IMPACT OF ROUGHNESS ON THE HYDRODYNAMIC BEHAVIOR OF INELASTIC SPHERES

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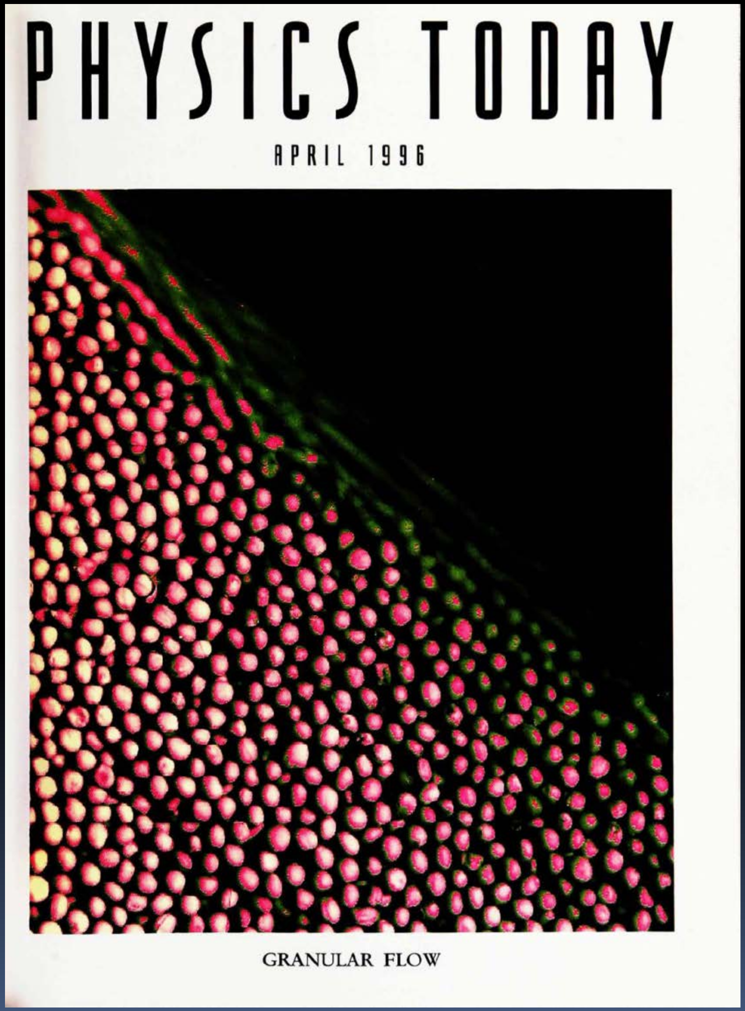
What is a granular material?

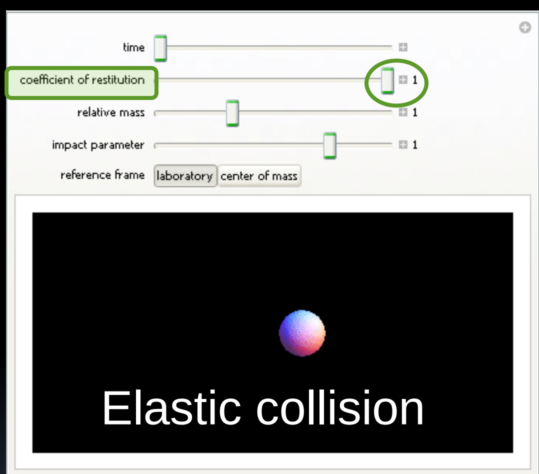
- It is a conglomeration of discrete solid, macroscopic particles characterized by a loss of energy whenever the grains collide.
- The constituents must be large enough such that they are not subject to thermal motion fluctuations. Thus, the lower size limit for grains is about 1 μm.

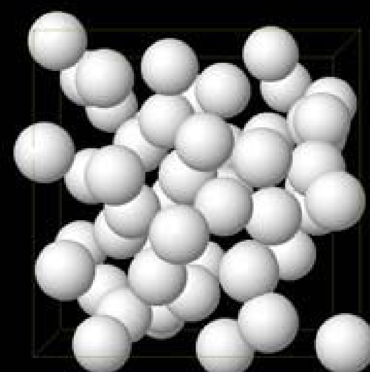
What is a granular *fluid*?

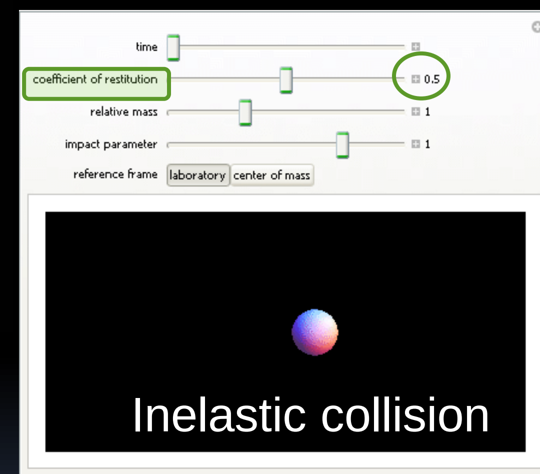
- When the granular matter is driven and energy is fed into the system (e.g., by shaking) such that the grains are not in constant contact with each other, the granular material is said to *fluidize*.



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



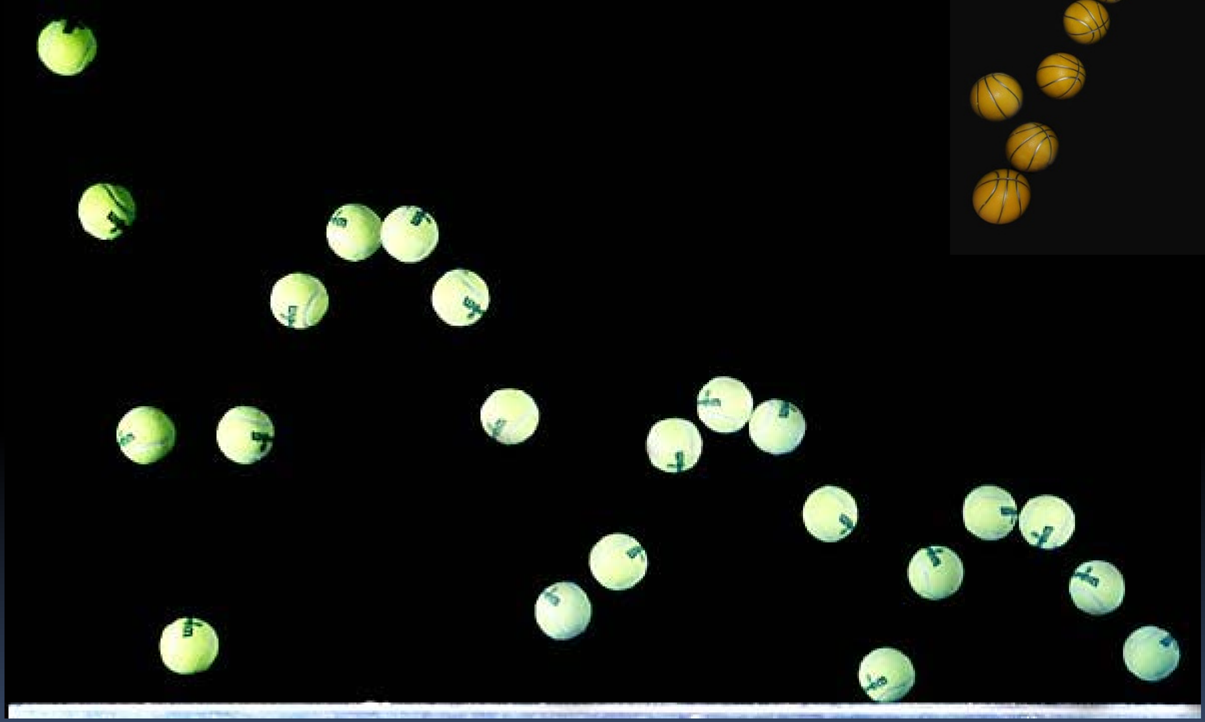




http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/

This minimal model ignores

Roughness



Simple model of a granular gas: A *collection* 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 of the talk

- 0. Collision rules for inelastic rough hard spheres.
- 1. Homogeneous cooling state. Velocity cumulants.
- 2. Navier-Stokes-Fourier transport coefficients.

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Material parameters:

- Mass m
- Diameter σ
- Moment of inertia I $(\kappa=4I/m\sigma^2)$
- Coefficient of normal restitution α
- Coefficient of tangential restitution β
- $\alpha=1$ for perfectly elastic particles
- $\beta=-1$ for perfectly smooth particles
- $\beta=+1$ for perfectly rough particles

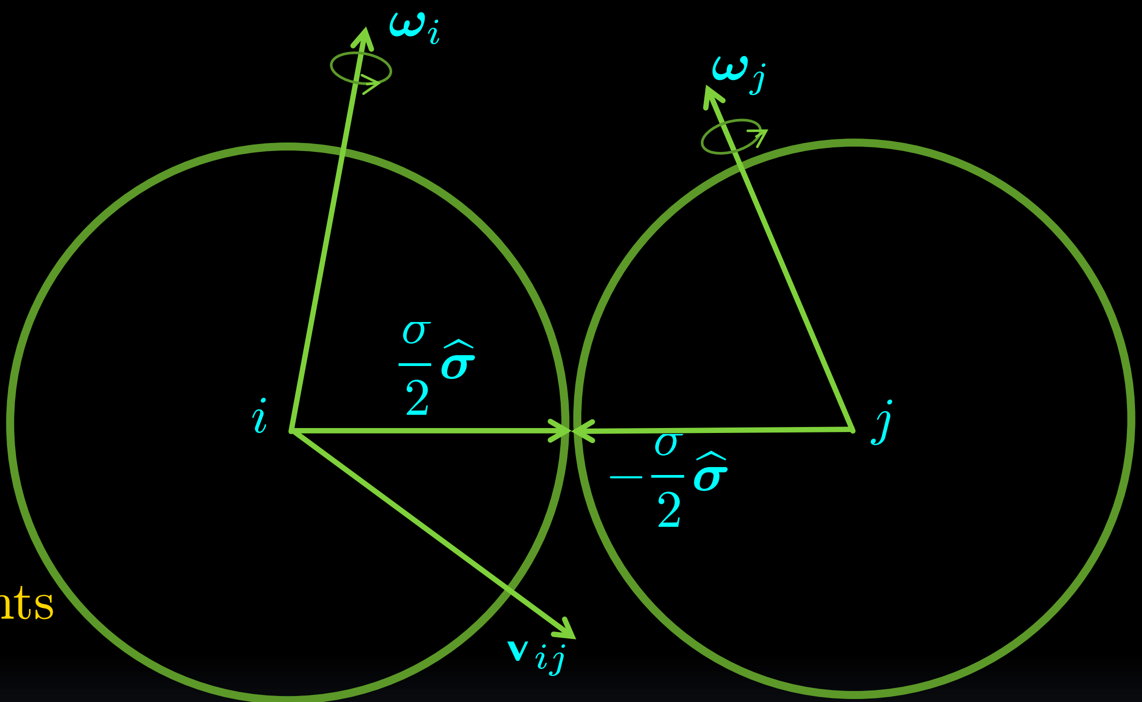
Collision rules

Cons. linear momentum:

$$\mathbf{v}_i' + \mathbf{v}_j' = \mathbf{v}_i + \mathbf{v}_j$$

Cons. angular momentum:

$$I\boldsymbol{\omega}_{i,j}' \mp m\frac{\sigma_i}{2}\widehat{\boldsymbol{\sigma}} \times \mathbf{v}_{i,j}'$$
$$= I\boldsymbol{\omega}_{i,j} \mp m\frac{\sigma_i}{2}\widehat{\boldsymbol{\sigma}} \times \mathbf{v}_{i,j}$$



Relative velocity of the points of the spheres at contact:

$$\overline{\mathbf{v}}_{ij} = \mathbf{v}_{ij} - \frac{\sigma}{2}\widehat{\boldsymbol{\sigma}} \times (\boldsymbol{\omega}_i + \boldsymbol{\omega}_j)$$

$$\widehat{\boldsymbol{\sigma}} \cdot \overline{\mathbf{v}}_{ij}' = -\alpha\widehat{\boldsymbol{\sigma}} \cdot \overline{\mathbf{v}}_{ij}, \quad \widehat{\boldsymbol{\sigma}} \times \overline{\mathbf{v}}_{ij}' = -\beta\widehat{\boldsymbol{\sigma}} \times \overline{\mathbf{v}}_{ij}$$

