INELASTIC AND FRICTIONAL HARD SPHERES AS A MODEL OF GRANULAR GASES

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What is a granular material?

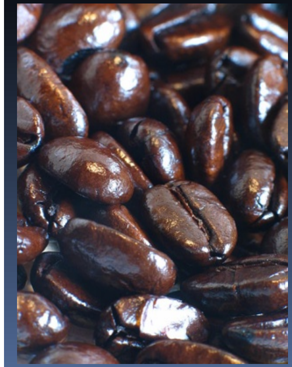
- It is a conglomeration of discrete solid, macroscopic particles characterized by a loss of energy whenever the grains collide.
- The constituents must be large enough such that they are not subject to thermal motion fluctuations. Thus, the lower size limit for grains is about 1 μm.

What is a granular material?

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

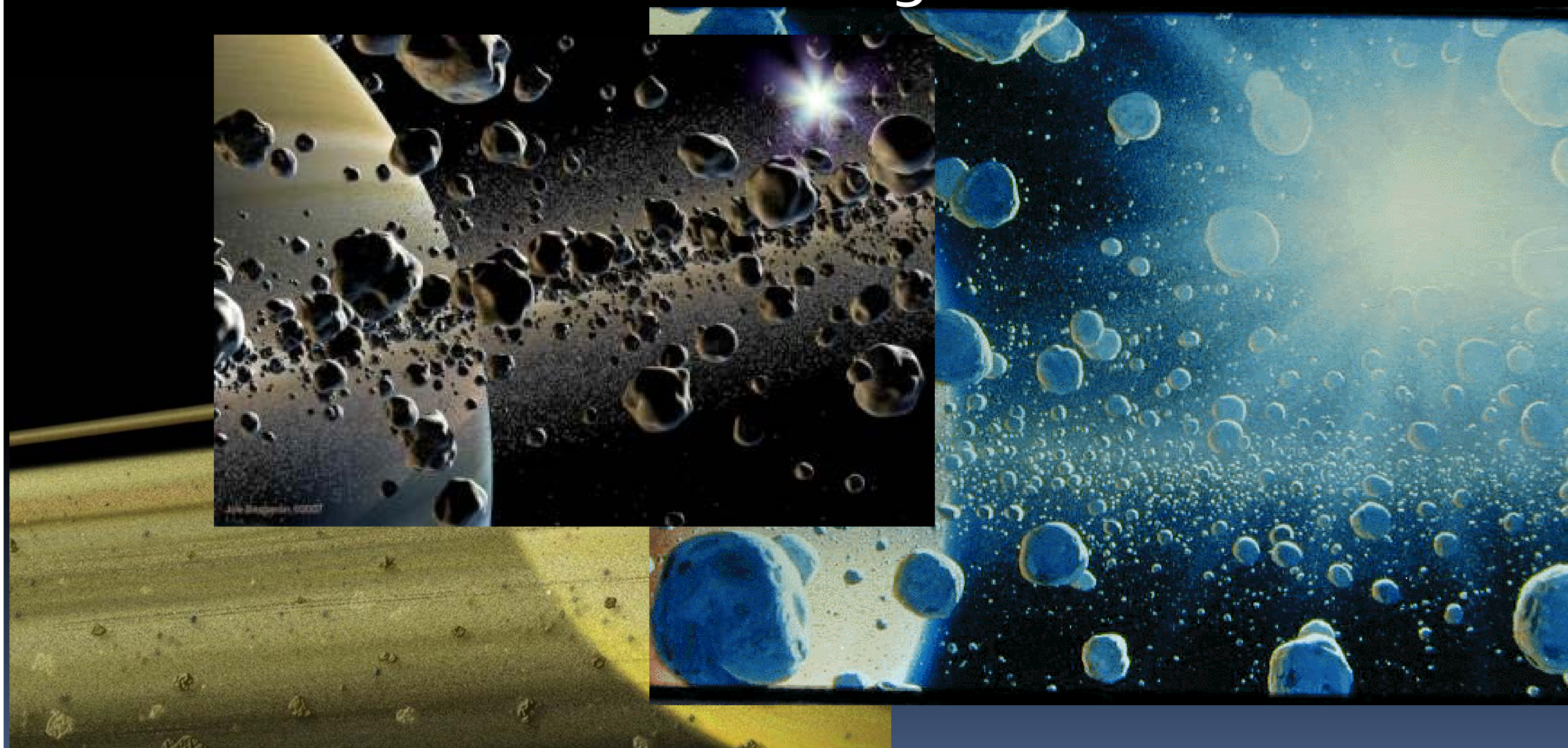






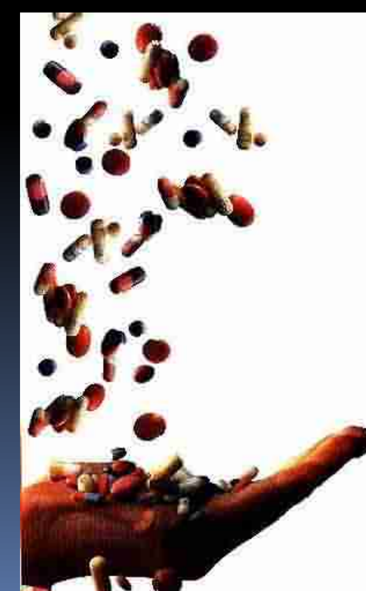
What is a granular material?

- … and even Saturn’s rings



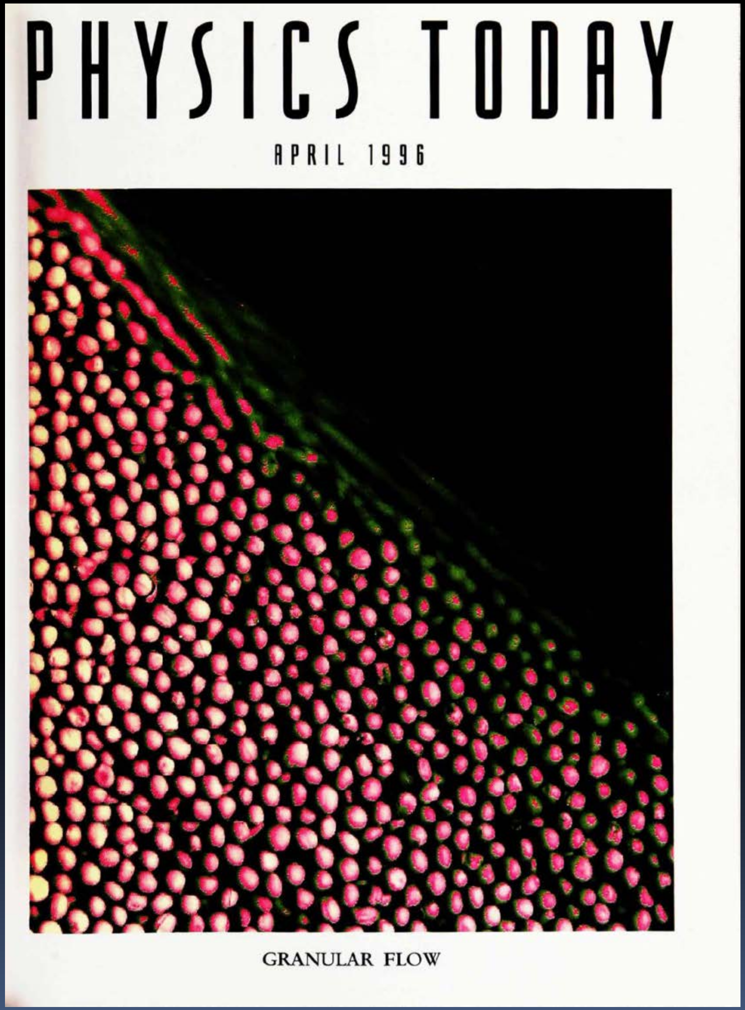
What is a granular material?

- 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).



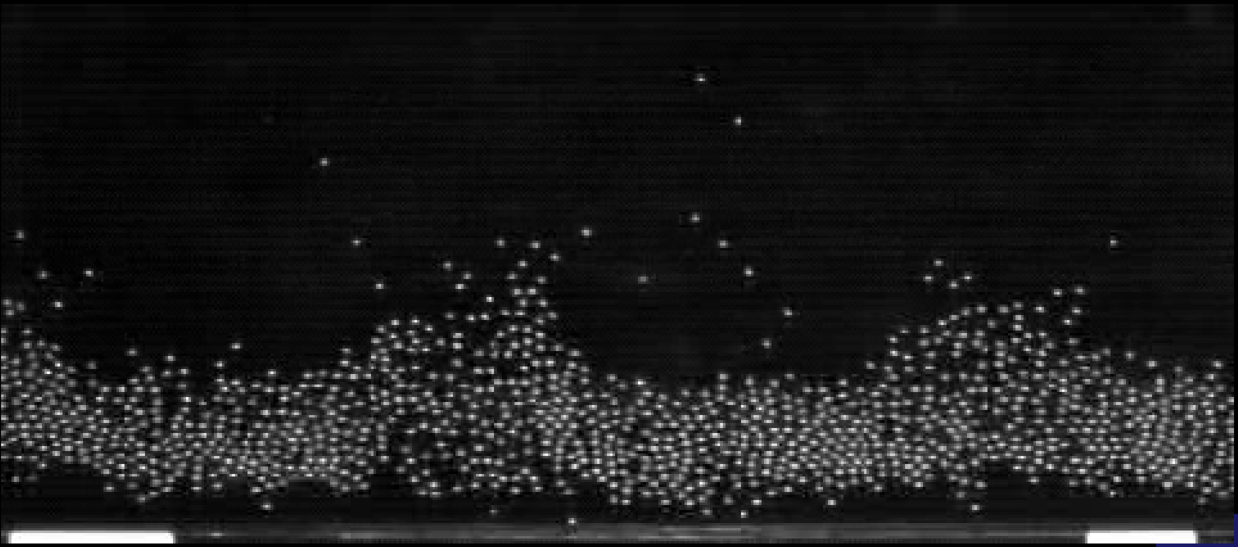
What is a granular *fluid*?

- 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*.

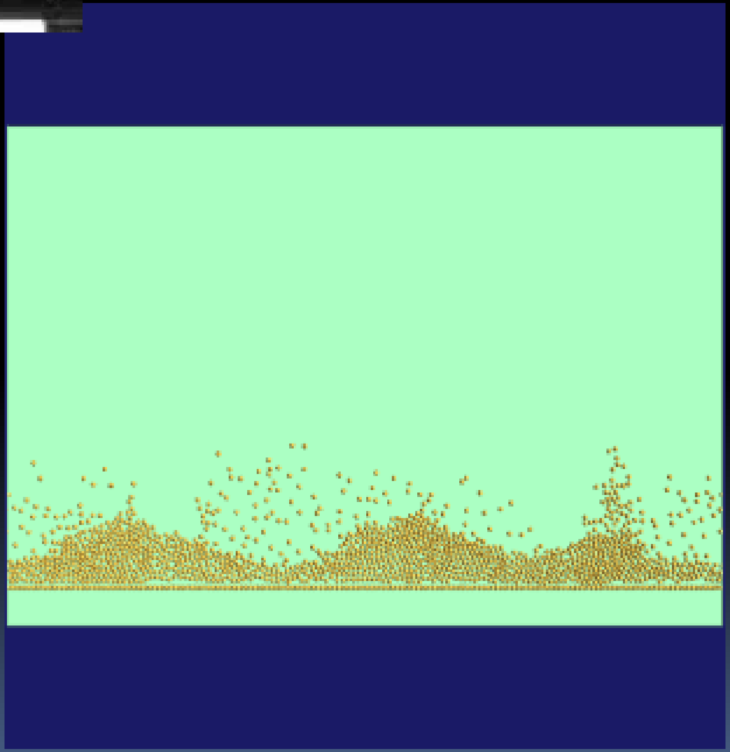


Granular fluids (or gases) exhibit many interesting phenomena:

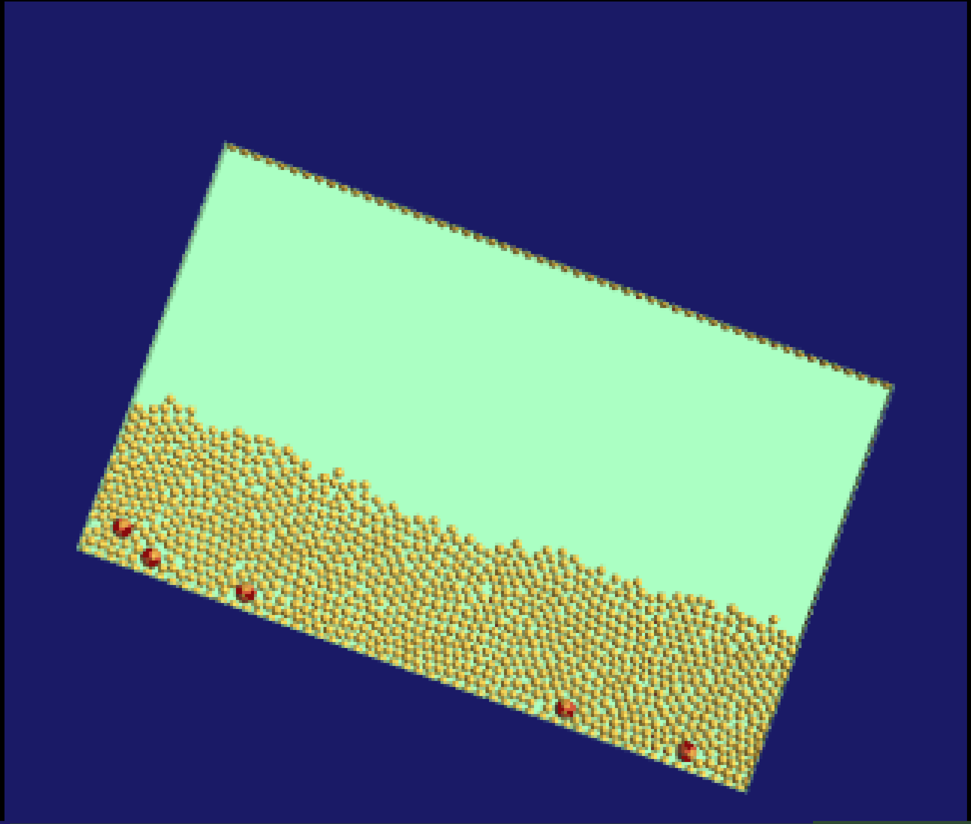
Granular eruptions (from University of Twente's group)



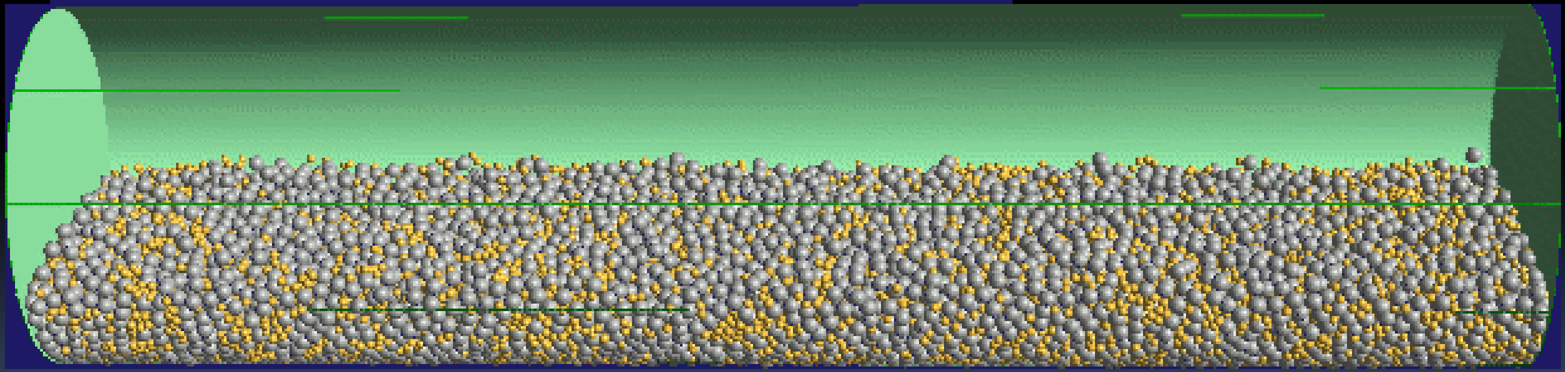
Wave patterns in a vibrated container
(from A. Kudrolli's group)



