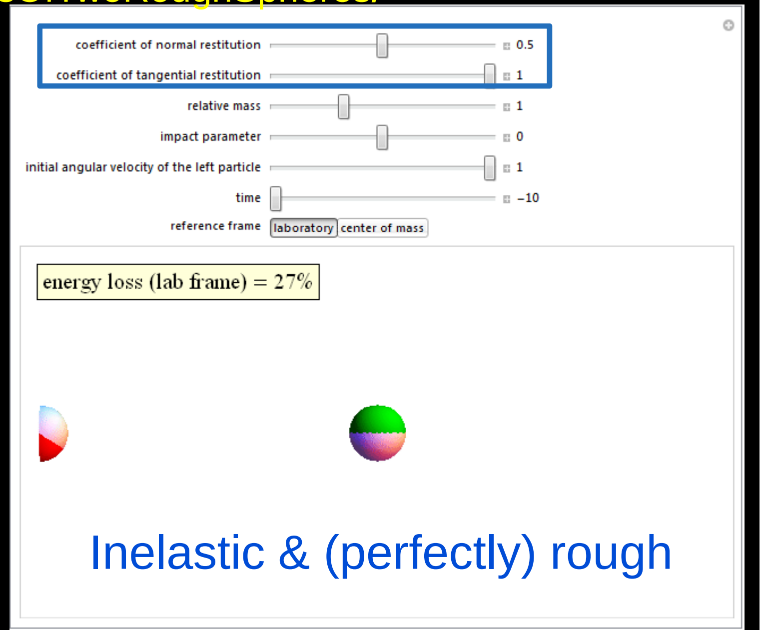


Inelastic & smooth

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



Elastic & (perfectly) rough



Inelastic & (perfectly) rough

Partial (granular) temperatures

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

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

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

Collisional rates of change for temperatures

Energy production rates:

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

Binary collisions

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

Net *cooling* rate:

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

Energy production rates. Scheme of the derivation

[A.S., G.M. Kremer, V. Garzó (2010)]

Collision rules

↓ 1st BBGKY equation

1. Formally exact expressions

↓ $f_{ij}^{(2)} \to \bar{f}_{ij}^{(2)} \equiv \langle f_{ij}^{(2)} \rangle_\Omega$

2. Two-body averages

↓ Information-theory estimate of $\bar{f}_{ij}^{(2)}$

3. Final results

Two-body velocity distribution function:

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

Molecular chaos+Maxwellian approx. for translational distribution

Final results.
Energy production rates

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

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

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

Final results.
Net cooling rate

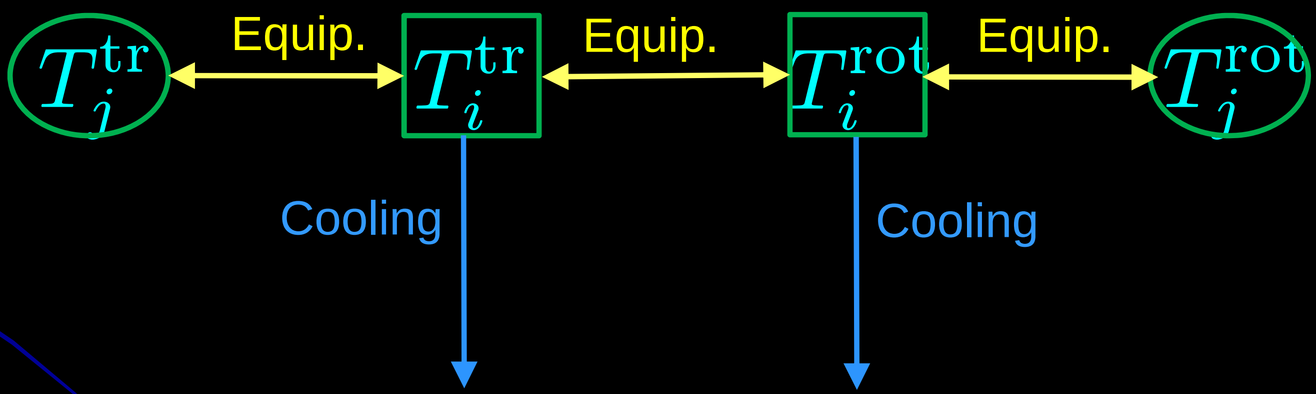
$$\zeta = \sum_i \frac{n_i}{2nT}\left(\xi_i^{\mathrm{tr}} T_i^{\mathrm{tr}} + \xi_i^{\mathrm{rot}} T_i^{\mathrm{rot}}\right)$$