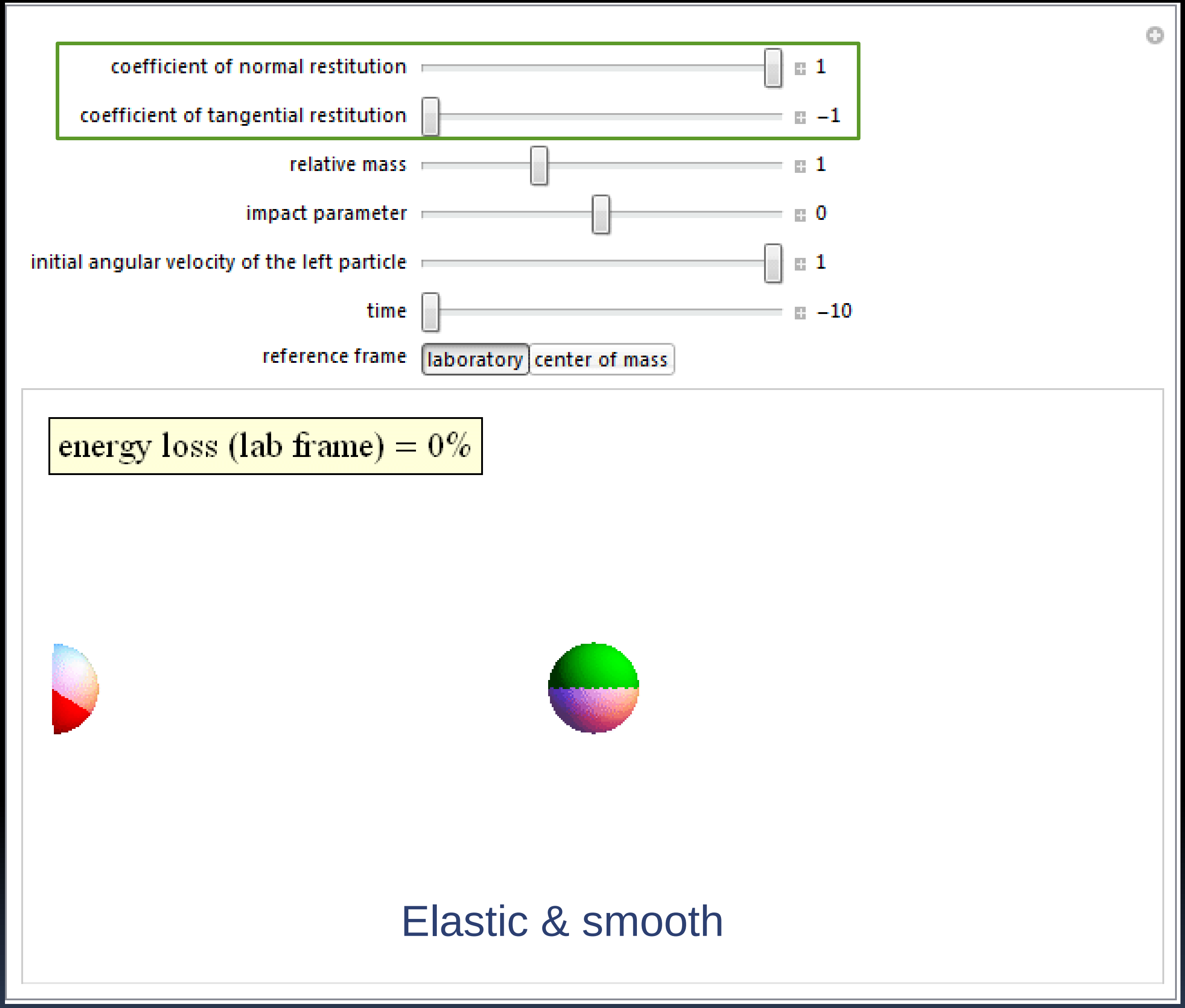
Energy collisional loss

$$E_{ij} = \frac{1}{2}mv_i^2 + \frac{1}{2}mv_j^2 + \frac{1}{2}I\omega_i^2 + \frac{1}{2}I\omega_j^2$$

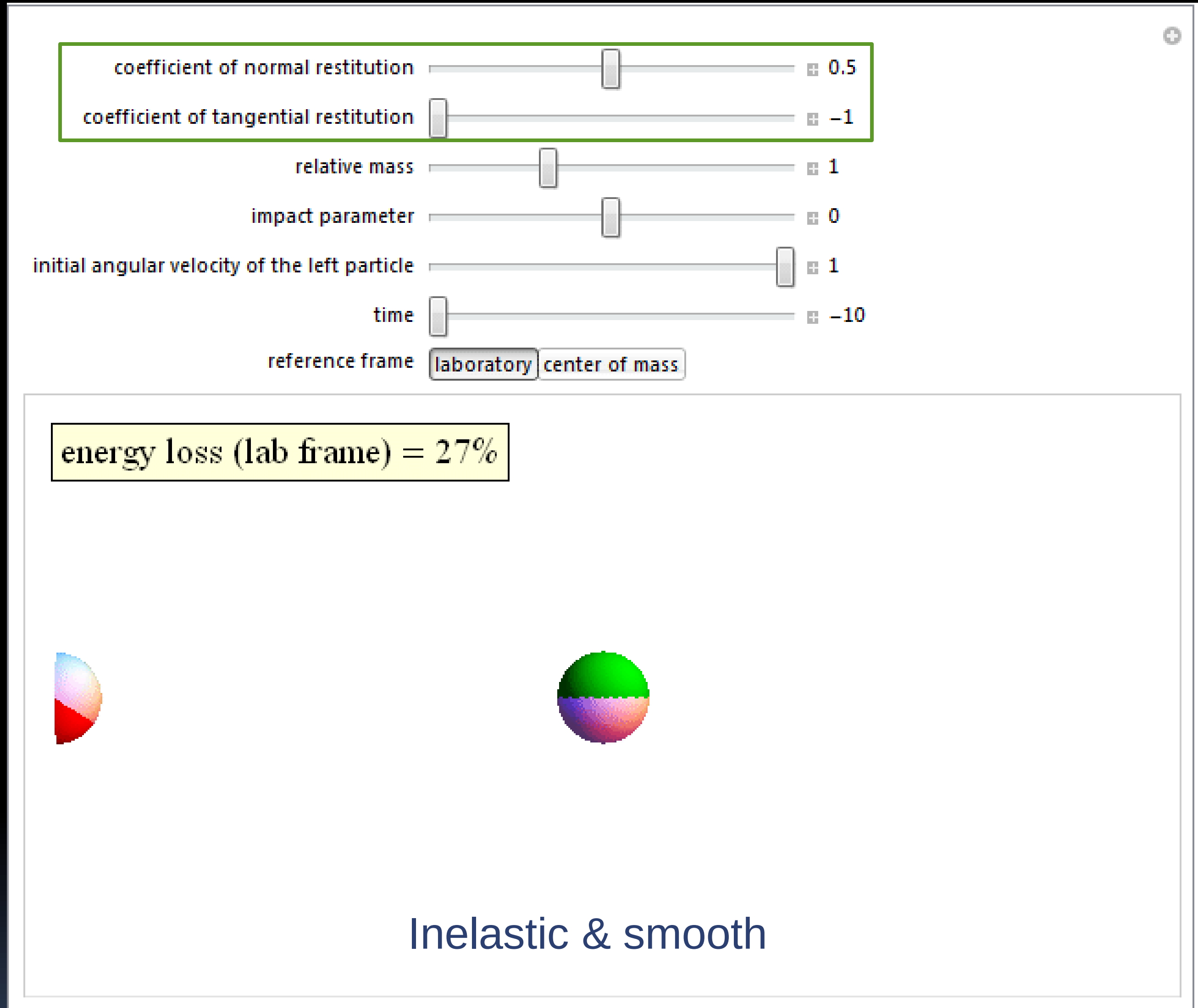
$$\begin{aligned} E'_{ij} - E_{ij} &= -(1-\alpha^2)\times\cdots \\ &\quad -(1-\beta^2)\times\cdots \end{aligned}$$

Energy is conserved *only* if the spheres are

- elastic (α=1) and
- either
  - perfectly smooth (β=-1) or
  - perfectly rough (β=+1)

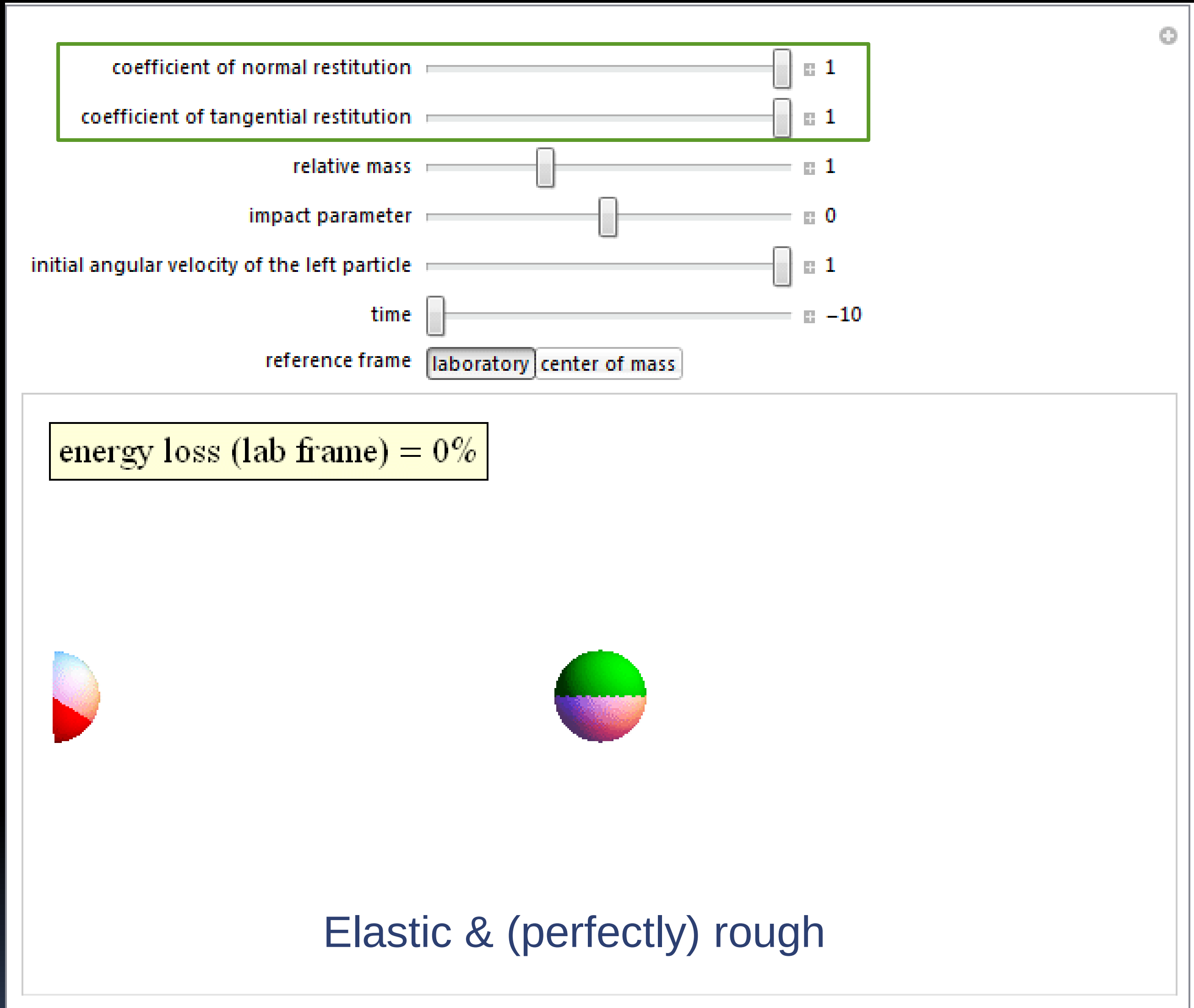


http://demonstrations.wolfram.com/InelasticCollisionsOfTwoRoughSpheres/



Inelastic & smooth

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



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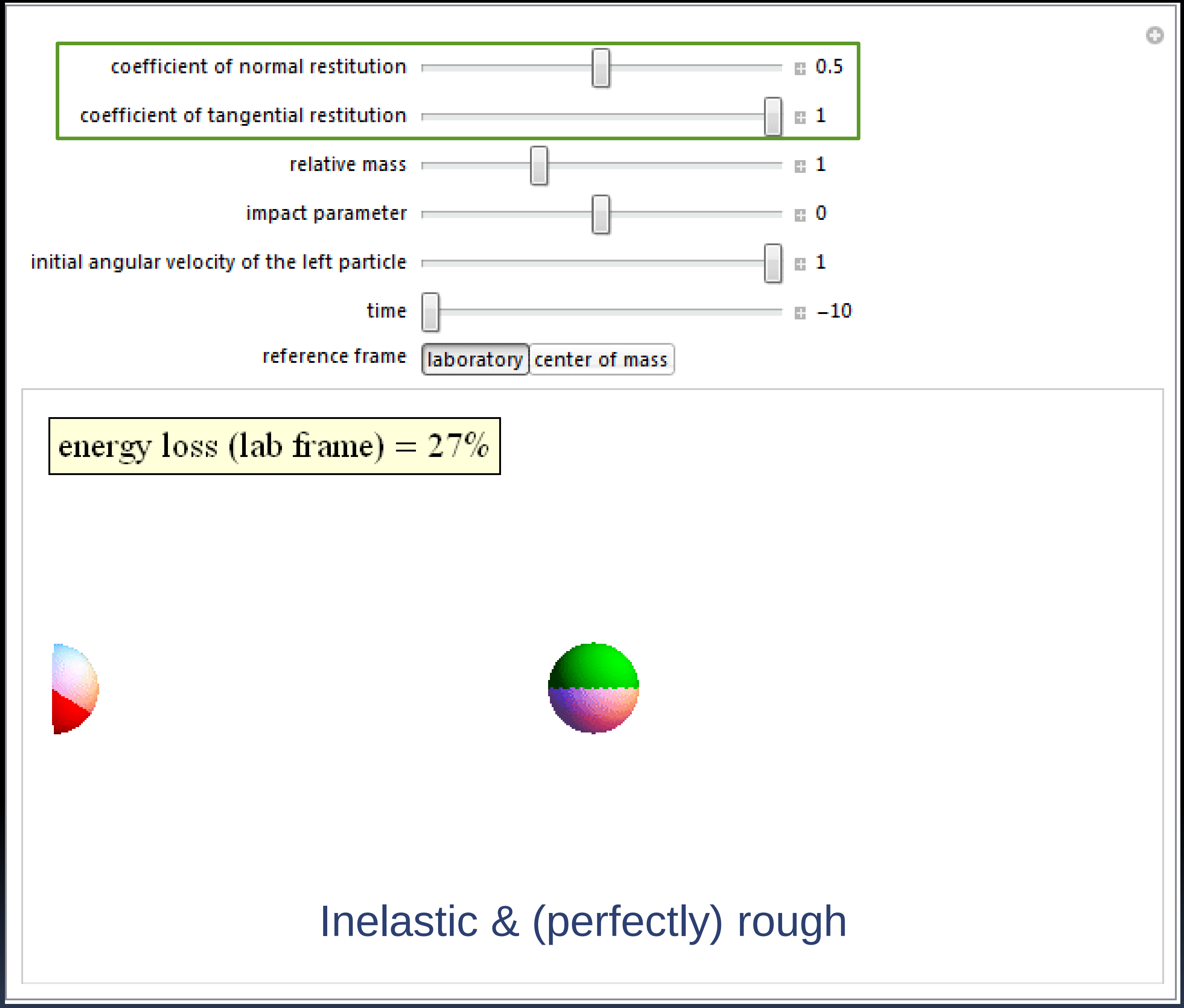

