HYDRODYNAMICS FOR A GRANULAR GAS OF INELASTIC ROUGH HARD SPHERES

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In collaboration with

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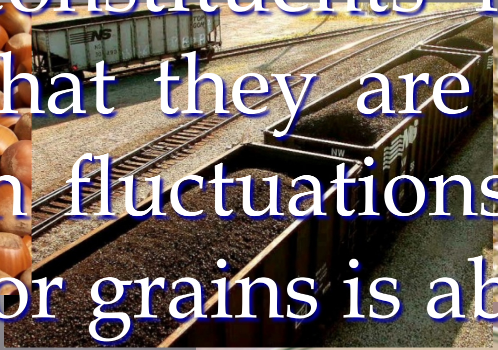
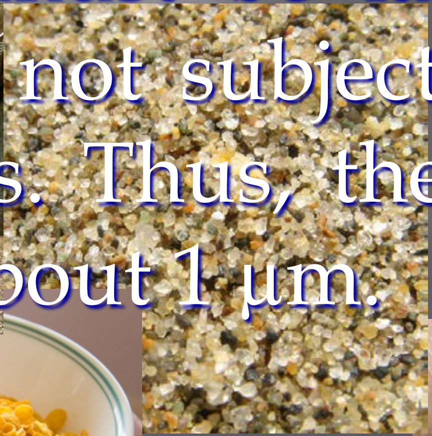
What is a granular material?

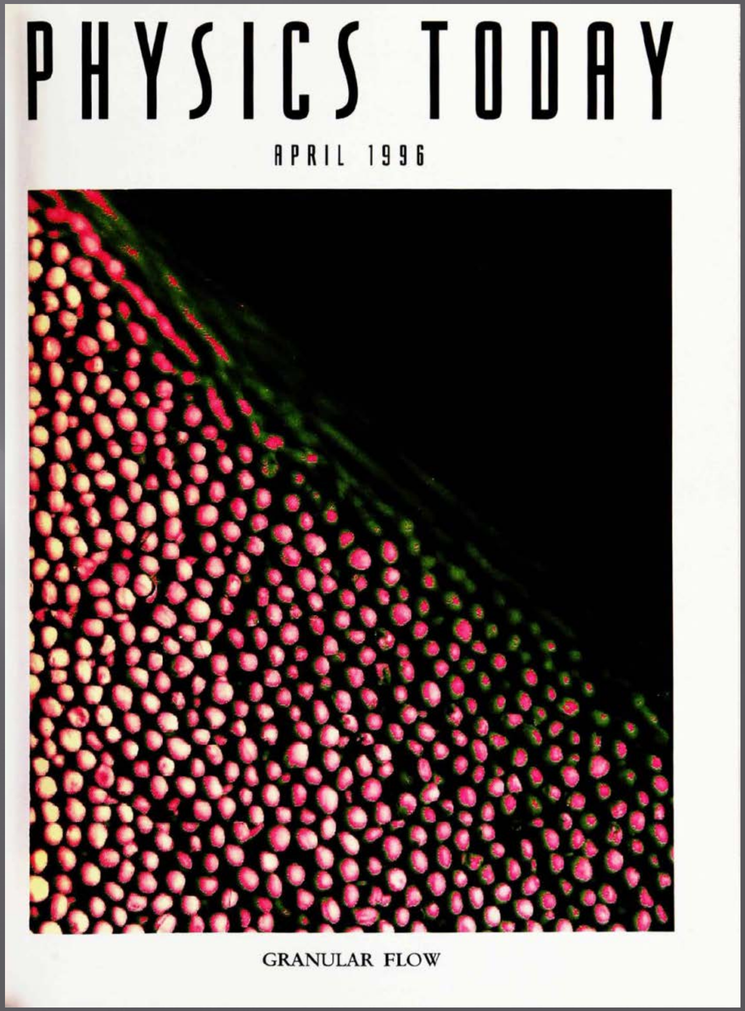
- It is a conglomeration of discrete solid, macroscopic particles characterized by a loss of energy whenever the grains collide.
- The constituents must be large enough such that they are not subject to thermal motion fluctuations. Thus, the lower size limit for grains is about 1 μm.

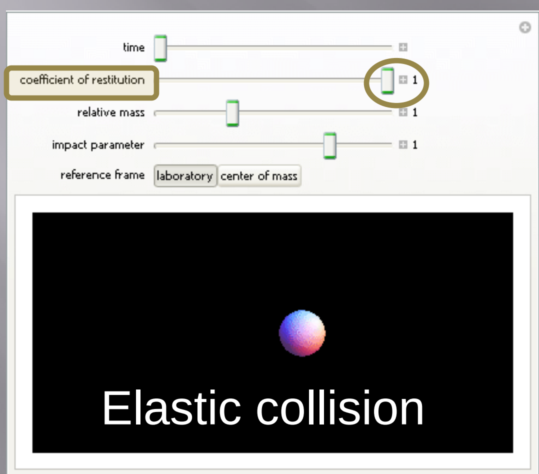


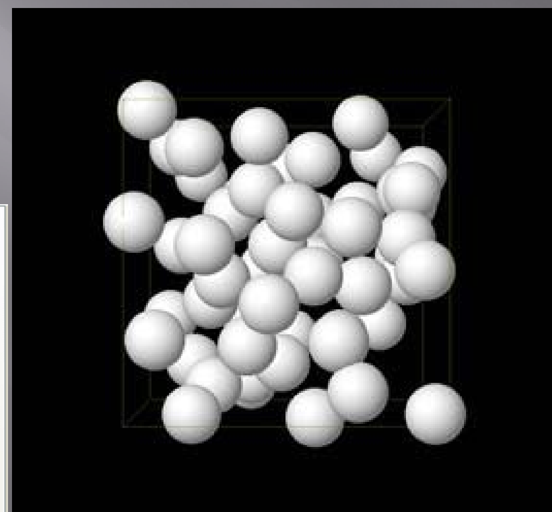
What is a granular *fluid*?

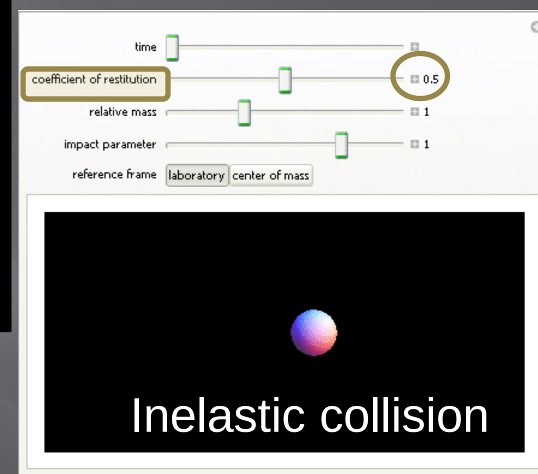
- When the granular matter is driven and energy is fed into the system (e.g., by shaking) such that the grains are not in constant contact with each other, the granular material is said to *fluidize*.



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

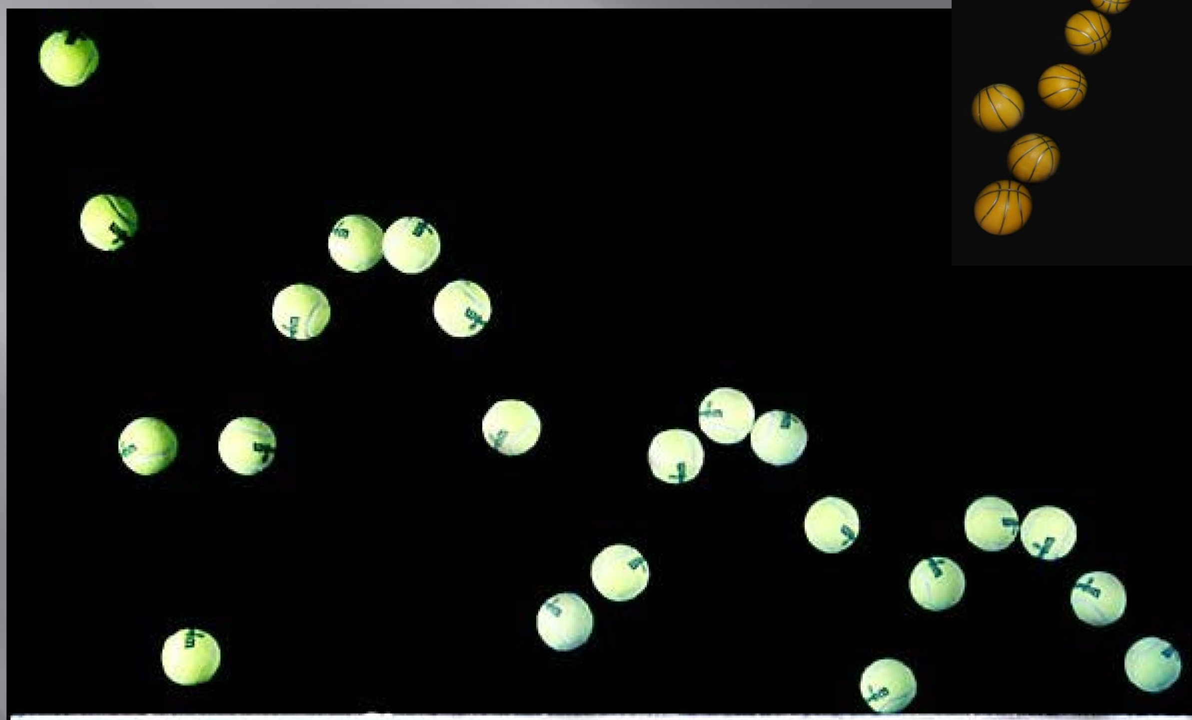






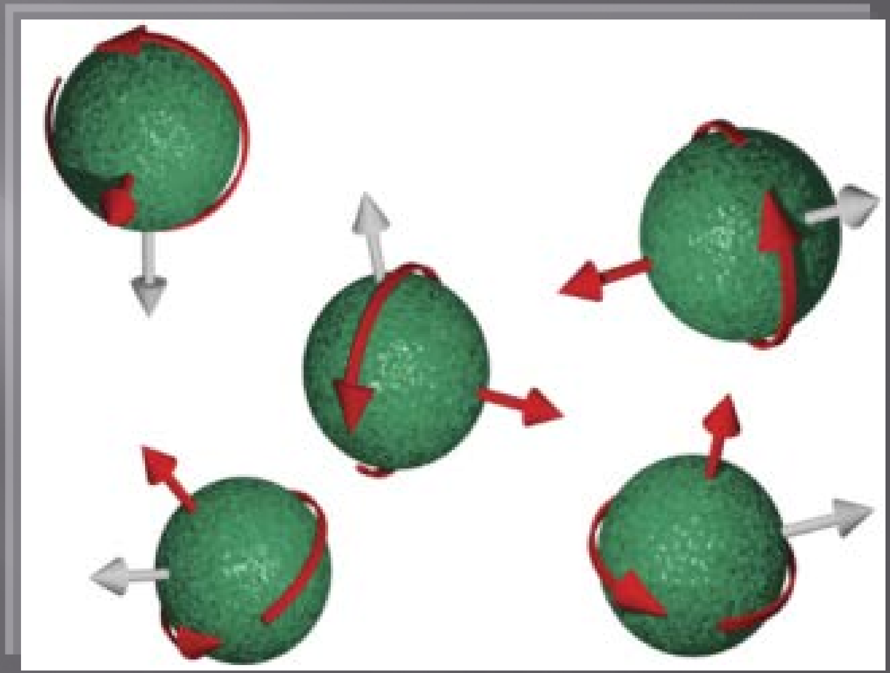
http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/

But this minimal model ignores *roughness* (spinning)



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



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

Outline of the talk

- 0. Collision rules for inelastic rough hard spheres
- 1. Navier-Stokes-Fourier transport coefficients
- 2. Stability analysis
- 3. Conclusions

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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

