A Model Kinetic Equation for a Granular Gas of Inelastic Rough Hard Spheres

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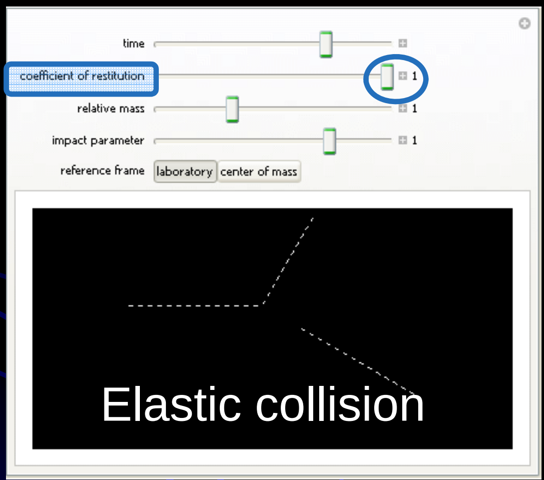
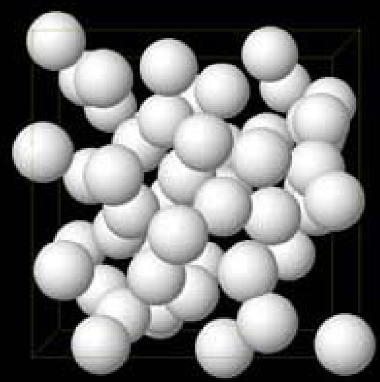
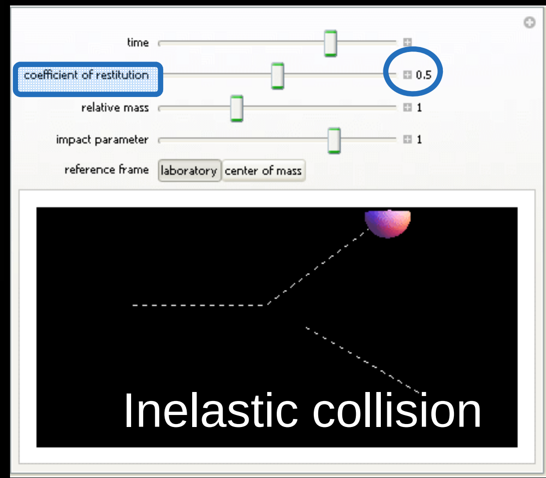
Minimal model of a granular gas:
A gas of *identical smooth inelastic* hard spheres



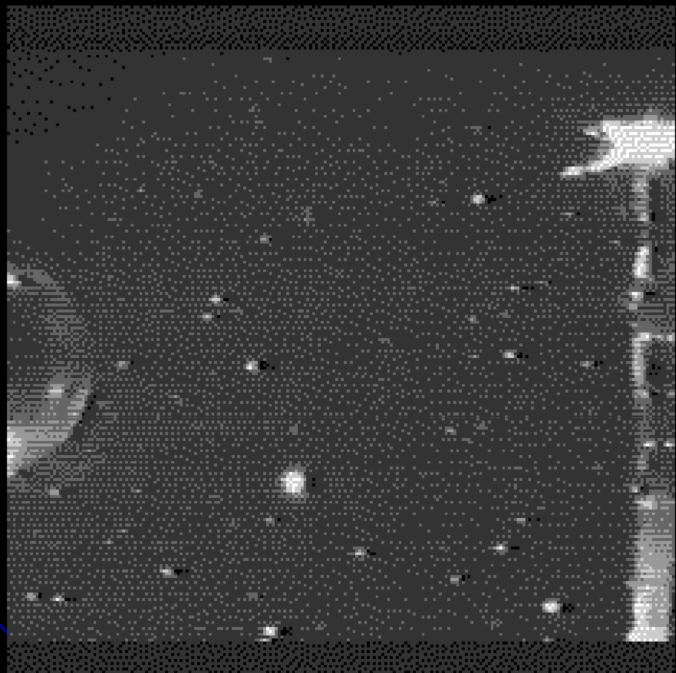




http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/

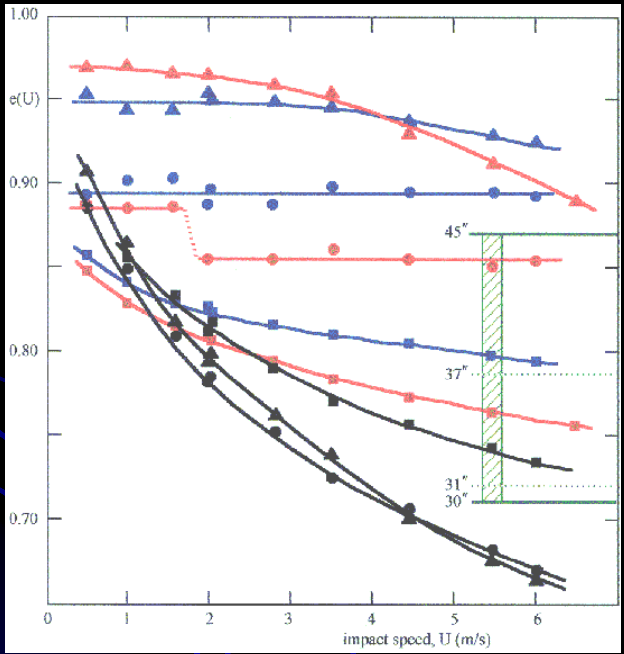
This minimal model ignores …

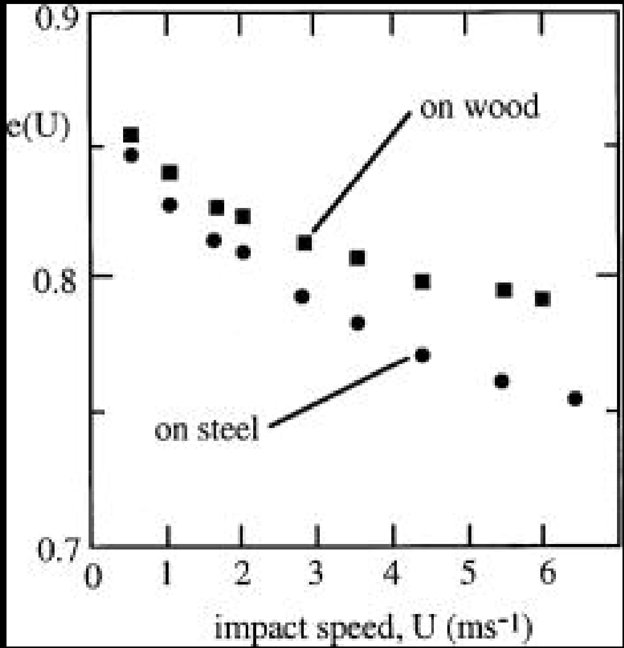
Interstitial fluid



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

Non-constant coefficient of restitution

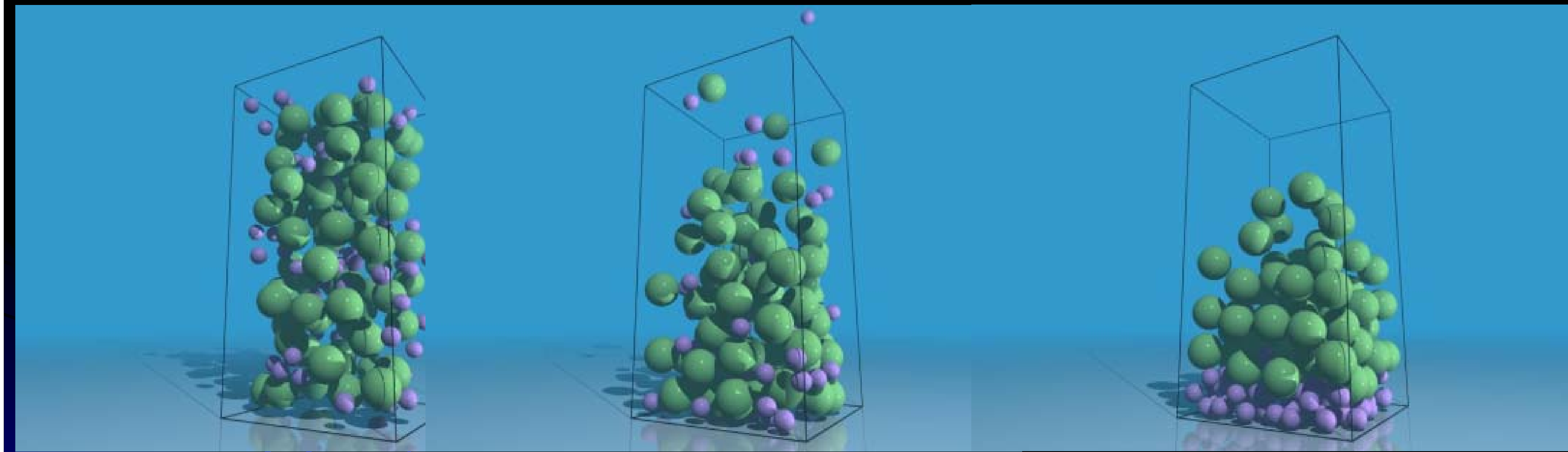




www.oxfordcroquet.com/tech/

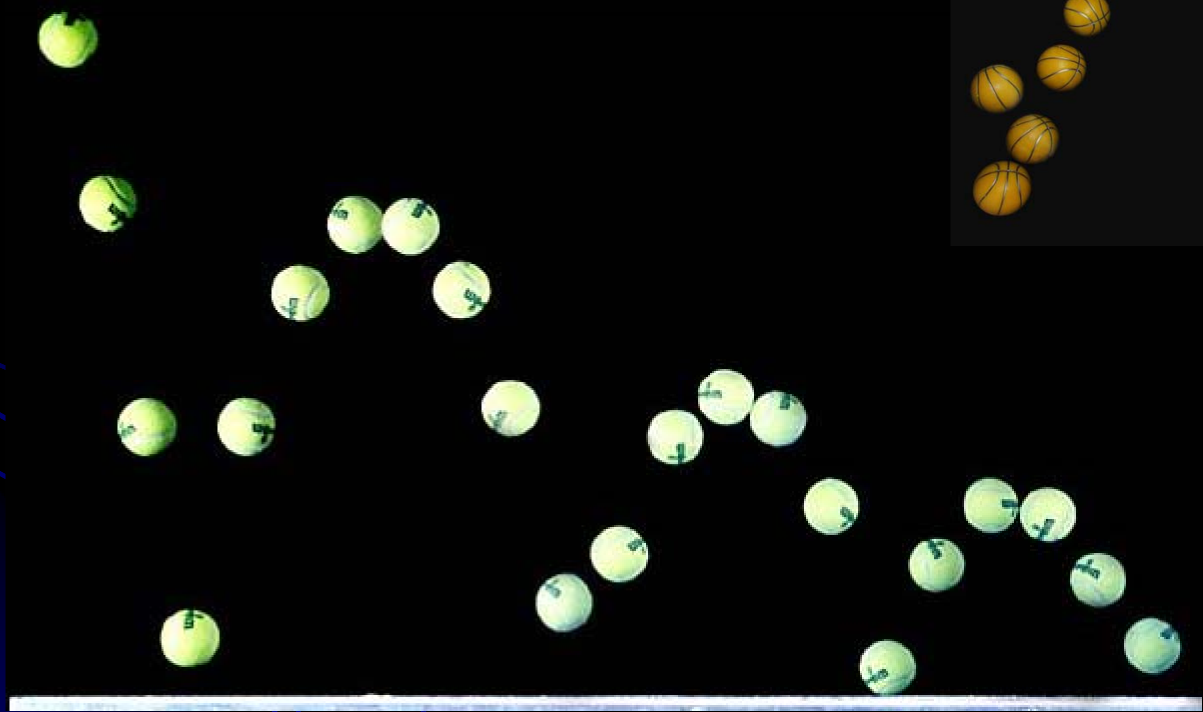
Non-spherical shape

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)

