Mechanical Systems Engineering

5th week (jamming and rheology of dense matters),
Frontiers in Non-equilibrium Physics 2024

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

Kinetic theory of moderately dense dry granular particles under a simple shear

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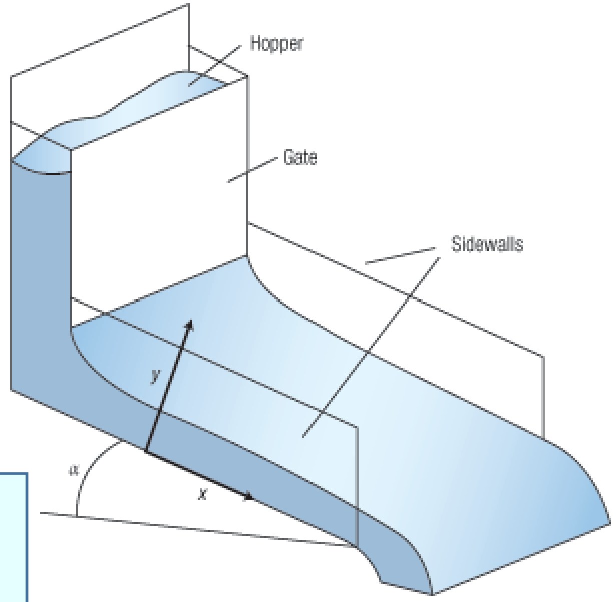
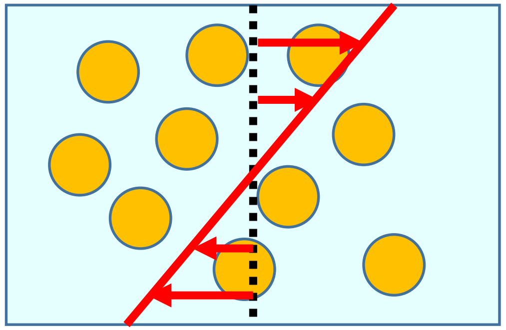
Introduction

- Understanding of rapid flow of dry granular particles is important.
- Our interest: Simple shear flow (e.g., bulk region of flow down inclined plane)
- Assumption:
  particles are frictionless and hard sphere (diameter σ, mass m)
  ⇒ Stress satisfies Bagnold's law
  $$\sigma_{xy} \sim m\dot{\gamma}^2/\sigma$$
- Kinetic theory (treating vel. dist. func.) is known to describe the flow.



shear

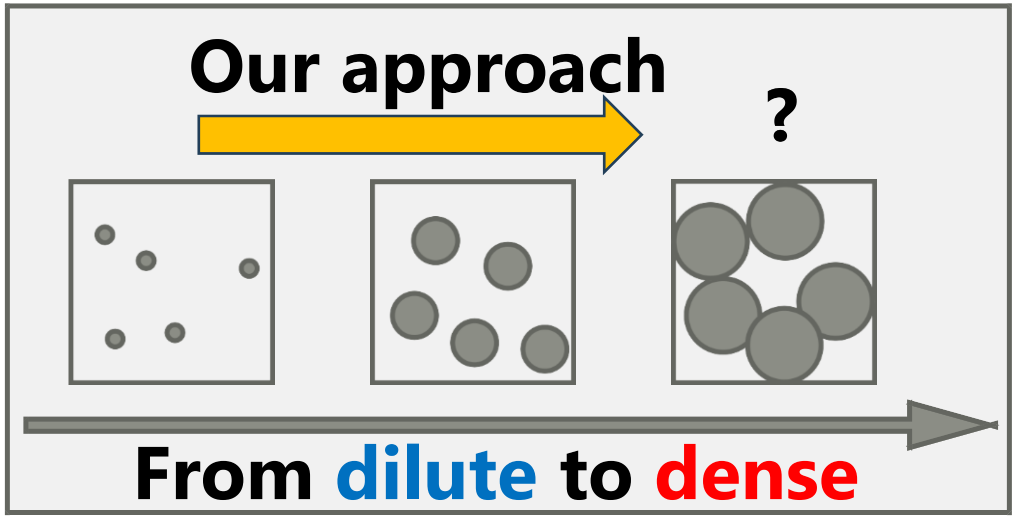


Our approach: hydrodynamic description

Try to derive hydrodyn. eqs.
for granular gas flows

Approach:
"From dilute to moderately dense"

- Dilute gases ($\varphi \ll 1$):
  inelastic Boltzmann equation
- Moderately dense gases ($\varphi \lesssim 0.5$):
  inelastic Enskog equation
- "Garzó and Dufty, PRE (1999)" is well-known.
  ⇒ Theory for homogeneous cooling state
  Many people use this theory "without doubt."

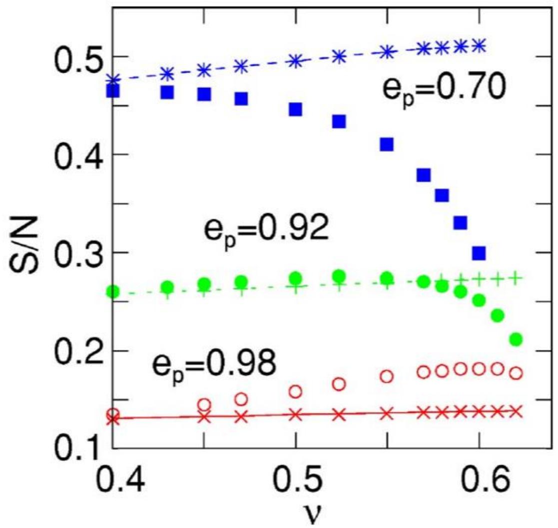


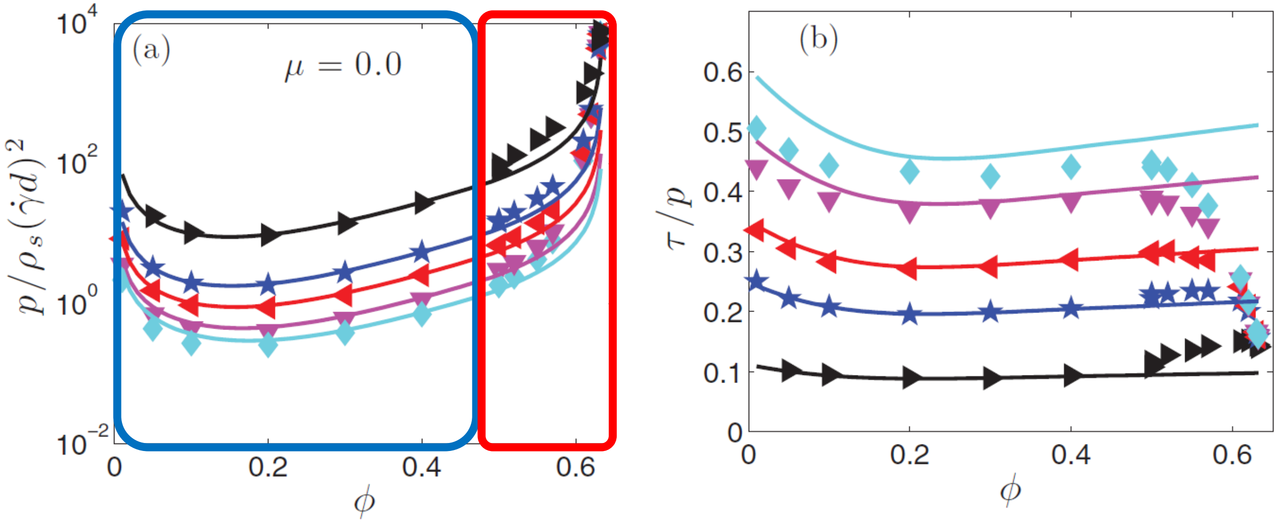
Boltzmann

Enskog

Validity of GD theory (Garzó and Dufty (1999))

- Validity of GD theory is examined by simulations.
  (e.g. Mitarai & Nakanishi (2007), Chialvo & Sundaresan (2013))





Theory seems to works well for $\varphi \lesssim 0.49$ (Alder transition).

- However, this theory is NOT applicable for sheared flows.
  ⇒ Why?