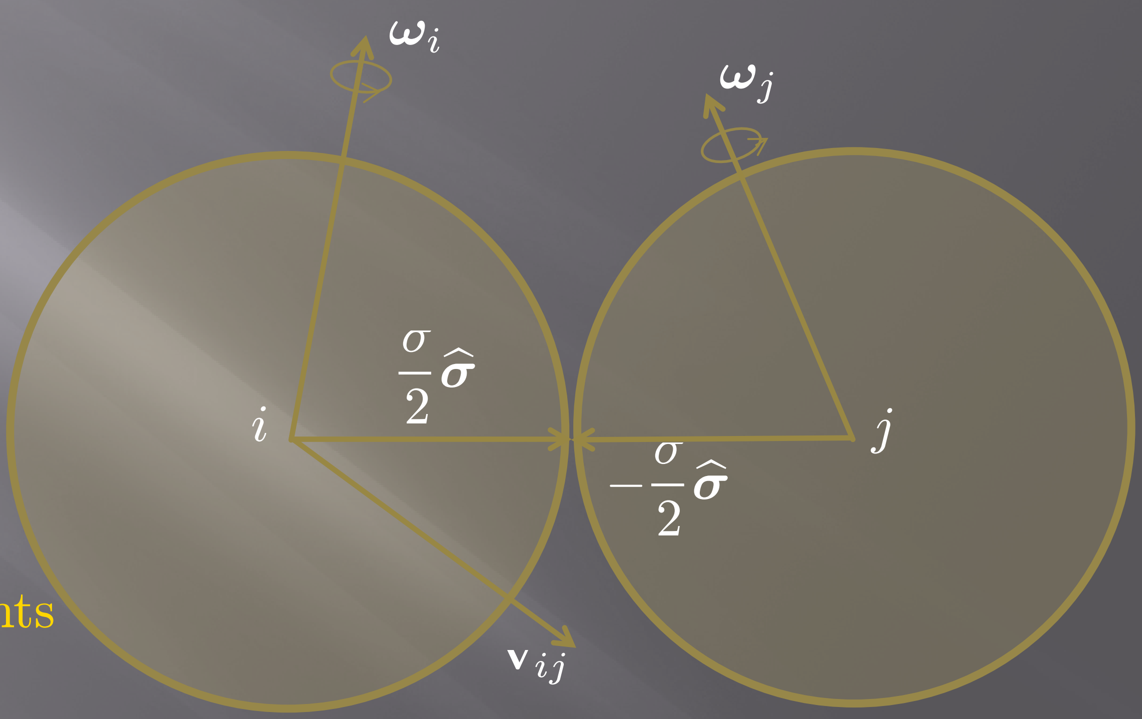
Cons. linear momentum:

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

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:

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

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

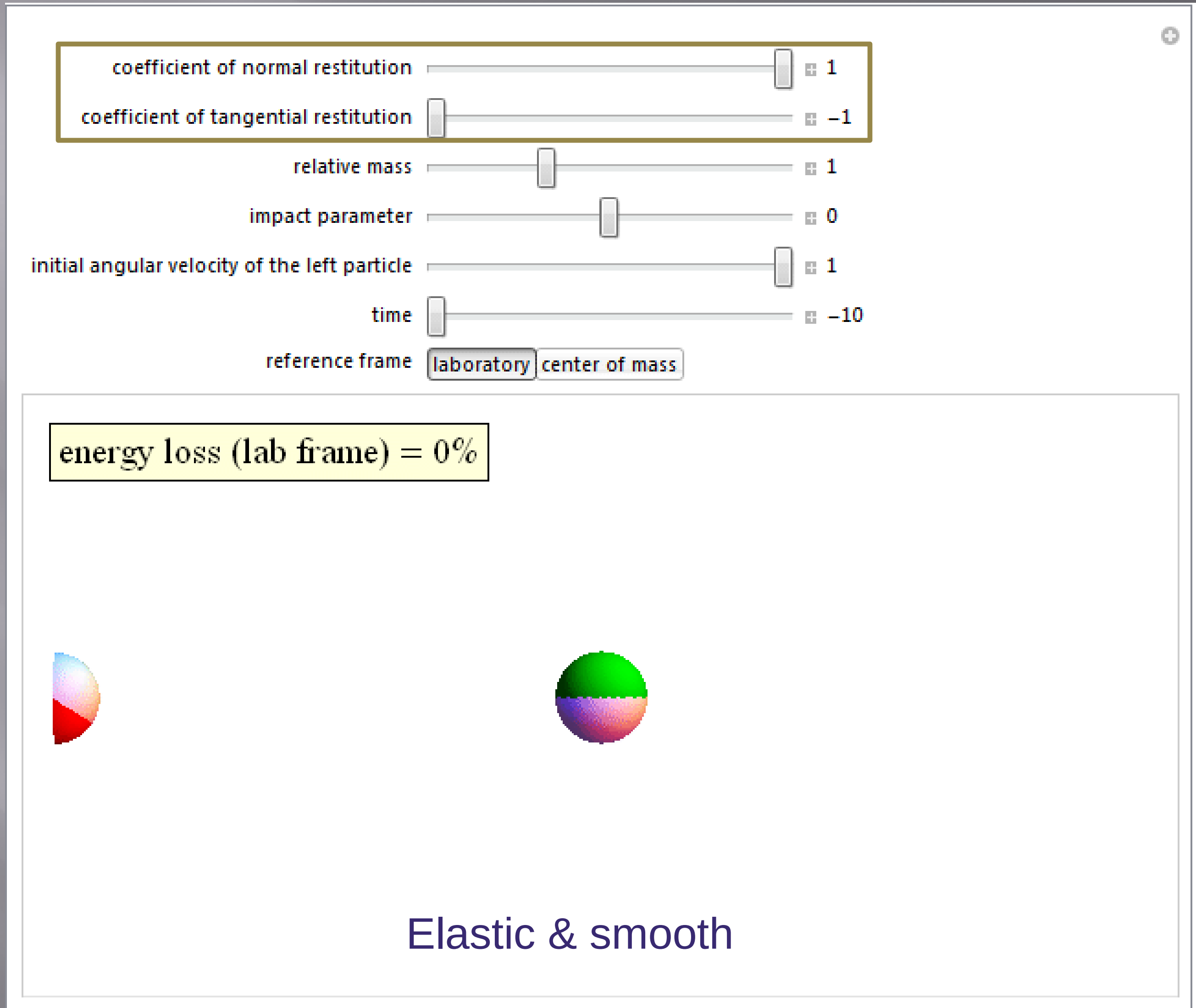
Energy collisional loss

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

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

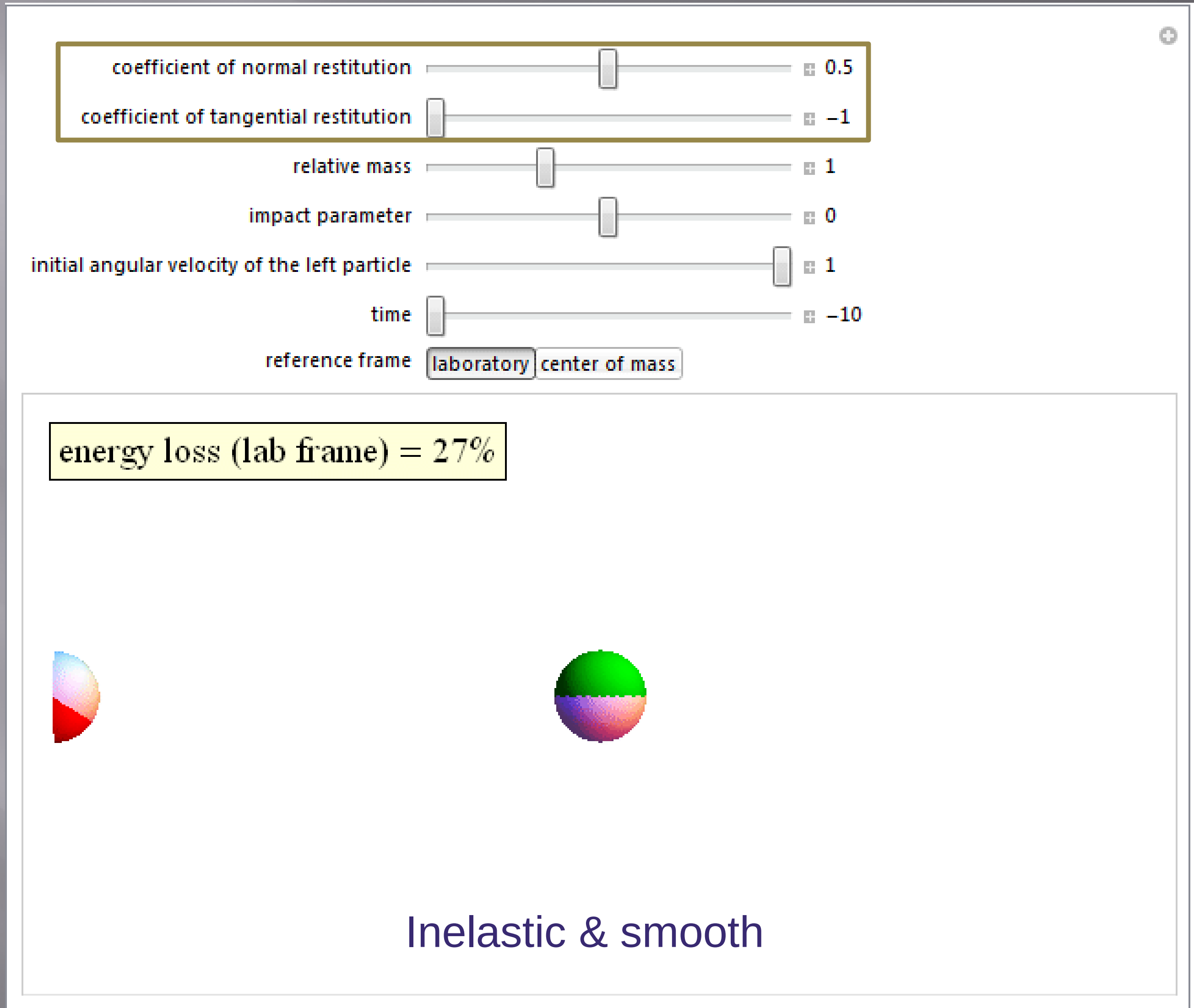
Energy is conserved *only* if the spheres are

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



Elastic & smooth

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



Inelastic & smooth

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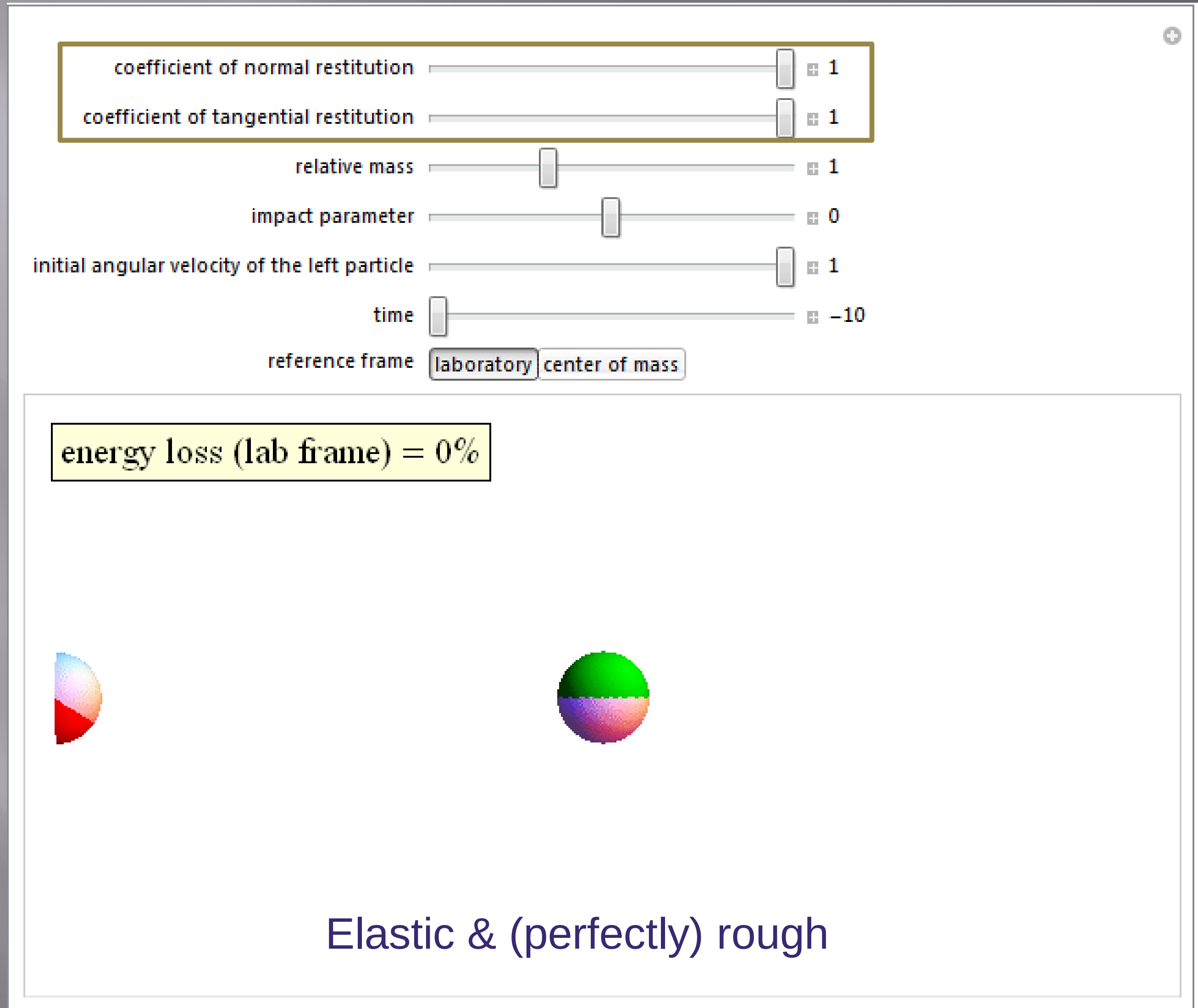

