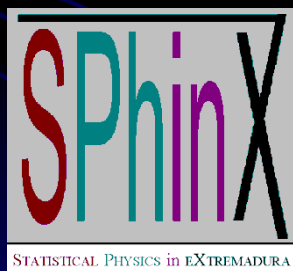
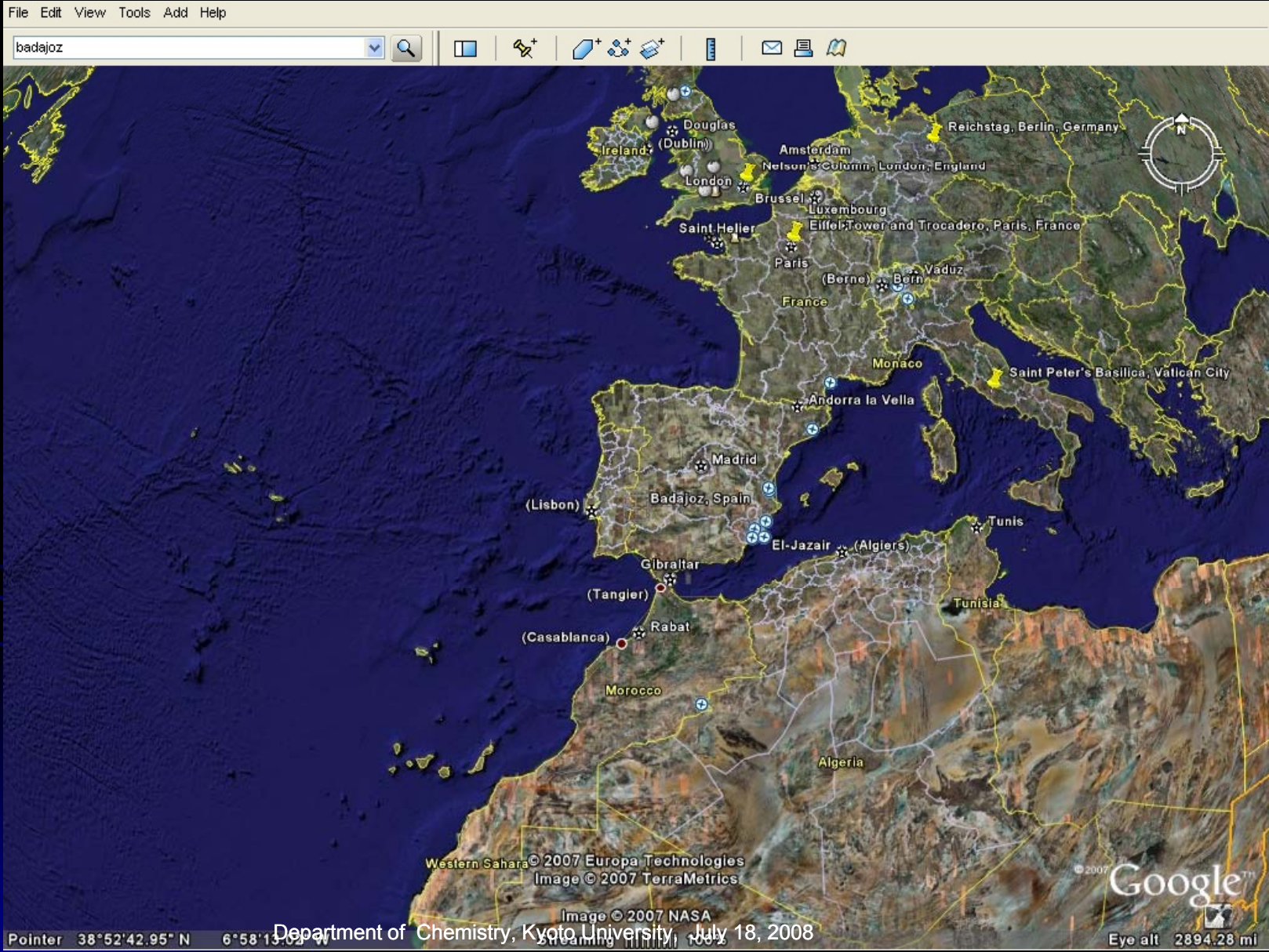


Hydrodynamics for granular gases beyond Navier-Stokes

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October 2003



Department of Chemistry, Kyoto University, July 18, 2008

Outline

- What is a granular material?
- A gas of inelastic hard spheres. The Boltzmann equation.
- Is hydrodynamics applicable to granular gases?
- A case study: The uniform shear flow.
- Does the Chapman-Enskog expansion converge?
- Conclusions.

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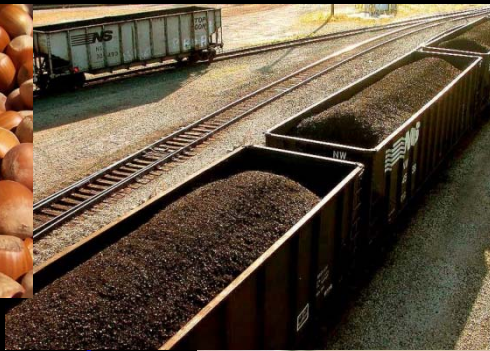
What is a granular material?

- 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 $1\ \mu\text{m}$.



What is a granular material?

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



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).

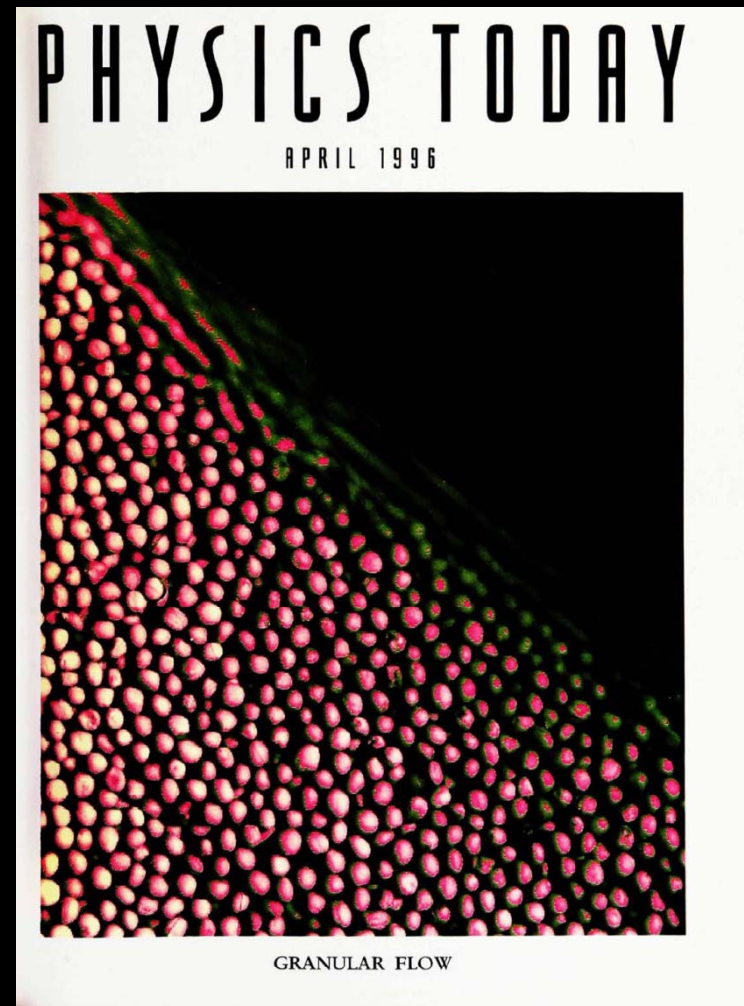


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What is a granular *fluid*?

- 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*.



