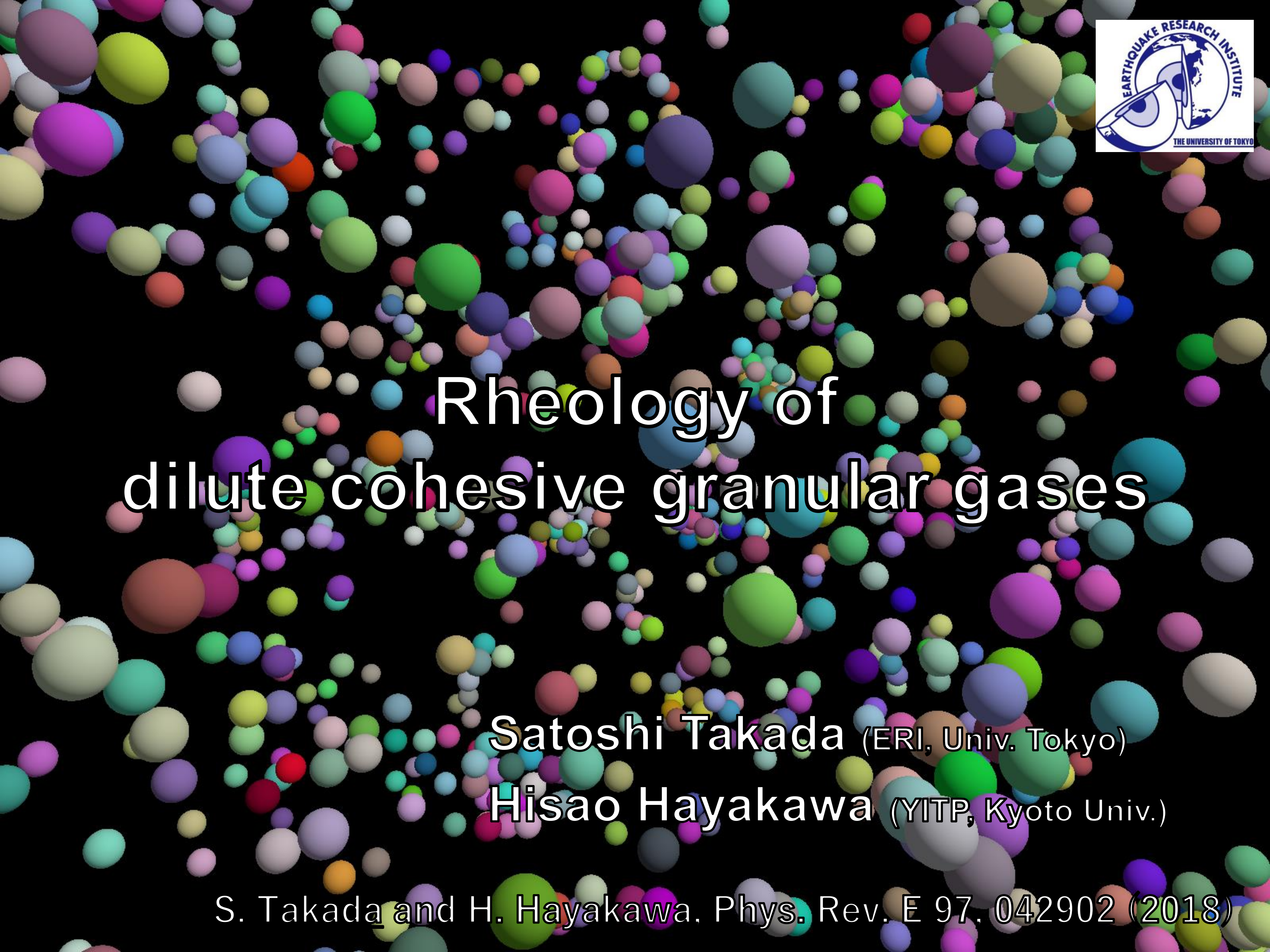


Rheology of dilute cohesive granular gases

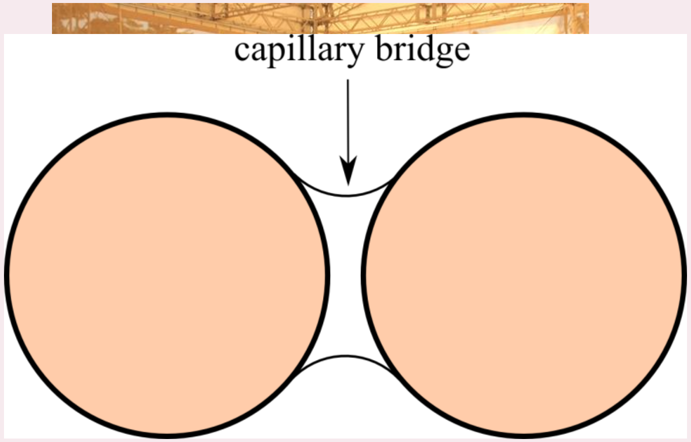
Satoshi Takada (ERI, Univ. Tokyo)
Hisao Hayakawa (YITP, Kyoto Univ.)

