Theory of dense granular flows for divergence of the viscosity

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Abstract

- This work is based on the collaboration with Dr. Koshiro Suzuki (Cannon Inc.).
- We have succeeded that the critical behavior in the vicinity of the jamming transition can be described by a microscopic theory based on the Liouville equation.
- The reference is K. Suzuki and H. Hayakawa, PRL in press (arXiv:1506. 02368).

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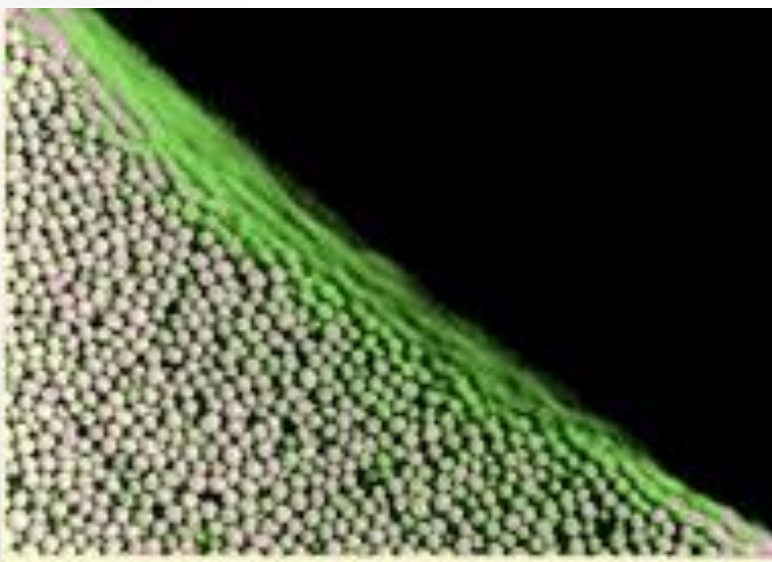
Introduction

- Granular materials behave as unusual solids and liquids.
- Jamming is an athermal solid-liquid transitions.



Flow of mustard seeds @Chicago group

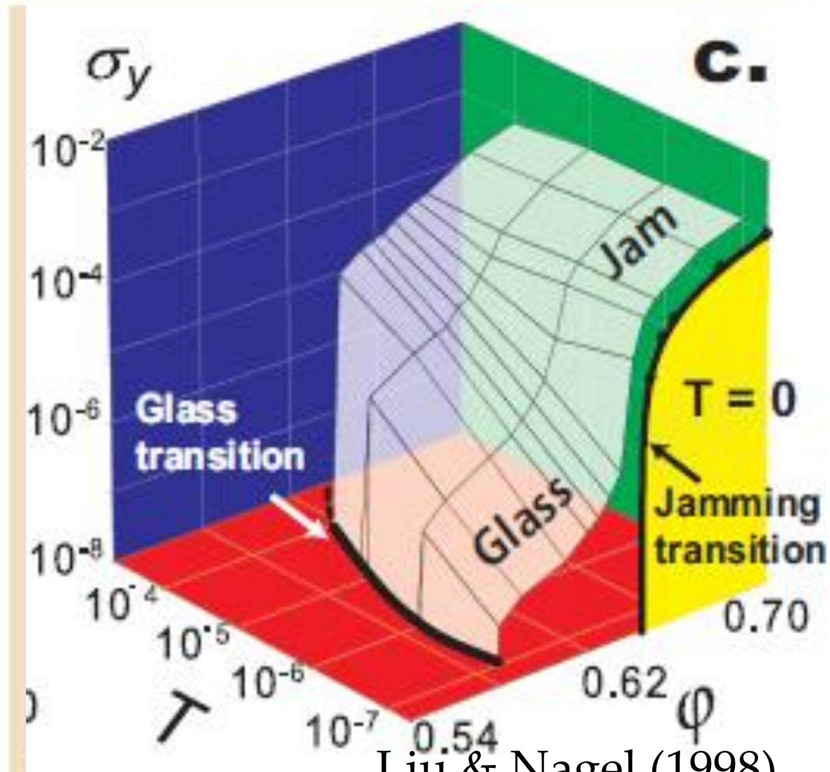
Kamigamo shrine (Kyoto!)

Characteristics of granular materials

- Most important characteristics is that each grain is dissipative.
- Thermal fluctuation does not affect any aspect of grains' motion.
- As a result, there is no equilibrium state.
- If we add an external force such as flow by gravity, air flow and shear, the system can reach a nonequilbrium steady state.
- Thus, to study granular materials is to study non-equilibrium statistical mechanics.

Jamming transition

- Above the critical density, the granules has rigidity and behaves as a solid.
- This transition is known as the jamming transition.



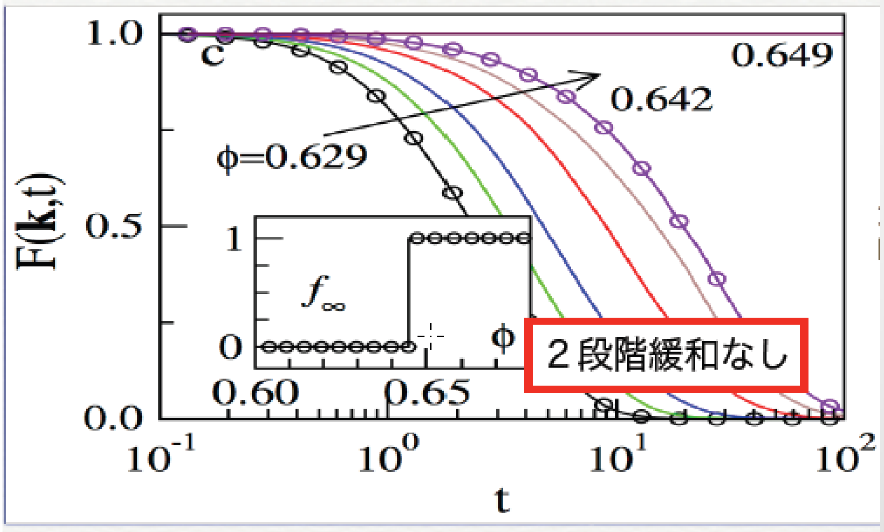
Liu & Nagel (1998)

Ikeda-Berthier-Sollich (2012)

Differences between jamming and glass transitions

- Although both describes the freezing of motion, there are some differences between two.
- Most important differences is that the jamming is the phase transition, but glass is not.
- There is no plateau of time correlation in the jamming.

