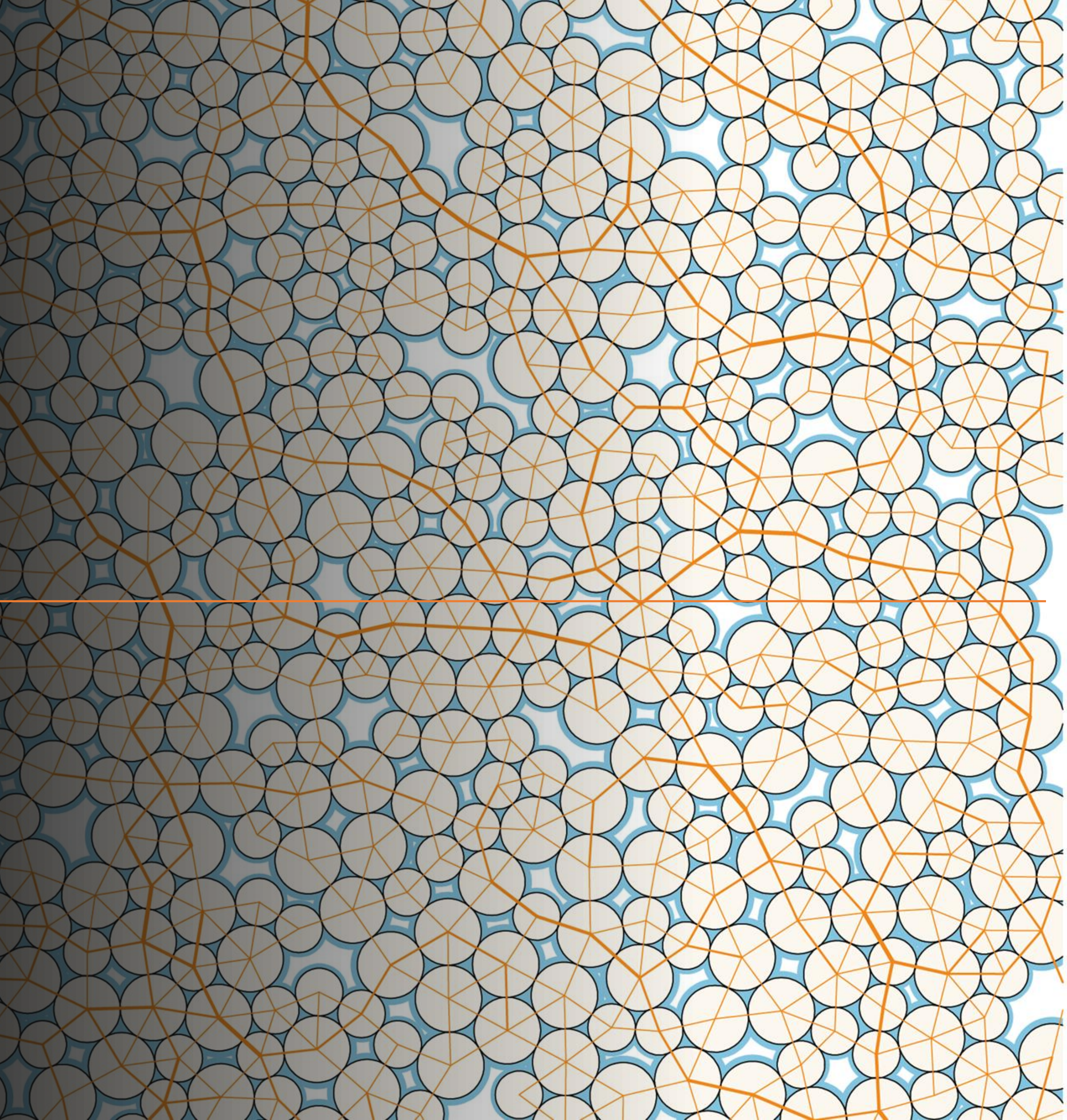
Shear-induced diffusion near jamming

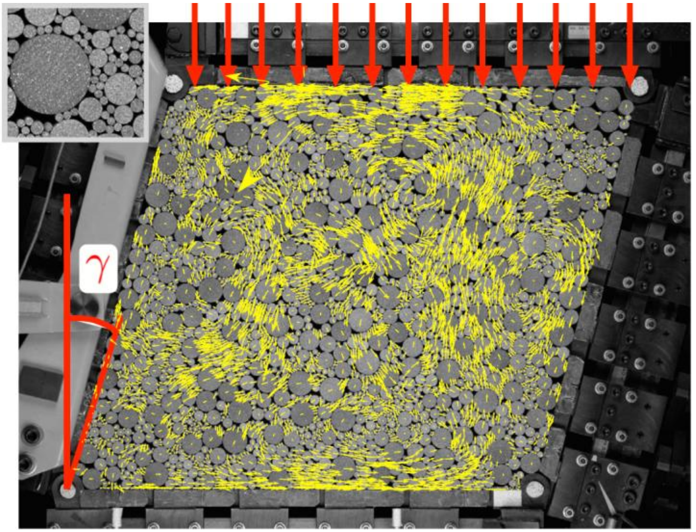
Kuniyasu Saitoh
Department of Physics, Faculty of Science, Kyoto Sangyo University, Japan