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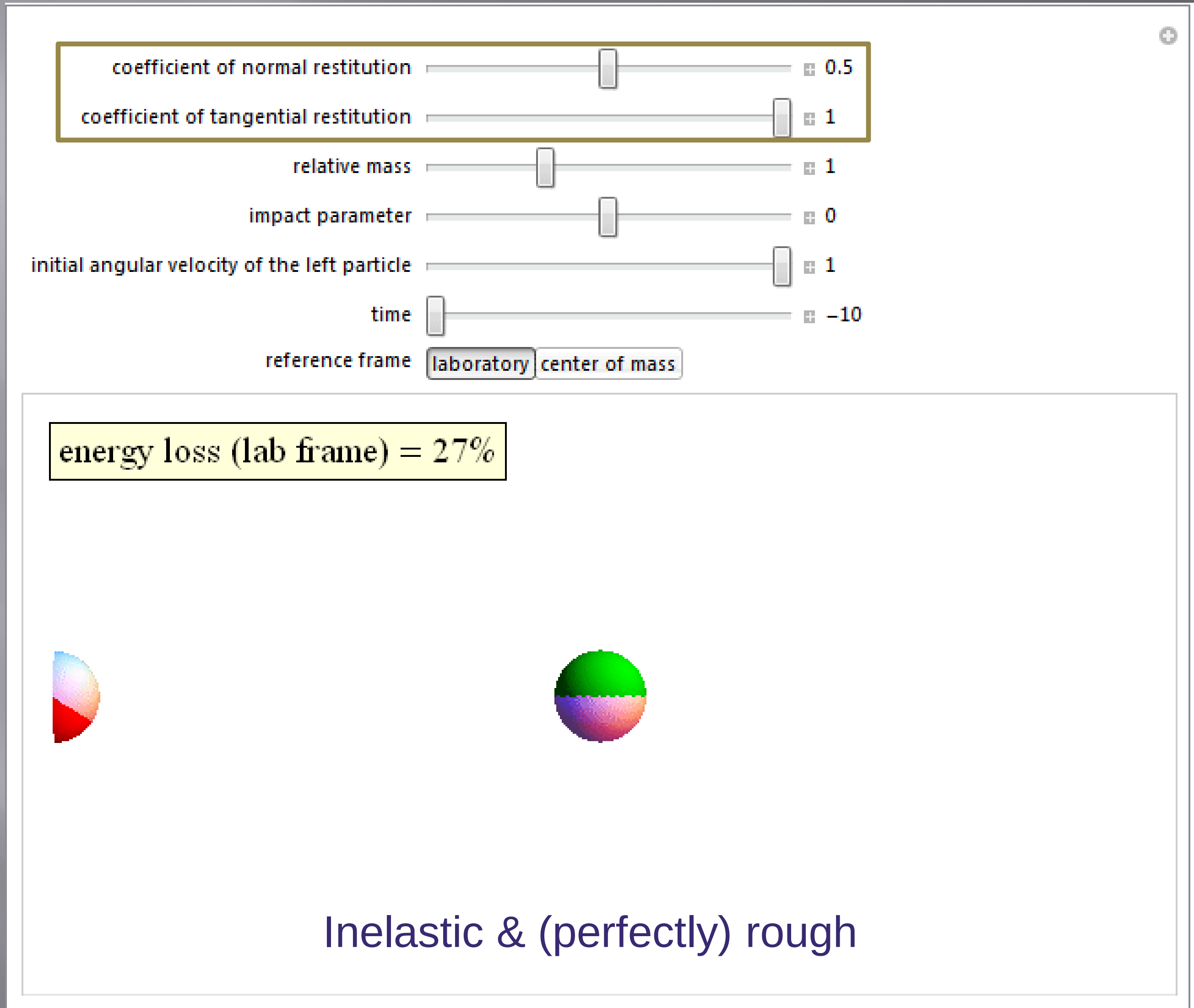

Inelastic & (perfectly) rough

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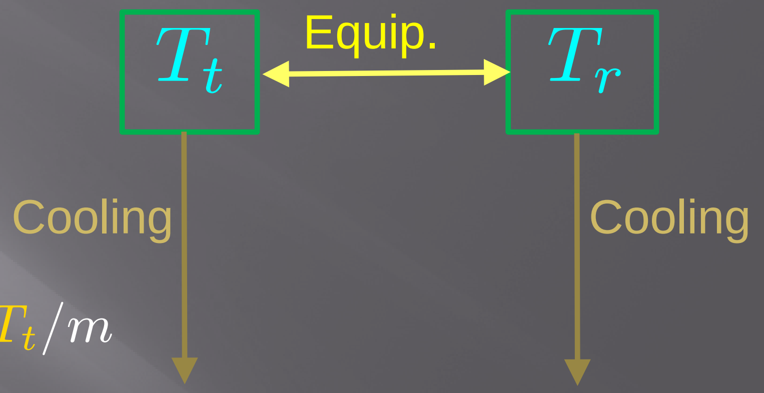
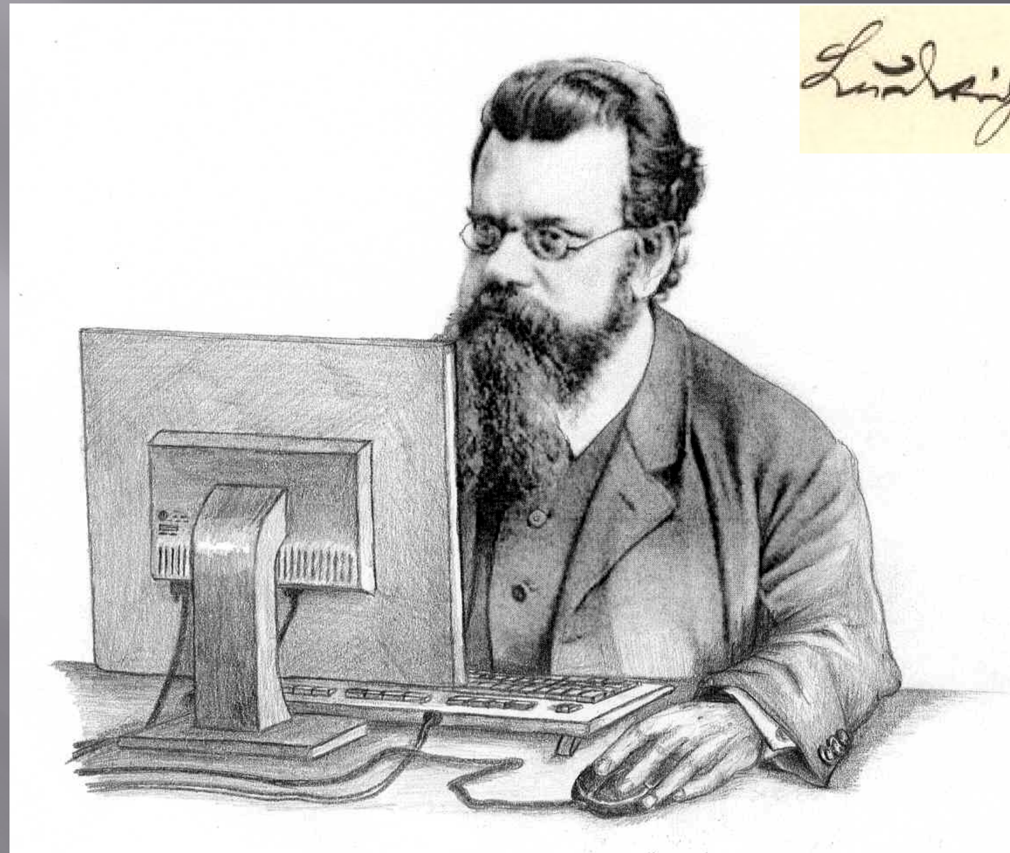
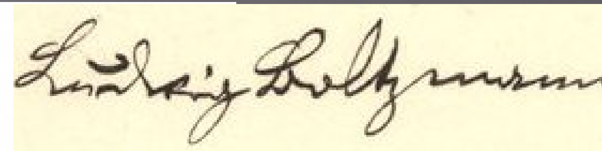
Homogeneous Cooling State (HCS)



- Translational temperature: $\langle(\mathbf{v}-\mathbf{u})^2\rangle = 3T_t/m$
- Rotational temperature: $\langle\omega^2\rangle = 3T_r/I$
- Temperature ratio: $\theta \equiv T_r/T_t$

$$T_t(t) \sim t^{-2}, \quad T_r(t)/T_t(t) \to \text{const} \neq 1$$





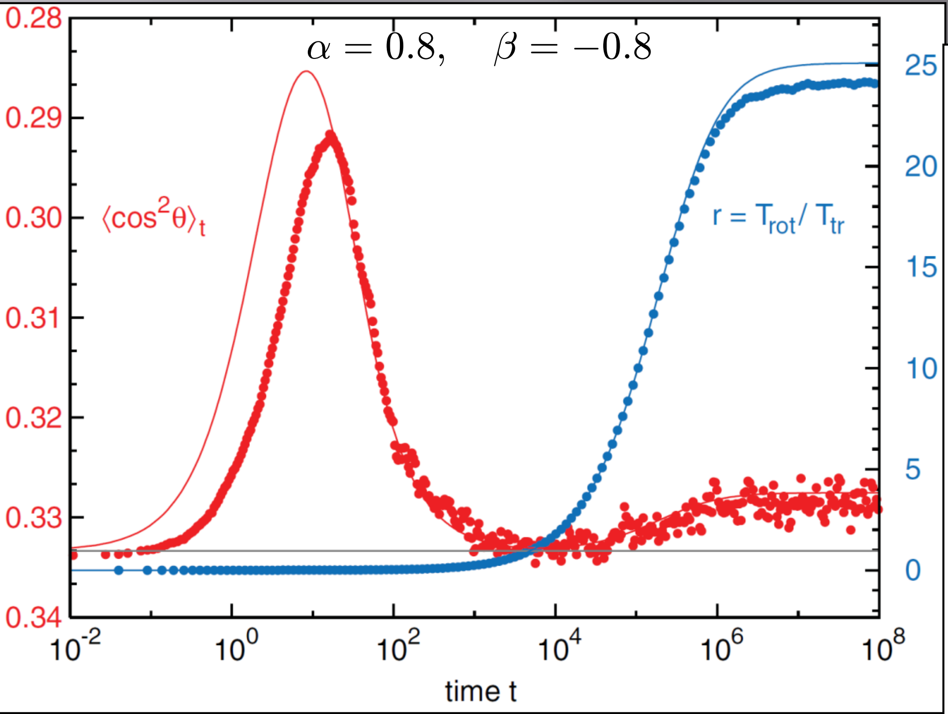
(1844-1906)