S. Takada and H. Hayakawa, Phys. Rev. E 97, 042902 (2018)

Introduction

Aerosols [1]

PM2.5 [2]



Fine powders

Ex)：PM2.5, aerosols, volcanic ashes…

Typical size $\sim\mu m$

Van der Waal force

Wet granular particles

Liquid bridges

Capillary force

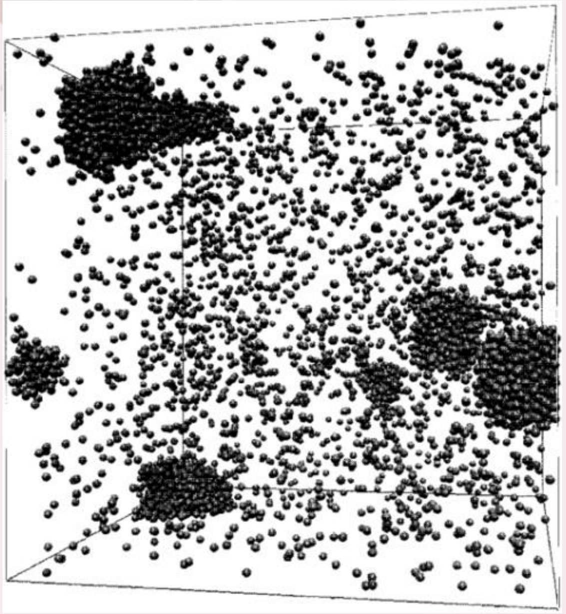
Gas-liquid or liquid-solid phase transition may occur.

[1] http://store.interstateproducts.com/images/spray-aerosols-cat.jpg

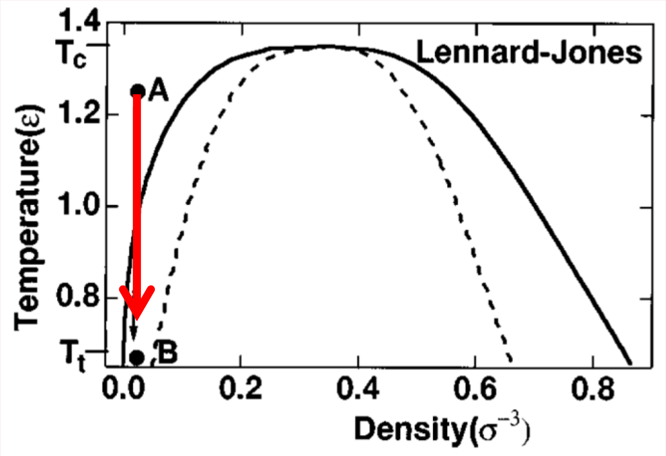
[2] http://china-pm25.com/

[3] http://www.sand-museum.jp

Cohesive particles

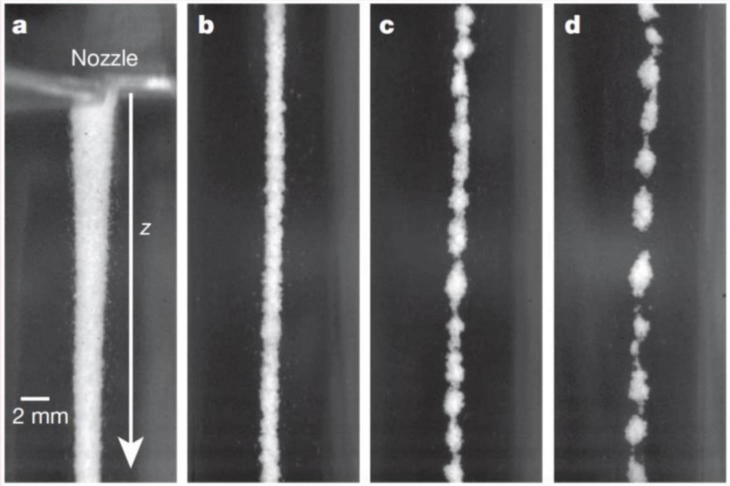


K. Yasuoka and M. Matsumoto,
J. Chem. Phys., **109** 8451 (1998)



When we control the temperature,
gas-liquid phase transition occurs after quench.

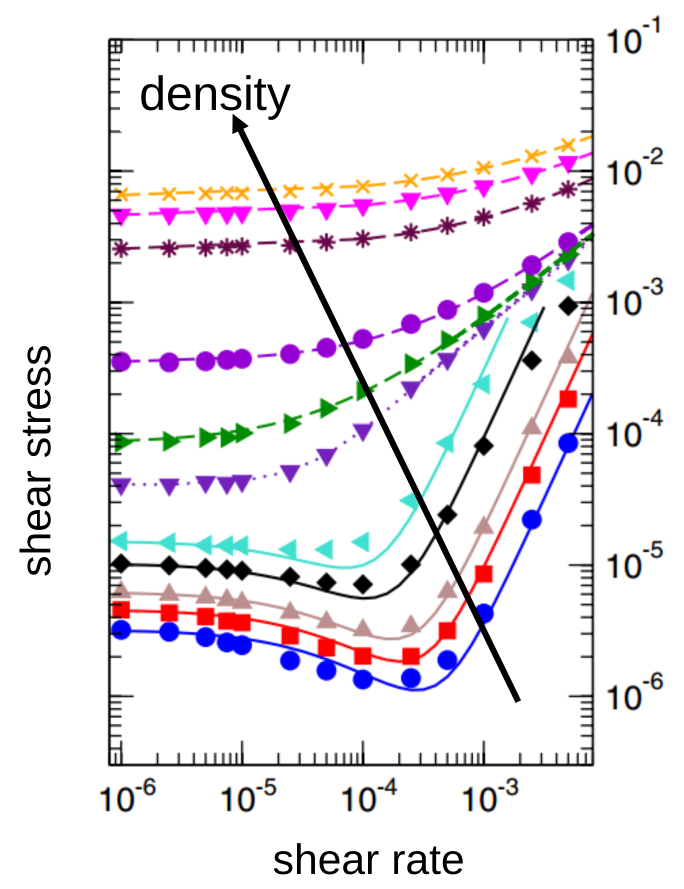
Freely falling wet granular particles
⇒ Clustering due to cohesive forces



Royer *et al.*, Nature, **459**, 1110, (2009)

Previous studies on rheology of (dense) cohesive systems

E. Irani, et al. PRL **112**, 188303 (2014)



If attractive interactions exist,
the rheology changes as
compared with non-cohesive systems.

