Three particle model for the complex shear modulus of frictional granular materials

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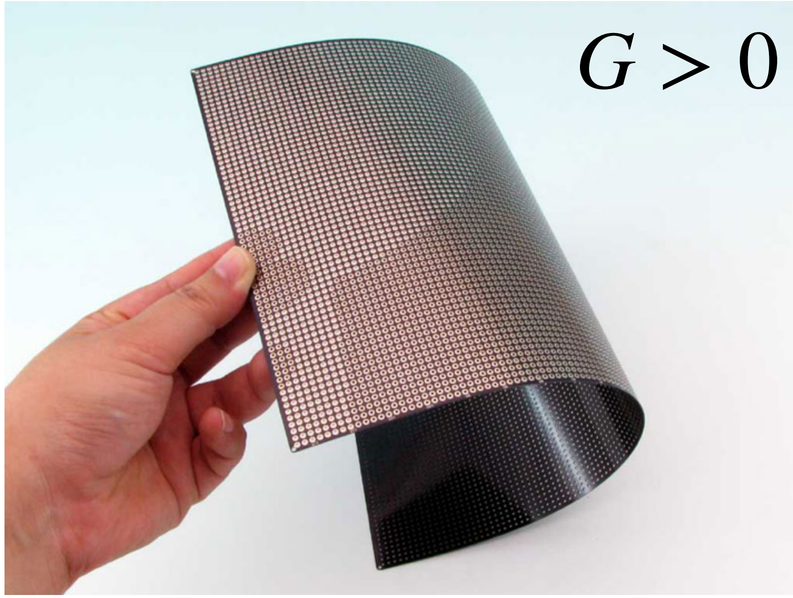
arXiv:2211.?????

Outline

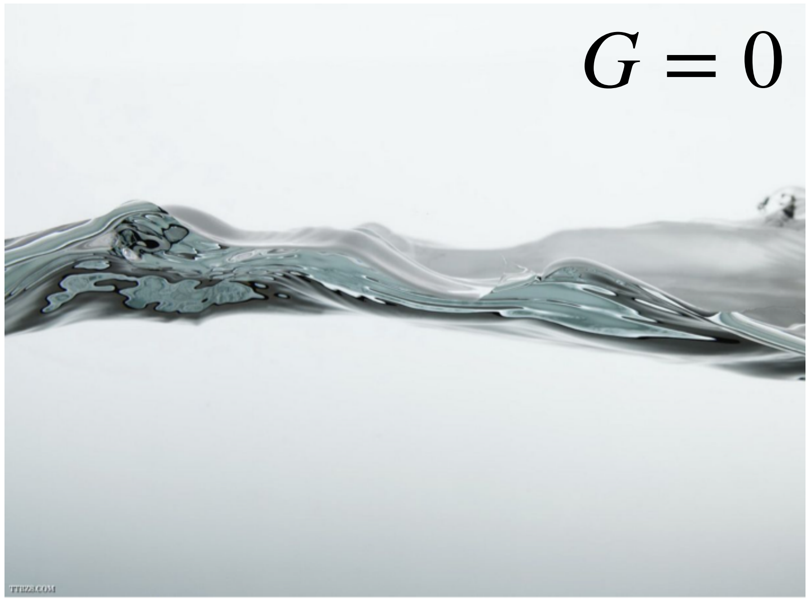
1. **Introduction : Mechanical response of granular materials**
2. Three-particle models (TPM)
3. Comparison with many-particle systems (MPS)
4. Summary

