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準静的剪断下における摩擦のあるアモルファス固体のヤコビアン行列による解析

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Introduction

Definition of Jacobian $J_{ij}^{\alpha\beta}$

$$J_{ij}^{\alpha\beta} = -\frac{\partial \tilde{F}_i^{\alpha}}{\partial q_j^{\beta}},$$

$\tilde{F}_i^{\alpha}$: α component of generalized force acting on i-th particle $\vec{\tilde{F}}_i = (F_i^x, F_i^y, T_i)^T$,

q_i^{α} : α component of generalized i-th particle coordinate $q_i := (r_i^x, r_i^y, \theta_i)$,

T_i : Torque of i th particle,

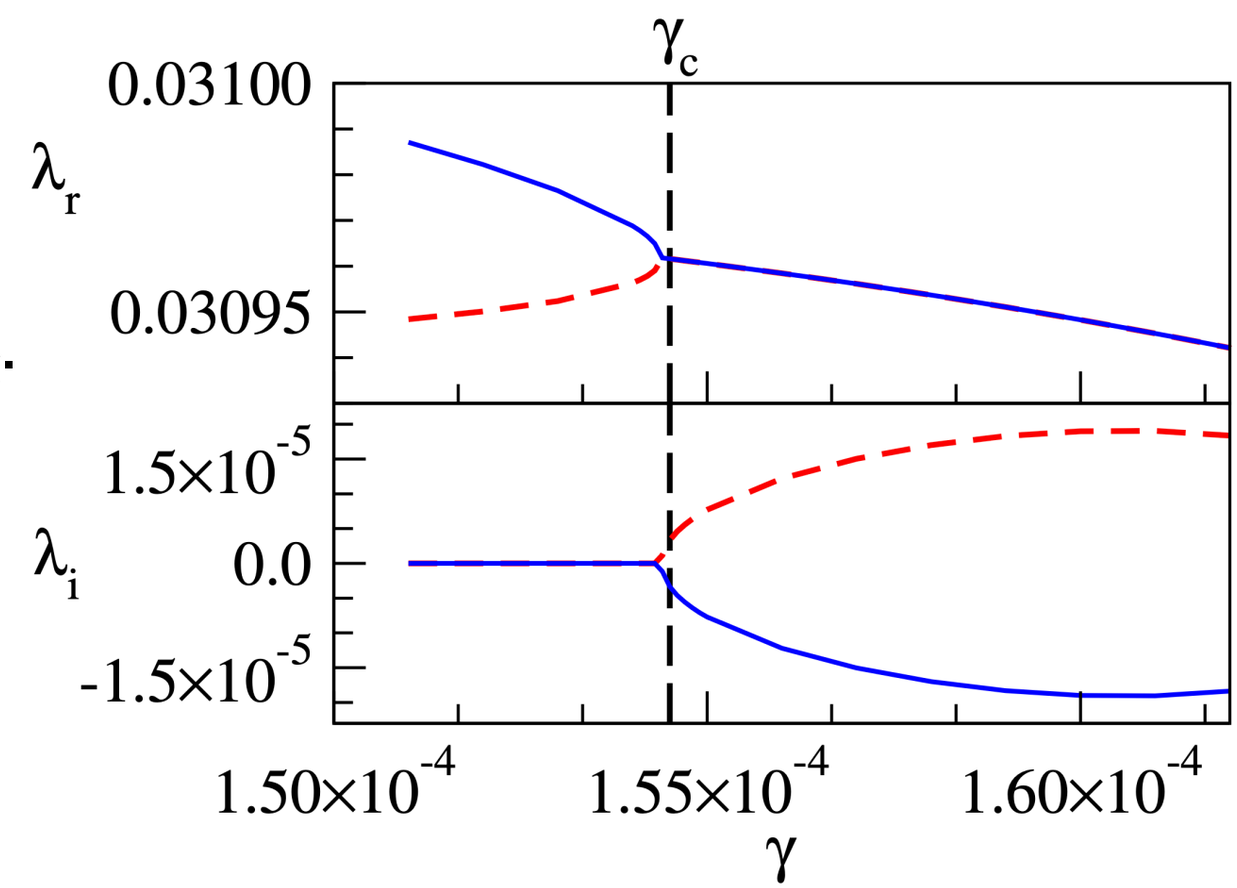
θ_i : Rotational degree of i th particle.