[M.P.Ciamarra, A.Coniglio, PRL**103** (2009) 23570



e=0.88

Divergence of viscosity

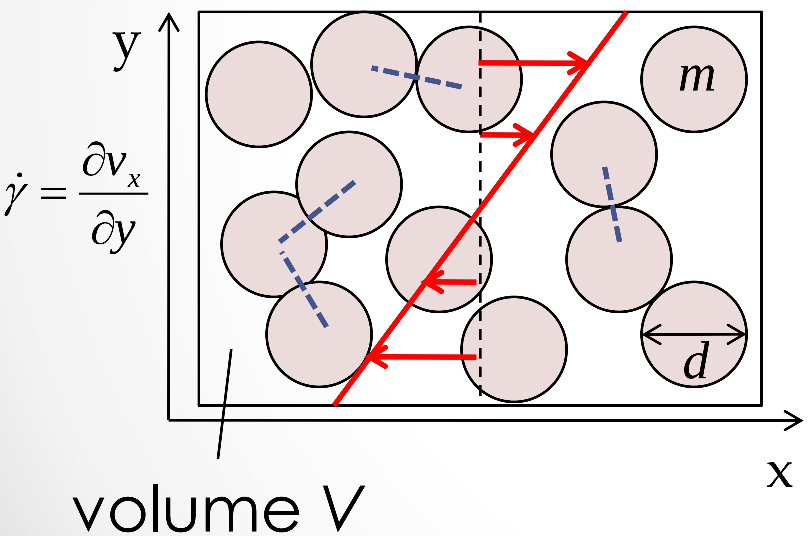
- Approach from below the jamming, the most important characteristics is the divergence of the viscosity at the jamming.

$$\eta \sim (\varphi_J - \varphi)^{-\lambda} \text{ with } \lambda \approx 2$$

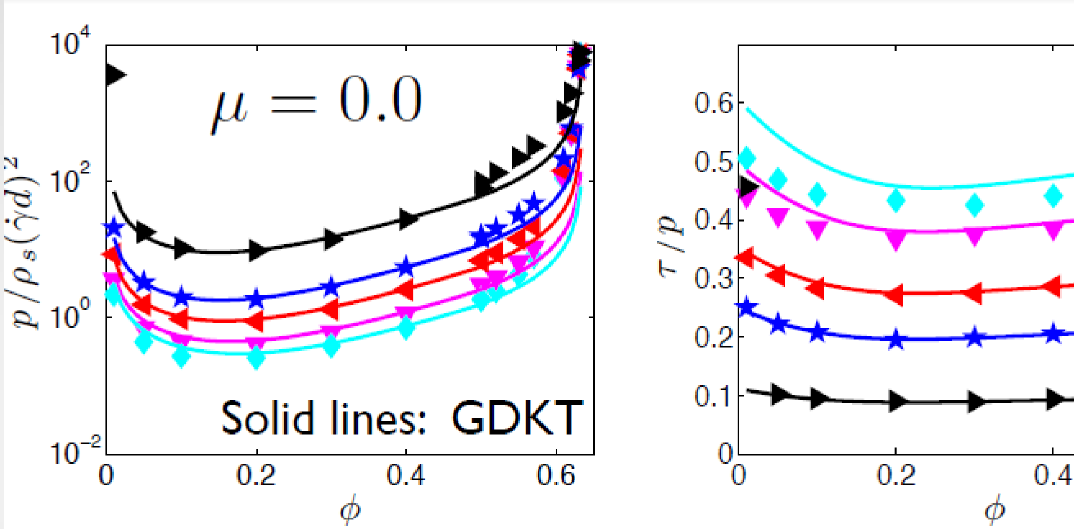
- Kawasaki et al estimated as $1.67 < \lambda < 2.5$.
- This divergence with $\lambda = 2$ is known even in colloid systems (see e.g. Brady 1993).
- However, some people indicated that λ for granular materials is larger than the estimated value.

Granular systems under a plane shear

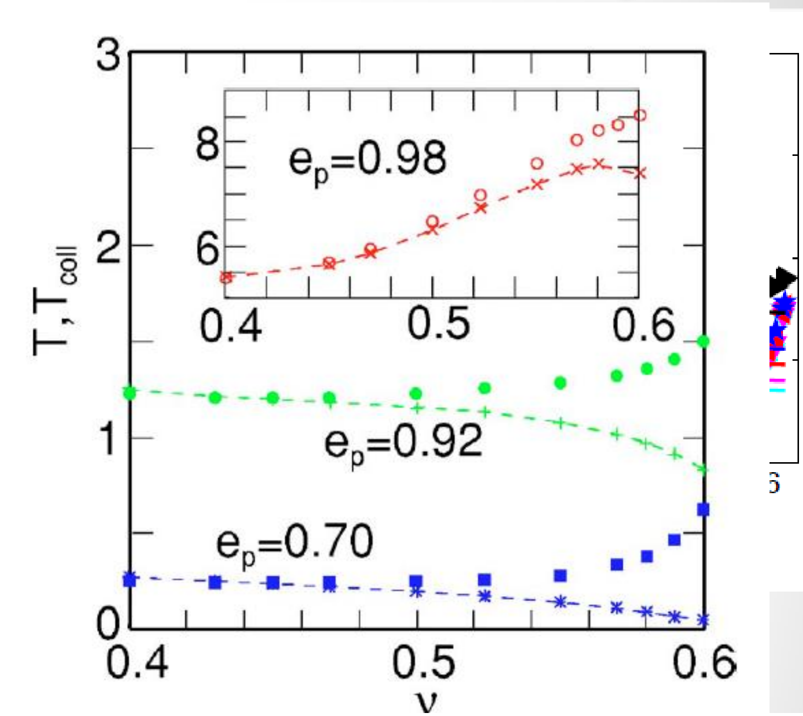
- Granular systems under uniform steady shear (SLLOD dynamics and Lees-Edwards boundary condition)