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

Decomposition

Energy production rates = Equipartition rates + Cooling rates

Net cooling rate = Σ Cooling rates



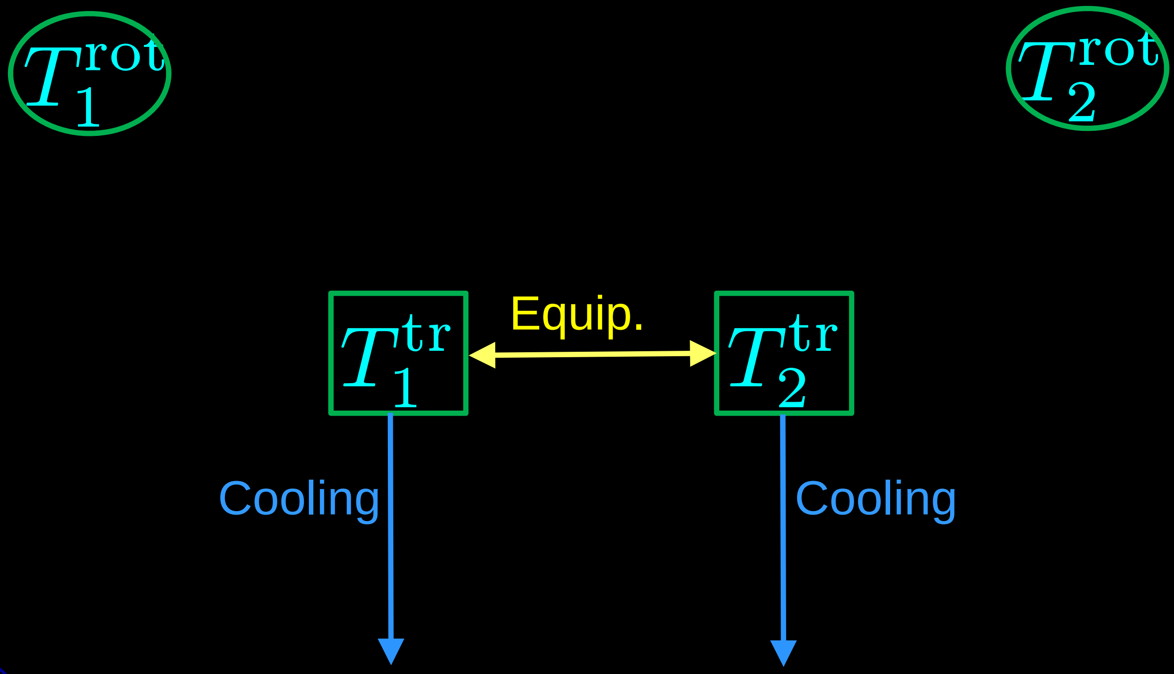
Simple application:
Homogeneous Free Cooling State

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

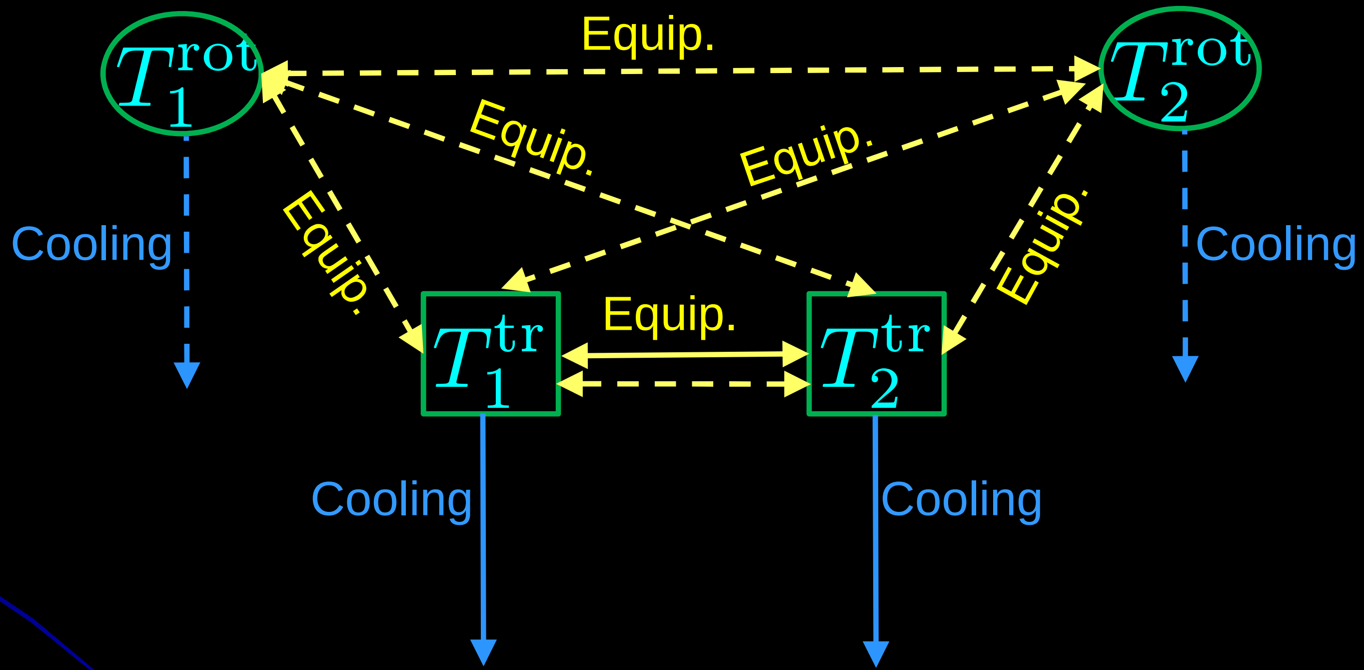
$$\frac{\partial}{\partial t}\frac{T_i^{\mathrm{tr}}}{T} = -\left(\xi_i^{\mathrm{tr}} - \zeta\right)\frac{T_i^{\mathrm{tr}}}{T}, \qquad \frac{\partial}{\partial t}\frac{T_i^{\mathrm{rot}}}{T} = -\left(\xi_i^{\mathrm{rot}} - \zeta\right)\frac{T_i^{\mathrm{rot}}}{T}$$