Collaborations with
Takeshi Kawasaki, The University of Osaka, Japan
Abhinendra Singh, Case Western Reserve University, US



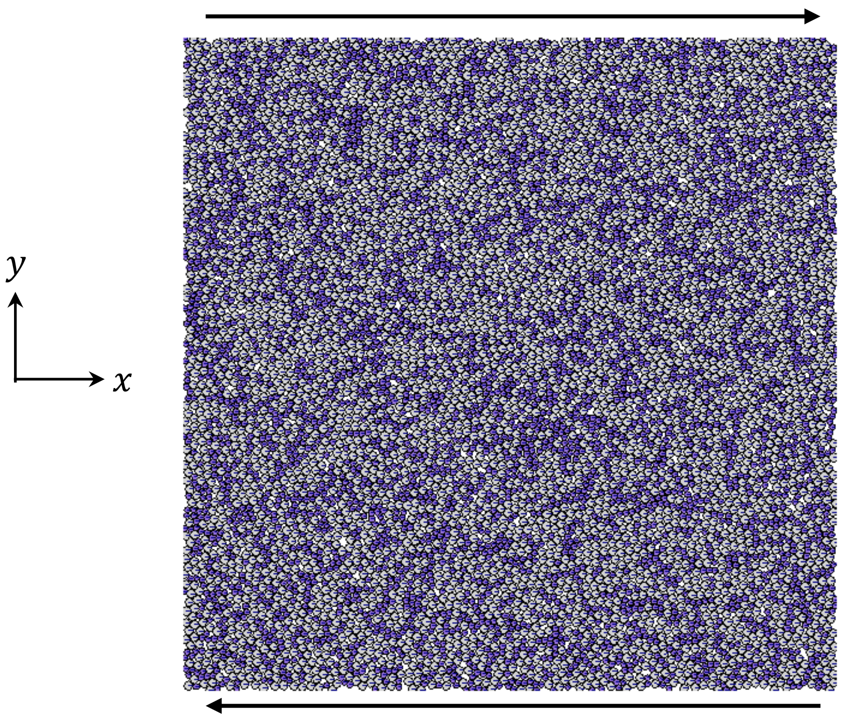
Granular materials under shear

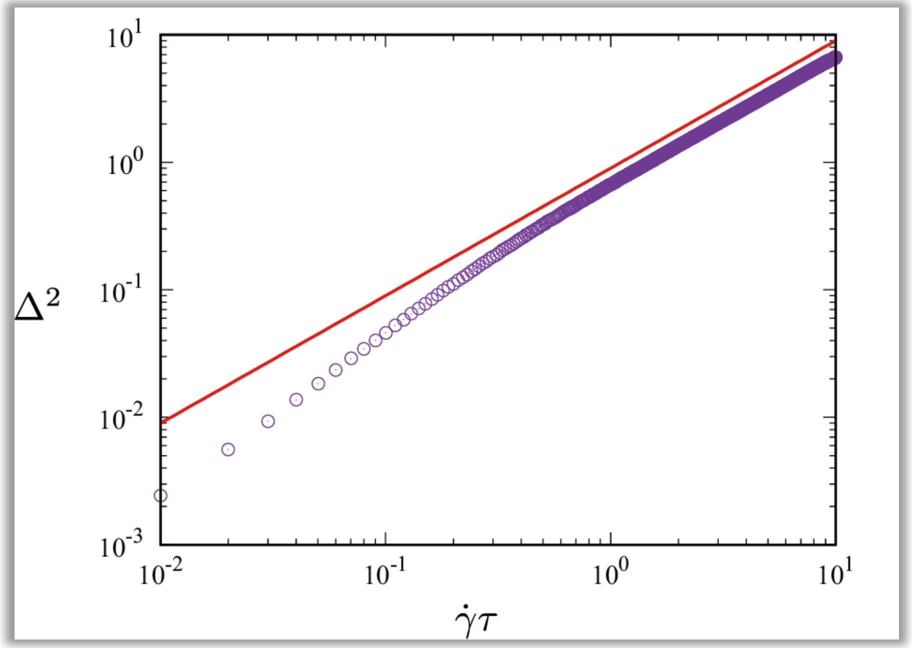
- **Constituent grains**
  - Macroscopic in size, from few μm to mm.
  - Thermal fluctuations are negligible, i.e., athermal.
  - Driven by mechanical deformations, e.g., simple shear.
- **Examples**
  - Mixing of foods, cosmetic and pharmaceutical products.
  - Geological hazards such as landslides and avalanches.
- **Experiments[1]**
  - Two-dimensional granular disks sheared under fixed pressure.
  - Complex non-affine displacements are observed (yellow arrows).



[1] G. Combe, V. Richefeu and M. Stasiak, and A.P.F. Atman, *Phys. Rev. Lett.* **115**, 238301 (2015).

