Numerical study on the time scales in jamming transition

2016/03/08 10:10 – 10:35

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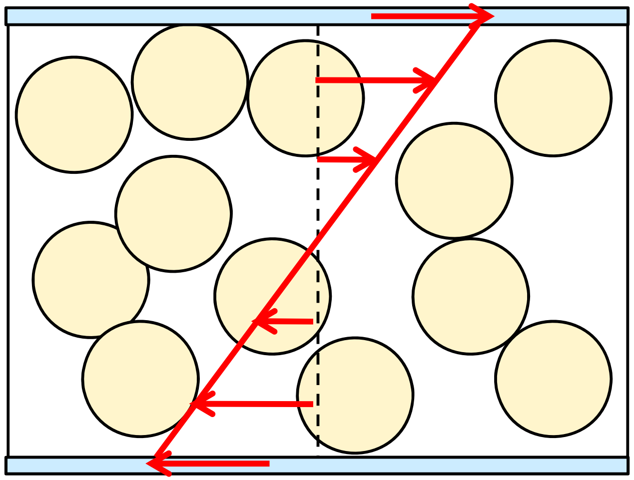
- Introduction
- Microscopic model
- Steady-state distribution function
- Relaxation time
- Steady-state temperature
- MD simulation
  - Shear stress, temperature
  - Relaxation time
  - Dissipation function
- Summary

Contents

Granular materials and jamming transition

- Dissipative, athermal, no equilibrium state
- Nonequilibrium steady state under external driving
- Emergence of rigidity at $\varphi > \varphi_J$ for disordered materials due to mechanical contact (granules, colloids, emulsions, foams, ...)
- Critical scaling behavior (stress, pressure, granular temperature, ...)

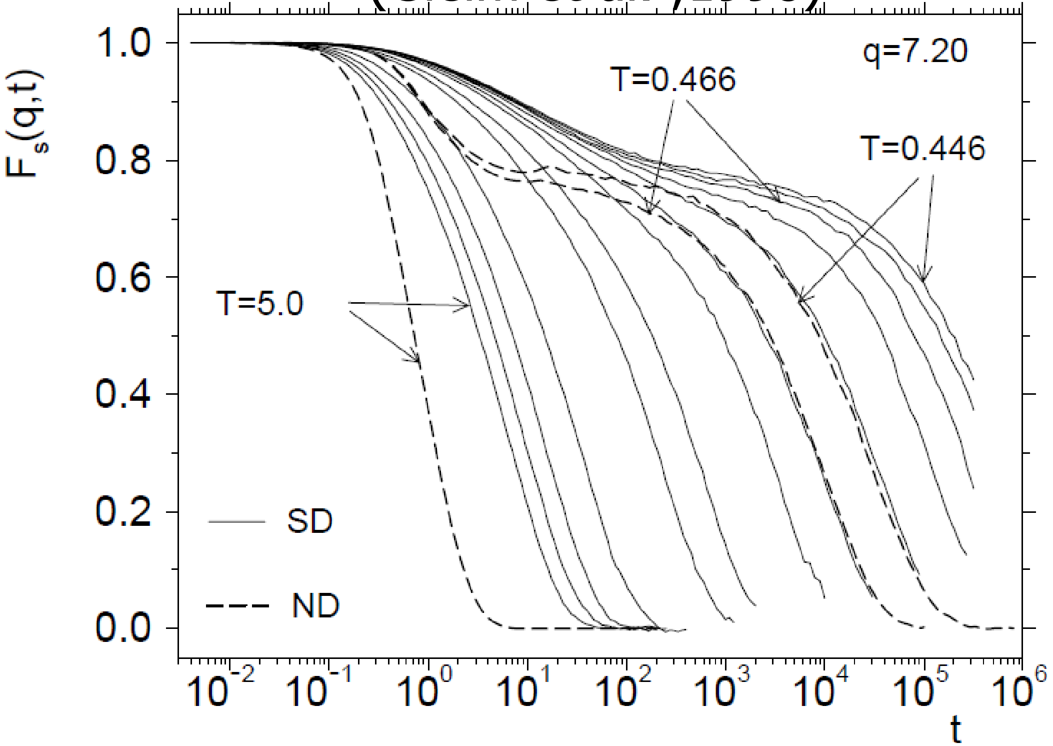


Jamming vs. glass transitions

- Relaxation of the density-density correlation
  - Glass: 2-step relaxation (cage effect)
  - Jamming: 1-step relaxation