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

Inelastic smooth spheres (β=-1)

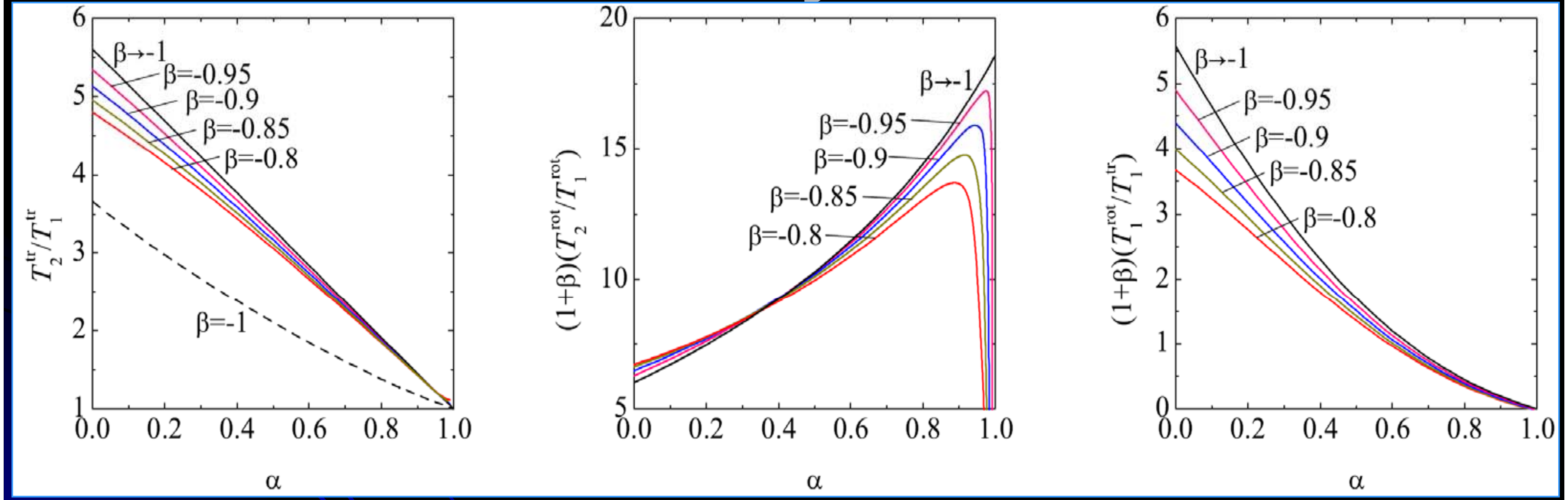


Inelastic quasi-smooth spheres ($\beta \lesssim$-1)