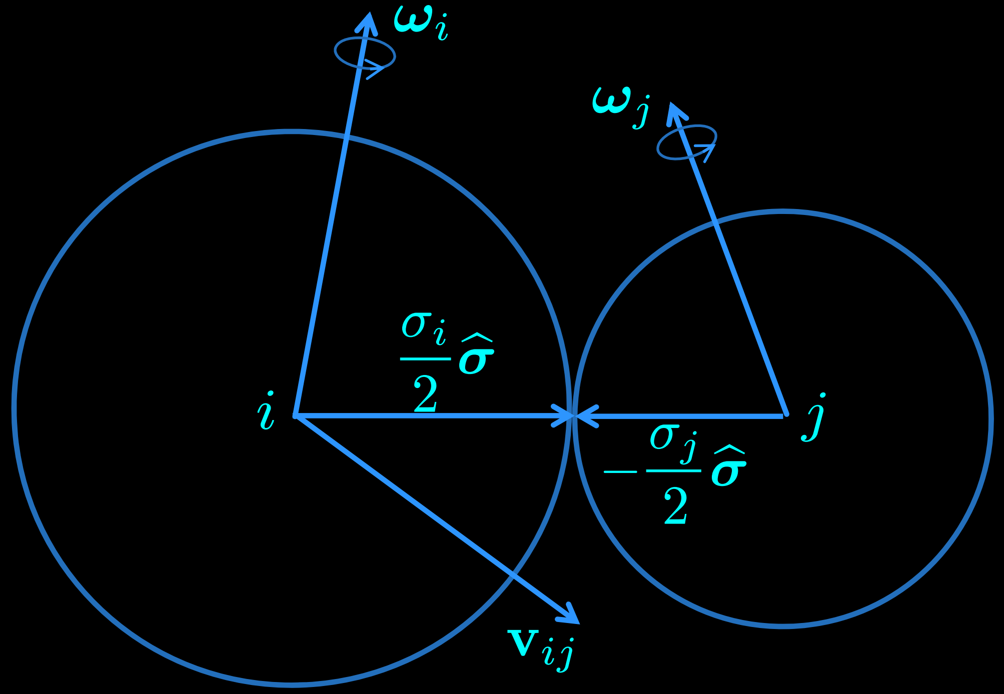
Outline

- 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.

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

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

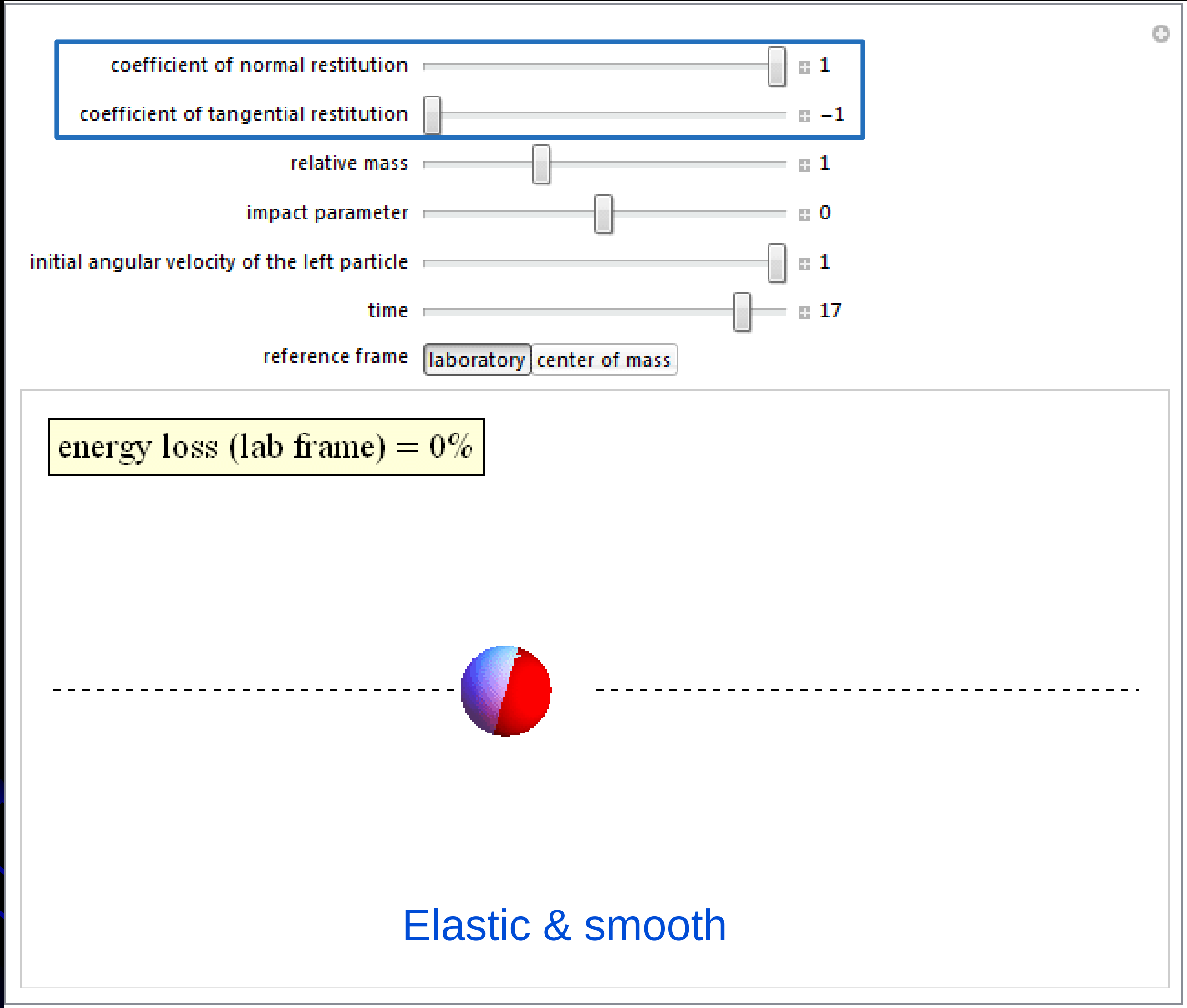
Energy collisional loss

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

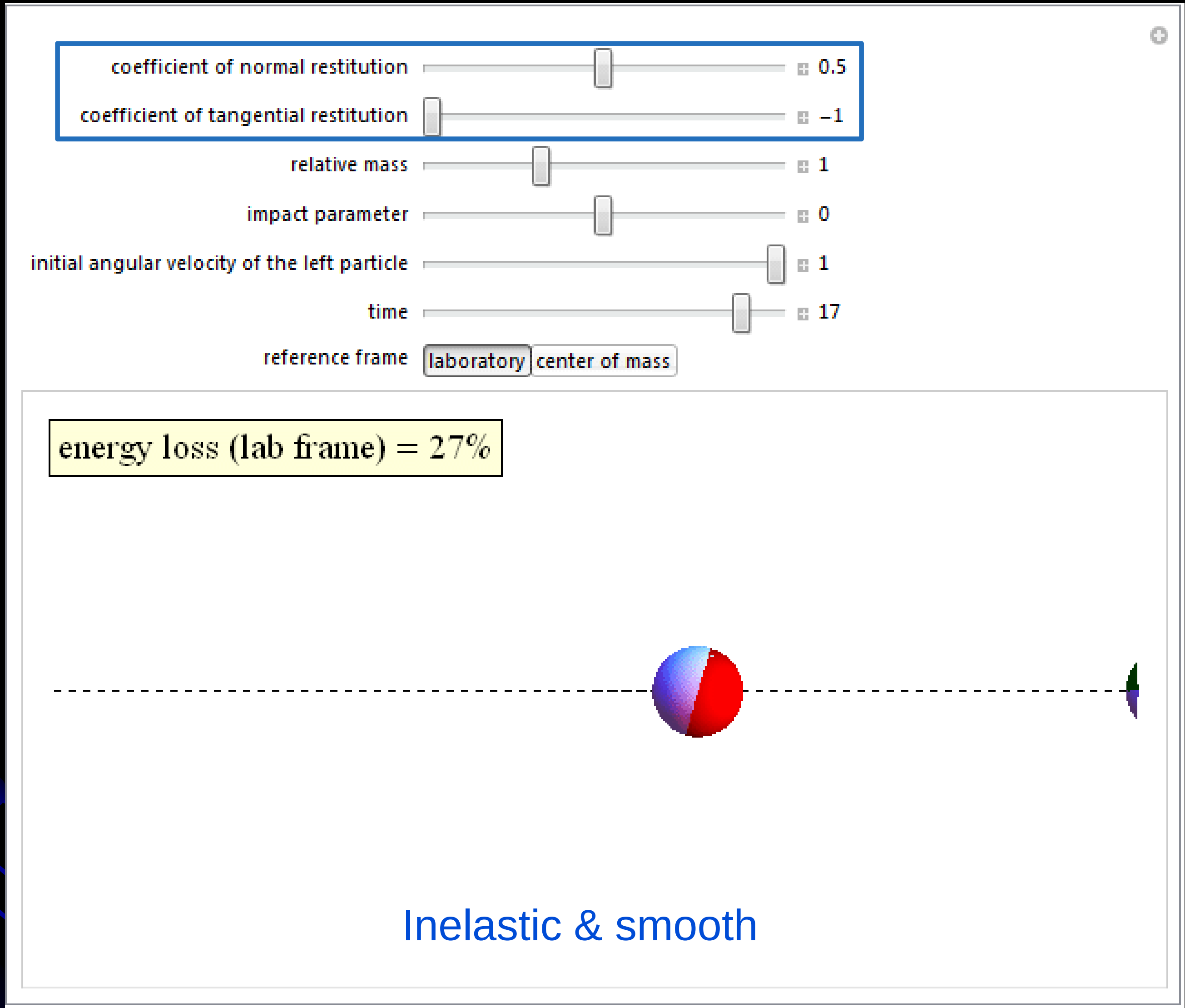
$$\begin{aligned} E'_{ij} - E_{ij} &= -(1-\alpha_{ij}^2) \times \cdots \\ & \quad -(1-\beta_{ij}^2) \times \cdots \end{aligned}$$