(Simulations by D. C. Rapaport)

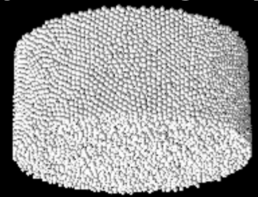


Segregation in sheared flow
(Simulations by D. C. Rapaport)

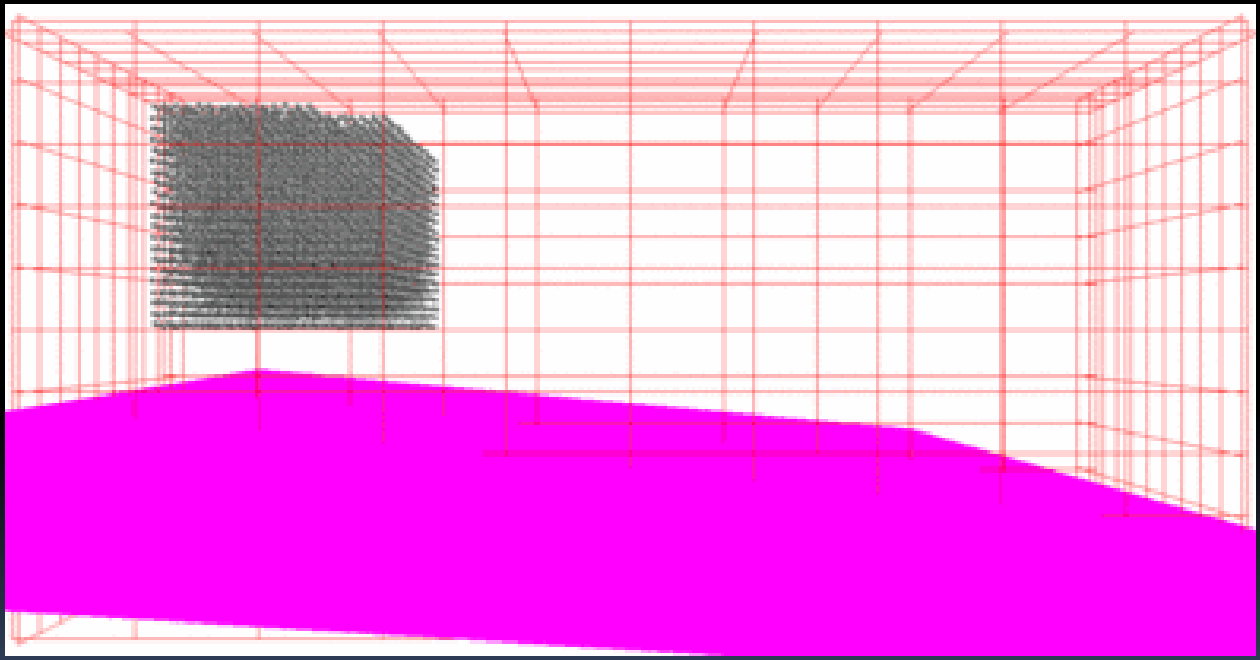


Segregation in a rotating cylinder
(Simulations by D. C. Rapaport)

Granular jet hitting a plane

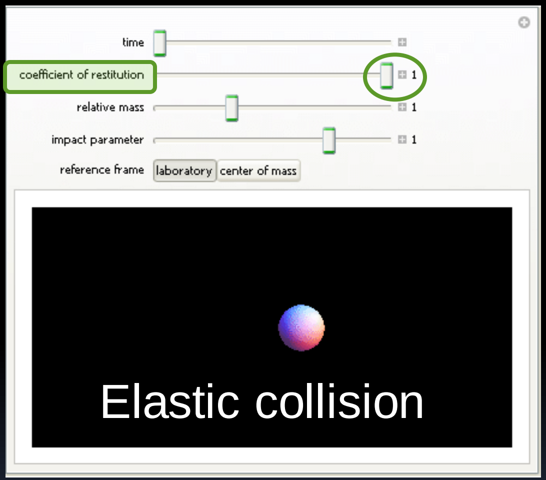


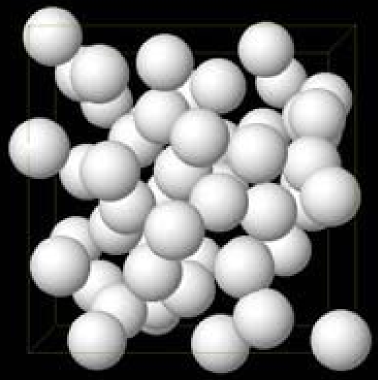
Particles falling on an inclined heated plane

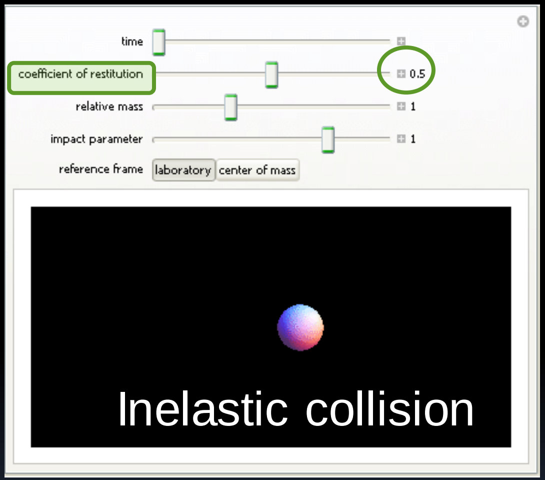


http://trevinca.ei.uvigo.es/~formella/

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



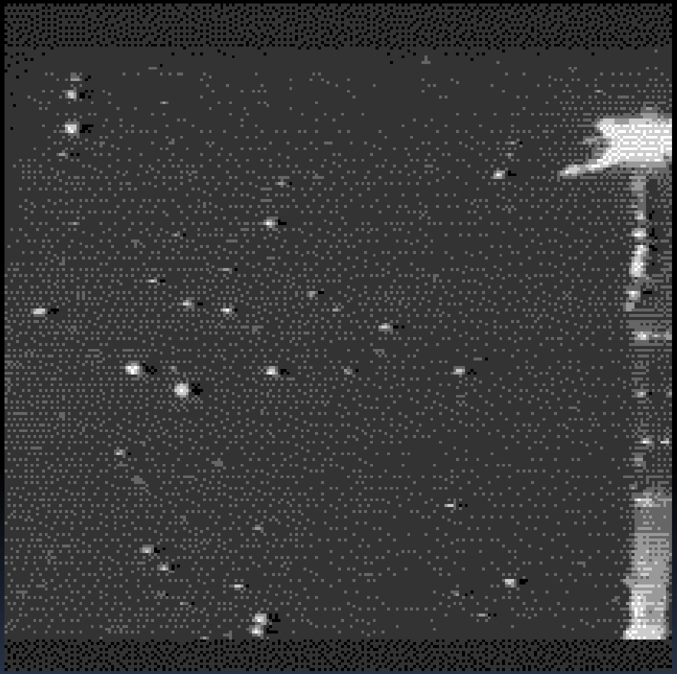




http://demonstrations.wolfram.com/InelasticCollisionsOfTwoSpheres/

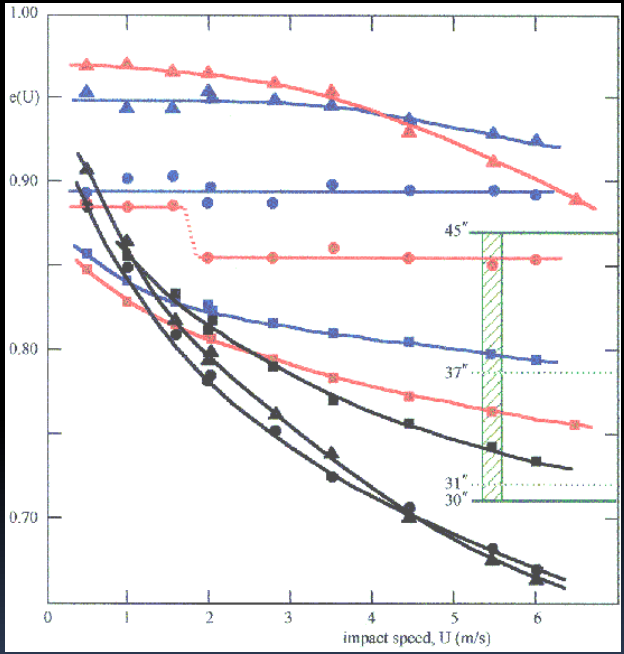
This minimal model ignores …

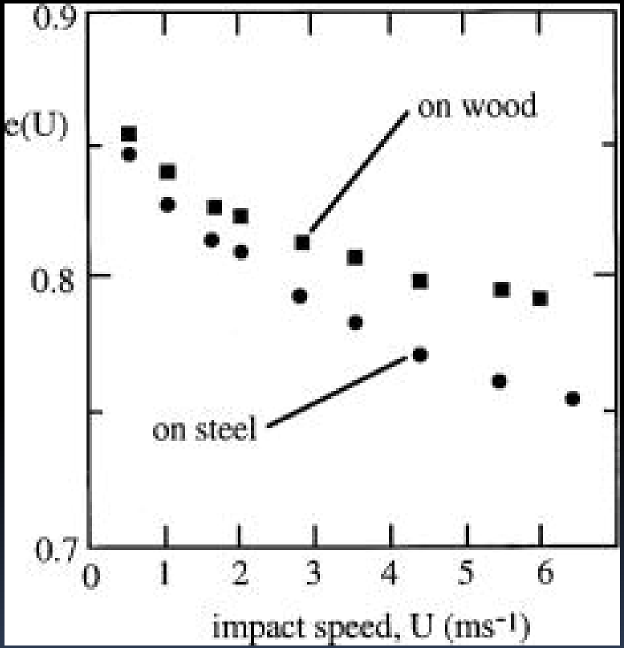
Interstitial fluid



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

Non-constant coefficient of restitution

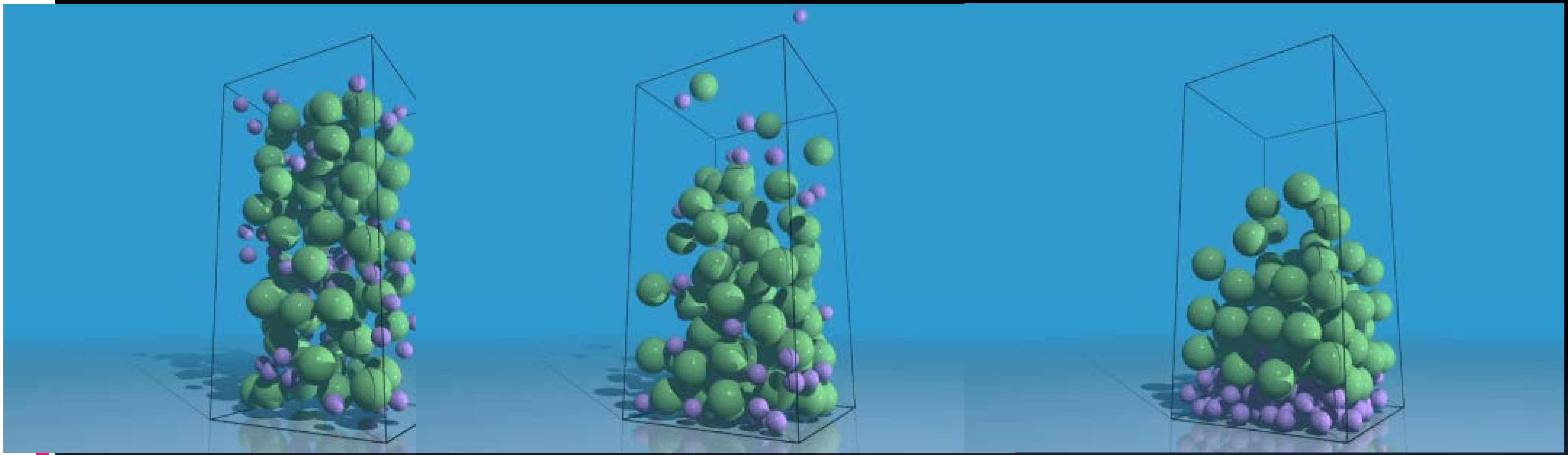




www.oxfordcroquet.com/tech/

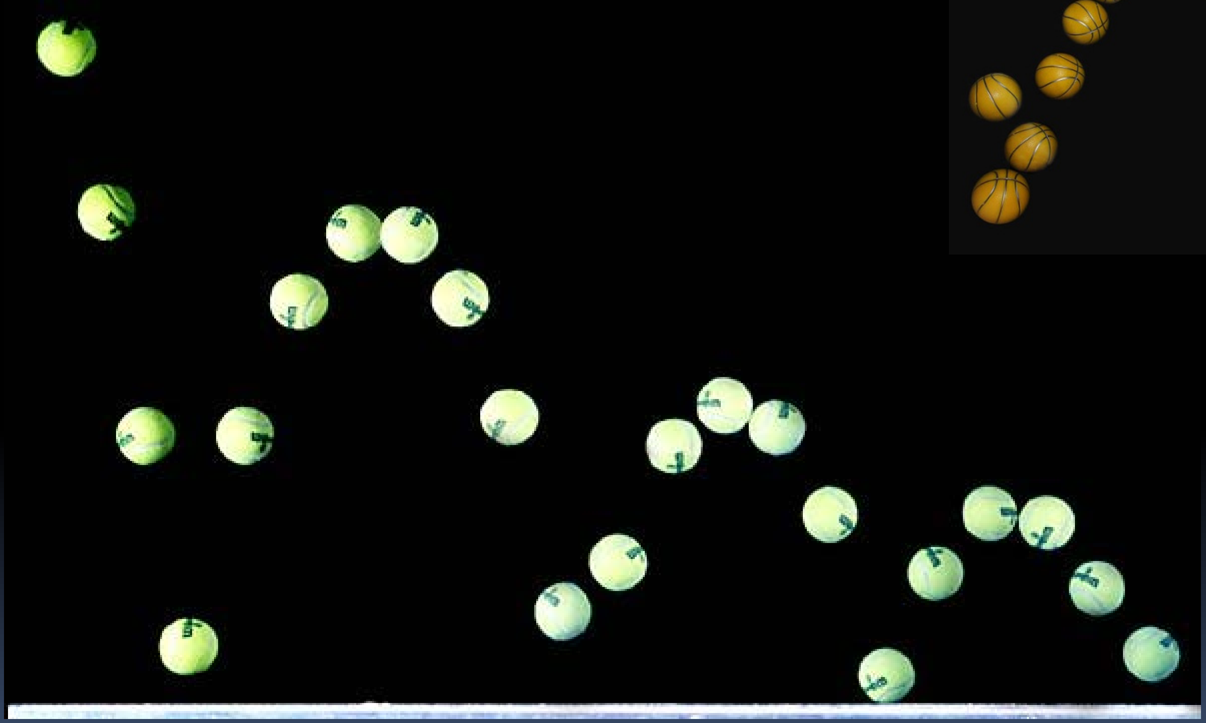
Non-spherical shape

Polydispersity



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

Roughness



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

- Collision rules for inelastic rough hard spheres. Statistical quantities.
- Homogeneous cooling state. Kinetic theory (Boltzmann-Enskog) description.
- Sonine approximation. Results.
- Conclusions and outlook.