Limitation of Kinetic Theory



S. Chialvo and S. Sundaresan, Phys. Fluid. **25**, 0
rate.



- Kinetic theory of Gai
  $\phi < 0.5$ (around Alder

N. Mitarai and H. Nakanishi, PRE75, 031305 (2007)
The agreement of the temperature is poor.

- So we need to construct a new approach for dense sheared granular flow.

Contents

Equation of motion

- Newton's equation (equivalent to Liouville equation)

$$m\ddot{\boldsymbol{r}}_i = \boldsymbol{F}_i^{(\mathrm{el})} + \boldsymbol{F}_i^{(\mathrm{vis})} \quad (i = 1, \cdots, N),$$

$$\boldsymbol{F}_i^{(\mathrm{el})} = -\partial U / \partial \boldsymbol{r}_i = \sum_{j \neq i} \boldsymbol{F}_{ij}^{(\mathrm{el})}$$

$$\boldsymbol{F}_{ij}^{(\mathrm{el})} = -\frac{\partial u(r_{ij})}{\partial \boldsymbol{r}_{ij}} = \Theta(d - r_{ij}) f(d - r_{ij}) \hat{\boldsymbol{r}}_{ij}$$

$$f(x) = \kappa x \quad (\kappa > 0)$$

$$\boldsymbol{F}_{ij}^{(\mathrm{vis})} = -\zeta \Theta(d - r_{ij}) \hat{\boldsymbol{r}}_{ij} (\boldsymbol{g}_{ij} \cdot \hat{\boldsymbol{r}}_{ij}). \qquad \boldsymbol{g}_{ij} \equiv \boldsymbol{v}_i - \boldsymbol{v}_j$$

Liouville equation

- Liouville equation is equivalent to Newton's equation.
- An arbitrary observable A($\Gamma(t)$) satisfies

$$\boldsymbol{\Gamma}(t) = \{\boldsymbol{r}_i(t), \boldsymbol{p}_i(t)\}_{i=1}^{N}$$

$$\frac{d}{dt}A(\boldsymbol{\Gamma}(t)) = \dot{\boldsymbol{\Gamma}} \cdot \frac{\partial}{\partial \boldsymbol{\Gamma}} A(\boldsymbol{\Gamma}(t)) \equiv i\mathcal{L}A(\boldsymbol{\Gamma}(t)).$$

- The distribution function satisfies

$$\frac{\partial \rho(\boldsymbol{\Gamma}, t)}{\partial t} = -\frac{\partial}{\partial \boldsymbol{\Gamma}} \cdot \left[\dot{\boldsymbol{\Gamma}} \rho(\boldsymbol{\Gamma}, t)\right] = -\left[\dot{\boldsymbol{\Gamma}} \cdot \frac{\partial}{\partial \boldsymbol{\Gamma}} + \Lambda(\boldsymbol{\Gamma})\right] \rho(\boldsymbol{\Gamma}, t)$$

$$\Lambda(\boldsymbol{\Gamma}) = -\frac{\zeta}{m} \sum_{i,j} \Theta(d - r_{ij}) < 0$$

Energy balance equation

- Hamiltonian

$$\mathcal{H}(\boldsymbol{\Gamma}) = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + {\sum_{i,j}}' u(r_{ij})$$

- Satisfies the energy balance equation

$$\dot{\mathcal{H}} = -\dot{\gamma} V \sigma_{xy} - 2\mathcal{R}.$$

$$\sigma_{\mu\nu}(\boldsymbol{\Gamma}) = \frac{1}{V} \sum_{i=1}^{N} \left[\frac{p_i^{\mu} p_i^{\nu}}{m} + r_i^{\nu} \left(F_i^{(\mathrm{el})\mu} + F_i^{(\mathrm{vis})\mu} \right) \right]$$

$$\mathcal{R}(\boldsymbol{\Gamma}) = -\frac{1}{2} \sum_{i=1}^{N} \dot{\boldsymbol{r}}_i \cdot \boldsymbol{F}_i^{(\mathrm{vis})} = -\frac{1}{4} {\sum_{i,j}}' \boldsymbol{g}_{ij} \cdot \boldsymbol{F}_{ij}^{(\mathrm{vis})}$$

Contents

Perturbation of the Liouville equation

- Liouville equation contains 6N dimensional distribution.
- This cannot be exactly solved because it contains too many degrees of freedom.
- Unperturbed state: canonical distribution (no dissipation)
    - This corresponds to the degenerated unperturbed state.
    - Zero-eigenmodes correspond to the density, momentum and energy conservations.
- Perturbation: inelasticity + shear => constant energy