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)



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



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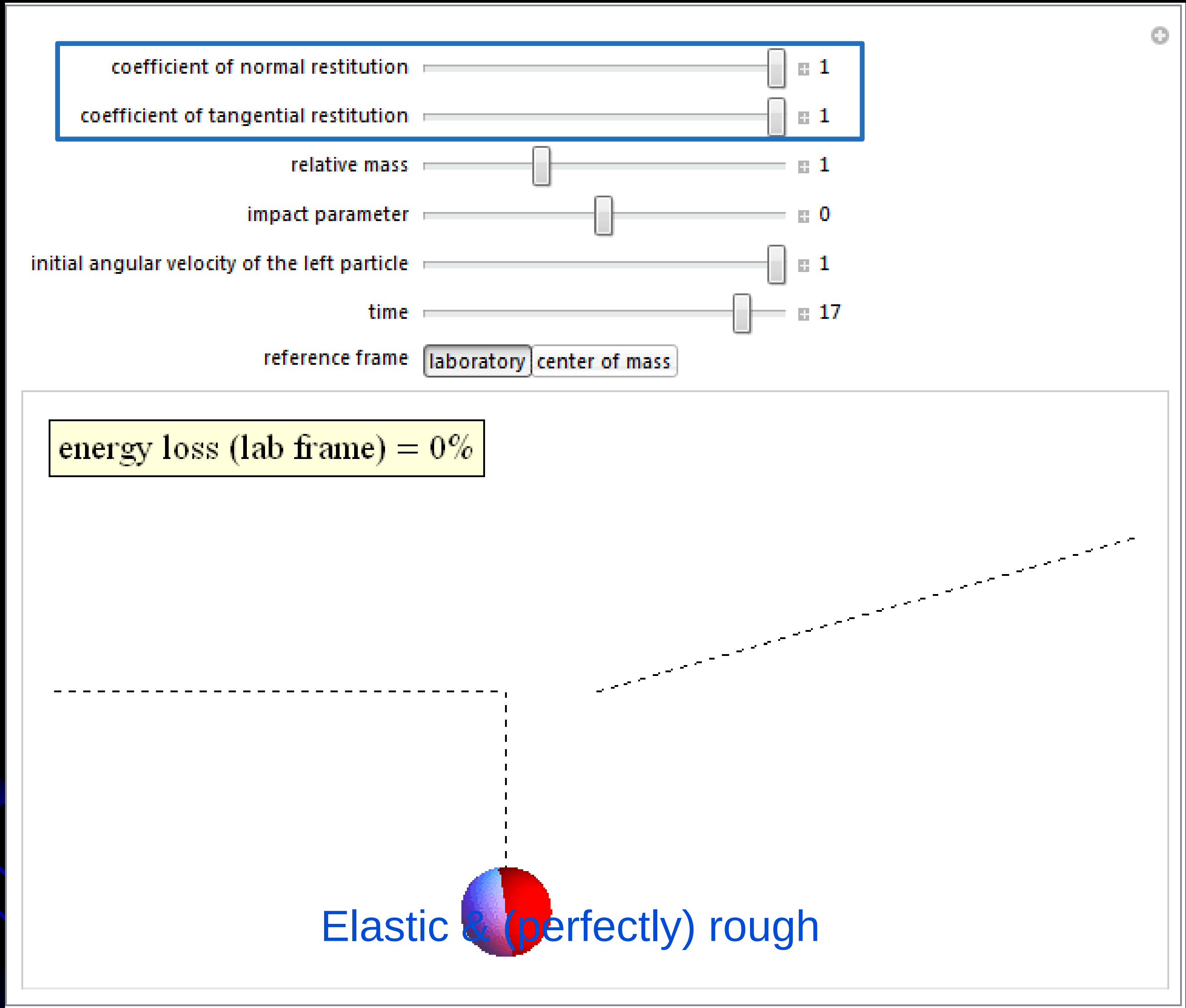
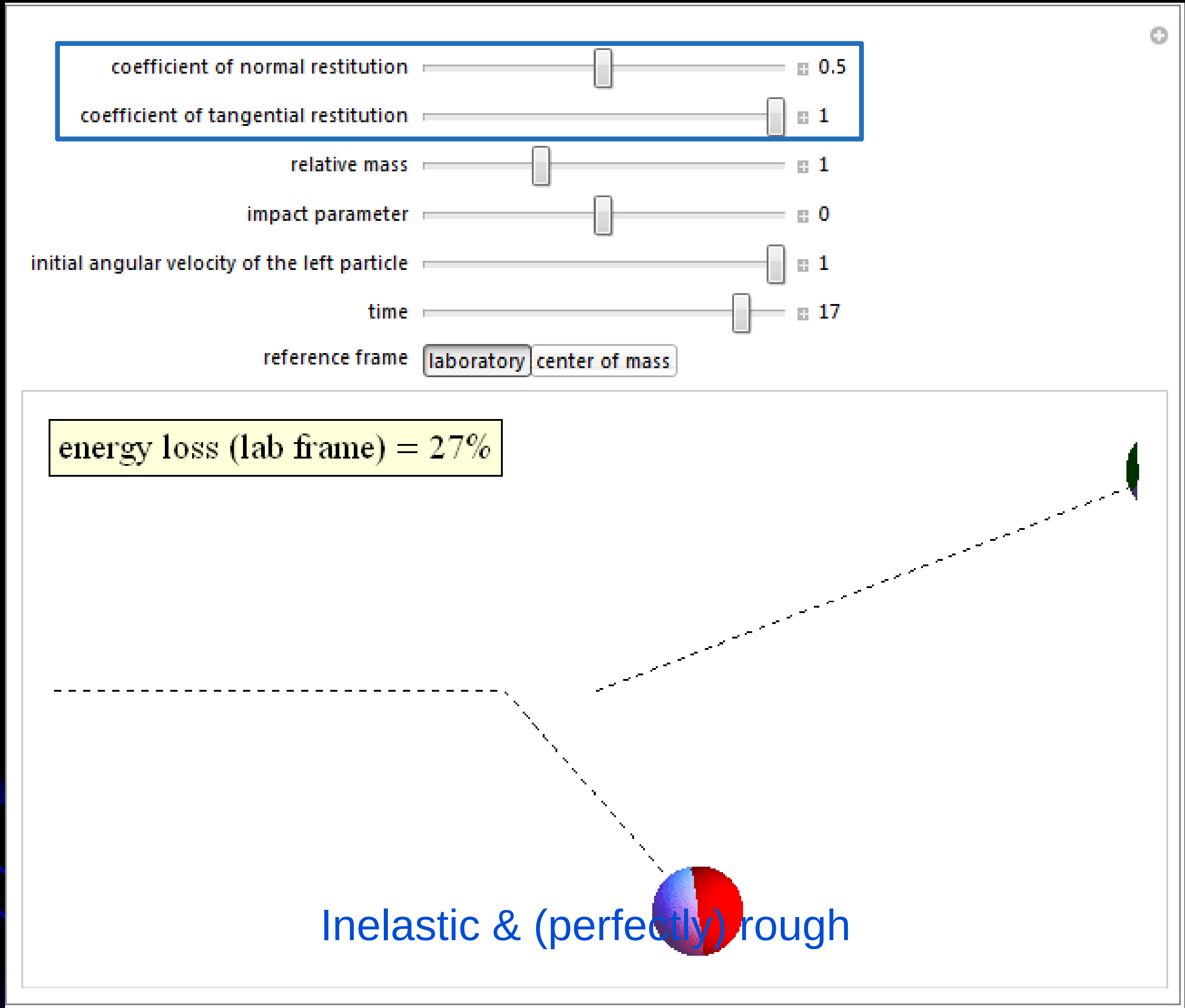