Material parameters:

- Mass m
- Diameter σ
- Moment of inertia I
- Coefficient of normal restitution α
- Coefficients of tangential restitution β
- $\alpha=1$ for perfectly elastic particles
- $\beta=-1$ for perfectly smooth particles
- $\beta=+1$ for perfectly rough particles

Collision rules

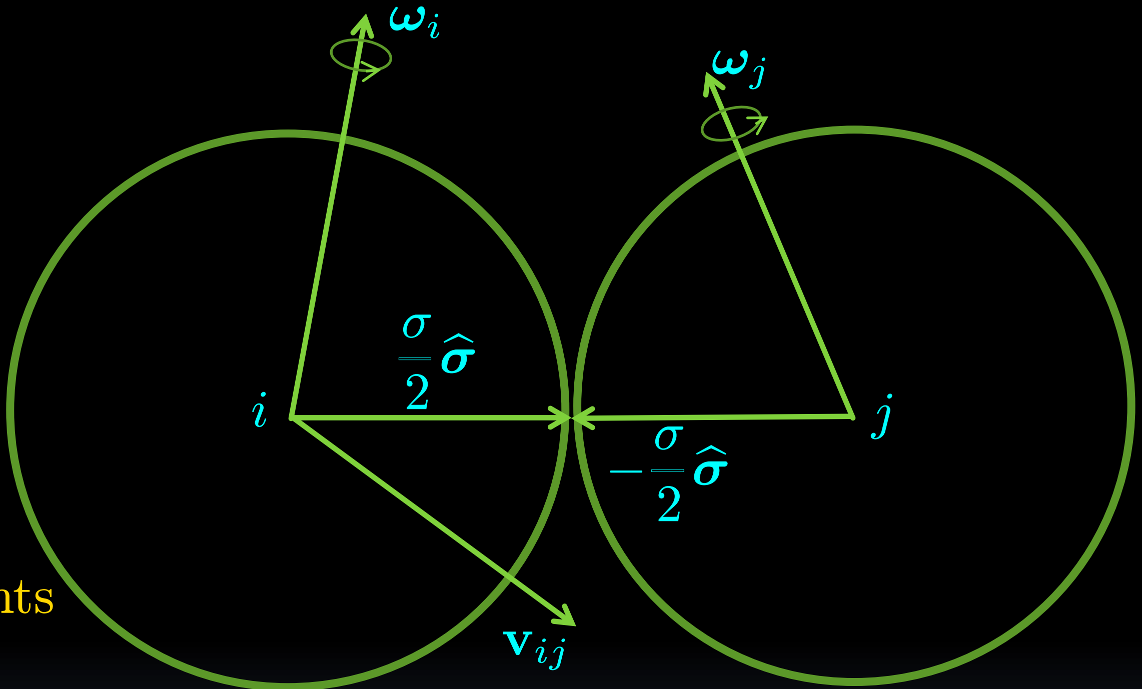
Cons. linear momentum:

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

Cons. angular momentum:

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

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



Relative velocity of the points of the spheres at contact:

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

$$\widehat{\boldsymbol{\sigma}} \cdot \boldsymbol{\mathcal{V}}_{ij}' = -\alpha\widehat{\boldsymbol{\sigma}} \cdot \boldsymbol{\mathcal{V}}_{ij}, \quad \widehat{\boldsymbol{\sigma}} \times \boldsymbol{\mathcal{V}}_{ij}' = -\beta\widehat{\boldsymbol{\sigma}} \times \boldsymbol{\mathcal{V}}_{ij}$$

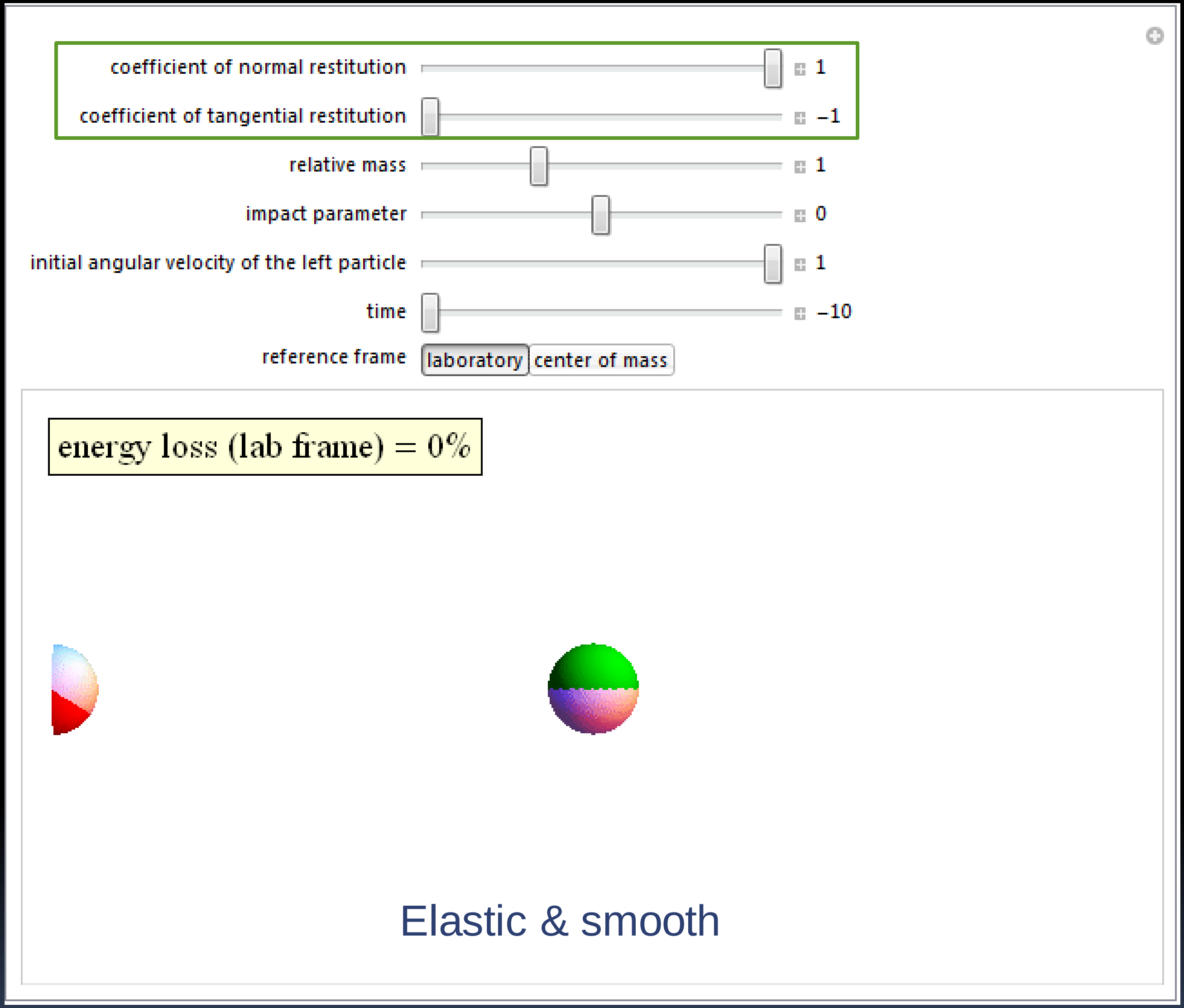
Energy collisional loss

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

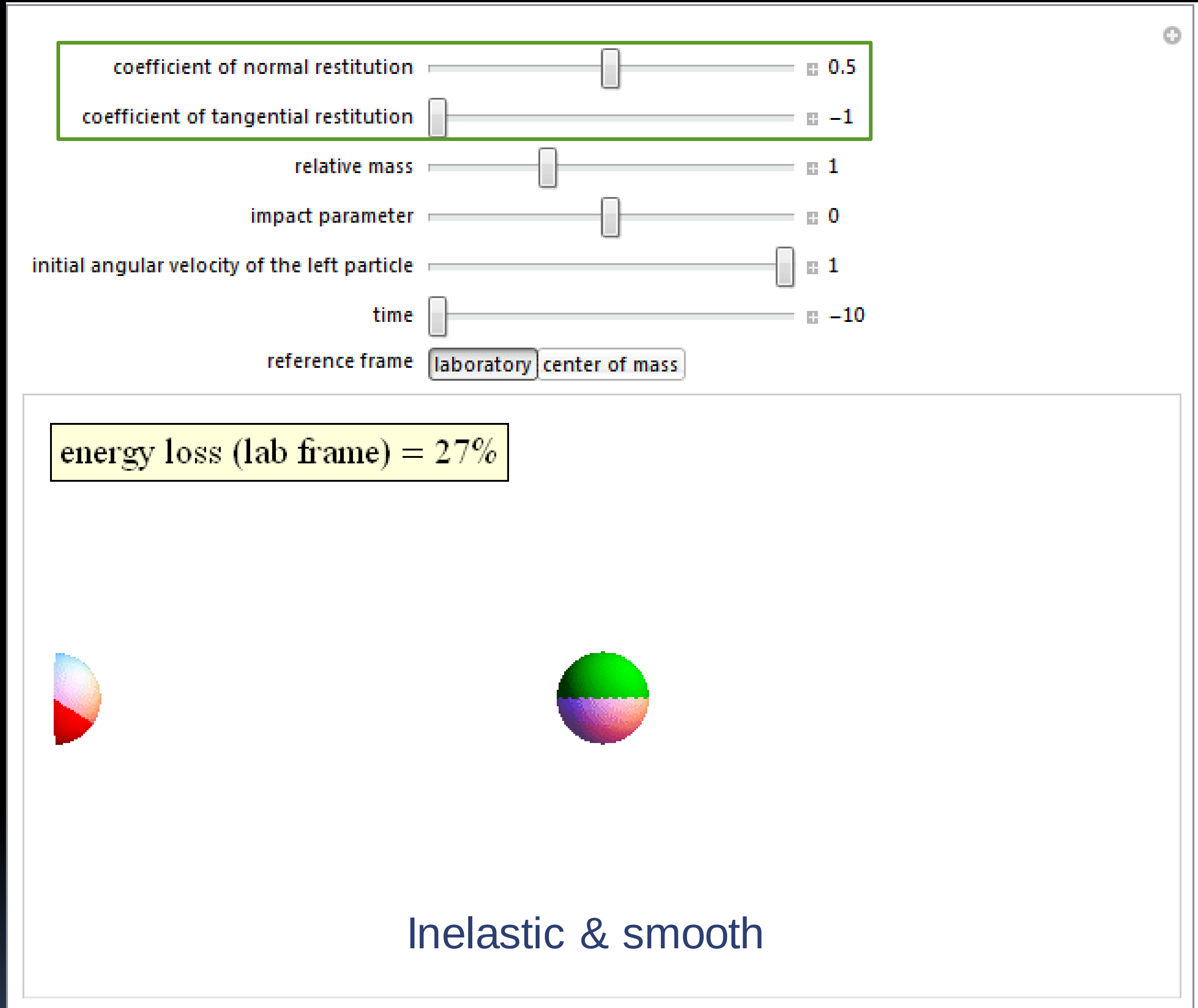
$$\begin{aligned} E'_{ij} - E_{ij} &= -(1-\alpha^2) \times \cdots \\ &\quad -(1-\beta^2) \times \cdots \end{aligned}$$