Jacobian is an asymmetric matrix.

->It has complex eigenvalue $\lambda = \lambda_r + i\lambda_i$.

->Imaginary parts contribute to oscillatory instability*.

AQS, Frictional particles



*J. Chattoraj et al., Phys. Rev. Lett. **123**, 098003 (2019).

Introduction

	Frictionless materials	Frictional materials
Tool for stability analysis (dynamical matrix)	Hessian: $H_{ij}^{\alpha\beta} = \dfrac{\partial^2 U}{\partial q_j^\alpha \partial q_j^\beta}$	Jacobian: $J_{ij}^{\alpha\beta} = -\dfrac{\partial \tilde{F}_i^\alpha}{\partial q_j^\beta}$
Oscillatory instability	×	○
Shear rigidity G formula with dynamical matrix	○	?

G can be obtained from $H_{ij}^{\alpha\beta}$, Hessian's eigenvalues & Hessian's eigenvectors*.

*A. Lemaître & C. Maloney, J. Stat. Phys. **123**, 2 (2006).

Question?

Can we predict G by Jacobian?

Purpose

To obtain the prediction of G in the limit $\gamma \to 0$

Our numerical protocol

Preparation of initial configuration

1. Preparing the frictionless configuration at density ϕ with energy minimization by FIRE*
2. Incorporating the tangential forces
3. Relaxation by drag force $-\eta \vec{v}_i$ until $|F_i^\alpha| < F_{\mathrm{Th}}$

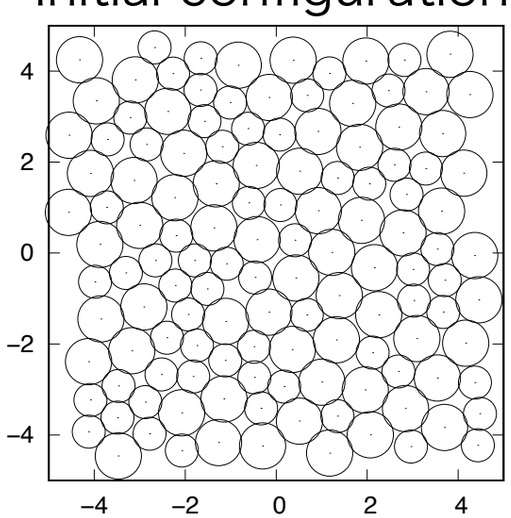
*E. Bitzek et al., Phys. Rev. Lett., 97, 170201 (2006).

Athermal quasistatic shear protocol

I. Applying affine shear deformation $\Delta\gamma$ to the system with Lees-Edwards periodic boundary condition

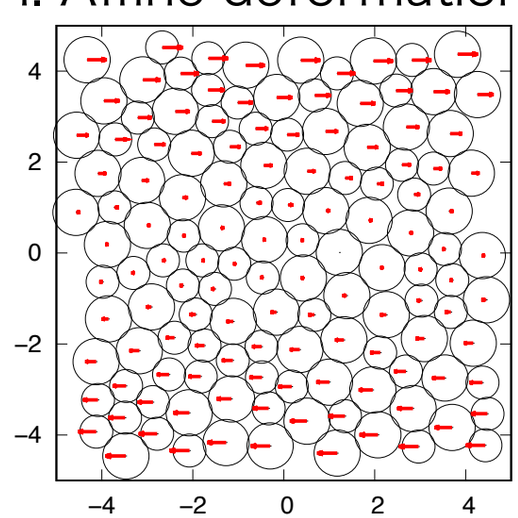
II. Relaxation by drag force $-\eta \vec{v}_i$ until $|F_i^\alpha| < F_{\mathrm{Th}}$