Elastic & (perfectly) rough

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



Inelastic & (perfectly) rough

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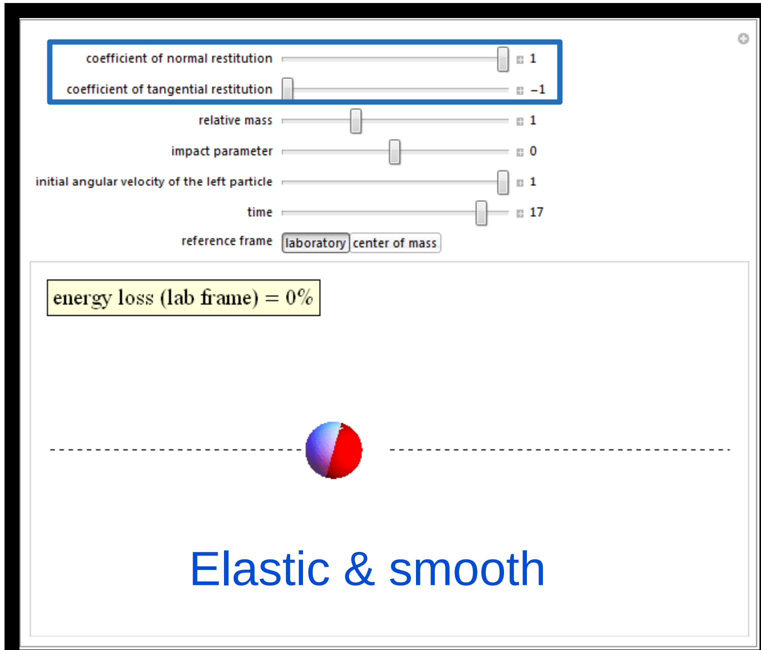
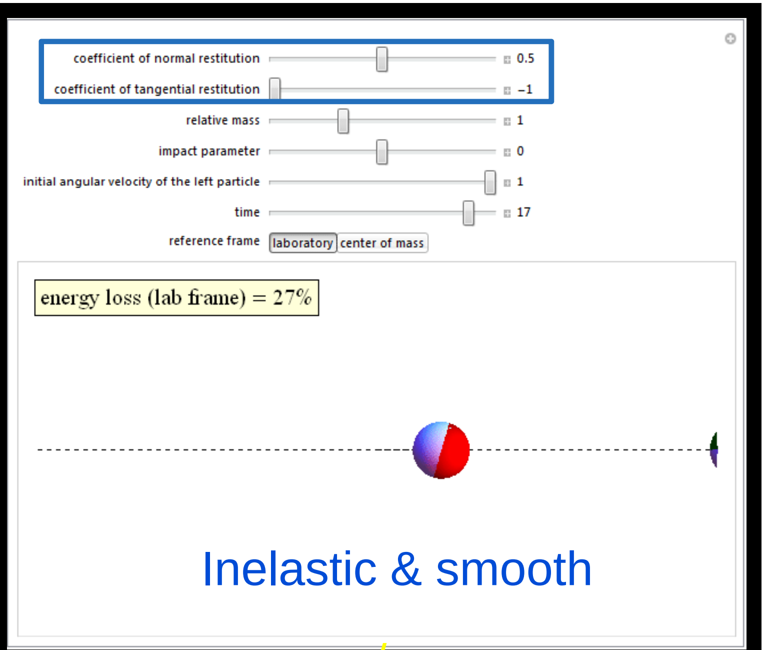
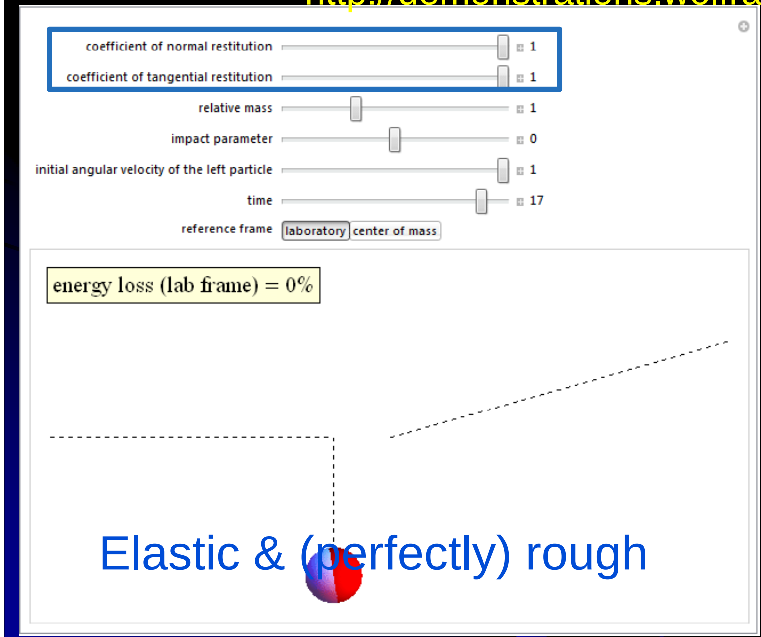


Elastic & smooth

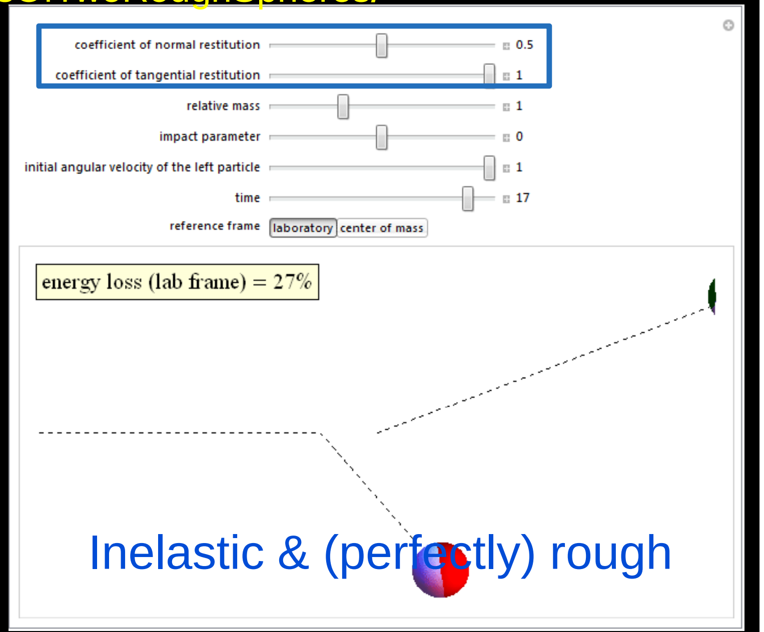


Inelastic & smooth

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



Elastic & (perfectly) rough



Inelastic & (perfectly) rough

Partial (granular) temperatures

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

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

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

Energy production rates:

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

Binary collisions

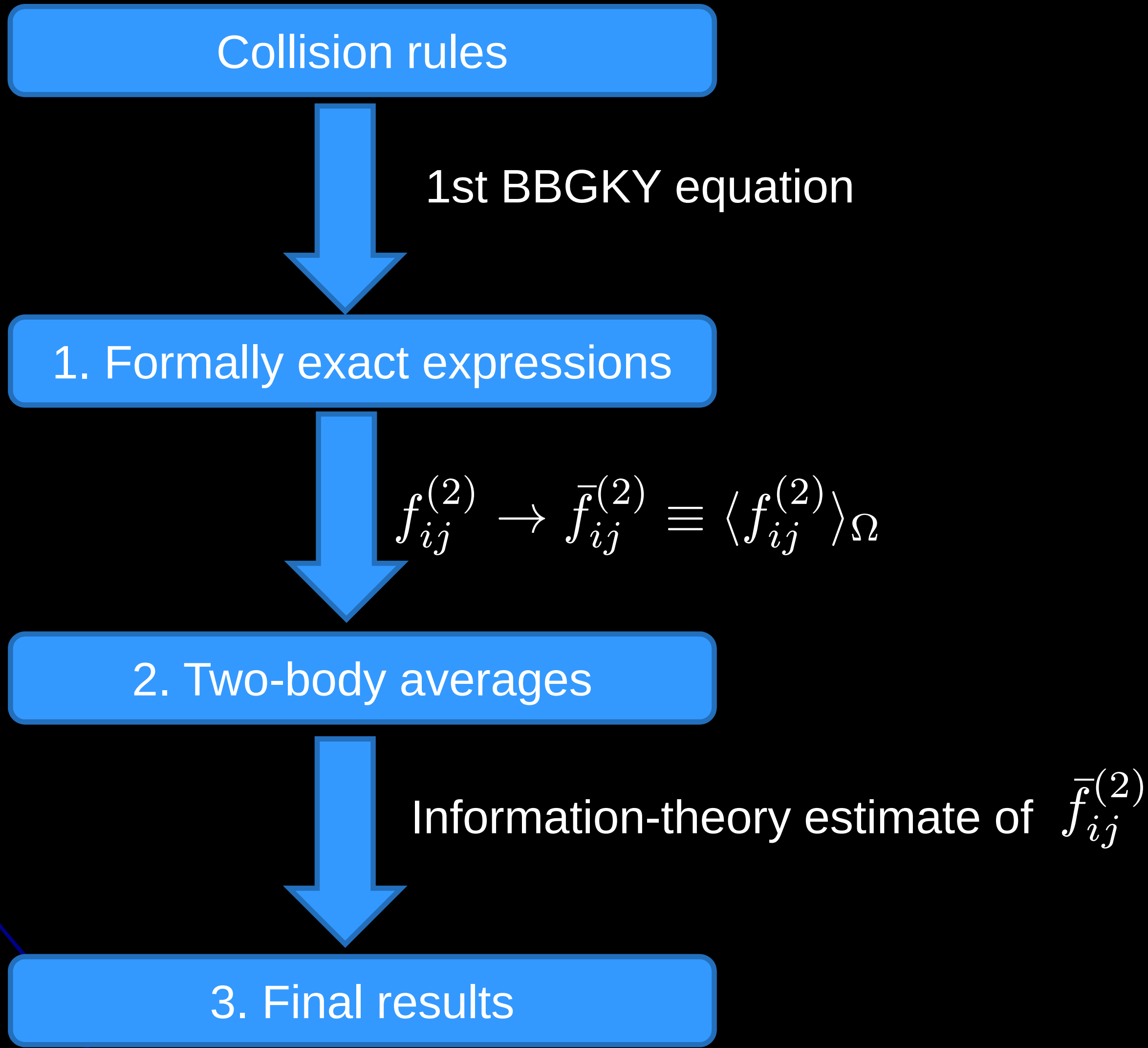
$$\xi_i^{\mathrm{rot}} = -\frac{1}{T_i^{\mathrm{rot}}}\left(\frac{\partial T_i^{\mathrm{rot}}}{\partial t}\right)_{\mathrm{coll}}, \quad \xi_i^{\mathrm{rot}} = \sum_j \xi_{ij}^{\mathrm{rot}}$$

Net *cooling* rate:

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

Energy production rates. Scheme of the derivation

(arXiv:0910.5614)



Final results. Energy production rates

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

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

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

Effective collision frequencies

Final results. Net cooling rate

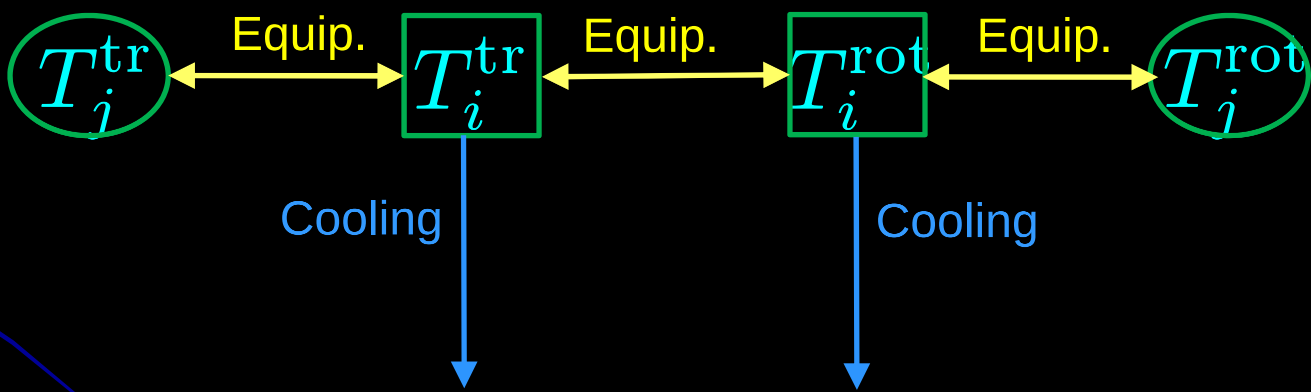
$$\zeta = \sum_i \frac{n_i}{2nT}\left(\xi_i^{\rm tr} T_i^{\rm tr} + \xi_i^{\rm rot} T_i^{\rm rot}\right)$$