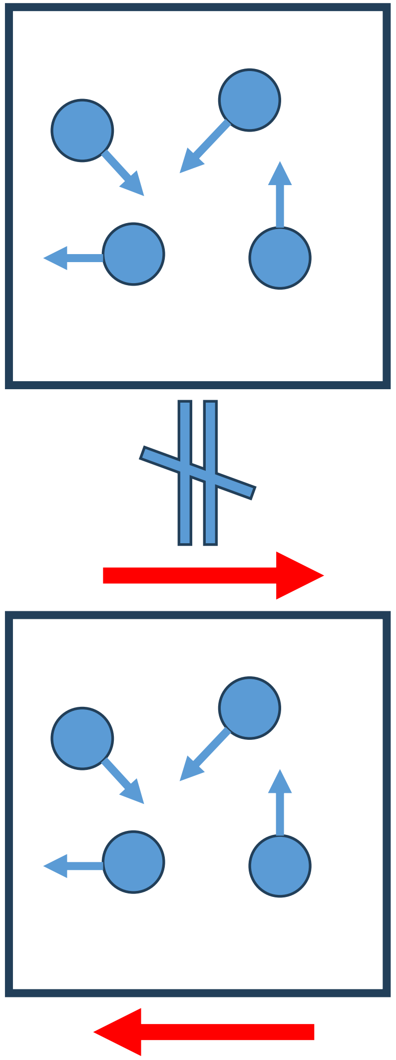
Difference between them

Answer: Base state is different!

- Garzó and Dufty's paper:
  = Homogenous cooling state (no external force)
  Base state is homogeneous and isotropic.
  ✓Viscosity: determined by the local fluctuation of velocity gradient

- Our interest = sheared flow
  Base state is homogeneous but anisotropic.
  ✓Viscosity: should be determined by homogeneous sheared state

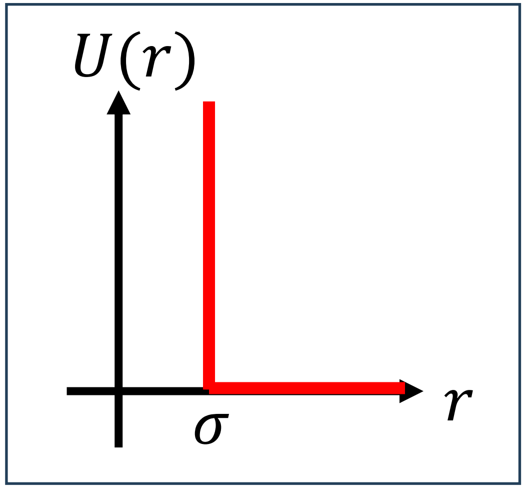
➡ **GD theory is NOT applicable as it is.**



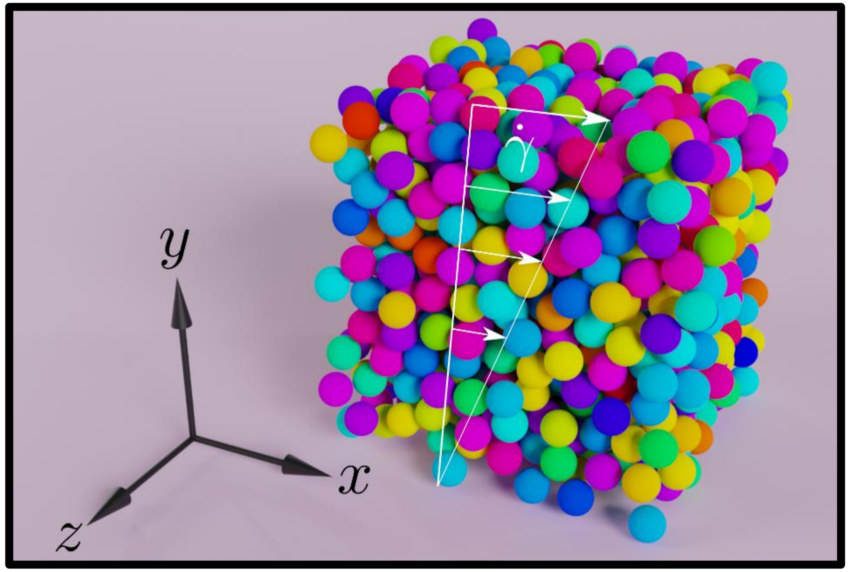
Our motivation:
To construct the theory by considering a proper base state.

Model and setup

- Particles:
  - monodisperse (mass m, diameter σ)
  - Frictionless hard-core potential
  - restitution coefficient $e(<1)$: constant



- Sheared periodic boundary condition (with SLLOD and Lees-Edwards)
  ⇒ no physical walls = "idealistic" condition
  But expected to be realized in the bulk region of the flow of inclined planes



- Event-driven simulations are also done to validate our theoretical results.

Kinetic theory of sheared granular flows

Starting equation (kinetic equation):

$$\left(\frac{\partial}{\partial t} - \dot{\gamma} V_y \frac{\partial}{\partial V_x}\right) f(\boldsymbol{V};t) = J\left(\boldsymbol{V}\middle|f^{(2)}\right)$$

shear — collisions

Time evol. of one-body vel. dist. func.

- **Collision integral: effect of binary collisions**

$$J\left[\boldsymbol{V}\middle|f^{(2)}\right] = \sigma^2 \int dv_2 \int d\hat{\sigma} \Theta(v_{12}\cdot\hat{\sigma})(v_{12}\cdot\hat{\sigma}) \left[\frac{1}{e^2} f^{(2)}(r, r-\sigma, v_1'', v_2'', t) - f^{(2)}(r, r+\sigma, v_1, v_2, t)\right]$$

$f^{(2)}(r_1, r_2, v_1, v_2, t)$: **two-body distribution function**

※ Kinetic eq. is not closed for one-body dist. func.

$$\int d\boldsymbol{V} m V_\alpha V_\beta \times (\text{kinetic eq.})$$

Time evol. of kinetic stress

$$\partial_t P^k_{\alpha\beta} + \dot{\gamma}\left(\delta_{\alpha x} P^k_{y\beta} + \delta_{\beta x} P^k_{y\alpha}\right) = -\Lambda_{\alpha\beta}$$

Kinetic part of the stress:

$$P^k_{\alpha\beta} \equiv m \int d\boldsymbol{V} V_\alpha V_\beta f(\boldsymbol{V}, t)$$

Collision moment:

$$\Lambda_{\alpha\beta} \equiv -m \int d\boldsymbol{V} V_\alpha V_\beta J\left(\boldsymbol{V}\middle|f^{(2)}\right)$$

Kinetic theory of sheared granular flows

Time evol. of kinetic stress

$$\partial_t P^k_{\alpha\beta} + \dot{\gamma}\left(\delta_{\alpha x} P^k_{y\beta} + \delta_{\beta x} P^k_{y\alpha}\right) = -\Lambda_{\alpha\beta}$$

Only xx, yy, zz, xy **components are important.**

Set of dynamic equations: for $T, \Delta T, \delta T, P^k_{xy}$

$$\partial_t T = -\frac{2}{3}\dot{\gamma} P^k_{xy} - \frac{1}{3}\Lambda_{\alpha\alpha}$$

$$\partial_t \Delta T = -\frac{2}{n}\dot{\gamma} P^k_{xy} - \frac{1}{n}\left(\Lambda_{xx} - \Lambda_{yy}\right)$$

$$\partial_t \delta T = -\frac{2}{n}\dot{\gamma} P^k_{xy} - \left(2\Lambda_{xx} + \Lambda_{yy} - \Lambda_{zz}\right)$$

$$\partial_t P^k_{xy} = -\dot{\gamma} P^k_{yy} - \Lambda_{xy}$$

Kinetic stress:

$$P^k_{\alpha\beta} \equiv m\int d\boldsymbol{V} V_\alpha V_\beta f(\boldsymbol{V}, t)$$

Temperature T **:**

$$T \equiv \frac{P^k_{xx} + P^k_{yy} + P^k_{zz}}{3n}$$

Anisotropic temperatures:

$$\Delta T \equiv \frac{P^k_{xx} - P^k_{yy}}{n}, \delta T \equiv \frac{P^k_{xx} - P^k_{zz}}{n}$$

Collisional contribution of stress:

$$P^c_{\alpha\beta} = \frac{1+e}{4} m g_0 \int dv_1 \int dv_2 \int d\hat{\sigma}\Theta(\hat{\sigma}\cdot v_{12})(\hat{\sigma}\cdot v_{12})^2 \hat{\sigma}_\alpha \hat{\sigma}_\beta \int_0^1 dx f^{(2)}(r - x\sigma, r + (1-x)\sigma, v_1, v_2; t)$$

Up to here, no approximation. BUT, not solvable!