⇩

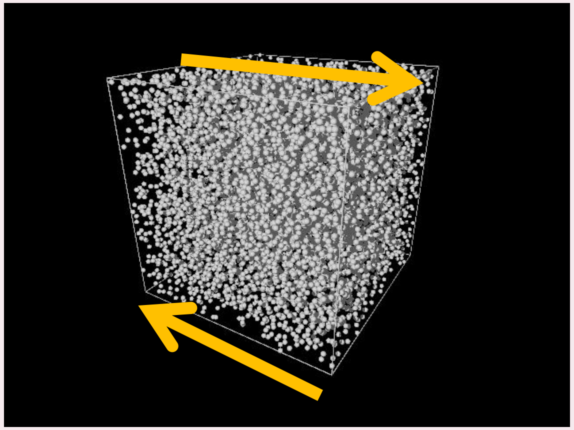
Clustering due to cohesive forces
may affect the rheology of the system.

Our previous studies

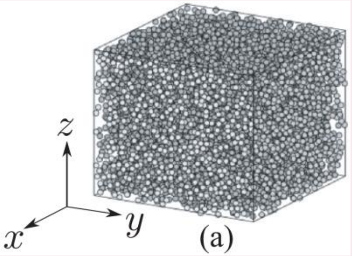
Lennard-Jones system

+ shear

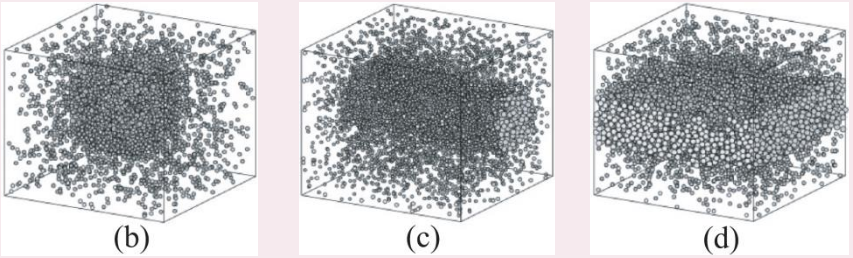
S. Takada, K. Saitoh, & H. Hayakawa,
Phys. Rev. E, **90**, 062207 (2014)



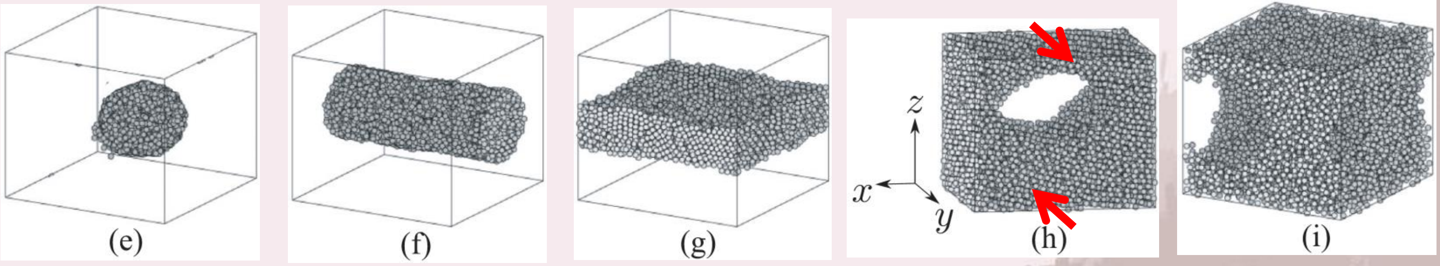
Uniform system



Coexistence system



Cluster phase



Motivation of this work

Theoretical explanation of the rheology of cohesive powders is poor.

Motivation:
How do attractive forces change the rheology?

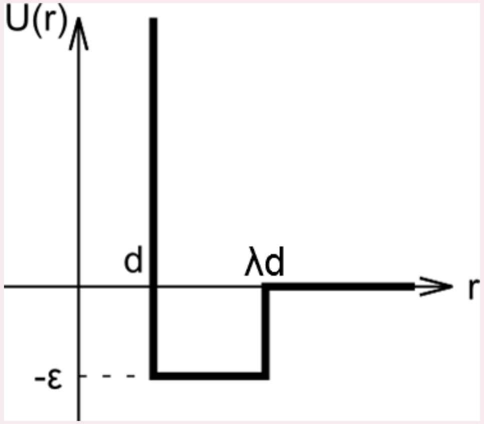
Especially, at the first step, we focus on

- cohesiveness from an attractive potential
- dilute case.

We study the rheology of cohesive powders numerically (MD simulation) and theoretically (kinetic theory).

Model

We perform event-driven molecular dynamics simulations by DynamO (open-source simulator).