Paradoxical "ghost" effect in the limit $\beta \to -1$ Stationary values

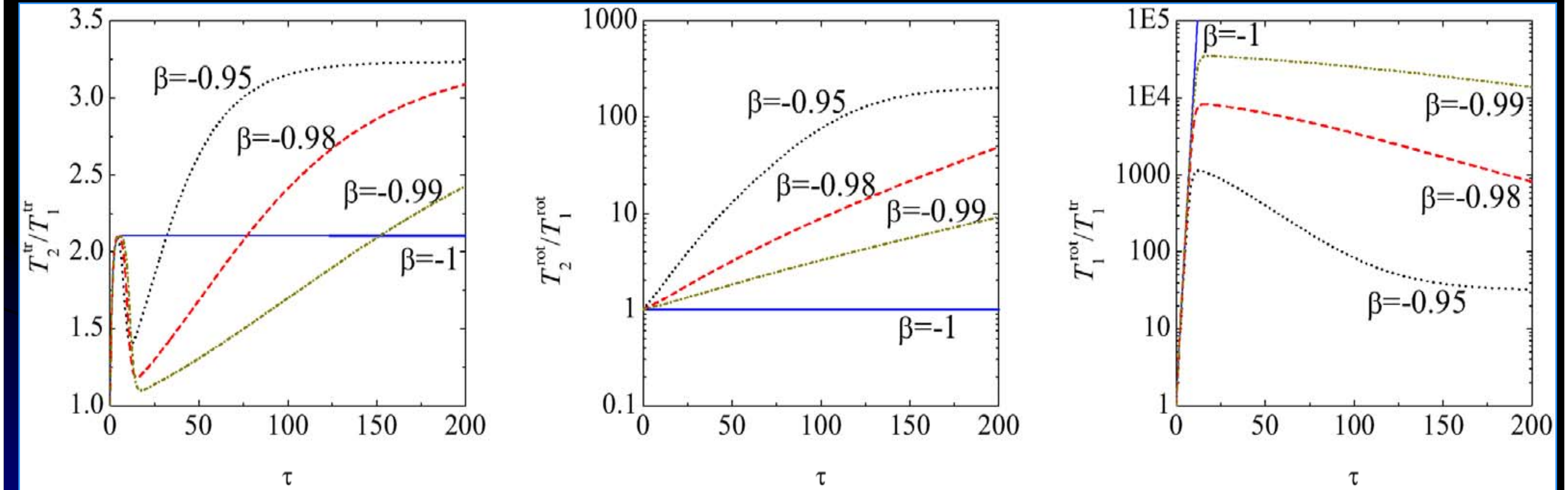
A.S. (2011)



$$n_2 = n_1, \quad m_2/m_1 = 8, \quad \sigma_2/\sigma_1 = 2, \quad \alpha = 0.5$$

Paradoxical "ghost" effect in the limit $\beta \to -1$ Time evolution

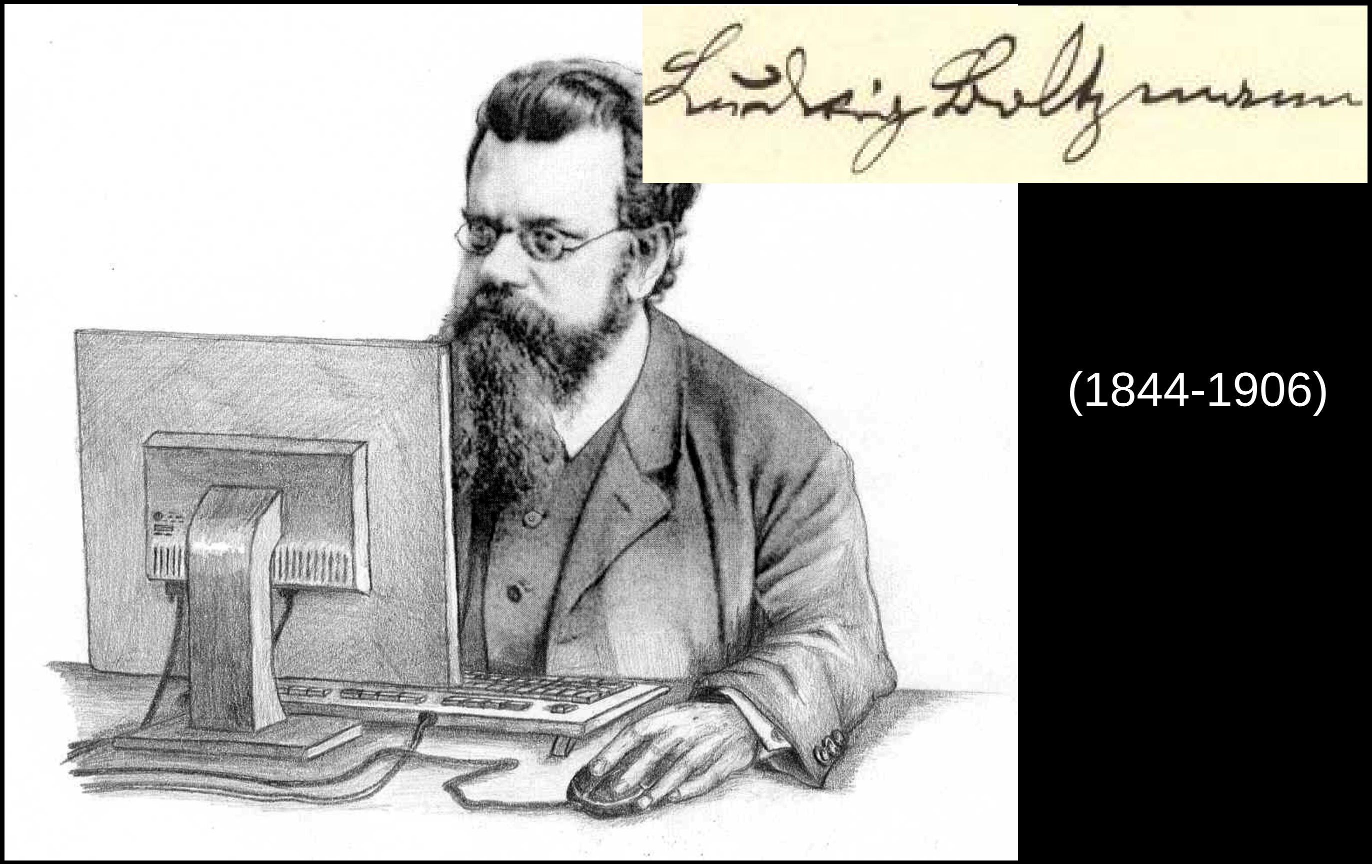
A.S. (2011)