Why? ⇒ not closed for the one-body distribution

Two-body distribution is included in

$$\Lambda_{\alpha\beta} \equiv -m\int d\boldsymbol{V} V_\alpha V_\beta J\left(\boldsymbol{V}\middle| f^{(2)}\right).$$

We need a closure.

Two approximations as closure

1. **Enskog's approximation:**
Two-body dist. ⇒ product of one-body dist. with radial dist. func.

$$f^{(2)}(r_1, r_1 \pm \sigma, v_1, v_2; t) \simeq g_0(|r_1 - r_2| = \sigma, \varphi) f(r_1, v_1, t) f(r_1 \pm \sigma, v_2, t)$$
$$\simeq g_0(\varphi) f(V_1; t) f\left(V_2 \mp \dot{\gamma} y \sigma \hat{\sigma}_y e_x; t\right)$$

Radial distribution at contact:
(Carnahan-Stirling formula and its denser extension)

$$g_0(\varphi) = \begin{cases} \dfrac{1 - \varphi/2}{(1-\varphi)^3} & (\varphi \le \varphi_{\mathrm{f}} = 0.49) \\ \dfrac{1 - \varphi_{\mathrm{f}}/2}{(1-\varphi_{\mathrm{f}})^3} \dfrac{\varphi_{\mathrm{J}} - \varphi_{\mathrm{f}}}{\varphi_{\mathrm{J}} - \varphi} & (\varphi_{\mathrm{f}} < \varphi < \varphi_{\mathrm{J}} = 0.639) \end{cases}$$

One-body dist.:
Assumption of uniform velocity profile
(System is uniform)

$$f(\boldsymbol{r} \pm \boldsymbol{\sigma}, \boldsymbol{v}_1, t) = f\left(\boldsymbol{V}_1 \mp \dot{\gamma} y \sigma \hat{\sigma}_y \boldsymbol{e}_x; t\right)$$

2. **Grad's approximation:**
expression of one-body dist.

$$f(\boldsymbol{V}; t) = f_{\mathrm{M}}(\boldsymbol{V}; t)\left(1 + \frac{m}{2T} \Pi_{\alpha\beta} V_\alpha V_\beta\right)$$

Maxwell distribution:

$$f_{\mathrm{M}}(\boldsymbol{V}; t) = n\left(\frac{m}{2\pi T}\right)^{3/2} \exp\left(-\frac{mV^2}{2T}\right)$$

Dimensionless kinetic stress:

$$\Pi_{\alpha\beta} \equiv \frac{P^k_{\alpha\beta}}{nT} - \delta_{\alpha\beta}$$

Dynamic equations

Dimensionless quantities:

$$\theta \equiv \frac{T}{m\sigma^2\dot{\gamma}^2}, \Delta\theta \equiv \frac{\Delta T}{m\sigma^2\dot{\gamma}^2}, \delta\theta \equiv \frac{\delta T}{m\sigma^2\dot{\gamma}^2}, \Pi_{xy}^* \equiv \frac{P_{xy}^k}{nm\sigma^2\dot{\gamma}^2}$$

After these two assumptions,

$\Lambda_{\alpha\beta}^*(\equiv \Lambda_{\alpha\beta}/nm\sigma^2\dot{\gamma}^3)$ **is closed for** $\theta, \Delta\theta, \delta\theta, \Pi_{xy}^*$.

Lower-order terms were already known ⇒

Santos, Montanero, Dufty, & Brey, PRE (1998)
Montanero, Garzó, Santos, & Brey, JFM (1999)
Takada, Hayakawa, Santos, & Garzó, PRE (2020)

This study: Full-order solutions are derived.

$$\Lambda_{\alpha\beta}^* = \frac{6\sqrt{2}}{\pi}(1+e)\varphi g_0 \theta^{3/2} \sum_{n=0}^{\infty} \theta^{-\frac{n}{2}} C_{\alpha\beta}^{(n)}(\theta, \Delta\theta, \delta\theta, \Pi_{xy}^*)$$

$1/\sqrt{\theta}$: expansion parameter

Set of closed dynamic equations:

$\tau \equiv \dot{\gamma} t$

$$\partial_\tau \theta = -\frac{2}{3}\Pi_{xy}^* - \frac{1}{3}\Lambda_{\alpha\alpha}^*$$

$$\partial_\tau \Delta\theta = -2\Pi_{xy}^* - (\Lambda_{xx}^* - \Lambda_{yy}^*)$$

$$\partial_\tau \delta\theta = -2\Pi_{xy}^* - (2\Lambda_{xx}^* + \Lambda_{yy}^* - \Lambda_{zz}^*)$$

$$\partial_\tau \Pi_{xy}^* = -\left(\theta - \frac{2}{3}\Delta\theta + \frac{1}{3}\delta\theta\right) - \Lambda_{xy}^*$$

Dynamics are determined by solving these coupled equations.

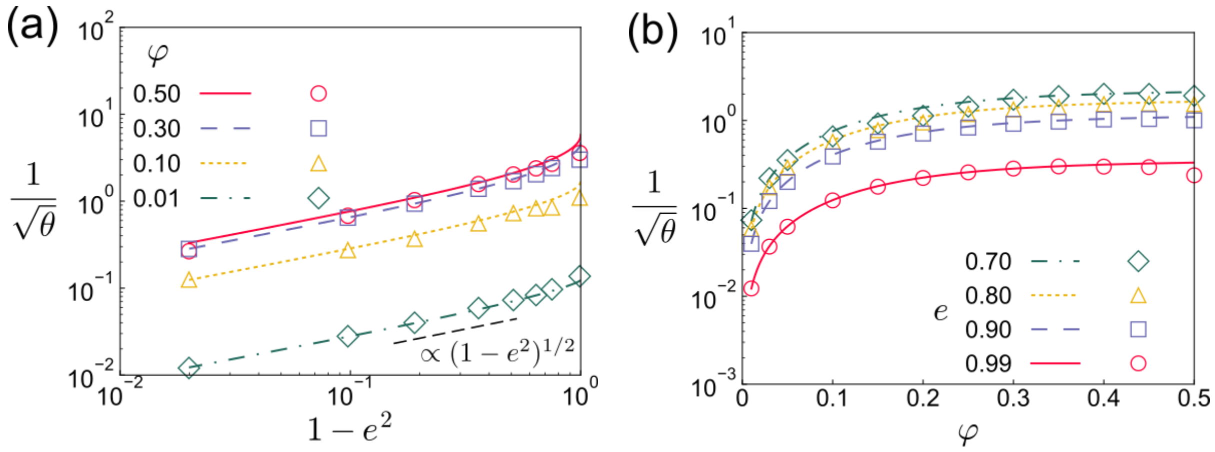
Collisional contribution of stress:

$$P_{\alpha\beta}^c(\boldsymbol{r},t) \approx \frac{1+e}{4} m\sigma^3 \int d\boldsymbol{V}_1 \int d\boldsymbol{V}_2 \int d\widehat{\boldsymbol{\sigma}} \Theta(\boldsymbol{V}_{12}\cdot\widehat{\boldsymbol{\sigma}})(\boldsymbol{V}_{12}\cdot\widehat{\boldsymbol{\sigma}})^2$$
$$\times \widehat{\sigma}_\alpha \widehat{\sigma}_\beta f\left(\boldsymbol{V}_1 + \frac{1}{2}\dot{\gamma}\sigma\widehat{\sigma}_y \boldsymbol{e}_x\right) f\left(\boldsymbol{V}_2 - \frac{1}{2}\dot{\gamma}\sigma\widehat{\sigma}_y \boldsymbol{e}_x\right)$$

Convergence of the expansion

Some previous studies treated only few terms...