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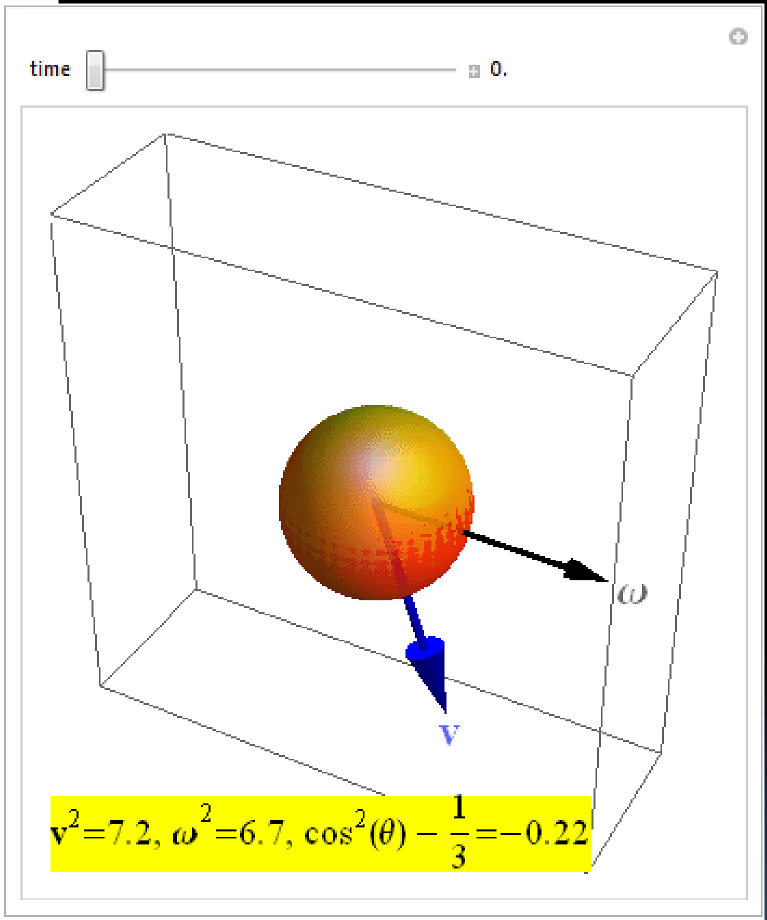
F. Vega Reyes, A. S., and G. M. Kremer, Phys. Rev. E **89**, 020202(R) (2014)

Francisco Vega Reyes

Gilberto M. Kremer

Granular temperatures, kurtoses, and correlations



translational temperature: $\langle v^2\rangle = \frac{3T_t}{m}$

rotational temperature: $\langle \omega^2\rangle = \frac{3T_r}{I}$

translational kurtosis: $\langle v^4\rangle = \frac{5}{3}\langle v^2\rangle^2\left(1+a_{20}^{(0)}\right)$

rotational kurtosis: $\langle \omega^4\rangle = \frac{5}{3}\langle \omega^2\rangle^2\left(1+a_{02}^{(0)}\right)$

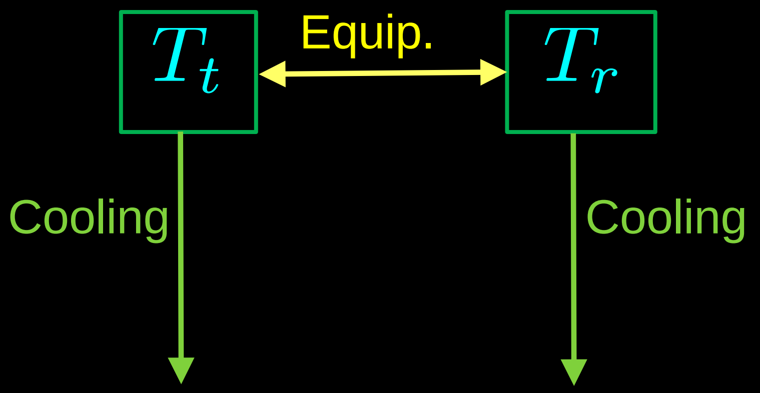
scalar correlations: $\langle v^2\omega^2\rangle = \langle v^2\rangle\langle \omega^2\rangle\left(1+a_{11}^{(0)}\right)$

angular correlations: $\langle(\mathbf{v}\cdot\boldsymbol{\omega})^2\rangle - \frac{1}{3}\langle v^2\omega^2\rangle \propto a_{00}^{(1)}$

Our aim:

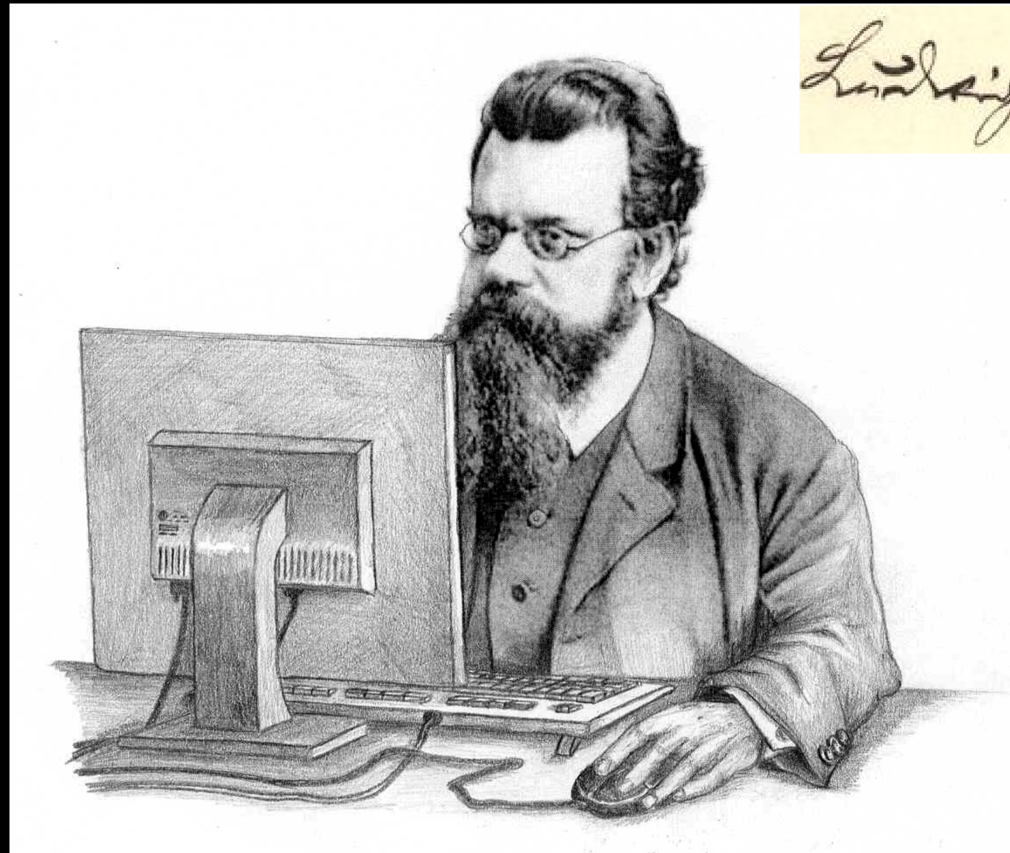
To measure

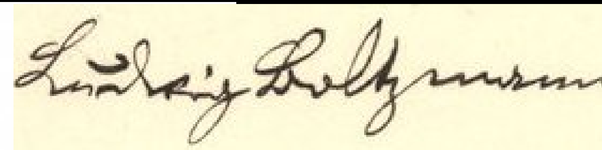
- Temperature ratio $\theta \equiv T_r/T_t$
- Kurtosis $a_{20}^{(0)}$
- Kurtosis $a_{02}^{(0)}$
- Correlation $a_{11}^{(0)}$
- Correlation $a_{00}^{(1)}$



in the Homogeneous Cooling State (HCS).

$$T_t(t) \sim t^{-2}, \quad T_r(t)/T_t(t) \to \text{const}$$





(1844-1906)

(Cartoon by Bernhard Reischl, University of Vienna)

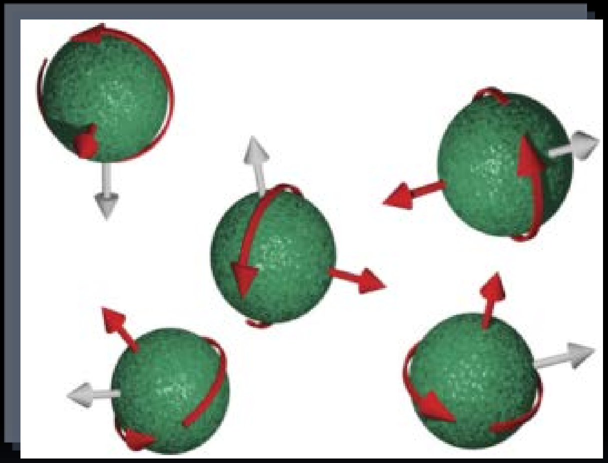
Boltzmann equation:

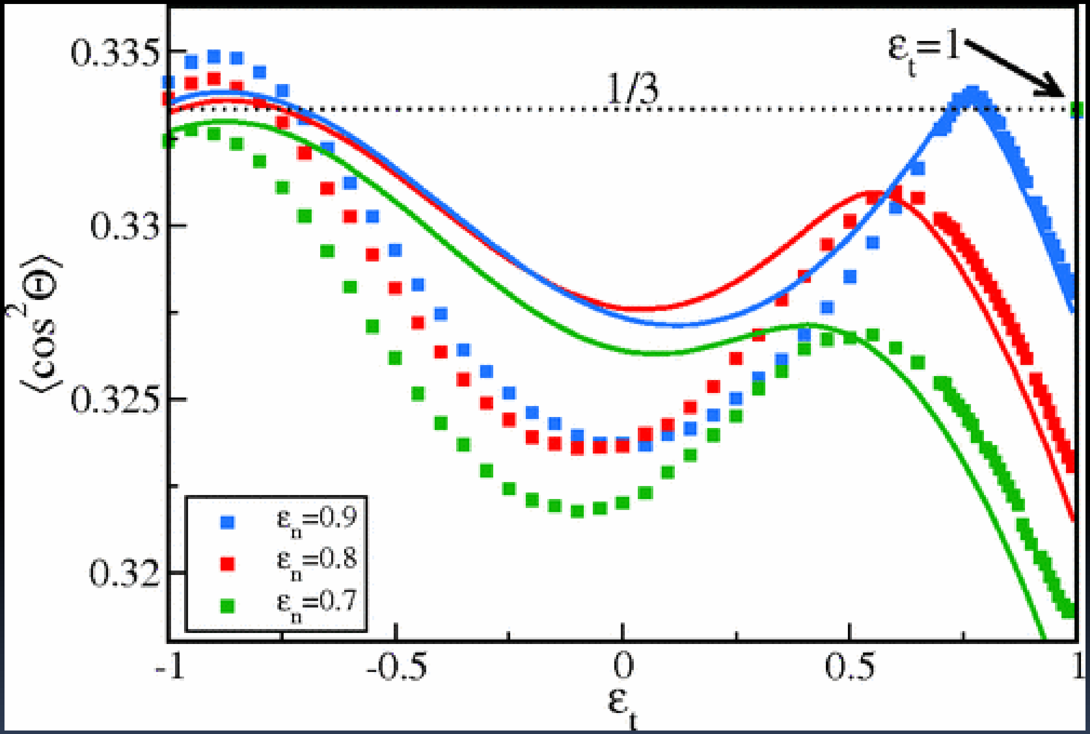
$$\partial_t f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) + \mathbf{v}\cdot\nabla f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) = J[\mathbf{r},\mathbf{v},\boldsymbol{\omega},t|f]$$