Energy is conserved *only* if the spheres are

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

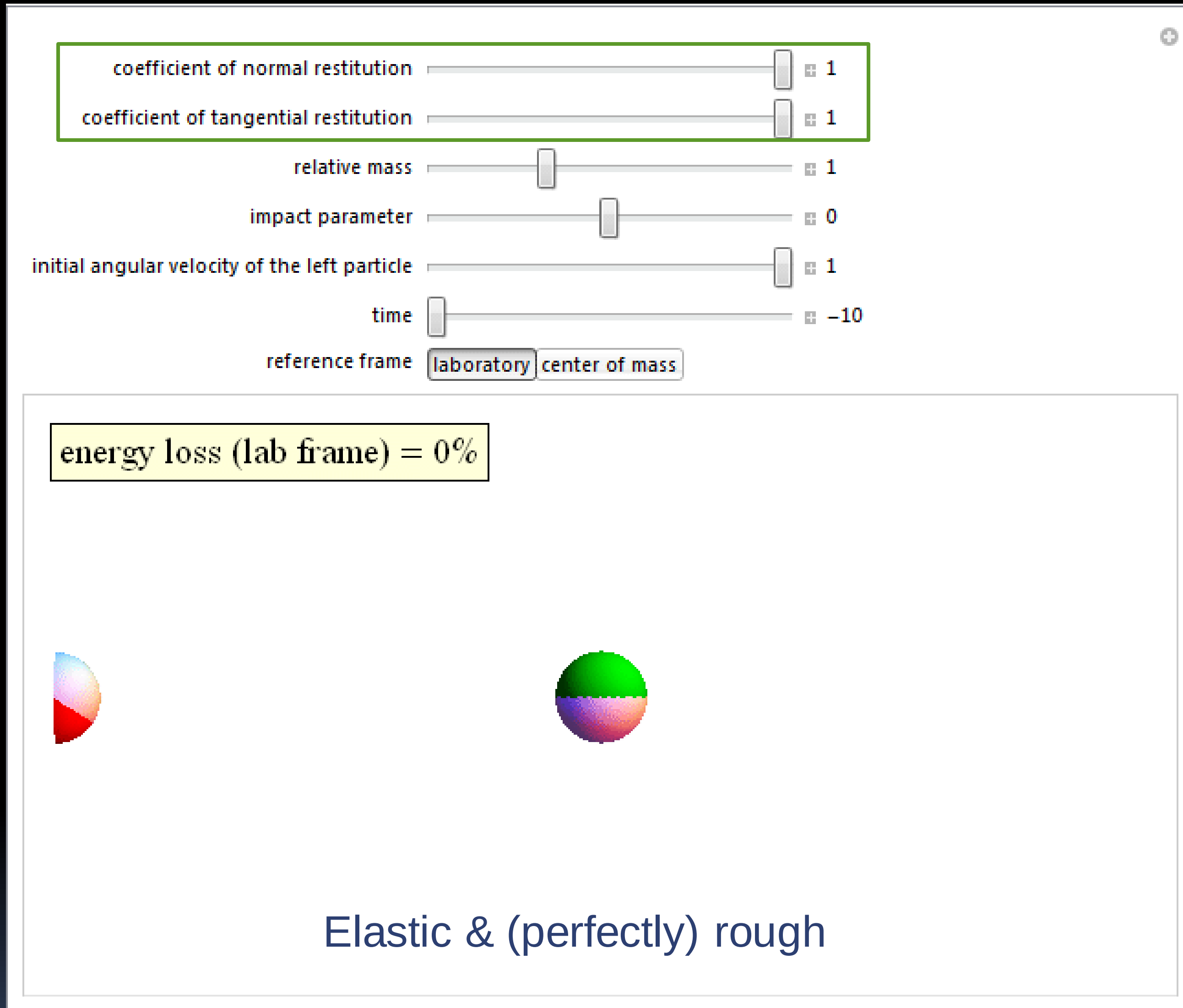


http://demonstrations.wolfram.com/InelasticCollisionsOfTwoRoughSpheres/



Inelastic & smooth

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



Elastic & (perfectly) rough

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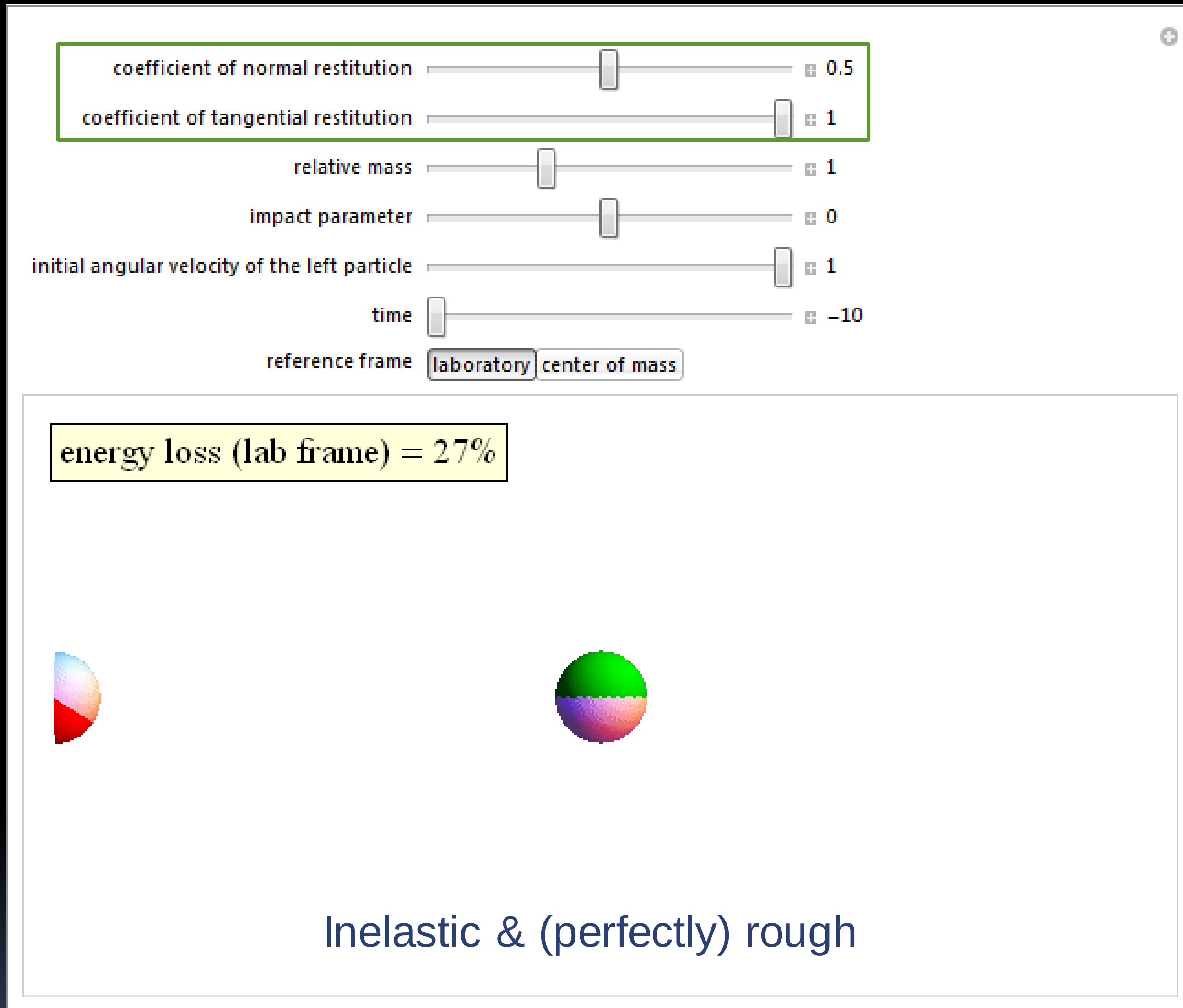

Inelastic & (perfectly) rough

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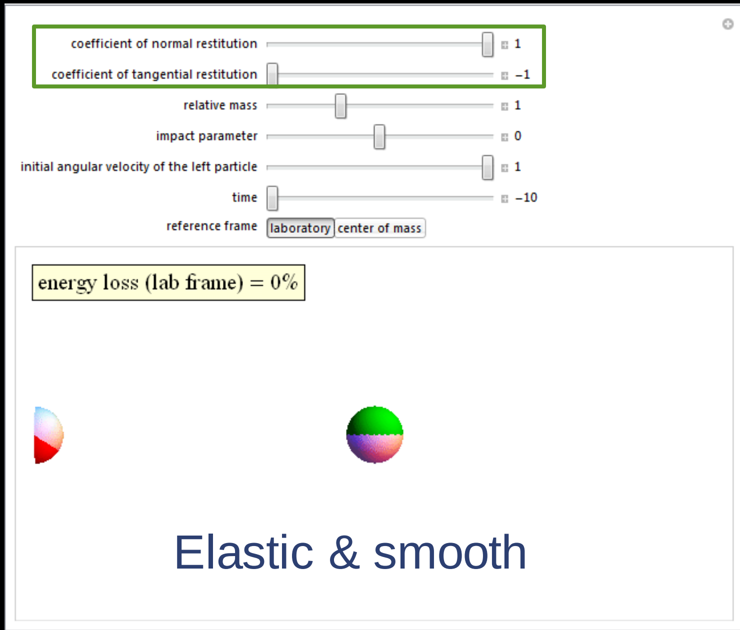
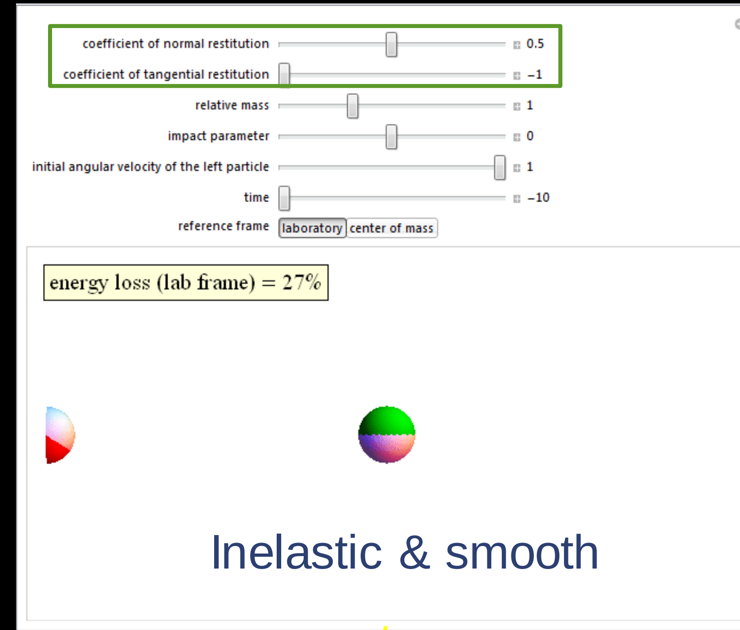


Elastic & smooth



Inelastic & smooth

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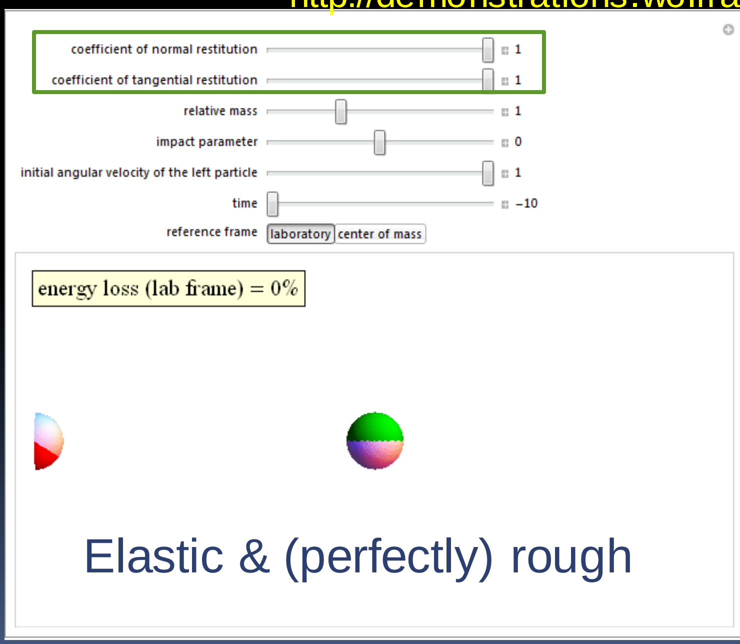
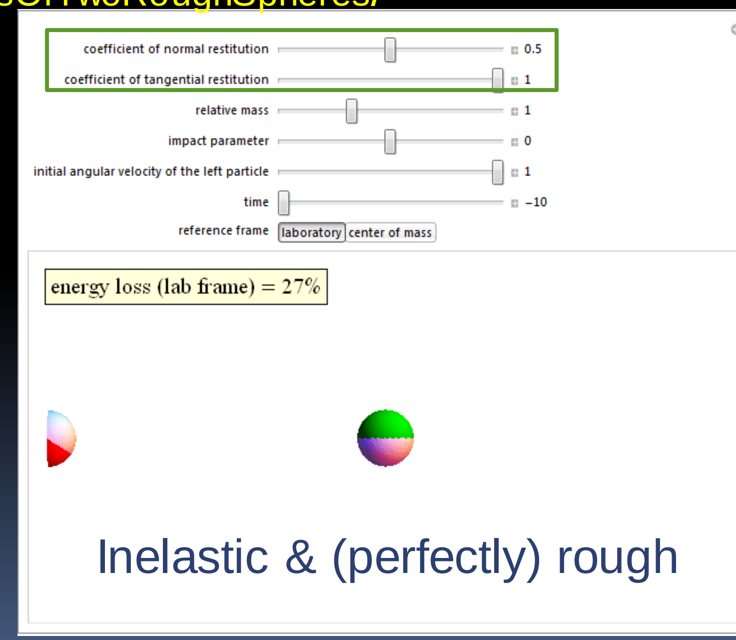
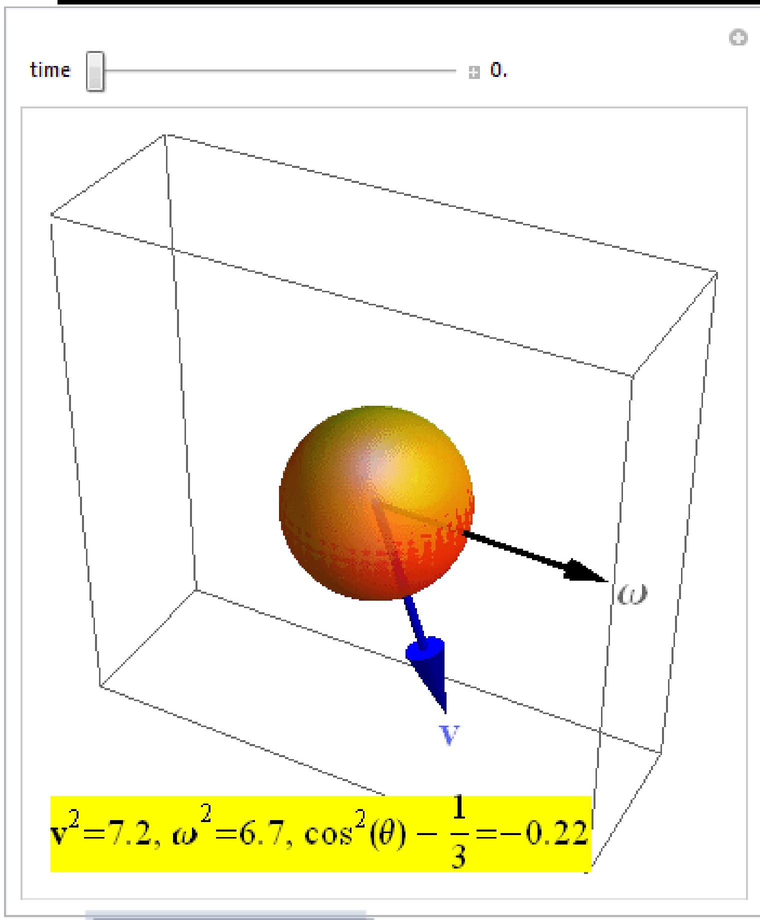


Elastic & (perfectly) rough



Inelastic & (perfectly) rough

Granular temperatures, kurtoses, and correlations



translational temperature: $\langle v^2\rangle = \dfrac{3T^{\rm tr}}{m}$

rotational temperature: $\langle \omega^2\rangle = \dfrac{3T^{\rm rot}}{I}$

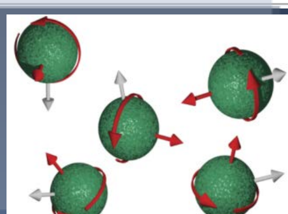
translational kurtosis: $\langle v^4\rangle = \frac{5}{3}\langle v^2\rangle^2(1+a_{20})$

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

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

angular correlations: $\langle(\mathbf{c}\cdot\mathbf{w})^2\rangle - \frac{1}{3}\langle c^2 w^2\rangle = \frac{5}{4}b$

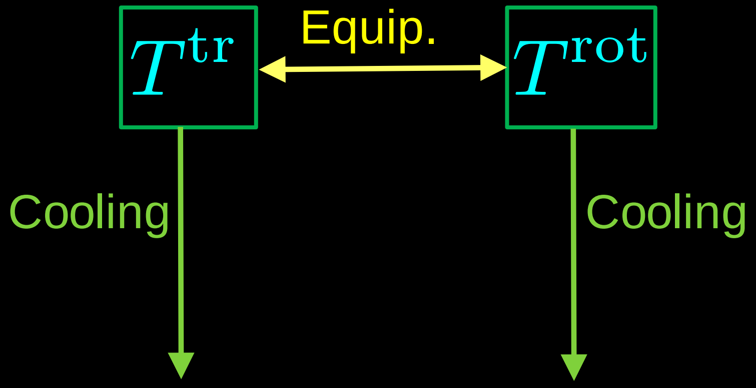
angular correlations: $\langle(\widehat{\mathbf{v}}\cdot\widehat{\boldsymbol{\omega}})^2\rangle - \frac{1}{3} = \frac{1}{5}b'$



Our aim:

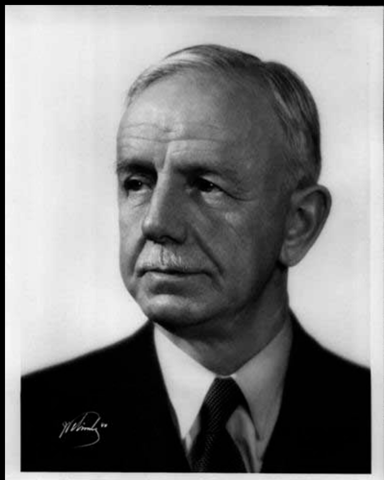
To measure

- Temperature ratio $T^{\mathrm{rot}}/T^{\mathrm{tr}}$
- Kurtosis a_{20}
- Kurtosis a_{02}
- Correlation a_{11}
- Correlation b