(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



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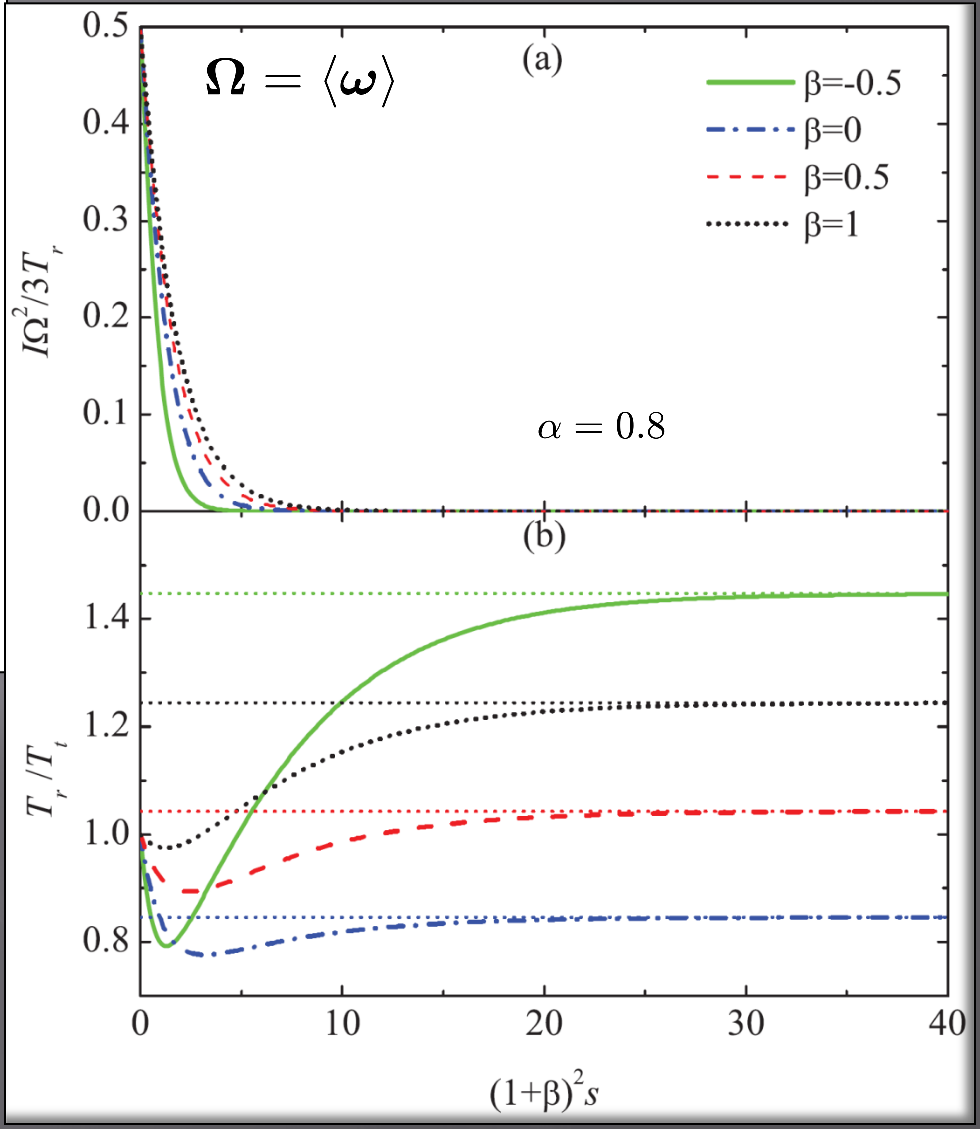


G. M. Kremer, A. S., and V. Garzó, Phys. Rev. E **90**, 022205 (2014)

Inhomogeneous states. Hydrodynamic fields

$$\text{Number density:} \quad n(\mathbf{r},t) = \int d\mathbf{v} \int d\boldsymbol{\omega}\, f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)$$

$$\text{Flow velocity:} \quad \mathbf{u}(\mathbf{r},t) = \frac{1}{n}\int d\mathbf{v} \int d\boldsymbol{\omega}\, \mathbf{v} f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)$$

$$\text{Temperature:} \quad T(\mathbf{r},t) = \frac{1}{2}\left[T_t(\mathbf{r},t) + T_r(\mathbf{r},t)\right]$$

$$= \frac{1}{3n}\int d\mathbf{v} \int d\boldsymbol{\omega} \left[m\left(\mathbf{v}-\mathbf{u}\right)^2 + I\omega^2\right] f(\mathbf{r},\mathbf{v},\boldsymbol{\omega},t)$$

Hydrodynamic fluxes

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

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

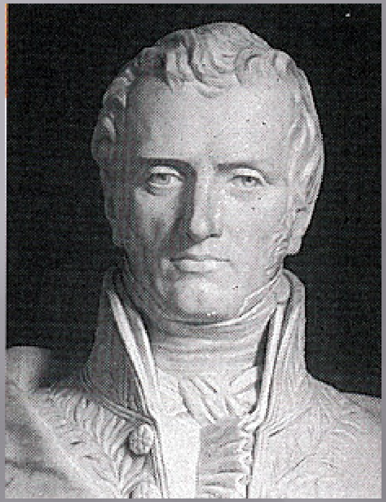
$$\begin{aligned}
\text{Cooling rate: } \zeta(\mathbf{r},t) &= \frac{T_t}{2T}\zeta_t(\mathbf{r},t)+\frac{T_r}{2T}\zeta_r(\mathbf{r},t) \\
&= -\frac{1}{6nT}\int d\mathbf{v} \int d\boldsymbol{\omega}\ \left[m(\mathbf{v}-\mathbf{u})^2 + I\omega^2\right] \\
&\quad \times J[\mathbf{r},\mathbf{v},\boldsymbol{\omega},t|f]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

Balance equations

$$\left.\begin{aligned} \mathcal{D}_t n + n\nabla\cdot\mathbf{u} &= 0 \\ \rho\mathcal{D}_t\mathbf{u} + \nabla\cdot\mathsf{P} &= 0 \\ \mathcal{D}_t T + \frac{1}{3n}\left(\nabla\cdot\mathbf{q} + \mathsf{P}:\nabla\mathbf{u}\right) &= -\zeta T \end{aligned}\right\}$$

$$(\mathcal{D}_t \equiv \partial_t + \mathbf{u}\cdot\nabla)$$

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

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

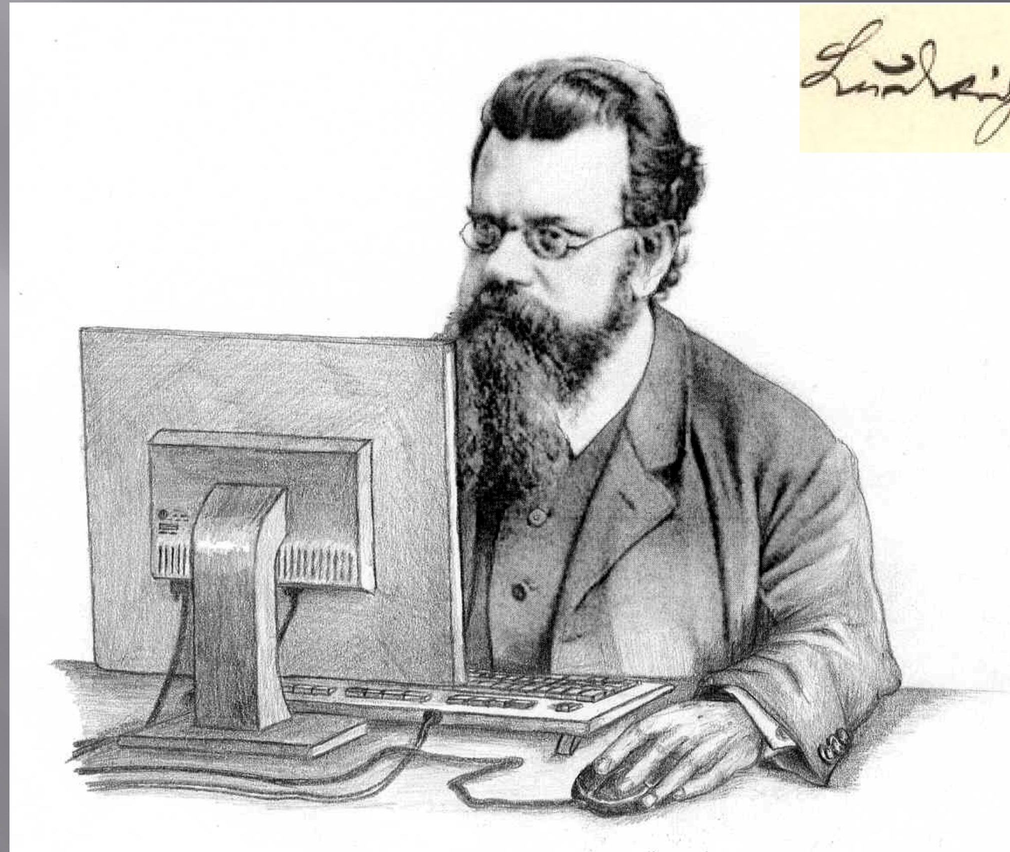
Thermal conductivity

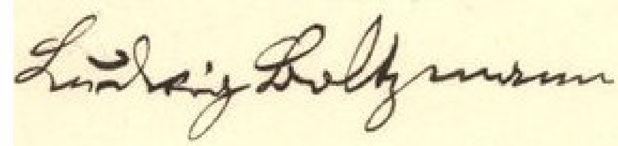
$$\zeta = \zeta^{(0)} - \xi\nabla\cdot\mathbf{u}$$

Cooling rate transport coefficient

Navier-Stokes-Fourier hydrodynamic equations

$$
\begin{aligned}
\mathcal{D}_t n + n\nabla\cdot\mathbf{u} &= 0 \\
\rho\mathcal{D}_t u_i + \nabla_i p^{(0)} &= \nabla_j\left[\eta\left(\nabla_i u_j + \nabla_j u_i - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{u}\right) + \eta_b\delta_{ij}\nabla\cdot\mathbf{u}\right] \\
\left(\mathcal{D}_t + \zeta^{(0)}\right)T + \frac{1}{3}T\tau_t\nabla\cdot\mathbf{u} &= \frac{1}{3n}\nabla\cdot\left(\lambda\nabla T + \mu\nabla n\right) \\
&\quad + \frac{1}{3n}\left[\eta\left(\nabla_i u_j + \nabla_j u_i - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{u}\right) + \eta_b\delta_{ij}\nabla\cdot\mathbf{u}\right] \\
&\quad \times\nabla_i u_j + T\xi\nabla\cdot\mathbf{u}
\end{aligned}
$$





(1844-1906)

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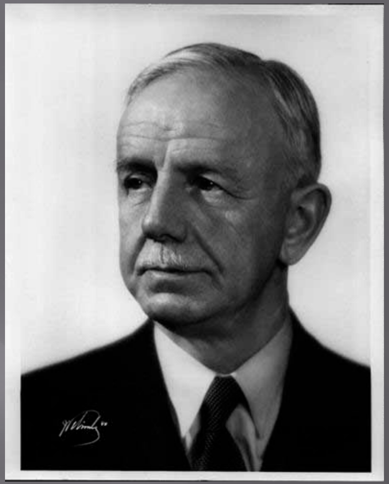
Inelastic+Rough collisions

Methodology: Chapman-Enskog method

Sydney Chapman
(1888-1970)



David Enskog
(1884-1947)

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

G. M. Kremer, A. S., and V. Garzó, Phys. Rev. E **90**, 022205 (2014)

Explicit expressions

HCS quantities

$$\widetilde{\alpha}=\frac{1+\alpha}{2},\ \widetilde{\beta}=\frac{1+\beta}{2}\frac{\kappa}{\kappa+1}$$

$$T_t^{(0)}/T=\tau_t=\frac{2}{1+\theta},\ T_r^{(0)}/T=\tau_r=\frac{2\theta}{1+\theta}$$

$$\theta=\sqrt{1+h^2}+h,\ h\equiv\frac{(1+\kappa)^2}{2\kappa(1+\beta)^2}\left[1-\alpha^2-(1-\beta^2)\frac{1-\kappa}{1+\kappa}\right]$$

$$\nu=\frac{16}{5}\sigma^2 n\sqrt{\pi\tau_t T/m}$$

$$\zeta^{(0)}/\nu=\zeta^*=\frac{5}{12}\frac{1}{1+\theta}\left[1-\alpha^2+(1-\beta^2)\frac{\theta+\kappa}{1+\kappa}\right]$$

NSF coefficients

$$\eta=(n\tau_t T/\nu)/(\nu_\eta^*-\tfrac{1}{2}\zeta^*)$$

$$\eta_b=(n\tau_t\tau_r T/\nu)\gamma_E$$

$$\lambda=\tau_t\lambda_t+\tau_r\lambda_r,\ \lambda_t=\frac{5}{2}(n\tau_t T/m\nu)\gamma_{A_t},\ \lambda_r=\frac{3}{2}(n\tau_t T/m\nu)\gamma_{A_r}$$

$$\mu=\mu_t+\mu_r,\ \mu_t=\frac{5}{2}(\tau_t^2T^2/m\nu)\gamma_{B_t},\ \mu_r=\frac{3}{2}(\tau_t\tau_r T^2/m\nu)\gamma_{B_r}$$

$$\xi=\frac{1}{2}(\tau_t\xi_t+\tau_r\xi_r)=\gamma_E\Xi,\ \xi_t=\gamma_E\Xi_t,\ \xi_r=\gamma_E\Xi_r$$