Inelastic+Rough collisions

Antecedents

N. V. Brilliantov, T. Pöschel, W. T. Kranz, and A. Zippelius, Phys. Rev. Lett. **98**, 128001 (2007)





SCALED QUANTITIES

Scaled velocities: $\mathbf{c}(t) \equiv \dfrac{\mathbf{v}}{\sqrt{2T_t(t)/m}}, \quad \mathbf{w}(t) \equiv \dfrac{\boldsymbol{\omega}}{\sqrt{2T_r(t)/I}}$

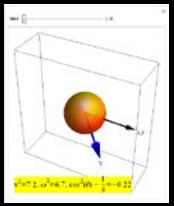
Scaled distribution function: $\phi(\mathbf{c},\mathbf{w}) \equiv \dfrac{1}{n}\left[\dfrac{4T_t(t)T_r(t)}{mI}\right]^{3/2} f(\mathbf{v},\boldsymbol{\omega},t)$

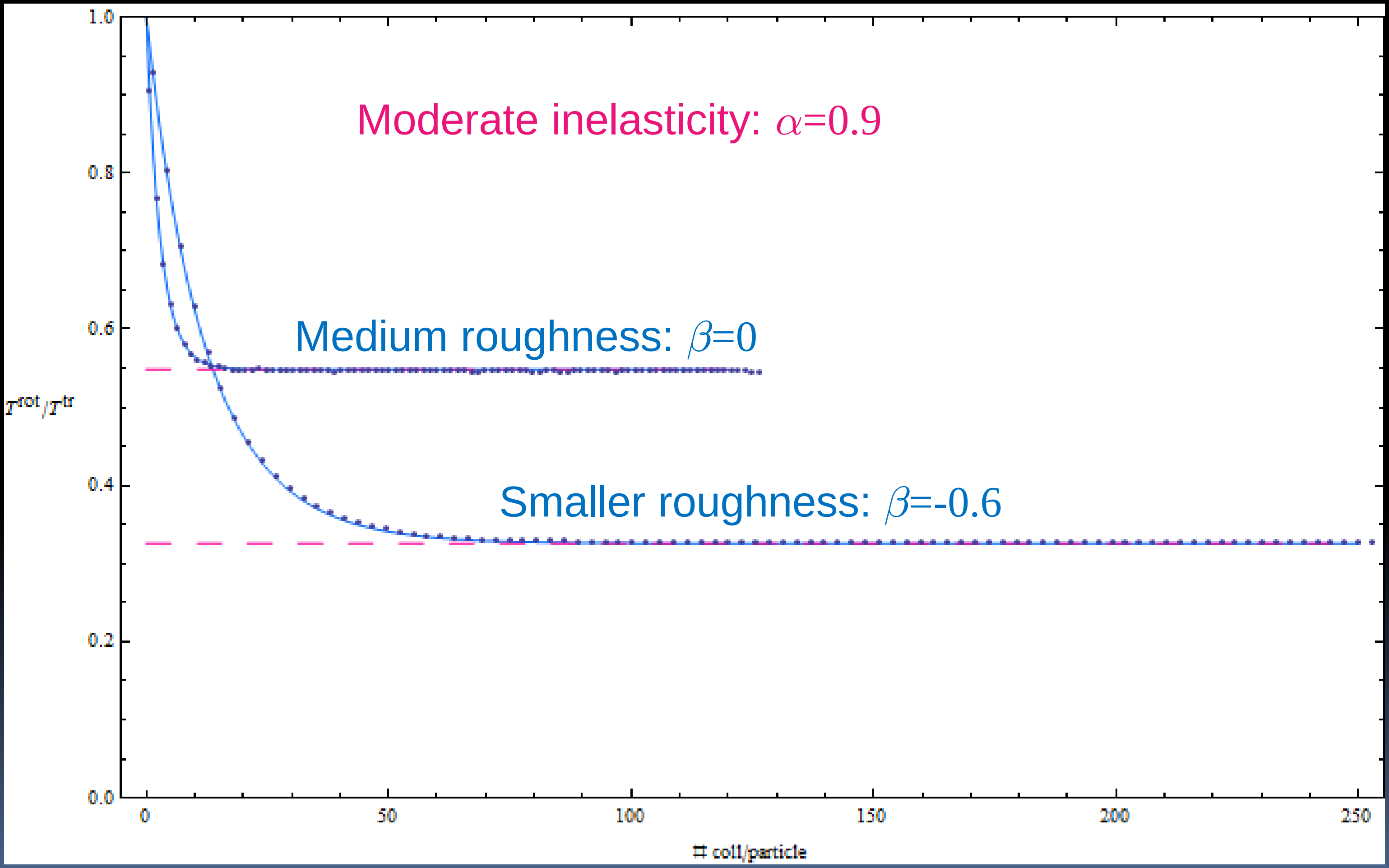
Linear Sonine approximation

$$\phi(\mathbf{c},\mathbf{w}) \simeq \pi^{-3}e^{-c^2-w^2}\left\{1 + a_{20}^{(0)}\frac{15-20c^2+4c^4}{8} + a_{02}^{(0)}\frac{15-20w^2+4w^4}{8} + a_{11}^{(0)}\frac{\left(3-2c^2\right)\left(3-2w^2\right)}{4} + a_{00}^{(1)}\frac{3(\mathbf{c}\cdot\mathbf{w})^2-c^2w^2}{2}\right\}$$

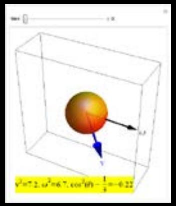
Results.
Comparison with Monte Carlo (DSMC) and molecular dynamics (MD) simulations