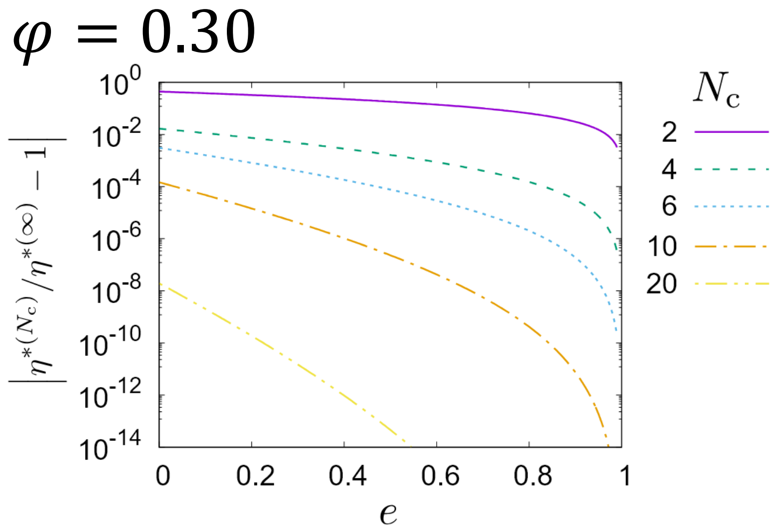
☞ Takada, Hayakawa, Santos, & Garzó PRE (2020)



Question:
How does the truncation of $\Lambda^*_{\alpha\beta}$ affect the results?

$$\Lambda^*_{\alpha\beta} = \frac{6\sqrt{2}}{\pi}(1+e)\varphi g_0 \theta^{3/2} \sum_{n=0}^{N_c} \mathcal{C}^{(n)}_{\alpha\beta} \left(\frac{1}{\sqrt{\theta}}\right)^n$$

For $e \ll 1$ (highly inelastic situation)
or finite φ (moderately dense situation),
the parameter $1/\sqrt{\theta}$ becomes larger.



Convergence is very slow.
⇒ needs a lot of terms

Steady dynamics

We now focus on the steady-state.

Set of dynamic eqs.:

$$0 = -\frac{2}{3}\Pi^*_{xy} - \frac{1}{3}\Lambda^*_{\alpha\alpha}$$

$$0 = -2\Pi^*_{xy} - (\Lambda^*_{xx} - \Lambda^*_{yy})$$

$$0 = -2\Pi^*_{xy} - \left(2\Lambda^*_{xx} + \Lambda^*_{yy} - \Lambda^*_{zz}\right)$$

$$0 = -\left(\theta - \frac{2}{3}\Delta\theta + \frac{1}{3}\delta\theta\right) - \Lambda^*_{xy}$$

List of scaled quantities:

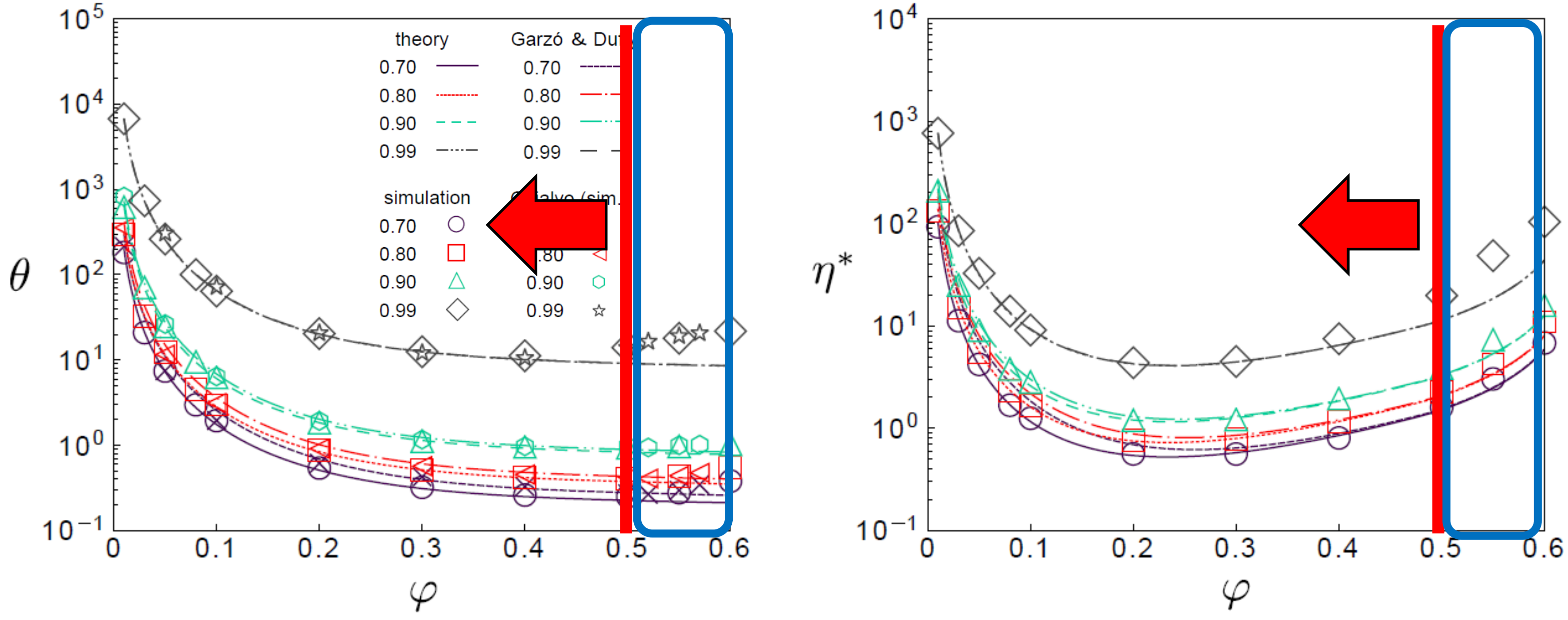
- **Temperature:** θ
- **Viscosity:** $\eta^* := -(\Pi^*_{xy} + \Pi^{c*}_{xy})$
- **Macroscopic friction coefficient:** $\mu := -P_{xy}/P$
- **Normal stress differences:** $N_1 := (P_{xx} - P_{yy})/P$, $N_2 := (P_{yy} - P_{zz})/P$

$$P^c_{\alpha\beta}(\boldsymbol{r},t) \approx \frac{1+e}{4} m\sigma^3 \int d\boldsymbol{V}_1 \int d\boldsymbol{V}_2 \int d\hat{\boldsymbol{\sigma}} \Theta(\boldsymbol{V}_{12}\cdot\hat{\boldsymbol{\sigma}})(\boldsymbol{V}_{12}\cdot\hat{\boldsymbol{\sigma}})^2 \times \hat{\sigma}_\alpha \hat{\sigma}_\beta f\left(\boldsymbol{V}_1 + \frac{1}{2}\dot{\gamma}\sigma\hat{\sigma}_y \boldsymbol{e}_x\right) f\left(\boldsymbol{V}_2 - \frac{1}{2}\dot{\gamma}\sigma\hat{\sigma}_y \boldsymbol{e}_x\right),$$

We will plot these quantities against the volume fraction φ and the restitution coefficient e.

Scaled kinetic temperature & viscosity

Plots of θ and η^* against the volume fraction φ (for various e)

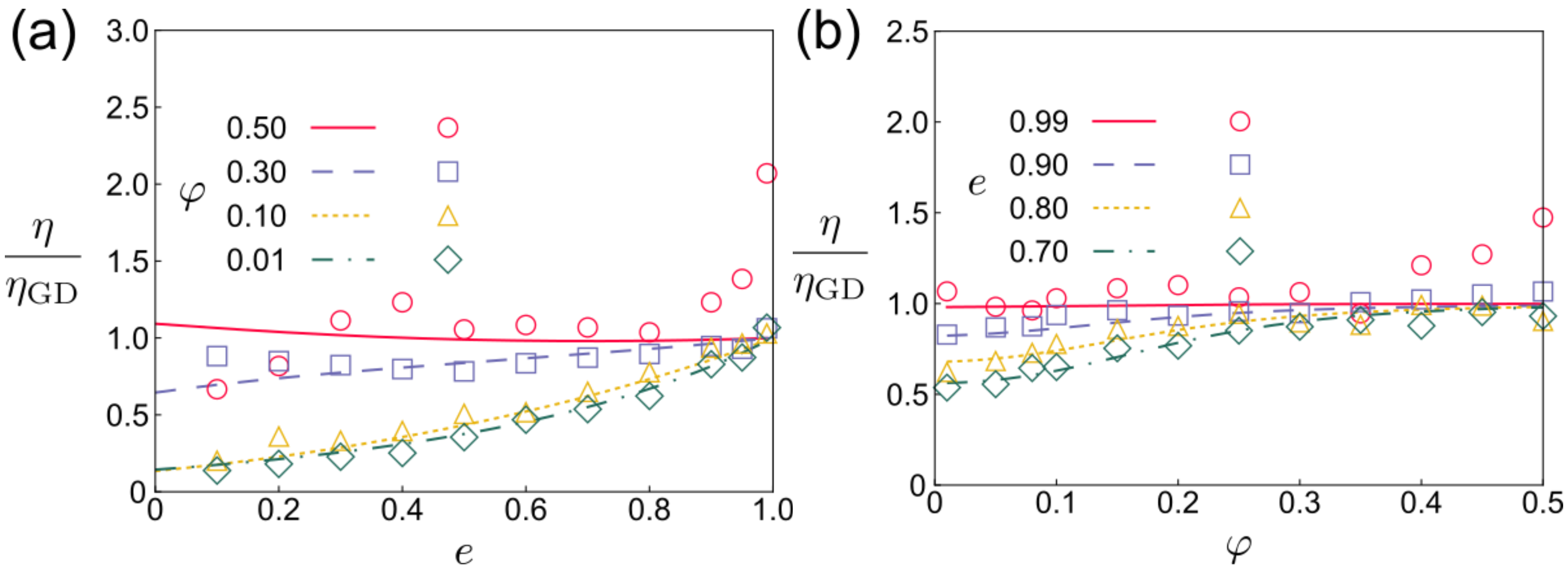


Shows good agreement with the MD simulations up to 50%.
But seems also good with the theory by Garzó and Dufty (1999)?
No difference? Why?