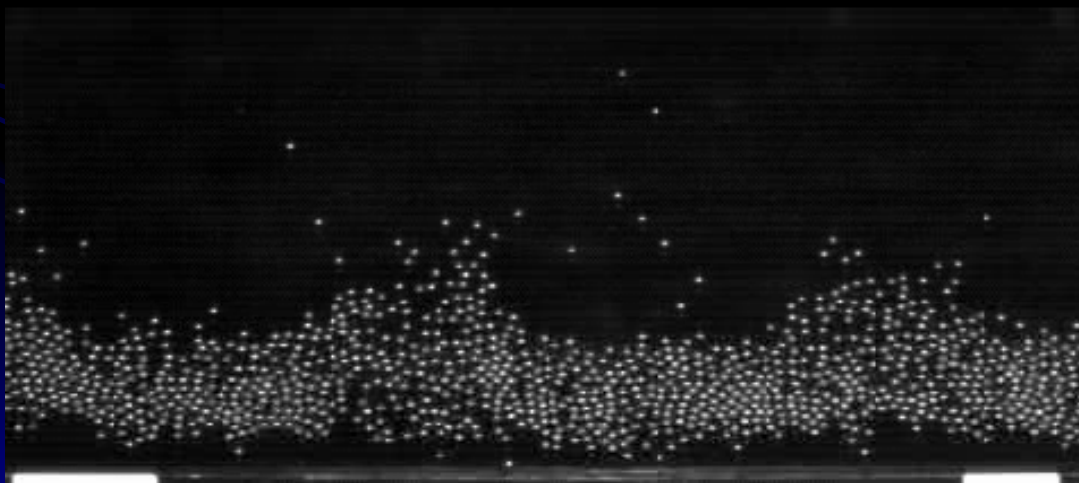
Granular fluids (or gases) exhibit many interesting phenomena:



Granular eruptions
(from University of Twente's
group)

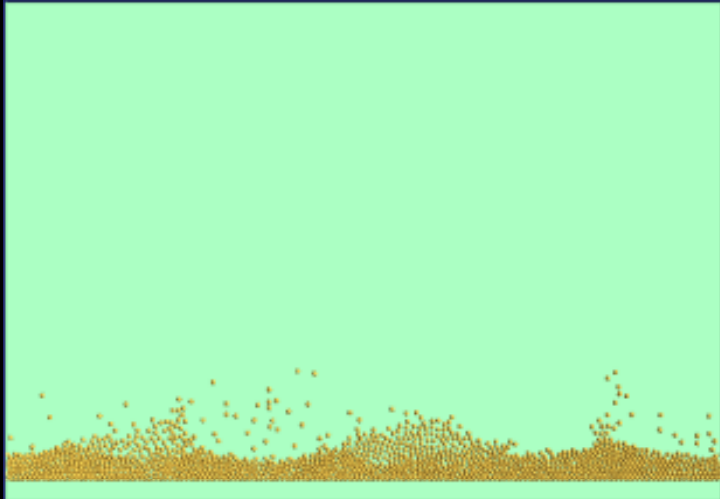


Clustering of dipolar magnetized particles in a vibrated container
(from A. Kudrolli's group)

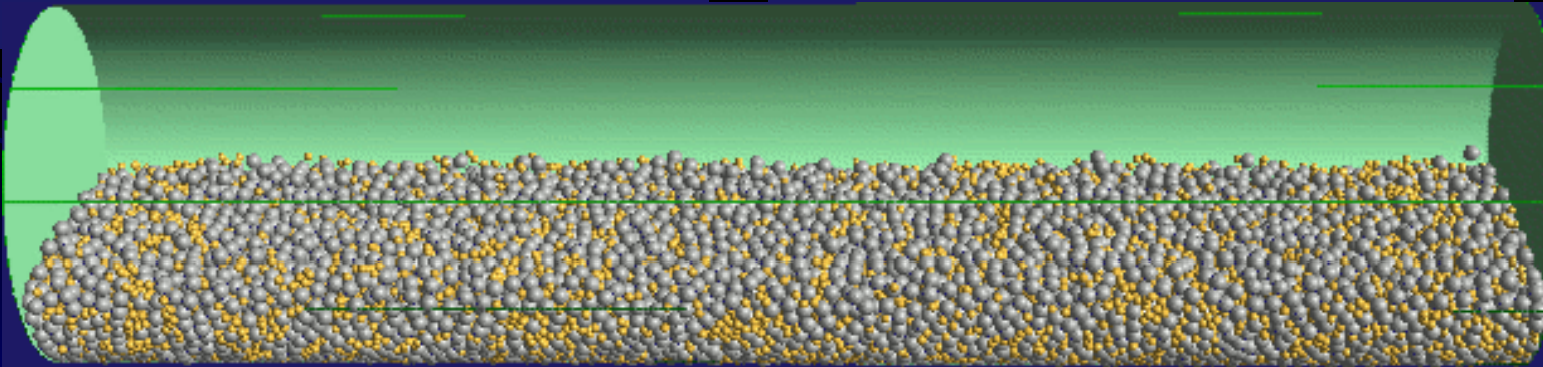
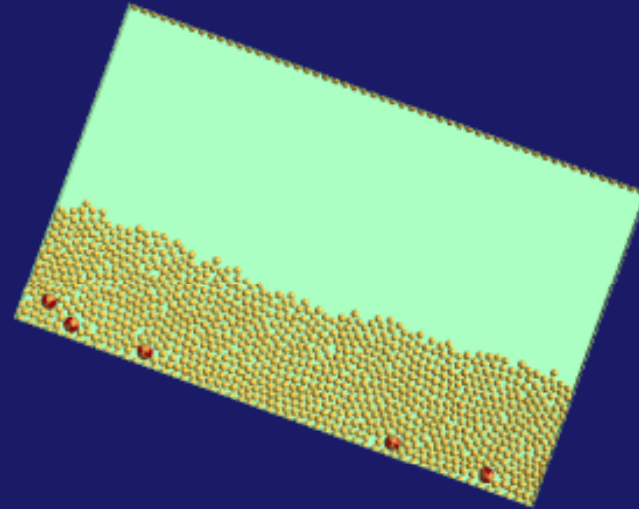


Wave patterns in a vibrated container
(from A. Kudrolli's group)

Wave patterns in a vibrated container
(Simulations by D. C. Rapaport)



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



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

Outline

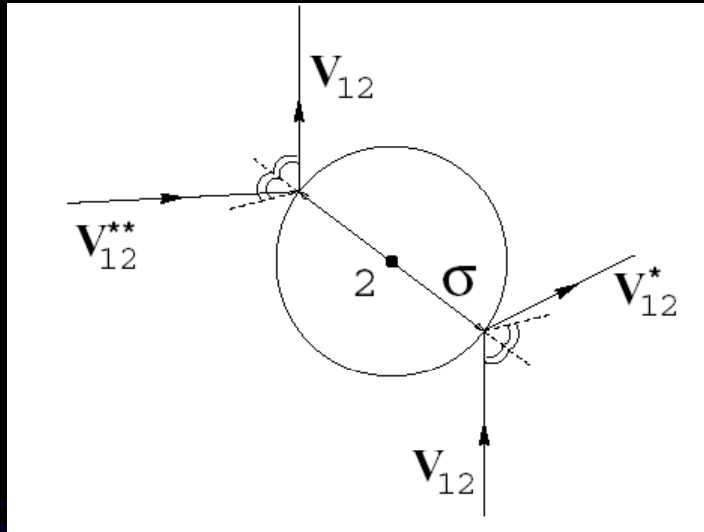
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Minimal model of a granular gas: A gas of (smooth) *inelastic* hard spheres



Several circles
(Kandinsky, 1926)

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



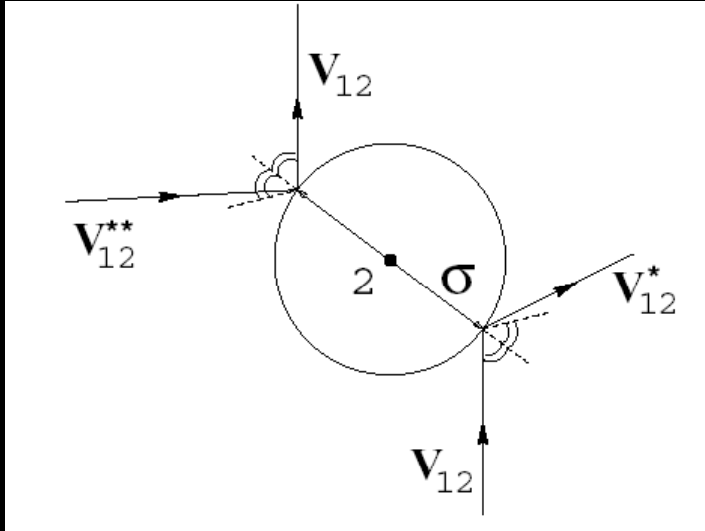
- Mass m
- Diameter σ
- Coefficient of normal restitution α
- $\alpha=1$ for elastic collisions

(After T.P.C. van Noije & M.H. Ernst)

Relative velocity

$$\text{Direct collision: } \mathbf{v}_1^* = \mathbf{v}_1 - \frac{1 + \alpha}{2} (\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}, \quad \mathbf{v}_2^* = \mathbf{v}_2 + \frac{1 + \alpha}{2} (\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}$$

$$\text{Restituting collision: } \mathbf{v}_1^{**} = \mathbf{v}_1 - \frac{1 + \alpha}{2\alpha} (\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}, \quad \mathbf{v}_2^{**} = \mathbf{v}_2 + \frac{1 + \alpha}{2\alpha} (\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}$$