Monodisperse gases (mass: m, diameter: d)

Potential = square-well potential

(well depth: ε, well width ratio: λ)

Dilute limit (packing fraction) $\phi \ll 1$

Nearly elastic limit (restitution coefficient) $e \lesssim 1$

Inelastic collision only occurs at $r = d$

We apply a shear by Lees-Edwards boundary condition (shear rate $\dot{\gamma}$)

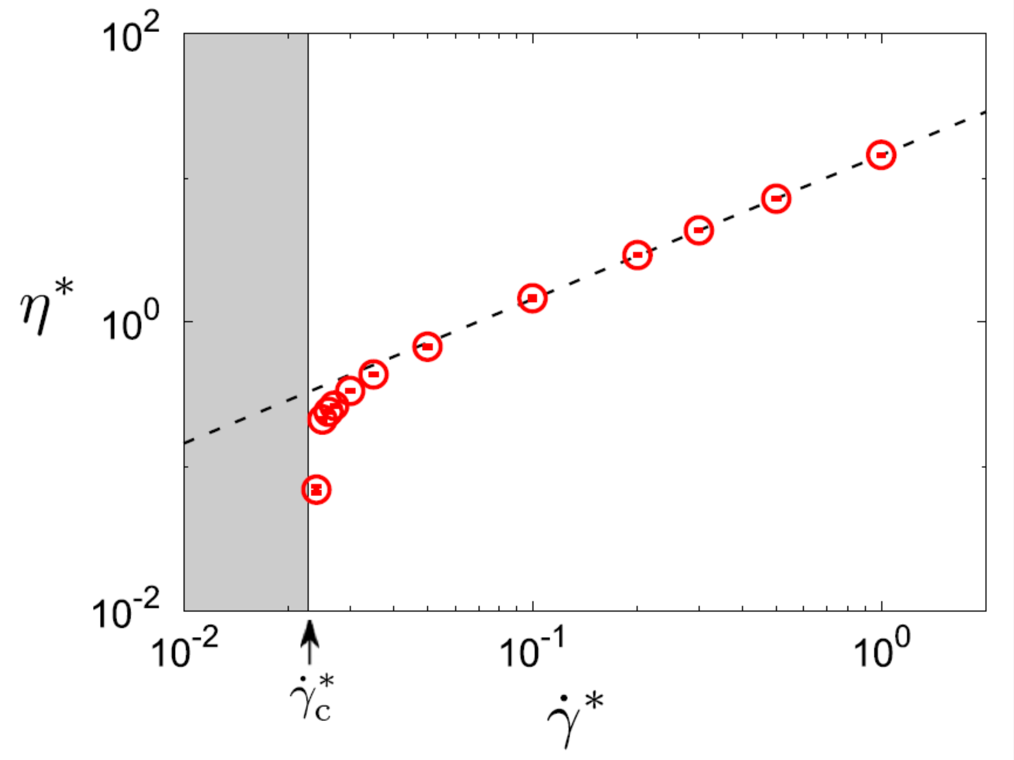
Parameters:
$\phi = 0.01$
$e = 0.99$
$\lambda = 1.5$

All quantities are nondimensionalized in terms of m, d, ε.

Numerical results

Results: high shear regime

Shear viscosity $\eta^* = -P^*_{xy}/\dot{\gamma}^*$ vs. shear rate $\dot{\gamma}^*$



- Existence of the critical shear rate $\dot{\gamma}_{\mathrm{c}}$ ($\dot{\gamma}^*_{\mathrm{c}} \simeq 0.02$)
- For $\dot{\gamma} \gtrsim \dot{\gamma}_{\mathrm{c}}$, there exists a steady state.

$\dot{\gamma} \gg \dot{\gamma}_{\mathrm{c}}$: consistent with Bagnoldian (hard-core limit)

$$\eta^* = \frac{5(2+e)}{72(1+e)^2(3-e)^3}\sqrt{\frac{5(2+e)}{3(1-e)}\frac{1}{\phi}}\dot{\gamma}^*$$

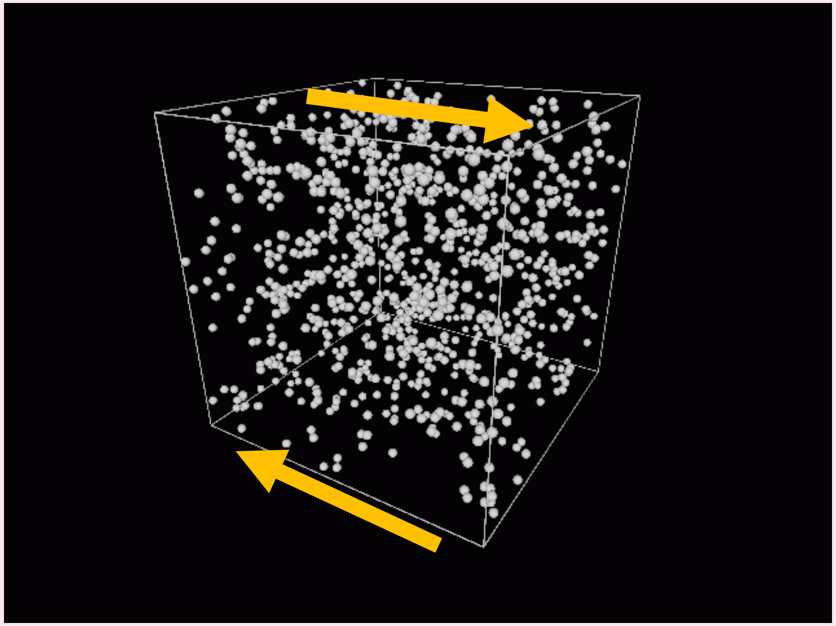
shear rate $\dot{\gamma}$: sufficiently high
⇒ temperature $T \gg$ well depth ε
⇒ Particles are hard-core like.