This is a log-plot magic!

Kinetic temperature & viscosity

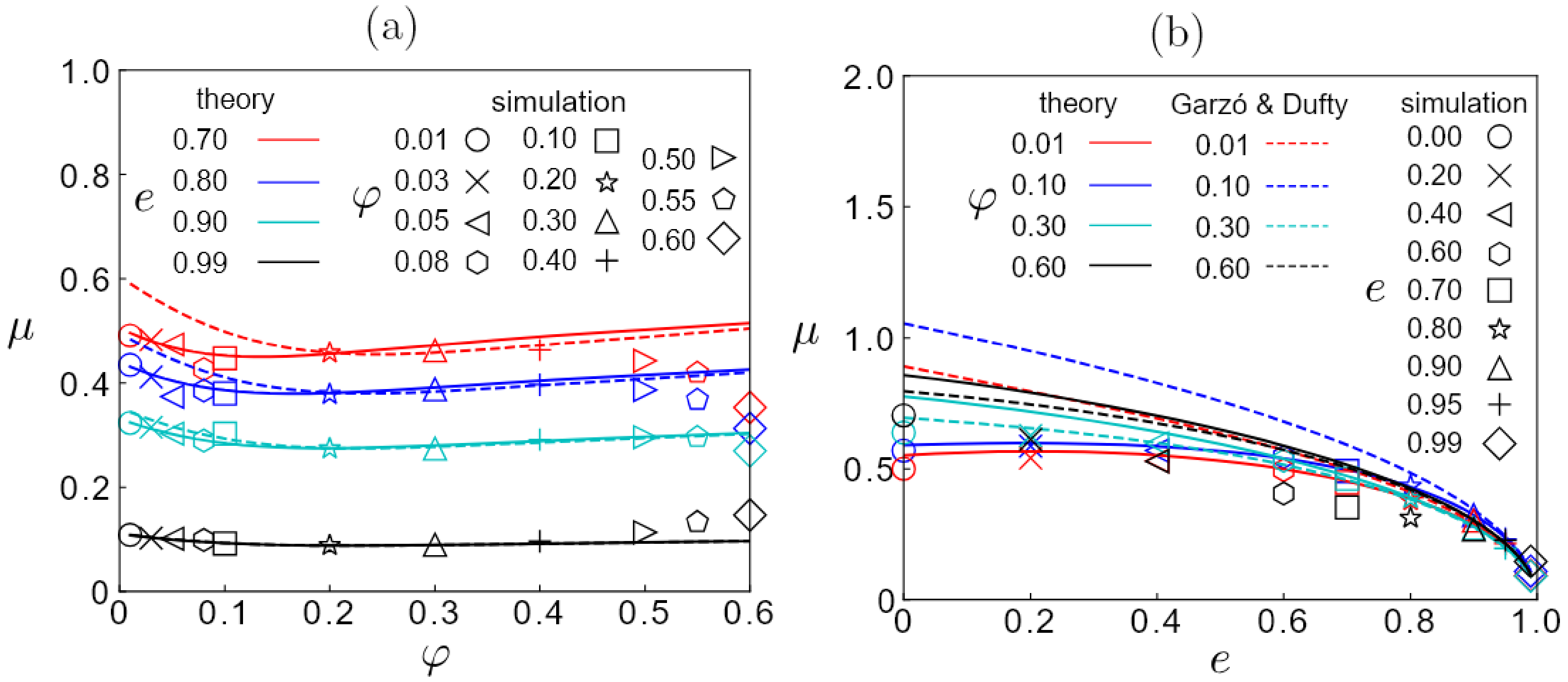
Ratio of the viscosity η from our theory to Garzó and Dufty's theory η_{GD} against the restitution coefficient e and the volume fraction φ



Garzó and Dufty's theory: deviations for $e \ll 1$ or $\varphi \ll 1$
⇒ Our theory can capture the behavior.
However…
Our theory: discrepancy appears for $\varphi \geq 0.4$ and $e \geq 0.9$
Why? This might be because $e = 1$ is singular.

(Macroscopic) friction coefficient

(Macroscopic) friction coefficient $\mu \equiv -P_{xy}/P$



Better agreement for dilute regime
Poor agreement for dense regime ($\varphi \geq 0.5$)

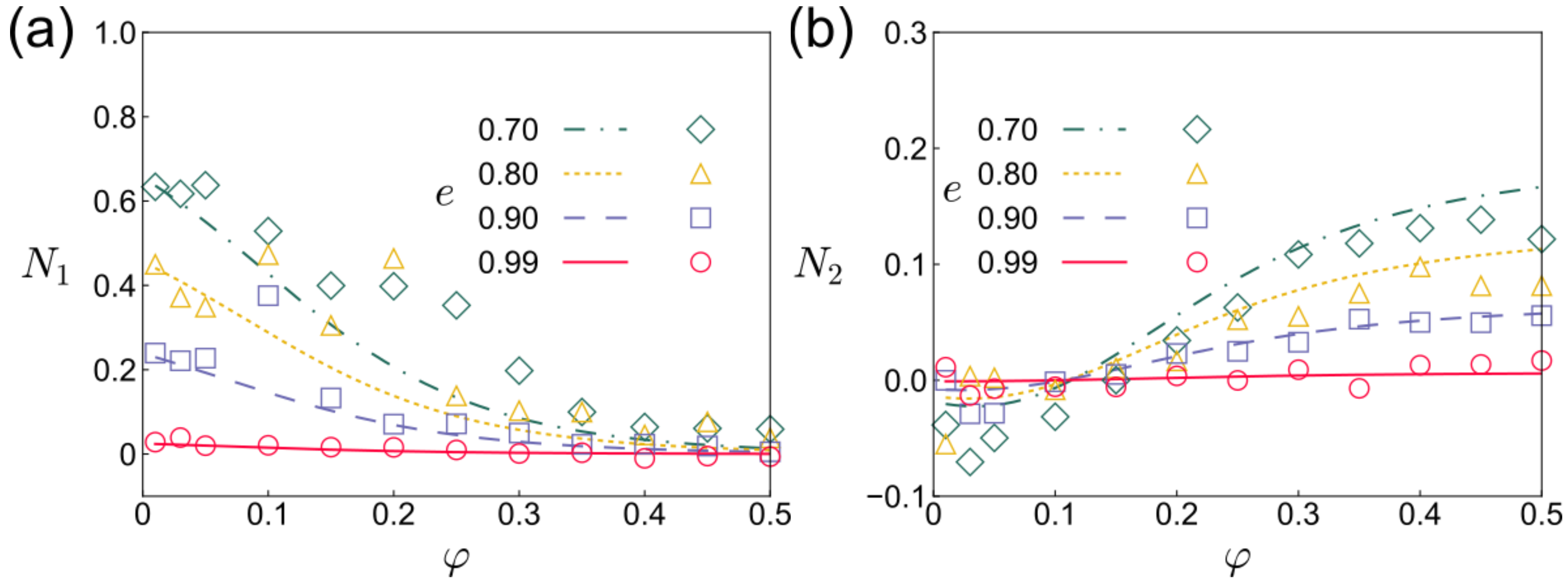
$\varphi_c \simeq 0.5$ might be the upper limit of the kinetic theory.