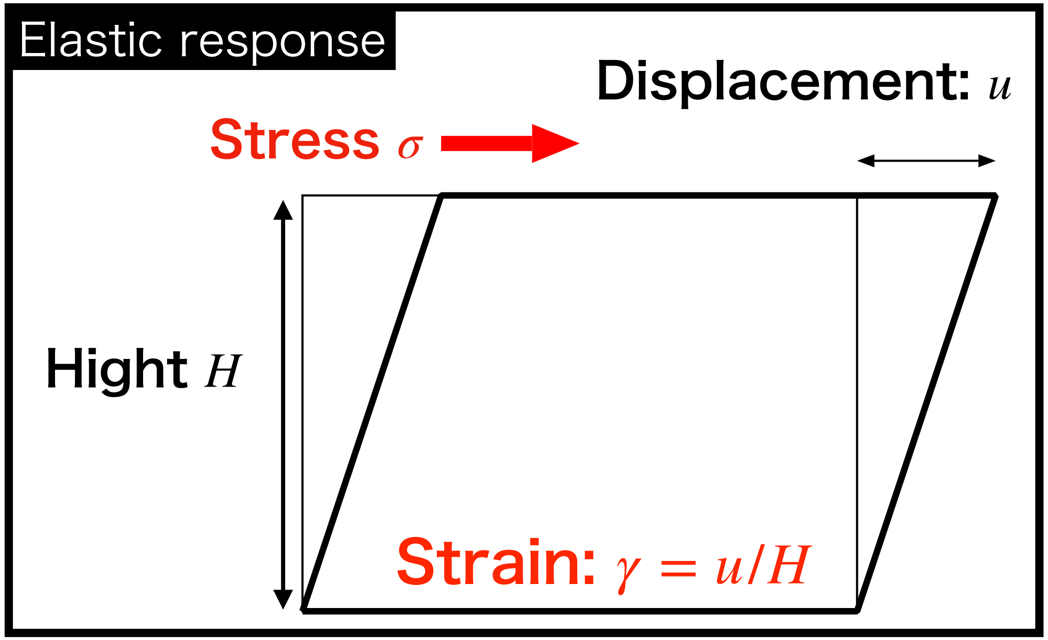
States of matters

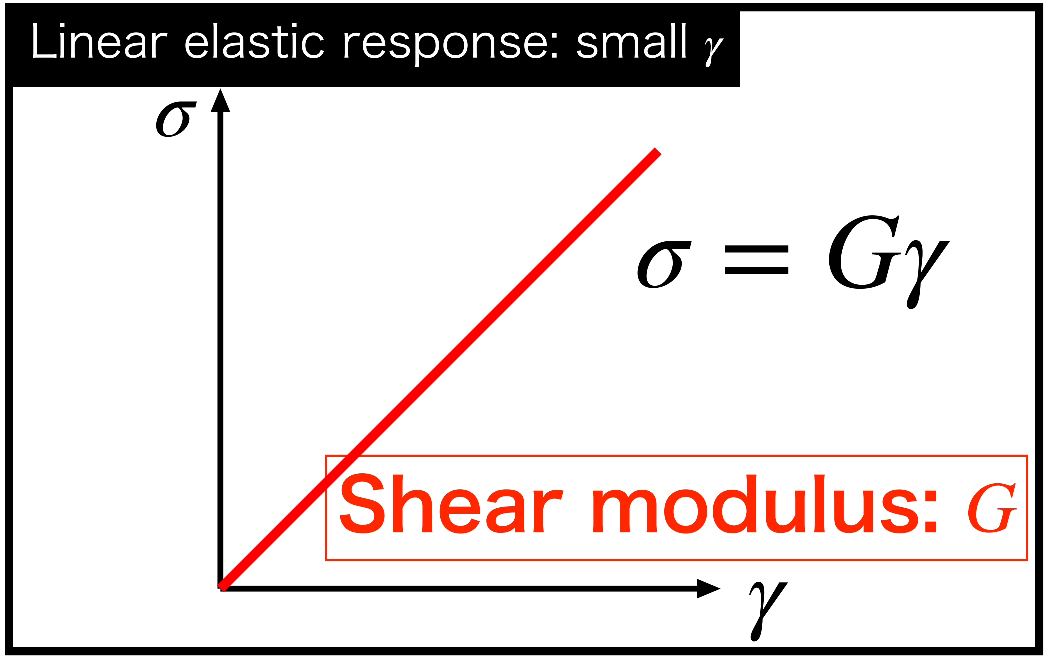
Solids



Fluids

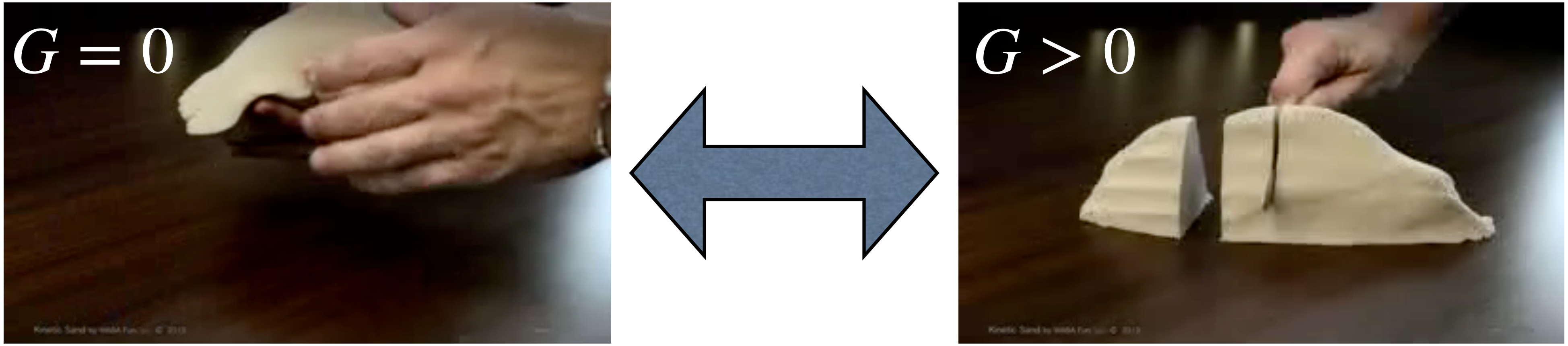






States of granular materials

- Granular materials: Collection of solid particles (powder, sand, etc).
- Jamming: The behavior depends on the density (packing fraction ϕ).
- Above the jamming point ϕ_J, elastic response with $G > 0$ is observed.



Low ϕ: Fluid | High ϕ: Solid

Jamming point: ϕ_J

Packing fraction ϕ

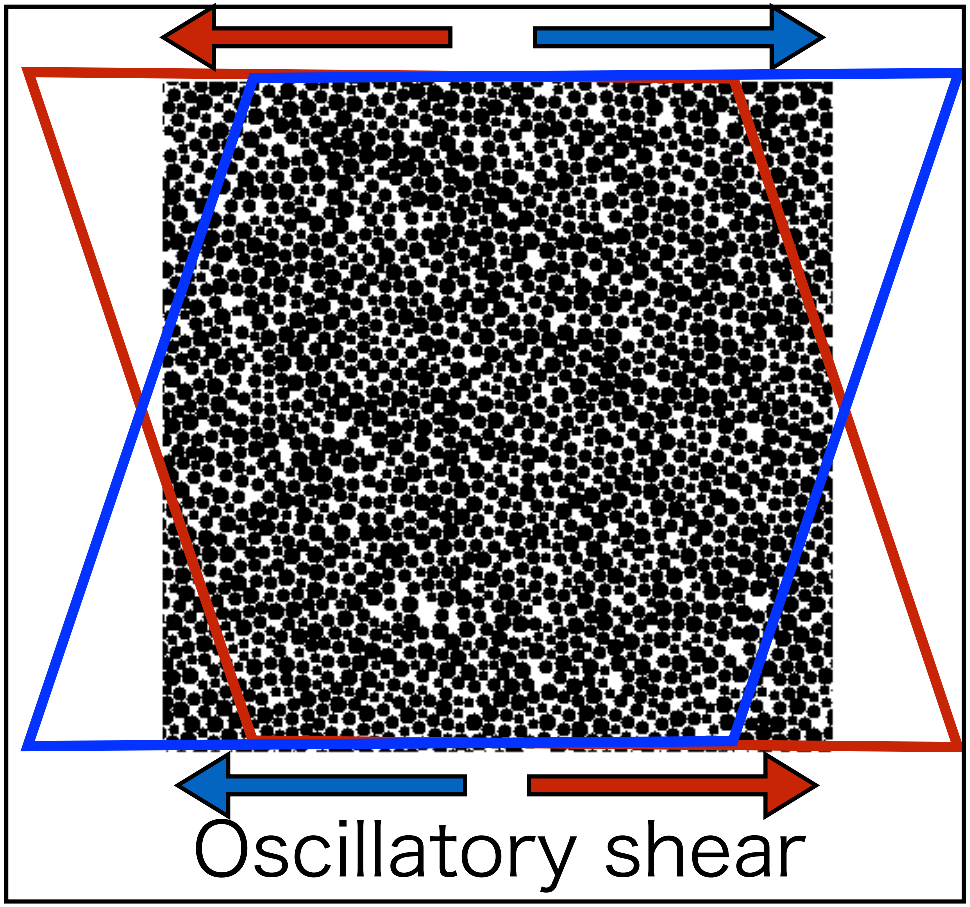
- **The shear modulus G characterizes the linear response for small γ.**
- **Mechanical response for large γ?**

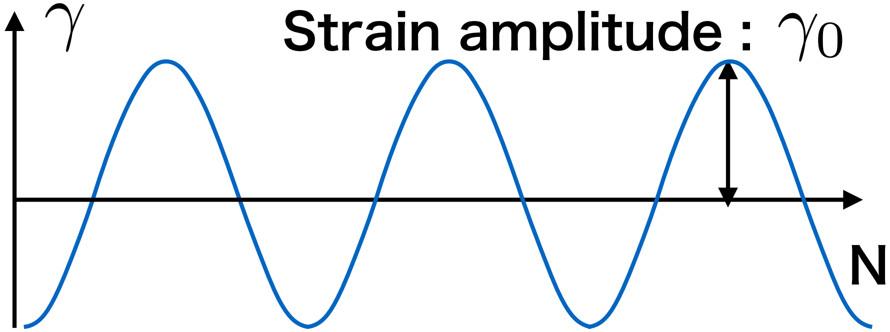
Nonlinear response?

- Dense granular materials with $\phi > \phi_J$ behave like solids for small γ.
- As γ increases, granular materials becomes soft.
- How do we characterize the nonlinear response depending on γ?

→ **Complex shear modulus**

Complex shear modulus





Strain : $\gamma(t) = \gamma_0 \sin(\omega t)$

Mechanical response under oscillatory shear

Shear strain: $\gamma(t) = \gamma_0 \sin(\omega t)$

γ_0: **Amplitude**, ω: **Frequency**

Shear stress:

$$\sigma(t) \simeq G' \sin(\omega t) + G'' \cos(\omega t)$$

Complex shear modulus

Storage modulus: elasticity

$$G' = \frac{\omega}{\pi} \int_0^{2\pi/\omega} d\theta \, \frac{\sigma(t)\sin(\omega t)}{\gamma_0}$$

