Can a system of *elastic* hard spheres mimic the transport properties of a granular gas?

A. Astillero and A. Santos
Universidad de Extremadura, Badajoz, Spain

Direct Simulation Monte Carlo: The Past 40 Years and the Future
Politecnico di Milano
June 3, 2003

OUTLINE

I. *Inelastic* hard spheres

II. "Equivalent" system of *elastic* hard spheres

III. Simple shear flow

IV. Applications and extensions

V. Conclusions

I. *Inelastic* hard spheres

- The prototype model for a *granular* medium in the *rapid flow* regime is a gas of *inelastic* hard spheres with a constant coefficient of normal restitution α.

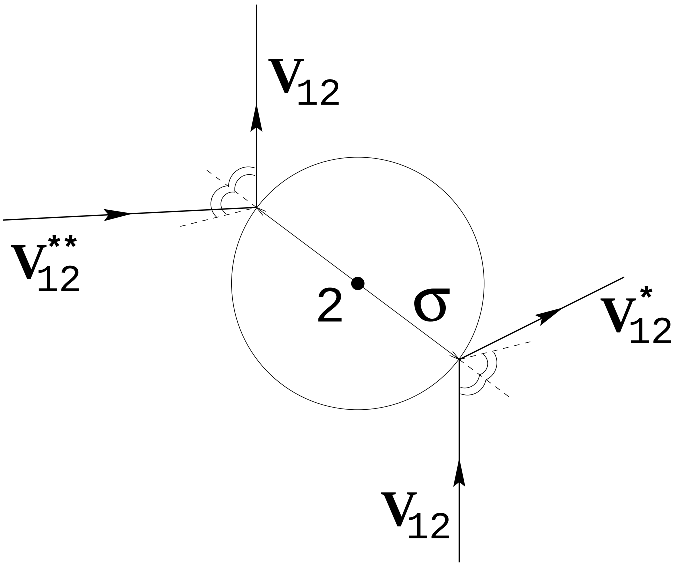

FIG. 1: Sketch of inelastic collisions (after T.P.C. van Noije & M.H. Ernst).

- Direct collision:

$$\left.\begin{array}{l} \widehat{b}\mathbf{v}_1 \equiv \mathbf{v}_1^* = \mathbf{v}_1 - \frac{1+\alpha}{2}\left(\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}}\right)\widehat{\boldsymbol{\sigma}} \\ \widehat{b}\mathbf{v}_2 \equiv \mathbf{v}_2^* = \mathbf{v}_2 + \frac{1+\alpha}{2}\left(\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}}\right)\widehat{\boldsymbol{\sigma}} \end{array}\right\} \Longrightarrow \mathbf{v}_{12}^*\cdot\widehat{\boldsymbol{\sigma}} = -\alpha\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}}$$

- Restituting collision:

$$\left.\begin{array}{l} \widehat{b}^{-1}\mathbf{v}_1 \equiv \mathbf{v}_1^{**} = \mathbf{v}_1 - \frac{1+\alpha^{-1}}{2}\left(\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}}\right)\widehat{\boldsymbol{\sigma}} \\ \widehat{b}^{-1}\mathbf{v}_2 \equiv \mathbf{v}_2^{**} = \mathbf{v}_2 + \frac{1+\alpha^{-1}}{2}\left(\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}}\right)\widehat{\boldsymbol{\sigma}} \end{array}\right\} \Longrightarrow \mathbf{v}_{12}^{**}\cdot\widehat{\boldsymbol{\sigma}} = -\alpha^{-1}\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}}$$

<u>Boltzmann equation</u> (molecular chaos)

$$\left(\partial_t + \mathbf{v}_1 \cdot \nabla\right) f(\mathbf{v}_1) = J^{(\alpha)}[\mathbf{v}_1|f],$$

$$J^{(\alpha)}[\mathbf{v}_1|f] = \sigma^{d-1} \int d\mathbf{v}_2 \int d\widehat{\boldsymbol{\sigma}}\, \Theta(\mathbf{v}_{12} \cdot \widehat{\boldsymbol{\sigma}})(\mathbf{v}_{12} \cdot \widehat{\boldsymbol{\sigma}}) \left(\alpha^{-2}\widehat{b}^{-1} - 1\right) f(\mathbf{v}_1) f(\mathbf{v}_2).$$

- Conservation of mass:

$$m \int d\mathbf{v}\, J^{(\alpha)}[\mathbf{v}|f] = 0.$$

- Conservation of momentum:

$$m \int d\mathbf{v}\, \mathbf{v} J^{(\alpha)}[\mathbf{v}|f] = \mathbf{0}.$$

- Energy decrease (collisional "cooling"):

$$\boxed{\frac{m}{dn} \int d\mathbf{v}\, V^2 J^{(\alpha)}[\mathbf{v}|f] = -\zeta(\alpha) T}, \quad \mathbf{V} \equiv \mathbf{v} - \mathbf{u},$$

$$T = \frac{m}{d}\langle V^2 \rangle\text{: Granular temperature,}$$

$$\zeta(\alpha) \propto (1-\alpha^2)\langle V_{12}^3 \rangle\text{: } \textit{Cooling rate.}$$

- Local equilibrium approximation:

$$\zeta(\alpha) \to \zeta_0(\alpha) = \frac{d+2}{4d} \nu_0 (1-\alpha^2),$$

$$\nu_0 \propto n\sigma^{d-1}(2T/m)^{1/2}\text{: (effective) collision frequency.}$$

II. "Equivalent" system of *elastic* hard spheres

- *Inelastic* hard spheres (IHS):

$$\left.\frac{\partial T}{\partial t}\right|_{\text{coll}} = -\zeta(\alpha)T.$$

- *Elastic* hard spheres (EHS):

$$\left.\frac{\partial T}{\partial t}\right|_{\text{coll}} = 0.$$

But ...

if a drag or friction force $\mathbf{F}_{\text{drag}} = -m\gamma\mathbf{V}$ exists, then

$$\left.\frac{\partial T}{\partial t}\right|_{\text{friction}} = -2\gamma T.$$

- Can a system of EHS with $\gamma = \frac{1}{2}\zeta_0(\alpha) \simeq \frac{1}{2}\zeta(\alpha)$ mimic the properties of a system of IHS?

$$\underbrace{J^{(\alpha)}[\mathbf{v}|f]}_{\text{inelastic collisions}} \to \beta(\alpha) \underbrace{J^{(1)}[\mathbf{v}|f]}_{\text{elastic collisions}} \underbrace{+\frac{1}{2}\zeta_0(\alpha)\frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{V}f)}_{\text{friction}}$$

$\beta(\alpha)$: parameter to modify the collision frequency of EHS relative to that of IHS ($\sigma_{\text{EHS}} \neq \sigma_{\text{IHS}}$).