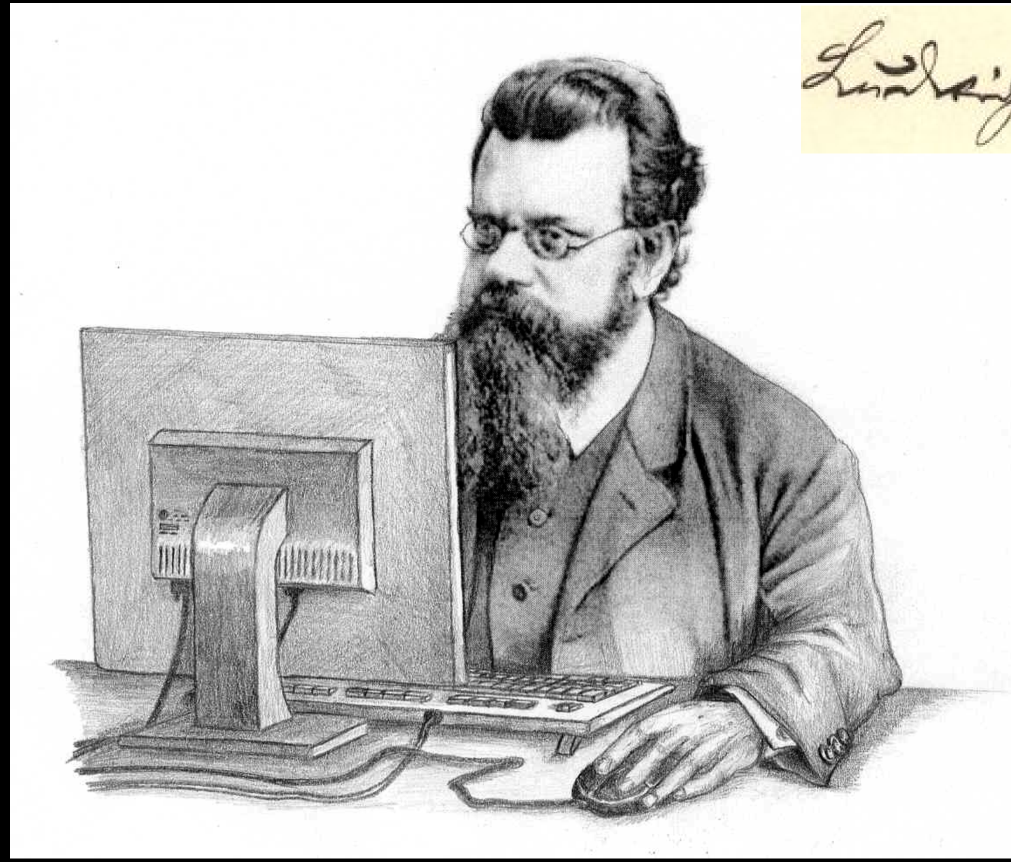


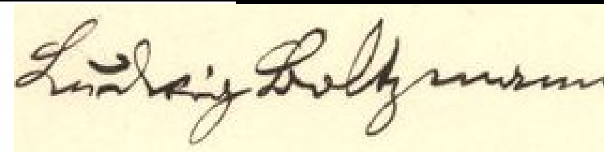
in the Homogeneous Cooling State (HCS).

$$T^{\mathrm{tr}}(t) \sim t^{-2}, \quad T^{\mathrm{rot}}(t)/T^{\mathrm{tr}}(t) \to \mathrm{const}$$



David Enskog
(1884-1947)





(1844-1906)

(Cartoon by Bernhard Reischl, University of Vienna)

Boltzmann-Enskog 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

SCALED QUANTITIES

Scaled velocities: $\mathbf{c}(t) \equiv \dfrac{\mathbf{v}}{\sqrt{2T^{\text{tr}}(t)/m}}, \quad \mathbf{w}(t) \equiv \dfrac{\boldsymbol{\omega}}{\sqrt{2T^{\text{rot}}(t)/I}}$

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

HCS: $\dfrac{\mu_{20}}{3}\dfrac{\partial}{\partial \mathbf{c}}\cdot(\mathbf{c}\phi) + \dfrac{\mu_{02}}{3}\dfrac{\partial}{\partial \mathbf{w}}\cdot(\mathbf{w}\phi) = J^*[\mathbf{c},\mathbf{w}|\phi]$

Collisional moments:

$$\mu_{pq} = -\int d\mathbf{c}\int d\mathbf{w}\, c^p w^q J^*[\mathbf{c},\mathbf{w}|\phi]$$

$$\mu_b = -\int d\mathbf{c}\int d\mathbf{w}\, (\mathbf{c}\cdot\mathbf{w})^2 J^*[\mathbf{c},\mathbf{w}|\phi]$$

Moment equations

$$\mu_{20} = \mu_{02}$$

$$5\mu_{20} = \frac{\mu_{40}}{1 + a_{20}}$$

$$\frac{3}{2}(\mu_{20} + \mu_{02}) = \frac{\mu_{22}}{1 + a_{11}}$$

$$5\mu_{02} = \frac{\mu_{04}}{1 + a_{02}}$$

$$\frac{5}{6}(\mu_{20} + \mu_{02})b = \mu_b - \frac{1}{3}\mu_{22}$$

Linear Sonine approximation

$$\phi(\mathbf{c},\mathbf{w}) \simeq \pi^{-3}e^{-c^2-w^2}\left\{1 + a_{20}S^{(2)}_{\frac{1}{2}}(c^2) + a_{02}S^{(2)}_{\frac{1}{2}}(w^2)\right.$$
$$\left. + a_{11}S^{(1)}_{\frac{1}{2}}(c^2)S^{(1)}_{\frac{1}{2}}(w^2) + b\left[(\mathbf{c}\cdot\mathbf{w})^2 - \frac{1}{3}c^2w^2\right]\right\}$$

Sonine (Laguerre) polynomials:

$$S^{(1)}_{\frac{1}{2}}(x) = \frac{3}{2} - x, \quad S^{(2)}_{\frac{1}{2}}(x) = \frac{1}{8}\left(15 - 20x + 4x^2\right)$$

And after tedious calculations …

$$\mu_{20} = 4\sqrt{2\pi}\left[\left(\widetilde{\alpha}(1-\widetilde{\alpha})+\widetilde{\beta}(1-\widetilde{\beta})\right)\left(1+\frac{3a_{20}}{16}\right)-\theta\frac{\widetilde{\beta}^2}{\kappa}\left(1-\frac{a_{20}}{16}+\frac{3a_{11}-b}{12}\right)\right],$$

$$\mu_{02} = 4\sqrt{2\pi}\frac{\widetilde{\beta}}{\kappa}\left[\left(1-\frac{\widetilde{\beta}}{\kappa}\right)\left(1-\frac{a_{20}}{16}+\frac{3a_{11}-b}{12}\right)-\frac{\widetilde{\beta}}{\theta}\left(1+\frac{3a_{20}}{16}\right)\right],$$

$$\begin{aligned}\mu_{40} = {} & 16\sqrt{2\pi}\Bigg\{\widetilde{\alpha}^3(2-\widetilde{\alpha})+\widetilde{\beta}^3(2-\widetilde{\beta})-\widetilde{\alpha}\widetilde{\beta}(1-\widetilde{\alpha}-\widetilde{\beta}+\widetilde{\alpha}\widetilde{\beta})+\frac{11}{8}(\widetilde{\alpha}+\widetilde{\beta})-\frac{19}{8}(\widetilde{\alpha}^2+\widetilde{\beta}^2)-\left[\widetilde{\alpha}\widetilde{\beta}\left(\frac{23}{15}-\widetilde{\alpha}-\widetilde{\beta}+\widetilde{\alpha}\widetilde{\beta}\right)-\frac{269}{120}(\widetilde{\alpha}+\widetilde{\beta})+\frac{357}{120}(\widetilde{\alpha}^2+\widetilde{\beta}^2)-\widetilde{\alpha}^3(2-\widetilde{\alpha})-\widetilde{\beta}^3(2-\widetilde{\beta})\right]\frac{15a_{20}}{16} \\ & -\frac{11\widetilde{\beta}^2\theta}{8\kappa}\left(1+\frac{41a_{20}}{176}+\frac{3a_{11}-b}{4}\right)+\frac{\widetilde{\beta}^2\theta}{\kappa}\left[\widetilde{\alpha}(1-\widetilde{\alpha})+2\widetilde{\beta}(1-\widetilde{\beta})\right]\left(1+\frac{3a_{20}}{16}+\frac{3a_{11}-b}{4}\right)-\frac{\widetilde{\beta}^4\theta^2}{\kappa^2}\left(1-\frac{a_{20}}{16}+\frac{a_{02}}{2}+\frac{3a_{11}-b}{6}\right)\Bigg\},\end{aligned}$$

$$\begin{aligned}\mu_{22} = {} & 3\sqrt{2\pi}\Bigg\{2\left[\widetilde{\alpha}(1-\widetilde{\alpha})+\widetilde{\beta}(1-\widetilde{\beta})-\frac{4\widetilde{\alpha}\widetilde{\beta}}{3\kappa}(1-\widetilde{\alpha})\left(1-\frac{\widetilde{\beta}}{\kappa}\right)-\frac{8\widetilde{\beta}^2}{3\kappa}\left(\frac{3}{4}-\widetilde{\beta}-\frac{\widetilde{\beta}}{\kappa}+2\frac{\widetilde{\beta}^2}{\kappa}\right)\right]\left(1+\frac{3a_{20}}{16}+\frac{3a_{11}-b}{4}\right)+\frac{7\widetilde{\beta}}{3\kappa}\left(1-\frac{\widetilde{\beta}}{\kappa}\right)\left(1+\frac{29a_{20}}{112}\right)-\frac{\widetilde{\beta}^2}{2\kappa\theta}a_{20}-\frac{8\widetilde{\beta}^2}{3\kappa\theta}\Bigg[\frac{9}{8}-\widetilde{\alpha}(1-\widetilde{\alpha}) \\ & -2\widetilde{\beta}(1-\widetilde{\beta})\Bigg]\left(1+\frac{15a_{20}}{16}\right)-\frac{\widetilde{\beta}^2\theta}{3\kappa}\left[5-8\frac{\widetilde{\beta}}{\kappa}\left(1-\frac{\widetilde{\beta}}{\kappa}\right)\right]a_{02}-8\frac{\widetilde{\beta}^2\theta}{3\kappa}\left[1-2\frac{\widetilde{\beta}}{\kappa}\left(1-\frac{\widetilde{\beta}}{\kappa}\right)\right] \\ & \times\left(1-\frac{a_{20}}{16}+\frac{3a_{11}-b}{6}\right)+\left[\frac{\widetilde{\beta}}{\kappa}\left(\frac{37}{12}-2\widetilde{\beta}-\frac{7\widetilde{\beta}}{4\kappa}\right)+\widetilde{\alpha}+\widetilde{\beta}-\frac{4\widetilde{\alpha}\widetilde{\beta}}{3\kappa}\right]\frac{3a_{11}-b}{3}+\left[5(\widetilde{\alpha}+\widetilde{\beta})-3(\widetilde{\alpha}^2+\widetilde{\beta}^2)+\frac{4\widetilde{\beta}}{\kappa}(1-\widetilde{\beta})-\frac{\widetilde{\beta}^2}{\kappa^2}(2+\kappa\theta)\right]\frac{b}{6}\Bigg\},\end{aligned}$$

$$\begin{aligned}\mu_{04} = {} & 4\sqrt{2\pi}\frac{\widetilde{\beta}}{\kappa}\Bigg\{\left(1-\frac{\widetilde{\beta}}{\kappa}\right)\left[5-4\frac{\widetilde{\beta}}{\kappa}\left(1-\frac{\widetilde{\beta}}{\kappa}\right)\right]\left(1-\frac{a_{20}}{16}\right)-\frac{\widetilde{\beta}}{\theta}\left[5-8\frac{\widetilde{\beta}}{\kappa}\left(1-\frac{\widetilde{\beta}}{\kappa}\right)\right]\left(1+\frac{3a_{20}}{16}+\frac{3a_{11}-b}{4}\right)-\frac{5}{2}\left(1-\frac{4\widetilde{\beta}}{5\kappa}\right)\frac{3a_{11}-b}{3}-\frac{4\widetilde{\beta}^3}{\kappa\theta^2}\left(1+\frac{15a_{20}}{16}\right)+ \\ & \left(5-\frac{13}{2}\frac{\widetilde{\beta}}{\kappa}+4\frac{\widetilde{\beta}^2}{\kappa^2}-2\frac{\widetilde{\beta}^3}{\kappa^3}\right)\left(a_{02}+\frac{3a_{11}-b}{3}\right)+\left(1-\frac{\widetilde{\beta}}{\kappa}-\frac{\widetilde{\beta}}{\theta}\right)\frac{b}{4}\Bigg\},\end{aligned}$$

$$\begin{aligned}\mu_b = {} & 2\sqrt{2\pi}\Bigg\{\left[\widetilde{\alpha}(1-\widetilde{\alpha})-\widetilde{\beta}^2\left(1+\frac{1}{\kappa^2}\right)\right]\left(1+\frac{3a_{20}}{16}+\frac{3a_{11}}{4}+\frac{b}{2}\right)+\frac{\widetilde{\alpha}}{2}\left(a_{11}+\frac{8b}{3}\right)+\widetilde{\beta}\left(1+\frac{1-\widetilde{\beta}}{\kappa}\right)\left(1+\frac{3a_{20}}{16}+\frac{5a_{11}}{4}+\frac{13b}{12}\right)+\widetilde{\beta}\left(\frac{3}{4}-\widetilde{\alpha}\right)\left(1+\frac{1}{\kappa}\right)b-\frac{\widetilde{\beta}^2}{2\kappa\theta}\left(1+\frac{7a_{20}}{16}\right) \\ & -\frac{\widetilde{\beta}^2\theta}{2\kappa}\left(1-\frac{a_{20}}{16}+\frac{3a_{11}-b}{6}\right)\Bigg\}.\end{aligned}$$

Inserting into the Moment equations

$$\mu_{20} = \mu_{02}$$

$$5\mu_{20} = \frac{\mu_{40}}{1 + a_{20}}$$

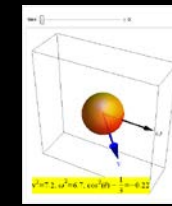
$$\frac{3}{2}(\mu_{20} + \mu_{02}) = \frac{\mu_{22}}{1 + a_{11}}$$

$$5\mu_{02} = \frac{\mu_{04}}{1 + a_{02}}$$

$$\frac{5}{6}(\mu_{20} + \mu_{02})b = \mu_b - \frac{1}{3}\mu_{22}$$

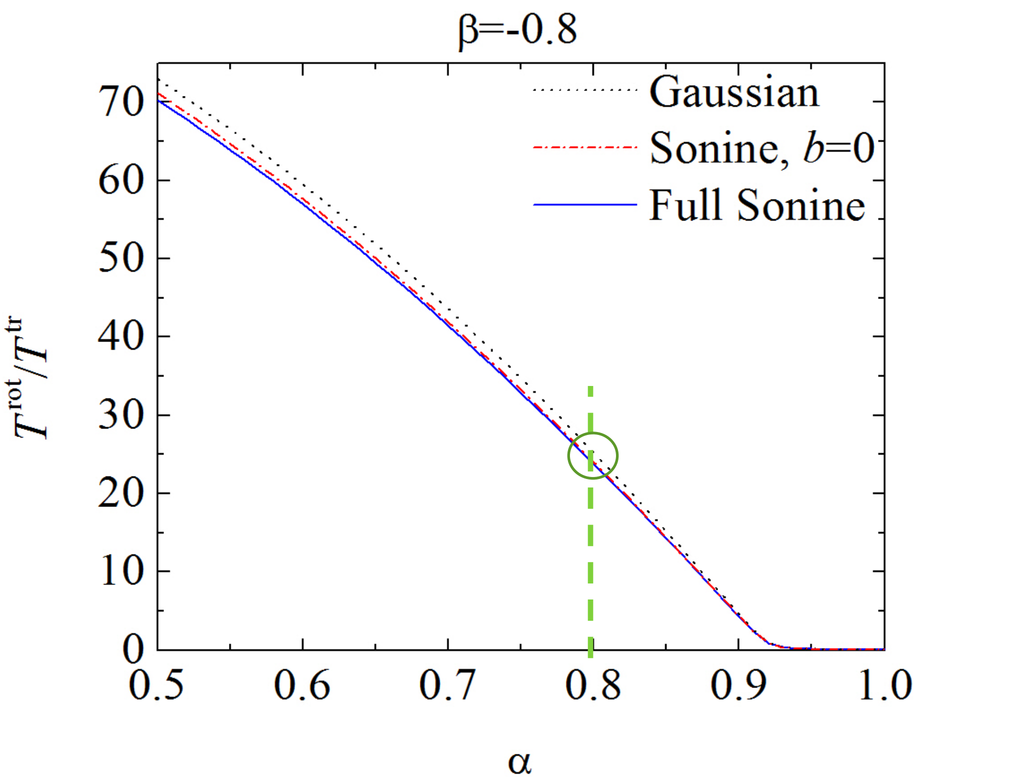
And neglecting terms nonlinear in a_{20}, a_{11}, a_{02} and b, we get a polynomial equation for $T^{\mathrm{rot}}/T^{\mathrm{tr}}$ and linear equations for a_{20}, a_{11}, a_{02} and b.