Time evolution.Temperature ratio



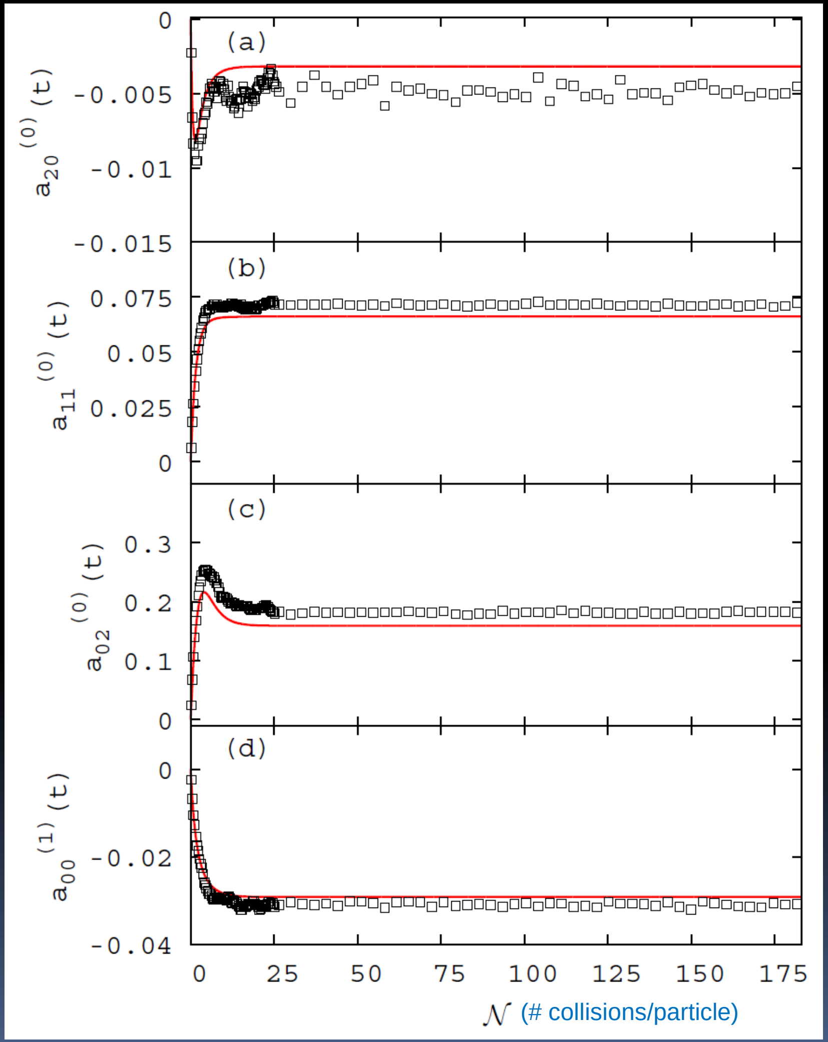


Time evolution. Cumulants

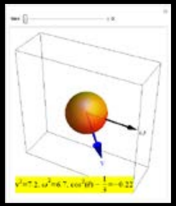


Moderate inelasticity: α=0.9

Medium roughness: β=0

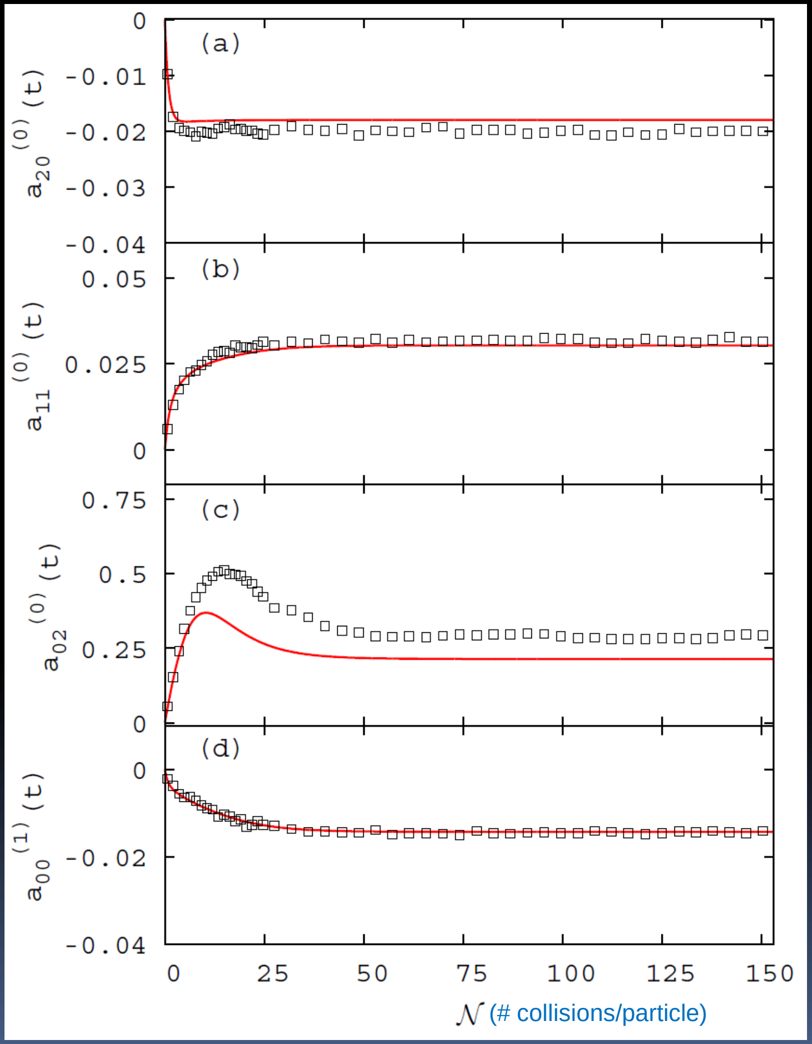


Time evolution. Cumulants

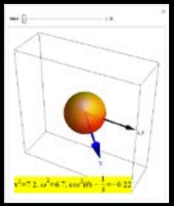


Moderate inelasticity: α=0.9

Smaller roughness: β=-0.6

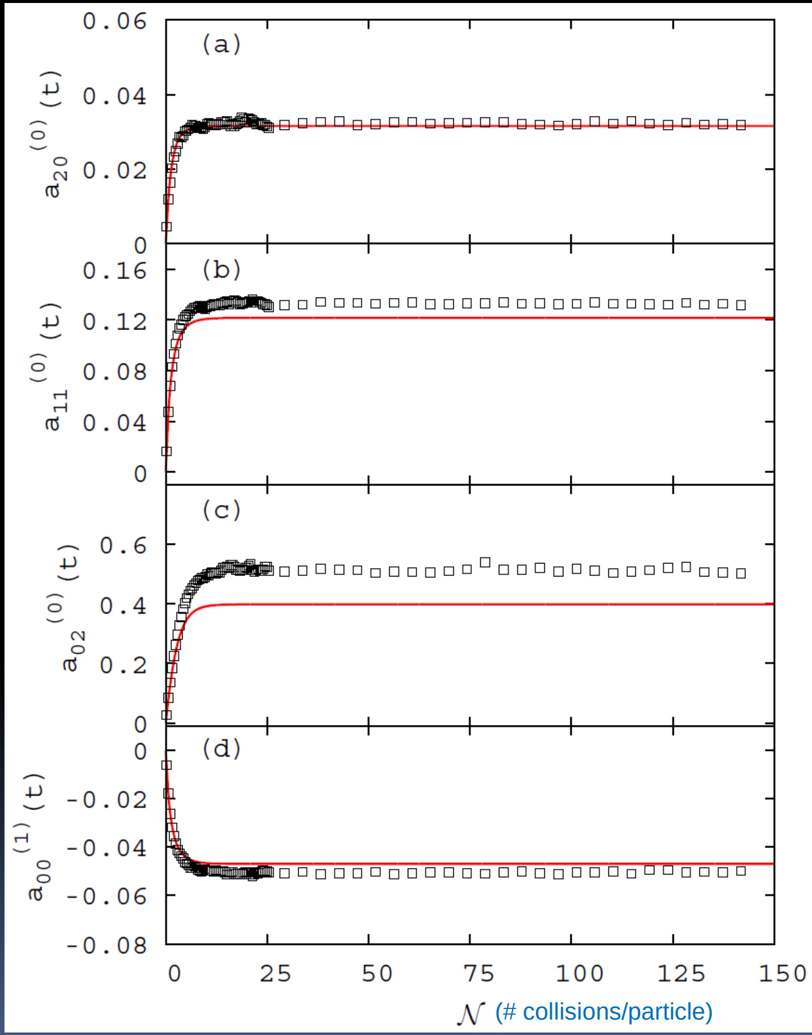


Time evolution. Cumulants

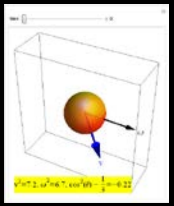


Larger inelasticity: α=0.7

Medium roughness: β=0

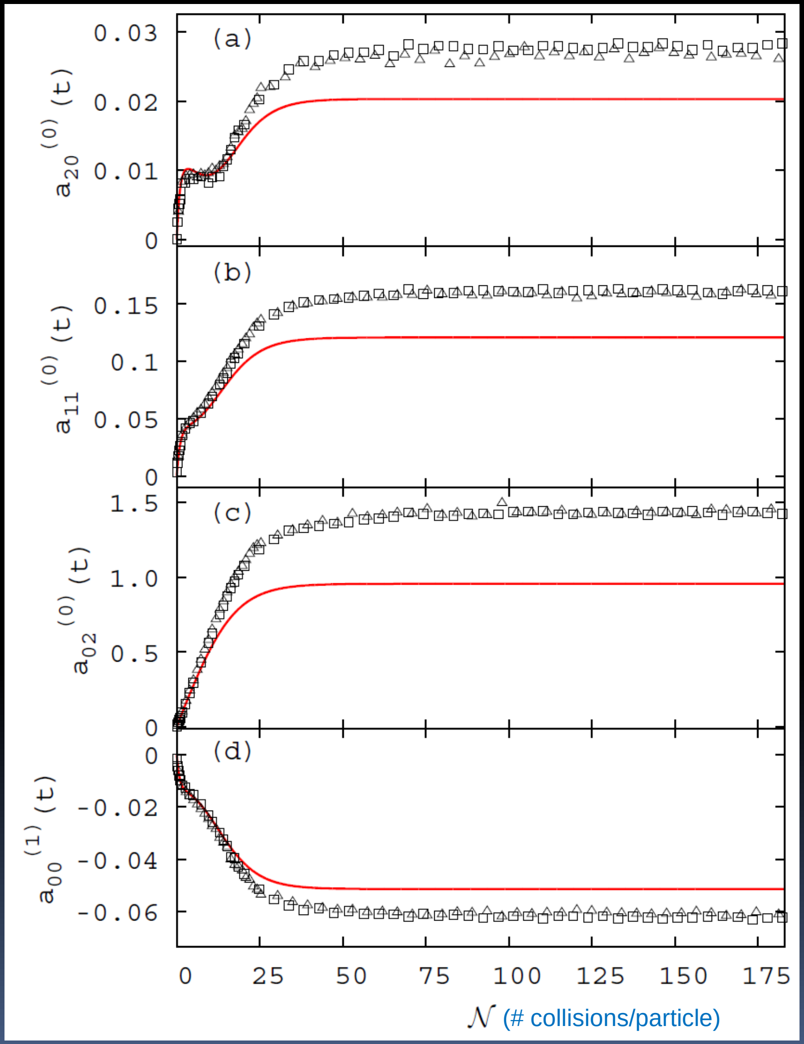


Time evolution. Cumulants

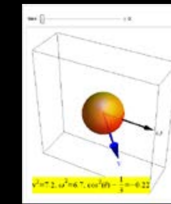


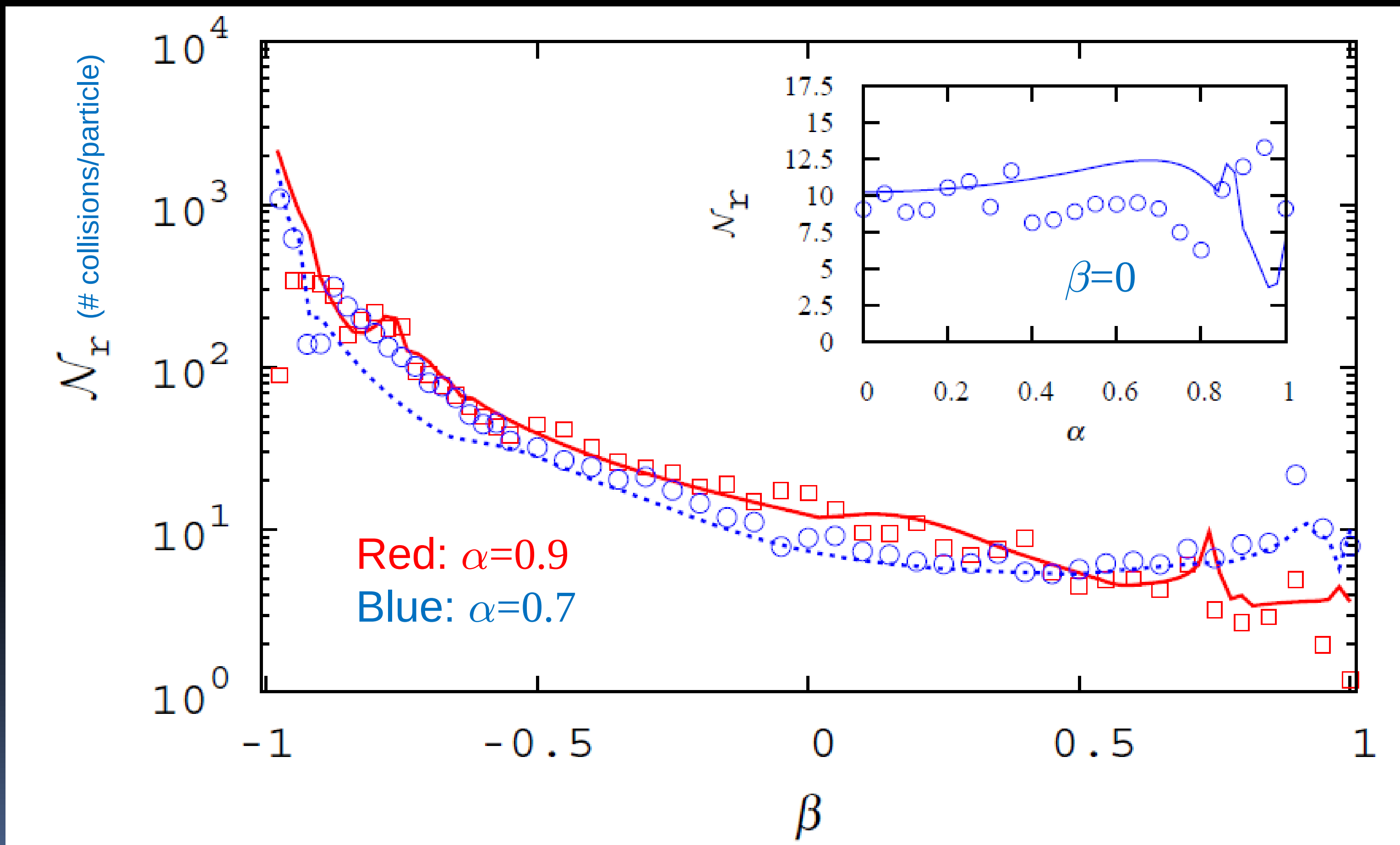
Larger inelasticity: α=0.7

Smaller roughness: β=-0.575

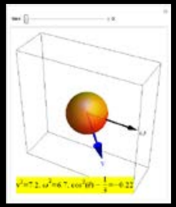


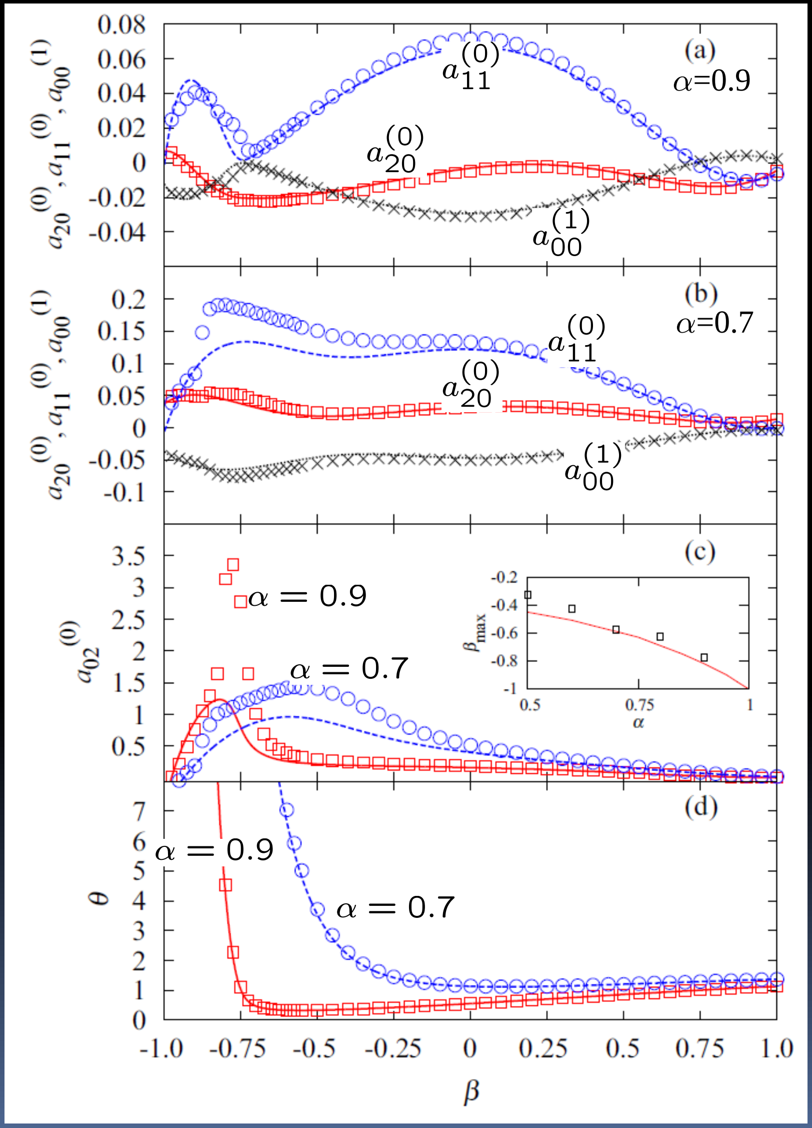
Relaxation time





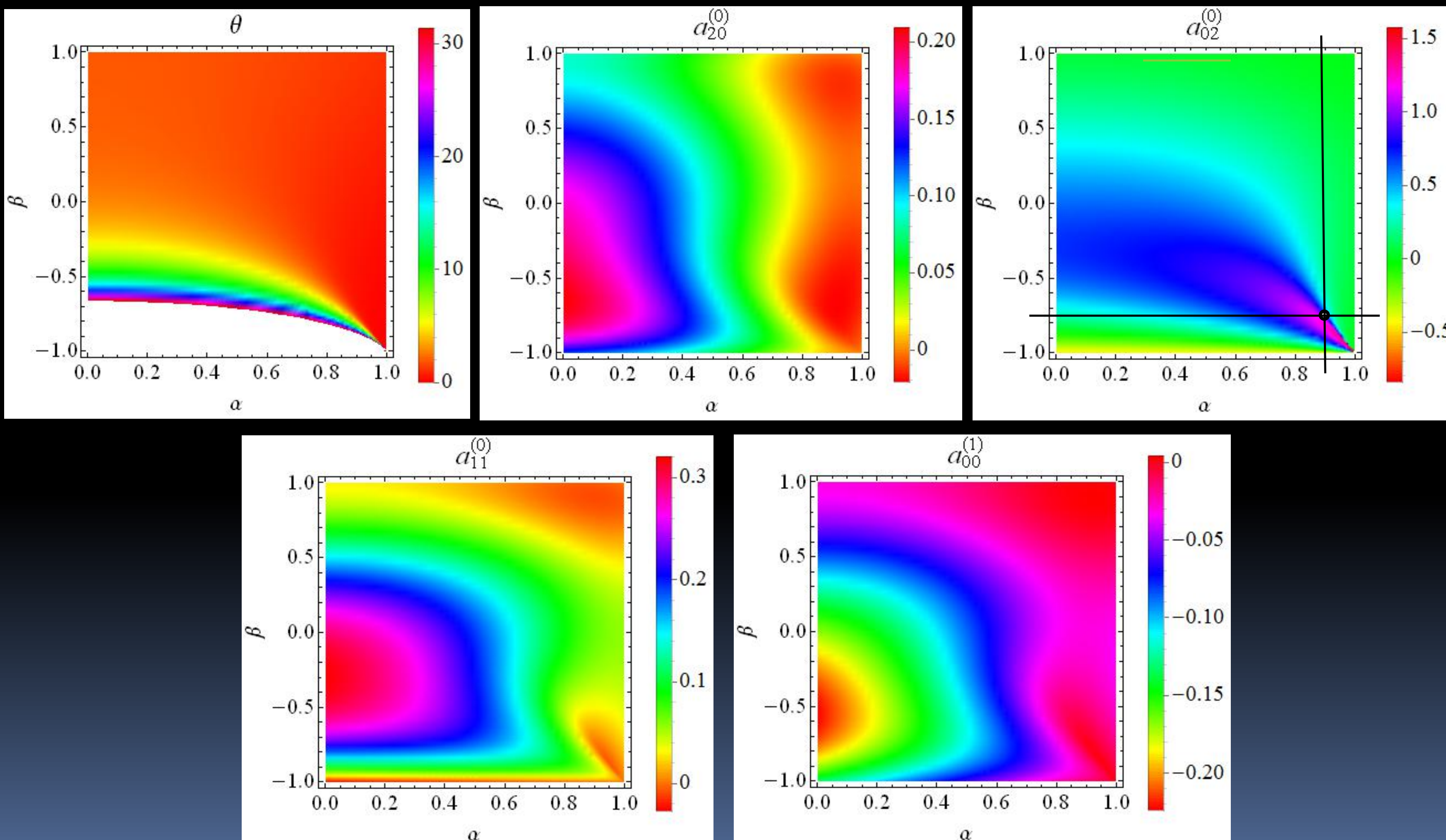
Stationary values



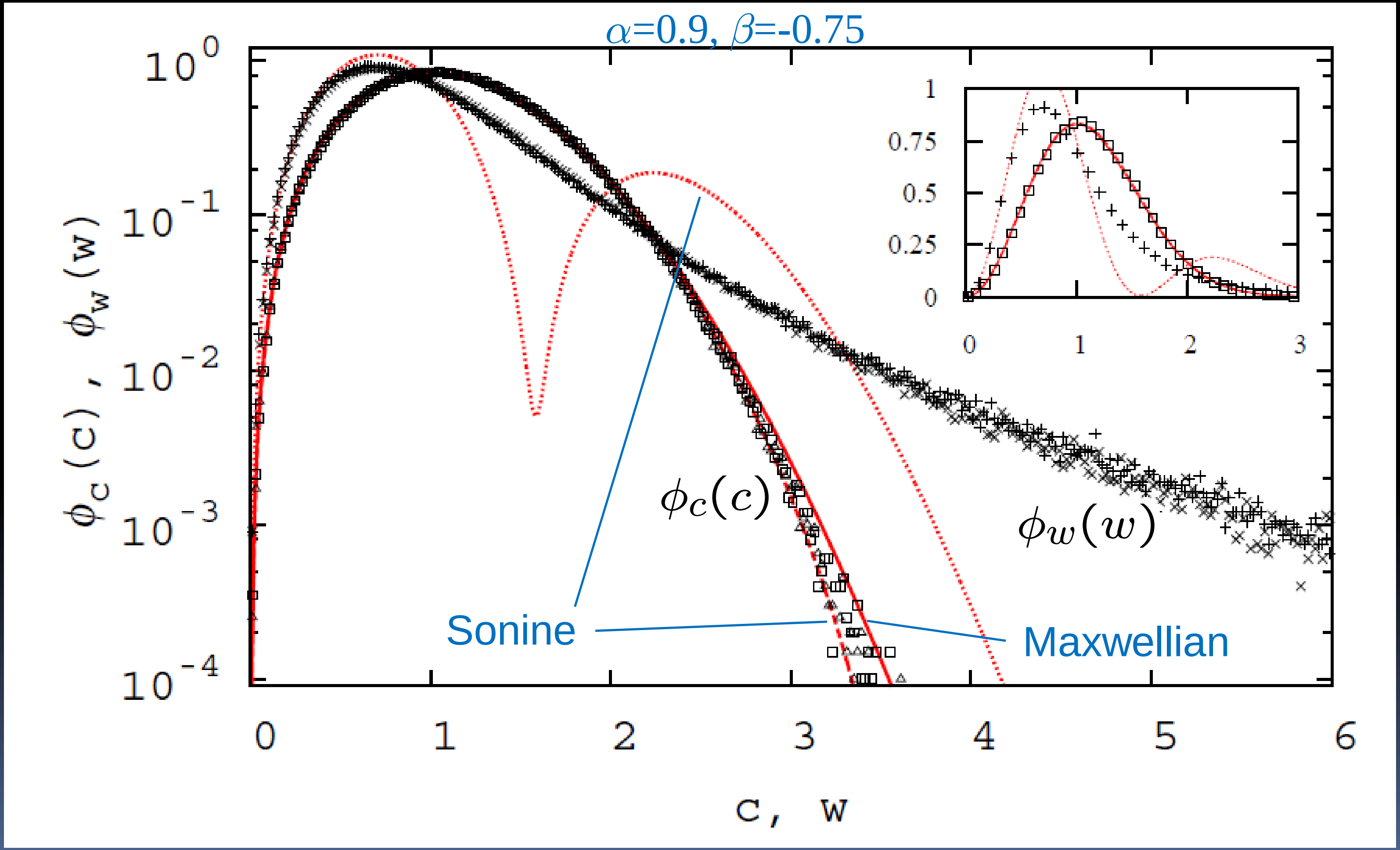


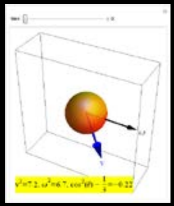
Stationary values

Density plots (Theory only)



(Marginal) velocity distributions





Conclusions (Part 1)

- The relaxation time is practically independent of the inelasticity coefficient α. However, it dramatically increases in the quasi-smooth limit ($\beta \to -1$).
- The linearized Sonine approximation theory provides an excellent description of the temperature ratio and the four velocity cumulants, *except* when the angular velocity kurtosis becomes large ($a_{02}^{(0)} > 0.3$).
- The cumulants are relatively small in the experimentally relevant regime $\beta > 0$.

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- 1. Homogeneous cooling state. Velocity cumulants.
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G. M. Kremer, A. S., and V. Garzó, in preparation

Gilberto M. Kremer

Vicente Garzó

Hydrodynamic fields

$$\begin{aligned}
\text{Number density:} \quad n(\mathbf{r},t) &= \int d\mathbf{v} \int d\boldsymbol{\omega}\, f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) \\
\text{Flow velocity:} \quad \mathbf{u}(\mathbf{r},t) &= \frac{1}{n} \int d\mathbf{v} \int d\boldsymbol{\omega}\, \mathbf{v} f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t) \\