Auxiliary quantities

$$\nu_\eta^*=(\widetilde{\alpha}+\widetilde{\beta})(2-\widetilde{\alpha}-\widetilde{\beta})+\widetilde{\beta}^2\theta/6\kappa$$

$$\gamma_E=\frac{2}{3}(\Xi_t-\Xi_r-\zeta^*)^{-1}$$

$$\Xi_t=\frac{5}{8}\tau_r\left[1-\alpha^2+(1-\beta^2)\frac{\kappa}{1+\kappa}-\frac{\kappa}{3}(\theta-5)\left(\frac{1+\beta}{1+\kappa}\right)^2\right]$$

$$\Xi_r=\frac{5}{8}\tau_t\frac{1+\beta}{1+\kappa}\left[\frac{\theta-2}{3}(1-\beta)+\frac{\kappa}{3}(\theta-5)\frac{1+\beta}{1+\kappa}\right]$$

$$\Xi=\frac{5}{16}\tau_t\tau_r\left[1-\alpha^2+(1-\beta^2)\left(1+\frac{1}{3}\frac{\theta-5}{1+\kappa}\right)\right]$$

$$\gamma_{A_t}=\frac{Z_r-Z_t-2\zeta^*}{(Y_t-2\zeta^*)(Z_r-2\zeta^*)-Y_rZ_t}$$

$$\gamma_{A_r}=\frac{Y_t-Y_r-2\zeta^*}{(Y_t-2\zeta^*)(Z_r-2\zeta^*)-Y_rZ_t}$$

$$\gamma_{B_t}=\zeta^*\frac{\gamma_{A_t}\left(Z_r-\frac{3}{2}\zeta^*\right)-\gamma_{A_r}Z_t}{\left(Y_t-\frac{3}{2}\zeta^*\right)\left(Z_r-\frac{3}{2}\zeta^*\right)-Y_rZ_t}$$

$$\gamma_{B_r}=\zeta^*\frac{\gamma_{A_r}\left(Y_t-\frac{3}{2}\zeta^*\right)-\gamma_{A_t}Y_r}{\left(Y_t-\frac{3}{2}\zeta^*\right)\left(Z_r-\frac{3}{2}\zeta^*\right)-Y_rZ_t}$$

$$Y_t=\frac{41}{12}\left(\widetilde{\alpha}+\widetilde{\beta}\right)-\frac{33}{12}\left(\widetilde{\alpha}^2+\widetilde{\beta}^2\right)-\frac{4}{3}\widetilde{\alpha}\widetilde{\beta}-\frac{7\theta}{12}\frac{\widetilde{\beta}^2}{\kappa}$$

$$Z_t=-\frac{5\theta}{6}\frac{\widetilde{\beta}^2}{\kappa}$$

$$Y_r=-\frac{25}{36}\frac{\widetilde{\beta}}{\kappa}\left(1-3\frac{\widetilde{\beta}}{\theta}-\frac{\widetilde{\beta}}{\kappa}\right)$$

$$Z_r=\frac{5}{6}\left(\widetilde{\alpha}+\widetilde{\beta}\right)+\frac{5}{18}\frac{\widetilde{\beta}}{\kappa}\left(7-3\frac{\widetilde{\beta}}{\kappa}-6\widetilde{\beta}-4\widetilde{\alpha}\right)$$

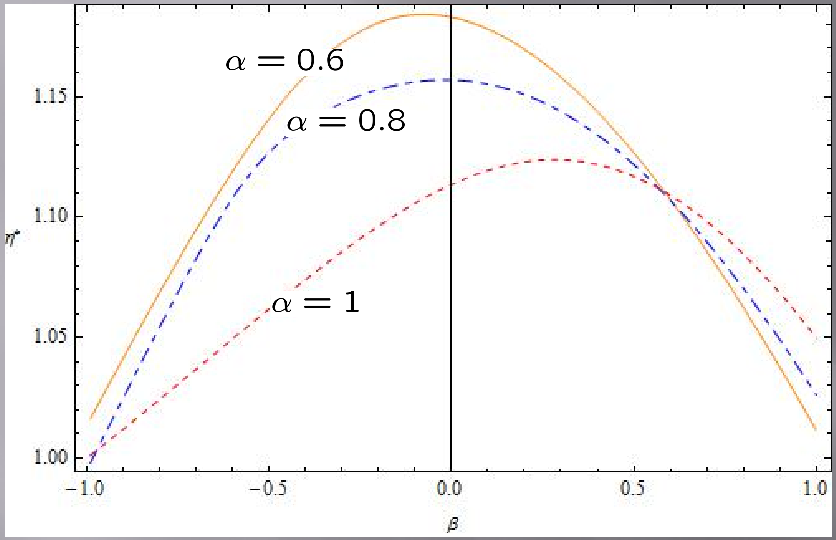
Special limiting cases

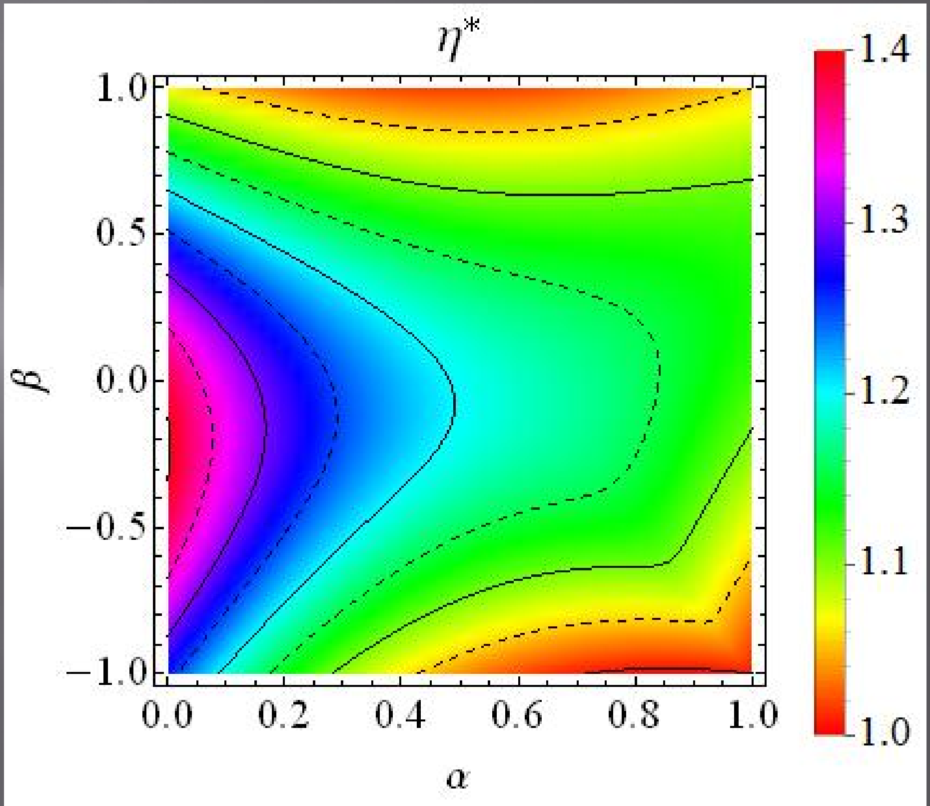
Quantity	Pure smooth ($\beta = -1$)	Quasi-smooth limit ($\beta \to -1$)	Perfectly rough and elastic ($\alpha = \beta = 1$)
η^*	$\frac{24}{(1+\alpha)(13-\alpha)}$	$\frac{24}{(1+\alpha)(19-7\alpha)}$	$\frac{6(1+\kappa)^2}{6+13\kappa}$
η_b^*	0	$\frac{8}{5(1-\alpha^2)}$	$\frac{(1+\kappa)^2}{10\kappa}$
λ^*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

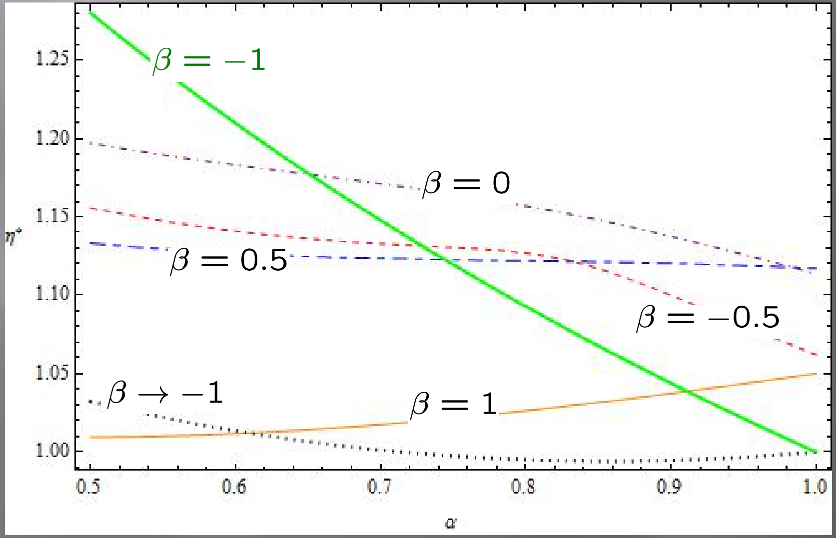
Brey, Dufty, Kim, Santos (1998)

Pidduck (1922)