$G' = G$ for small γ_0

Loss modulus: dissipation

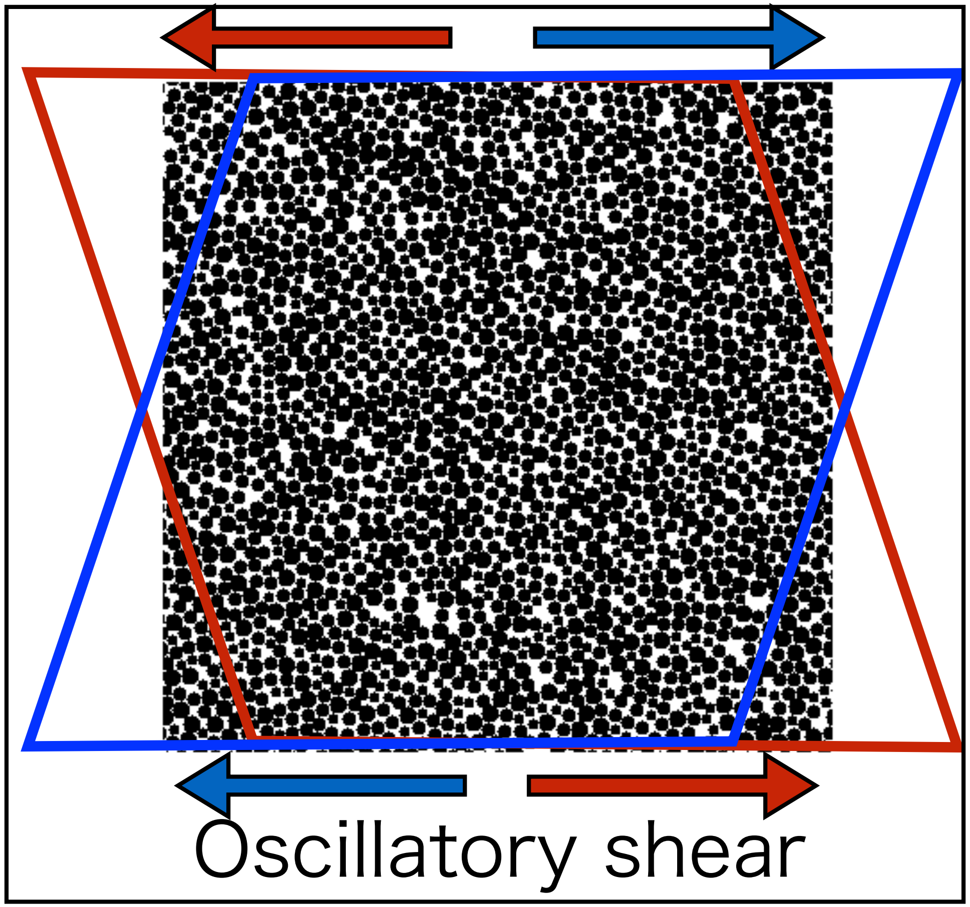
$$G'' = \frac{\omega}{\pi} \int_0^{2\pi/\omega} d\theta \, \frac{\sigma(t)\cos(\omega t)}{\gamma_0}$$

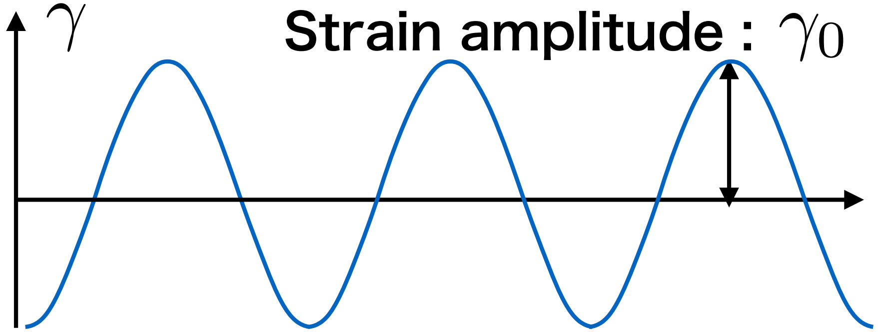
Nonlinear response: G' **and** G'' **depending on** γ_0

G' **and** G'' **has been numerically studied.**

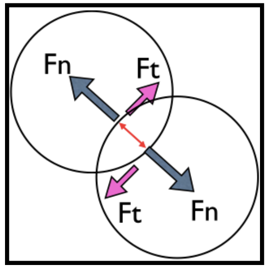
Previous studies on G' and G'' : Model

MO and H. Hayakawa, Phys. Rev. E 95, 062902 (2017)





Strain : $\gamma(t) = \gamma_0 \sin(\omega t)$



F_n : Normal repulsive force

F_t : Tangential friction

Coulomb's law $F_t \leq \mu F_n$

μ : Friction coefficient

SLLOD eq. : Newton's second law with shear

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m_i} + \dot{\gamma}(t) r_{i,y} \hat{\boldsymbol{x}},$$

$$\frac{d\boldsymbol{p}_i}{dt} = \sum_{j \neq i} \boldsymbol{F}_{ij} - \dot{\gamma}(t) p_{i,y} \hat{\boldsymbol{x}},$$

Complex shear modulus: **Shear stress:** $\sigma(t)$

Storage modulus: elasticity

$$G' = \frac{\omega}{\pi} \int_0^{2\pi/\omega} d\theta \, \frac{\sigma(t)\sin(\omega t)}{\gamma_0}$$

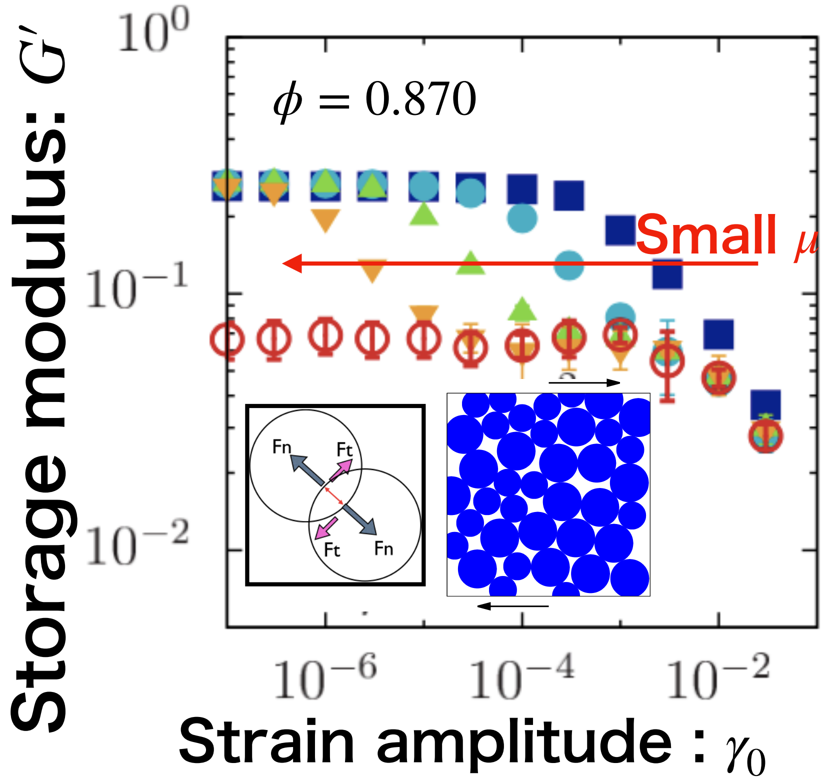
$G' = G$ for small γ_0

Loss modulus: dissipation

$$G'' = \frac{\omega}{\pi} \int_0^{2\pi/\omega} d\theta \, \frac{\sigma(t)\cos(\omega t)}{\gamma_0}$$

Previous studies on G' and G''