Shear-induced diffusion

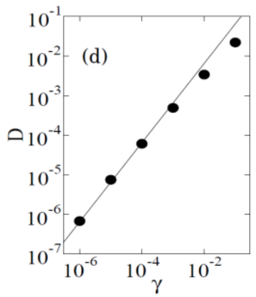
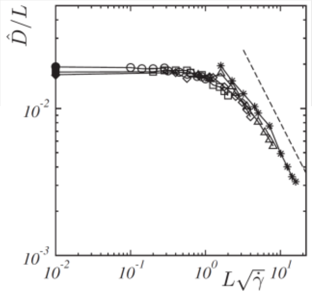




- **Molecular dynamics (MD) simulations of sheared frictional disks**
  - The transverse y-component of particle displacement, $\Delta y_i(\tau)$.
  - The mean squared displacement (MSD) is defined as $\Delta^2(\tau) = N^{-1}\sum_{i=1}^{N} \Delta y_i(\tau)^2$.
  - The MSD is linear in τ (normal diffusion) if the strain exceeds unity.

Previous works

- Shear-induced diffusion coefficient $D = \lim_{\tau \to \infty} \Delta^2(\tau)/2\tau$ depends on both packing fraction ϕ and shear rate $\dot{\gamma}$.
- *Rigid clusters*[2] – D is linear in a correlation length ξ as $D \sim d_0 \xi \dot{\gamma}$ with the mean particle diameter d_0.

	$\boldsymbol{\phi < \phi_J}$	$\boldsymbol{\phi \approx \phi_J}$	$\boldsymbol{\phi > \phi_J}$
Overdamped MD P. Olsson (2010)	$D \propto \dot{\gamma}$	$D \propto \dot{\gamma}^{0.78}$ $D \propto \lvert\Delta\phi\rvert \dot{\gamma}^{0.515}$	$D \propto \dot{\gamma}^{0.68}$
Underdamped MD T. Hatano (2011) I.K. Ono et al. (2003)		$D \propto \begin{cases} \dot{\gamma} & (\dot{\gamma} < \dot{\gamma}_D) \\ \dot{\gamma}^{0.8} & (\dot{\gamma} > \dot{\gamma}_D) \end{cases}$ $\xi \propto \dot{\gamma}^{-0.23}$	
P. Kharel & P. Rognon (2017)			$D \propto \dot{\gamma}^{1/2}$ $\xi \propto \dot{\gamma}^{-1/2}$
A. Lemaitre & C. Caroli (2009)			$D \propto \begin{cases} \dot{\gamma} L & (\dot{\gamma} < \dot{\gamma}_D) \\ \dot{\gamma}^{1/2} & (\dot{\gamma} > \dot{\gamma}_D) \end{cases}$ $\xi \propto \dot{\gamma}^{-1/2}$

[2] P. Kharel and P. Rognon, *Phys. Rev. Lett.* **119**, 178001 (2017).

Critical scaling of diffusion coefficient

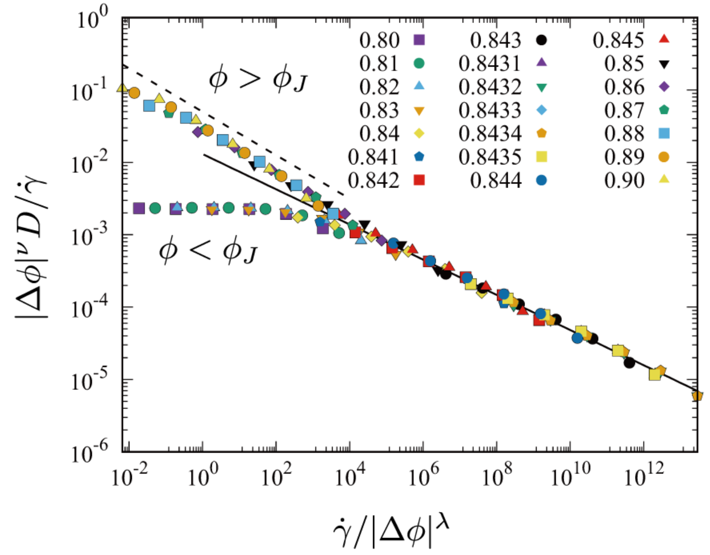
- **Overdamped MD simulations**
  - The same model with Olsson & Teitel (2007)[3].
- **Data collapses**[4]
  - Critical scaling of diffusion coefficient, $D(\phi, \dot{\gamma})$.
  - We numerically confirmed $D(\phi, \dot{\gamma}) \sim d_0 \xi(\phi, \dot{\gamma}) \dot{\gamma}$.

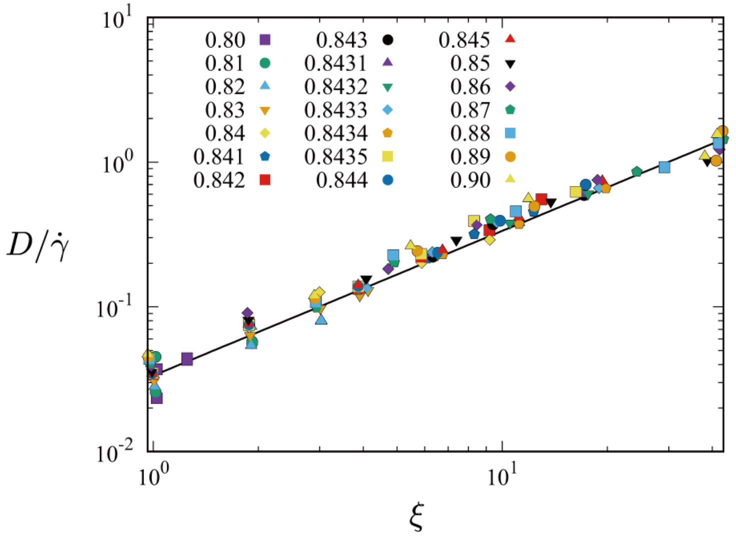
$$|\Delta\phi|^{\nu} D/\dot{\gamma} \sim \mathcal{F}_{\pm}\left(\frac{\dot{\gamma}}{|\Delta\phi|^{\lambda}}\right)$$ where $\nu \approx 0.939$ and $\lambda \approx 3.87$.