Results: Temperature ratio

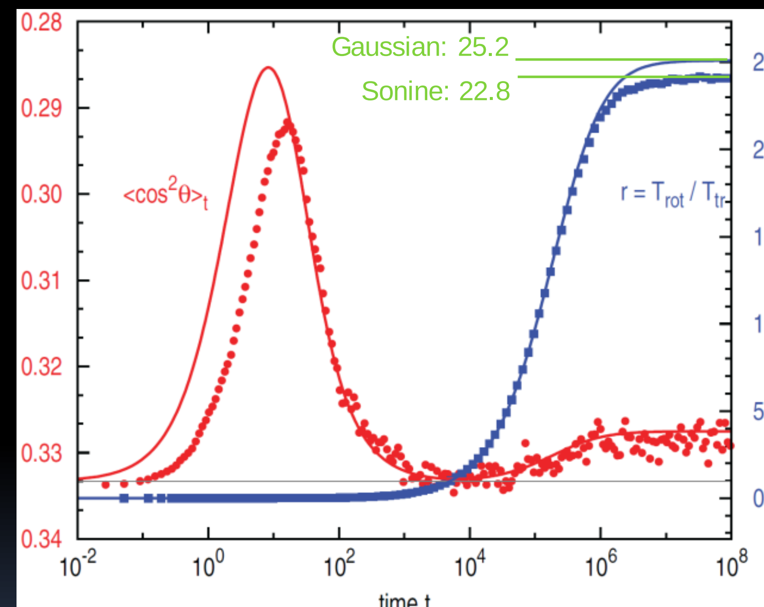


Weak roughness

$$\langle v^2 \rangle = \frac{3T^{\rm tr}}{m}, \quad \langle \omega^2 \rangle = \frac{3T^{\rm rot}}{I}$$

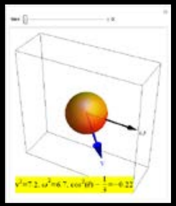


α=0.8, β=-0.8



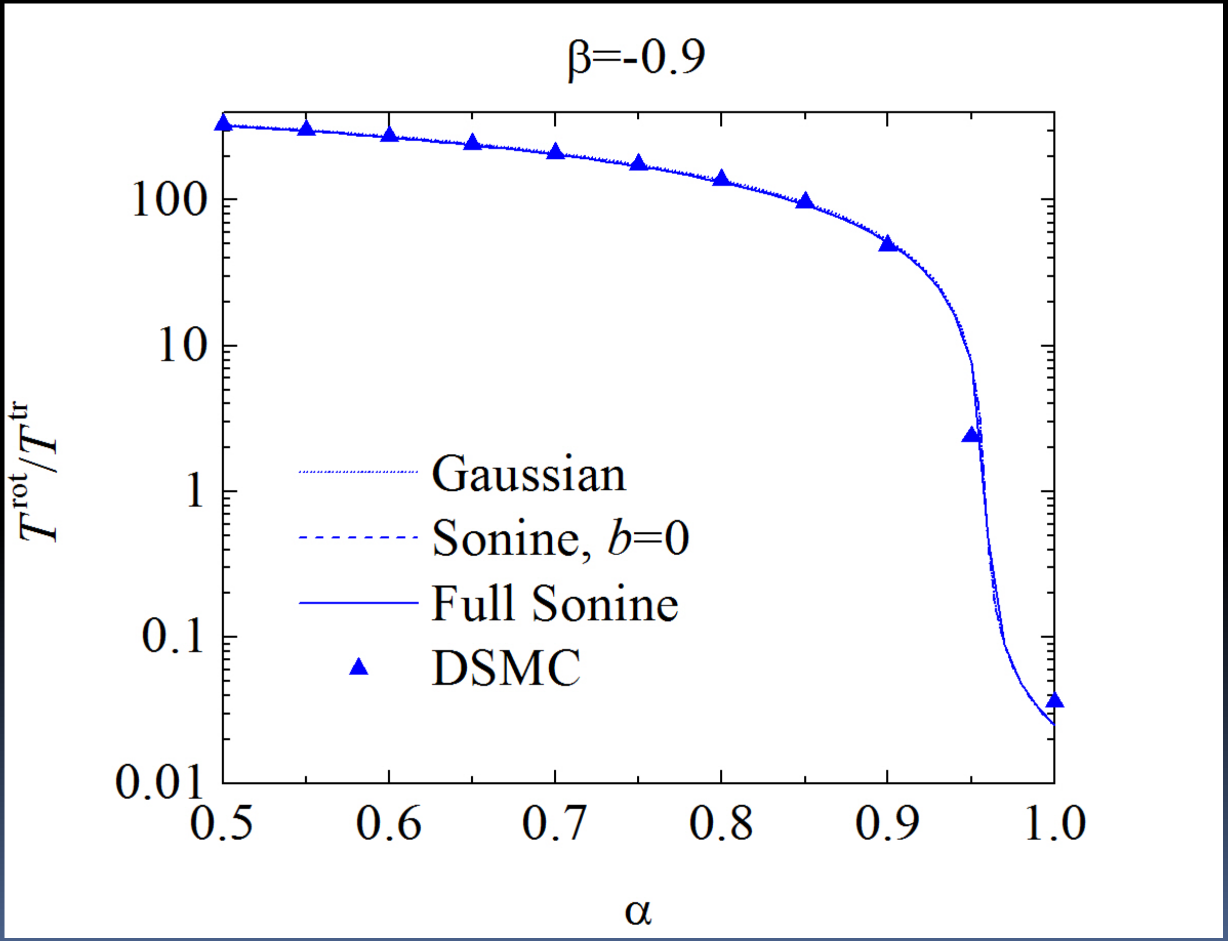
N. V. Brilliantov,[1,2] T. Pöschel,[3] W. T. Kranz,[4] and A. Zippelius[4] PRL **98,** 128001 (2007)

Results: Temperature ratio

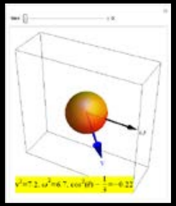


$$\langle v^2 \rangle = \frac{3T^{\rm tr}}{m}, \quad \langle \omega^2 \rangle = \frac{3T^{\rm rot}}{I}$$

Weak roughness

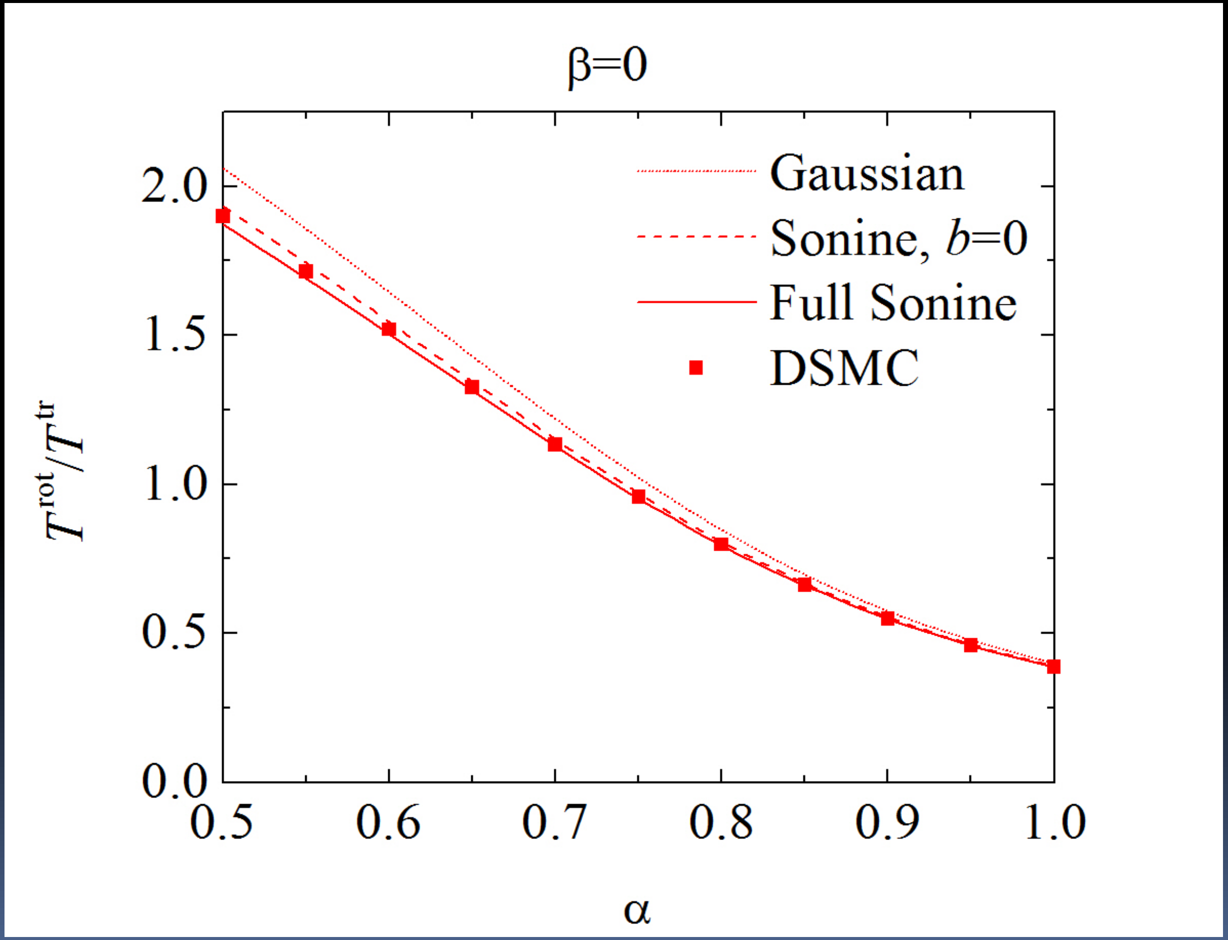


Results: Temperature ratio

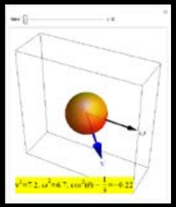


$$\langle v^2 \rangle = \frac{3T^{\mathrm{tr}}}{m}, \quad \langle \omega^2 \rangle = \frac{3T^{\mathrm{rot}}}{I}$$

Medium roughness

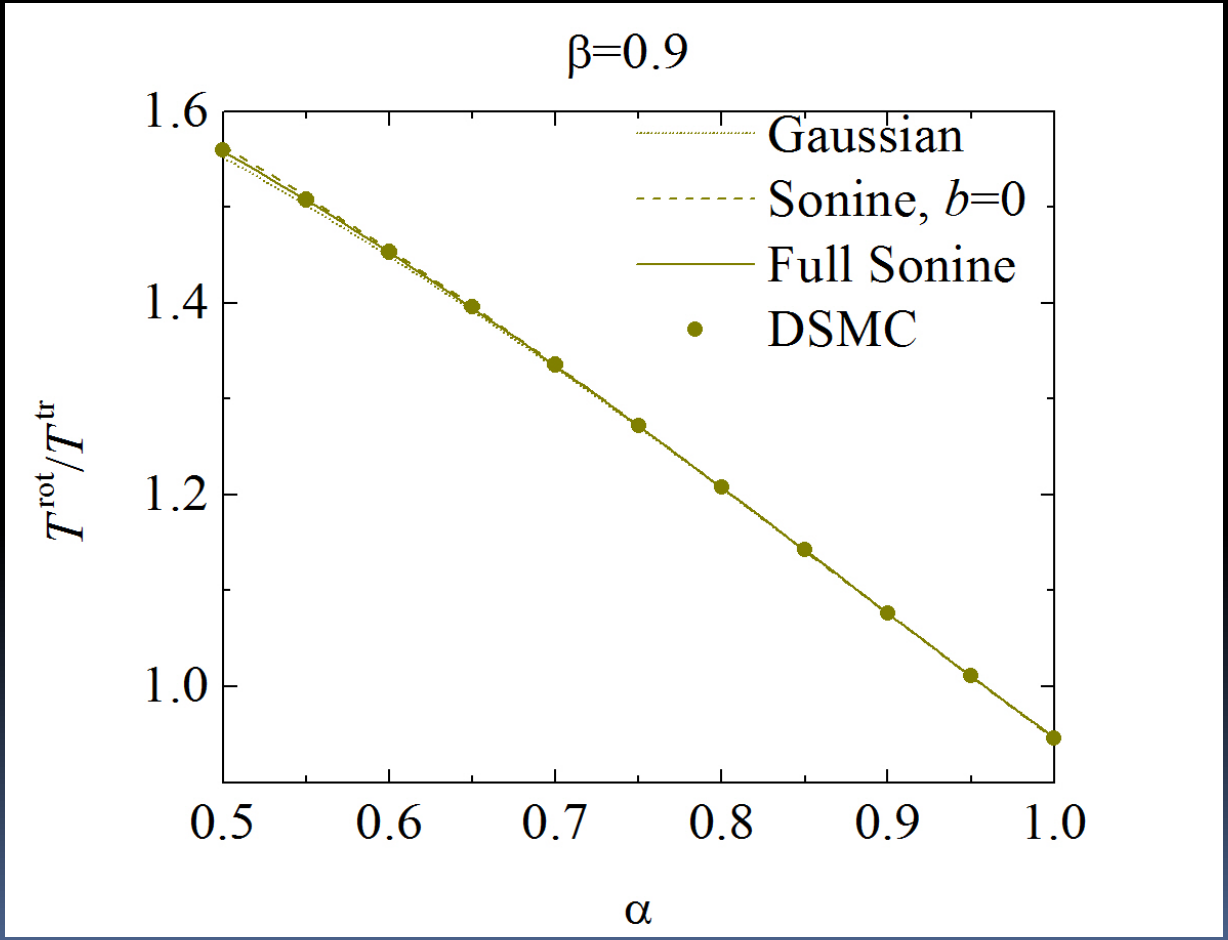


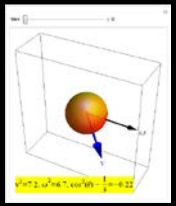
Results: Temperature ratio



$$\langle v^2 \rangle = \frac{3T^{\text{tr}}}{m}, \quad \langle \omega^2 \rangle = \frac{3T^{\text{rot}}}{I}$$