Normal stress differences

Normal stress differences:

$$\mathcal{N}_1 \equiv \frac{P_{xx} - P_{yy}}{P}, \mathcal{N}_2 \equiv \frac{P_{yy} - P_{zz}}{P}$$

- Because the system is anistropic, the normal stress differences are also important.
- GD theory cannot explain these quantities.



Qualitatively agree with each other.
However, the theory underestimates $\mathcal{N}_2$ for $\varphi \ll 1$.
Why?

Comparison with similar approach

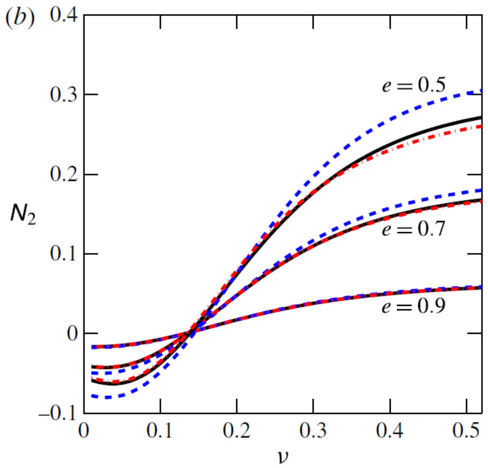
- Saha & Alam JFM (2016) constructed the theory in terms of the anisotropic Gaussian model.

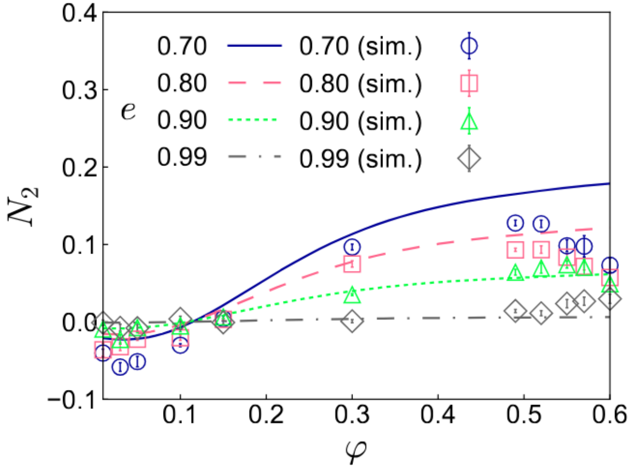
$$f(\boldsymbol{c}, \boldsymbol{x}, t) = \frac{n}{(8\pi^3|\boldsymbol{M}|)^{1/2}} \exp\left(-\frac{1}{2}\boldsymbol{C}\cdot\boldsymbol{M}^{-1}\cdot\boldsymbol{C}\right)$$

Grad's approximation:

$$f(\boldsymbol{V};t) = f_{\mathrm{M}}(\boldsymbol{V};t)\left(1+\frac{m}{2T}\Pi_{\alpha\beta}V_\alpha V_\beta\right)$$

- Behaviors of almost of the quantities are similar.





Their theory captures the behavior of N_2 in the dilute regime.
⇒ Their theory seems superior to our theory.
⇒ Other corrections are needed in our theory?

Modification: Effect of non-Gaussianity

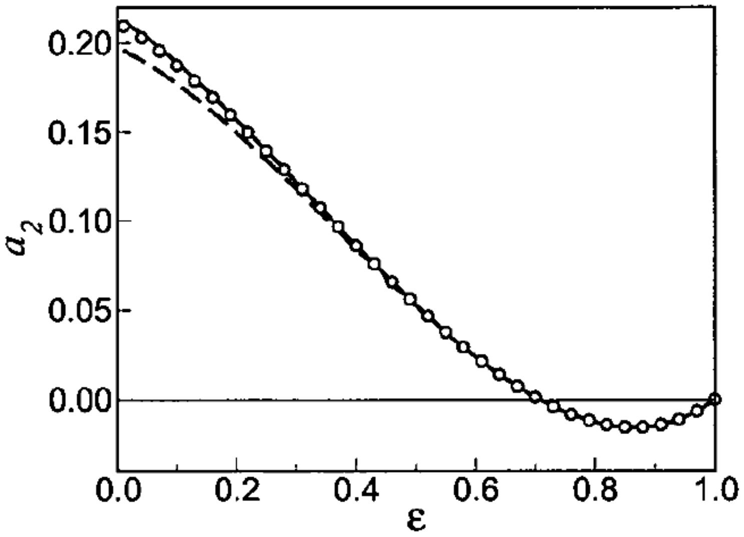
Our present approach:
Expansion around the Maxwellian

$$f(\boldsymbol{V};t) = f_{\mathrm{M}}(\boldsymbol{V};t)\left(1+\frac{m}{2T}\Pi_{\alpha\beta}V_\alpha V_\beta\right)$$

Maxwell distribution:

$$f_{\mathrm{M}}(\boldsymbol{V};t) = n\left(\frac{m}{2\pi T}\right)^{3/2}\exp\left(-\frac{mV^2}{2T}\right)$$

"Non-Gaussianity" is important even in homogeneous cooling state!
(Sonine polynomials are often used as polynomial expansion.)

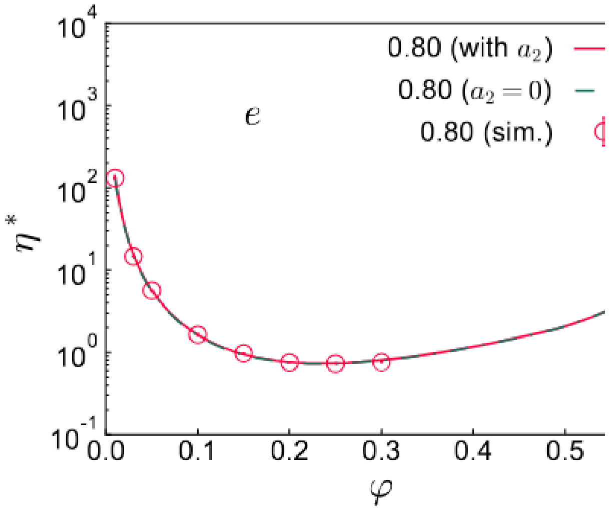


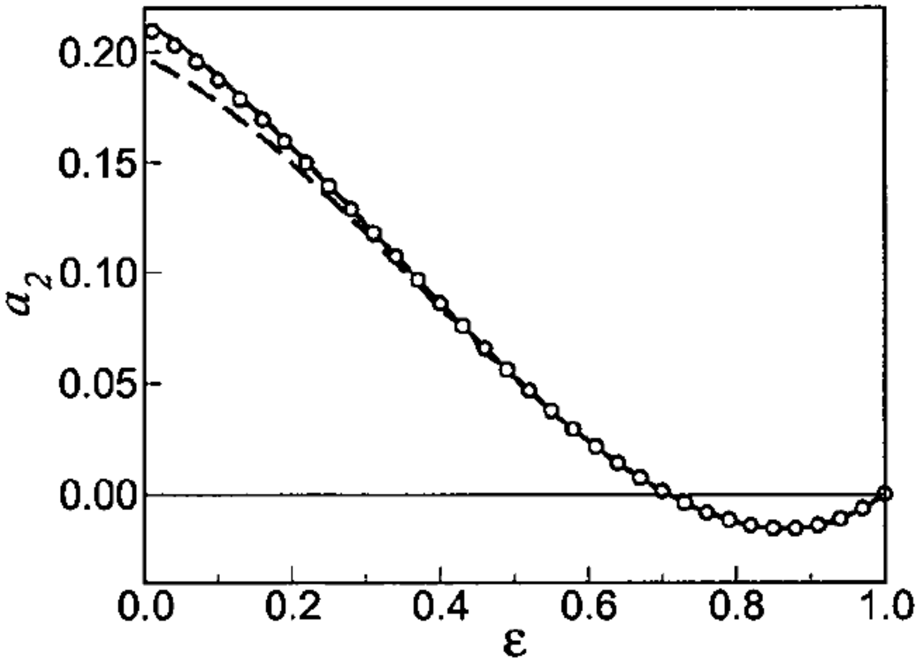
$$f(\boldsymbol{V};t) = f_{\mathrm{M}}(\boldsymbol{V};t)\left\{1+a_2\left[\frac{1}{2}\left(\frac{mV^2}{2T}\right)^2-\frac{5}{2}\frac{mV^2}{2T}+\frac{15}{8}\right]\right\}\left(1+\frac{m}{2T}\Pi_{\alpha\beta}V_\alpha V_\beta\right)$$

a_2 determines the magnitude of non-Gaussianity.
(van Noije & Ernst (1998))

a_2 changes the results?