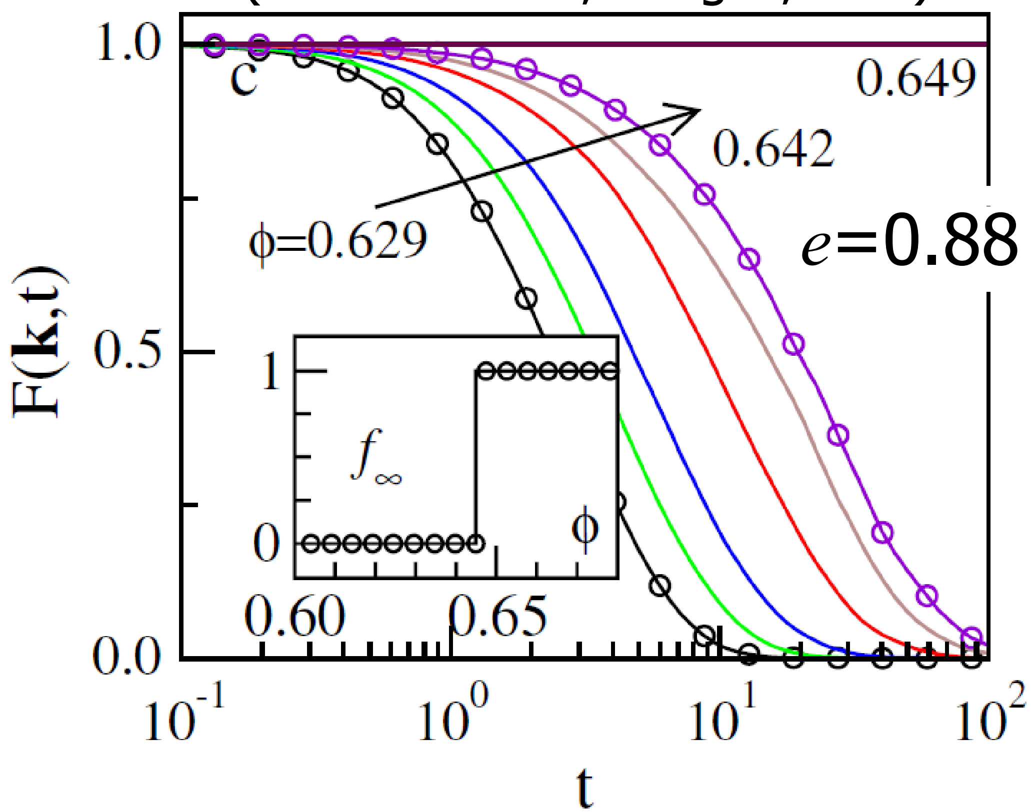
glass

(Gleim et al. ,1998)



jamming

(Pica Ciamarra,Coniglio,2009)

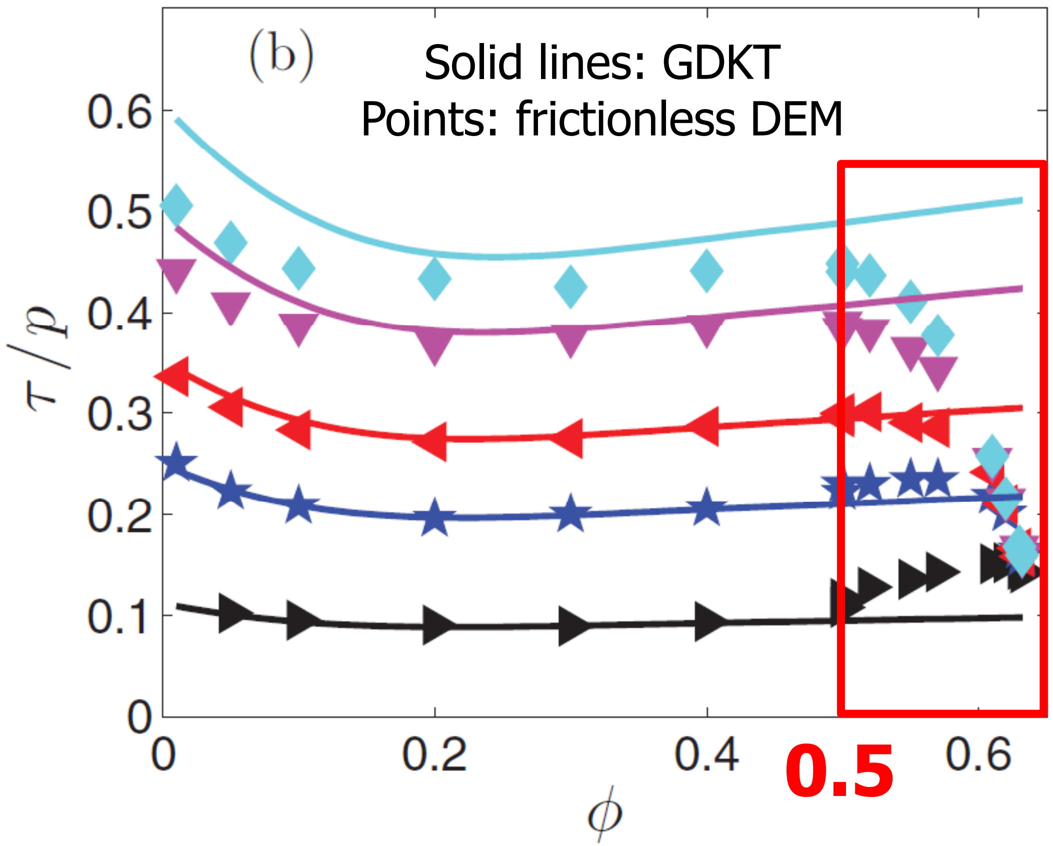


Theoretical approach

- Kinetic theory for inelastic spheres (Garzo,Dufty,1999)
  - breaks down at $\varphi > 0.5$ (Chialvo,Sundaresan,2013)

see also (Mitarai,Nakanishi,2007)

shear stress ratio



Aim of the study / Contents

- Aim of the study
  - Construct a microscopic theory valid in the dense regime up to the jamming point

- Contents
  - Microscopic model
  - Steady-state distribution function
  - Steady-state temperature
  - MD simulation
    - shear stress, temperature
    - relaxation time
    - dissipation function

Contents

Microscopic model

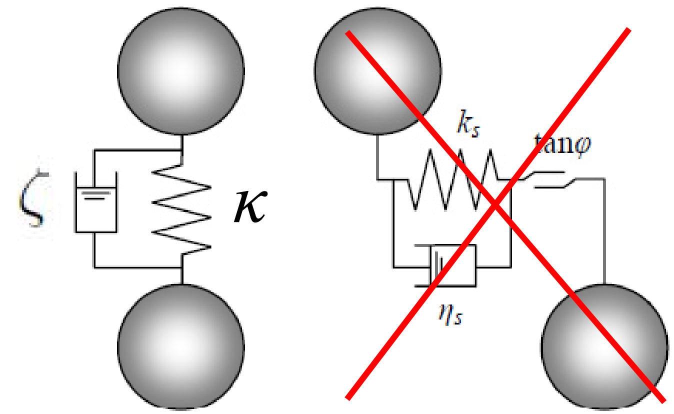
- Equation of motion

$$\dot{\boldsymbol{r}}_i = \frac{\boldsymbol{p}_i}{m} + \dot{\gamma}\,(y,0,0)^T$$