Collisions conserve momentum, but not kinetic energy:

$$\begin{aligned}\Delta E &= \frac{1}{2}m(v_1^{*2} + v_2^{*2} - v_1^2 - v_2^2) \\ &= -\frac{m}{2}(1 - \alpha^2)(\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}})^2\end{aligned}$$

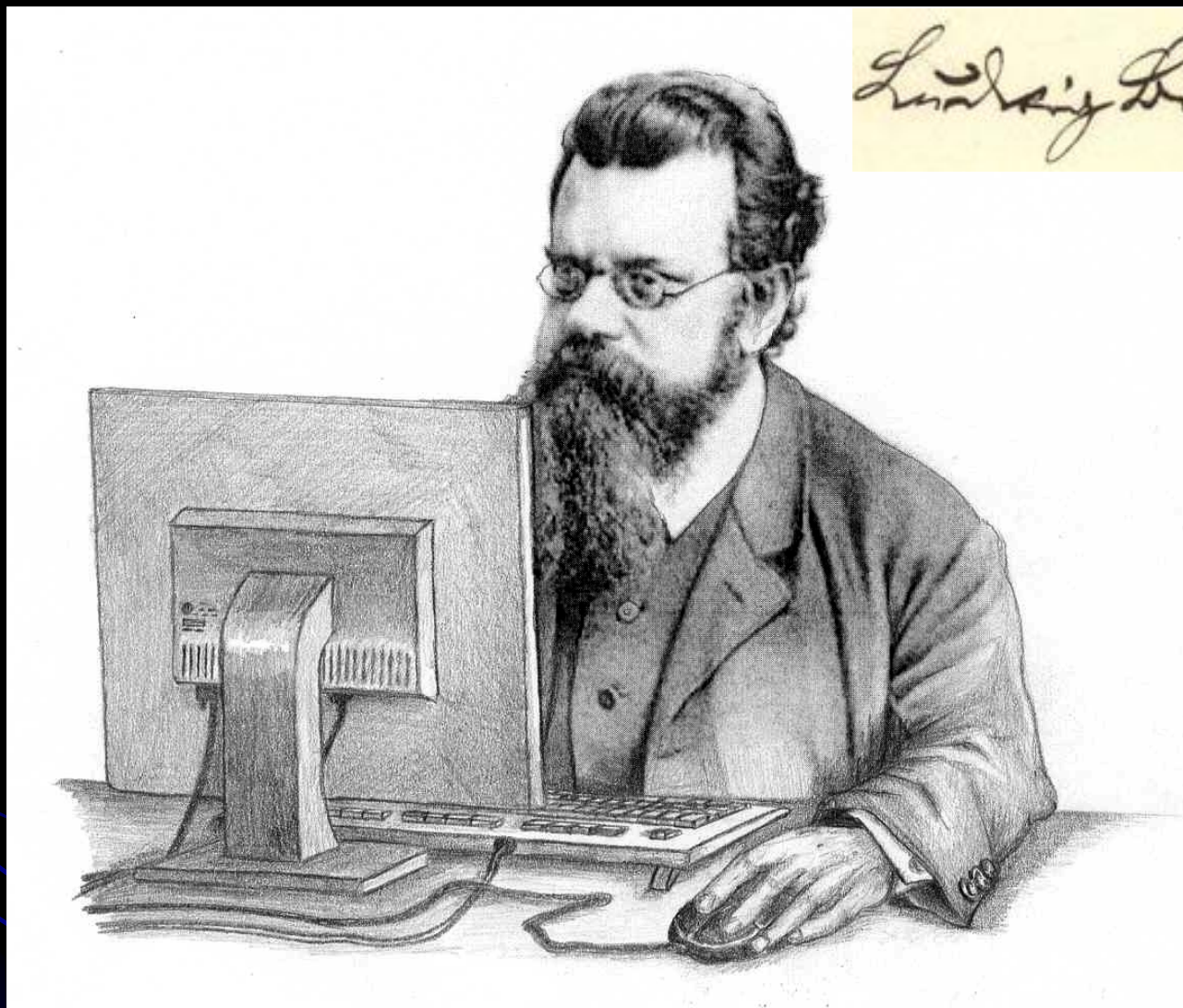
“Granular” temperature: $T = \frac{m}{3} \langle (\mathbf{v} - \mathbf{u})^2 \rangle$, $\mathbf{u} = \langle \mathbf{v} \rangle$

$$\left. \frac{\partial T}{\partial t} \right|_{\text{coll}} = -\zeta T, \quad \zeta \propto 1 - \alpha^2$$

“Cooling” rate

Kinetic theory description

- Velocity distribution function:
- $f(\mathbf{r}, \mathbf{v}, t) d\mathbf{r} d\mathbf{v}$: Average number of particles that at time t are located between \mathbf{r} and $\mathbf{r}+d\mathbf{r}$ and move with velocities between \mathbf{v} and $\mathbf{v}+d\mathbf{v}$.
- Closed equation for f : Boltzmann equation.



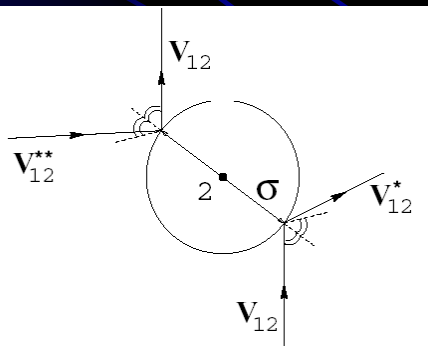
(1844-1906)

(Cartoon by Bernhard Reischl, University of Vienna)

Boltzmann equation (inelastic collisions)

$$\partial_t f + \mathbf{v}_1 \cdot \nabla f = J[f, f] \quad \text{Collision operator}$$

$$J[f, f] = \sigma^2 \int d\mathbf{v}_2 \int d\hat{\sigma} \Theta(\mathbf{v}_{12} \cdot \hat{\sigma}) (\mathbf{v}_{12} \cdot \hat{\sigma}) \\ \times \left[\alpha^{-2} f(\mathbf{v}_1^{**}) f(\mathbf{v}_2^{**}) - f(\mathbf{v}_1) f(\mathbf{v}_2) \right]$$



$$\mathbf{v}_1^{**} = \mathbf{v}_1 - \frac{1 + \alpha}{2\alpha} (\mathbf{v}_{12} \cdot \hat{\sigma}) \hat{\sigma}, \quad \mathbf{v}_2^{**} = \mathbf{v}_2 + \frac{1 + \alpha}{2\alpha} (\mathbf{v}_{12} \cdot \hat{\sigma}) \hat{\sigma}$$

Collisional Balance

$$\int d\mathbf{v} \begin{Bmatrix} 1 \\ \mathbf{v} \\ (\mathbf{v} - \mathbf{u})^2 \end{Bmatrix} J[f, f] = \begin{Bmatrix} 0 \\ \mathbf{0} \\ -\frac{3}{m} \zeta n T \end{Bmatrix}$$

Cooling rate

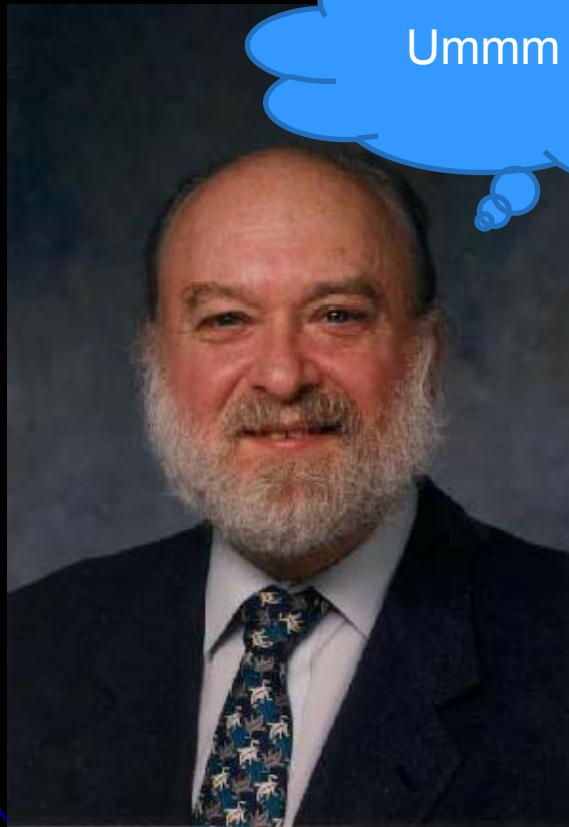
- Conservation of mass
- Conservation of momentum
- *Energy sink*

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Is a hydrodynamic description applicable to granular gases?