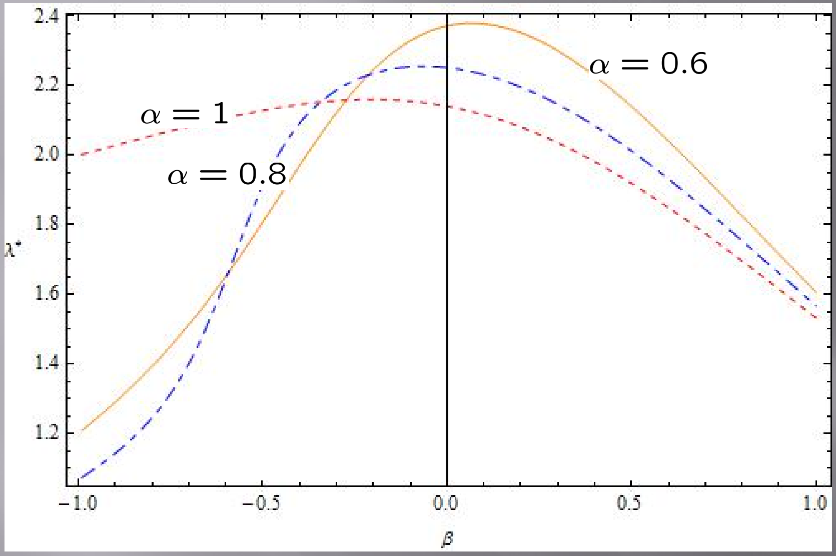
Shear viscosity

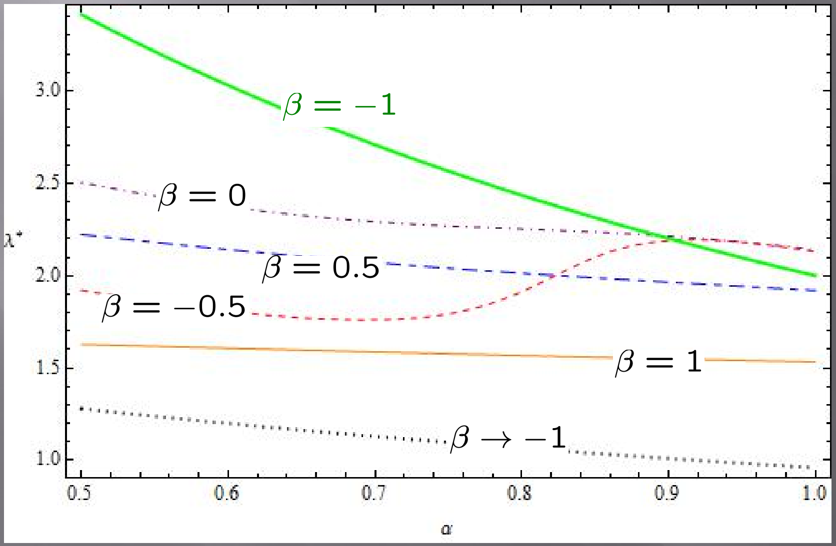


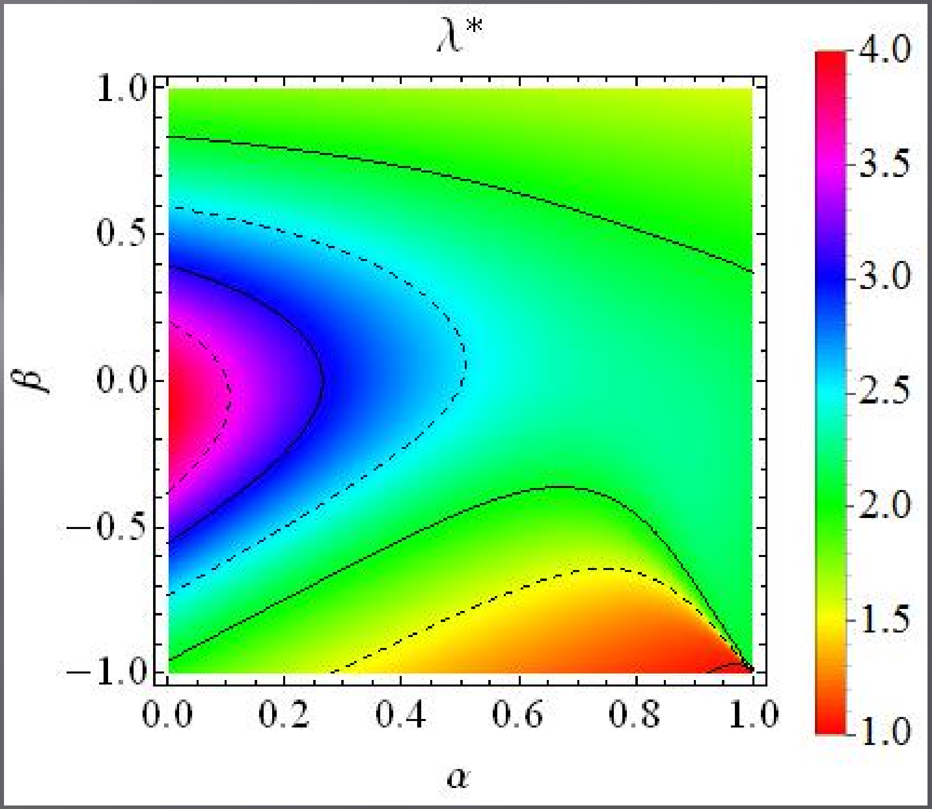




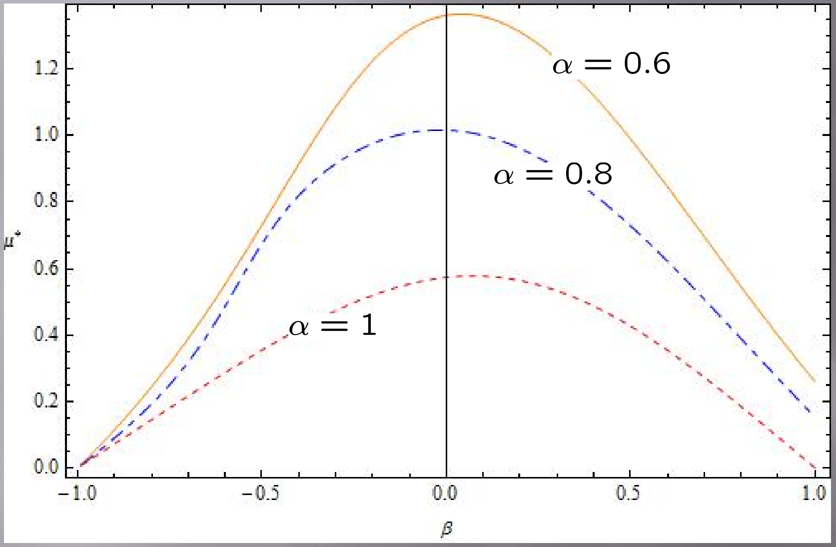
Thermal conductivity

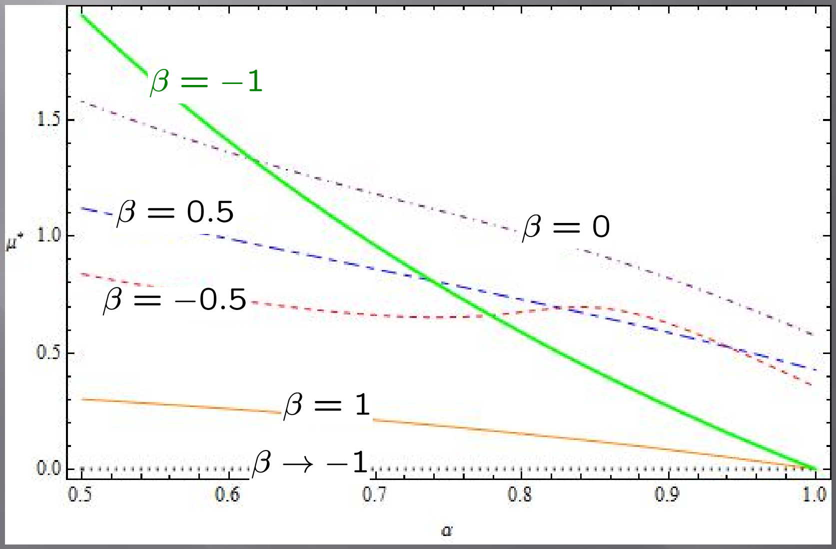


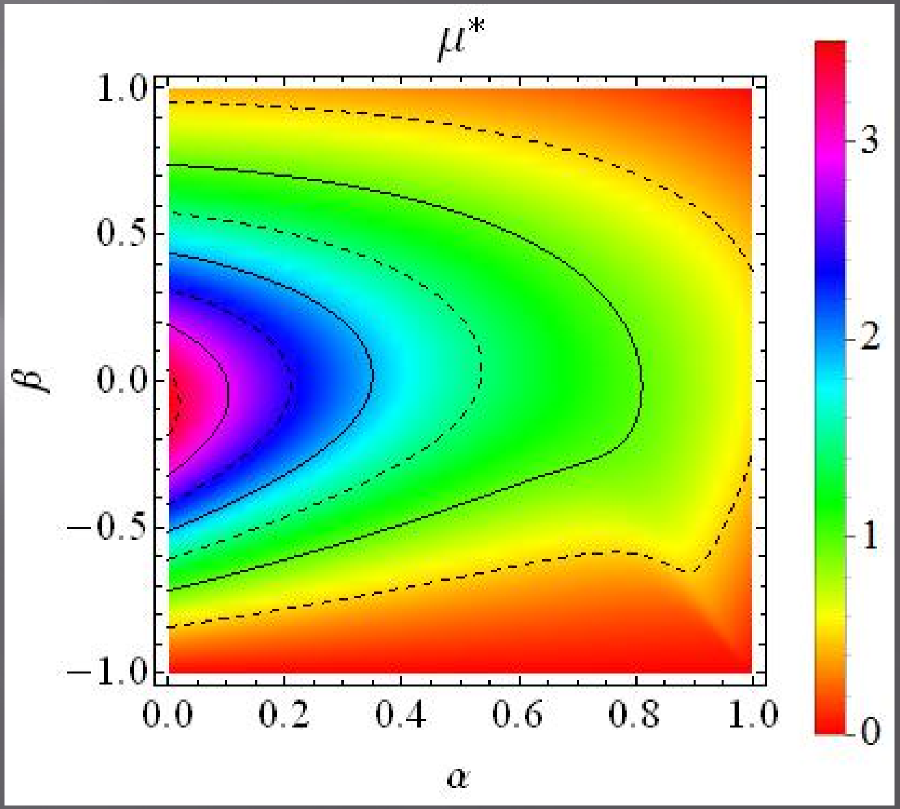




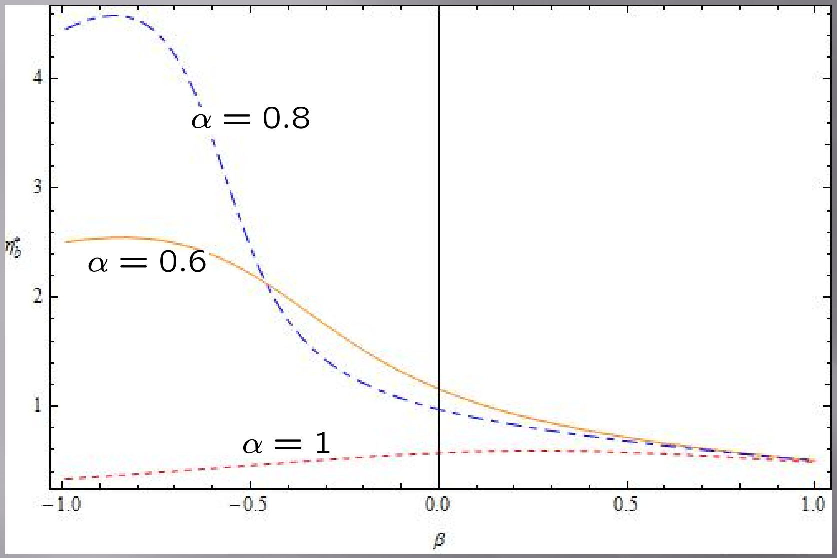
Dufour-like coefficient

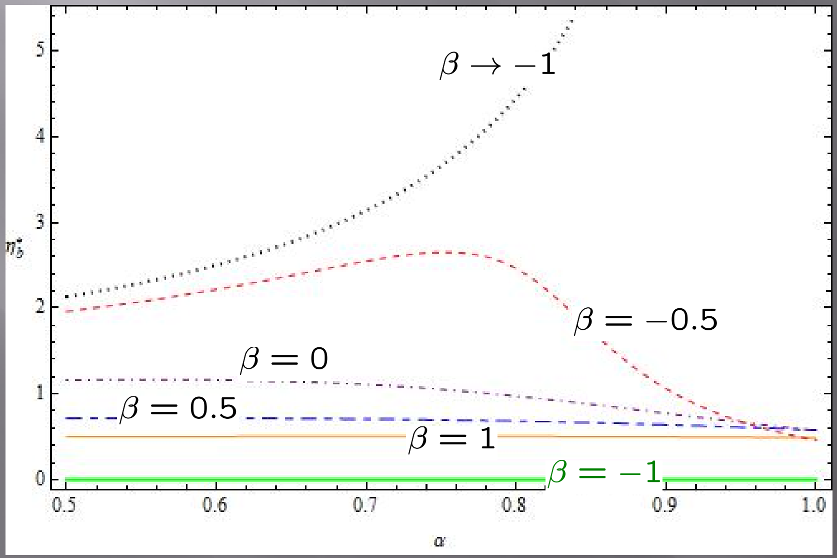


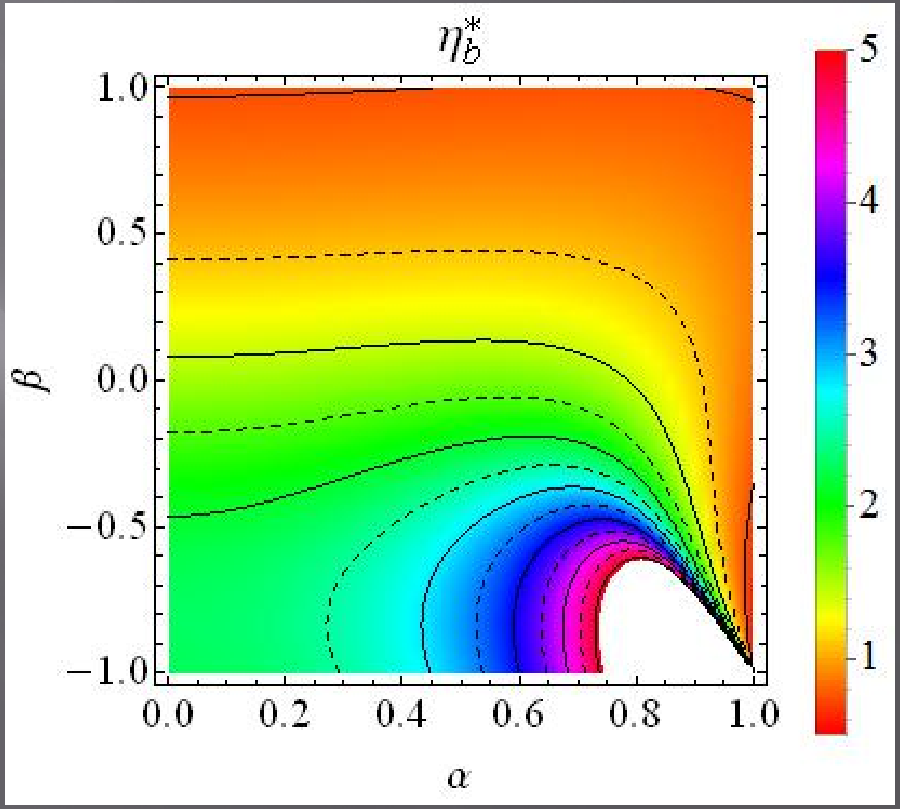




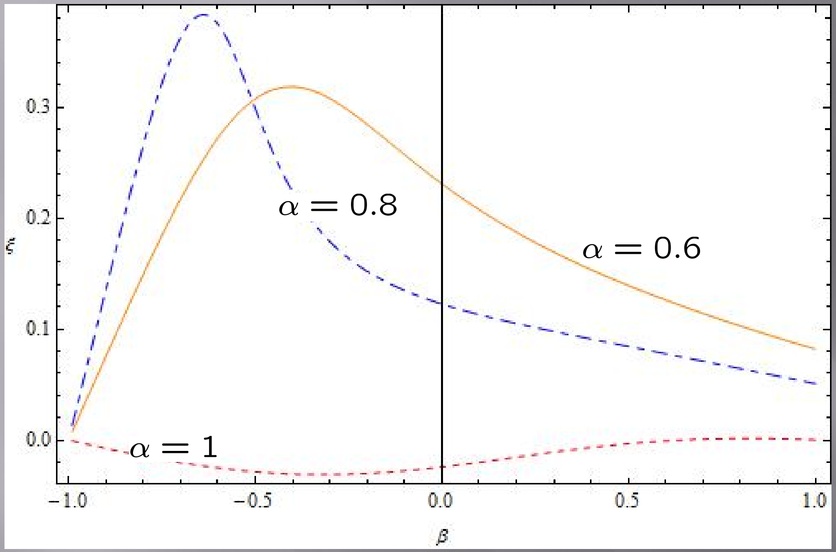
Bulk viscosity

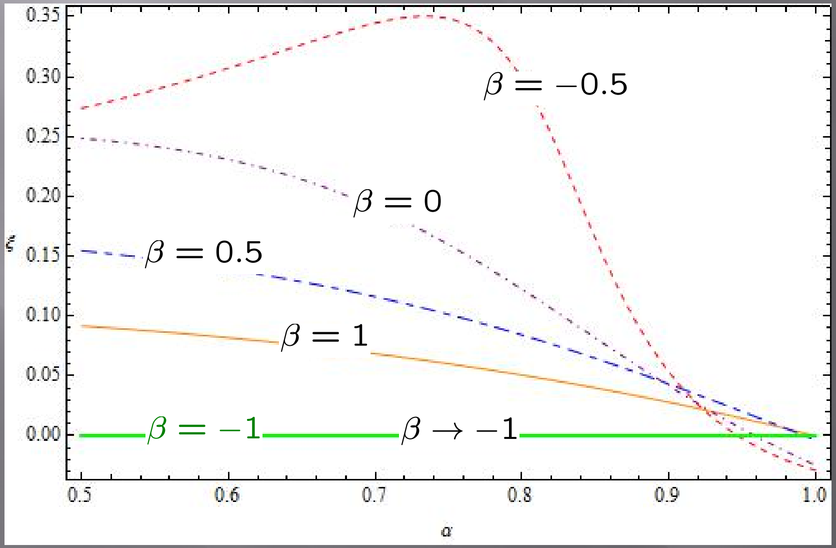


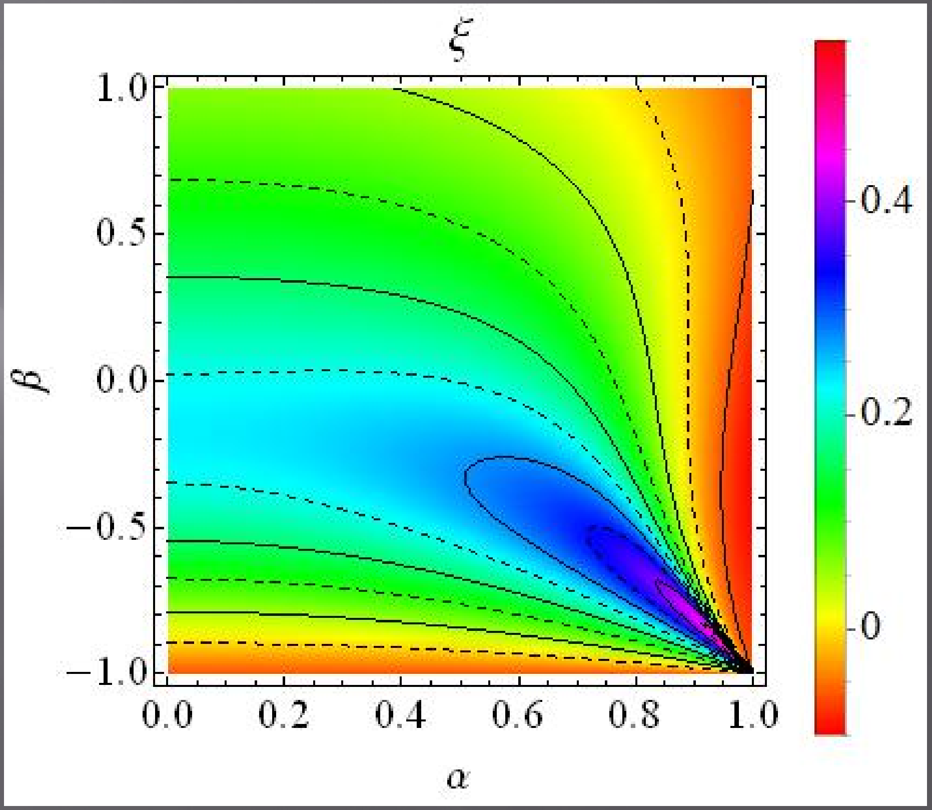




Cooling rate coefficient







Outline of the talk

- 0. Collision rules for inelastic rough hard spheres
- 1. Navier-Stokes-Fourier transport coefficients
- 2. Stability analysis
- 3. Conclusions

Instability of the HCS

J. Fluid Mech. (2013), vol. 729, pp. 484–495. © Cambridge University Press 2013 484
doi:10.1017/jfm.2013.328

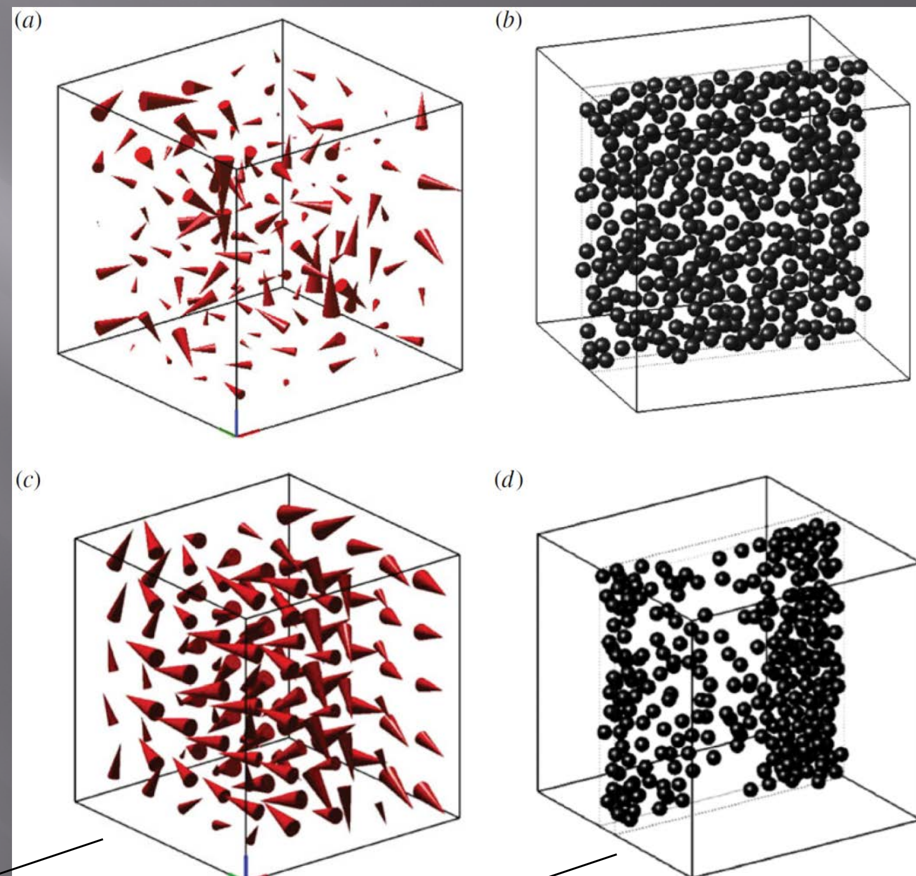
Dual role of friction in granular flows: attenuation versus enhancement of instabilities

Peter P. Mitrano, Steven R. Dahl, Andrew M. Hilger, Christopher J. Ewasko and Christine M. Hrenya†

$\alpha = 0.7, \quad \beta = -0.7$

volume fraction $\phi = 0.3$

$L/\sigma = 10$



4 collisions per particle

100 collisions per particle

Vortices

Clustering

Nonlinear NSF hydrodynamic equations

$$