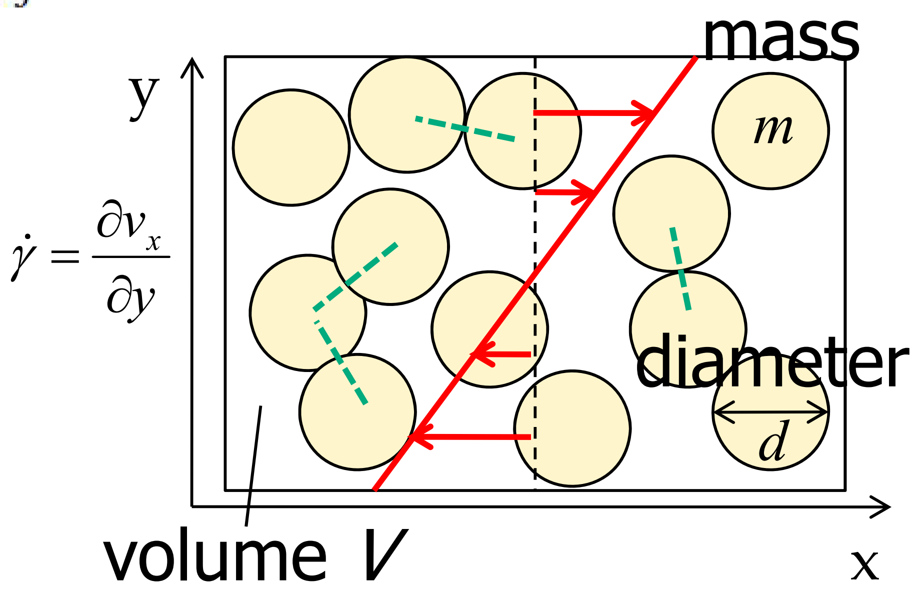
$$\dot{\boldsymbol{p}}_i = \boldsymbol{F}_i^{(\mathrm{el})} + \boldsymbol{F}_i^{(\mathrm{vis})} - \dot{\gamma}\,(p_{iy},0,0)^T$$

$$\boldsymbol{F}_i^{(\mathrm{el})} = \boxed{\kappa}\sum_{j\neq i} \underline{\Theta(d-r_{ij})}(d-r_{ij})\hat{\boldsymbol{r}}_{ij}$$

$$\boldsymbol{F}_i^{(\mathrm{vis})} = -\boxed{\zeta}\sum_{j\neq i} \underline{\Theta(d-r_{ij})}\,(\dot{\boldsymbol{r}}_{ij}\cdot\hat{\boldsymbol{r}}_{ij})\,\hat{\boldsymbol{r}}_{ij}$$



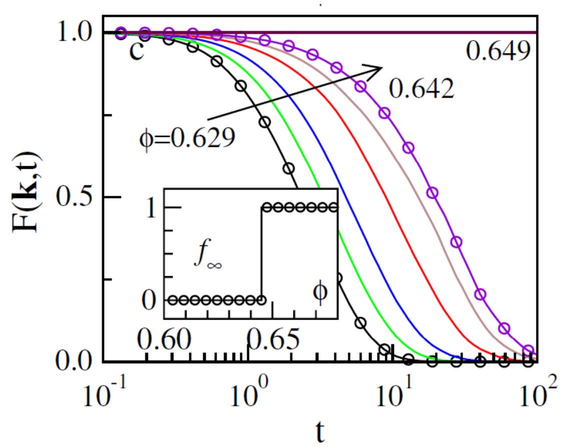
- normal contact forces
  - elastic : linear spring
  - dissipative : viscous
- no thermal noises



Contents

Steady-state distribution function

- Approximate expression
  - Derived from Liouville eq.
  - Relaxation time approximation



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

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

$$\Omega_{\mathrm{SS}}(\boldsymbol{\Gamma}) = -\beta_{\mathrm{SS}}[\dot{\gamma}V\sigma^{(\mathrm{el})}_{xy}(\boldsymbol{\Gamma}) + 2\Delta\mathcal{R}^{(1)}_{\mathrm{SS}}(\boldsymbol{\Gamma})]$$

$$\Delta\mathcal{R}^{(1)}_{\mathrm{SS}}(\boldsymbol{\Gamma}) = \mathcal{R}^{(1)}(\boldsymbol{\Gamma}) + \frac{T_{\mathrm{SS}}}{2}\Lambda(\boldsymbol{\Gamma}),\ \ \mathcal{R}^{(1)}(\boldsymbol{\Gamma}) = \frac{\zeta}{4}{\sum_{i,j}}'\left(\frac{\boldsymbol{p}_{ij}}{m}\cdot\hat{\boldsymbol{r}}_{ij}\right)^2\Theta(d-r_{ij})$$

  - Depends only on $T_{\mathrm{SS}} = \beta_{\mathrm{SS}}^{-1}$
  - Constitutes of "canonical term" + "correction"
  - T_{SS} : determined by the energy balance