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

Decomposition

Energy production rates = Equipartition rates + Cooling rates

Net cooling rate = $\sum$ Cooling rates



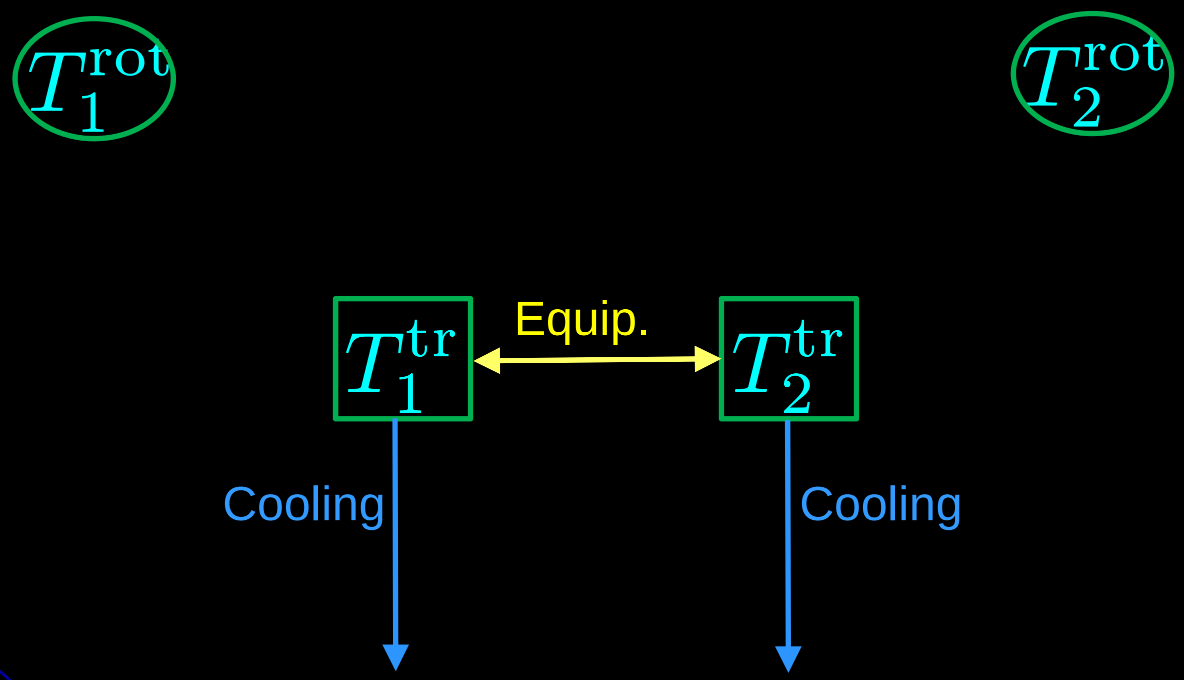
Simple application: Homogeneous Free Cooling State

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

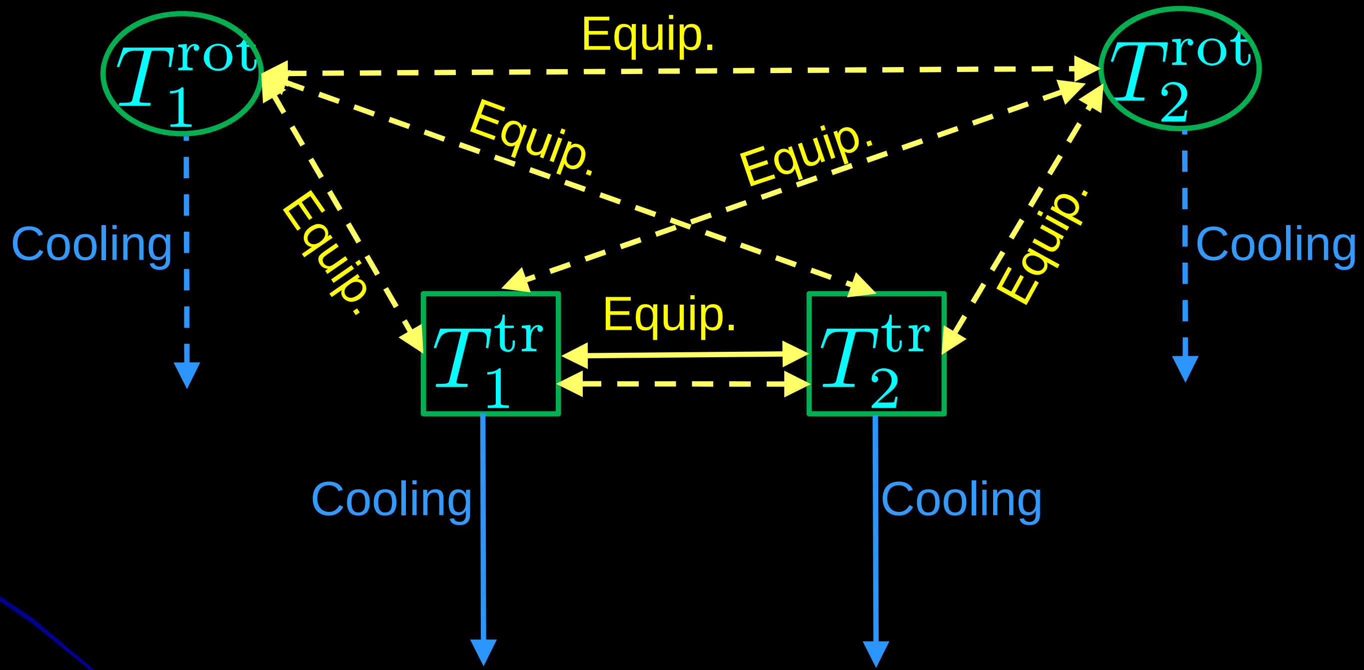
$$\frac{\partial}{\partial t}\frac{T_i^{\rm tr}}{T} = -\left(\xi_i^{\rm tr} - \zeta\right)\frac{T_i^{\rm tr}}{T}, \qquad \frac{\partial}{\partial t}\frac{T_i^{\rm rot}}{T} = -\left(\xi_i^{\rm rot} - \zeta\right)\frac{T_i^{\rm rot}}{T}$$

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

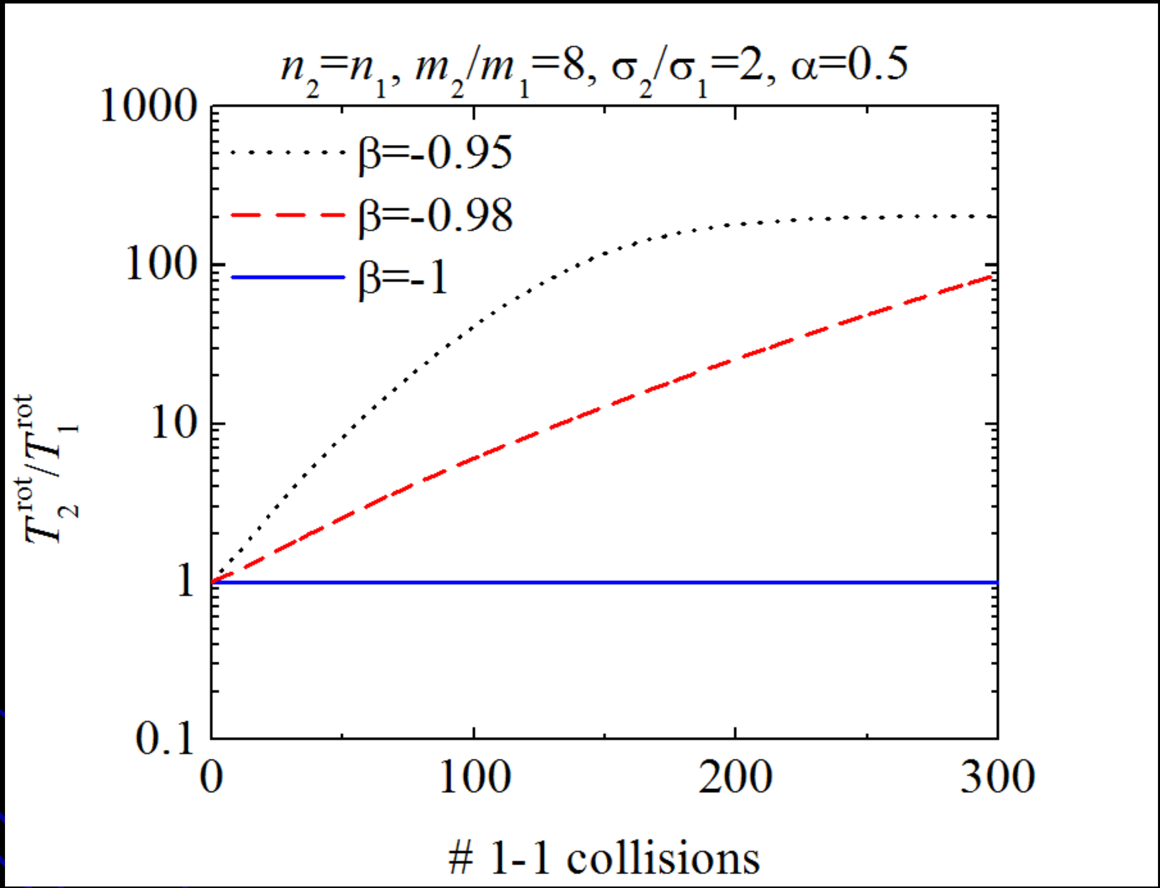
Inelastic smooth spheres (β=-1)