Leo P. Kadanoff
(b. 1937)



Ummm ... I think not

L. P. Kadanoff, *Built upon sand: Theoretical ideas inspired by granular flows*, Rev. Mod. Phys. **71**, 435 (1999):

- Can a granular material be described by hydrodynamic equations, most specifically those equations which apply to an ordinary fluid?
- It seems to me that the answer is “no!”.
- The study of collisions and flow in these materials requires new theoretical ideas beyond those in the standard statistical mechanics or hydrodynamics.
- One might even say that the study of granular materials gives one a chance to reinvent statistical mechanics in a new context.

Hydrodynamic description in *ordinary* gases

- Conservation equations (mass, momentum, and energy):

$$\underbrace{\partial_t y_i(\mathbf{r}, t)}_{\text{Hydrodynamic fields}} + \nabla \cdot \underbrace{\mathbf{J}_i(\mathbf{r}, t)}_{\text{Fluxes}} = 0$$

- Constitutive equations:

$$\mathbf{J}_i(\mathbf{r}, t) = \mathcal{F}_i[\{y_j\}]$$

Closed set
of equations



Claude-Louis Navier
(1785-1836)



George Gabriel Stokes
(1819-1903)

Navier-Stokes constitutive equations

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

Stress tensor Viscosity

$$\boxed{\mathbf{q}} = -\boxed{\kappa} \nabla T$$

Heat flux Thermal conductivity

Hydrodynamic description in *ordinary* gases

Navier-Stokes:

$$\mathbf{J}_i(\mathbf{r}, t) = \mathbf{J}_i^{\text{le}}(\mathbf{r}, t) - \sum_j \lambda_j(\mathbf{r}, t) \nabla y_j(\mathbf{r}, t)$$

Transport coefficients

... but a hydrodynamic description is not restricted to the Navier-Stokes constitutive equations (non-Newtonian behavior, rheological properties, ...)

$$\mathbf{J}_i(\mathbf{r}, t) = \mathcal{F}_i[\{y_j\}]$$

Hydrodynamics beyond Navier-Stokes: the Chapman-Enskog method



Sydney Chapman
(1888-1970)

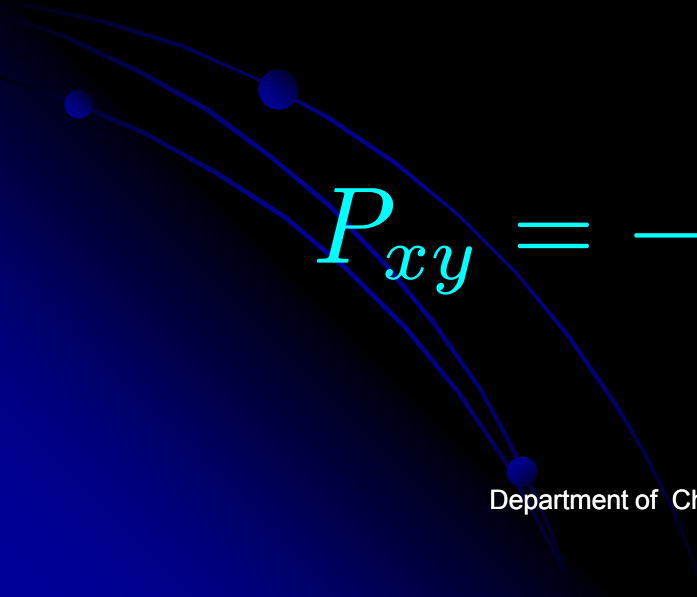


David Enskog
(1884-1947)

Weak hydrodynamic gradients \rightarrow
Chapman-Enskog expansion

$\epsilon \sim \nabla$: uniformity parameter

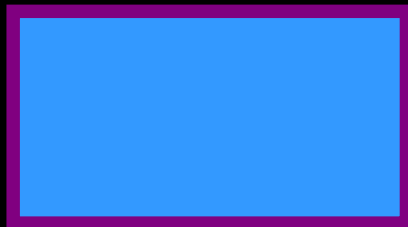
$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \dots$$


$$P_{xy} = - \sum_{k=0}^{\infty} \eta_k \left(\frac{\partial u_x}{\partial y} \right)^{2k+1}$$

“Aging” to hydrodynamics in *ordinary* gases



$t = 0$



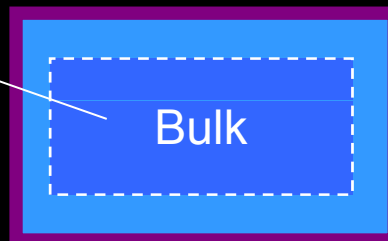
$t \sim 1$ mean free time



\sim Mean free path



$t \gg 1$ mean free time



Hydrodynamic description

Low-density (*ordinary*) gases: Aging from the Boltzmann equation

$$\left. \begin{aligned} \partial_t f + \mathbf{v} \cdot \nabla f &= J[f, f] \\ f(\mathbf{r}, \mathbf{v}, 0) &= f_0(\mathbf{r}, \mathbf{v}) \\ \text{boundary conditions} & \end{aligned} \right\} \Rightarrow f(\mathbf{r}, \mathbf{v}, t) = \mathcal{F}[f_0; \mathbf{r}, \mathbf{v}, t]$$

1. Kinetic stage ($t \sim 1$ mean free time):

- Sensitive to the initial preparation

2. Hydrodynamic stage ($t \gg 1$ mean free time) \Rightarrow

“Hydrodynamic” solution: $f(\mathbf{r}, \mathbf{v}, t) = \mathcal{F}[\{y_i\}; \mathbf{v}]$

“Aging” to hydrodynamics in *granular* gases?

- Does the conventional aging scenario (short kinetic stage followed by slow hydrodynamic stage) still apply to *granular*?
- Energy is intrinsically not conserved!

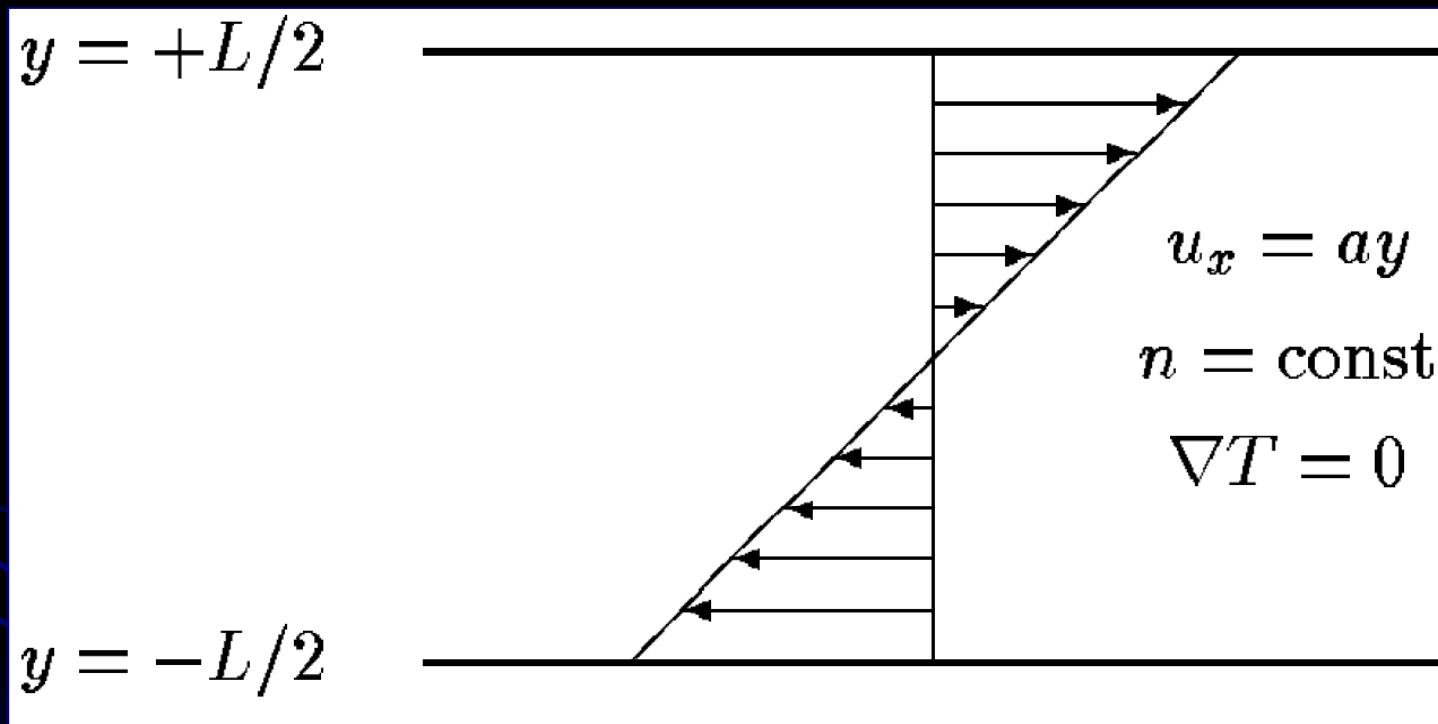
$$\left. \frac{\partial T(t)}{\partial t} \right|_{\text{coll}} = -\zeta(t)T(t)$$