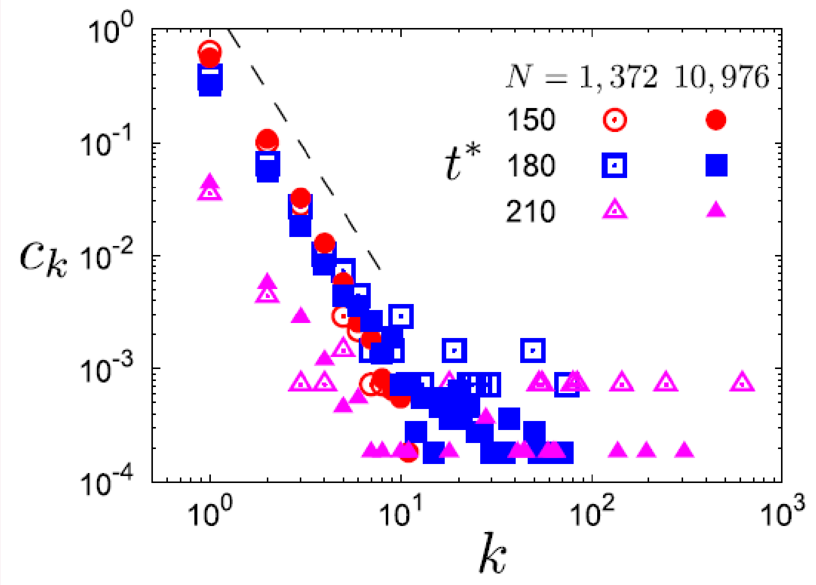
$\dot{\gamma} \simeq \dot{\gamma}_{\mathrm{c}}$: deviation from Bagnoldian

Results:
low shear regime

- For $\dot{\gamma} \lesssim \dot{\gamma}_\mathrm{c}$, no steady state

What happens? ⇨ Clustering

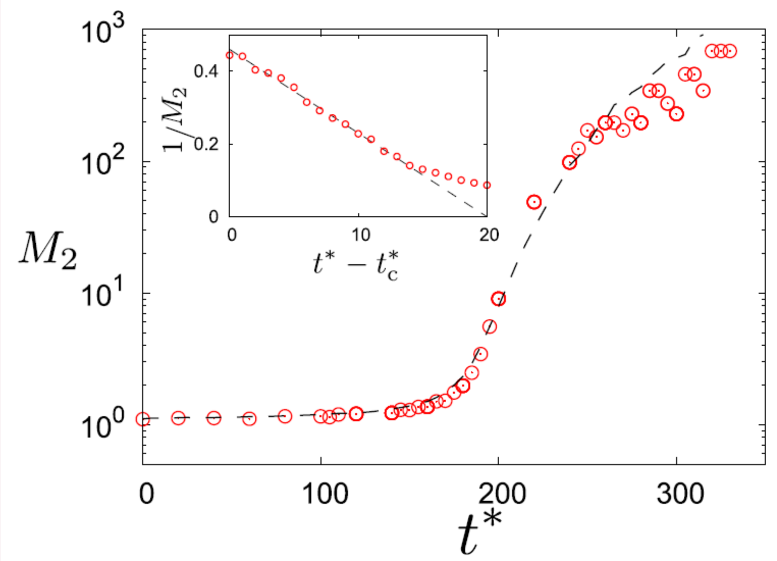




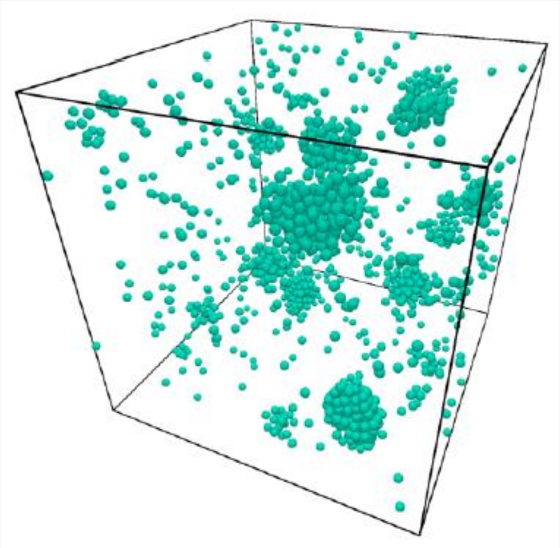
cluster size distribution

$c_k \propto k^{-2.67}$

Mean cluster size $M_2 = \sum_k k^2 c_k$ grows as time goes on.



Results: low shear regime



Q. Can we modify the theory
in terms of this cluster size?

Effective quantities

Assumption:

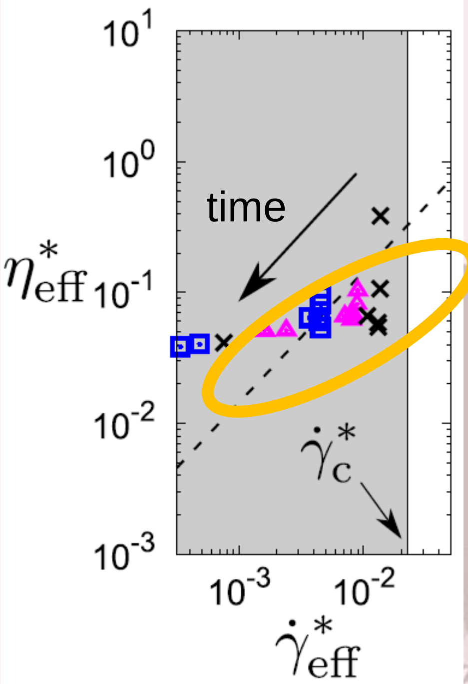
(a) All clusters are the same size M_2

(b) Cluster is spherical (mass $m_{\mathrm{cl}} \sim M_2$, diameter $d_{\mathrm{cl}} \sim M_2^{1/3}$)

effective shear viscosity & effective shear rate

$$\dot{\gamma}_{\mathrm{eff}} = \dot{\gamma}^* \sqrt{\frac{\varepsilon}{m_{\mathrm{cl}} d_{\mathrm{cl}}^2}} = \dot{\gamma} M_2^{-5/6}$$