Contents

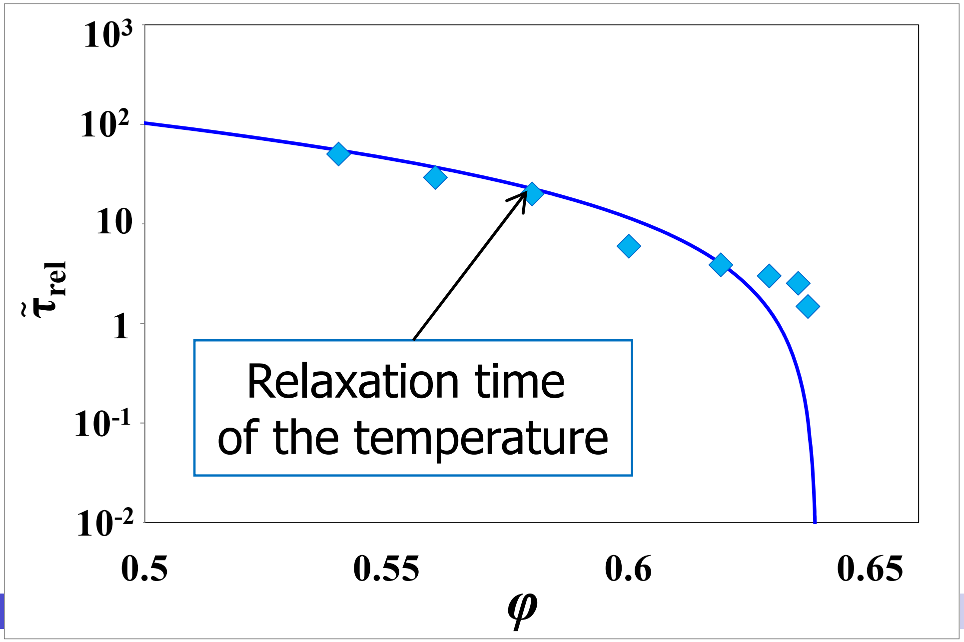
Relaxation time

- Relaxation time $\tau_{\rm rel}$
  - Eigenvalue of the perturbation of the Liouville eq.

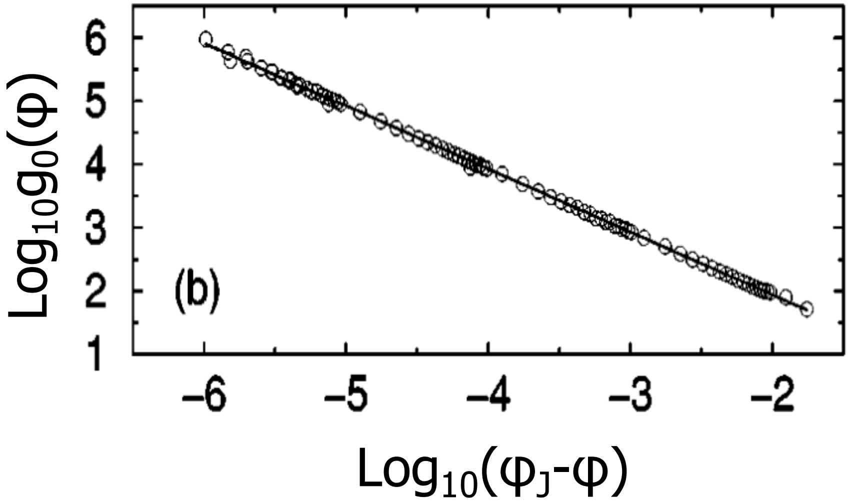
$$\tau^*_{\rm rel} \approx -\frac{1}{\epsilon \tilde{z}^{(1)}_\alpha} = \left[\frac{2}{3}\epsilon \mathscr{G}\right]^{-1} \to \left[\frac{2\sqrt{\pi}}{3}\epsilon\, \omega^*_E(T^*)\right]^{-1}$$ (hard-core limit)

$$\epsilon \equiv \zeta/\sqrt{\kappa m}$$

$$\omega_E(T) = 4\sqrt{\pi}\, n\sqrt{T/m}\, g_0(\varphi) d^2$$: collision (Enskog) frequency



$$g_0(\varphi) \approx (\varphi_J - \varphi)^{-1}, \quad \varphi_J \approx 0.639$$



(O'Hern et.al,2003)

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Steady-state temperature

- Steady-state condition (energy balance)

$$\left\langle \dot{\mathcal{H}}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} = -\dot{\gamma} V \left\langle \sigma_{xy}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} - 2 \left\langle \mathcal{R}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} = 0$$

- Energy dissipation rate

$$\left\langle \tilde{\mathcal{R}}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} \approx \left\langle \tilde{\mathcal{R}}^{(1)}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} = \frac{\sqrt{\pi}}{2} N T^*_{\mathrm{SS}} \tilde{\omega}_E (T^*_{\mathrm{SS}})$$

  - Retain only the leading canonical term ⇒ check later

Steady-state temperature

- Shear stress

$$\langle \tilde{\sigma}_{xy}(\mathbf{\Gamma}) \rangle_{\rm SS} = -\tilde{\tau}_{\rm rel} \dot{\tilde{\gamma}} \beta^*_{\rm SS} V^* \underline{\langle \tilde{\sigma}_{xy}(\mathbf{\Gamma}) \tilde{\sigma}_{xy}(\mathbf{\Gamma}) \rangle_{\rm eq}}$$
$$\approx -\tilde{\tau}_{\rm rel} \dot{\tilde{\gamma}} n^* T^*_{\rm SS} S(\varphi),$$

  - Approximate 4-body correlation by a product of 2-body correlations

$$\langle \tilde{\sigma}_{xy}(\mathbf{\Gamma}) \tilde{\sigma}_{xy}(\mathbf{\Gamma}) \rangle_{\rm eq} \approx \frac{n^*}{V^*} T^{*2}_{\rm SS} S(\varphi), \quad S(\varphi) \approx \frac{3\pi^3}{160} n^{*3} g_0(\varphi)^3$$