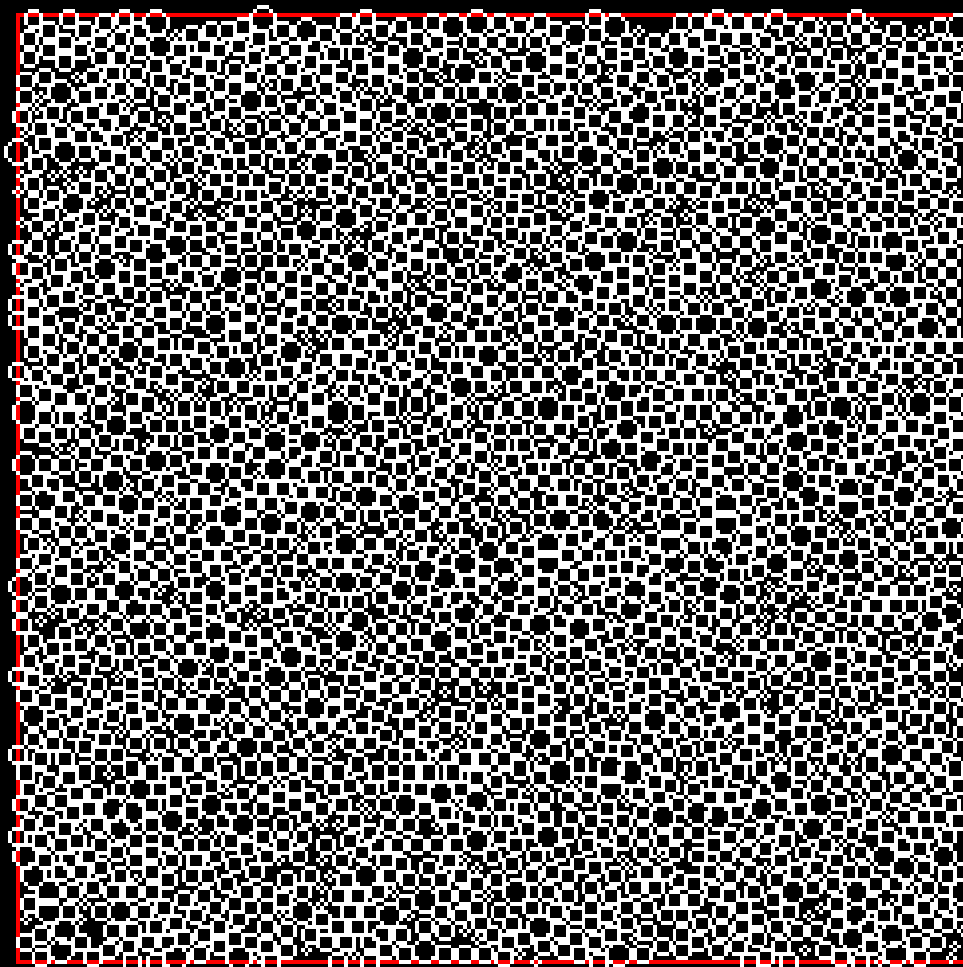
Cooling rate

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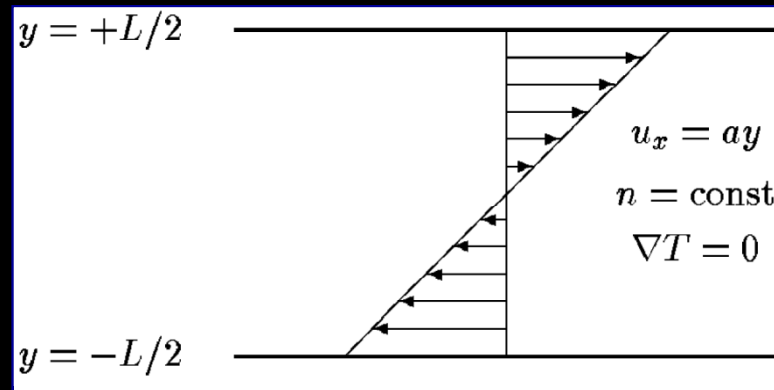
Paradigmatic nonequilibrium state: Simple or Uniform Shear Flow (USF)





Computer simulations
by UCSB's group

Uniform shear flow of a granular gas



$$\partial_t T = \underbrace{-\frac{2a}{3n} P_{xy}}_{\text{Viscous heating}} - \underbrace{\zeta T}_{\text{Inelastic cooling}} \Rightarrow T(t) \text{ reaches a stationary value}$$

Scaled shear rate: $a^*(t) \equiv \frac{a}{\nu(t)}$

Effective collision frequency

Coefficient of restitution: $\alpha = \text{const}$

“Aging” to hydrodynamics

$$f(\mathbf{r}, \mathbf{v}, t) = \mathcal{F}[f_0; \mathbf{r}, \mathbf{v}, t] \rightarrow \mathcal{F}[\{y_i\}; \mathbf{v}]$$

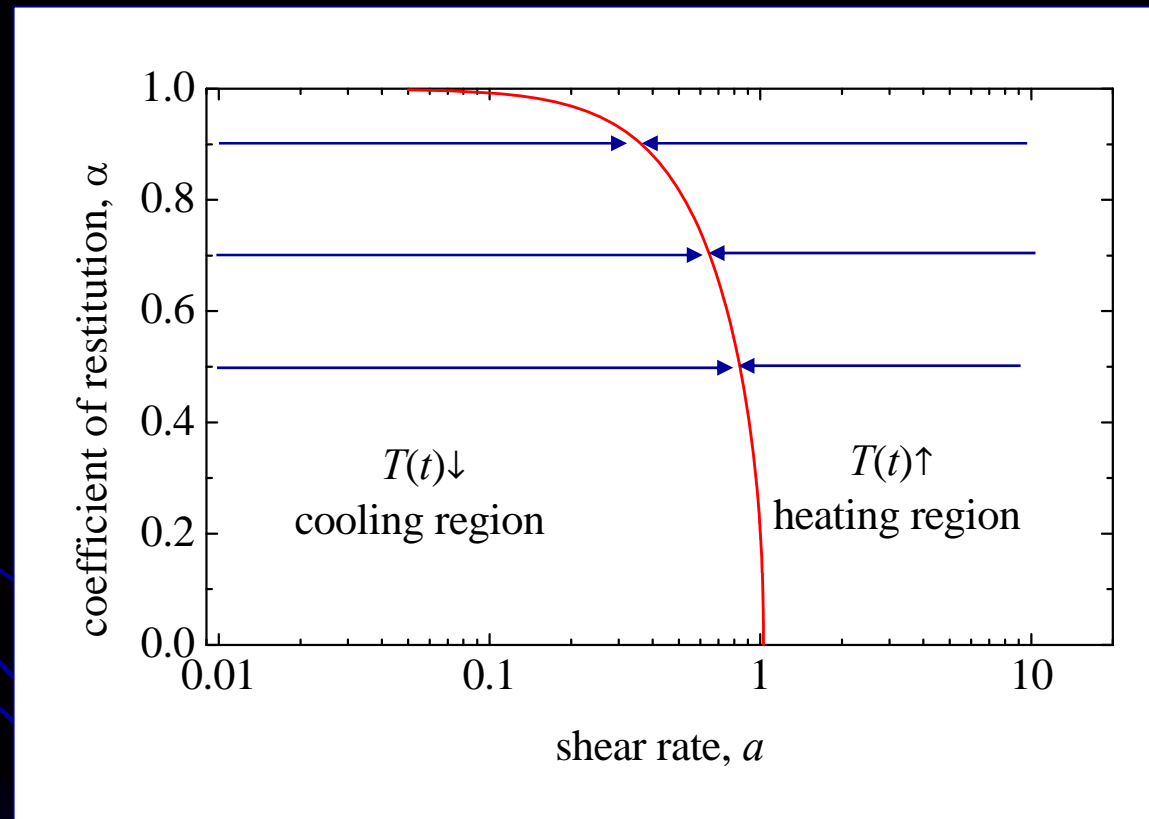
$$\text{USF} \Rightarrow f(\mathbf{r}, \mathbf{v}, t) \rightarrow n \left[\frac{m}{2T(t)} \right]^{3/2} f^*(\mathbf{C}(t); a^*(t))$$

$$\mathbf{C}(t) \equiv \frac{\mathbf{v} - \mathbf{u}(\mathbf{r})}{\sqrt{2T(t)/m}}$$

$$\eta(t) \equiv -\frac{P_{xy}(t)}{a} \rightarrow \frac{nT(t)}{\nu(t)} \eta^*(a^*(t), \alpha)$$