$$\mathcal{F}_{-}(x) = \text{const.} \quad \therefore D \propto |\Delta\phi|^{-\nu}\dot{\gamma} \quad (\phi < \phi_c)$$

$$\mathcal{F}_{+}(x) = x^{-0.3} \quad \therefore D \propto |\Delta\phi|^{0.3\lambda-\nu}\dot{\gamma}^{0.7} \quad (\phi > \phi_c)$$

Critical regime (solid line) $\quad \mathcal{F}_{\pm}(x) = x^{-\nu/\lambda} \quad \therefore D \propto \dot{\gamma}^{1-\nu/\lambda}$

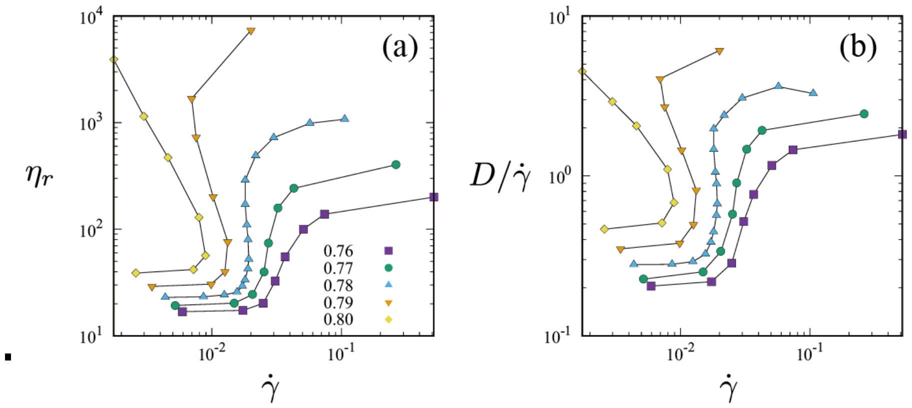




[3] P. Olsson and S. Teitel, *Phys. Rev. Lett.* **99**, 178001 (2007).
[4] K.S. and T. Kawasaki, *Front. Phys.* **8**, 99 (2020).

Relation to shear viscosity

- **Overdamped MD simulations**[5]
  - Frictional non-Brownian particles in two dimensions.
  - The system is sheared by the Lees-Edwards boundaries.
  - Discontinuous shear thickening (DST) is observed.
  - As the viscosity, $D/\dot{\gamma}$ also exhibits the characteristic "S-shape".

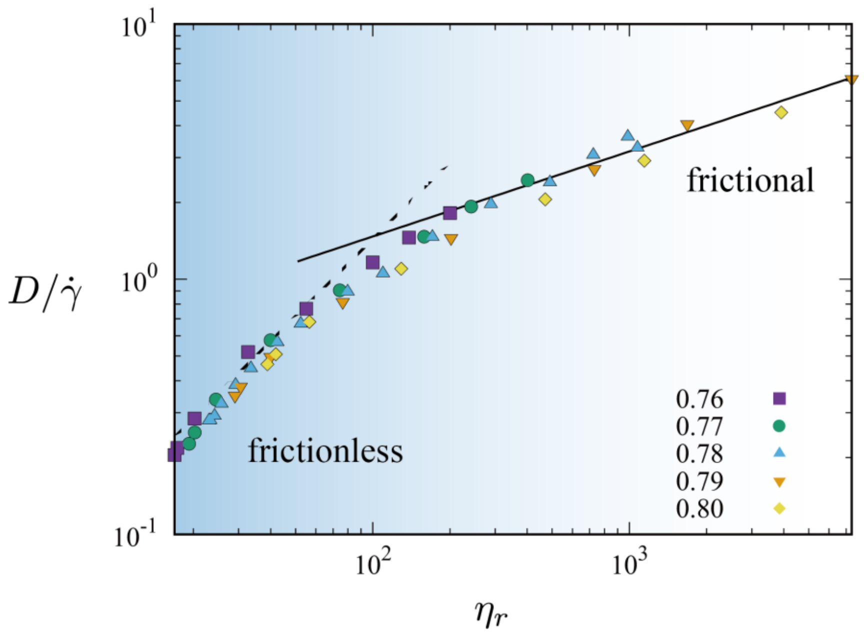


- **Energy balance equation**
  - Small/large shear stress ⟺ frictionless/frictional state
  - The rate of energy dissipation scales as

$$\Gamma \propto \begin{cases} (\xi\dot{\gamma})^2 & \text{(frictionless)} \\ \xi^3\dot{\gamma}^2 & \text{(frictional)} \end{cases}$$