  - 1st peak value of the radial distribution function

$$g_0(\varphi) = g_{\rm CS}(\varphi_f)(\varphi_f - \varphi_J)/(\varphi - \varphi_J), \qquad \varphi_f < \varphi < \varphi_J$$

$$\Rightarrow \quad T^*_{\rm SS} \approx \frac{3\dot{\tilde{\gamma}}^2}{32\pi^2} n^* g_0(\varphi)$$

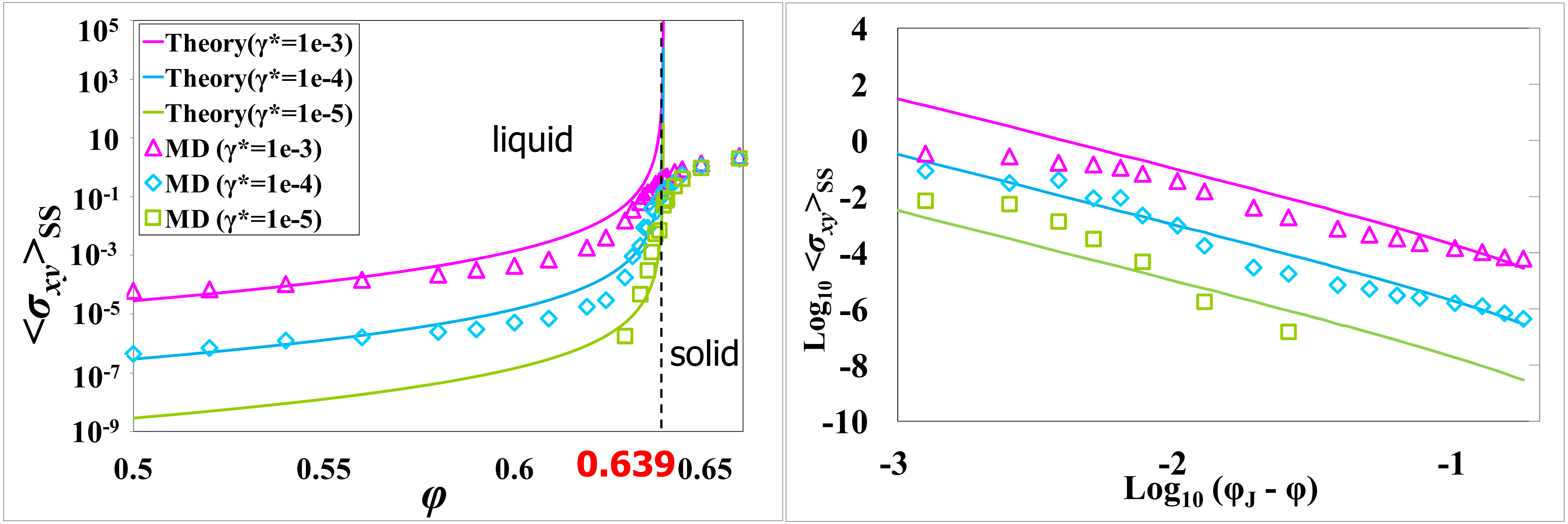
Contents

MD simulation

- Frictionless grains
- Uniform shear (SLLOD + Lees-Edwards b.c.)
- Units
  - Mass : m, length: d, time: $(m/k)^{1/2}$
- Parameters
  - $N = 2000$, $\Delta t^* = 0.01$, $\epsilon = 0.018375$ ($e=0.96$)
  - $0.50 < \varphi < 0.66$, $\dot{\gamma}^* = 10^{-3}, 10^{-4}, 10^{-5}$
- Procedure
  - Initial thermalization ($\dot{\gamma} = 0$, $\boldsymbol{F}^{(\mathrm{vis})} = 0$)
  - Switch on shear & dissipation
  - Start measurement of the stress after the relaxation of $T(t) = \sum_{i=1}^{N} \boldsymbol{p}_i(t)^2/(3Nm)$

Shear stress

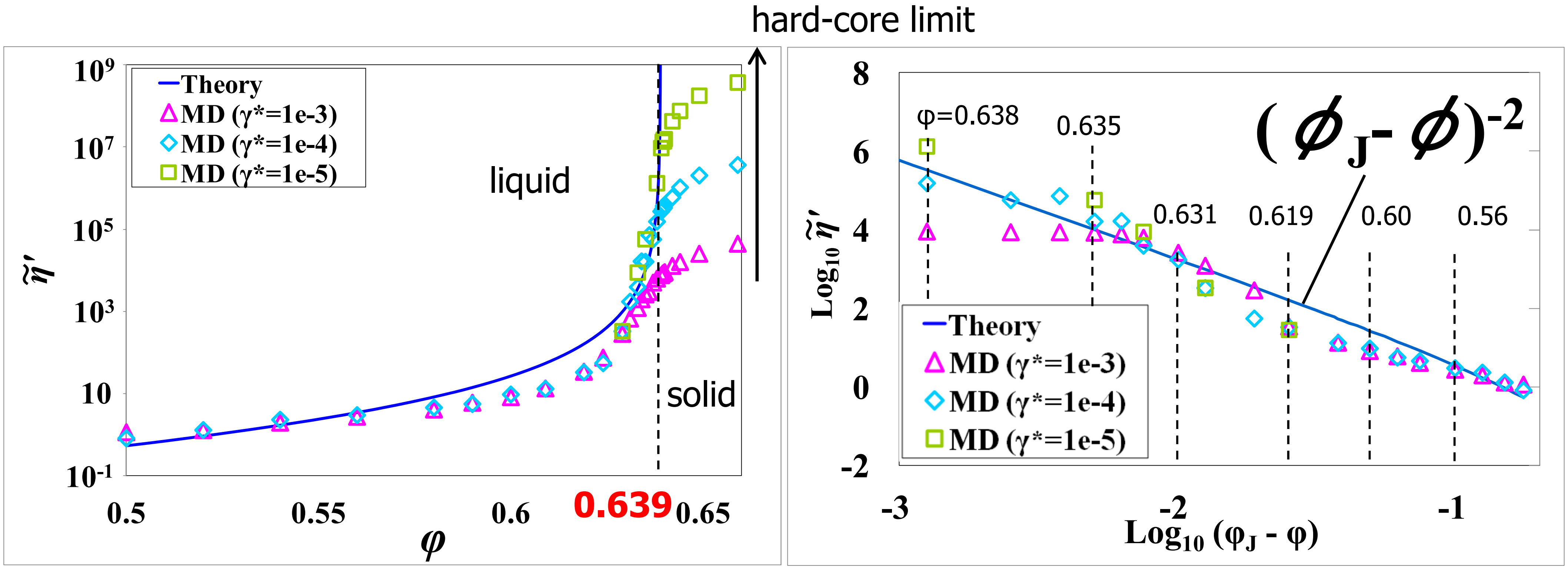
$$\langle\tilde{\sigma}_{xy}(\Gamma)\rangle_{\rm SS} \approx \tilde{\dot{\gamma}}^2 n^{*\frac{7}{2}} g_0(\varphi)^{\frac{5}{2}} \sim (\varphi_J - \varphi)^{-\frac{5}{2}}$$