Scaled shear viscosity

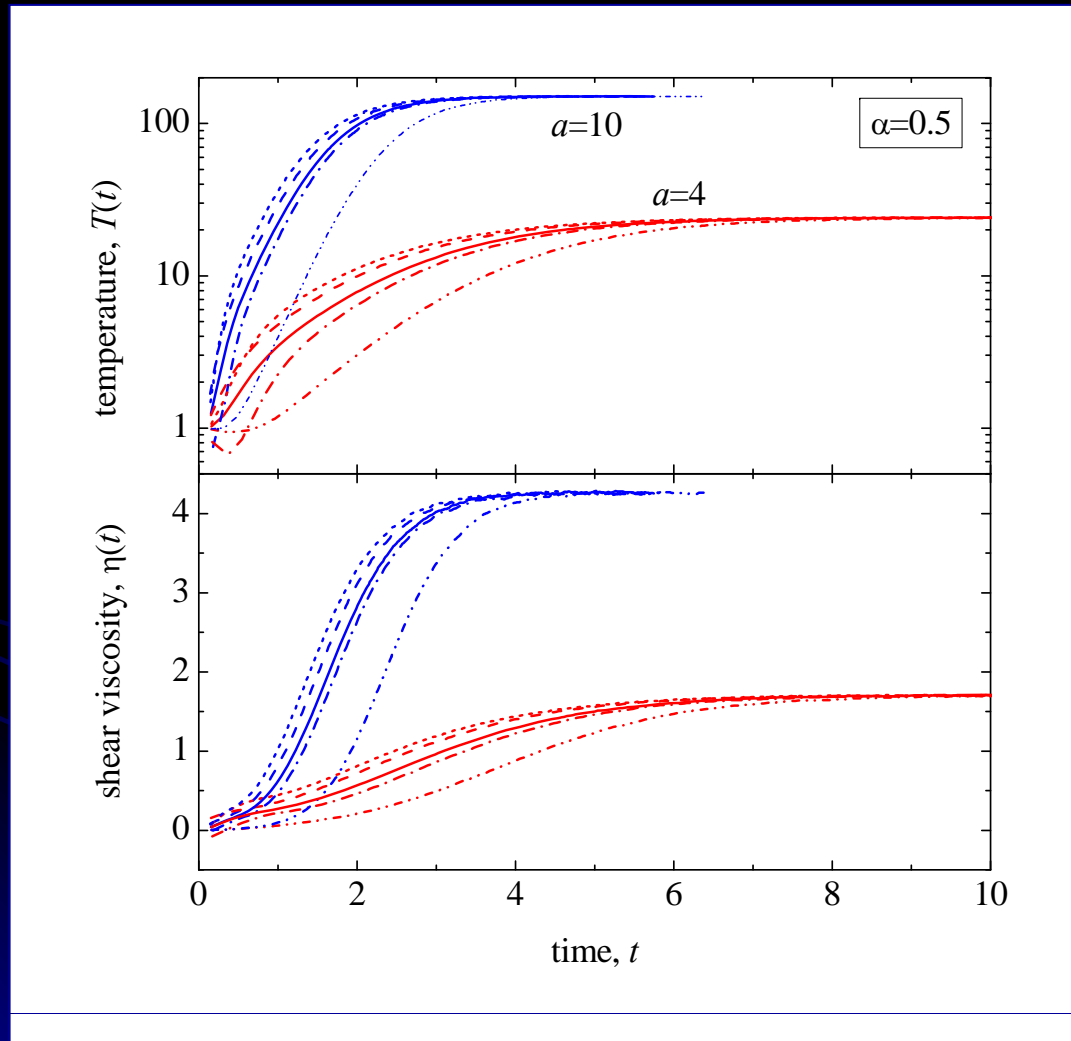
“Phase diagram”: Competition between inelastic cooling and viscous heating



For each one of the 12 pairs (a^*, α) , 5 different initial conditions

Monte Carlo simulations

Relaxation toward the steady state

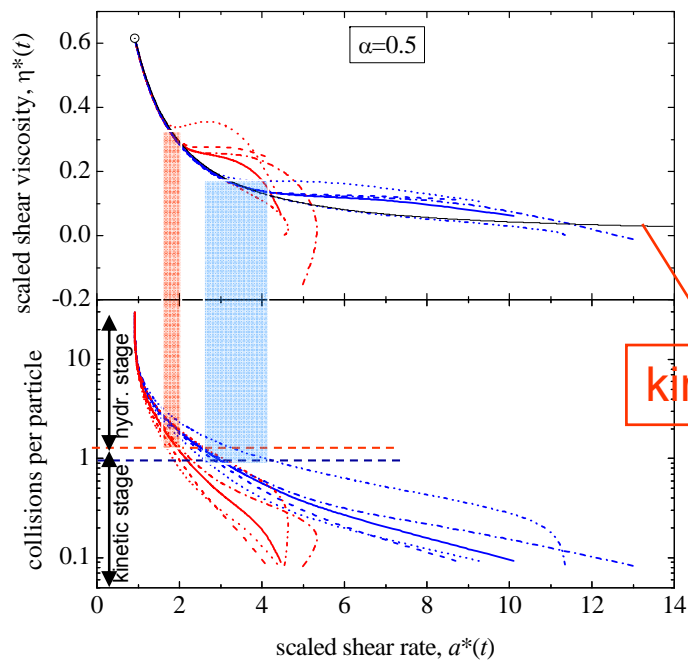


$$T(t) \rightarrow T_s(a, \alpha)$$
$$\eta(t) \rightarrow \eta_s(a, \alpha)$$

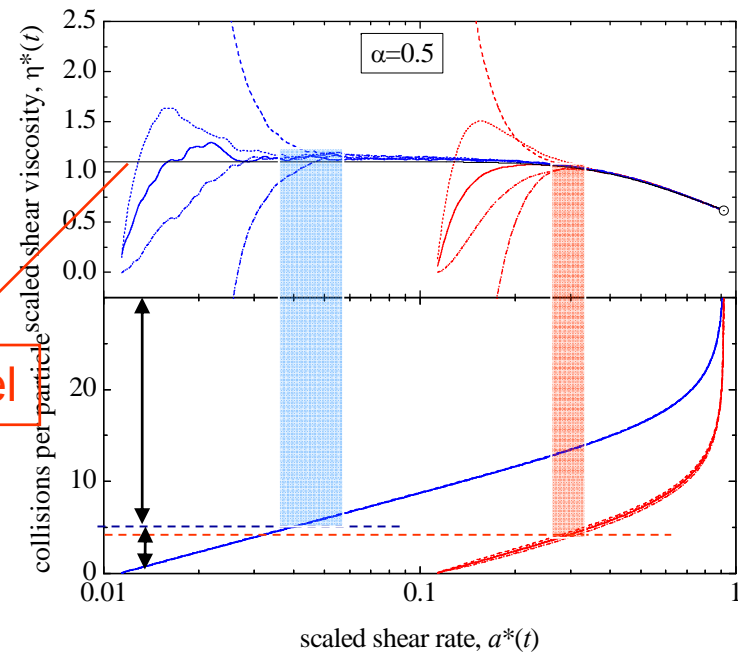
$$a^*(t) \rightarrow a_s^*(\alpha)$$
$$\eta^*(t) \rightarrow \eta_s^*(\alpha)$$

Monte Carlo simulations

Unsteady hydrodynamic regime prior to the steady state?