$$n_2 = n_1, \quad m_2/m_1 = 8, \quad \sigma_2/\sigma_1 = 2, \quad \alpha = 0.5$$

II. A simple kinetic model for *monodisperse* inelastic rough hard spheres

(Cartoon by Bernhard Reischl, University of Vienna)



(1844-1906)

Boltzmann equation:

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

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]

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

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

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

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

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

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

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

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

The kinetic model. Joint distribution

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

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

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

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

A simpler version. Marginal distributions

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

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

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

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

An even simpler version. Translational distribution

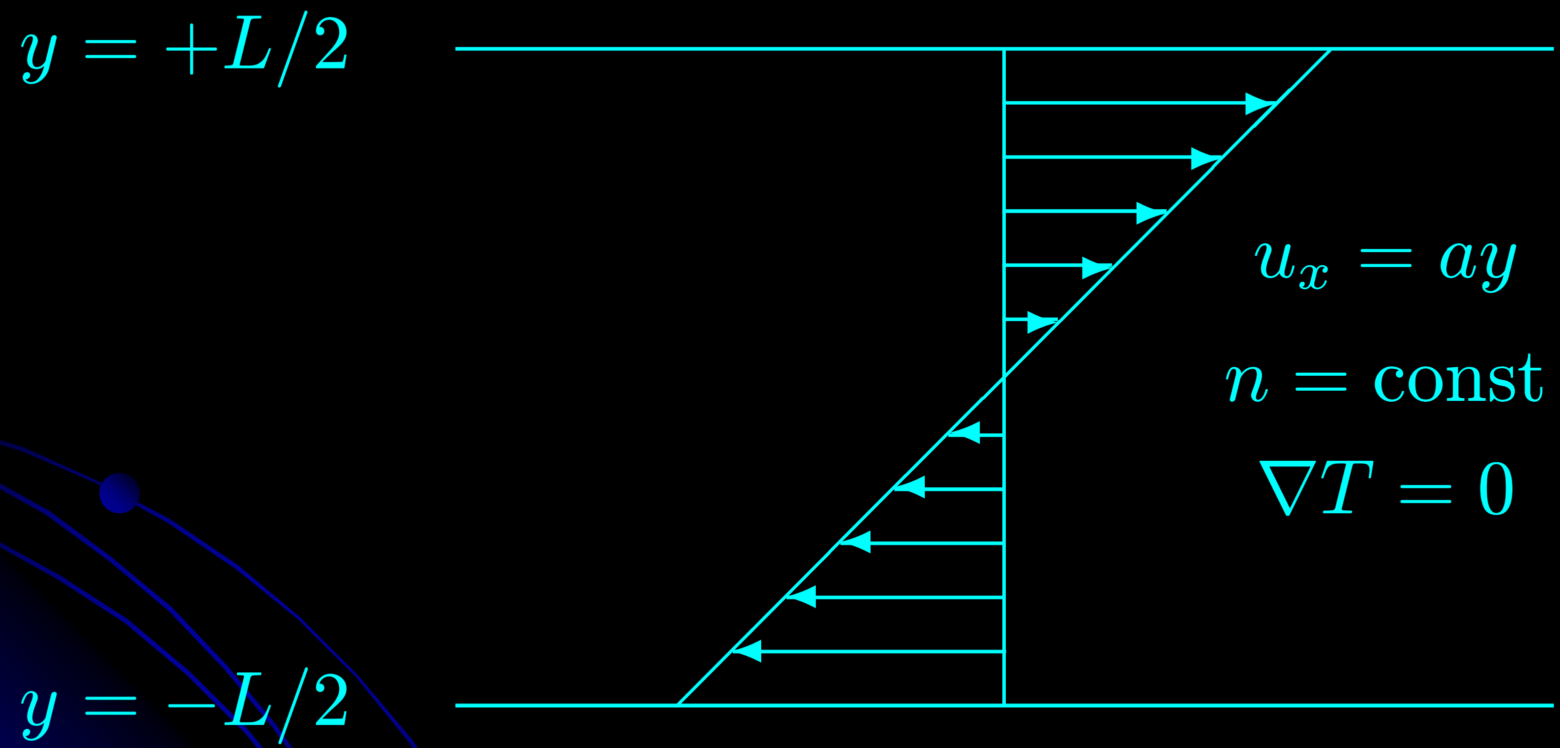
$$f^{\rm tr} = \int d\boldsymbol{\omega}\, f, \quad \boldsymbol{\Omega} = \frac{1}{n}\int d\mathbf{v}\int d\boldsymbol{\omega}\,\boldsymbol{\omega} f, \quad T^{\rm rot} = \frac{I}{3n}\int d\mathbf{v}\int d\boldsymbol{\omega}\,\omega^2 f$$