\begin{aligned}
\mathcal{D}_t n + n\nabla\cdot\mathbf{u} &= 0 \\
\rho\mathcal{D}_t u_i + \nabla_i p^{(0)} &= \nabla_j\left[\eta\left(\nabla_i u_j + \nabla_j u_i - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{u}\right) + \eta_b\delta_{ij}\nabla\cdot\mathbf{u}\right] \\
\left(\mathcal{D}_t + \zeta^{(0)}\right)T + \frac{1}{3}T\tau_t\nabla\cdot\mathbf{u} &= \frac{1}{3n}\nabla\cdot(\lambda\nabla T + \mu\nabla n) \\
&\quad + \frac{1}{3n}\left[\eta\left(\nabla_i u_j + \nabla_j u_i - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{u}\right) + \eta_b\delta_{ij}\nabla\cdot\mathbf{u}\right] \\
&\quad \times\nabla_i u_j + T\xi\nabla\cdot\mathbf{u}
\end{aligned}
$$

Linear stability analysis

$$\left.\begin{aligned} n(\mathbf{r},t) &= n_H\left[1+\delta n^*(\mathbf{r},t)\right] \\ \mathbf{u}(\mathbf{r},t) &= \mathbf{u}_H + v_H(t)\delta\mathbf{u}^*(\mathbf{r},t) \\ T(\mathbf{r},t) &= T_H(t)\left[1+\delta T^*(\mathbf{r},t)\right] \end{aligned}\right\} \delta y_\alpha(\mathbf{r},t), \quad \alpha = 1,\dots,5$$

Fourier-Laplace transform:

$$\delta y_\alpha(\mathbf{r},t) = \delta y_{\alpha;\mathbf{k},\omega} e^{i\mathbf{k}\cdot\mathbf{r}^*} e^{-\omega(k)s} \qquad \left[\mathbf{r}^* \equiv \frac{\mathbf{r}}{\mathrm{m.f.p.}}, \quad s \equiv \frac{1}{2}\int_0^t dt'\,\nu_H(t')\right]$$

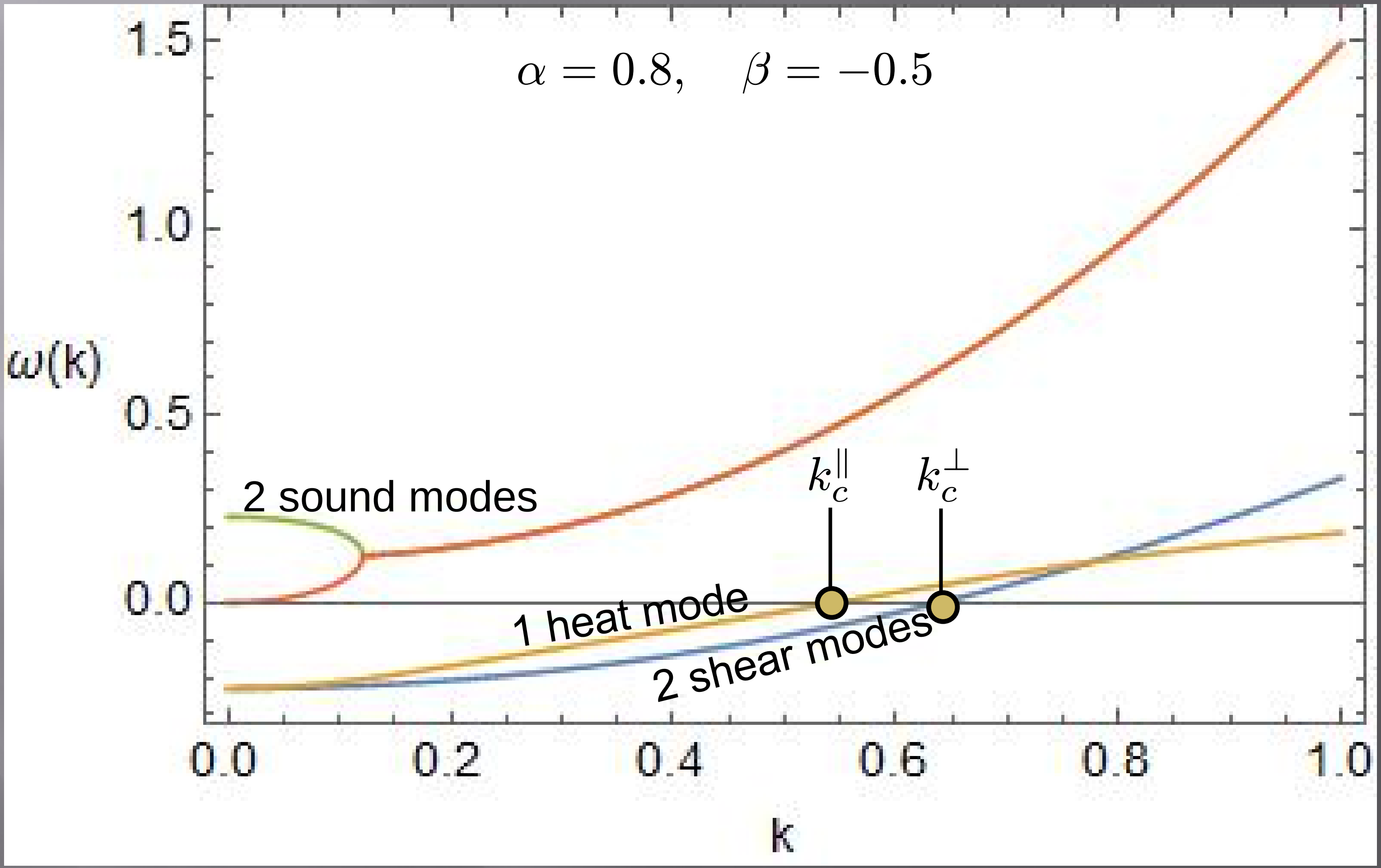
Characteristic equation:

$\det\left[\mathsf{M}(k) - \omega(k)\mathsf{I}\right] = 0 \Rightarrow$ Dispersion relation

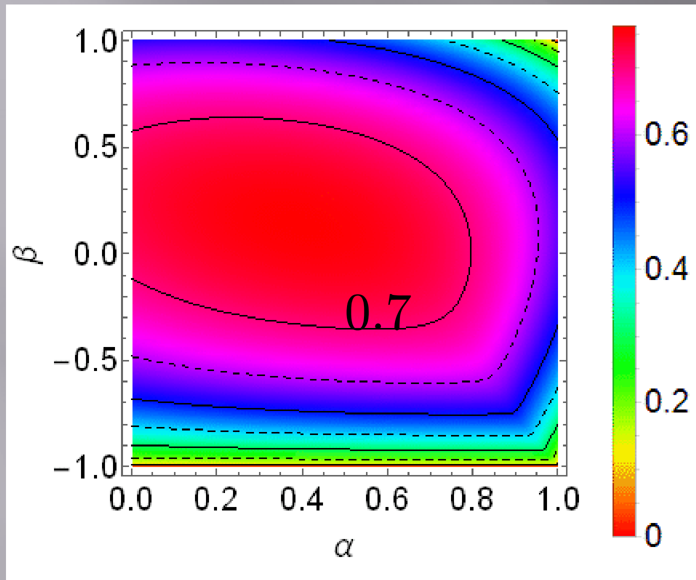
$\omega(k) < 0 \Rightarrow$ Instability

V. Garzó, A. S., and G. M. Kremer, in preparation

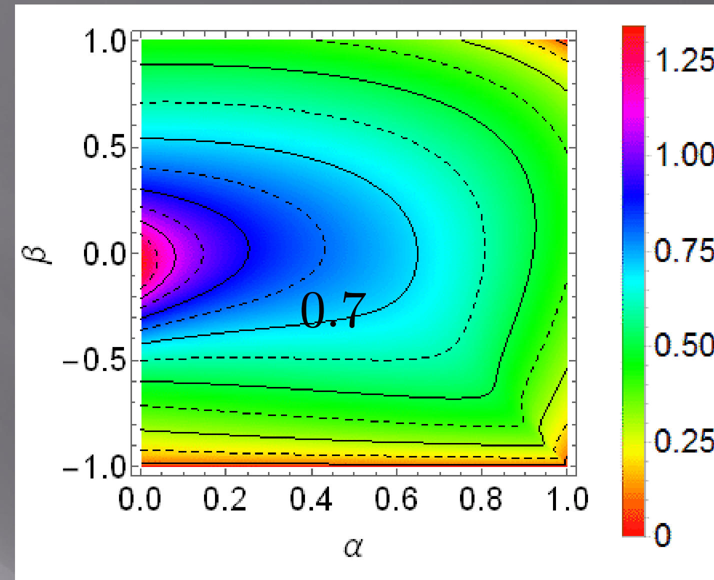
Dispersion relations



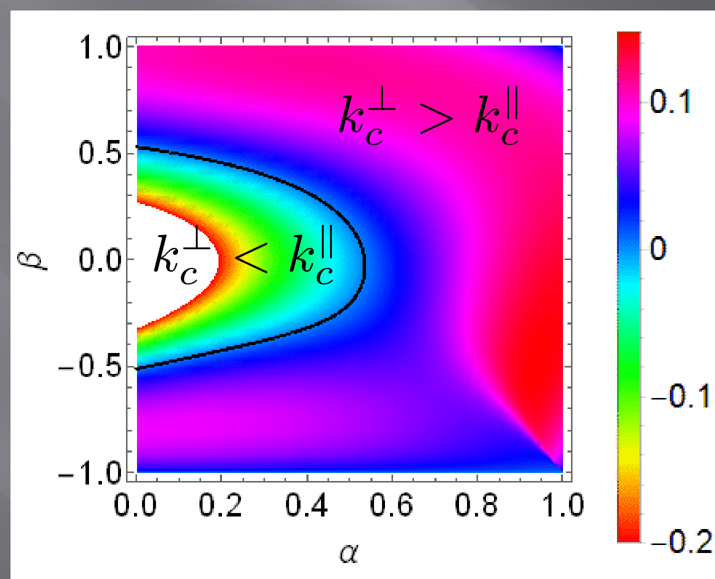
$k_c^{\perp}(\alpha,\beta)=\sqrt{2\zeta^*/\eta^*}$



$k_c^{\parallel}(\alpha,\beta)=\sqrt{8\zeta^*/5(\lambda^*-\mu^*)}$



The shear modes (vortices) are more unstable than the heat mode (clusters), except for high inelasticity and medium roughness

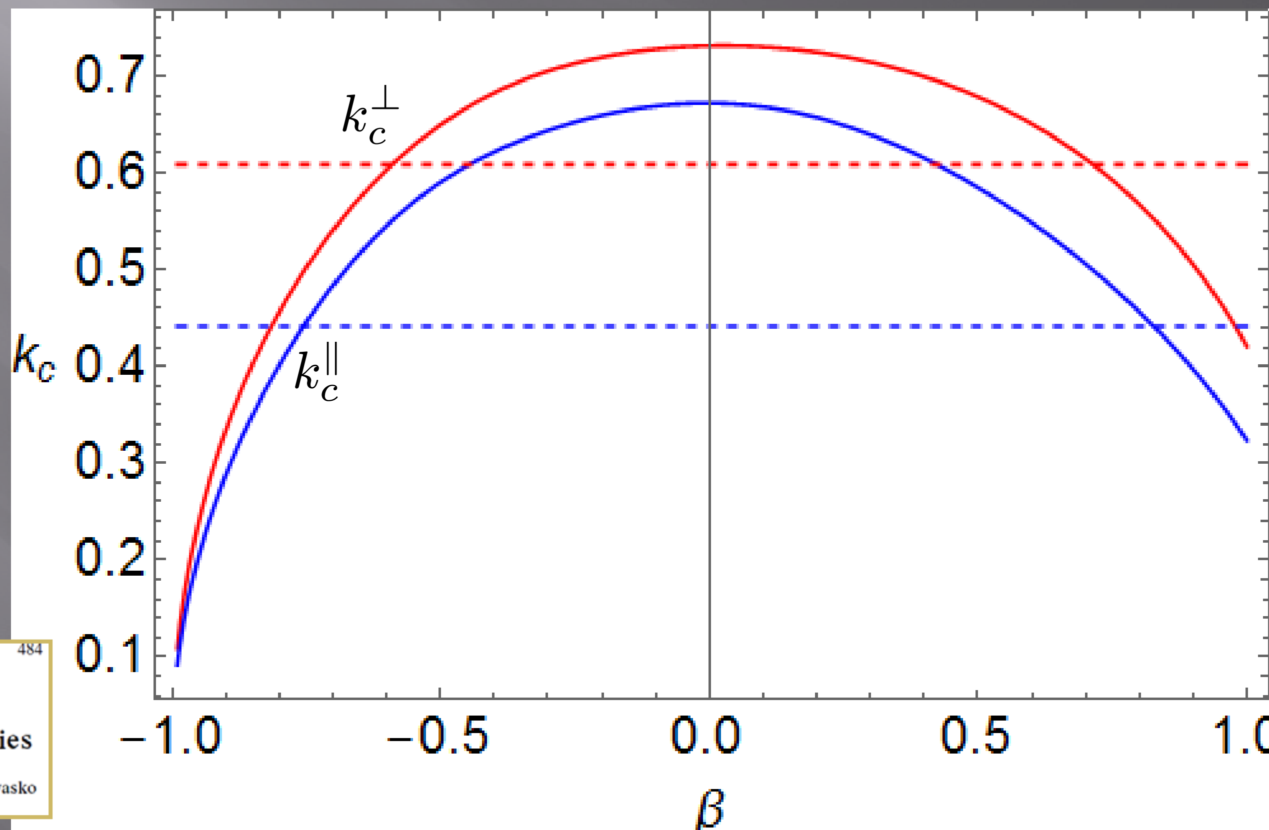


$k_c^{\perp}(\alpha,\beta)-k_c^{\parallel}(\alpha,\beta)$

Comparison with the pure smooth case

$\alpha = 0.7$

Medium roughness enhances instabilities, while small and high levels of roughness attenuate it



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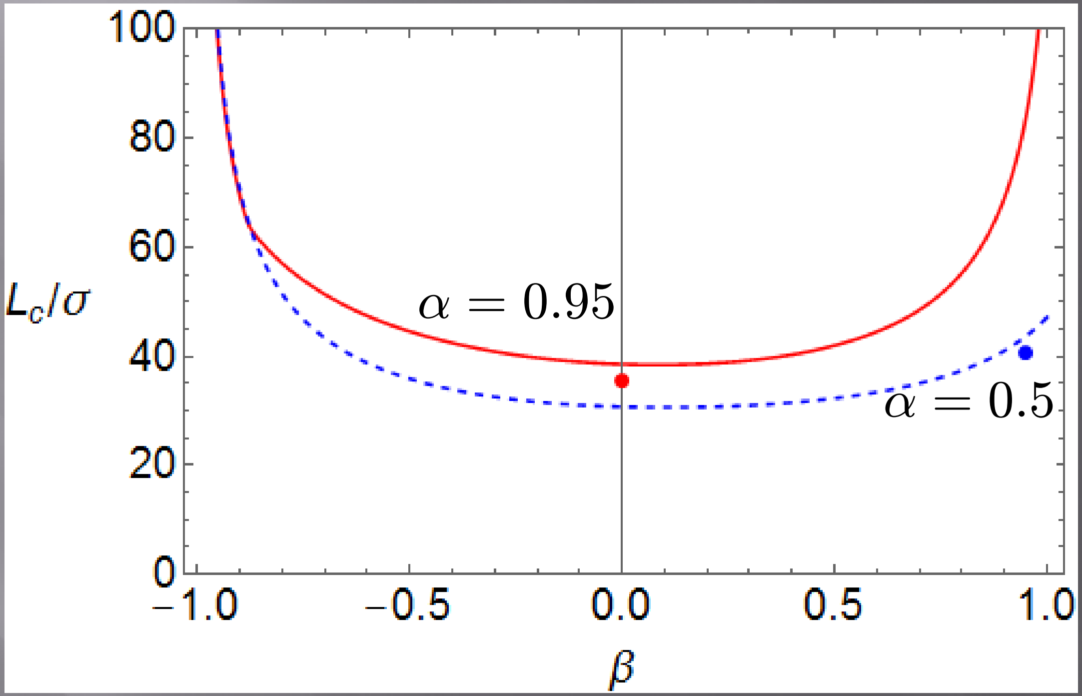
Comparison with preliminary MD simulations

volume fraction $\phi = 0.05$



(MD points, courtesy of Peter Mitrano)

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Conclusions

- 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.
- Medium roughness enhances instabilities; small and large levels of roughness attenuate it.

Thank you for your attention!

Origin of the singular behavior in the quasi-smooth limit