kinetic model

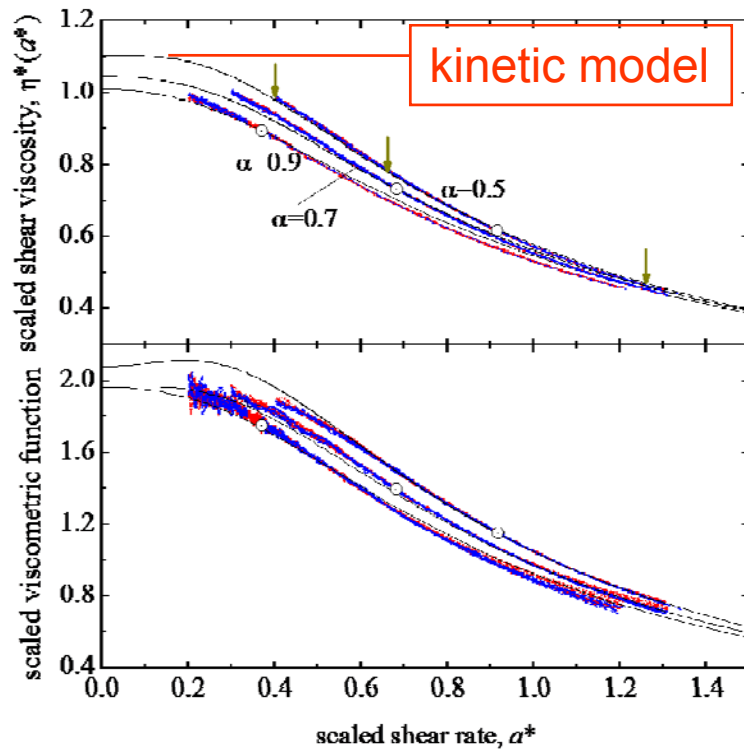


A. Astillero & A. Santos, Europhys. Lett. **78**, 24002 (2007)

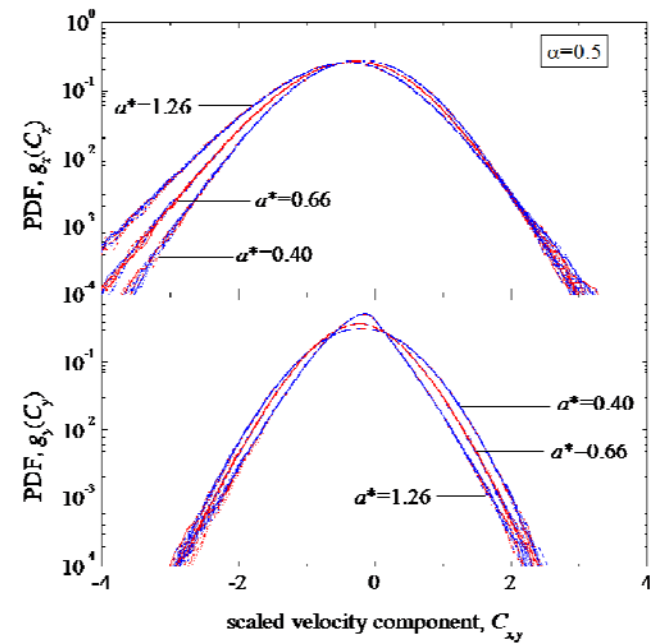
Department of Chemistry, Kyoto University, July 18, 2008

Monte Carlo simulations

Rheological quantities



Velocity distribution



A. Astillero & A. S., Europhys. Lett. **78**, 24002 (2007)

Department of Chemistry, Kyoto University, July 18, 2008

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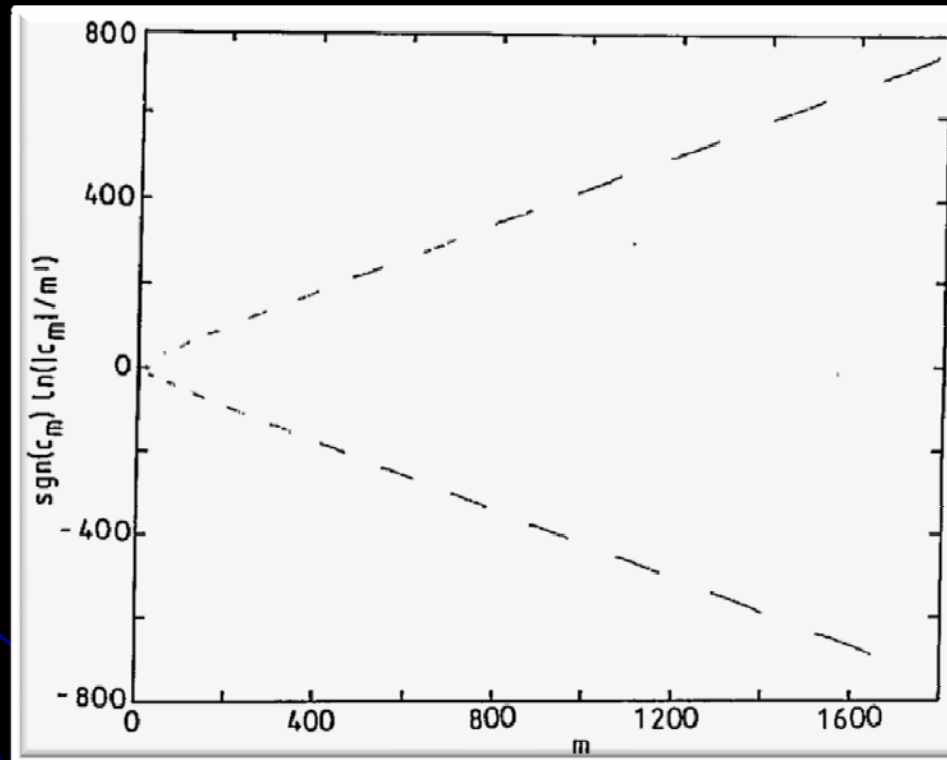
Is the Chapman-Enskog (CE) expansion convergent?

$$P_{xy} = - \sum_{k=0}^{\infty} \eta_k \left(\frac{\partial u_x}{\partial y} \right)^{2k+1}$$

$$\eta^*(a^*, \alpha) = \sum_{k=0}^{\infty} c_k(\alpha) a^{*2k}$$

It diverges for *ordinary* gases

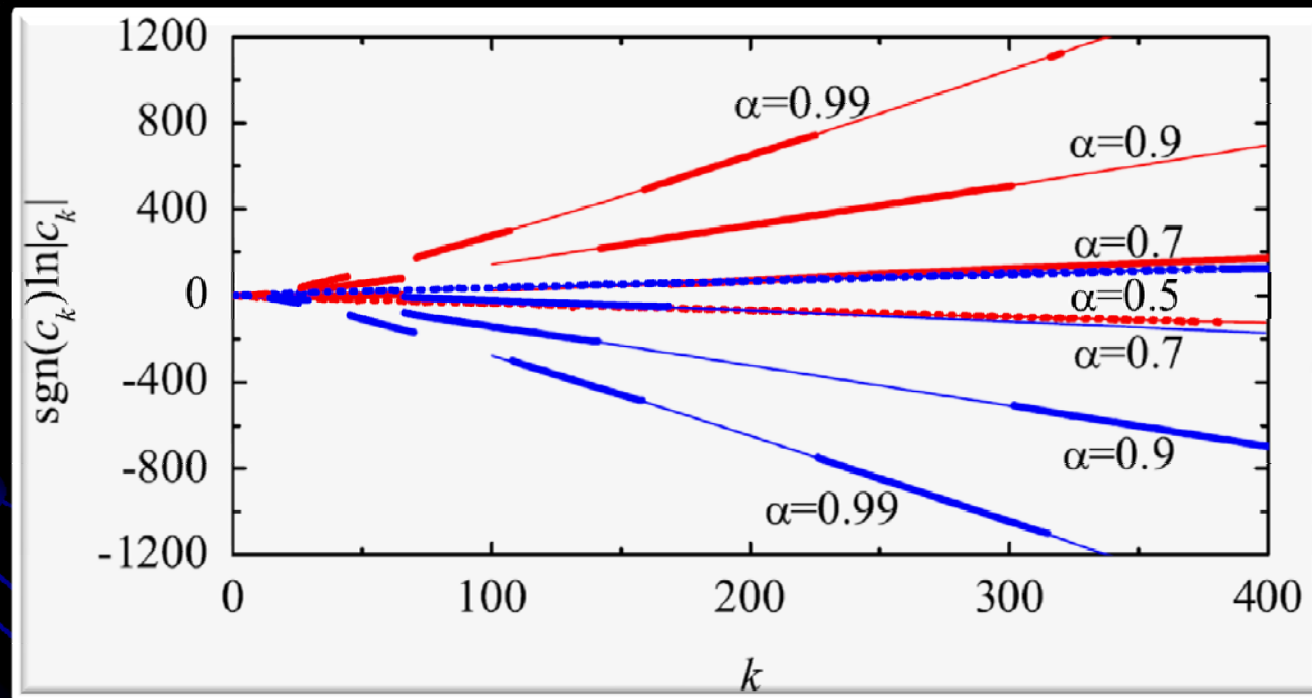
$$|c_k| \sim (2/3)^k k!$$



A.S., J. J. Brey, & J. W. Dufty, Phys. Rev. Lett. **56**, 1571 (1986)

Does the CE series diverge even more rapidly for granular gases?