  - Because of $\dot{\gamma}\sigma \sim \Gamma$, the viscosity $\eta = \sigma/\dot{\gamma}$ scales as

$$\eta \propto \begin{cases} \xi^2 \\ \xi^3 \end{cases} \quad \therefore D/\dot{\gamma} \propto \begin{cases} \eta & \text{(frictionless)} \\ \eta^{1/3} & \text{(frictional)} \end{cases}$$

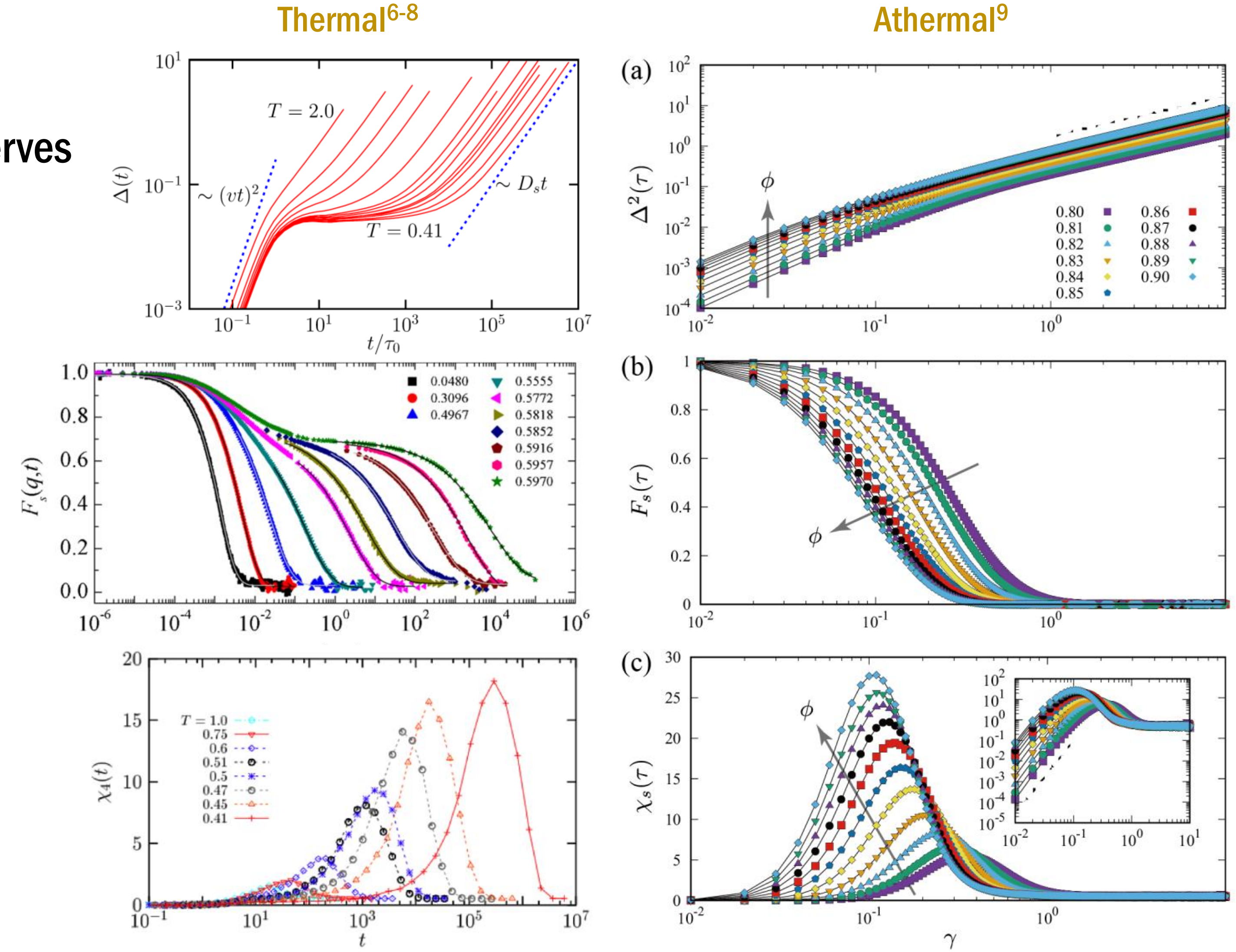


[5] A. Singh and K.S., *Soft Matter* **19**, 6631 (2023).

Dynamic heterogeneities

- **Glasses[6-8]**
  - Approaching the glass transition, one observes
    - ✓ A plateau develops in MSD,
    - ✓ Relaxation time increases,
    - ✓ Heterogeneities also increases.

- **Shear-induced diffusion[9]**
  - Distinct from the glassy dynamics.
  - Increasing ϕ/decreasing $\dot{\gamma}$, we find
    - ✓ No plateau in MSD (no cage),
    - ✓ Relaxation time *decreases*,
    - ✓ Though heterogeneities increases.



[6] L. Berthier and G. Biroli, *Rev. Mod. Phys.* **83**, 587 (2011).
[7] G. Brambilla et al., *Phys. Rev. Lett.* **102**, 085703 (2009).
[8] L. Berthier, *Physics* **4**, 42 (2011).
[9] K.S. and T. Kawasaki, *Front. Phys.* **10**, 992239 (2022).