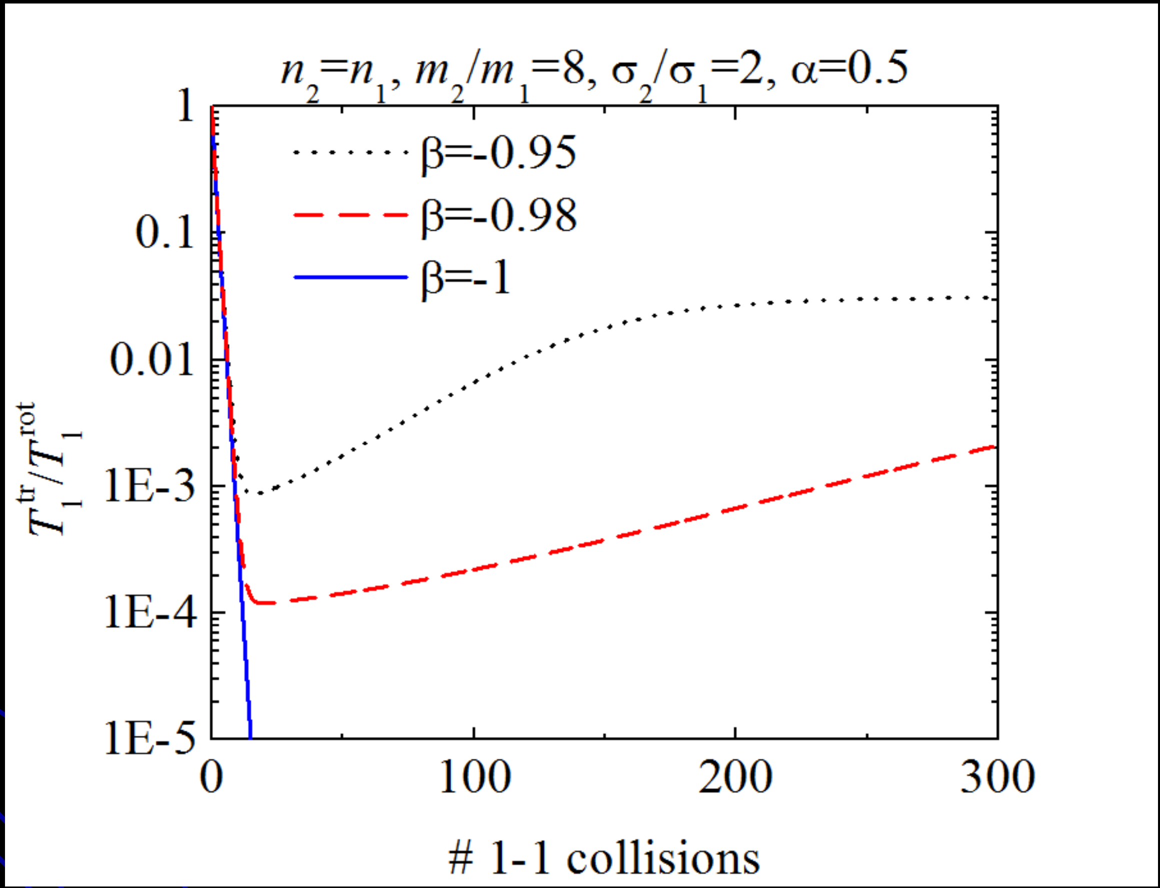
Inelastic quasi-smooth spheres ($\beta \lesssim$-1)



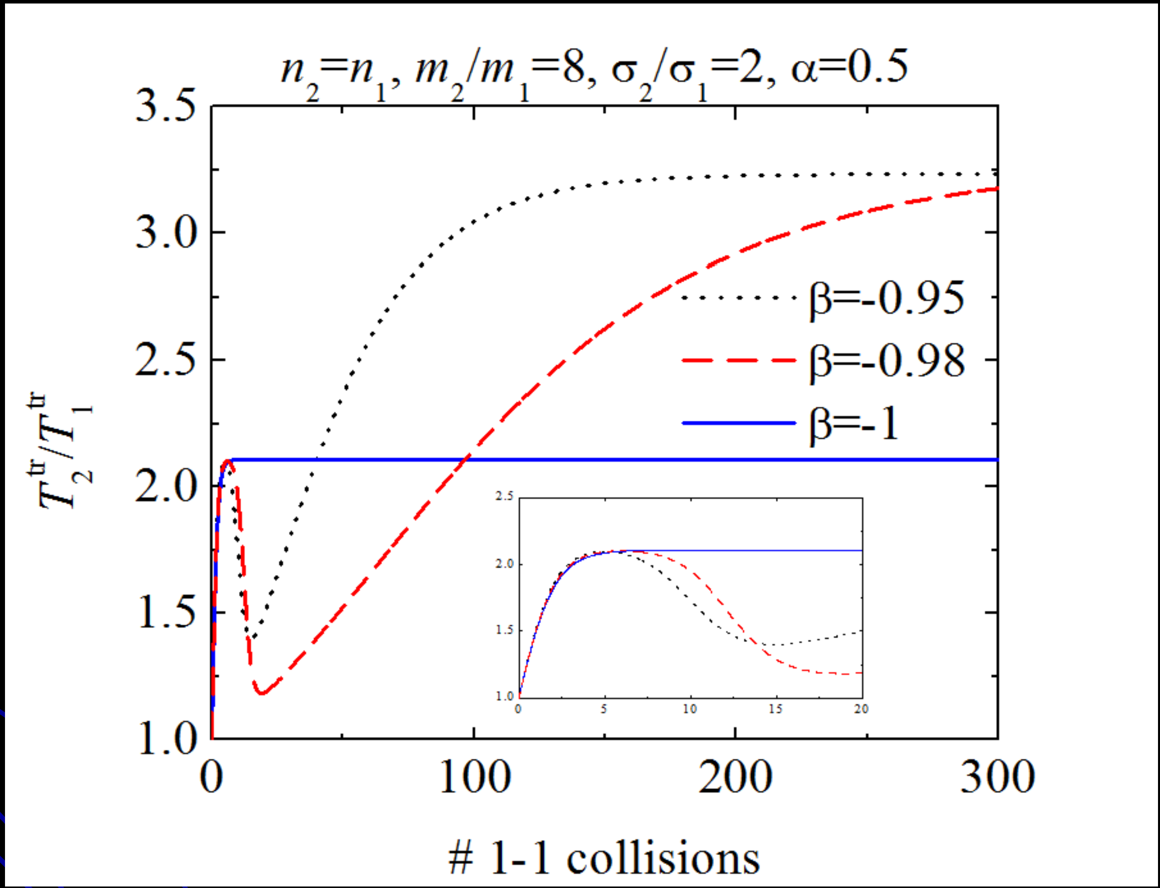
Rotational/Rotational. Time evolution



Rotational/Rotational. Time evolution

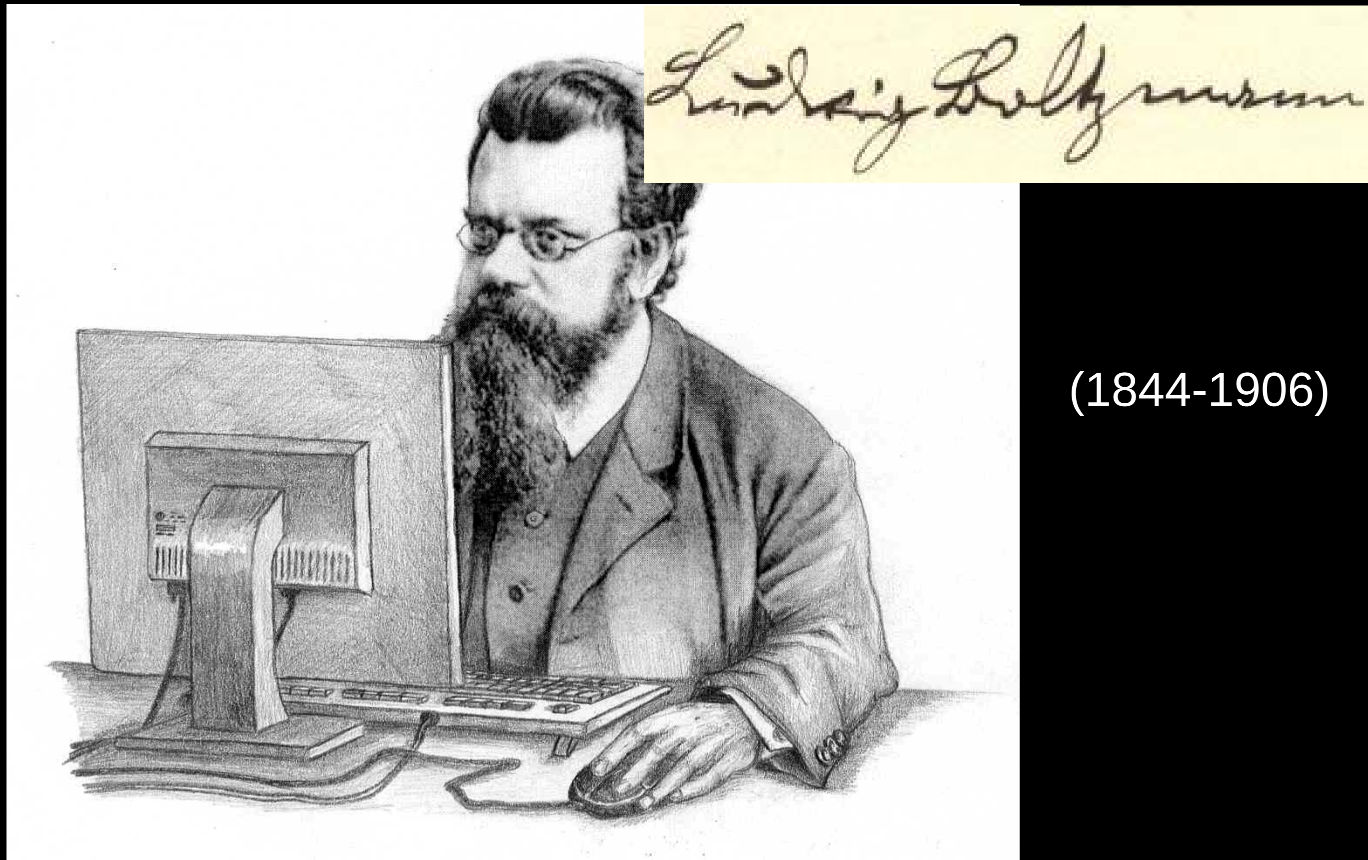


Translational/Translational. Time evolution



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

(Cartoon by Bernhard Reischl, University of Vienna)



(1844-1906)

Boltzmann equation:

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

Binary collisions

Antecedents for *smooth* particles

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

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

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

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

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

Simple kinetic model for *monodisperse* inelastic rough hard spheres

Three key ingredients we want to keep:

1. $(\partial_t T^{\text{tr}})_{\text{coll}} = -\xi^{\text{tr}} T^{\text{tr}}$
2. $(\partial_t T^{\text{rot}})_{\text{coll}} = -\xi^{\text{rot}} T^{\text{rot}}$
3. $\int d\mathbf{v}_i \int d\boldsymbol{\omega}_i \, \mathbf{v}_i J_{ij}[\mathbf{v}_i, \boldsymbol{\omega}_i | f_i, f_j] = \lambda_{ij} \underbrace{\int d\mathbf{v}_i \int d\boldsymbol{\omega}_i \, \mathbf{v}_i J_{ij}[\mathbf{v}_i, \boldsymbol{\omega}_i | f_i, f_j] \Big|_{\substack{\alpha_{ij}=1 \\ \beta_{ij}=-1}}}_{\text{Elastic smooth spheres}}$

$$\lambda_{ij} \equiv \frac{1+\alpha_{ij}}{2} + \frac{\kappa_{ij}}{1+\kappa_{ij}} \frac{1+\beta_{ij}}{2}$$