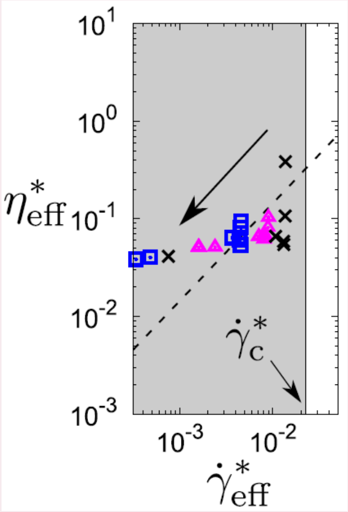
$$\eta_{\mathrm{eff}} = \eta M_2^{-1/6}$$

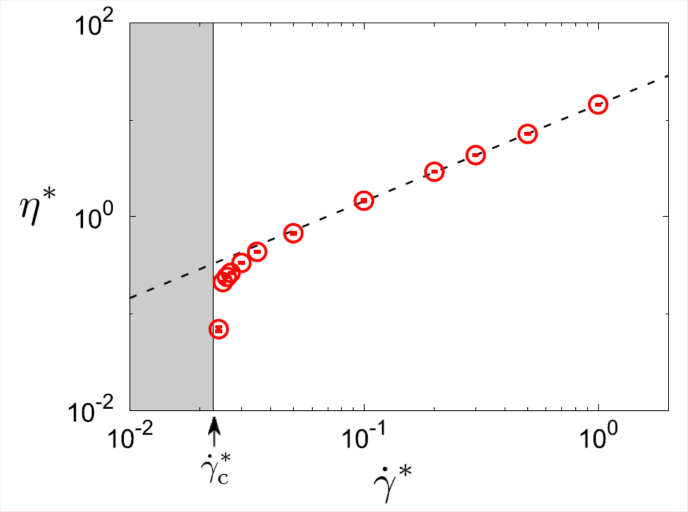


→ Effective rheology curve for the viscosity is partially consistent with Bagnoldian expression!

Short summary of simulation results

We have performed event-driven molecular dynamics simulations of granular gases having the square-well potential under a shear.





$\dot\gamma \gg \dot\gamma_{\rm c} \Rightarrow$ Bagnold
$\dot\gamma \simeq \dot\gamma_{\rm c} \Rightarrow$ Deviation from Bagnold
$\dot\gamma \lesssim \dot\gamma_{\rm c} \Rightarrow$ no steady state the "effective" Bagnold

Question:
What determines the critical shear rate $\dot\gamma_{\rm c}$?
Can we explain the deviation from Bagnoldian expression?

We analyze the Boltzmann equation under a shear.

Theoretical results

Boltzmann equation under plane shear

Starting point:

$$\left(\frac{\partial}{\partial t} - \dot{\gamma} V_y \frac{\partial}{\partial V_x}\right) f(\mathbf{V}, t) = I(f, f)$$

Effect of shear

Santos et al. PRE, **69** 061303 (2004)

$f(\boldsymbol{V}, t)$: velocity distribution
$I(f, f)$: collision integral

Equation of state $p^k = nT$ (ideal gas)

Assumption

H. Grad, Comm. Pure Appl. Math. **2**, 331–407 (1949).

Velocity distribution = Grad’s 13 moment method

$$f(\boldsymbol{V}) = f_{\mathrm{M}}(\boldsymbol{V})\left[1 + \frac{m}{2T}\left(\frac{P_{ij}^{k}}{p^{k}} - \delta_{ij}\right) V_i V_j\right]$$

$f_{\mathrm{M}}(V)$: Maxwell distribution

Collision geometry

refractive index $\nu = \sqrt{1 + \dfrac{4\varepsilon}{mv^2}}$

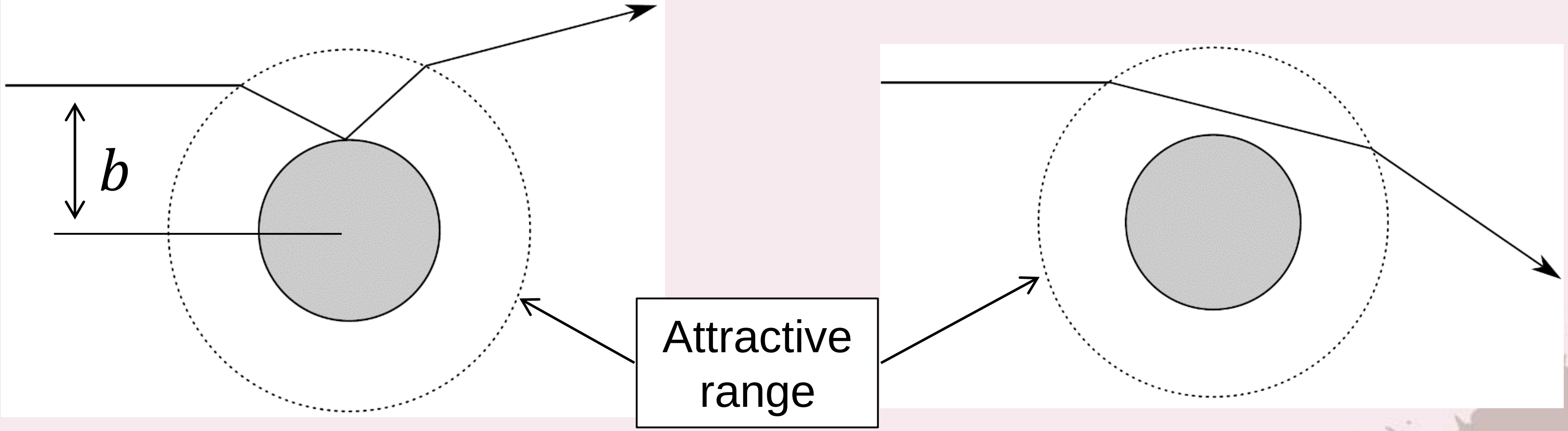
☛ Landau Lifshitz “Mechanics”