\text{Temperature:} \quad T(\mathbf{r},t) &= \frac{1}{2}\left[T_t(\mathbf{r},t) + T_r(\mathbf{r},t)\right] \\
&= \frac{1}{3n} \int d\mathbf{v} \int d\boldsymbol{\omega}\, \left[m\left(\mathbf{v}-\mathbf{u}\right)^2 + I\omega^2\right] f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)
\end{aligned}$$

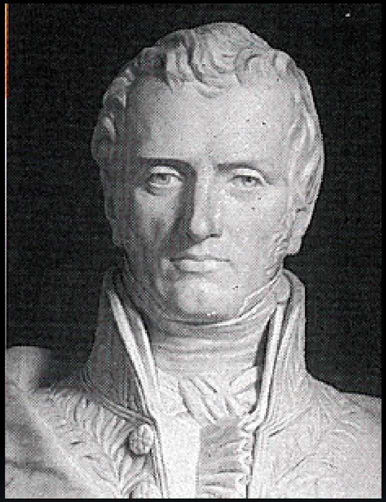
Hydrodynamic fluxes

$$\text{Pressure tensor: } \mathsf{P}(\mathbf{r},t) = \int d\mathbf{v} \int d\boldsymbol{\omega}\; (\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u})\, f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)$$

$$\begin{aligned}
\text{Heat flux: } \mathbf{q}(\mathbf{r},t) &= \mathbf{q}_t(\mathbf{r},t) + \mathbf{q}_r(\mathbf{r},t) \\
&= \frac{1}{2}\int d\mathbf{v} \int d\boldsymbol{\omega}\, \left[m\,(\mathbf{v}-\mathbf{u})^2 + I\omega^2\right] \\
&\quad \times (\mathbf{v}-\mathbf{u})\, f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)
\end{aligned}$$

$$\begin{aligned}
\text{Cooling rate: } \zeta(\mathbf{r},t) &= \frac{T_t}{2T}\zeta_t(\mathbf{r},t) + \frac{T_r}{2T}\zeta_r(\mathbf{r},t) \\
&= -\frac{1}{6nT}\int d\mathbf{v} \int d\boldsymbol{\omega}\, \left[m\,(\mathbf{v}-\mathbf{u})^2 + I\omega^2\right] \\
&\quad \times J[\mathbf{r},\mathbf{v},\boldsymbol{\omega},t|f]
\end{aligned}$$

Navier-Stokes-Fourier constitutive equations



Claude-Louis Navier
(1785-1836)

George Gabriel Stokes
(1819-1903)

Jean-Baptiste Joseph Fourier
(1768-1830)

Navier-Stokes-Fourier constitutive equations

$$P_{ij} = n\tau_t T\delta_{ij} - \eta\left(\nabla_i u_j + \nabla_j u_i - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{u}\right) - \eta_b\delta_{ij}\nabla\cdot\mathbf{u}$$

Shear viscosity

Bulk viscosity

Dufour-like coefficient

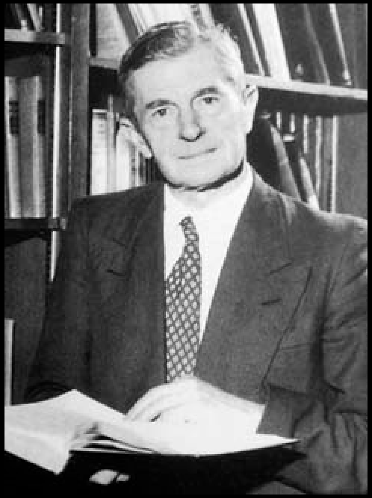
$$\mathbf{q} = -\lambda\nabla T - \mu\nabla n$$

Thermal conductivity

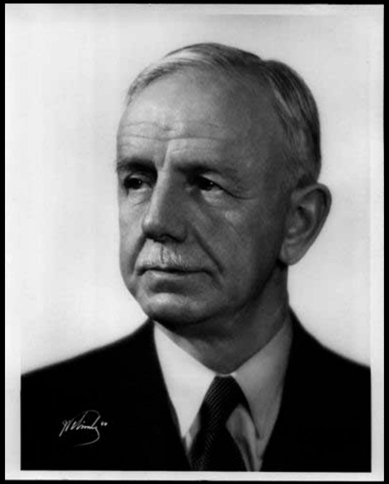
$$\zeta = \zeta^{(0)} - \xi\nabla\cdot\mathbf{u}$$

Cooling rate transport coefficient

Methodology: Chapman-Enskog method



Sydney Chapman
(1888-1970)



David Enskog
(1884-1947)

$$\boxed{f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \cdots}, \quad \epsilon \sim \nabla$$