- Liquid branch: OK, solid branch: NG

Shear viscosity

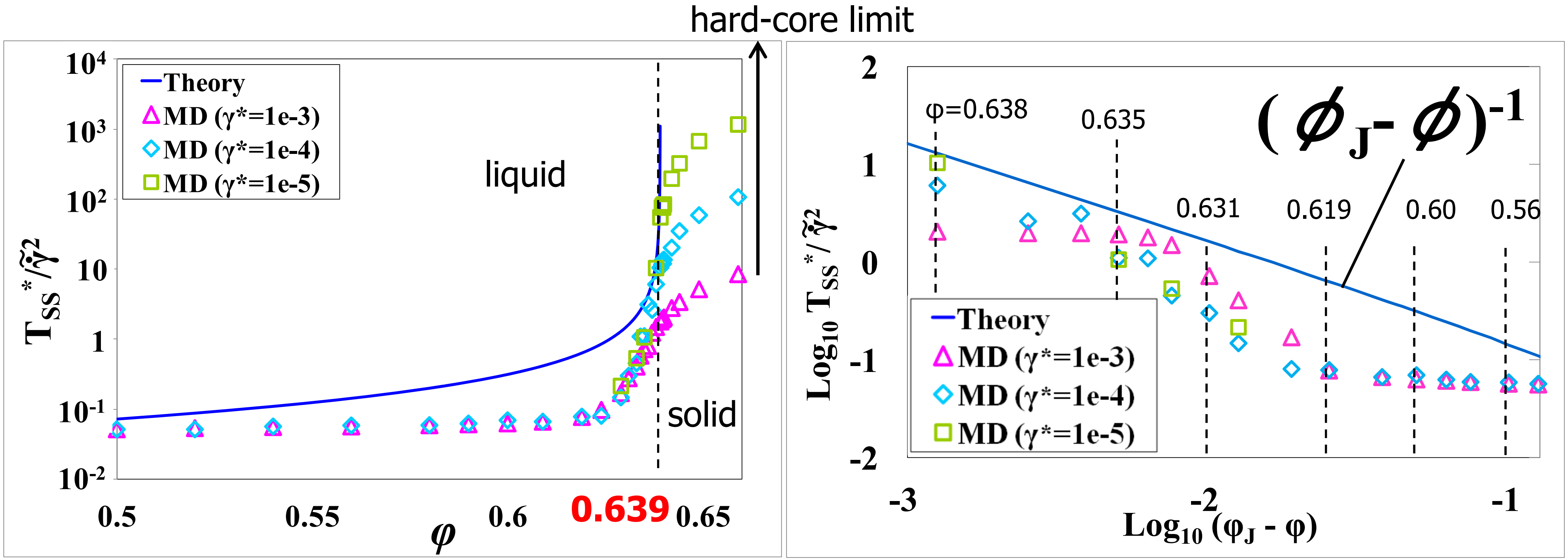
$$\tilde{\eta}' \equiv -\langle \sigma_{xy}(\Gamma)\rangle_{SS} / (\tilde{\dot{\gamma}}\sqrt{T_{SS^*}}) \approx n^{*3} g_0(\varphi)^2 \sim (\varphi_J - \varphi)^{-2}$$



- Agrees well in the hard-core limit
- Exponent = -2 “in average”
- Cross-over at φ=0.62 for MD

Granular temperature

$$T^*_{\mathrm{SS}} \approx \tilde{\dot{\gamma}}^2 n^* g_0(\varphi) \sim (\varphi_J - \varphi)^{-1}$$



- Relatively poor agreement
- Cross-over at φ=0.62 for MD

KS and H.Hayakawa, PRL **115**, 098001 (2015)

Discussions

- Problem
  - Is the relaxation time coincident to the collision time ?

$$\langle \sigma_{xy}(\mathbf{\Gamma}) \rangle_{\rm SS} \approx \tau_{\rm rel} \dot{\gamma} \beta_{\rm SS} V \left\langle \sigma_{xy}(\mathbf{\Gamma}(0)) \sigma_{xy}(\mathbf{\Gamma}(0)) \right\rangle_{\rm eq}$$

$$\langle \sigma_{xy}(\mathbf{\Gamma}) \rangle_{\rm SS} = \dot{\gamma} \beta_{\rm SS} V \int_0^\infty dt \, \left\langle \sigma_{xy}(\mathbf{\Gamma}(t)) \sigma_{xy}(\mathbf{\Gamma}(0)) \right\rangle_{\rm eq}$$

$$\left\langle \sigma_{xy}(\mathbf{\Gamma}(t)) \sigma_{xy}(\mathbf{\Gamma}(0)) \right\rangle_{\rm eq} \approx \left\langle \sigma_{xy}(\mathbf{\Gamma}(0)) \sigma_{xy}(\mathbf{\Gamma}(0)) \right\rangle_{\rm eq} e^{-t/\tau_{\rm rel}}$$