Initial configuration



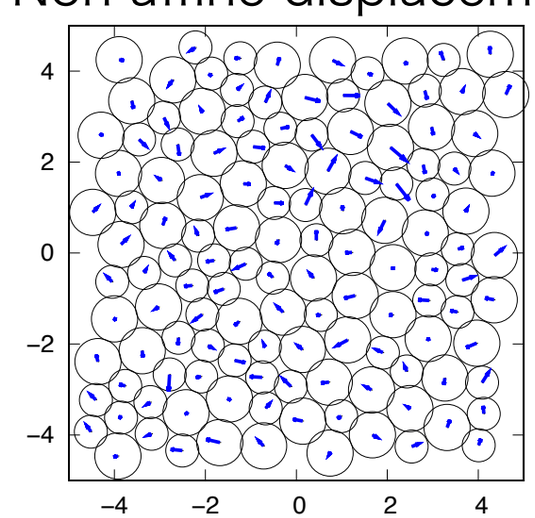
Step strain $\Delta\gamma$

I. Affine deformation



Relaxation by $-\eta \vec{v}_i$

II. Non affine displacement



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Numerical methods

Equation of motion

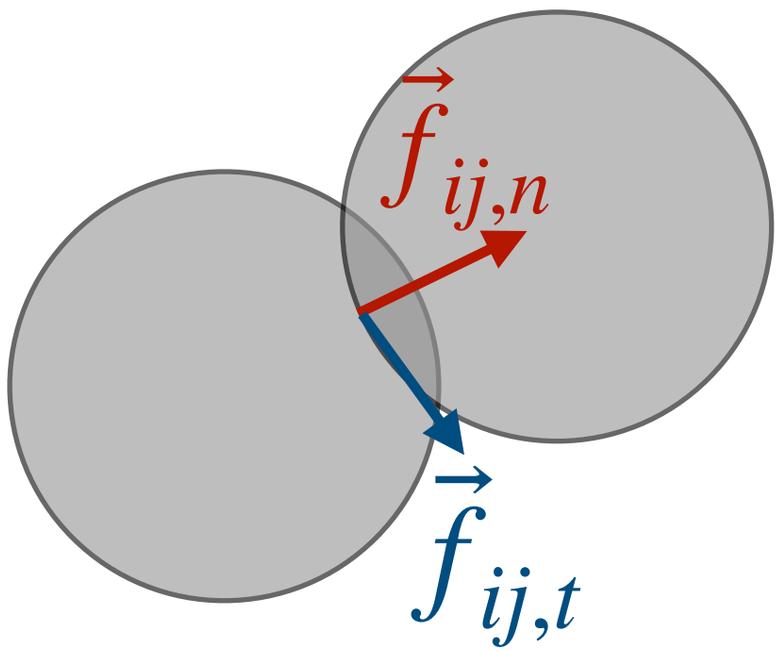
$$m_i \frac{d^2 \vec{x}_i}{dt^2} = \vec{F}_i^c - \eta \frac{d\vec{x}_i}{dt},$$

$$I_i \frac{d^2 \theta_i}{dt^2} = T_i^c - \eta \frac{d\theta_i}{dt}$$

$\vec{F}_i^c$: Contact force of i particle

T_i^c : Torque of i particle

θ_i : rotational degree of i particle



$$\vec{F}_i^c = \sum_j \left(\vec{f}_{ij,n} + \vec{f}_{ij,t} \right) \Theta(a_i + a_j - r_{ij}),$$

$$\vec{f}_{ij,n} = k_n \xi_{ij,n}^{3/2} \vec{n}_{ij},$$

$$\vec{f}_{ij,t} = -k_t \xi_{ij,n}^{1/2} \vec{\xi}_{ij,t}$$

*nonslip model

Our simulated system

2 dimensional binary disks ($N = 128$),

Step strain: $\Delta\gamma = 10^{-10}$,

Threshold value of mechanical equilibrium condition: $F_{\mathrm{Th}}/(k_n d_0) = 10^{-14}$,

Density $0.80 \leq \phi \leq 0.90$, Tangential ratio $0.0 \leq k_t/k_n \leq 10.0$.

Expression of G by J

We obtain shear modulus G by J:

$$G(0) = \frac{1}{2L^2} \sum_{i,j(i\neq j)} \left[\underline{y_{ij}^2(0) J_{N,ij}^{xx}(0)} + \underline{\sum_{\kappa=x,y} y_{ij}(0) J_{ij}^{\kappa x}(0) \frac{du_{ij}^{\kappa}(0)}{d\gamma} + y_{ij}(0) J_{ij}^{\ell x}(0) \left(\frac{du_i^{\ell}(0)}{d\gamma} + \frac{du_j^{\ell}(0)}{d\gamma} \right)} \right] \quad \cdots \quad (1)$$

Affine shear modulus Non affine shear modulus

with $J_{ij}^{\alpha\beta} = -\frac{\partial f_{ij}^{\beta}}{\partial q_i^{\alpha}}$, $J_{N,ij}^{\alpha\beta} = -\frac{\partial f_{N,ij}^{\beta}}{\partial q_i^{\alpha}}$, $u_{ij}^{\alpha} := u_i^{\alpha} - u_j^{\alpha}$, $u_i^{\alpha}(0) = q_i^{\alpha}(\Delta\gamma) - q_i^{\alpha}(0) - \Delta\gamma\delta_{\alpha x}$: non affine displacement.