- Both systems (IHS and EHS+friction) yield the same *hydrodynamic* balance equations (except for the approximation $\zeta \to \zeta_0$).

  However, the *microscopic* dynamics is quite different.

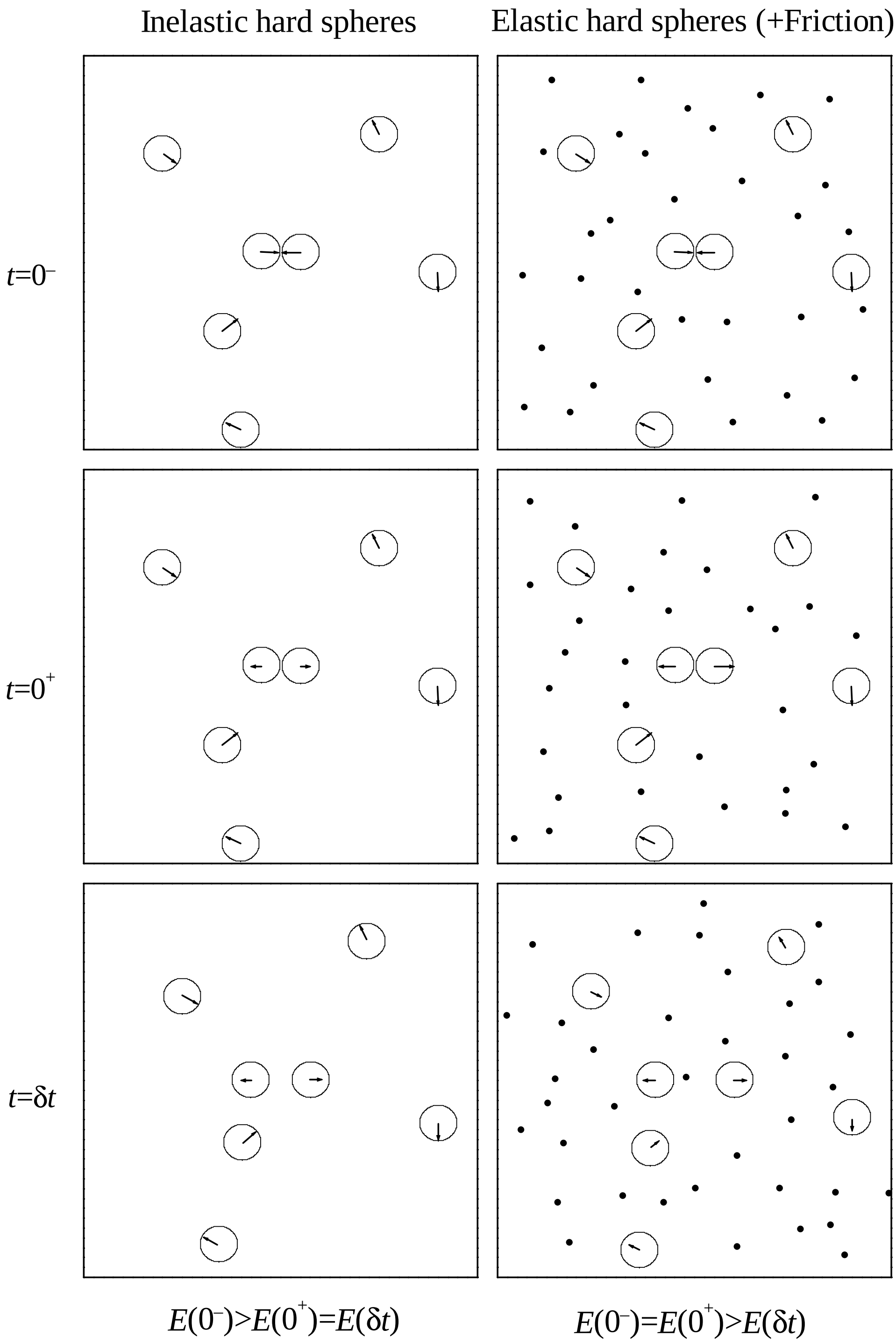

FIG. 2: Sketch of IHS and EHS

Homogeneous cooling state

- Haff's law:

$$T = \frac{T_0}{\left(1 + \frac{1}{2}\zeta_{t=0}t\right)^2}.$$

- Scaling solution:

$$f^*(\mathbf{c}) = \frac{1}{n}\left(\frac{2T}{m}\right)^{d/2} f(\mathbf{v}), \quad \mathbf{c} = \mathbf{v}/(2T/m)^{1/2}.$$

- EHS:

$$f^*(\mathbf{c}) = \pi^{-d/2}e^{-c^2}.$$

- IHS:

$$f^*(\mathbf{c}) \neq \pi^{-d/2}e^{-c^2},$$

$$\text{second cumulant (kurtosis): } a_2 \equiv \frac{4}{d(d+2)}\langle c^4\rangle - 1 \neq 0,$$

$$\text{high energy tail: } f^*(\mathbf{c}) \sim e^{-Ac} \Rightarrow G(\mathbf{c}) \equiv e^{Ac}f^*(\mathbf{c}) \to \text{const.}$$