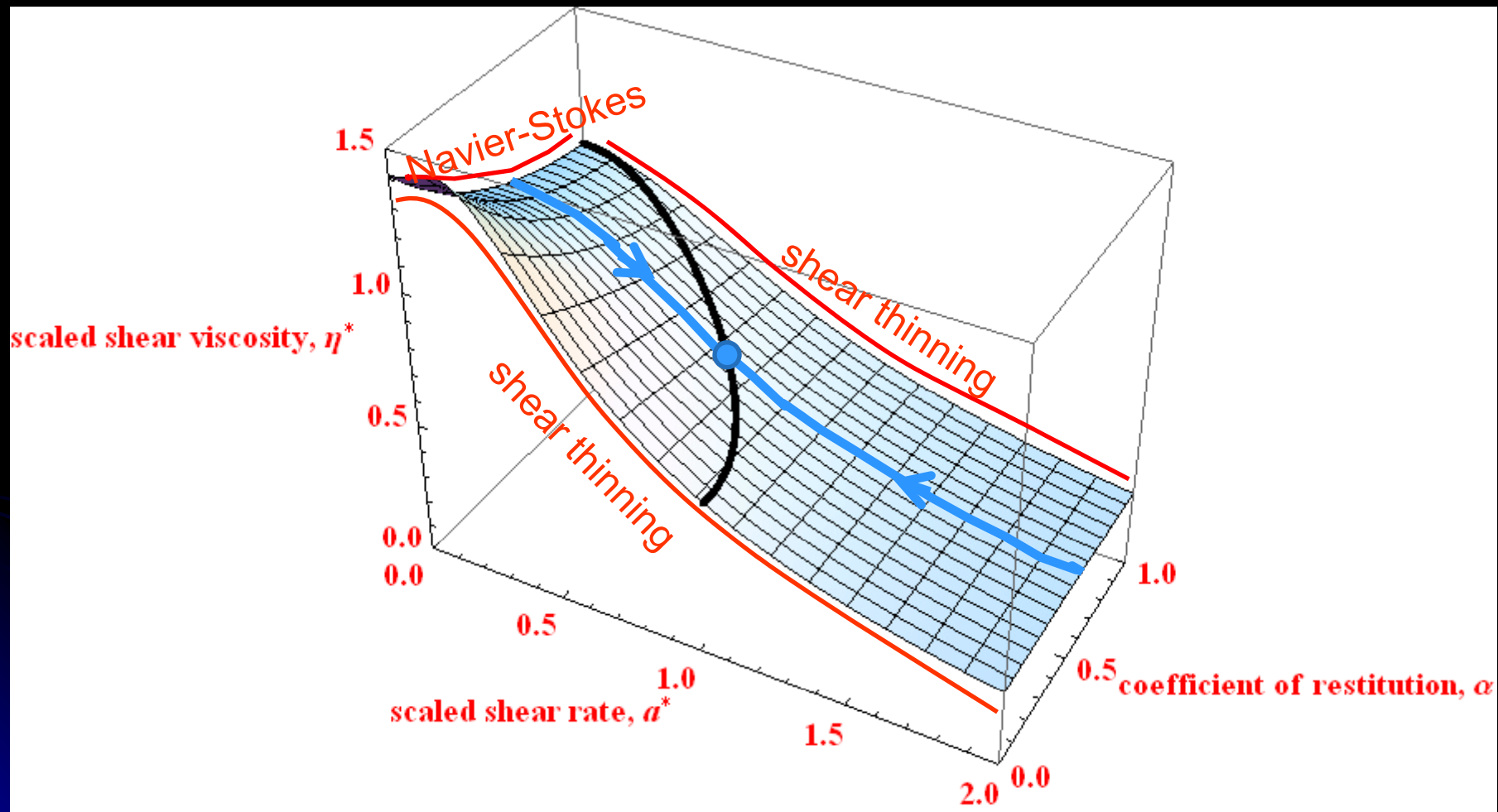
$$|c_k| \sim a_s^{*-2k}$$



A.S., Phys. Rev. Lett. **100**, 078003 (2008)

- The Chapman-Enskog series diverges for *elastic* collisions.
- But it converges for *inelastic* collisions!
- In fact, the stronger the inelasticity, the larger the radius of convergence.
- Can this paradoxical result be understood by physical arguments?

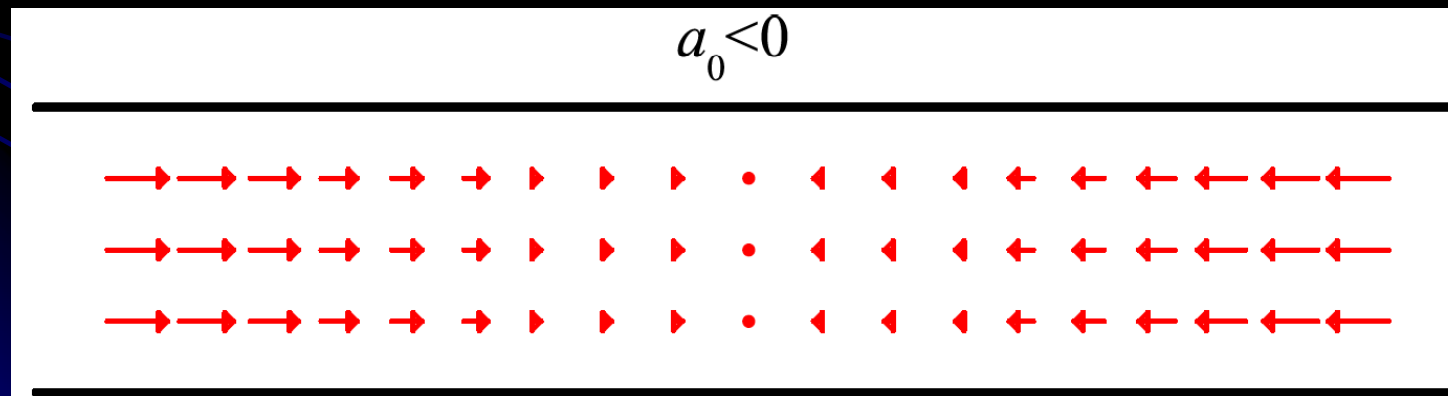
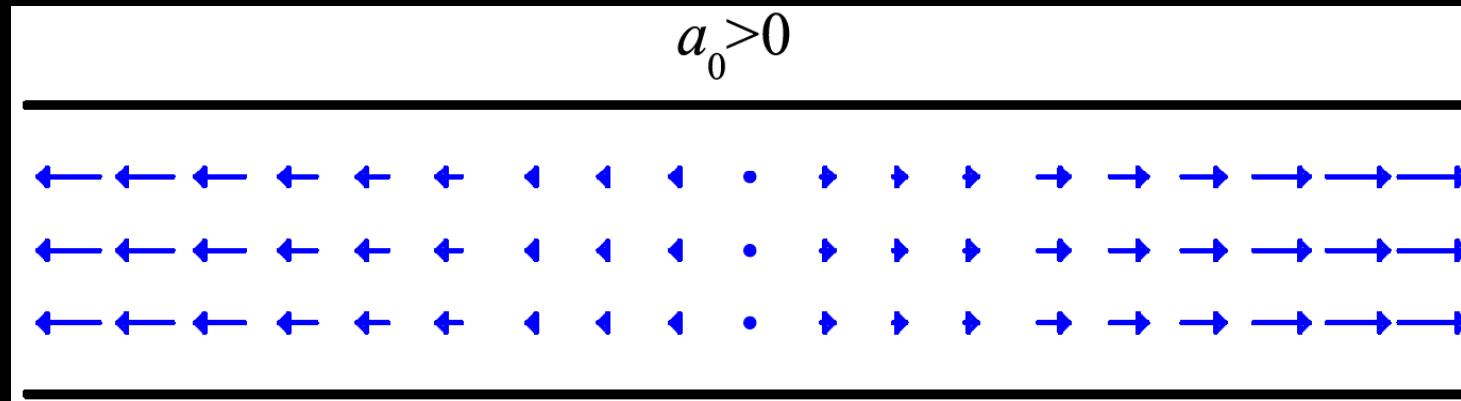
$$\eta^*(a^*, \alpha)$$



$$\eta^*(a^*, \alpha) = \sum_{k=0}^{\infty} c_k(\alpha) a^{*2k}$$

- The reference homogeneous state ($a^*=0$) is an *attractor* of the evolution of $a^*(t)$ for elastic collisions \Rightarrow The CE expansion goes against the arrow of time \Rightarrow The CE series diverges.
- The state $a^*=0$ is a *repeller* of $a^*(t)$ for inelastic collisions \Rightarrow The CE series converges.

A similar case: longitudinal flow



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Conclusions

- The conventional scenario of aging to hydrodynamics seems to remain essentially valid for granular gases, even for non-Newtonian states.
- At a given value of α , the (scaled) nonlinear shear viscosity $\eta^*(a^*)$ moves on a certain rheological curve, the steady-state value $\eta_s^* = \eta^*(a_s^*)$ representing just one point.
- The Chapman-Enskog expansion of $\eta^*(a^*)$ diverges for ordinary gases (elastic collisions) but converges for granular gases (inelastic collisions).
- Last but not least ... granular fluids are fun!

Thanks for your attention!



Japanese granular matter