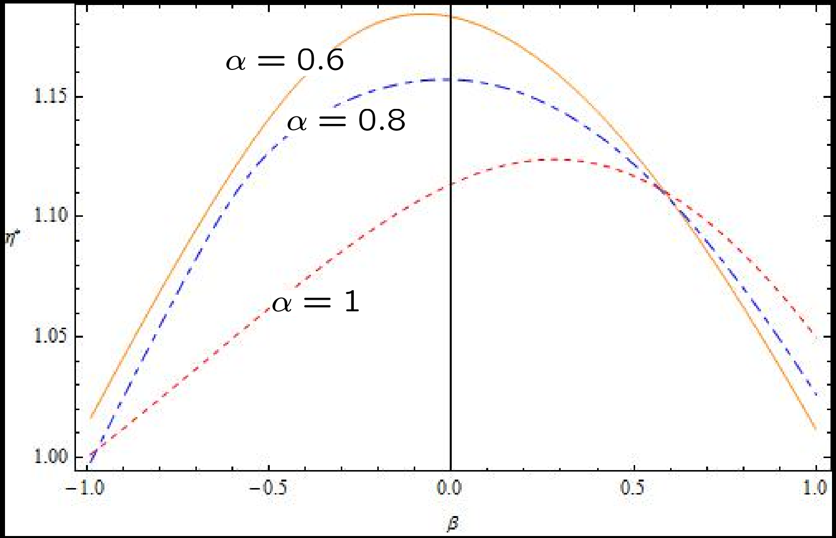
Special limiting cases

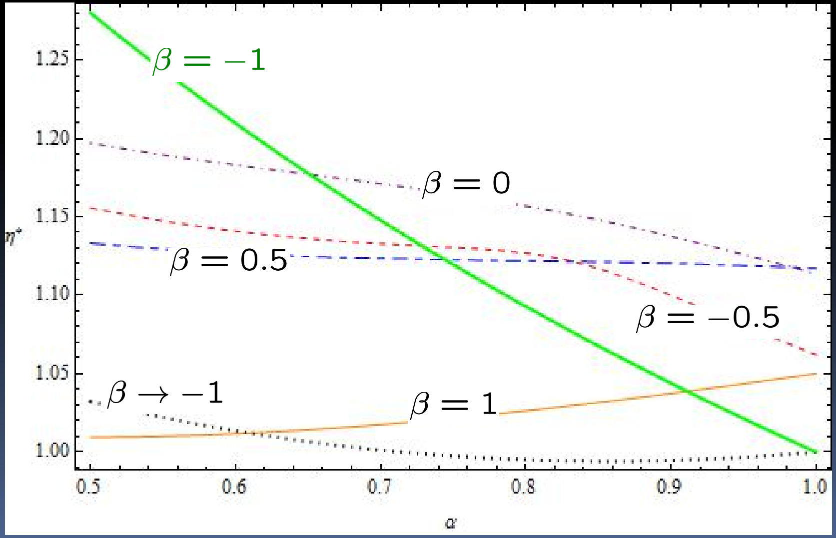
Quantity	Pure smooth ($\beta = -1$)	Quasi-smooth limit ($\beta \to -1$)	Perfectly rough and elastic ($\alpha = \beta = 1$)
η^*	$\frac{24}{(1+\alpha)(13-\alpha)}$	$\frac{24}{(1+\alpha)(19-7\alpha)}$	$\frac{6(1+\kappa)^2}{6+13\kappa}$
η_b^*	0	$\frac{8}{5(1-\alpha^2)}$	$\frac{(1+\kappa)^2}{10\kappa}$
λ^*	$\frac{64}{(1+\alpha)(9+7\alpha)}$	$\frac{48}{25(1+\alpha)}$	$\frac{12(1+\kappa)^2\left(37+151\kappa+50\kappa^2\right)}{25\left(12+75\kappa+101\kappa^2+102\kappa^3\right)}$
μ^*	$\frac{1280(1-\alpha)}{(1+\alpha)(9+7\alpha)(19-3\alpha)}$	0	0
ξ	0	0	0

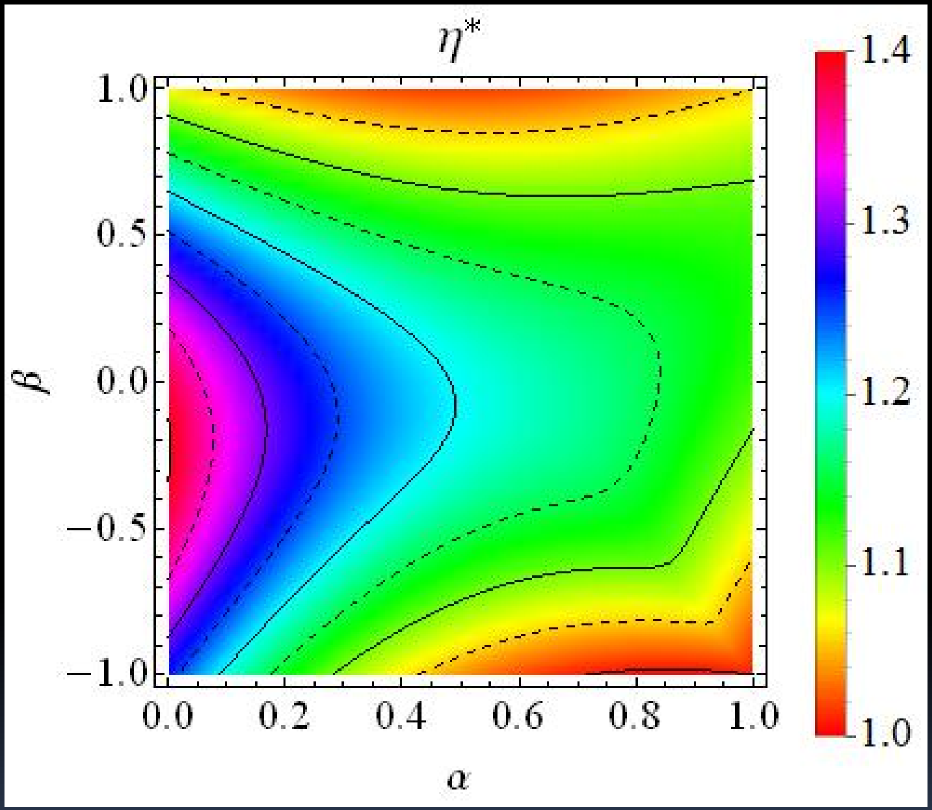
Brey, Dufty, Kim, Santos (1998)

Pidduck (1922)