Expansion parameters & restitution constant

- Perturbation parameter

$$\epsilon = \frac{\zeta}{\sqrt{\kappa m}} \ll 1.$$

- Restitution constant

$$e = \exp\left[-\zeta t_c/m\right]$$

$$t_c = \pi/\sqrt{2\kappa/m - (\zeta/m)^2}$$

duration time

$$\epsilon \approx \sqrt{2}(1-e)/\pi \ \text{ for } e \approx 1$$

Perturbative spectrum analysis

$$\Psi_n(\mathbf{\Gamma}) = \int_{-\infty}^{0} dt\, e^{-z_n t} \rho(\mathbf{\Gamma}, t)$$

$$\Psi_n^*(\mathbf{\Gamma}) = \rho_{\rm eq}^*(\mathbf{\Gamma}) \left[\Psi_n^{(0)*}(\mathbf{\Gamma}) + \epsilon \tilde{\Psi}_n^{(1)}(\mathbf{\Gamma}) \right] + \mathcal{O}(\epsilon^2)$$

$$z_n^* = z_n^{(0)*} + \epsilon \tilde{z}_n^{(1)} + \mathcal{O}(\epsilon^2),$$

$$i\,\mathcal{L}\,\Psi_n = z_n\,\Psi_n$$

Unperturbed canonical state

$$i\mathcal{L}^{(\rm eq)*}(\mathbf{\Gamma}) \rho_{\rm eq}^*(\mathbf{\Gamma}) = 0$$

Zero-eigenmodes

$$i\mathcal{L}^{(\rm eq)*}(\mathbf{\Gamma}) \phi_\alpha^*(\mathbf{\Gamma}) = 0 \quad (\alpha = 1, \cdots, 5).$$

$$\phi_\alpha^*(\mathbf{\Gamma}) \propto \left\{ 1, \sum_{i=1}^{N} p_i^{*x}, \sum_{i=1}^{N} p_i^{*y}, \sum_{i=1}^{N} p_i^{*z}, \mathcal{H}^*(\mathbf{\Gamma}) \right\}$$

Map onto the zero modes

- There are five zero modes in the base state.

$$\phi_1^*(\mathbf{\Gamma}) = 1,$$

$$\phi_2^*(\mathbf{\Gamma}) = \frac{1}{\sqrt{\frac{3}{2}NT^*}}\left(\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^{*2}}{2} - \frac{3}{2}NT^*\right)$$

$$\phi_\alpha^*(\mathbf{\Gamma}) = \frac{1}{\sqrt{NT^*}}\sum_{i=1}^{N} p_{i,\lambda}^*$$

- We expand the zero eigenvector in terms of the bases:

$$\Psi_\alpha^{(0)*}(\mathbf{\Gamma}) = \sum_{\alpha'=1}^{5} c_{\alpha\alpha'}\phi_{\alpha'}^*(\mathbf{\Gamma})$$

Eigenvalue

- Lowest eigenvalues are easily obtained as

$$\tilde{z}_1^{(1)} = 0,$$

$$\tilde{z}_\alpha^{(1)} = -\frac{2}{3}\mathscr{G} \quad (\alpha = 2, 3, 4, 5),$$

- Where

Radial distribution function

$$\mathscr{G} = n^* \int d^3\boldsymbol{r}^*\, g(r^*, \varphi)\Theta(1 - r^*)$$

- In the hard-core limit, the relaxation time is

$$\tau_{\mathrm{rel}}^* \approx -\frac{1}{\epsilon \tilde{z}_\alpha^{(1)}} = \left[\frac{2}{3}\epsilon\,\mathscr{G}\right]^{-1} \Rightarrow \mathscr{G} \to \sqrt{\pi}\,\omega_E^*(T^*),$$

hard core limit

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Steady distribution

$$\rho_{\rm SS}^{\rm (ex)}(\boldsymbol{\Gamma}) = \exp\left[\int_{-\infty}^{0} d\tau\, \Omega_{\rm eq}(\boldsymbol{\Gamma}(-\tau))\right] \rho_{\rm eq}(\boldsymbol{\Gamma}(-\infty))$$

$$\boxed{\exp\left[\int_{-\infty}^{0} d\tau\, \Omega_{\rm eq}(\boldsymbol{\Gamma}(-\tau))\right] \approx e^{\tau_{\rm rel}\Omega_{\rm SS}(\boldsymbol{\Gamma})}}$$

$$\tau_{\rm rel}^* = \left[\frac{2\sqrt{\pi}}{3}\epsilon\, \omega_E^*(T^*)\right]^{-1}$$

$$\tilde{\Omega}_{\rm SS}(\boldsymbol{\Gamma}) = -\beta_{\rm SS}^*\left[\tilde{\dot{\gamma}} V^* \tilde{\sigma}_{xy}^{\rm (el)}(\boldsymbol{\Gamma}) + 2\Delta\tilde{\mathcal{R}}_{\rm SS}^{(1)}(\boldsymbol{\Gamma})\right]$$

$$\Delta\mathcal{R}_{\rm eq}^{(1)}(\boldsymbol{\Gamma}) \equiv \mathcal{R}^{(1)}(\boldsymbol{\Gamma}) + \frac{T_{\rm eq}}{2}\Lambda(\boldsymbol{\Gamma})$$

$$\mathcal{R}^{(1)}(\boldsymbol{\Gamma}) \equiv \frac{\zeta}{4}\sum_{i,j}\left(\frac{\boldsymbol{p}_{ij}}{m}\cdot\hat{\boldsymbol{r}}_{ij}\right)^2 \Theta(d - r_{ij})$$

Thus, we obtain the effective Hamiltonian in NESS.