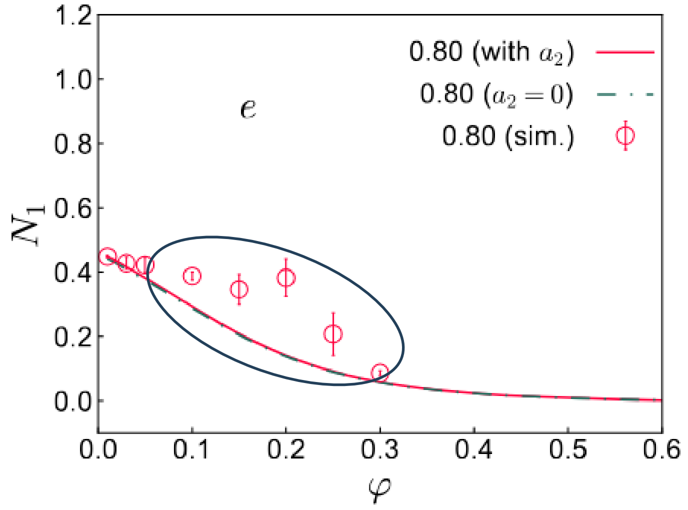
a_2 correctio… …lasticity)

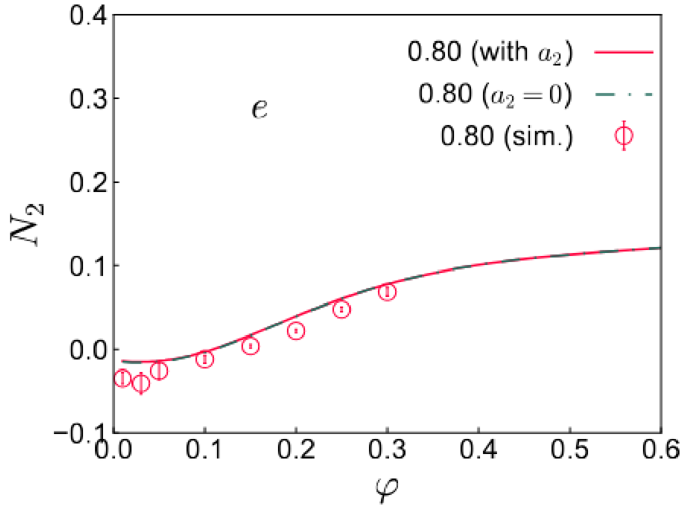




…iscosity & frict. coeff.
…e insensitive to a_2.

…ood agreements,
…ut the correction is invisible.

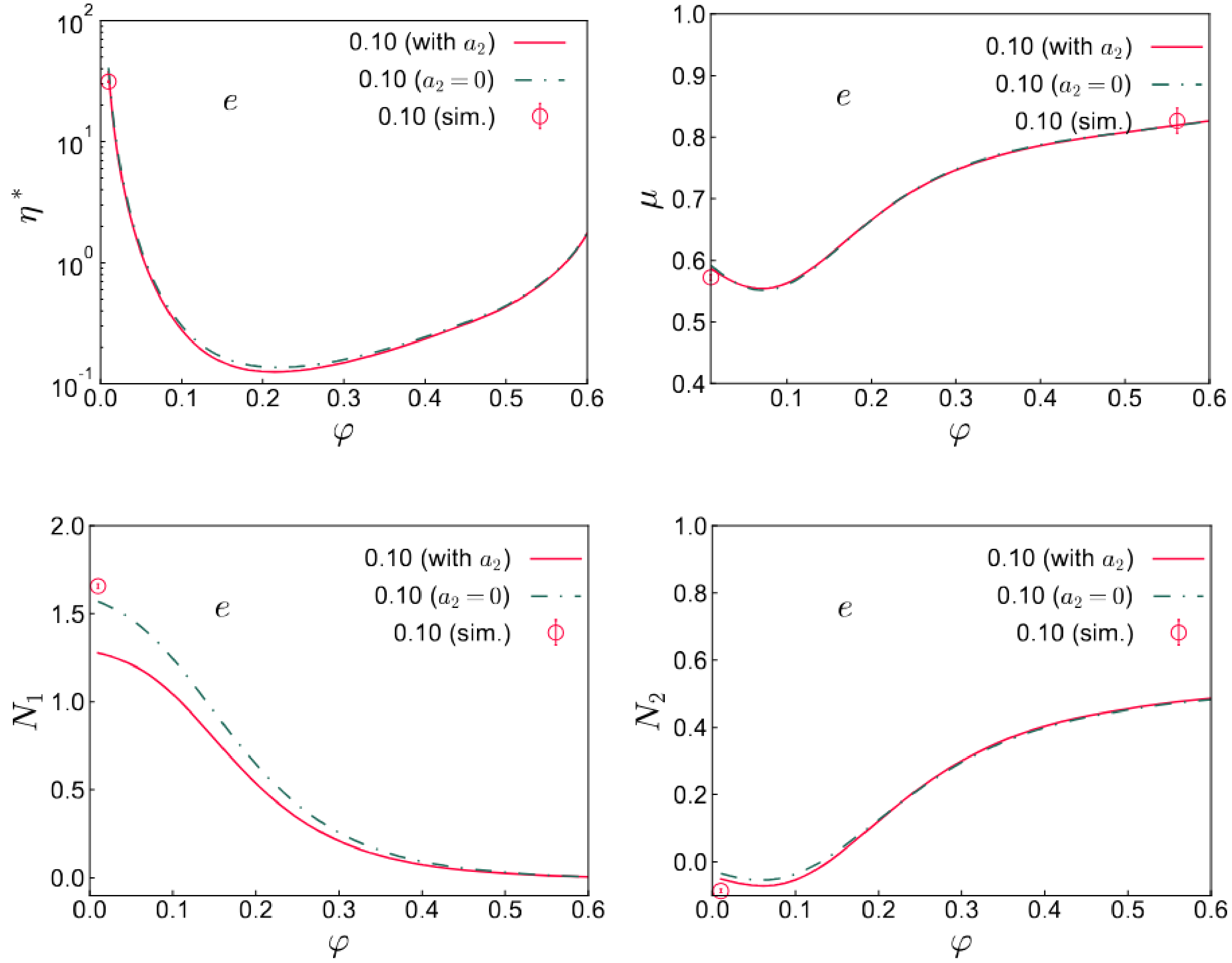




Still poor agreements
Why?

Non-Gaussianity $a_2 \simeq 0$
for $e \simeq 0.8$
What happens for
strong inelastic case?

a_2 correction : $e \simeq 0.1$ (strong inelasticity)



Viscosity & frict. coeff. are still insensitive to a_2.

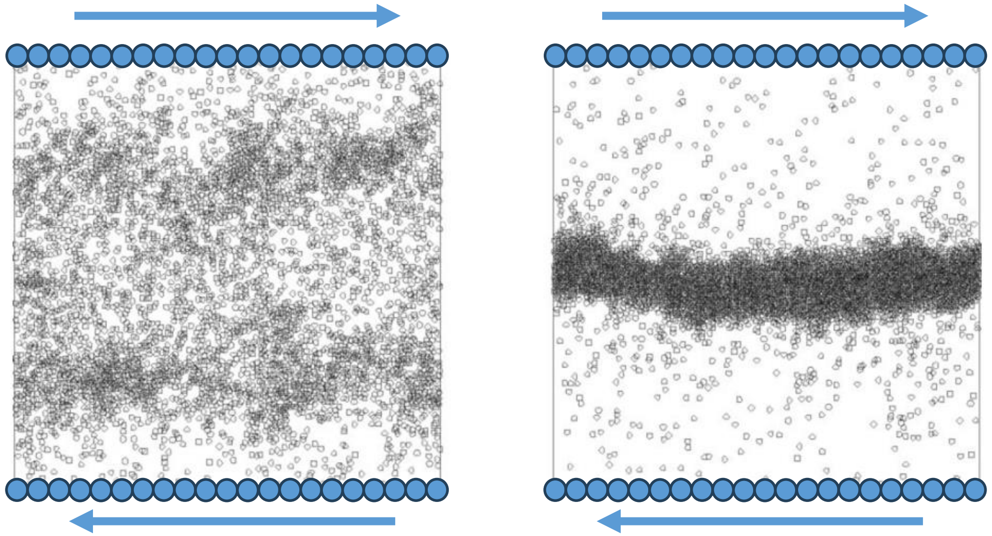
⇕

Normal stress diffs. are sensitive to a_2.