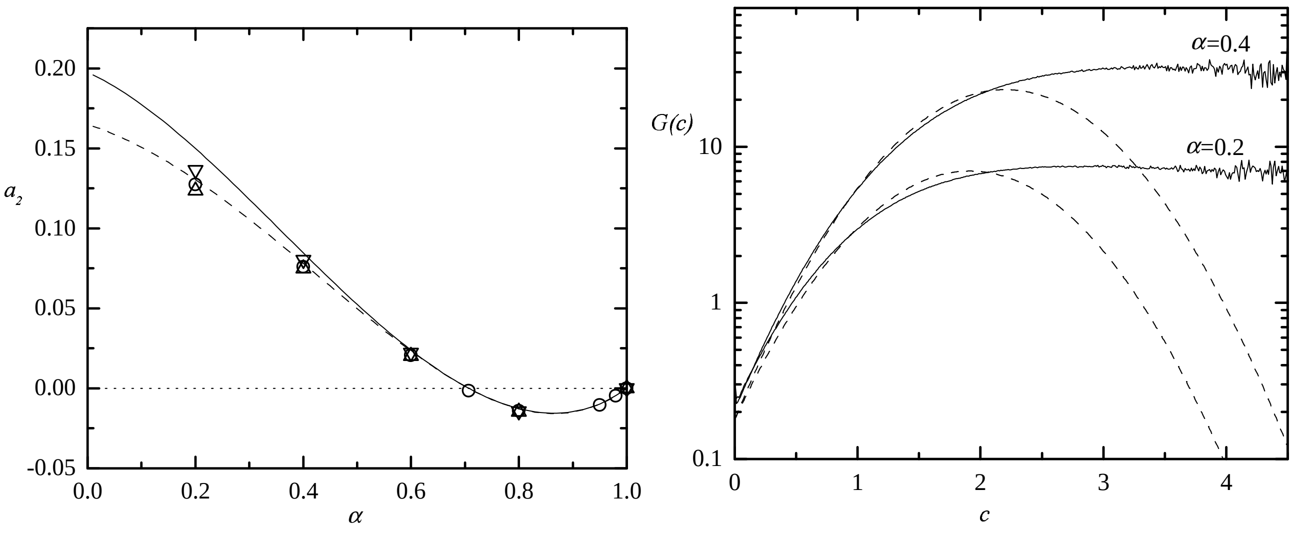

FIG. 3: $d = 3$ [J. M. Montanero & A.S., Gran. Matt. **2**, 53 (2000)]

- What happens in *inhomogeneous* states?

Transport coefficients (Chapman–Enskog method)

- So far, $\beta(\alpha)$ remains undetermined.
- A comparison between the transport coefficients for IHS and EHS shows that the optimal choice for the *shear viscosity* is

$$\beta(\alpha) = \frac{1+\alpha}{2}\left[1 - \frac{d-1}{2d}(1-\alpha)\right] \equiv \beta_\eta(\alpha),$$

while the optimal choice for the *thermal conductivity* is

$$\beta(\alpha) = \frac{1+\alpha}{2}\left[1 + \frac{3}{8}\frac{4-d}{d-1}(1-\alpha)\right] \equiv \beta_\kappa(\alpha).$$

- This suggests to take

$$\boxed{\beta(\alpha) = \frac{1+\alpha}{2}}$$

as the *simplest* choice.

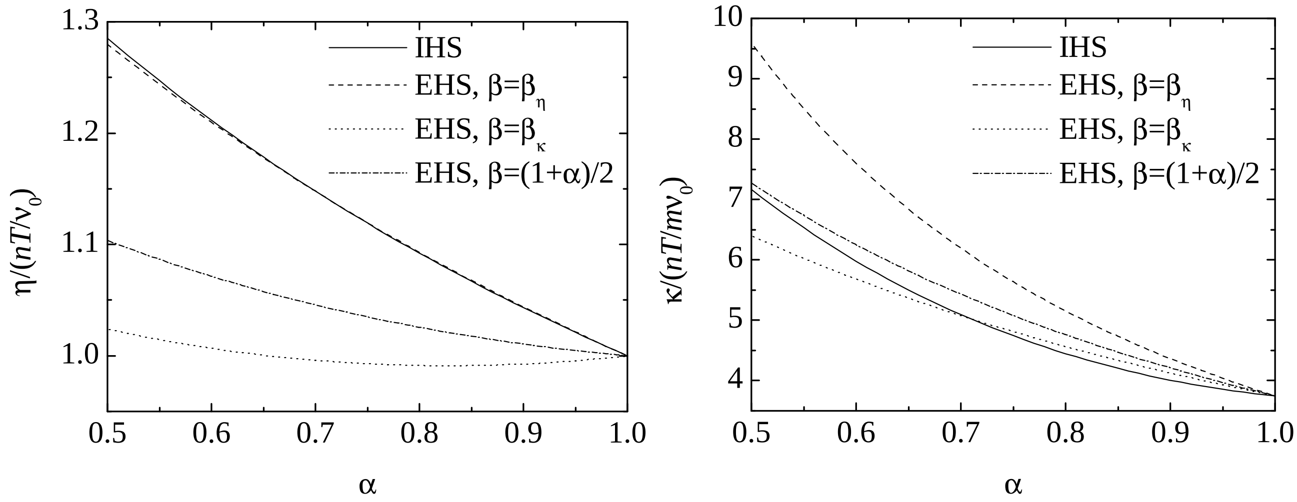

FIG. 4: Shear viscosity and thermal conductivity ($d = 3$).