  - We measure the stress-stress time correlation function by MD simulation

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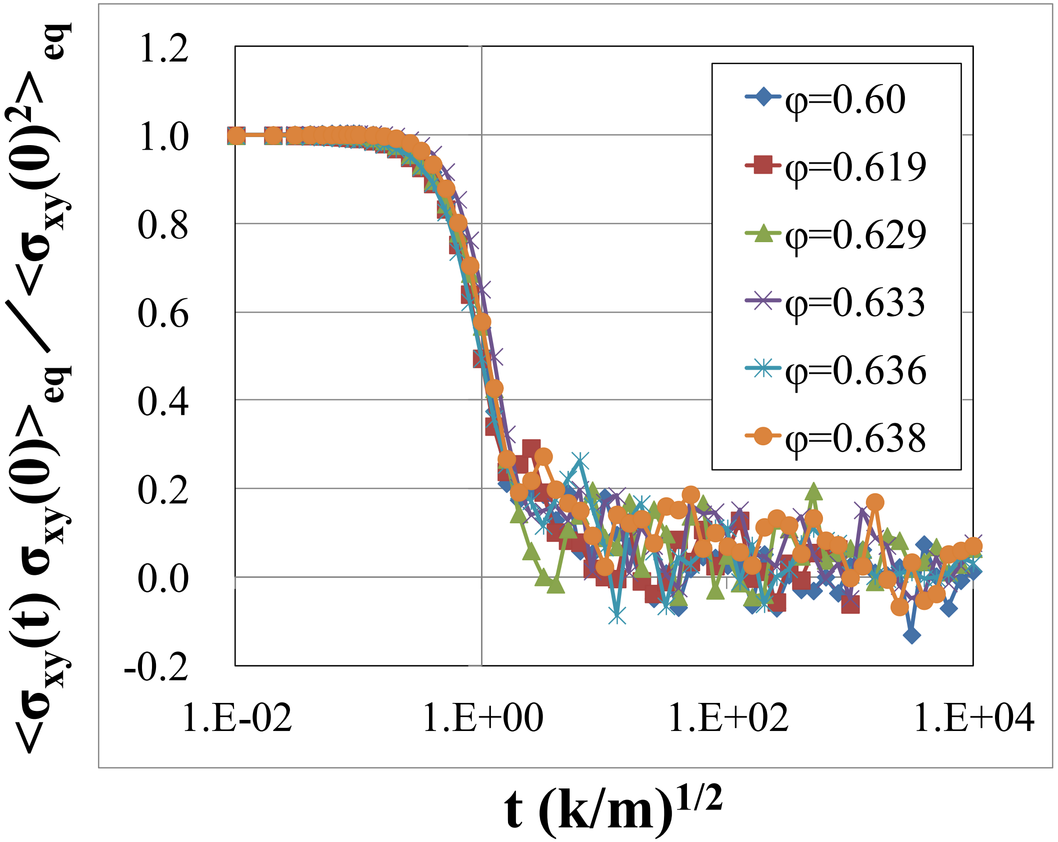
Relaxation time

- Stress time correlation function (MD)



Conditions

$\dot{\gamma}^* = 2.12 \times 10^{-6}$

$\zeta^* = 4.50 \times 10^{-4}$ (e=0.999)

N = 1000

200 samples

Time scales

- ✓ shear rate $\dot{\gamma}^{-1}$
- ✓ dissipation (collision time) ω_E^{-1}
- ✓ contact duration $\sqrt{m/k}$

- Independent of the density
- Determined by the contact duration time

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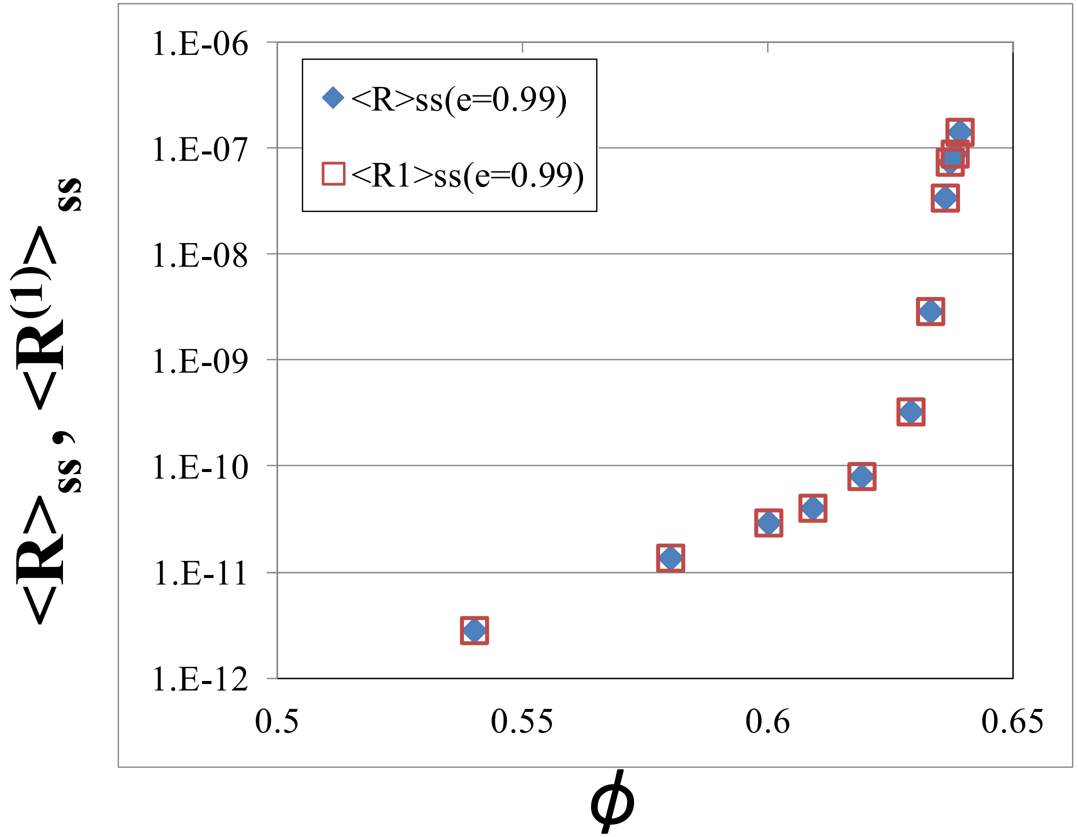
Dissipation function