Although the simulation data are insufficient, the trend of N_2 seems good, but that of N_1 seems bad.
⇒ I have no idea.

Discussion: Existence of physical walls

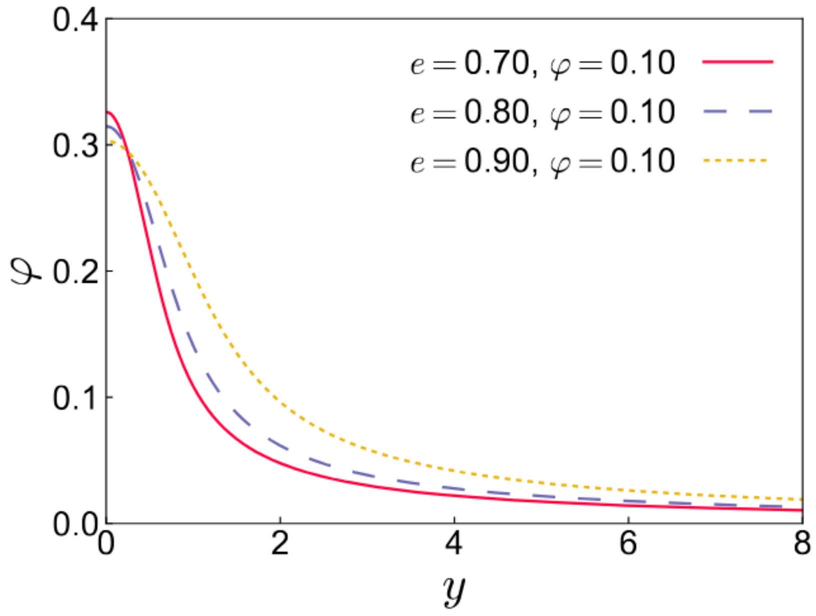
Physical (bumpy) wall "kicks" particles inward.
⇒ Walls violate homogeneity of the system.



Saitoh & Hayakawa,
Phys. Rev. E **75**, 021302 (2007)

2D case was solved by Saitoh & Hayakawa.
Particles gather in the center of the system.

Assumption used in the previous part (homogeneity) becomes invalid.



We should solve the hydrodynamic eqs. more seriously!

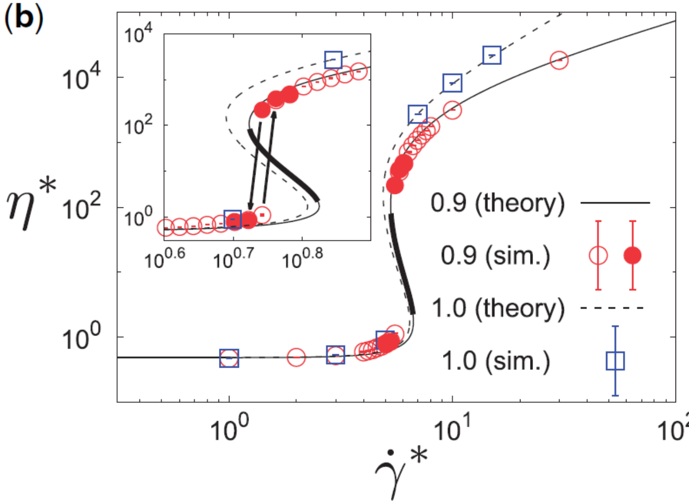
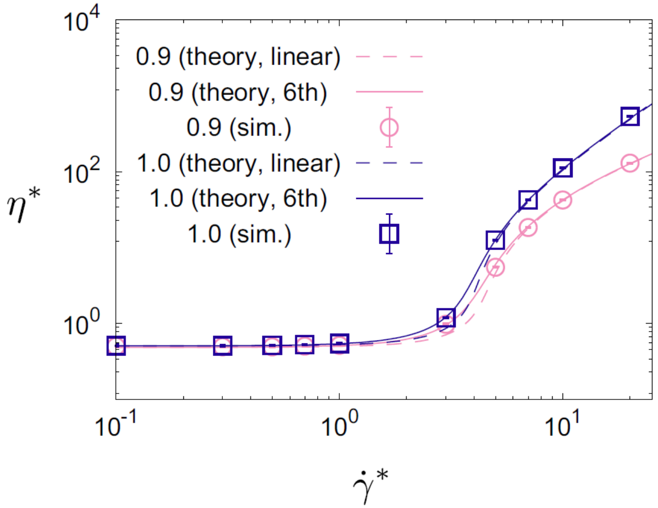
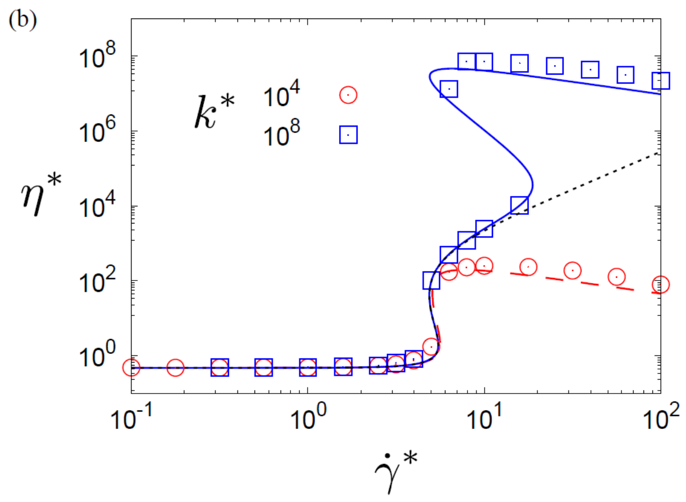
$$D_t\rho = -\rho\nabla\cdot\boldsymbol{v},$$

$$\rho D_t\boldsymbol{v} = -\nabla\cdot\boldsymbol{P},$$

$$\rho D_t T = -\boldsymbol{P}:(\nabla\boldsymbol{v}) - \nabla\cdot\boldsymbol{q} - \chi,$$

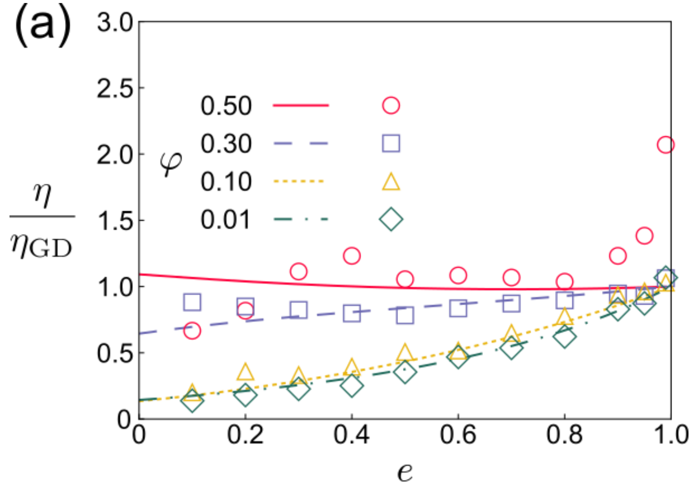
Kinetic theoretical treatments to different systems

- Similar approach for inertial suspensions
  ⇒ Good agreements with simulations

Hard-core		Soft-core
 **Discontinuous jump of viscosity for $\varphi \ll 1$** Hayakawa & Takada, PTEP **2019**, 083J01 (2019)	 **Discontinuous to continuous as $\varphi \nearrow$** Hayakawa, Takada, & Garzó, Phys. Rev. E **96**, 042903 (2017) Takada, Hayakawa, Santos, & Garzó, Phys. Rev. E **102**, 022907 (2020)	 **Two-step discontinuous jump** Sugimoto & Takada, J. Phys. Soc. Jpn. **89**, 084803 (2020)

Summary

- We have revisited the kinetic theory for sheared granular flows.
  - We have constructed the theory using a proper base state.
  - Full-order solution of the collision moment is derived.
- Results
  - Kinetic theory well describes sheared granular flows at least for $\varphi \lesssim 0.5$.
  - Friction coefficient μ is well reproduced, but normal stress differences are not.



- Questions (and future work)
  - Non-Gaussianity of the vel. dist. func. is important for $e \ll 1$?
  - Physical wall violates homogeneity.