III. Simple shear flow

- Steady state:

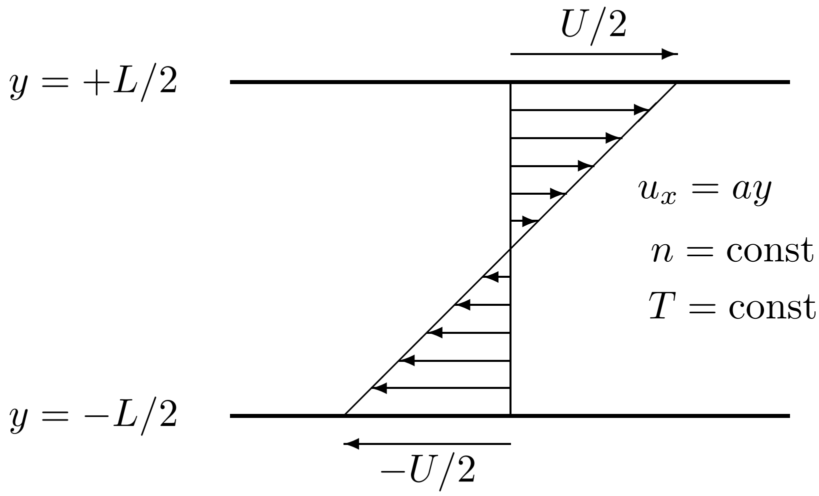

FIG. 5: Sketch of the simple shear flow

$$a = \frac{U}{L} = \text{(constant) shear rate.}$$

- Energy balance equation:

$$\frac{\partial}{\partial t}T = \underbrace{-\frac{2}{d}aP_{xy}}_{\text{viscous heating}} + \underbrace{(-\zeta T)}_{\text{inelastic cooling (or friction)}} = 0,$$

$$P_{ij} = mn\langle V_i V_j \rangle\text{: pressure tensor.}$$

- Test case:

$$d = 3,$$

$$a = 4\tau_0^{-1}, \quad \tau_0 = \text{initial m.f.t. of the IHS gas,}$$

$$L = 2.5\lambda, \quad \lambda = \text{average m.f.p. of the IHS gas,}$$

$$U = aL = 10v_0, \quad v_0 = \lambda/\tau_0 = \text{initial thermal velocity}$$

- Initial conditions:
  - *Total* equilibrium.
  - *Local* equilibrium.

- DSMC details:

$$N = 10^4 \text{ particles},$$

$$50 \text{ layers} \Rightarrow \Delta L = 0.05\lambda$$

$$\text{Time step: } \delta t = 10^{-3}\tau_0\sqrt{T_0/T}$$

- IHS: Inelastic collisions with $\alpha = 0.9$.
- EHS: Elastic collisions (rate reduced by a factor $\beta = \frac{1+\alpha}{2} = 0.95$) + Friction.

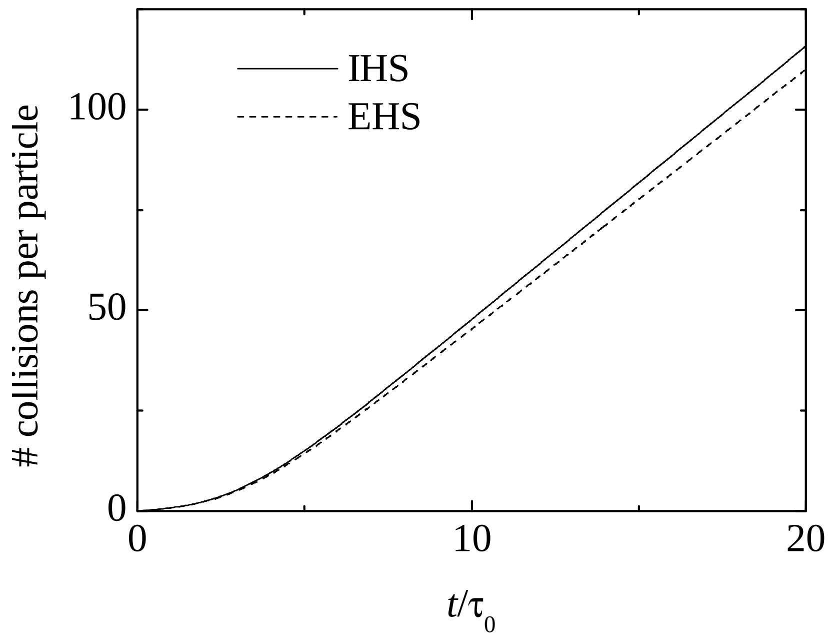

FIG. 6: Number of collisions per particle

• Initial condition: Total equilibrium

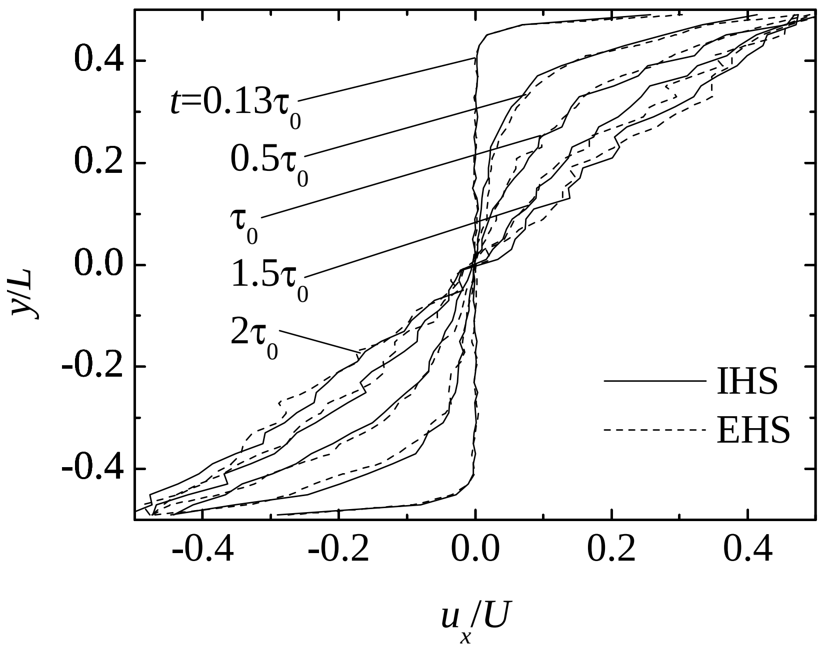

FIG. 7: Velocity profiles.