Average under NESS

- Average is calculated by

$$\langle \cdots \rangle_{\mathrm{SS}} \equiv \int d\mathbf{\Gamma}\, \rho_{\mathrm{SS}}(\mathbf{\Gamma}) \cdots$$

$$\rho_{\mathrm{SS}}(\mathbf{\Gamma}) = \frac{e^{-I_{\mathrm{SS}}(\mathbf{\Gamma})}}{\int d\mathbf{\Gamma} e^{-I_{\mathrm{SS}}(\mathbf{\Gamma})}} \qquad \boxed{I_{\mathrm{SS}}(\mathbf{\Gamma}) = \beta_{\mathrm{SS}} \mathcal{H}(\mathbf{\Gamma}) - \tau_{\mathrm{rel}} \Omega_{\mathrm{SS}}(\mathbf{\Gamma})}$$

- β_{ss} is determined by the energy balance equation.

$$\boxed{\rho_{\mathrm{SS}}(\mathbf{\Gamma}) \approx \frac{e^{-\beta^*_{\mathrm{SS}} \mathcal{H}^*(\mathbf{\Gamma})} \left[1 + \tilde{\tau}_{\mathrm{rel}} \tilde{\Omega}_{\mathrm{SS}}(\mathbf{\Gamma})\right]}{\mathcal{Z}}}$$

$$\mathcal{Z} \approx \int d\mathbf{\Gamma}\, e^{-\beta^*_{\mathrm{SS}} \mathcal{H}^*(\mathbf{\Gamma})} \left[1 + \tilde{\tau}_{\mathrm{rel}} \tilde{\Omega}_{\mathrm{SS}}(\mathbf{\Gamma})\right]$$

Shear stress

$$\boxed{\langle A(\mathbf{\Gamma})\rangle_{\mathrm{SS}} \approx \langle A(\mathbf{\Gamma})\rangle_{\mathrm{eq}} + \tilde{\tau}_{\mathrm{rel}} \left\langle A(\mathbf{\Gamma})\tilde{\Omega}_{\mathrm{SS}}(\mathbf{\Gamma}) \right\rangle_{\mathrm{eq}}}$$

$$\langle \cdots \rangle_{\mathrm{eq}} = \int d\mathbf{\Gamma}\, e^{-\beta^*_{\mathrm{SS}}\mathcal{H}^*(\mathbf{\Gamma})} \ldots$$

$$\langle \tilde{\sigma}_{xy}(\mathbf{\Gamma})\rangle_{\mathrm{SS}} \approx -\tilde{\tau}_{\mathrm{rel}}\tilde{\dot{\gamma}}\beta^*_{\mathrm{SS}}V^* \left\langle \tilde{\sigma}^{(\mathrm{el})}_{xy}(\mathbf{\Gamma})\tilde{\sigma}^{(\mathrm{el})}_{xy}(\mathbf{\Gamma}) \right\rangle_{\mathrm{eq}}$$

- This corresponds to Kubo formula under the exponential relaxation.

$$\left\langle \tilde{\mathcal{R}}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} \approx \left\langle \tilde{\mathcal{R}}^{(1)}(\mathbf{\Gamma}) \right\rangle_{\mathrm{eq}} - 2\tilde{\tau}_{\mathrm{rel}}\beta^*_{\mathrm{SS}} \left\langle \tilde{\mathcal{R}}^{(1)}(\mathbf{\Gamma})\Delta\tilde{\mathcal{R}}^{(1)}_{\mathrm{SS}}(\mathbf{\Gamma}) \right\rangle_{\mathrm{eq}} .$$

Contents

The evaluation of multi-body correlations

- We have to evaluate 3-body and 4-body static correlation functions.
- We adopt the Kirkwood approximation in which the mult-body correlation can be represented by a product of two-body correlations.

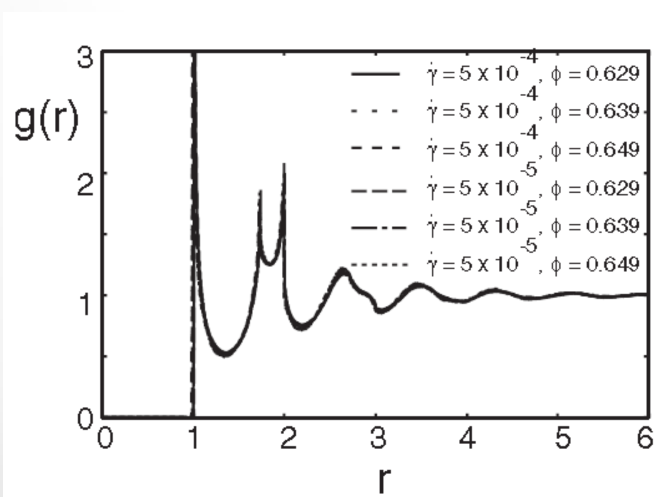
Radial distribution at contact

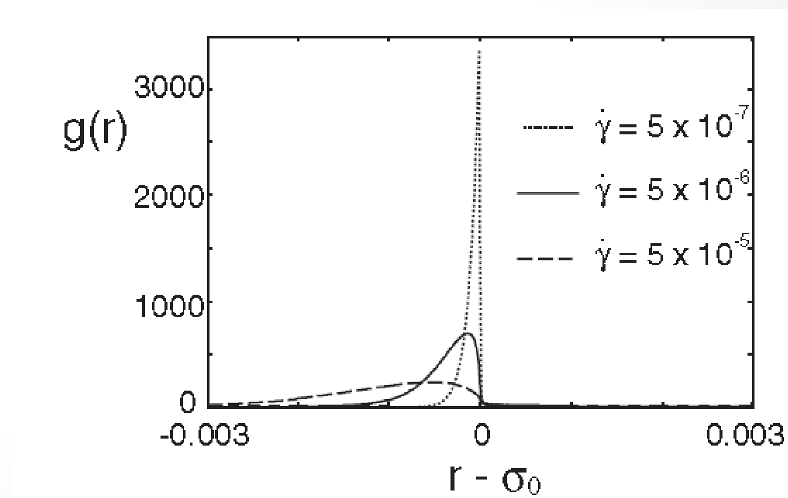
- We use the empirical formula for the radial distribution at contact

$$g(\varphi) = \mathscr{G}_{\mathrm{CS}}(\varphi_f)(\varphi_f - \varphi_J)/(\varphi - \varphi_J)$$

$$\mathscr{G}_{\mathrm{CS}}(\varphi) = (1 - \varphi/2)/(1 - \varphi)^3$$

$$\varphi_f < \varphi < \varphi_J, \text{ where } \varphi_f = 0.49 \text{ and } \varphi_J = 0.639$$