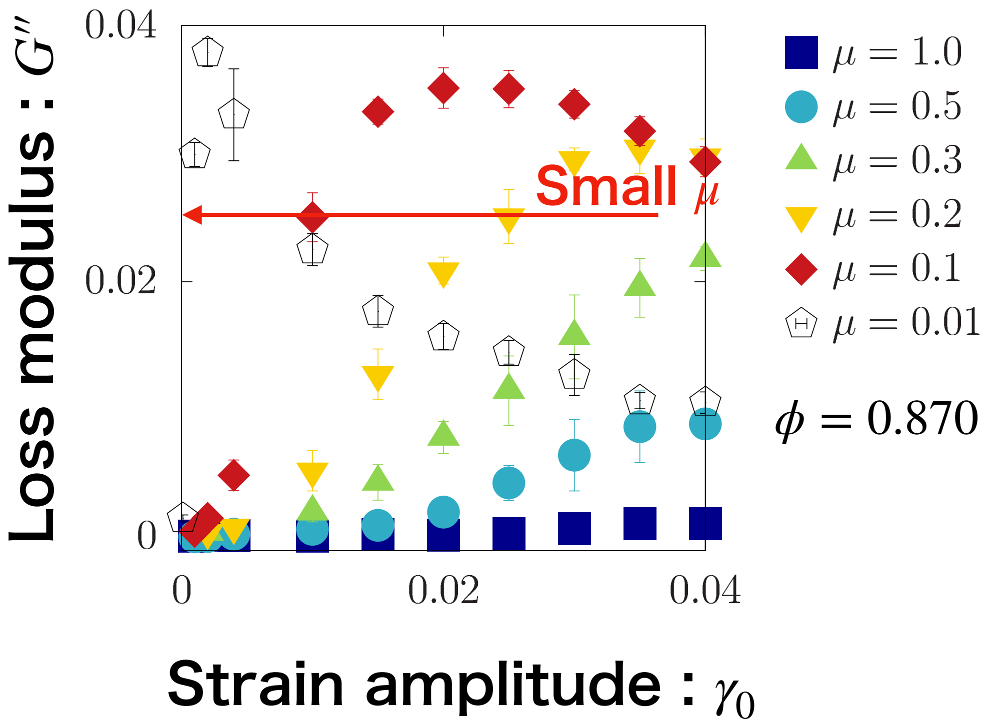
μ: Friction coefficient



MO and H. Hayakawa, Phys. Rev. E 95, 062902 (2017)

- G' decreases as γ_0 increases.
- The critical strain depends on μ.
- G' exhibits two step relaxation.

The number of grains : $N \geq 1000$



MO and H. Hayakawa, Eur. Phys. J. E 44, 106 (2021)

- G'' becomes finite as γ_0 increases.
- The critical strain depends on μ.
- G'' has a peak for small μ.

Theoretical analysis is difficult.

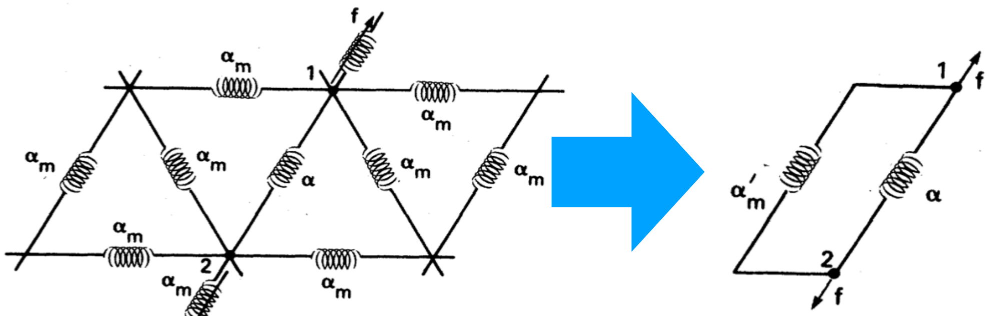
Many body systems, friction, etc.

Approach: simple effective model

Example: Mean field theory for Ising model

Elastic response of amorphous solid

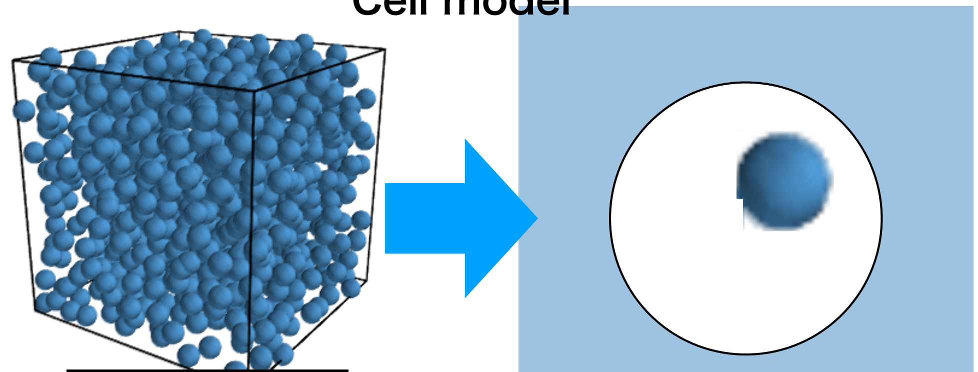
Effective medium theory



Feng, Thorpe, and Garboczi, Phys. Rev. B 31, 276 (1995)

Gas-liquid transition

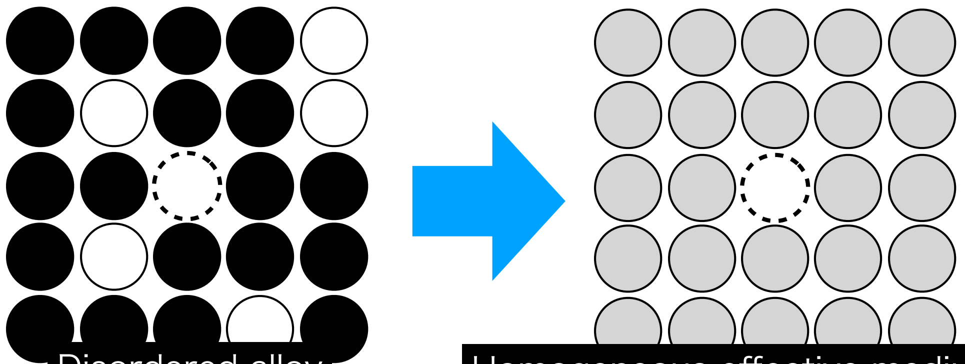
Cell model



Lennard-Jones, Devonshire, Proc. R. Soc. Lond A 63, 53 (1937)

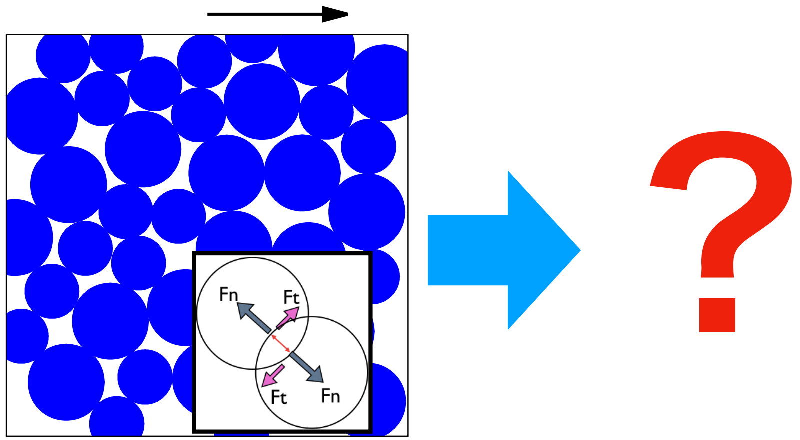
Electric band structure for disordered solid

Coherent potential approximation



Yonezawa, Morigaki, Prog. Theor. Supple. 53, 1 (1973)

Response of frictional grains under shear



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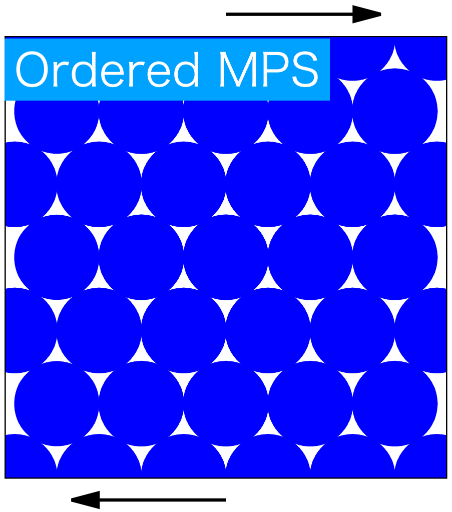
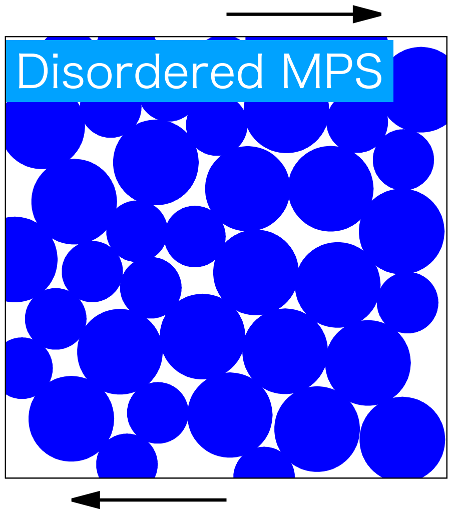
Three particle model: Dynamics