Calculation methods of G

Cauchy's expression

$$G = \frac{d\sigma_{xy}}{d\gamma}, \quad \sigma_{xy} = -\frac{1}{L^2} \sum_i \sum_{j>i} f_{ij}^x y_{ij},$$

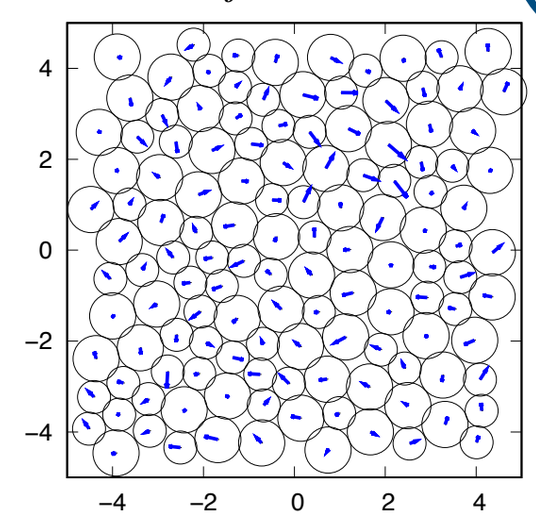
f_{ij}^x : x component of forces from j to i particle,

y_{ij} : y component of displacements from j to i particle.

It needs $f_{ij}^x(0)$, $y_{ij}(0)$, $f_{ij}^x(\Delta\gamma)$, $y_{ij}(\Delta\gamma)$.