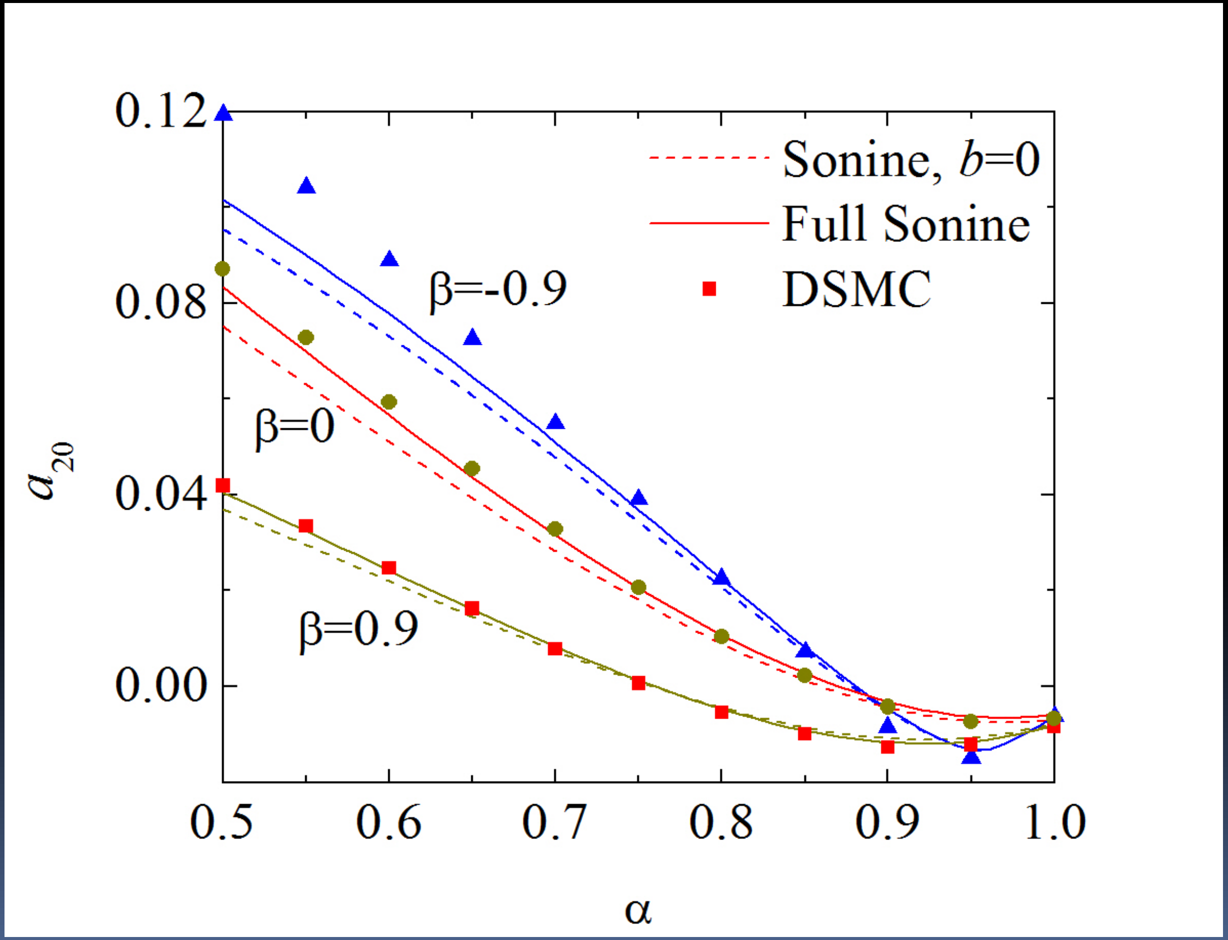
Strong roughness



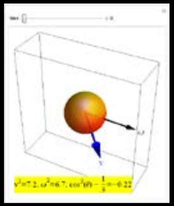


Results: Translational kurtosis

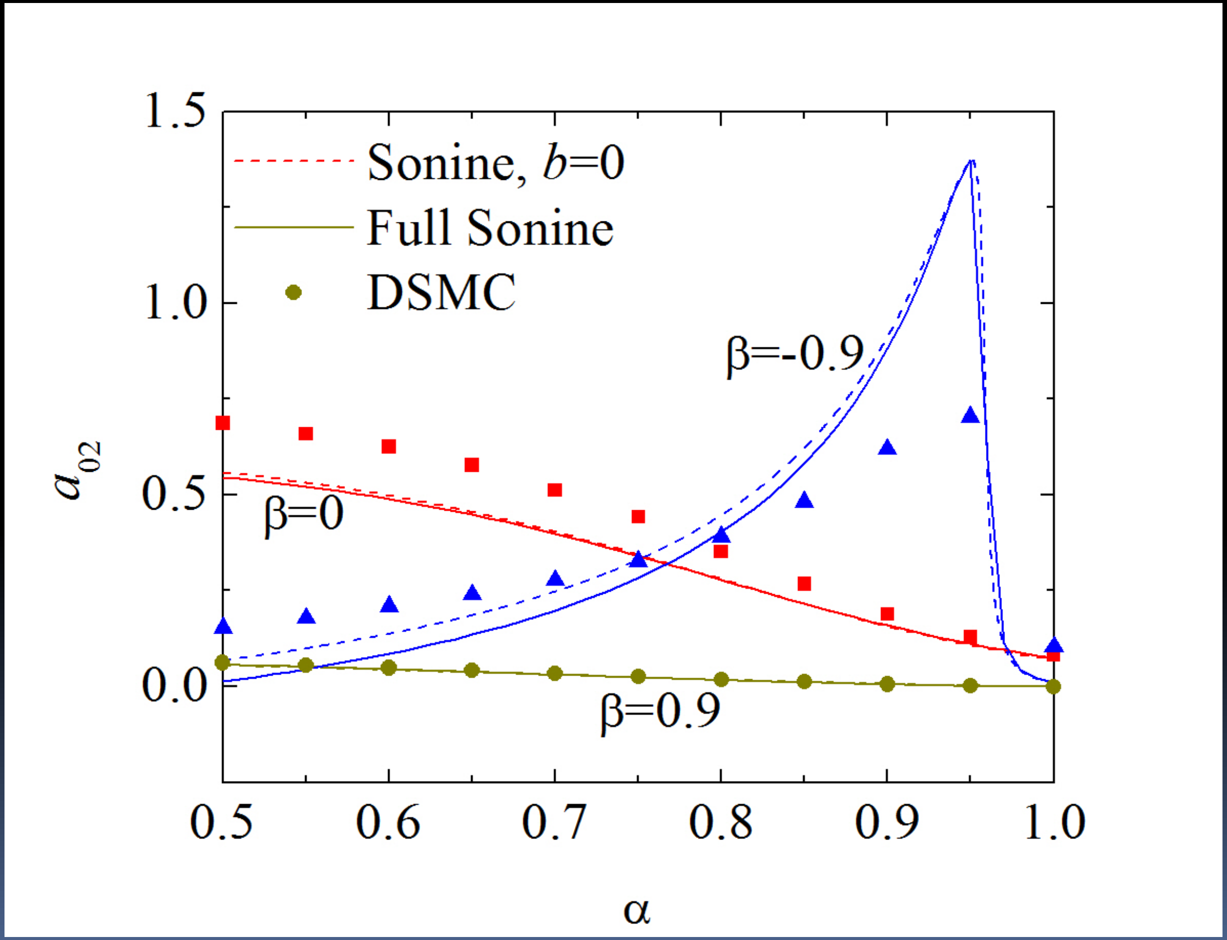
$$\langle v^4 \rangle = \frac{5}{3} \langle v^2 \rangle^2 (1 + a_{20})$$

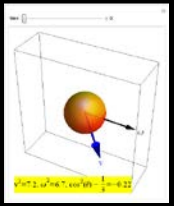


Results: Rotational kurtosis



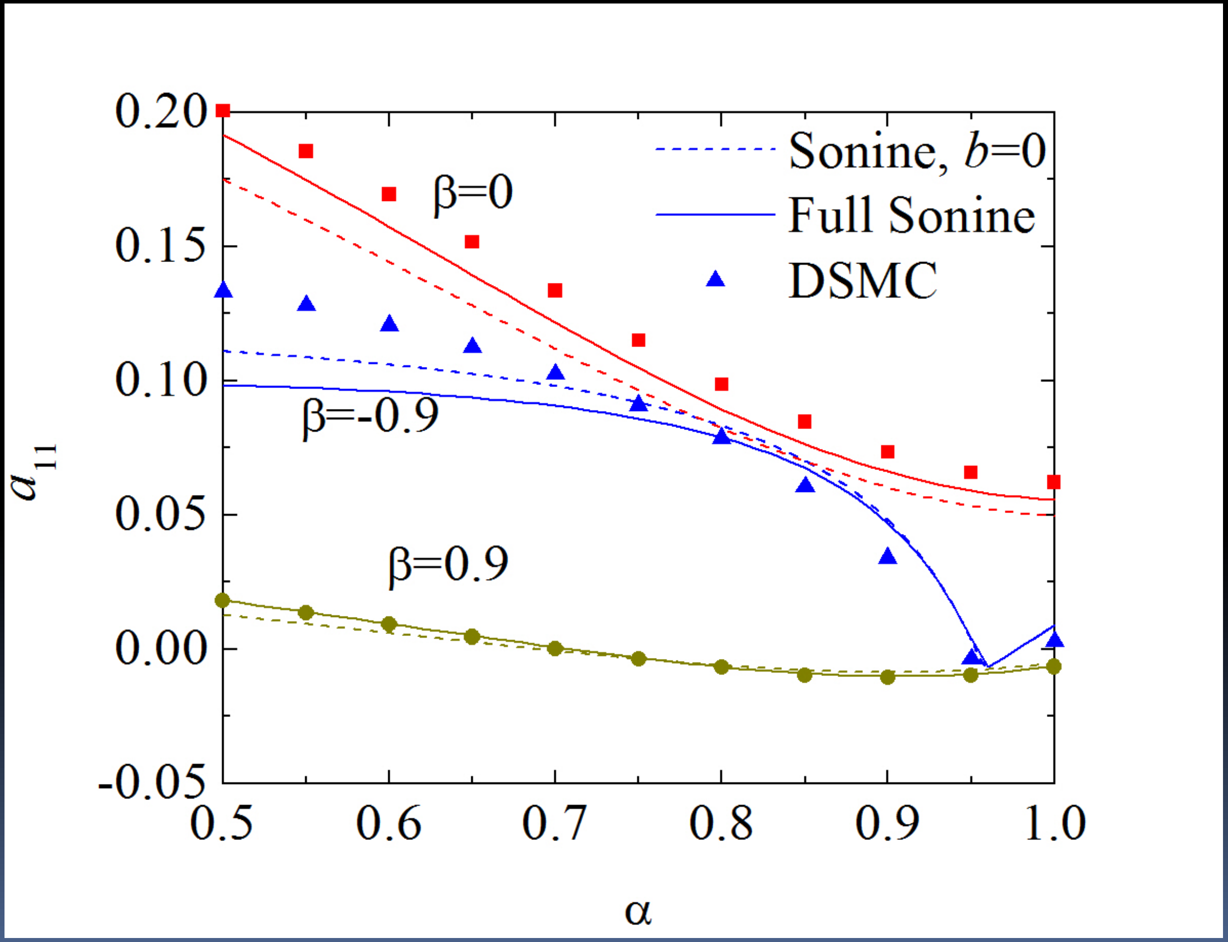
$$\langle \omega^4 \rangle = \frac{5}{3} \langle \omega^2 \rangle^2 (1 + a_{02})$$





Results: Scalar correlations

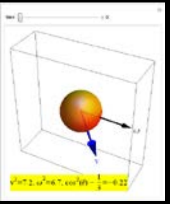
$$\langle v^2\omega^2\rangle = \langle v^2\rangle\langle\omega^2\rangle(1 + a_{11})$$

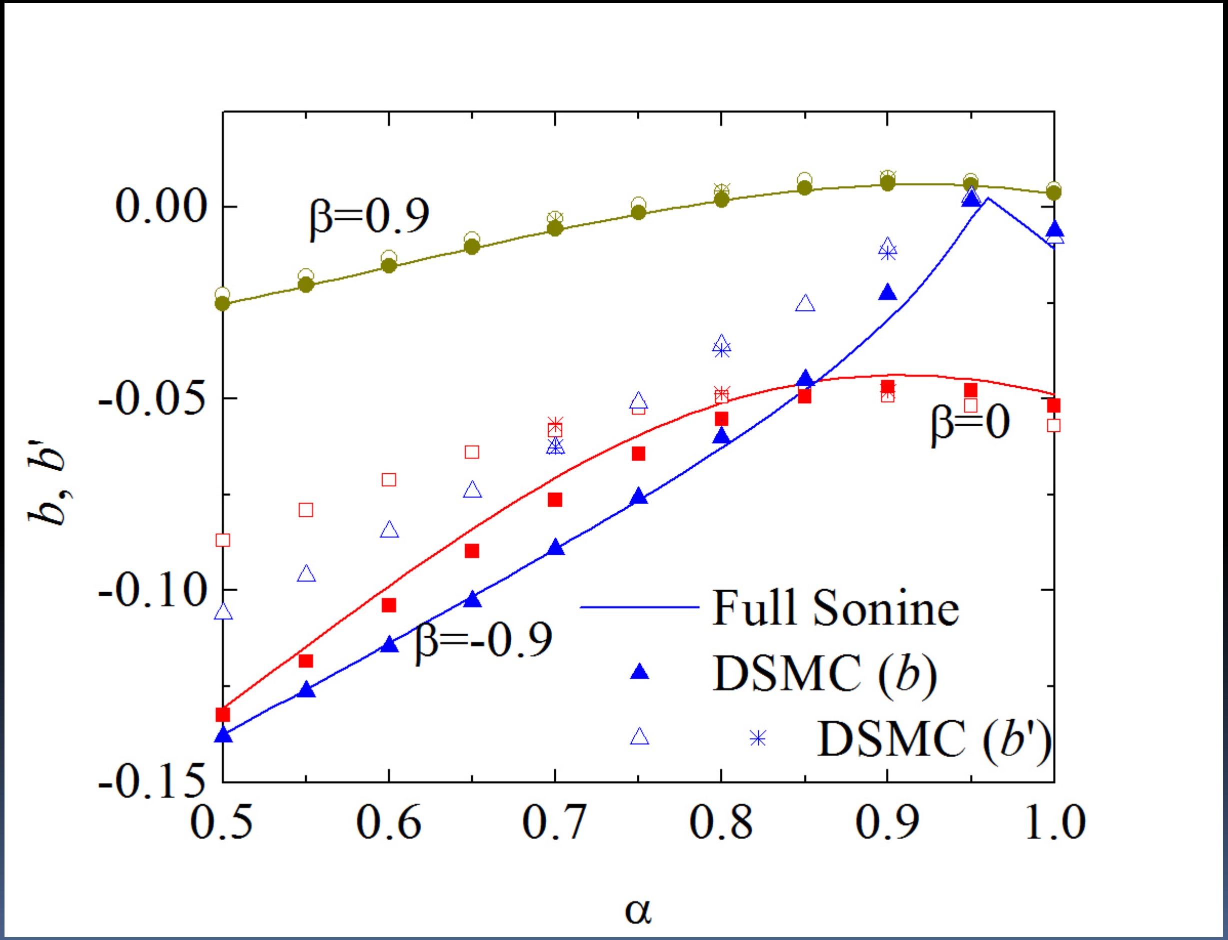


Results: Angular correlations

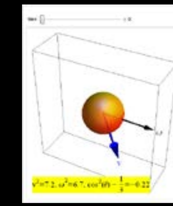
$$\langle(\hat{\mathbf{v}}\cdot\hat{\boldsymbol{\omega}})^2\rangle - \frac{1}{3} = \frac{1}{5}b'$$

$$\langle(\mathbf{c}\cdot\mathbf{w})^2\rangle - \frac{1}{3}\langle c^2 w^2\rangle = \frac{5}{4}b$$