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- Liouville equation= Newton's equation
- Eigenvalue equation for perturbed Liouville equation
- NESS in sheared granular systems and Kubo formula
- Evaluation of correlations
- Results for viscosity and granular temperature
- Comparison with simulation
- Discussion
- Conclusions

Granular temperature and shear stress

- From the energy balance and Kirkwood approximation, we obtain

$$\boxed{T^*_{\rm SS} = \frac{3\tilde{\dot\gamma}^2}{32\pi}\frac{S}{R}}$$

where S and R are given by

$$S = 1 + \mathscr{S}_2\, n^* g(\varphi) + \mathscr{S}_3\, n^{*2} g(\varphi)^2 + \mathscr{S}_4\, n^{*3} g(\varphi)^3$$
$$R = \mathscr{R}'_2\, n^* g(\varphi) + \mathscr{R}'_3\, n^{*2} g(\varphi)^2,$$

with $\mathscr{R}'_2 = -3/4$, $\mathscr{R}'_3 = 7\pi/16$ $\mathscr{S}_2 = 2\pi/15$, $\mathscr{S}_3 = -\pi^2/20$, $\mathscr{S}_4 = 3\pi^3/160$

$$\boxed{\langle\tilde\sigma_{xy}(\Gamma)\rangle_{\rm SS} = -\frac{3}{8\pi}\tilde{\dot\gamma}\, T^{*1/2}_{\rm SS}\frac{S}{g(\varphi)} = -\frac{3\sqrt{6}}{64\pi^{3/2}}\tilde{\dot\gamma}^2\frac{S^{3/2}}{R^{1/2}g(\varphi)}.}$$

Near the jamming point

- Near the jamming point, the radial distribution function diverges linearly. Thus, we extract the most divergent term:

$$T^*_{\mathrm{SS}} \approx \frac{3\tilde{\dot{\gamma}}^2}{32\pi}\frac{\mathscr{S}_4}{\mathscr{R}'_3} n^* g(\varphi) = \frac{9\pi}{2240}\tilde{\dot{\gamma}}^2 n^* g(\varphi),$$

$$\langle\tilde{\sigma}_{xy}(\mathbf{\Gamma})\rangle_{\mathrm{SS}} \approx -\frac{9\pi^2}{1280}\tilde{\dot{\gamma}}\, T^{*\,1/2}_{\mathrm{SS}} n^{*3} g(\varphi)^2$$

$$= -\frac{27\pi^{5/2}}{10240\sqrt{35}}\tilde{\dot{\gamma}}^2 n^{*7/2} g(\varphi)^{5/2}.$$

- The power law dependences are

$$T^*_{\mathrm{SS}} \sim g(\varphi) \sim (\varphi_J - \varphi)^{-1}$$

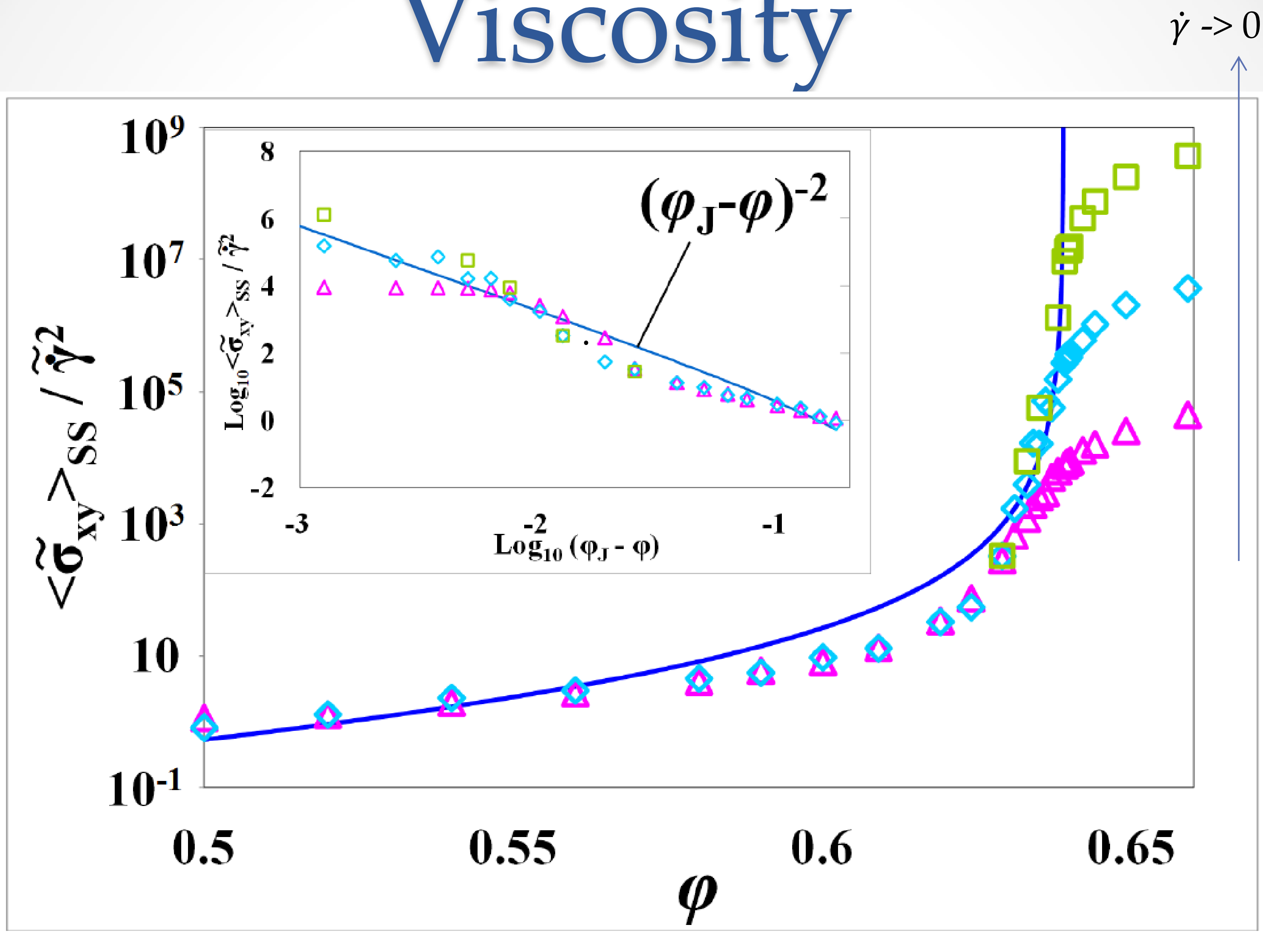
$$\boxed{\tilde{\eta}' = -\langle\tilde{\sigma}_{xy}\rangle_{\mathrm{SS}}/\tilde{\dot{\gamma}}^2 \propto -\langle\tilde{\sigma}_{xy}\rangle_{\mathrm{SS}}/(\tilde{\dot{\gamma}}\sqrt{T^*_{\mathrm{SS}}}) \sim (\varphi_J - \varphi)^{-2}}$$