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

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

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

Application to simple shear flow (steady state)



$$u_x = ay$$

$$n = \mathrm{const}$$

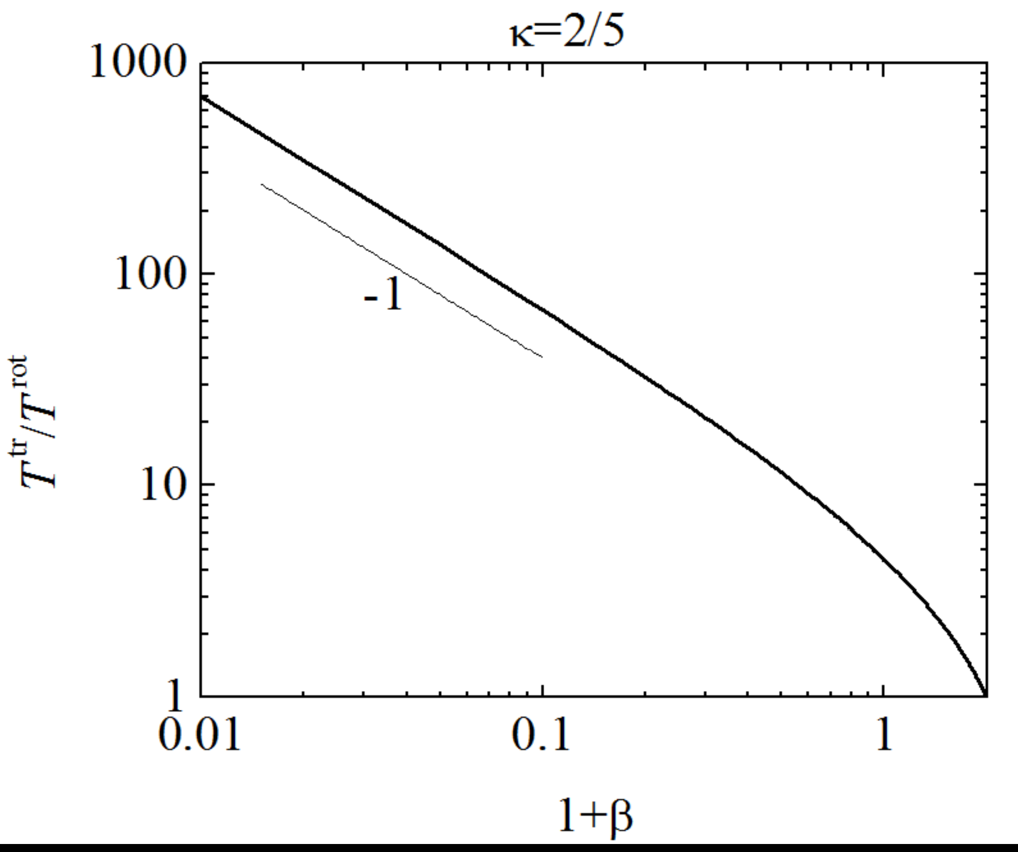
$$\nabla T = 0$$

Application to simple shear flow

Translational/Rotational temperature ratio

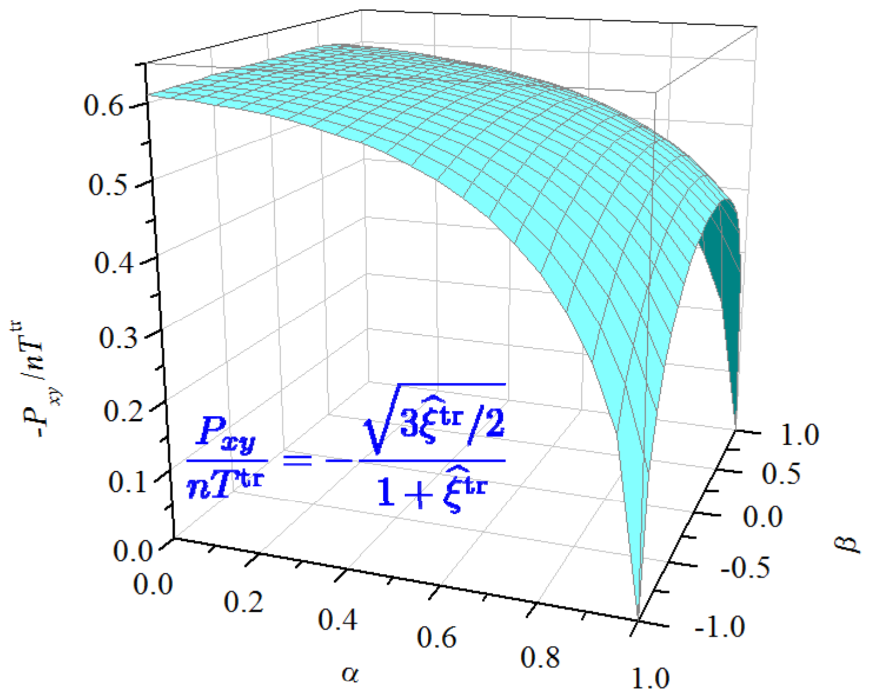
$$\xi^{\mathrm{rot}} = 0 \Rightarrow \boxed{\frac{T^{\mathrm{tr}}}{T^{\mathrm{rot}}} = \frac{2\kappa + 1 - \beta}{\kappa(1+\beta)}}$$