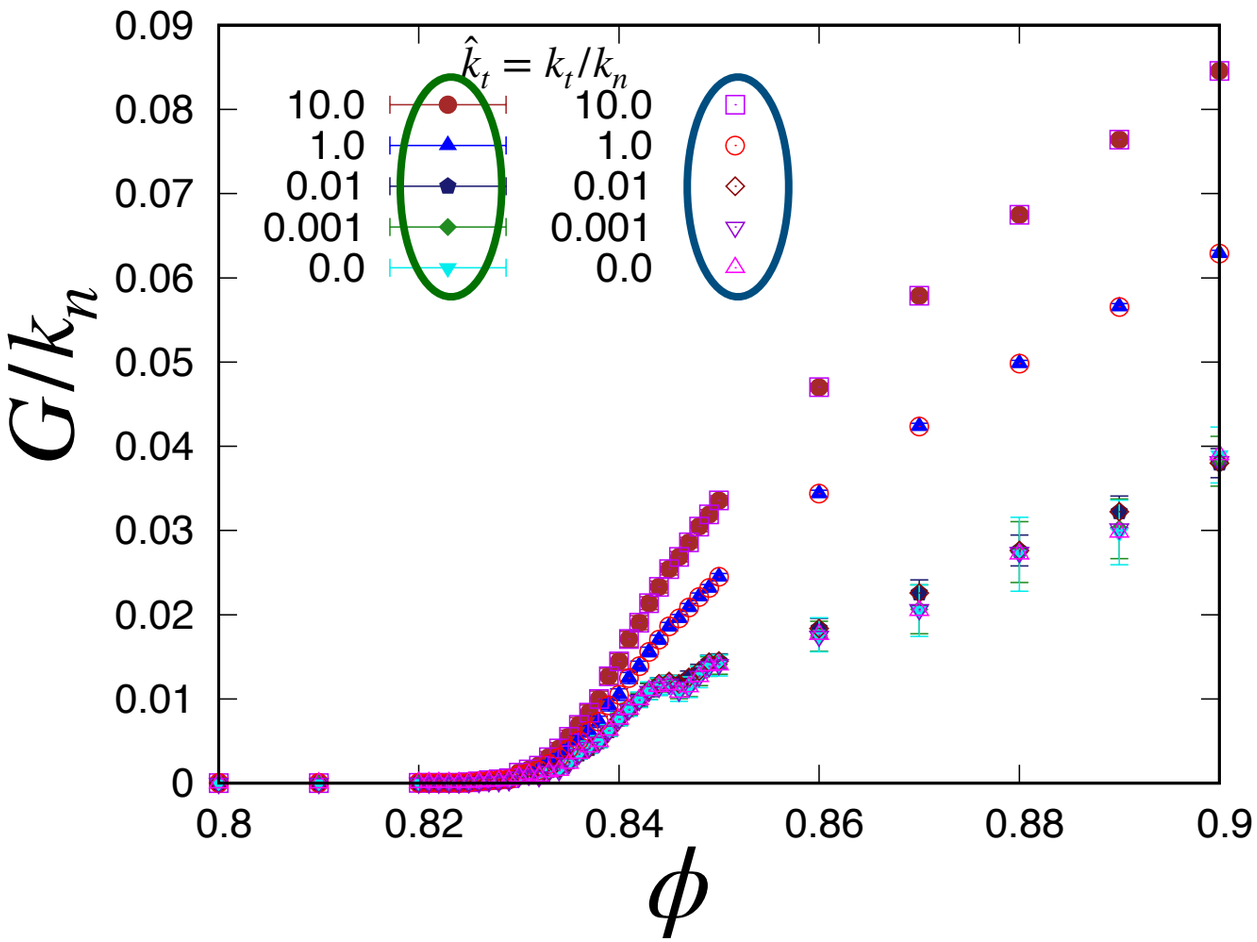
Jacobian's expression

Eq. (1) needs $J_{ij}^{\alpha\beta}(0)$, $y_{ij}(0)$, $u_i^{\alpha}(0)$

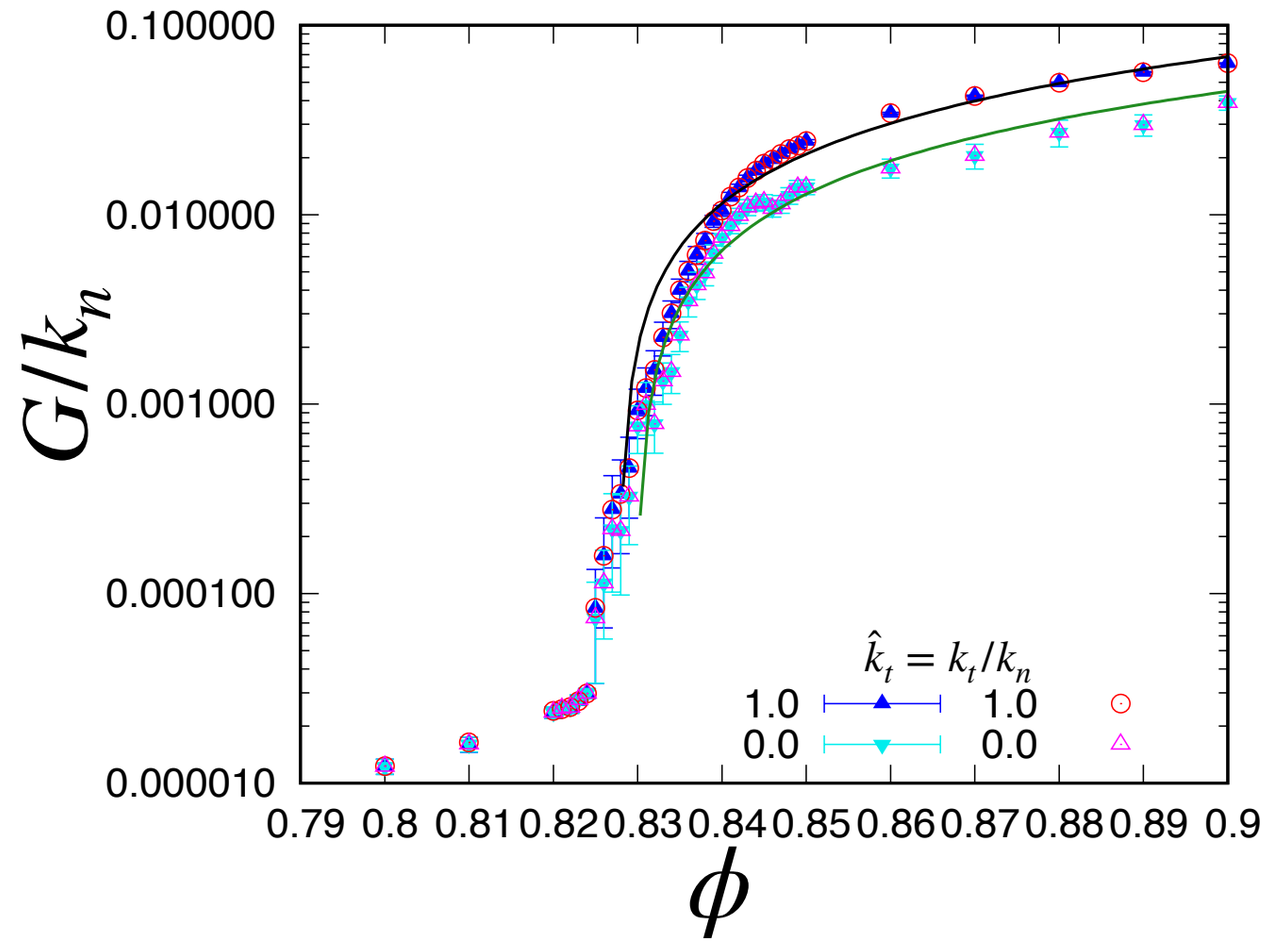


Non affine displacement: $u_i^{\alpha}(0)$

ϕ-dependence



Fitted by $G(\phi) = G_0 + c(\phi - \phi_J)^\alpha$ with $\alpha = 1$

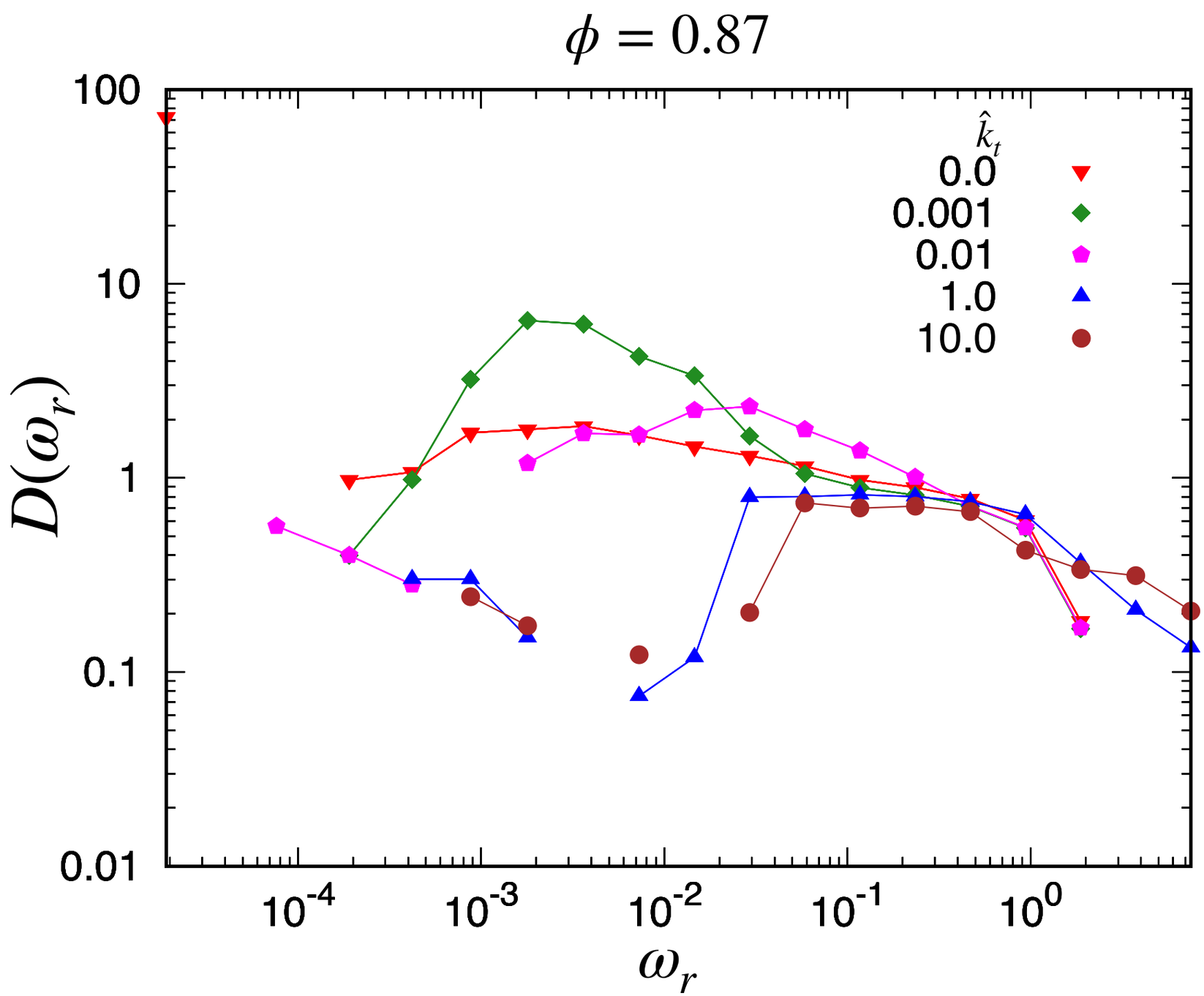


Jacobian's expression reproduces ϕ dependence.