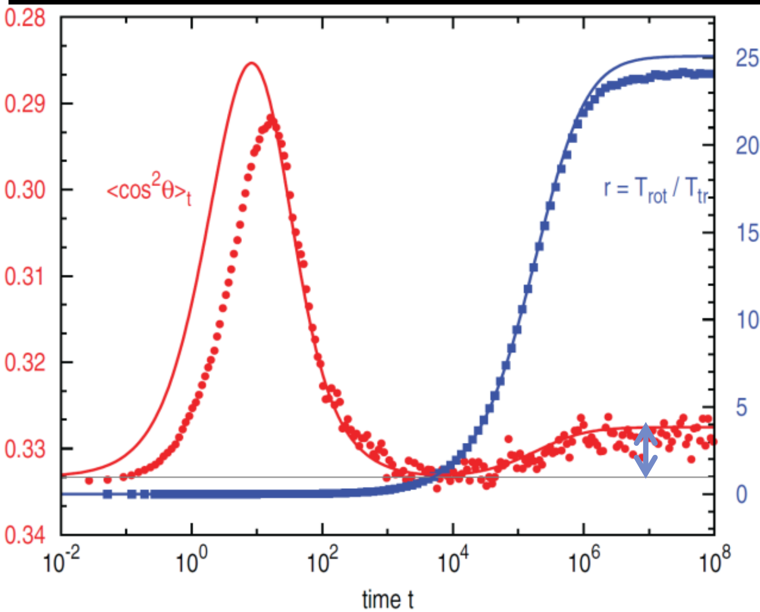




Results: Angular correlations



α=0.8, β=-0.8



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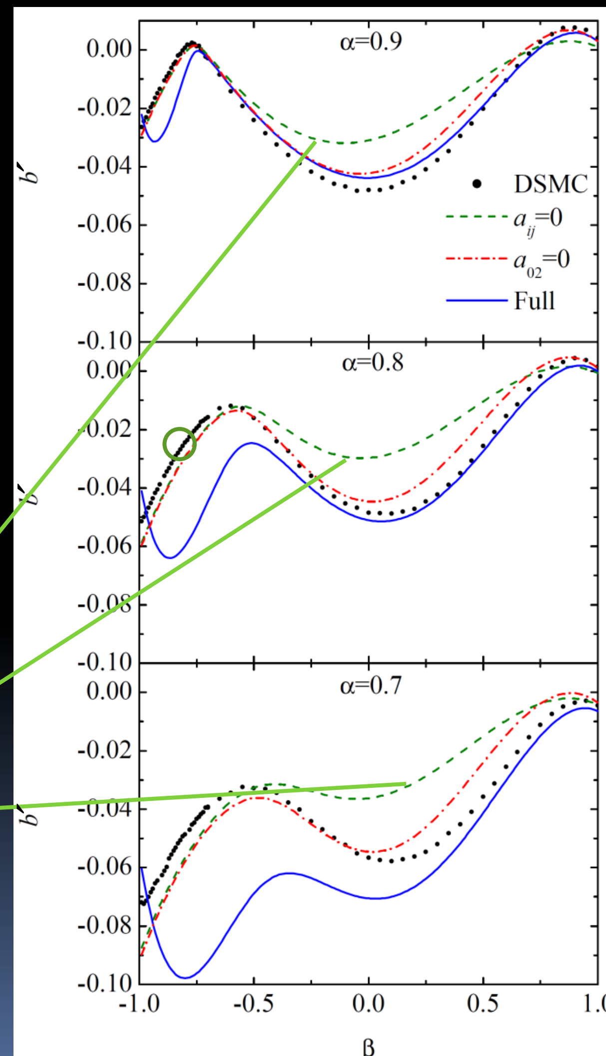
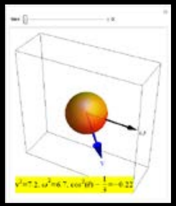
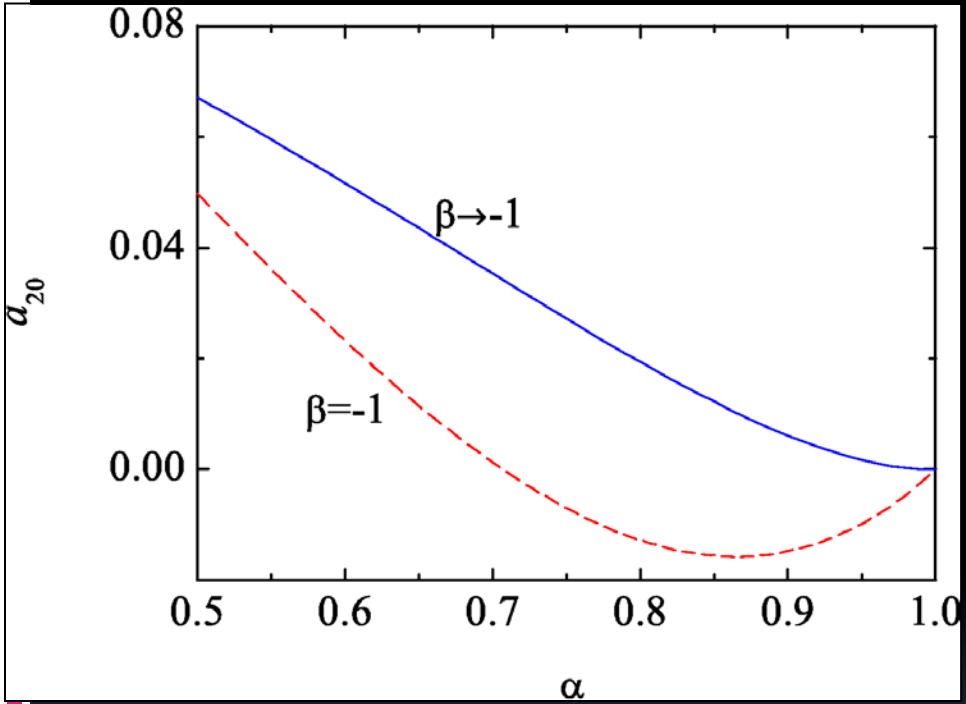
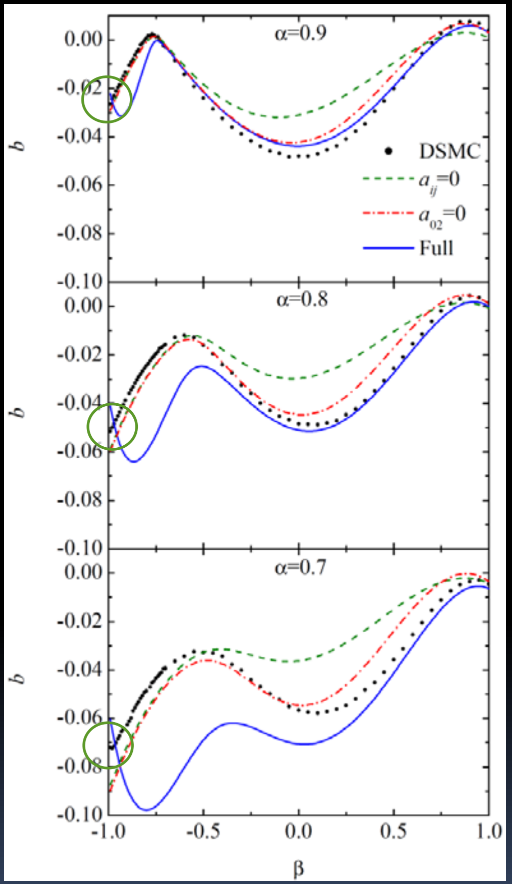


$$\langle (\widehat{\mathbf{v}} \cdot \widehat{\boldsymbol{\omega}})^2 \rangle - \frac{1}{3} = \frac{1}{5} b'$$

Results: Singular behavior in the quasi-smooth limit





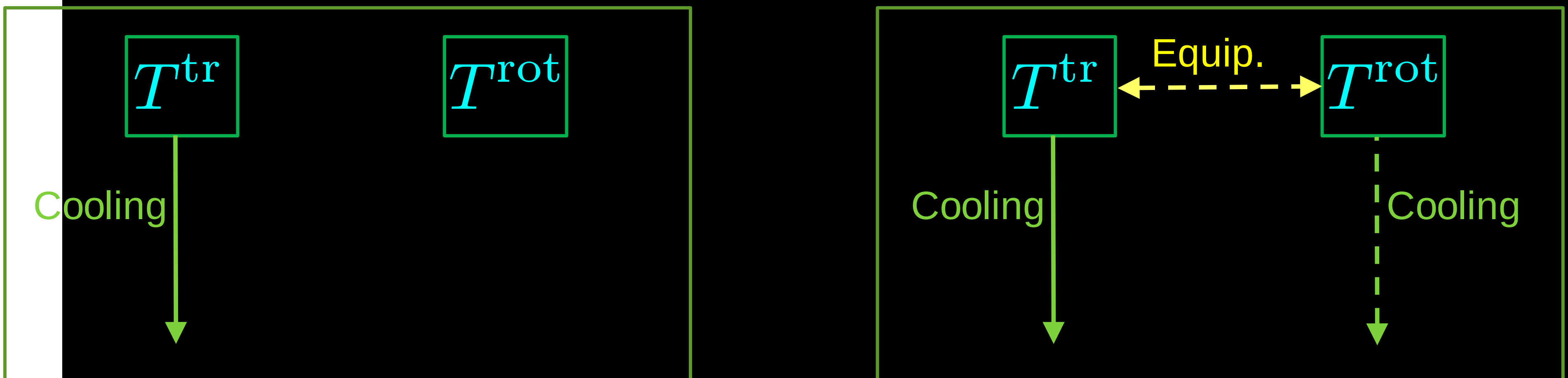


$$\langle v^4\rangle = \frac{5}{3}\langle v^2\rangle^2(1+a_{20})$$

$$\langle(\widehat{\mathbf{v}}\cdot\widehat{\boldsymbol{\omega}})^2\rangle - \frac{1}{3} = \frac{1}{5}b'$$

Origin of this paradoxical singular behavior in the quasi-smooth limit

$\beta = -1$ $\qquad\qquad$ $\beta \gtrsim -1$

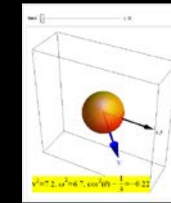


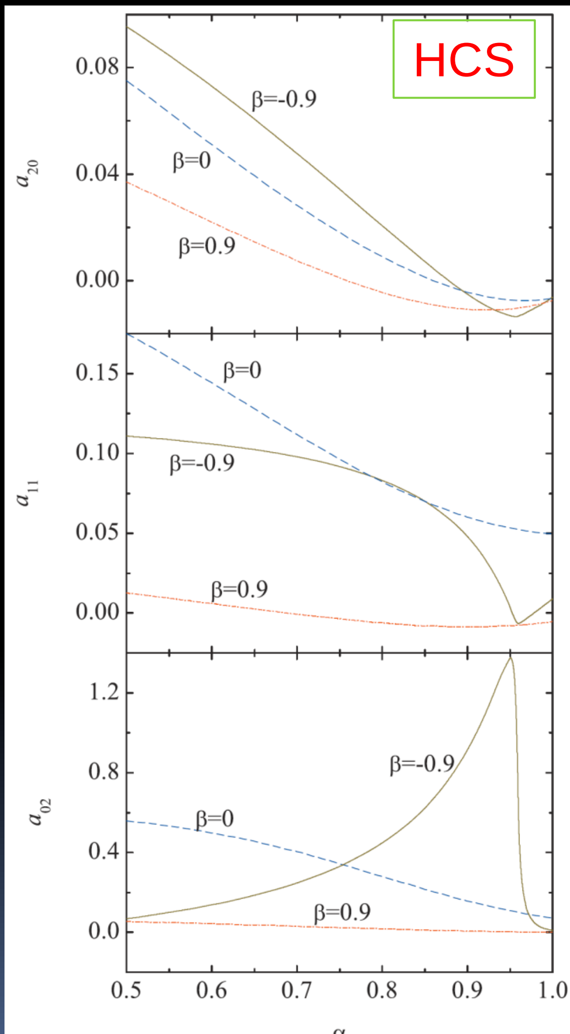
Conclusions and outlook

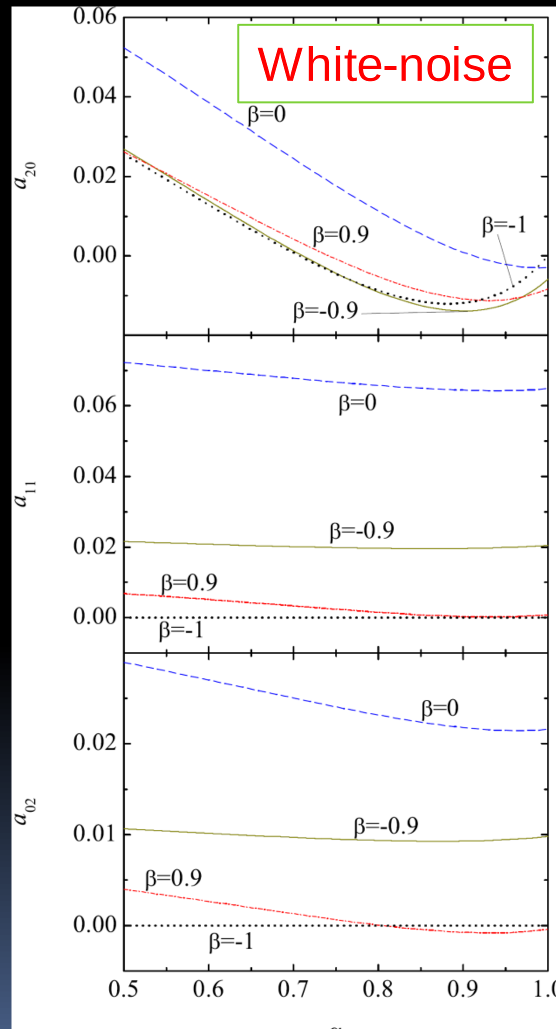
- The Sonine approximation for the temperature ratio successfully corrects the Gaussian prediction.
- While $|a_{20}|$, $|a_{11}|$, and $|b|$ are always small, the cumulant $|a_{02}|$ may take relatively large values, thus invalidating the linear approach (at a quantitative level).
- Comparison with simulation data shows a general good agreement, except perhaps in the cases of a_{02} and b' for weak-medium roughness.
- Interesting singular phenomenon in the quasi-elastic limit.
- Simulations planned for steady states (e.g., white-noise thermostat).

Thank you for your attention!

Results: kurtoses & scalar correlations







$$\langle v^4 \rangle = \frac{5}{3} \langle v^2 \rangle^2 (1 + a_{20})$$

$$\langle \omega^4 \rangle = \frac{5}{3} \langle \omega^2 \rangle^2 (1 + a_{02})$$

$$\langle v^2 \omega^2 \rangle = \langle v^2 \rangle \langle \omega^2 \rangle (1 + a_{11})$$