Independent of α

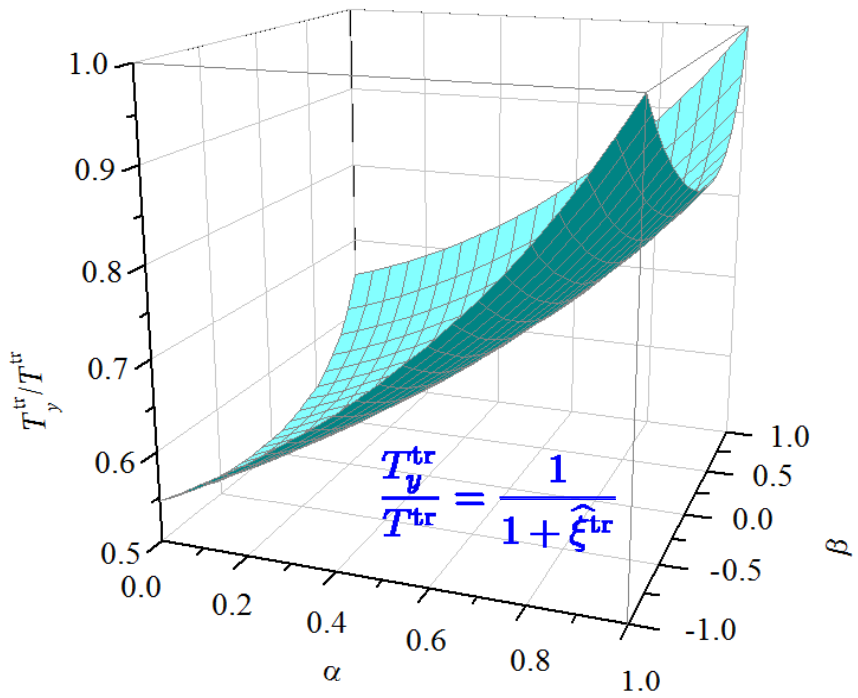


Application to simple shear flow

Shear stress



Anisotropic translational temperature



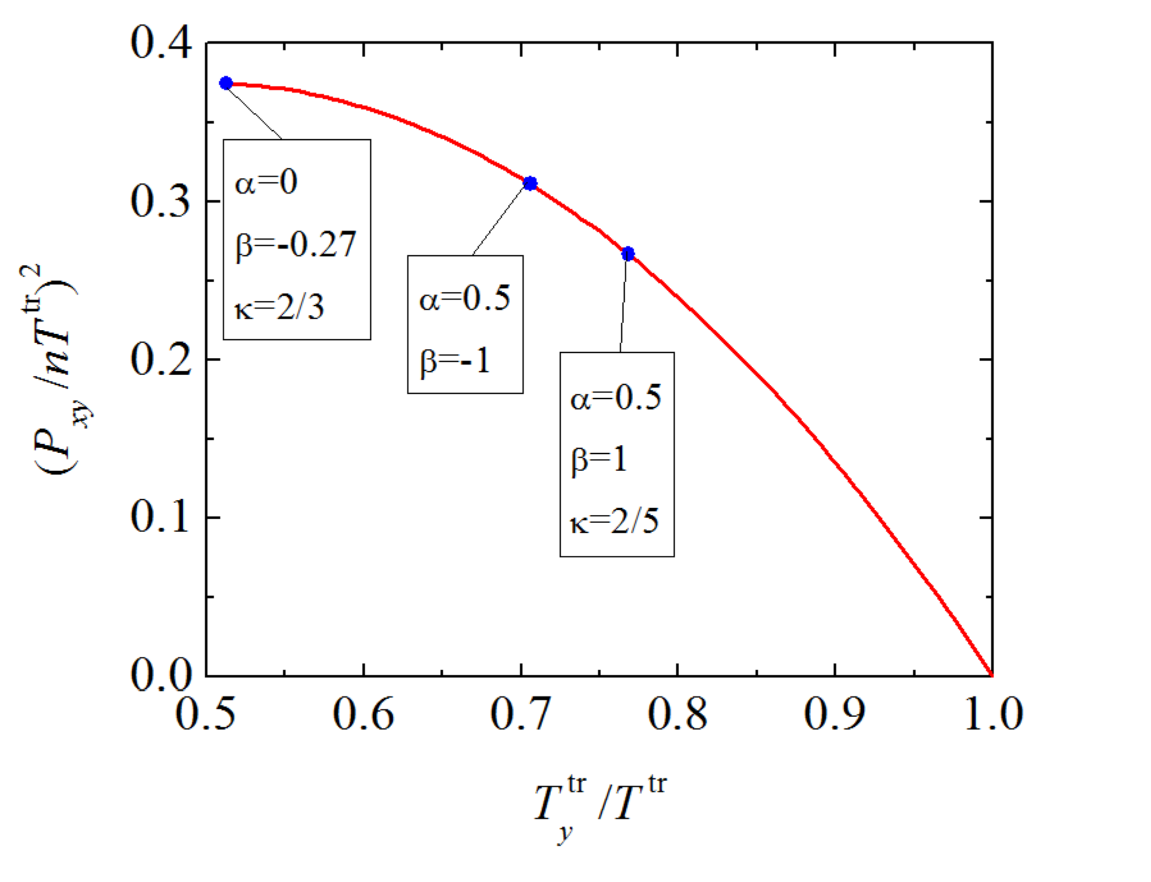
Scaled energy production rate

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

Application to simple shear flow

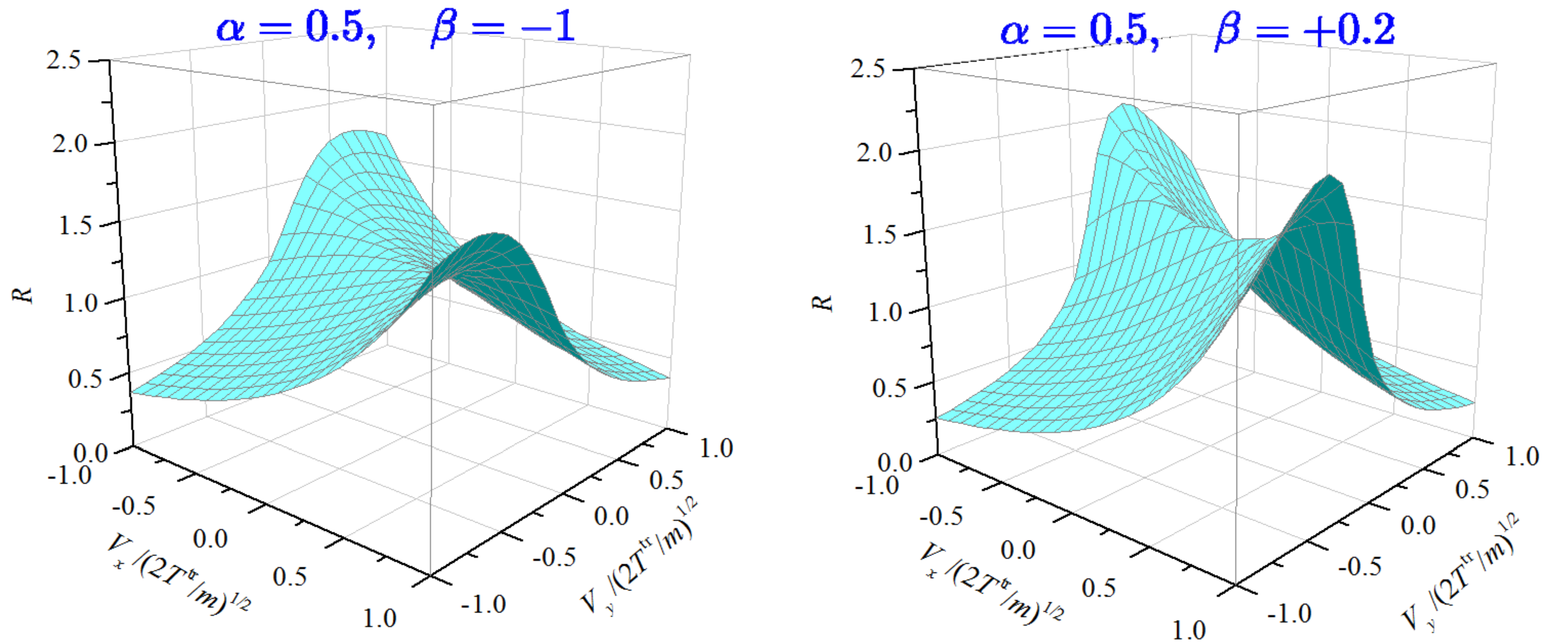
"Universal" relationship

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



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.
- Interesting non-equipartition phenomena in the homogeneous free 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.
- Derivation of the Navier-Stokes constitutive equations.

Thanks for your attention!