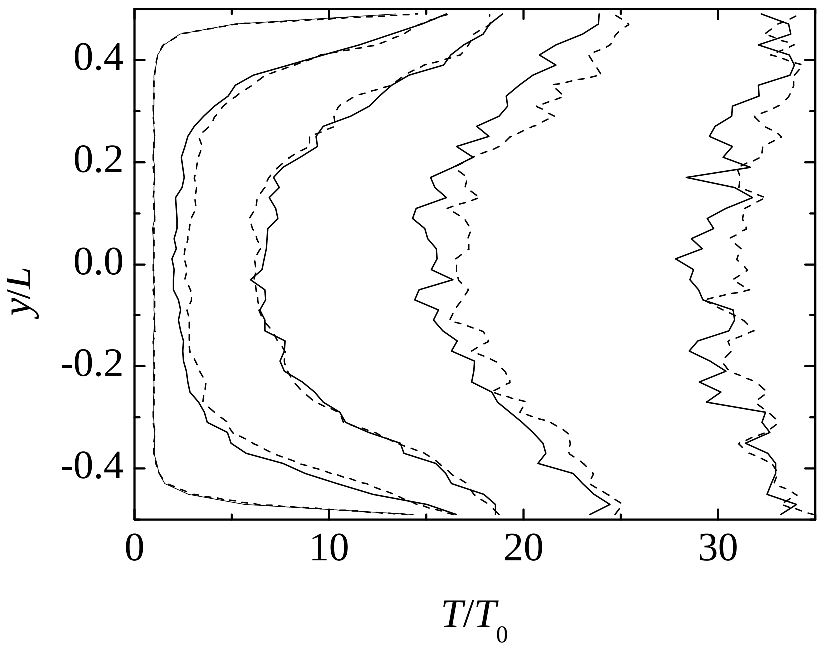

FIG. 8: Temperature profiles.

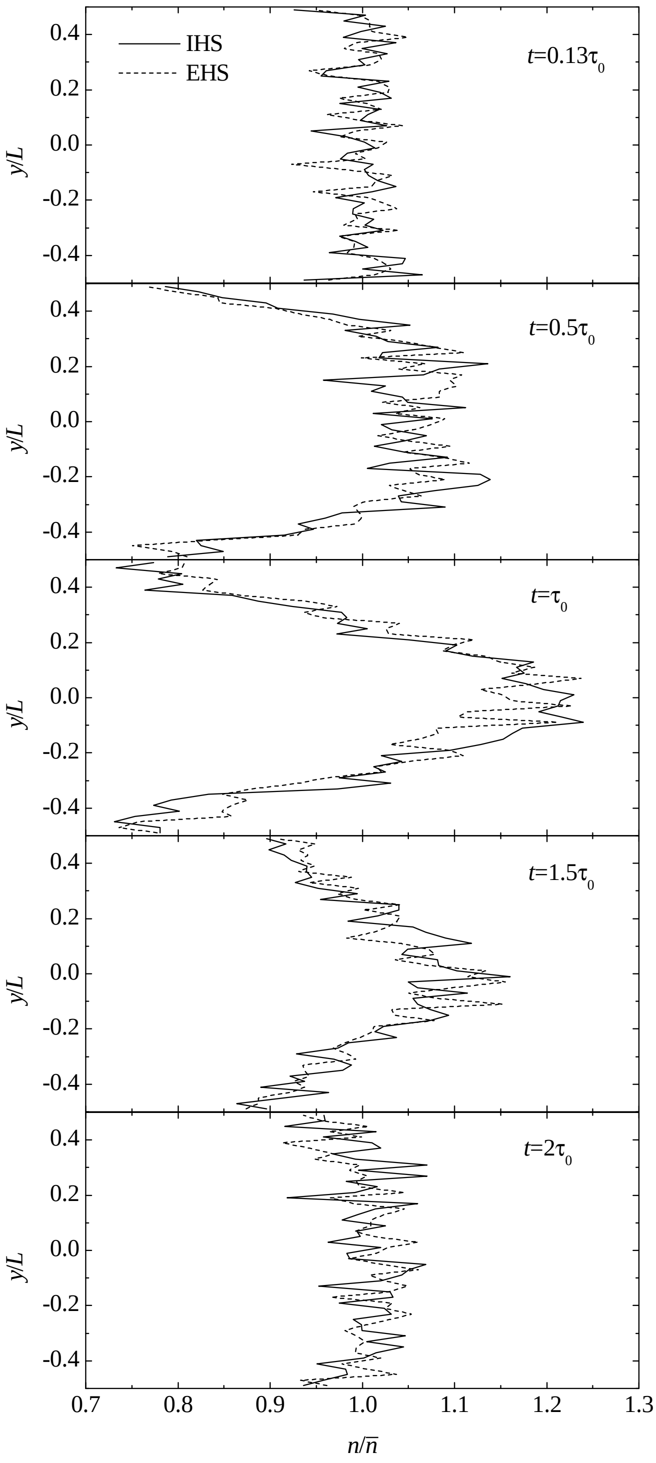

FIG. 9: Density profiles.