Two types of collisions depending on b, v

(a) inelastic collision

(b) grazing collision (no dissipation)

Acceleration in the potential well



(a) Inelastic collision ($b < \nu d$)

(b) Grazing collision ($\nu d < b < \lambda d$)

⇒ The collision integral has two terms:

$$I(f,f) = I_{\text{hard-core}}(f,f) + I_{\text{grazing}}(f,f)$$

Boltzmann equation under plane shear

Starting point:

$$\left(\frac{\partial}{\partial t}-\dot{\gamma}V_y\frac{\partial}{\partial V_x}\right)f(\mathbf{V},t)=I(f,f)$$

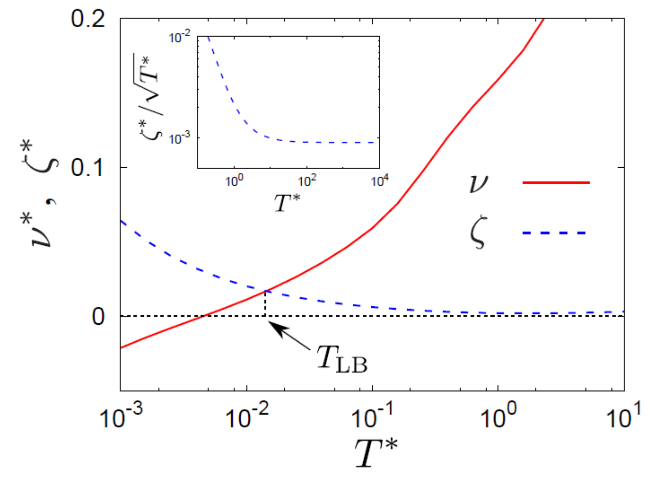
Santos et al. PRE, **69** 061303 (2004)

$f(\boldsymbol{V},t)$: velocity distribution
$I(f,f)$: collision integral

Time evolution of the stress tensor

$$\partial_t P_{ij}^k+\dot{\gamma}\left(\delta_{ix}P_{yj}^k+\delta_{jx}P_{ij}^k\right)$$
$$=-\nu\left(P^k-p^k\delta_{ij}\right)-\zeta p^k\delta_{ij}$$

Two different frequencies



Time evolution of the stress tensor

$$\partial_t P^k_{ij} + \dot{\gamma}\left(\delta_{ix} P^k_{yj} + \delta_{jx} P^k_{ij}\right) = -\nu\left(P^k - p^k \delta_{ij}\right) - \zeta p^k \delta_{ij}$$

We need to solve the simultaneous equations for three parameters:

$$\begin{cases} \partial_t p^k + \dfrac{2}{3}\dot{\gamma} P^k_{xy} = -\zeta p^k & \text{Static pressure} \\ \partial_t \Delta P^k + 2\dot{\gamma} P^k_{xy} = -\nu \Delta P^k & \text{Pressure difference } \Delta P = P^k_{xx} - P^k_{yy} \\ \partial_t P^k_{xy} + \dot{\gamma}\left(p^k - \dfrac{1}{3}\Delta P^k\right) = -\nu P^k_{xy} & \text{Shear stress} \end{cases}$$