$G(\phi)$ has a linear dependence of $\phi - \phi_J$*.

*C. S. O'Hern et al., Phys. Rev. Lett., **88**, 7 (2002),
E. Somfai et al., Phys. Rev. E, **75**, 020301(R) (2007).

Density of State



An isolated band at low frequency* appears for $\hat{k}_t \geq 0.01$.

*C. F. Schreck et al., Phys. Rev. E, **85**, 061305 (2012).

Summary

Frictional amorphous solids under quasi-static shear are analyzed using the Jacobian.

Shear modulus G in the limit $\gamma \to 0$

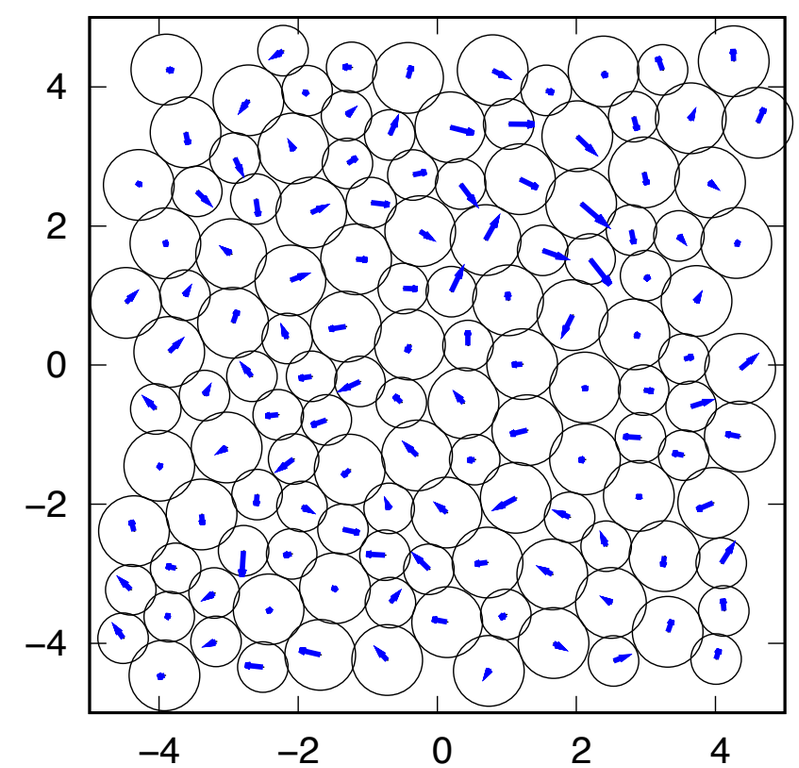
- **Jacobain's representation can reproduce G.**

Density of state $D(\omega_r)$ in the limit $\gamma \to 0$

- **An isolated band at low frequency appears for $\hat{k}_t \geq 0.01$.**

Future work

- Expanding non affine displacements $u_i^\alpha(0)$ by eigenfunctions of Jacobian



Non affine displacement: $u_i^\alpha(0)$