Divergence of shear-induced diffusion coefficient

- **Shear-induced diffusion**[10]

If the system is in a quasi-static regime above jamming, i.e., $\dot{\gamma} t_0 \ll 1$ and $\phi > \phi_c$, the correlation length reaches the system length, $\xi \sim L$.

$$\therefore D \sim d_0 L \dot{\gamma} \rightarrow \infty \text{ in the thermodynamic limit, } L \rightarrow \infty.$$

- **Long-time tail in two dimensions**

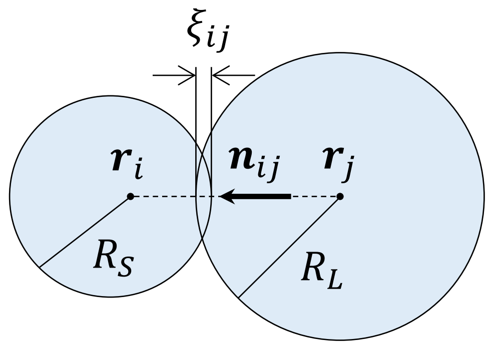
It is known that velocity auto-correlation functions in fluid systems exhibit long-time tails.

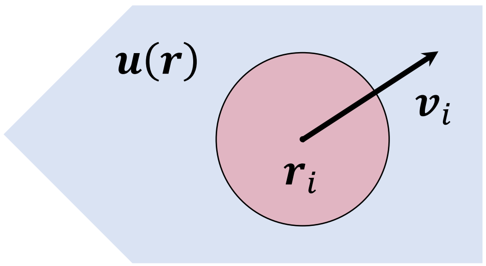
$$\therefore D \rightarrow \infty \text{ in two dimensions.}$$

Is there a link between the divergence of shear-induced diffusion coefficient and long-time tails?

[10] A. Lemaitre and C. Caroli, *Phys. Rev. Lett.* **103**, 065501 (2009).

Overdamped MD simulations

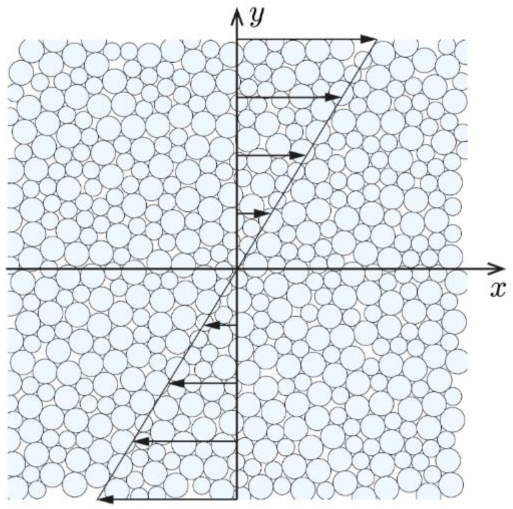




Soft particles

- $N = 8192$ soft particles in two dimensions.
- A 50:50 binary mixture with size ratio $R_L/R_S = 1.4$.

Numerical model



- Repulsive force is linear in overlap as $\boldsymbol{f}_{ij} = k\xi_{ij}\boldsymbol{n}_{ij}$.
- Damping force is given by the deviation from mean flow field,

$$\boldsymbol{F}_i^{\mathrm{d}} = -\mu\{\boldsymbol{v}_i - \boldsymbol{u}(\boldsymbol{r}_i)\}$$

- Imposing $\boldsymbol{u}(\boldsymbol{r}) = \dot{\gamma} y \boldsymbol{e}_x$, we numerically solve overdamped dynamics,

$$\boldsymbol{0} = k\sum_{j\neq i}\boldsymbol{f}_{ij} + \boldsymbol{F}_i^{\mathrm{d}} \qquad \therefore \boldsymbol{v}_i = \boldsymbol{u}(\boldsymbol{r}_i) + \mu^{-1}\sum_{j\neq i}\boldsymbol{f}_{ij}$$

- Units of length and time are given by $d_0 \equiv R_L + R_S$ and $t_0 \equiv \mu/k$, respectively.