- Check the approximation (MD)

$$\left\langle \tilde{\mathcal{R}}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} \approx \left\langle \tilde{\mathcal{R}}^{(1)}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} = \frac{\sqrt{\pi}}{2} N T^*_{\mathrm{SS}} \tilde{\omega}_E(T^*_{\mathrm{SS}})$$



Conditions

$\dot{\gamma}^* =$ 6.73 x 10^{-6}

$\zeta^* =$ 4.52 x 10^{-3} (e=0.99)

N = 2000

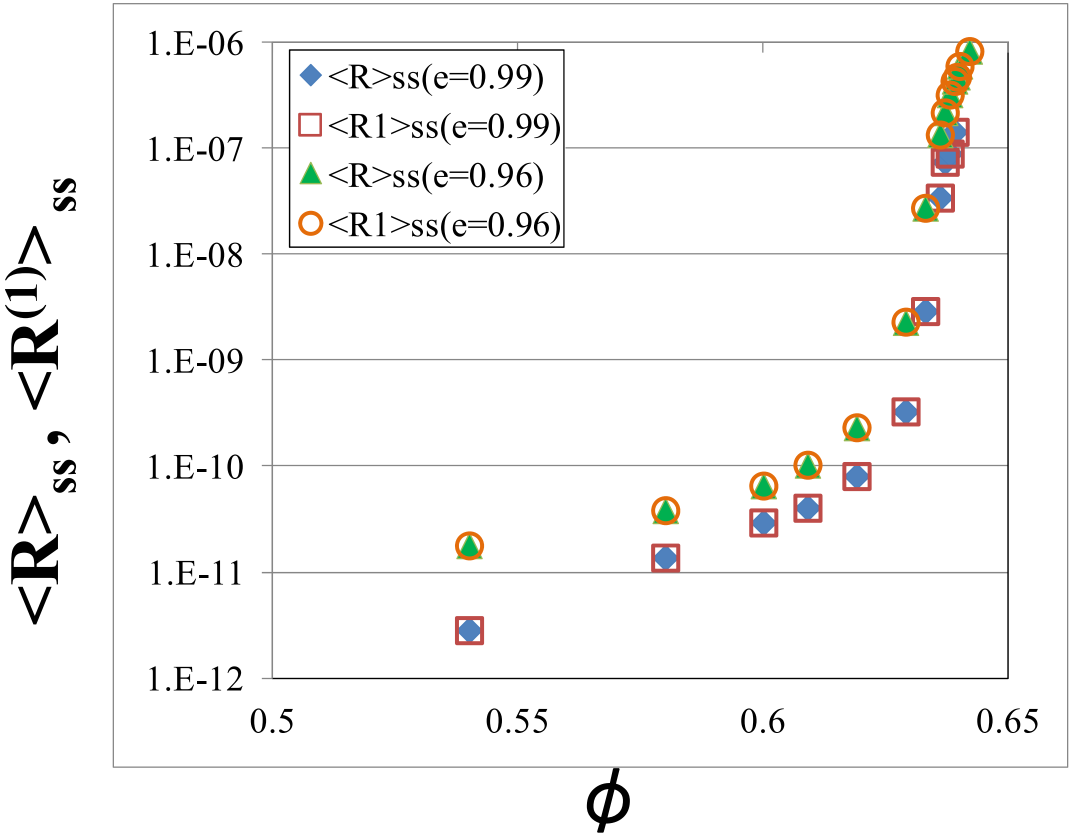
Error < 0.1-0.2 %

- Dissipation is determined by the collision time

Dissipation function

- Check the approximation (MD)

$$\left\langle \tilde{\mathcal{R}}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} \approx \left\langle \tilde{\mathcal{R}}^{(1)}(\mathbf{\Gamma}) \right\rangle_{\mathrm{SS}} = \frac{\sqrt{\pi}}{2} N T^*_{\mathrm{SS}} \tilde{\omega}_E (T^*_{\mathrm{SS}})$$



Conditions

$\dot{\gamma}^* = 1.36 \times 10^{-5}$

$\zeta^* = 1.84 \times 10^{-2}$ (e=0.96)

N = 2000

⇒ Error < 1-2 %

- Approximation is valid for e=0.96

Contents

Summary

- The theory for sheared granular materials is based on the assumption that the relaxation time is given by the collision time.
- The relaxation time for the stress time correlation function is numerically estimated. It is determined by the contact duration.
- There are two time-scales: contact duration (stress) and collision time (dissipation).
- The implications to the theory are now under investigation.