Many particle system (MPS)





SLLOD eq.：Newton's second law with shear

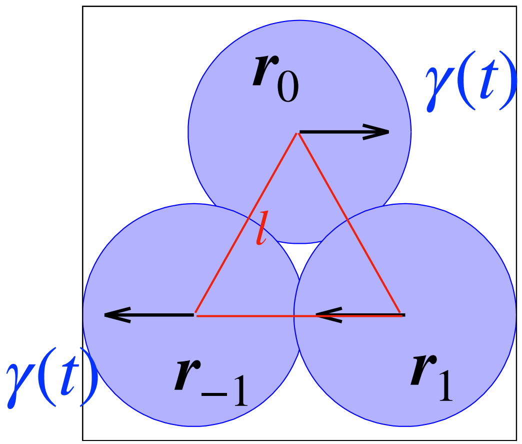
$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\boldsymbol{p}_i}{m_i} + \dot{\gamma}(t) r_{i,y}\hat{\boldsymbol{x}},$$

$$\frac{d\boldsymbol{p}_i}{dt} = \sum_{j \neq i} \boldsymbol{F}_{ij} - \dot{\gamma}(t) p_{i,y}\hat{\boldsymbol{x}},$$

Shear strain: $\gamma(t) = \gamma_0 \sin(\omega t)$

γ_0: **Amplitude**, ω: **Frequency**

Three particle model (TPM):



$l = d(1-\epsilon)$ **: Initial distance**

d **: diameter of grains**

ϵ **: compressive strain** $\propto \phi - \phi_J$

$$\boldsymbol{r}_0 = (\sqrt{3}\gamma(t)l/4,\ \sqrt{3}l/4)$$

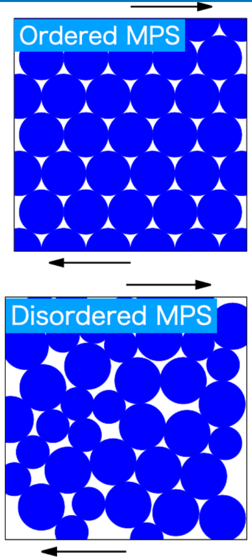
$$\boldsymbol{r}_{\pm 1} = (\pm l/2 - \sqrt{3}\gamma(t)l/4,\ -\sqrt{3}l/4)$$

Shear strain: $\gamma(t) = \gamma_0 \sin(\omega t)$

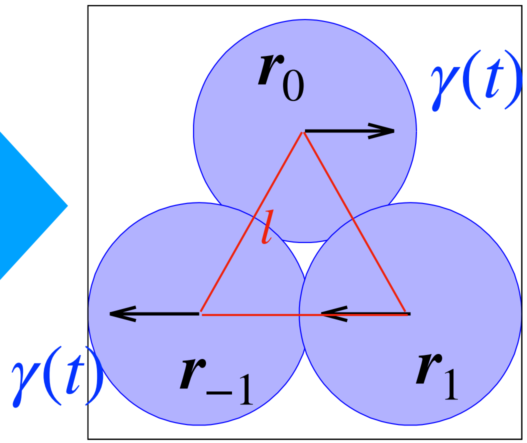
γ_0: **Amplitude**, ω: **Frequency**

Three particle model: Interaction force

Many particle system



Three particle model:



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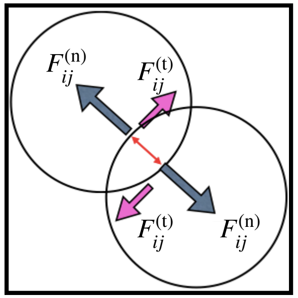
γ_0**: Amplitude**, ω**: Frequency**

Particle interaction



The force is the same as that for usual simulations.

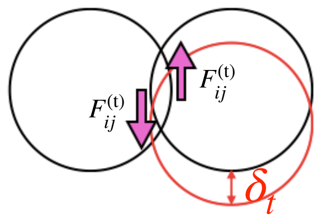
$F_{ij}^{(n)}$ **: Normal repulsive force**

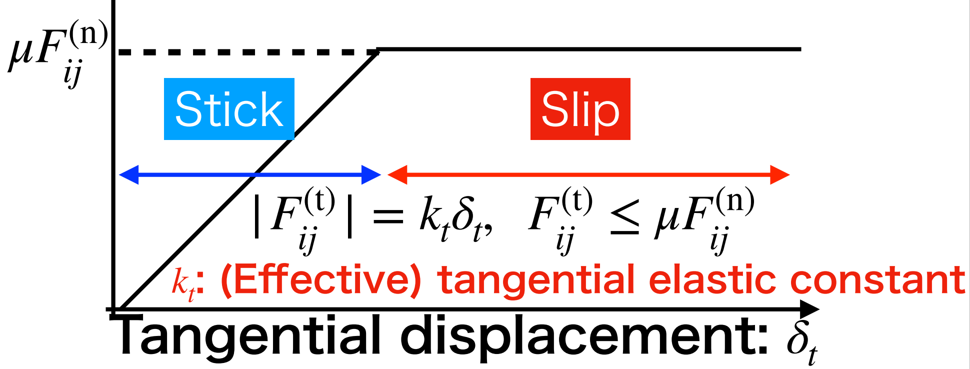
$F_{ij}^{(t)}$ **: Tangential friction**

Coulomb's law $F_{ij}^{(t)} \le \mu F_{ij}^{(n)}$

μ **: Friction coefficient**

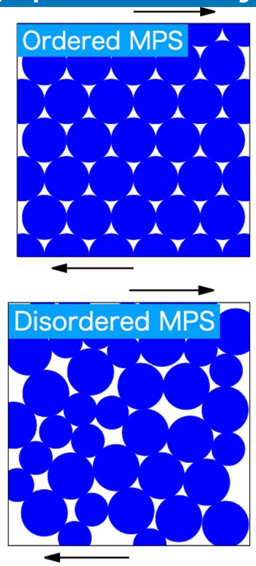
Tangential friction:



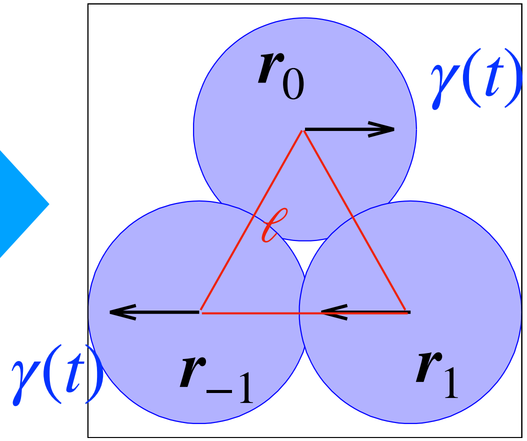


Shear modulus in three-particle model

Many particle system



Three particle model:



$l = d(1-\epsilon)$ **: Initial distance**

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$\boldsymbol{r}_0 = (\sqrt{3}\gamma(t)l/4,\ \sqrt{3}l/4)$

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Shear strain: $\gamma(t) = \gamma_0 \sin(\omega t)$