• Initial condition: Local equilibrium

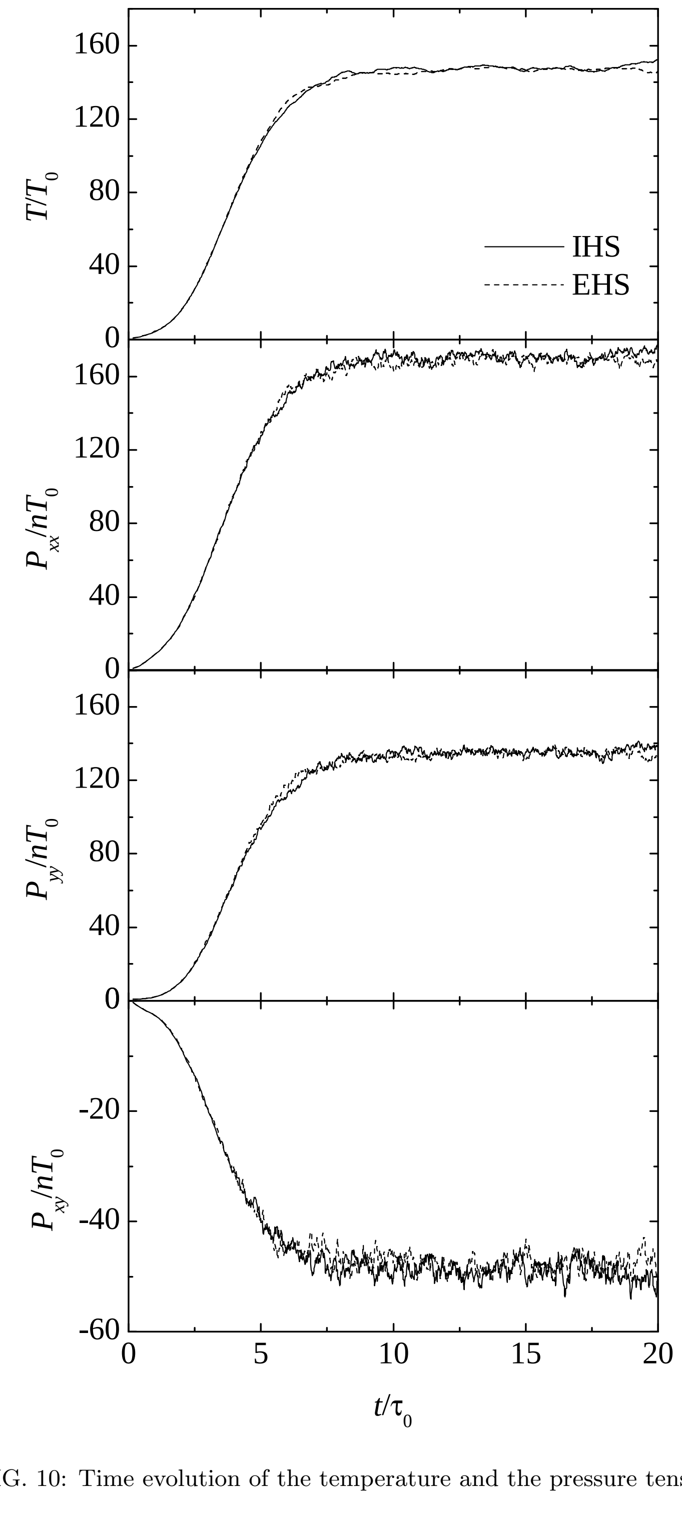

FIG. 10: Time evolution of the temperature and the pressure tensor.

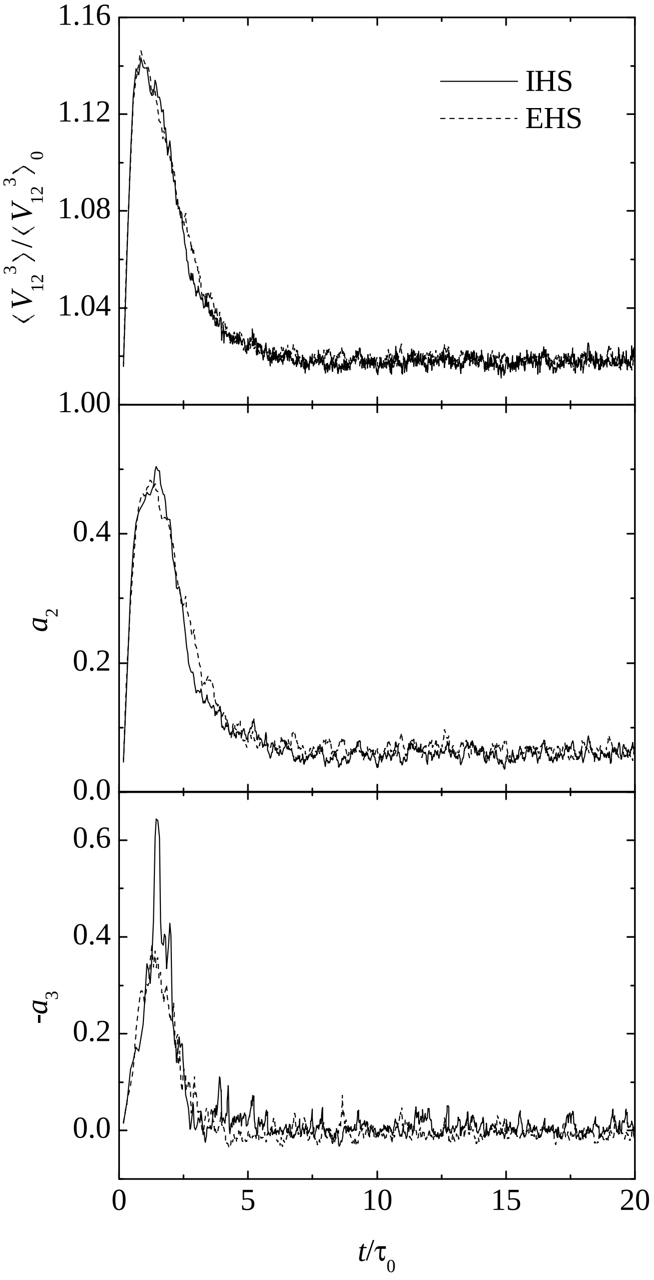

FIG. 11: Time evolution of $\langle V_{12}^3\rangle/\langle V_{12}^3\rangle_0$, and the second and third cumulants.

$$a_2 = \frac{4}{15}\langle C^4\rangle - 1, \quad -a_3 = \frac{8}{105}\langle C^4\rangle - 1 - 3a_2.$$