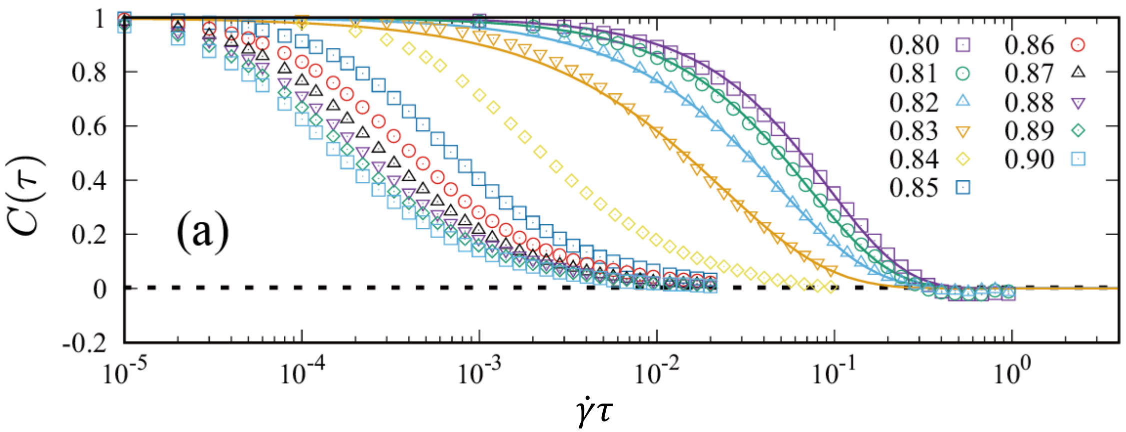
The Green-Kubo formula

- **Diffusion coefficient**
  - We examine the Green-Kubo (GK) formula,

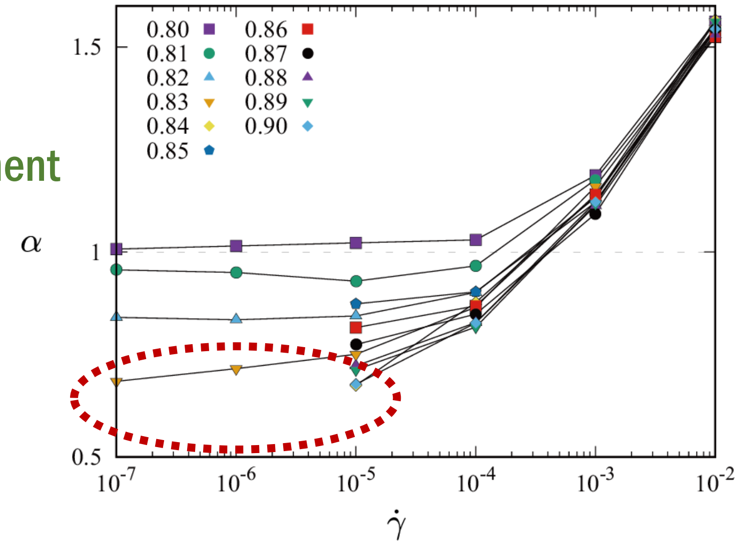
$$D = \langle {v_y}^2 \rangle \int_0^\infty C(\tau)\, d\tau$$

  - Mean squared velocity, $\langle {v_y}^2 \rangle$.
  - Normalized velocity auto-correlation function,

$$C(\tau) = \frac{\langle v_y(\tau) v_y(0) \rangle}{\langle {v_y}^2 \rangle}$$



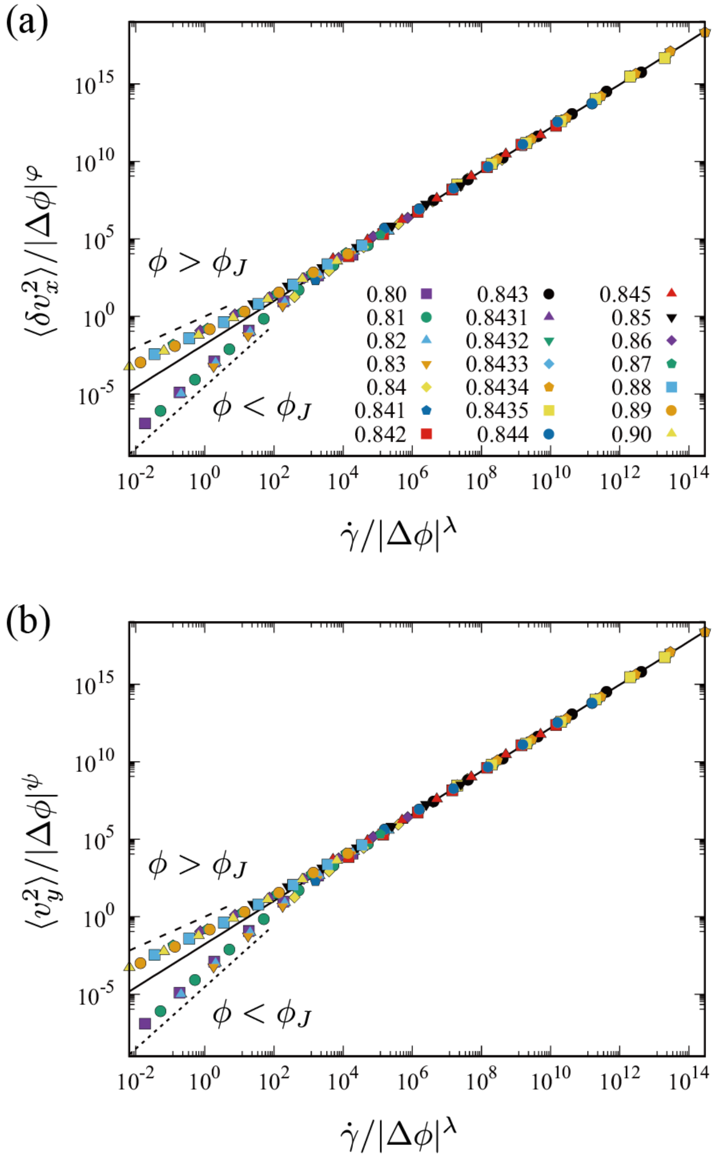
Stretching exponent



- **Stretched exponential function**
  - Data are fitted to $C(\tau) = \exp[-(\tau/\tau_*)^\alpha]$ (solid lines).
  - In the quasi-static regime above jamming, i.e., $\dot{\gamma} t_0 \ll 1$ and $\phi > \phi_c$, $C(\tau)$ cannot be fitted to the stretched exponential.