γ_0**: Amplitude**, ω**: Frequency**

$\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j = (x_{ij}, y_{ij})$

Interaction force: $F_{ij}^{(\mathrm{n})}, F_{ij}^{(\mathrm{t})}$

Stress: $\sigma = -\frac{1}{A}\sum_i \sum_j \left(\frac{x_{ij}y_{ij}}{r_{ij}} F_{ij}^{(\mathrm{n})} + \frac{x_{ij}^2 - y_{ij}^2}{r_{ij}} F_{ij}^{(\mathrm{n})} \right)$

Pressure: $P = \frac{1}{A}\sum_i \sum_j r_{ij} F_{ij}^{(\mathrm{n})}$

A : the area of the system

Storage modulus (Elasticity)

$$G' = \frac{\omega}{\pi}\int_0^{2\pi/\omega} d\theta\ \frac{\sigma(t)\sin(\omega t)}{\gamma_0}$$

Loss modulus (Dissipation)

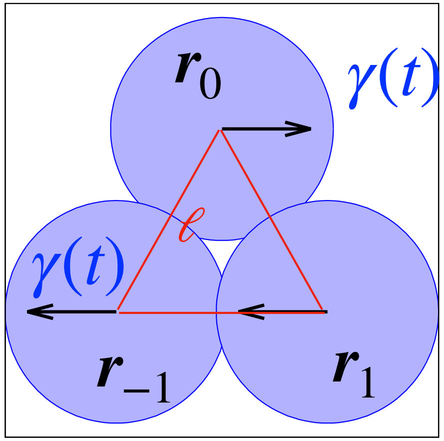
$$G'' = \frac{\omega}{\pi}\int_0^{2\pi/\omega} d\theta\ \frac{\sigma(t)\cos(\omega t)}{\gamma_0}$$

Analytical solution: stress σ

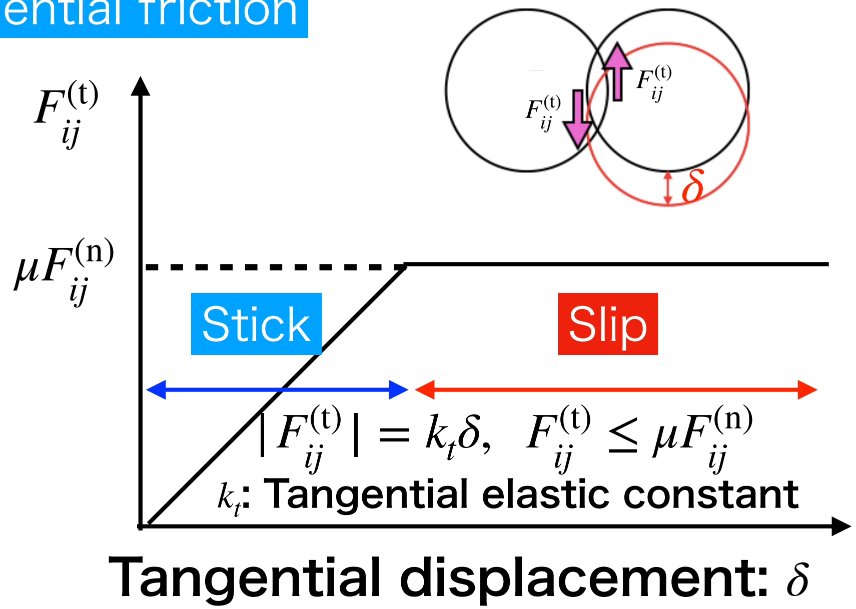
Assumption: $\gamma_0 \ll 1$

Three-particle model:

$$\boldsymbol{r}_0 = (\sqrt{3}\gamma(t)l/4,\ \sqrt{3}l/4)$$
$$\boldsymbol{r}_{\pm 1} = (\pm l/2 - \sqrt{3}\gamma(t)l/4,\ -\sqrt{3}l/4)$$



Tangential friction



Transition to slip state when γ becomes large

Displacement for slip: $\delta_c = \mu F_{ij}^{(n)}/k_t$

Pressure: $P \sim F_{ij}^{(n)}/d$

Normal force: $F_{ij}^{(n)}$, **Diameter of grain**: d

Critical strain: $\gamma_c \sim \delta_c/d \sim \mu P/k_t$

Analytical solution for γ_c

$$\gamma_c(\mu) = \frac{4}{3\sqrt{3}}\frac{\mu P}{k_t}$$

Analytical solution for σ

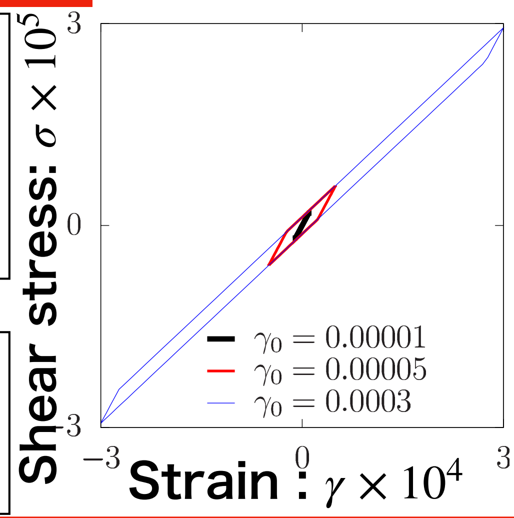
$\gamma_0 < \gamma_c(\mu)$: **no slip**

$$\sigma(t) = \frac{\sqrt{3}(k_n + k_t)}{4}\gamma(t)$$

k_n: elastic constant for $F_{ij}^{(n)}$

$\gamma_0 \ge \gamma_c(\mu)$: **slip**

$\sigma(t)$ **exhibits loops.**



→ **Calculation of G' and G''**

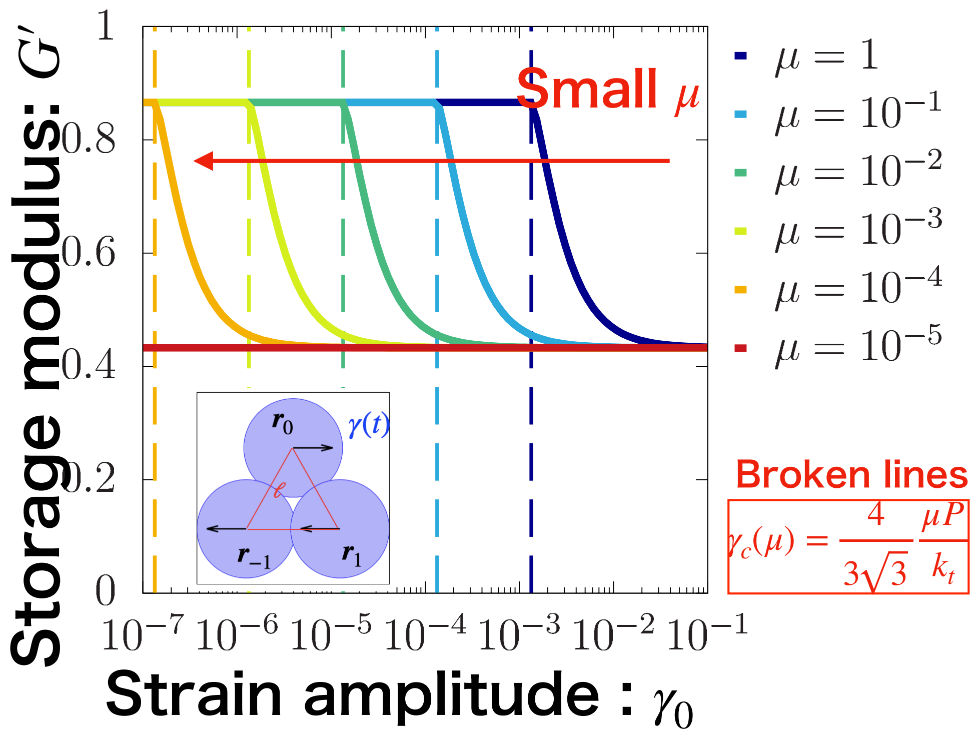
Analytical solution: G' and G''