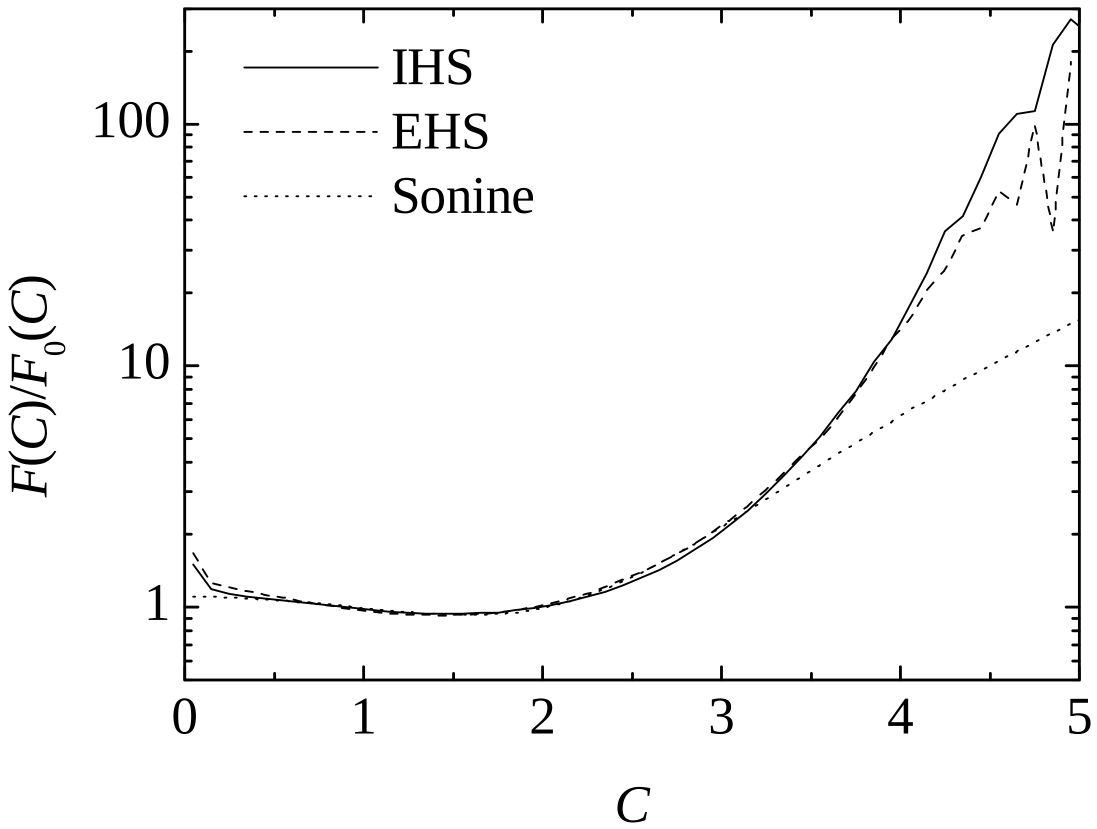

FIG. 12: Steady-state distribution function for the magnitude of $\mathbf{C} = \mathbf{V}/\sqrt{2T/m}$.

$$F(C) = C^2 \int \mathrm{d}\widehat{\mathbf{C}}\, f^*(\mathbf{C}), \quad F_0(C) = 4\pi^{-1/2} C^2 e^{-C^2}.$$

IV. Applications and extensions

Kinetic modeling

- The mapping IHS↔EHS allows one to extend to granular gases those kinetic models originally proposed for conventional gases.
- Bhatnagar–Gross–Krook (BGK) model:

$$J^{(1)}[\mathbf{v}|f] \to -\nu_0[f(\mathbf{v}) - f_0(\mathbf{v})], \quad f_0(\mathbf{v}) = n\left(\frac{m}{2\pi T}\right)^{d/2} \exp\left(-\frac{mV^2}{2T}\right),$$

$$\boxed{(\partial_t + \mathbf{v}\cdot\nabla) f(\mathbf{v}) = -\beta(\alpha)\nu_0[f(\mathbf{v}) - f_0(\mathbf{v})] + \frac{1}{2}\zeta_0(\alpha)\frac{\partial}{\partial \mathbf{v}}\cdot[\mathbf{V}f(\mathbf{v})]}.$$

[J.J. Brey, J.W. Dufty & A.S., J. Stat. Phys. **97**, 281 (1999).]

However, Prandtl number in the elastic limit: $\mathrm{Pr} = 1 \neq \frac{d-1}{d}$.

- Ellipsoidal statistical (ES) model:

$$(\partial_t + \mathbf{v}\cdot\nabla) f(\mathbf{v}) = -\beta(\alpha)\frac{d-1}{d}\nu_0[f(\mathbf{v}) - f_R(\mathbf{v})] + \frac{1}{2}\zeta_0(\alpha)\frac{\partial}{\partial \mathbf{v}}\cdot[\mathbf{V}f(\mathbf{v})],$$

$$f_R(\mathbf{v}) = n\left(\frac{mn}{2\pi}\right)^{d/2}(\det \mathsf{R})^{-1/2}\exp\left(-\frac{mn}{2}\mathsf{R}^{-1}:\mathbf{V}\mathbf{V}\right),$$