Contents

MD simulation

- To verify the validity of our theoretical prediction, we perform MD (or DEM) for frictionless grains.
- Parameters; N=2000, $\epsilon = 0.018375$ ($e = 0.96$)
  $\dot{\gamma}^* = 10^{-3}, 10^{-4}, 10^{-5}$
- Sllod + Lees-Edwards boundary condition

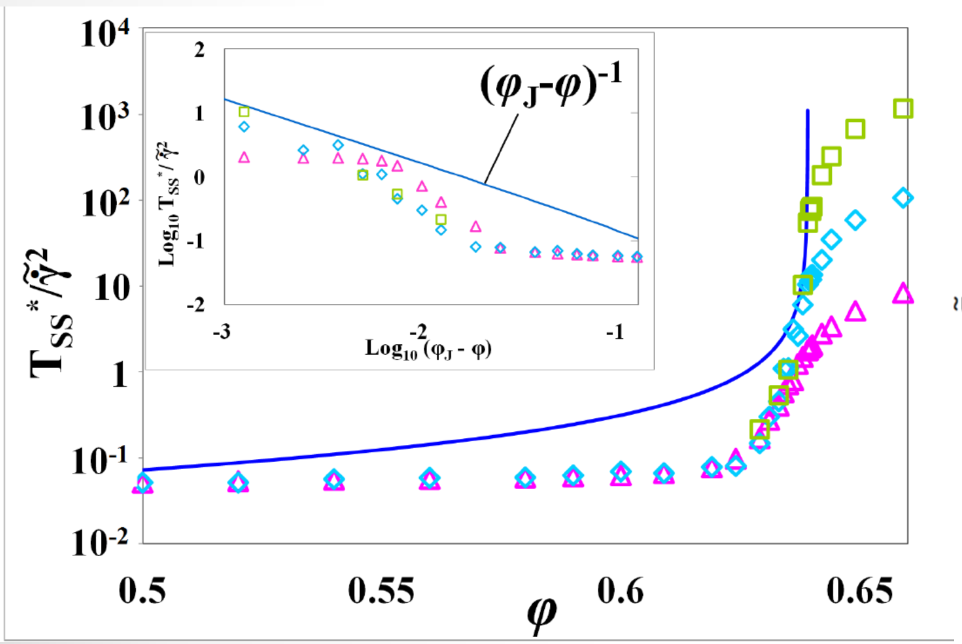
Viscosity

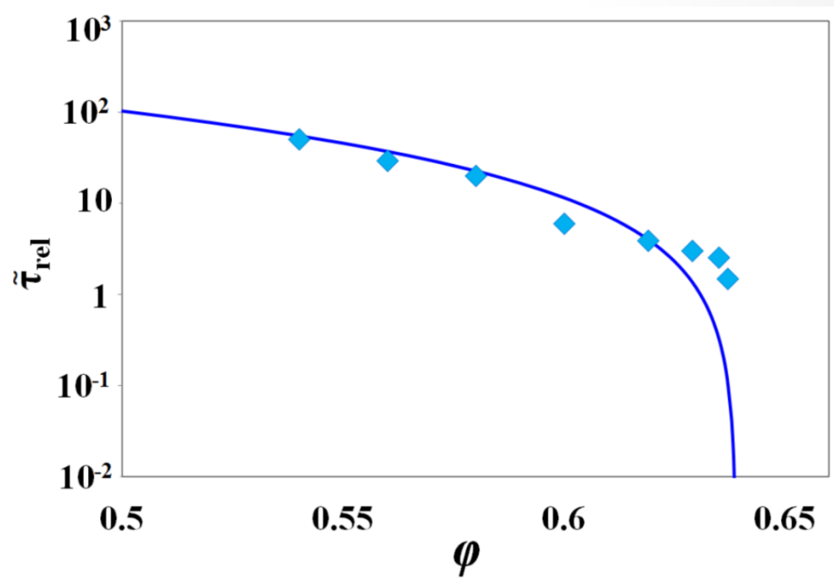


$\dot{\gamma}$ -> 0
10^9
10^7
10^5
10^3
10
10^{-1}
0.5
0.55
0.6
0.65
φ
$\langle\tilde{\sigma}_{xy}\rangle_{SS} / \tilde{\dot{\gamma}}^2$
$(\varphi_J-\varphi)^{-2}$
8
6
4
2
0
-2
-3
-2
-1
$Log_{10}\langle\tilde{\sigma}_{xy}\rangle_{SS} / \tilde{\dot{\gamma}}^2$
$Log_{10}(\varphi_J - \varphi)$

Granular temperature & relaxation time

- Agreement of granular temperature is relatively poor.
- The relaxation time is good.