Storage modulus

$\epsilon = 0.001$

$$G' = \begin{cases} \dfrac{\sqrt{3}(k_\mathrm{n} + k_\mathrm{t})}{4}, & \gamma_0 < \gamma_c(\mu) \\ \dfrac{\sqrt{3}}{4}\left\{k_\mathrm{n} + \dfrac{k_\mathrm{t}}{\pi}(\Theta(\gamma_0) - \sin\Theta(\gamma_0)\cos\Theta(\gamma_0)\right\}, & \gamma_c(\mu) \le \gamma_0 \end{cases}$$

$$\Theta(\gamma_0) = \cos^{-1}\left(1 - 2\gamma_c(\mu)/\gamma_0\right)$$



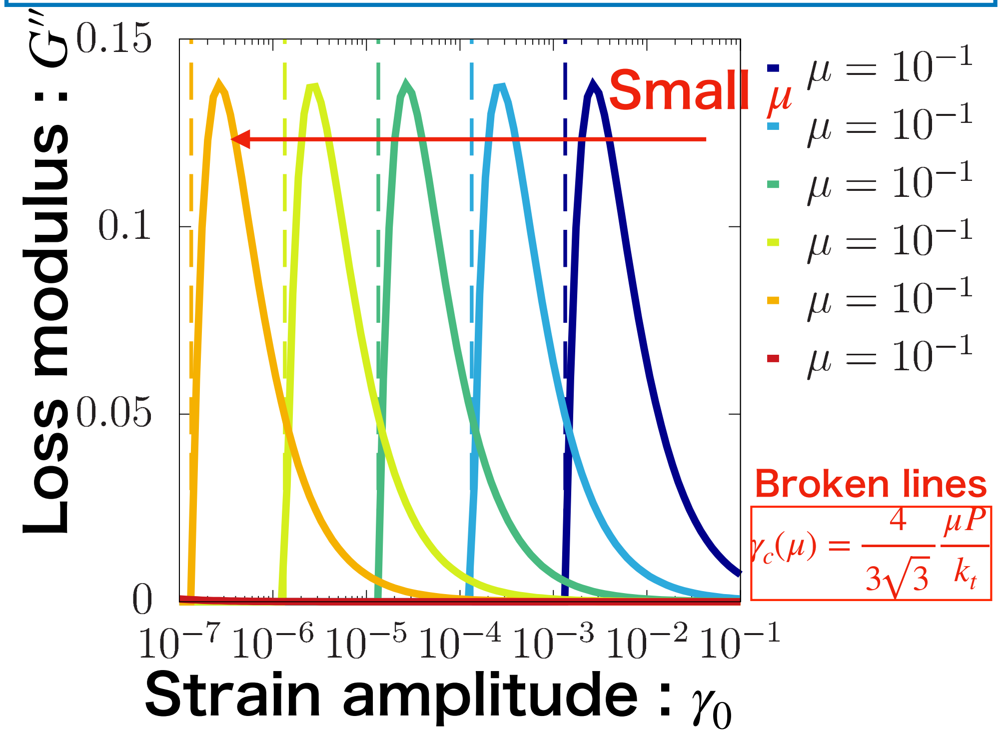
- G' decreases as γ_0 exceeds $\gamma_c(\mu)$.
- The critical strain depends on μ.
- G' exhibits a second plateau.

Loss modulus

$\epsilon = 0.001$

$$G'' = \begin{cases} 0, & \gamma_0 < \gamma_c(\mu) \\ \dfrac{\sqrt{3}k_\mathrm{t}}{4\pi}\left\{1 - \cos^2\Theta(\gamma_0)\right\}, & \gamma_c(\mu) \le \gamma_0 \end{cases}$$

$$\Theta(\gamma_0) = \cos^{-1}\left(1 - 2\gamma_c(\mu)/\gamma_0\right)$$



- G'' becomes non-zero for $\gamma_0 > \gamma_c(\mu)$.
- The critical strain depends on μ.
- G'' has a peak.

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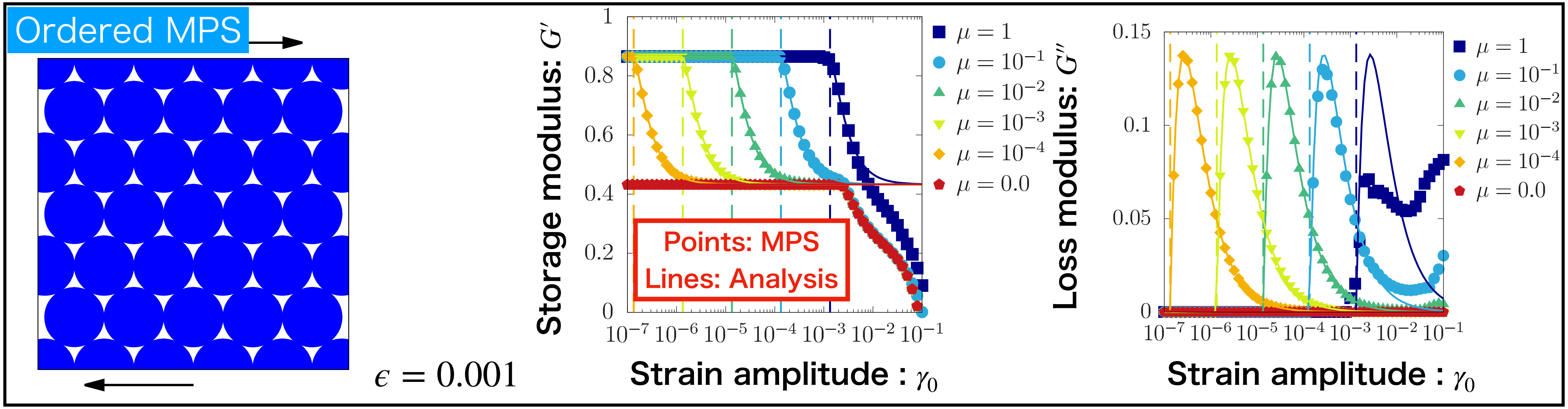
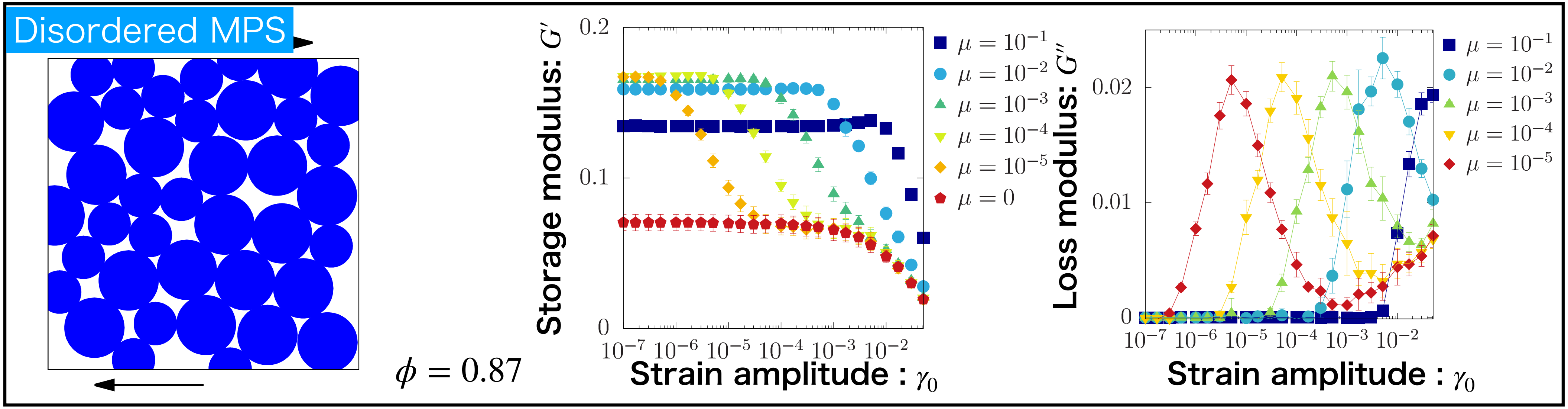
Comparison with many-particle systems





- The analytical results for TPM perfectly agree with ordered MPS except for large γ_0.
- The analytical results qualitatively reproduce those of disordered MPS.