The kinetic model. Joint distribution

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

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

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

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

A simpler version. Marginal distributions

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

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

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

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

An even simpler version. Translational distribution

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

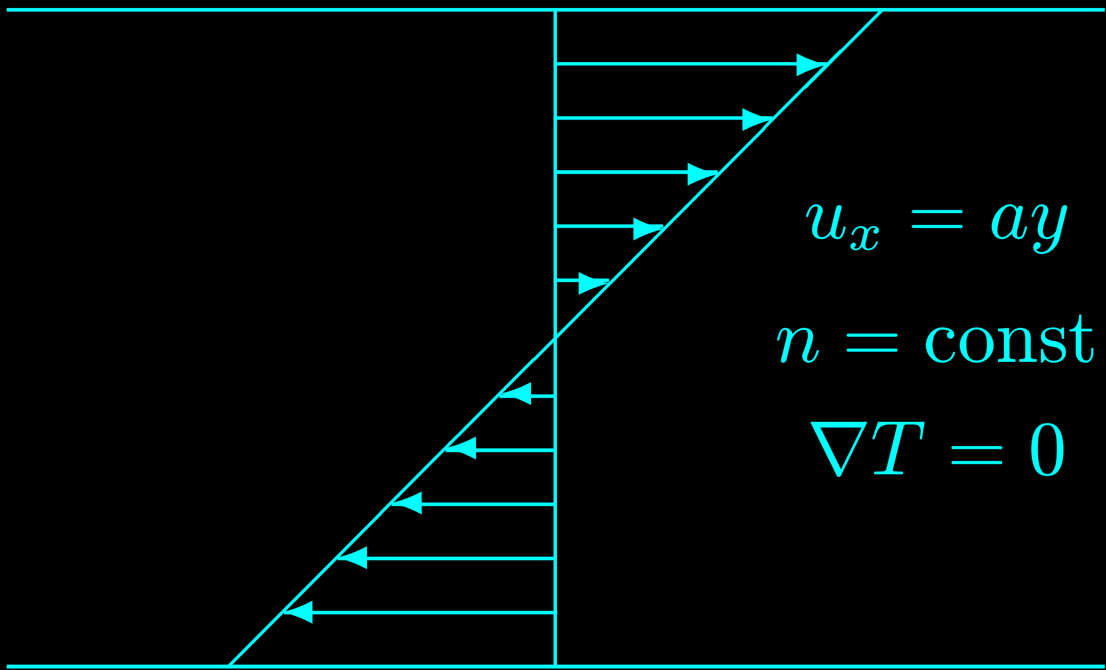
$$\partial_t f^{\mathrm{tr}}+\mathbf{v}\cdot\nabla f^{\mathrm{tr}}=-\lambda\nu_0\left(f^{\mathrm{tr}}-f_0^{\mathrm{tr}}\right)+\frac{\xi^{\mathrm{tr}}}{2}\frac{\partial}{\partial\mathbf{v}}\cdot\left[(\mathbf{v}-\mathbf{u})f^{\mathrm{tr}}\right]$$

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

$$\partial_t T^{\mathrm{rot}}+\mathbf{u}\cdot\nabla T^{\mathrm{rot}}=-\xi^{\mathrm{rot}}T^{\mathrm{rot}}$$

Application to simple shear flow (steady state)