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Discussion

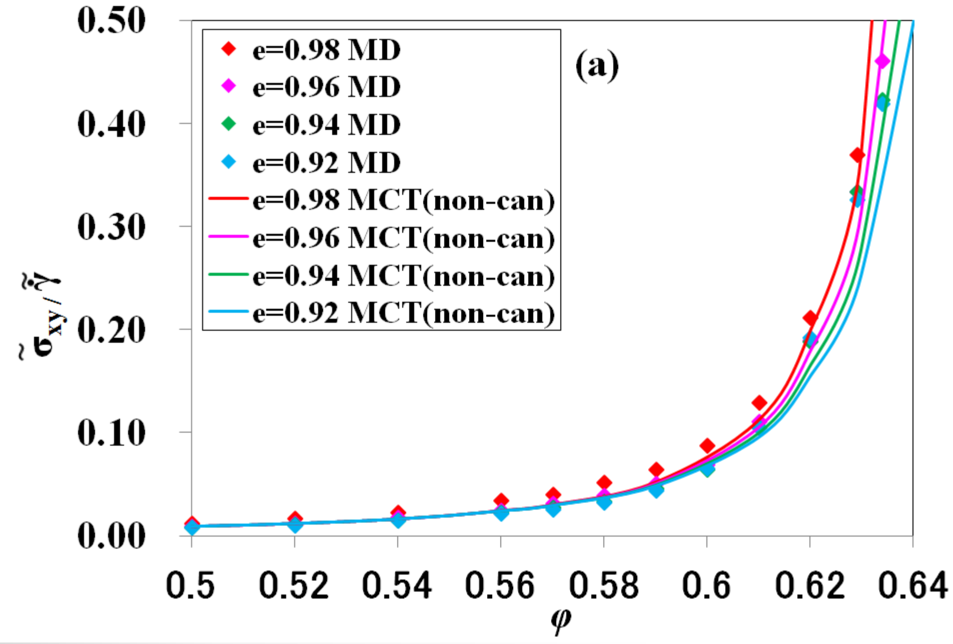
- Constitutive equation still obeys Bagnold's scaling.
- For example, if we assume $\sigma_{xy} \sim |\varphi - \varphi_J|$, then $\sigma_{xy} \sim \dot{\gamma}^{4/7}$, which is close to the simulation value.
- Based on the nonequilibrium steady distribution, we may discuss above the jamming point (by using replica)=> Now in progress.
- The effects of rotation and tangential friction mainly appear in the radial distribution at contact.=> Now in progress
- Our method is generic. Thus, we can apply it to many other systems.

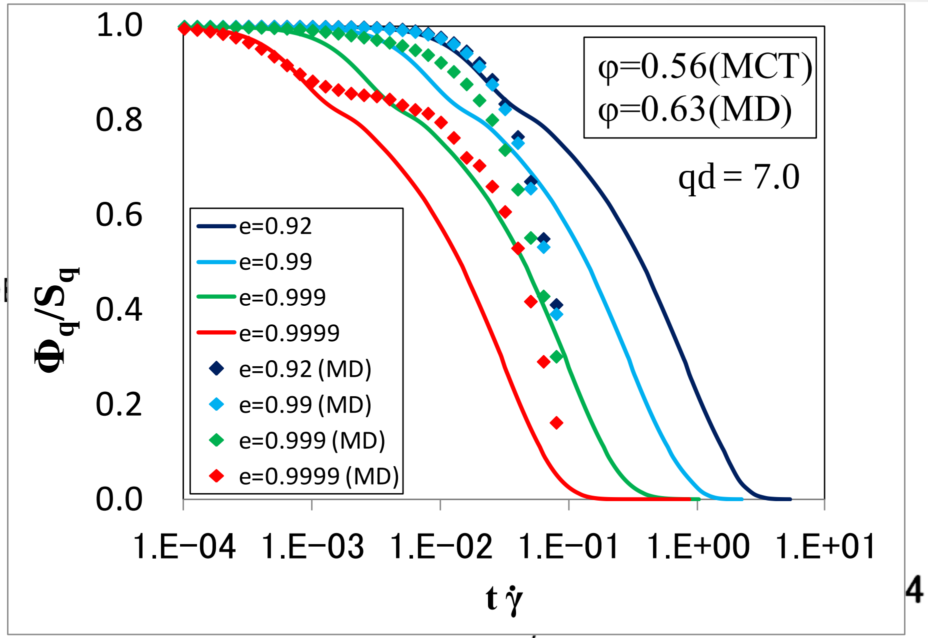
Discussion on MCT

- We had used MCT to analyze dense granular flows, and got reasonable results.
- The disadvantages of MCT are, however,
  - complicated which requires numerical treatment of MCT equation,
  - predicts two-step relaxation in density correlation, which has never been observed in granular systems,
  - needs the shift of the density,
  - and then, cannot use the divergence of the first peak of the radial distribution function.
- We conclude that MCT is not necessary for granular flows.

Achievement of MCT

- We obtain qualitatively nice results.
- However, the divergence of viscosity is unrelated to the divergence of the first peak of radial distribution.





$\Delta\varphi = 0.07$

* Temperature is multiplied by 0.6 for fitting.

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Summary

- We have developed the theory of dense sheared granular flow (frictionless grains).
- We obtain the steady distribution, which can be regarded as the effective Hamilitonian in the non-equilibrium steady state.
- Then, we can evaluate the viscosity and the granular temperature analytically.
- The result of the viscosity gives the quantitatively precise result.
- The granular temperature is not good.
- See PRL in press (arXiv:1506.02368) for details.