Prediction: critical scaling law

Analytical solution of TPM:

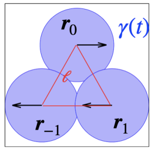
Assumption: $\gamma_0 \ll 1$

$$G'' = \begin{cases} 0, & \gamma_0 < \gamma_c(\mu) \\ \frac{\sqrt{3}k_t}{4\pi}\left\{1-\cos^2\Theta(\gamma_0)\right\}, & \gamma_c(\mu) \le \gamma_0 \end{cases} \qquad \Theta(\gamma_0) = \cos^{-1}\left(1 - 2\gamma_c(\mu)/\gamma_0\right) \qquad \gamma_c(\mu) = \frac{4}{3\sqrt{3}}\frac{\mu P}{k_t}$$

Prediction: Scaling laws for G' and G''

$$G'(\gamma_0, \mu) = G'_M(\mu)\ \mathcal{F}_1\left(\frac{k_t\gamma_0}{\mu P(\mu)}\right) \sim \gamma_0/\gamma_c$$

$$G''(\gamma_0, \mu) = G''_M(\mu)\ \mathcal{F}_2\left(\frac{k_t\gamma_0}{\mu P(\mu)}\right)$$



μ: Friction coefficient **P: Pressure**

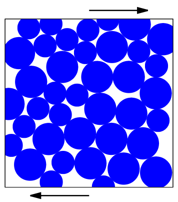
k_t: Tangential elastic constant

$G'_M(\mu)$: Maximum value of G'

$G''_M(\mu)$: Maximum value of G''

$\mathcal{F}_1(x)$, $\mathcal{F}_2(x)$: Scaling functions

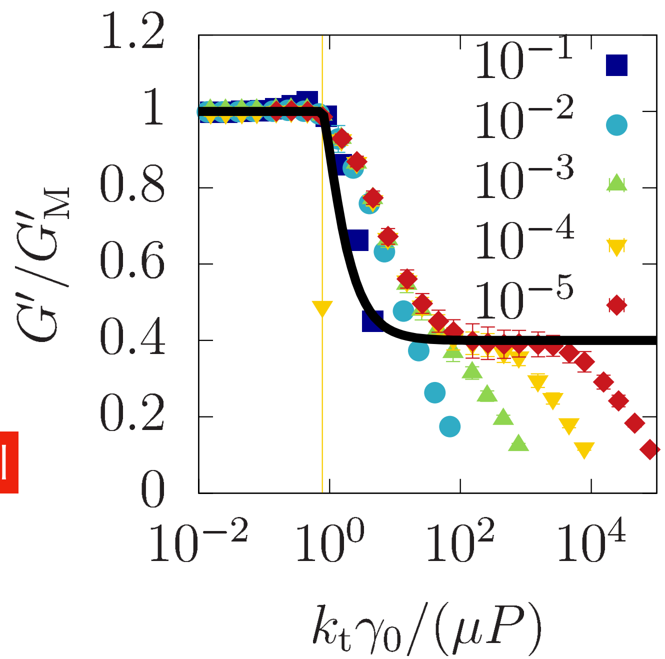
Disordered MPS

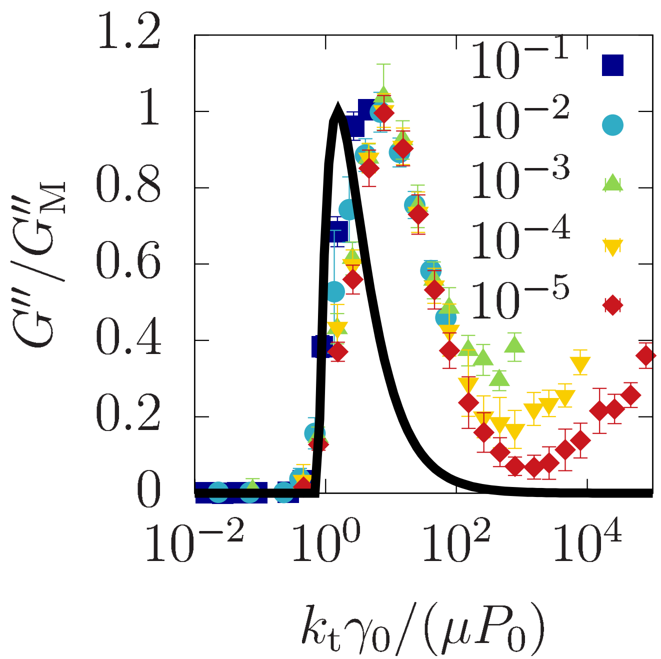


Scaling laws are satisfied in MPS.

Solid line: three particle model

k_t is used as a fitting parameter.





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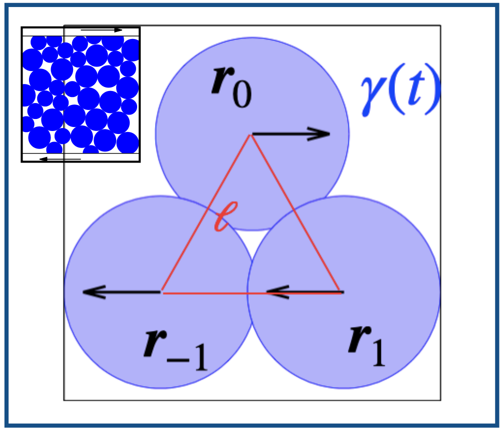
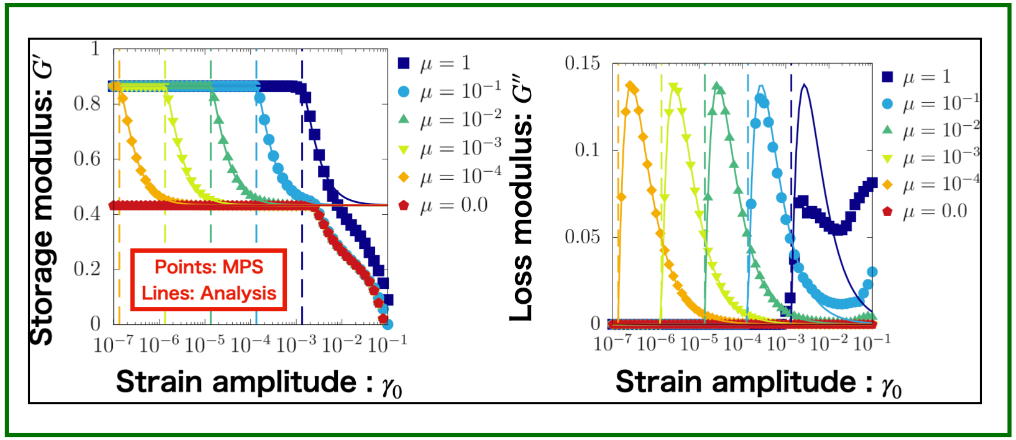
Summary

- Topic : Non-linear response of frictional granular materials.
- We have proposed three-particle model.
- Three-particle model perfectly reproduces G' and G'' in ordered MPS.
- Three-particle model qualitatively reproduces G' and G'' in disordered MPS.
- We derive scaling laws, which are satisfied even in disordered MPS.
- Problem: we need a fitting parameter for disordered MPS.
- Future work: Self-consistent determination of a fitting parameter.





Scaling laws:

$$G' = G'_M \; F_1\left(\frac{k_t \gamma_0}{\mu P(\mu)}\right)$$

$$G'' = G''_M \; \mathscr{F}_2\left(\frac{k_t \gamma_0}{\mu P(\mu)}\right)$$