$$y = +L/2$$



$$u_x = ay$$

$$n = \text{const}$$

$$\nabla T = 0$$

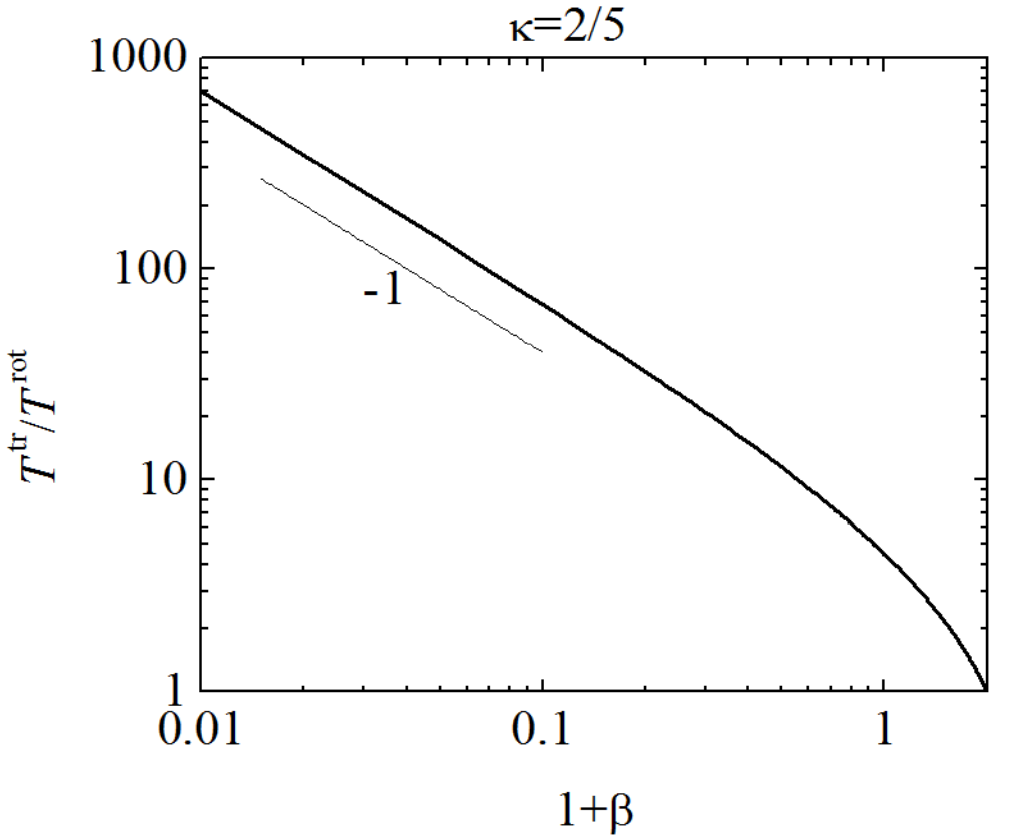
$$y = -L/2$$

Application to simple shear flow

Translational/Rotational temperature ratio

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

Independent of α



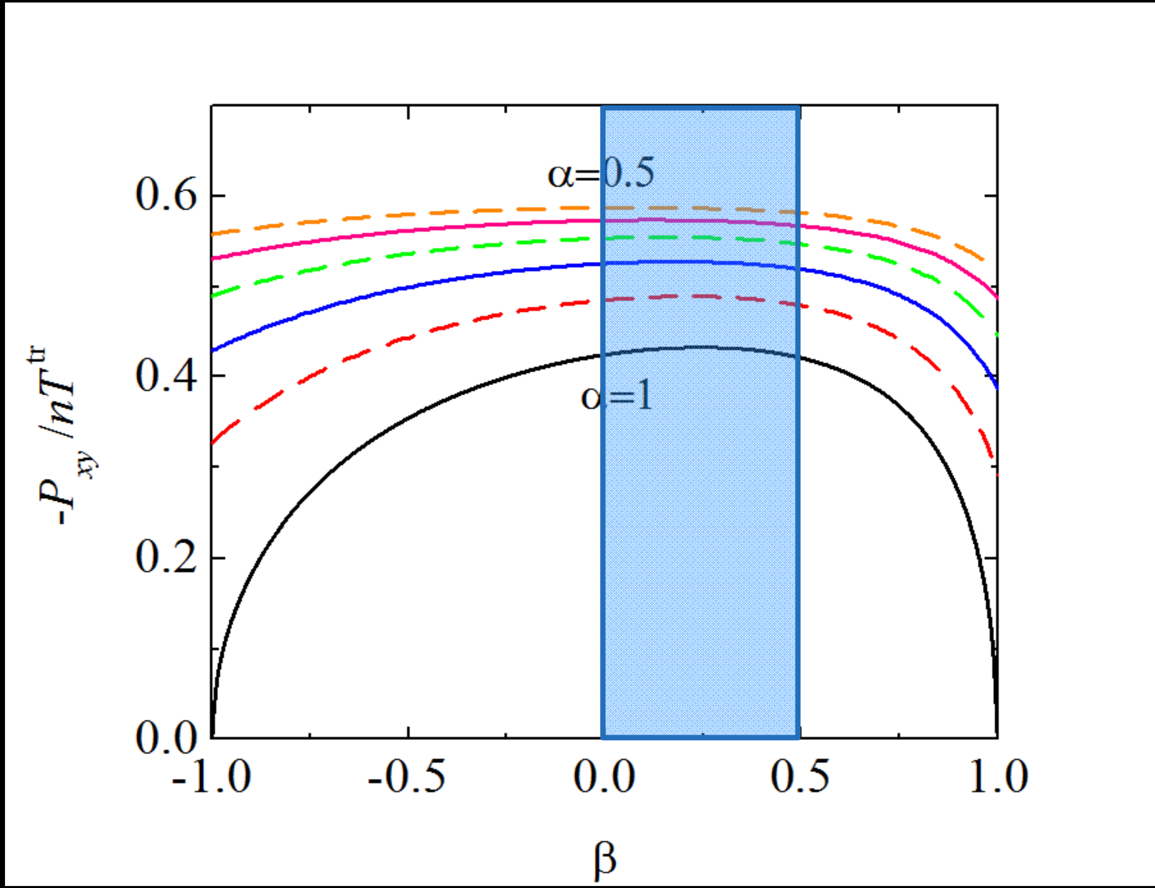
Application to simple shear flow

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 energy production rate

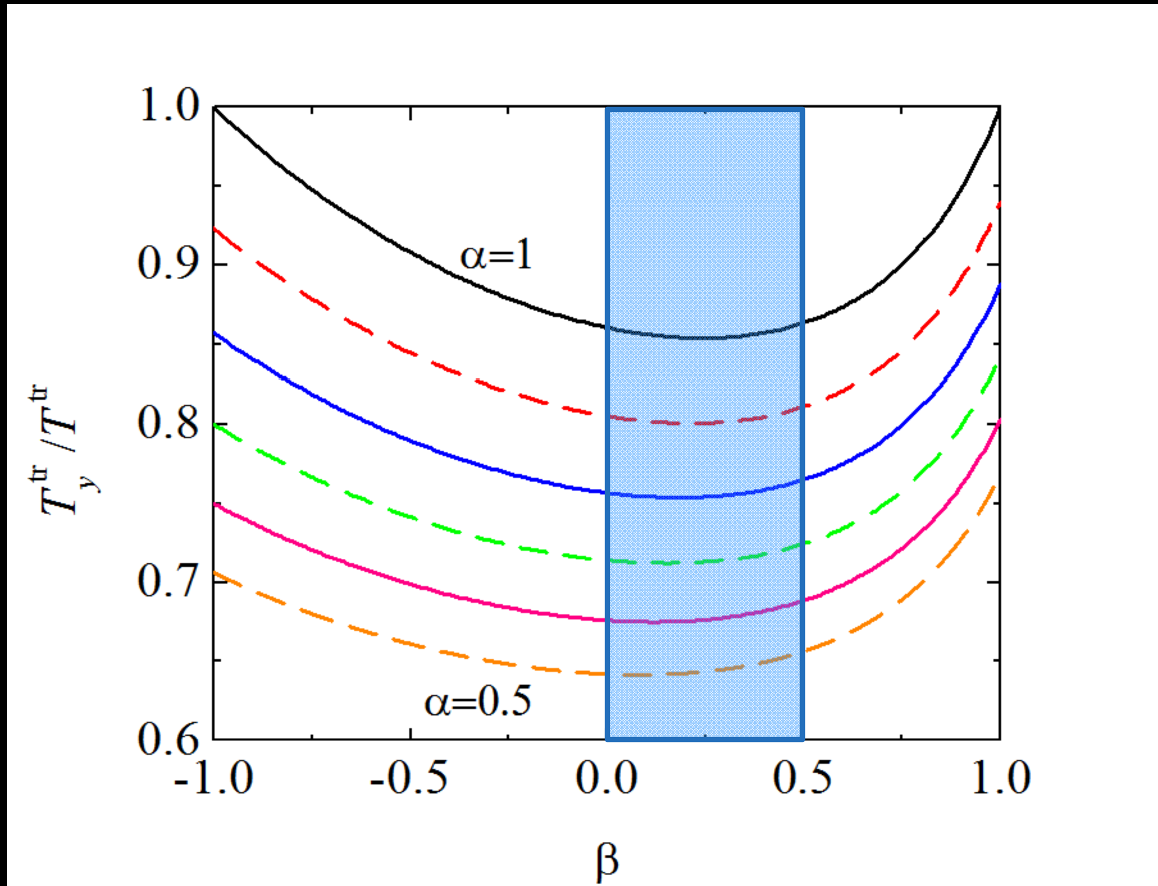


Application to simple shear flow

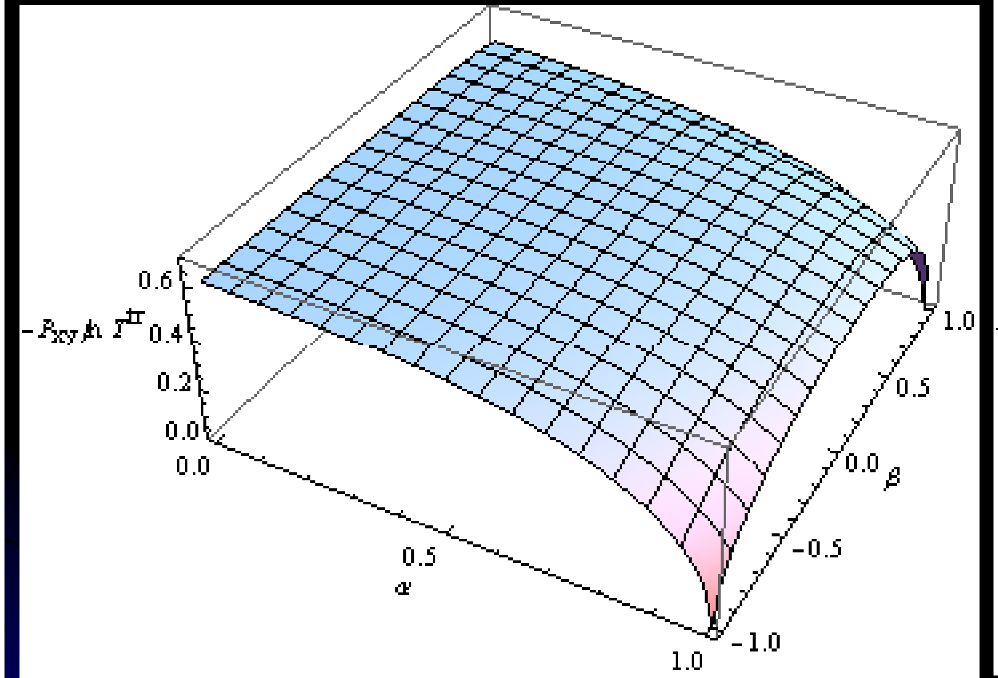
Anisotropic translational temperatures

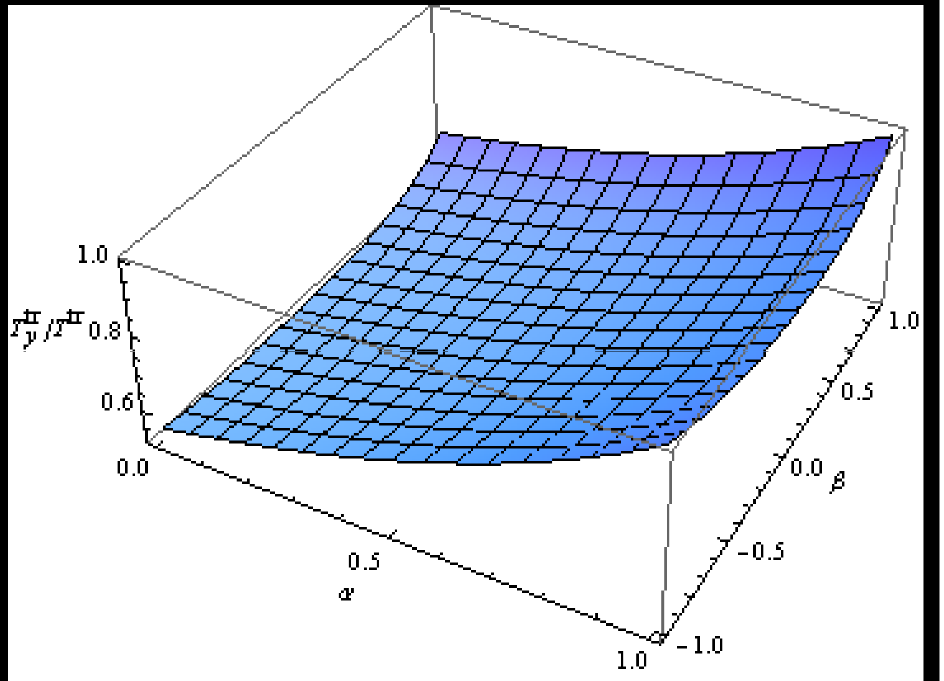
$$\frac{T_y^{\rm tr}}{T^{\rm tr}} = \frac{T_z^{\rm tr}}{T^{\rm tr}} = \frac{1}{1+\widehat{\xi}^{\rm tr}}$$

$$\frac{T_x^{\rm tr}}{T^{\rm tr}} = 3 - 2\frac{T_y^{\rm tr}}{T^{\rm tr}}$$



Application to simple shear flow

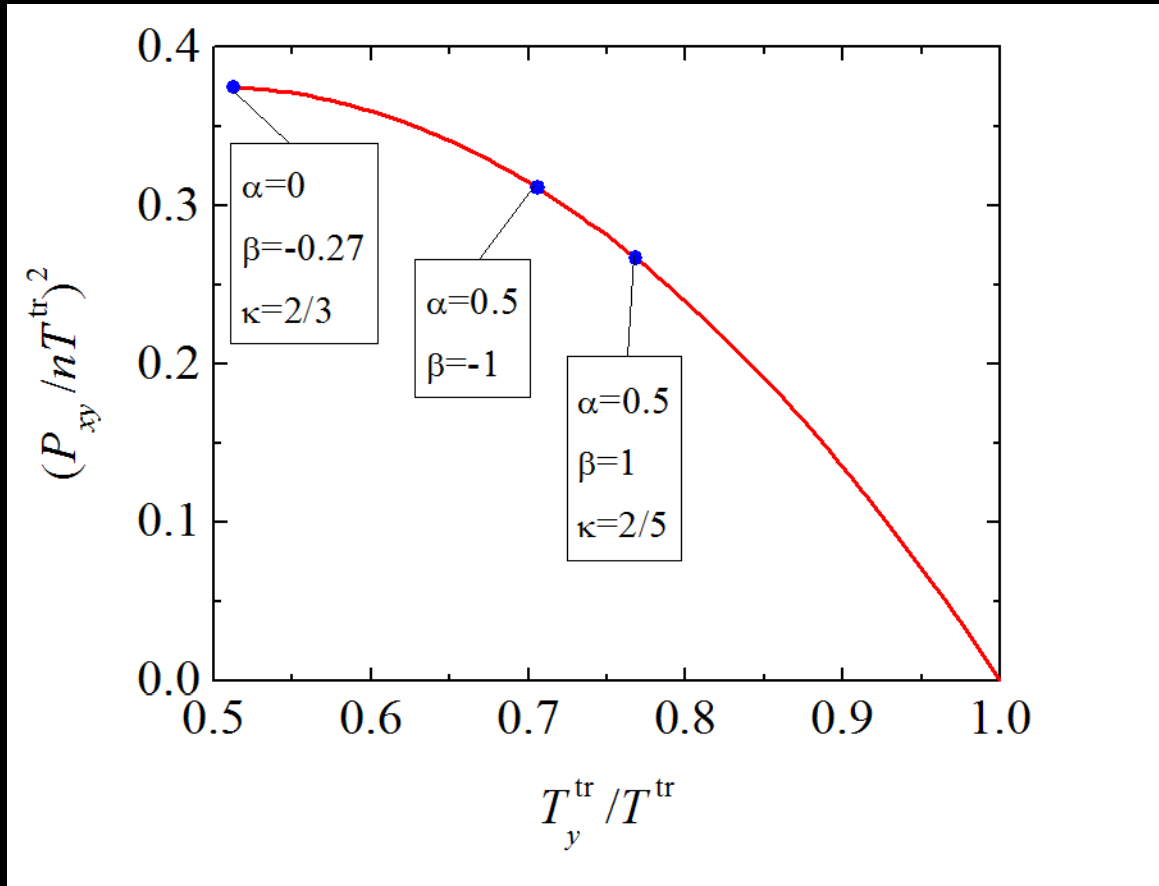




Application to simple shear flow

"Universal" relationship

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



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!