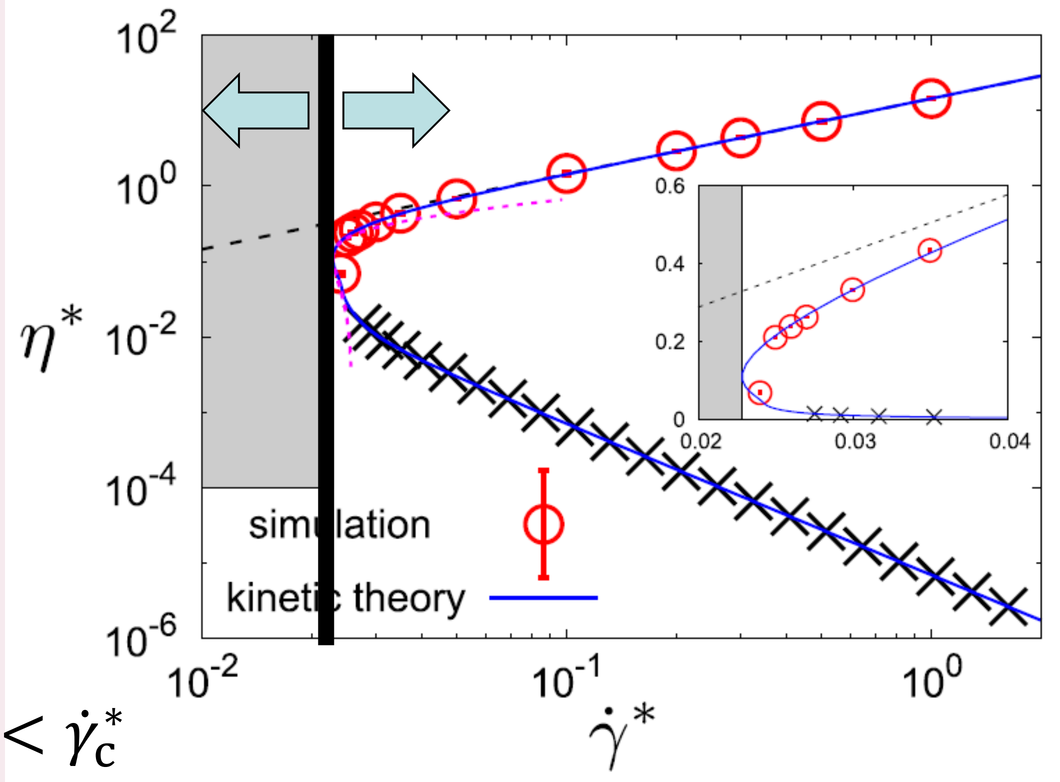
In a steady state ➡

Steady state solution

- Shear rate $\dot{\gamma} = \sqrt{\frac{3}{2}\frac{\nu^2\zeta}{\nu-\zeta}}$, Pressure difference $\Delta P^k = \frac{3\zeta}{\nu} p^k$
- Shear stress $P^k_{xy} = -\frac{p^k}{\nu}\sqrt{\frac{3}{2}\zeta(\nu-\zeta)}$

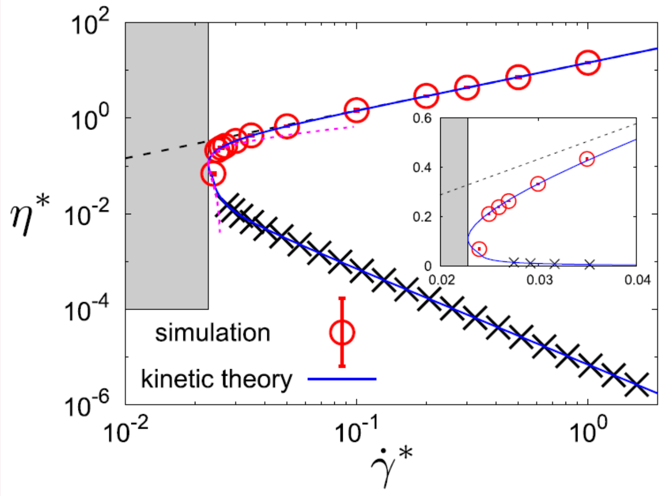
All quantities can be represented as a function of the temperature. ⇒ Parametric plot of T.

Result: viscosity vs. shear rate

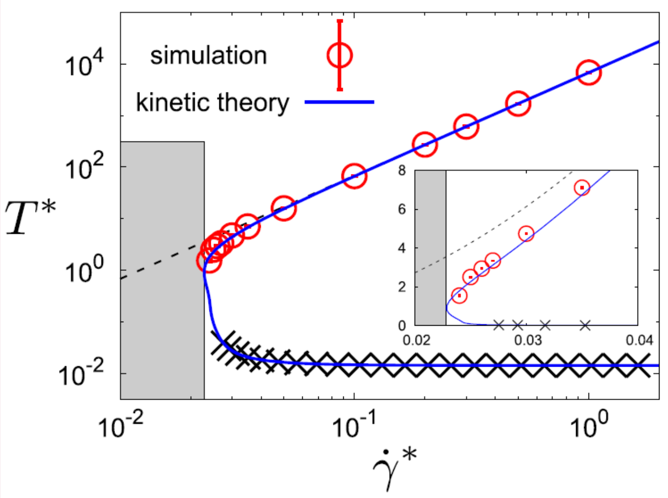


- Existence of the critical shear rate $\dot\gamma_c^*$ ⇒ Consistent with the simulation result
- No steady solution for $\dot\gamma < \dot\gamma_c^*$
- Two branches for $\dot\gamma > \dot\gamma_c^*$
  1. Upper branch well reproduces simulation results including the vicinity of $\dot\gamma_c^*$ (Even when we use linear plot)
  2. Lower branch is linearly unstable

Discussion



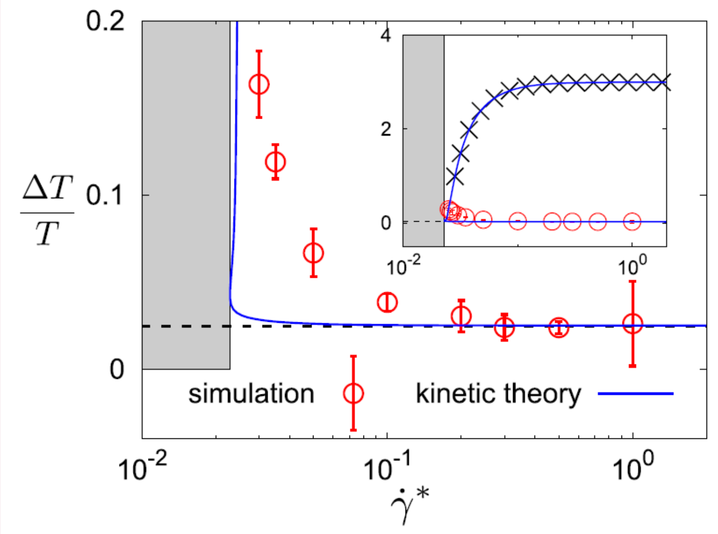
The shear viscosity and the temperature obtained by kinetic theory show good agreements with those of simulations.



BUT, the temperature difference

$$\Delta T \equiv \frac{P_{xx}^k - P_{yy}^k}{n}$$

shows a poor agreement!



Why?
We have no idea.

Summary

We have

(numerically)

- performed event-driven molecular dynamics simulations of granular gases having the square-well potential under a shear.
- found the consistency of the rheology curve with the Bagnold expression for high shear.
- not found any steady state in the low shear rate regime, but the effective rheology curve for the viscosity is consistent with the Bagnoldian expression.

(theoretically)

- constructed the kinetic theory of dilute cohesive granular gases under a shear.
- obtained the **consistent** results with simulations.