$$R_{ij} = \frac{d}{d-1}p\,\delta_{ij} - \frac{1}{d-1}P_{ij}.$$

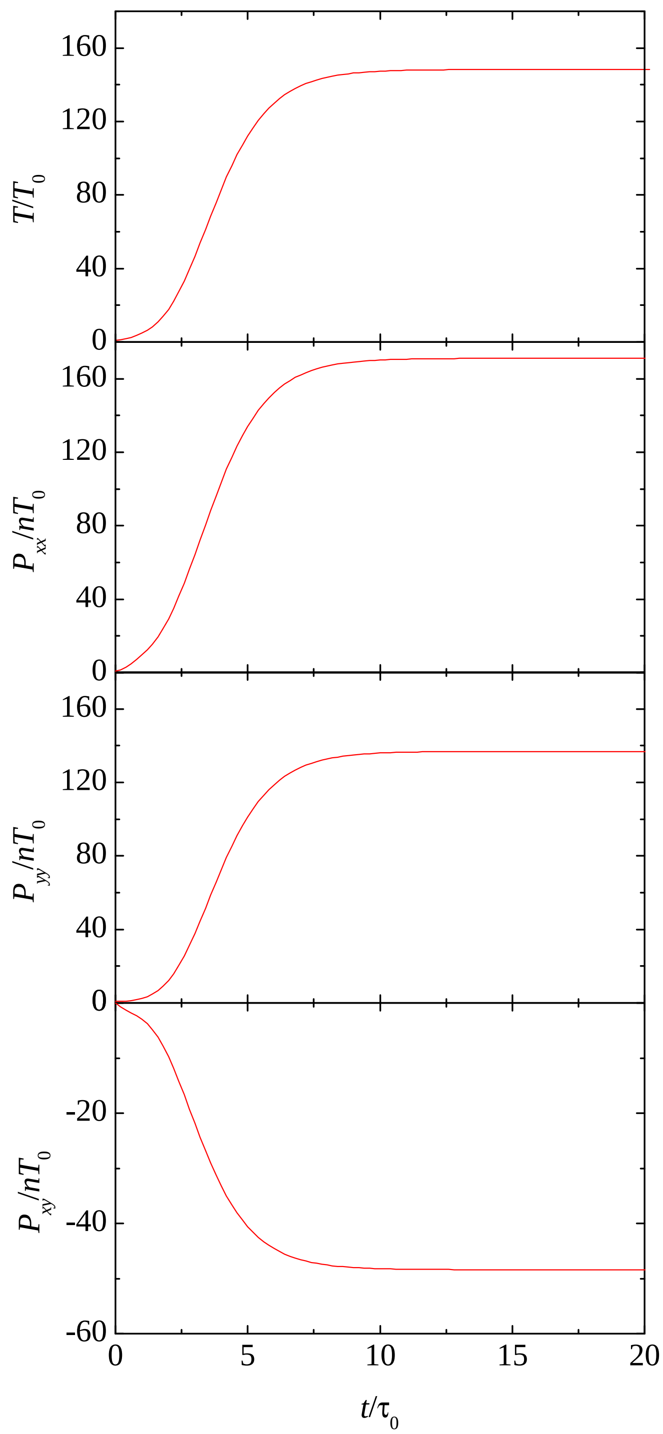

FIG. 13: Time evolution of the temperature and the pressure tensor.

Mixtures

- Boltzmann equation:

$$(\partial_t + \mathbf{v}_1 \cdot \nabla)\, f_i(\mathbf{v}_1) = \sum_j J_{ij}^{(\alpha_{ij})}[\mathbf{v}_1|f_i, f_j],$$

$$J_{ij}^{(\alpha_{ij})}[\mathbf{v}_1|f_i, f_j] = \sigma^{d-1} \int \mathrm{d}\mathbf{v}_2 \int \mathrm{d}\widehat{\boldsymbol{\sigma}}\, \Theta(\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}})(\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}}) \left(\alpha_{ij}^{-2}\widehat{b}_{ij}^{-1} - 1\right) f_i(\mathbf{v}_1) f_j(\mathbf{v}_2),$$

$$\left.\begin{array}{l} \widehat{b}_{ij}\mathbf{v}_1 = \mathbf{v}_1 - \mu_{ji}(1+\alpha_{ij})(\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}})\widehat{\boldsymbol{\sigma}} \\ \widehat{b}_{ij}\mathbf{v}_2 = \mathbf{v}_2 + \mu_{ij}(1+\alpha_{ij})(\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}})\widehat{\boldsymbol{\sigma}} \end{array}\right\} \Longrightarrow \widehat{b}_{ij}\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}} = -\alpha_{ij}\mathbf{v}_{12}\cdot\widehat{\boldsymbol{\sigma}},$$

$$\mu_{ij} \equiv \frac{m_i}{m_i + m_j}.$$

- “Equivalent” system of elastic particles:

$$\underbrace{J_{ij}^{(\alpha_{ij})}[\mathbf{v}|f_i, f_j]}_{\text{inelastic collisions}} \to \beta_{ij}(\alpha_{ij})\, \underbrace{J_{ij}^{(1)}[\mathbf{v}_1|f_i, f_j]}_{\text{elastic collisions}} + \underbrace{\frac{1}{2}\zeta_{ij}(\alpha_{ij})\frac{\partial}{\partial\mathbf{v}}\cdot\left[(\mathbf{v}-\mathbf{u}_i)\, f_i(\mathbf{v})\right]}_{\text{friction}}$$

- Simplest choice:

$$\beta_{ij}(\alpha_{ij}) = \frac{1+\alpha_{ij}}{2},$$

$$\zeta_{ij}(\alpha_{ij}) = \frac{d+2}{4d}\nu_{ij}(1-\alpha_{ij}^2),$$

$$\nu_{ij} \propto n_j \mu_{ji}^2 \sigma_{ij}^{d-1} \left(\frac{2T_i}{m_i}\right)^{1/2} \left(1 + \frac{m_i T_j}{m_j T_i}\right)^{3/2}.$$

- This choice preserves the collision integrals

$$\int \mathrm{d}\mathbf{v} \left\{ \begin{array}{c} \mathbf{v} \\ v^2 \end{array} \right\} J_{ij}^{(\alpha_{ij})}[\mathbf{v}|f_i, f_j]$$

  in the (multi-temperature) local equilibrium approximation.

- As before, kinetic models (e.g. Gross–Krook, Garzó–Santos–Brey, Andries–Aoki–Perthame, …) for *elastic* mixtures can be extended to *inelastic* mixtures.

V. Conclusions

- A system of elastic hard spheres with a friction force succeeds in capturing the main nonequilibrium *transport* properties of a granular gas (at least in a coarse-grained way).

- To disguise as a granular gas, the elastic particles must reduce their collision rate by a factor $\beta(\alpha)$.

  This is equivalent to assume that the EHS have a size smaller than the IHS: $\sigma_{\text{EHS}} = \beta^{1/(d-1)}\sigma_{\text{IHS}}$.

- It is sufficient to take

  $$\beta(\alpha) = \frac{1+\alpha}{2}$$

  and the *local equilibrium* approximation

  $$\gamma = \frac{1}{2}\zeta_0(\alpha).$$

- Of course, the "equivalent" system of EHS is unable to retain finer details of the true system of IHS (e.g., high energy tails, velocity correlations,...).

- Further work:
  - Study of other nonequilibrium states.
  - Extension to *dense* granular gases (Enskog equation).