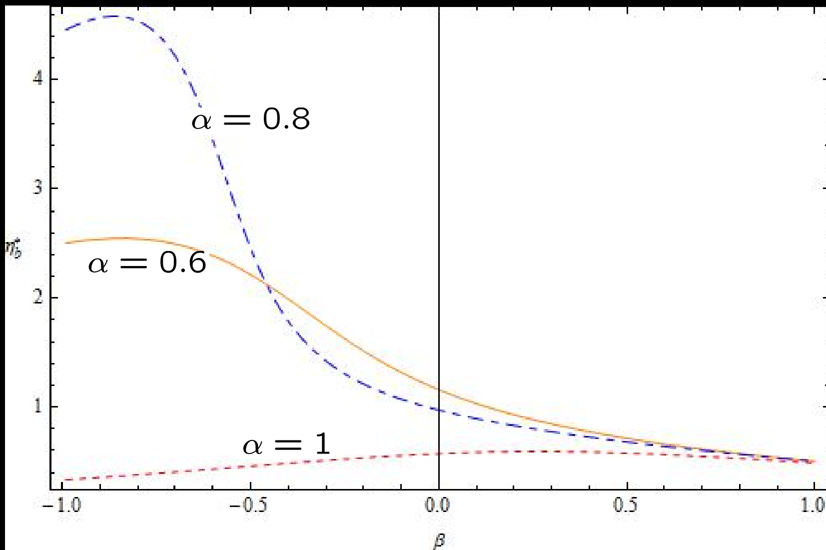
Shear viscosity

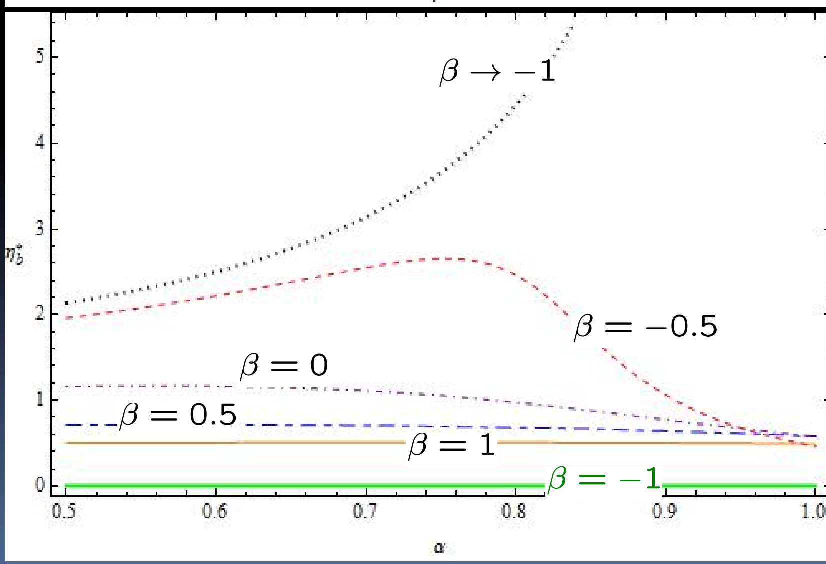


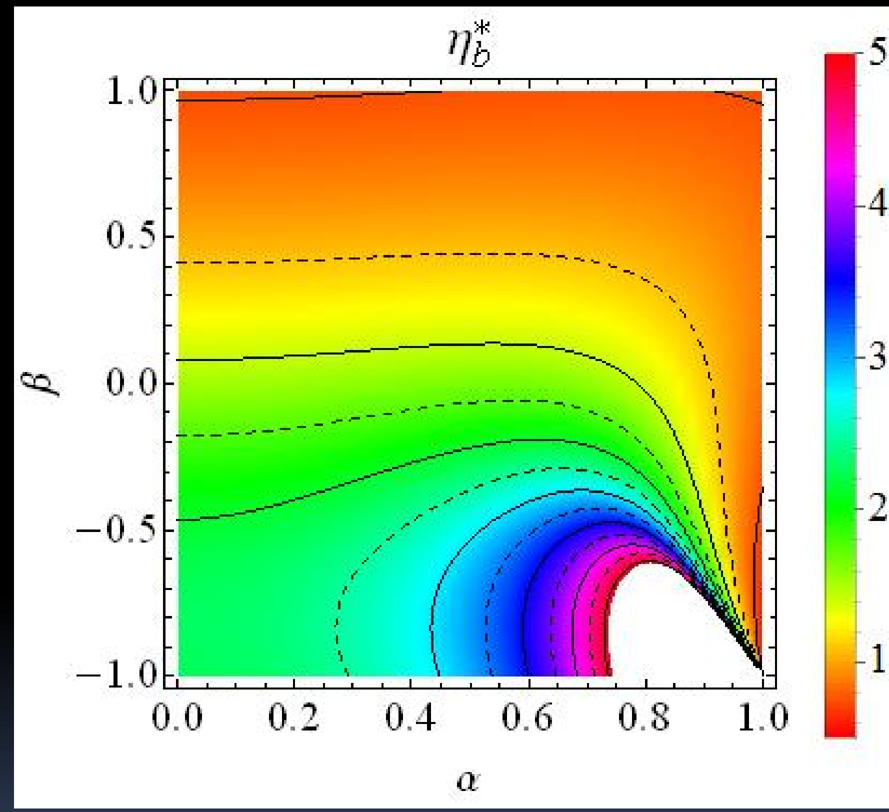




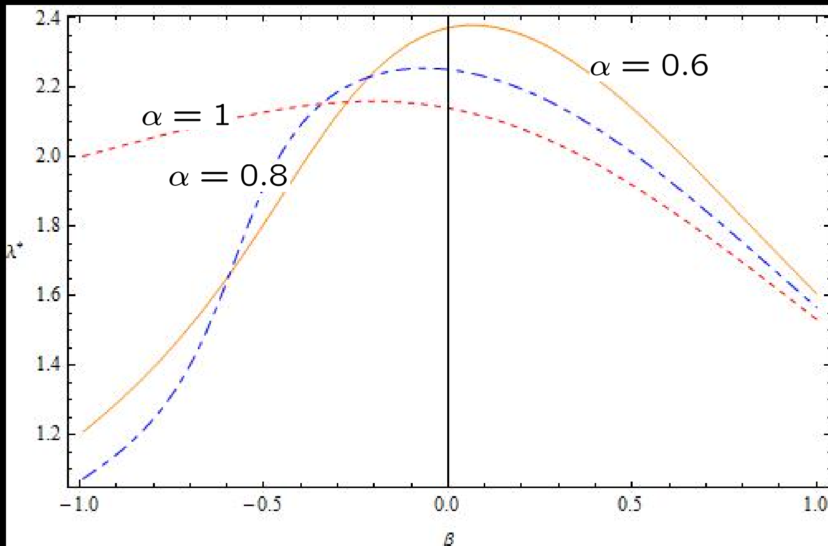
Bulk viscosity

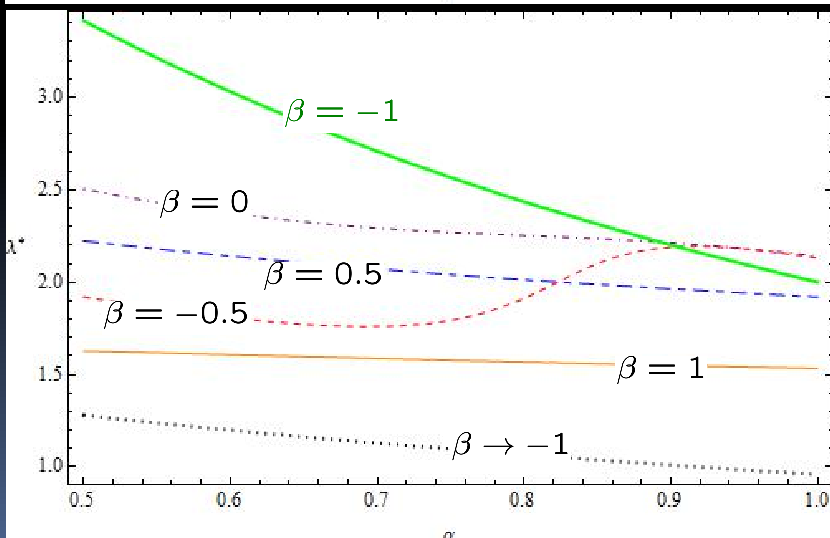


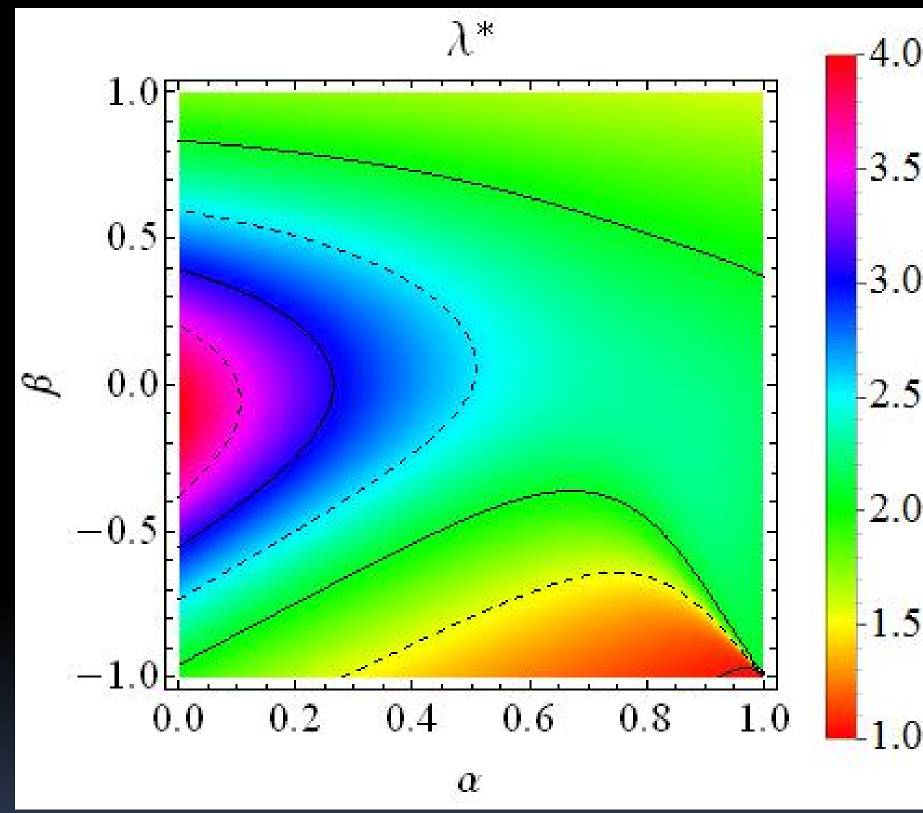




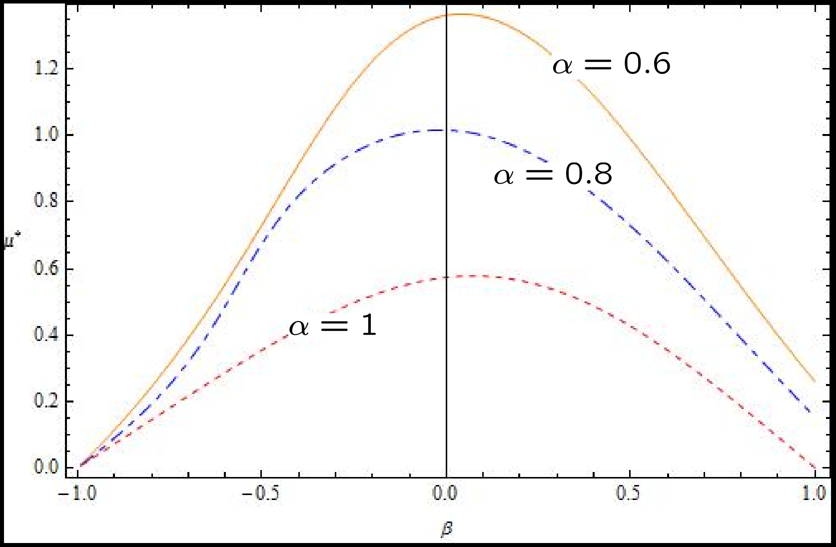
Thermal conductivity

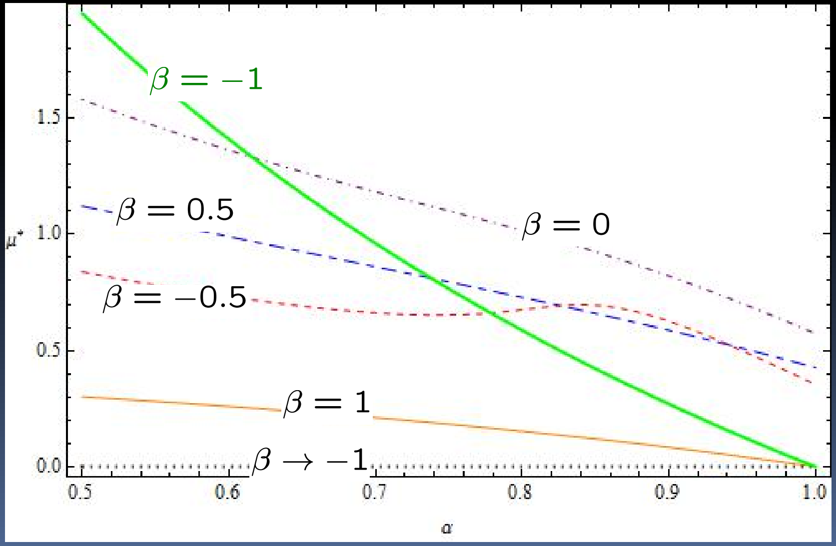


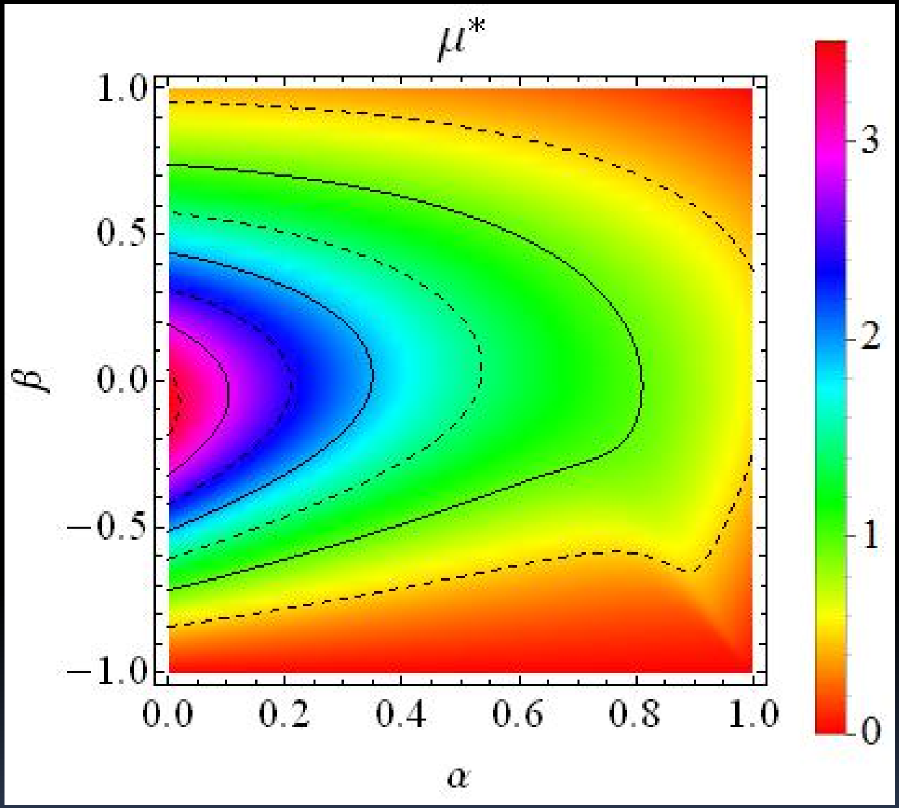




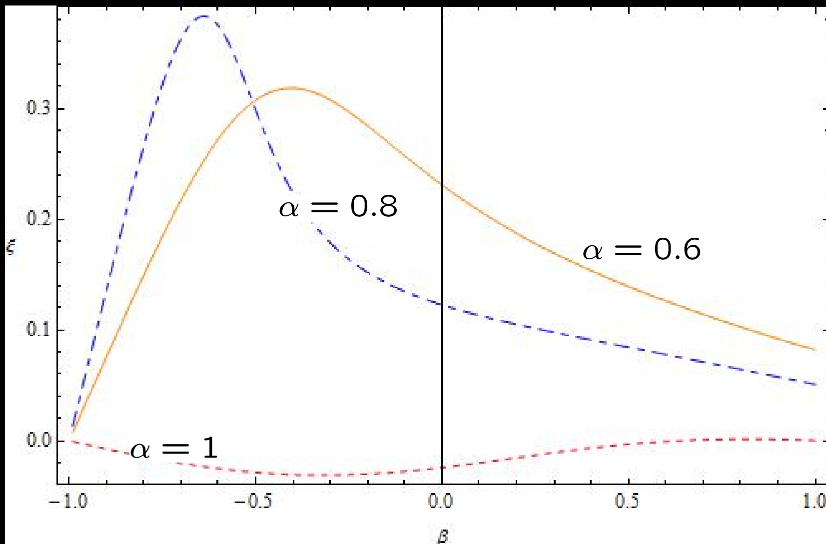
Dufour-like coefficient

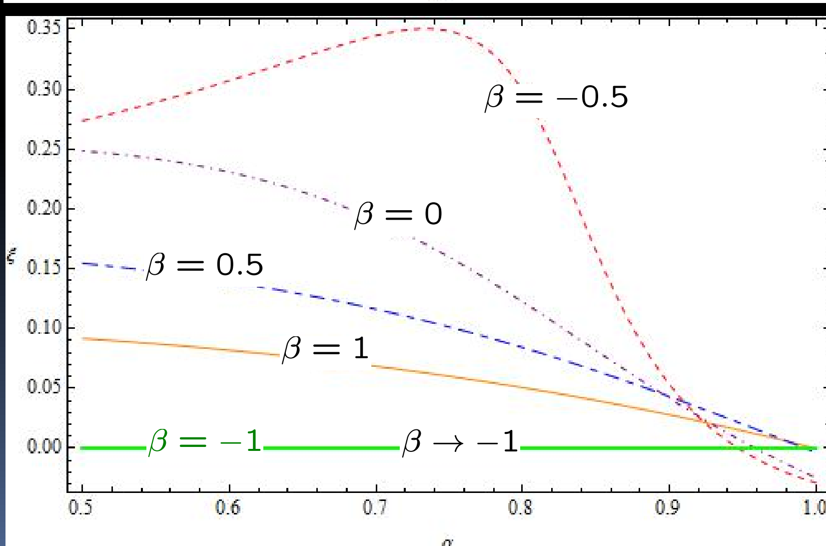


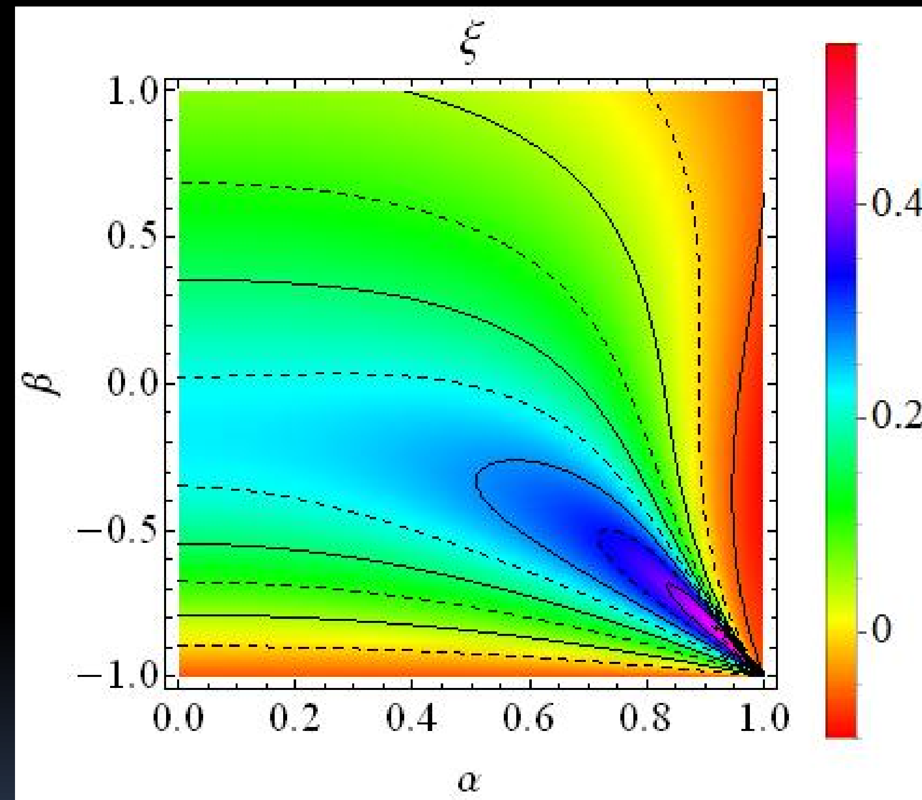




Cooling rate coefficient







Conclusions (Part 2)

- Roughness induces two extra transport coefficients (η_b, ξ), not present in the case of a (dilute) gas of smooth spheres.
- Typically, at fixed α the coefficients have a maximum at an intermediate value of β.
- In general, the dependence of the coefficients on α is weaker than in the case of smooth spheres.
- Future application: Stability analysis of the HCS.

Thank you for your attention!