Mean squared velocity

- **Dependence on ϕ and $\dot{\gamma}$**
  - Data are nicely collapsed as $\dfrac{\langle {v_y}^2 \rangle}{|\Delta\phi|^{\psi}} \sim F_{\pm}\left(\dfrac{\dot{\gamma}}{|\Delta\phi|^{\lambda}}\right)$.
  - We estimate the scaling exponents *quantitatively*[11].
  - $\psi = 5.39$ and λ is the same with that for D.
- **Scaling functions**[12]
  - In $\phi < \phi_c$, consistent with the viscosity divergence,
    $F_{-}(x) = x^2 \quad \therefore \langle {v_y}^2 \rangle \propto |\Delta\phi|^{\psi - 2\lambda}\dot{\gamma}^2 \approx |\Delta\phi|^{-2.35}\dot{\gamma}^2$
  - In $\phi > \phi_c$, consistent with the yield stress near jamming,
    $F_{+}(x) = x \quad \therefore \langle {v_y}^2 \rangle \propto |\Delta\phi|^{\psi - \lambda}\dot{\gamma} \approx |\Delta\phi|^{1.52}\dot{\gamma}$
  - $\Delta\phi$-independent critical regime (solid line),
    $F_{\pm}(x) = x^{\psi/\lambda} \quad \therefore \langle {v_y}^2 \rangle \propto \dot{\gamma}^{\psi/\lambda} \approx \dot{\gamma}^{1.39}$



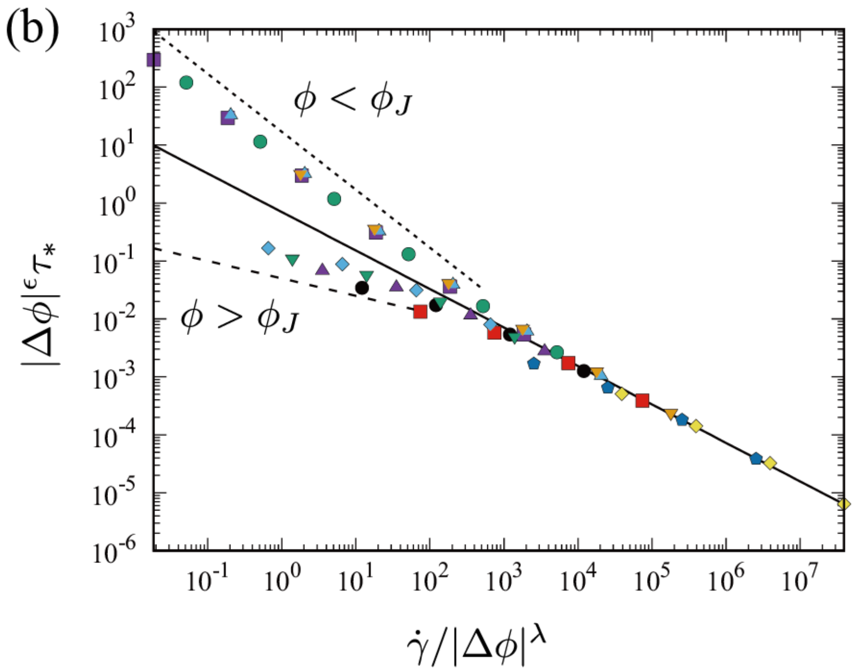
[11] M. Otsuki and H. Hayakawa, *Phys. Rev. E* **86**, 031505 (2012).

[12] Since $\dot{\gamma}\sigma \sim \Gamma$ and $\Gamma \sim \langle {v_y}^2 \rangle$, $\langle {v_y}^2 \rangle \sim \eta\dot{\gamma}^2$ below jamming and $\langle {v_y}^2 \rangle \sim \sigma_Y \dot{\gamma}$ above jamming.

Relaxation time below jamming

- **Dependence on ϕ and $\dot{\gamma}$**
  - Except for $\dot{\gamma} t_0 \ll 1$ and $\phi > \phi_c$, data are well collapsed as $|\Delta\phi|^{\epsilon}\tau_* \sim G_{\pm}\left(\frac{\dot{\gamma}}{|\Delta\phi|^{\lambda}}\right)$.
  - We *quantitatively* estimate the scaling exponents as $\epsilon = 2.57$ and λ is the same with that for D.

- **Scaling functions**
  - In $\phi < \phi_c$, $\quad G_{-}(x) = x^{-1}$
    $\therefore \tau_* \propto |\Delta\phi|^{\lambda-\epsilon}\dot{\gamma}^{-1} \approx |\Delta\phi|^{1.30}\dot{\gamma}^{-1}$
  - In $\phi > \phi_c$, $\quad G_{+}(x) = x^{-0.3}$
    $\therefore \tau_* \propto |\Delta\phi|^{0.3\lambda-\epsilon}\dot{\gamma}^{-0.3} \approx |\Delta\phi|^{-1.41}\dot{\gamma}^{-0.3}$
  - $\Delta\phi$-independent critical regime (solid line),
    $G_{\pm}(x) = x^{-\epsilon/\lambda} \quad \therefore \tau_* \propto \dot{\gamma}^{-\epsilon/\lambda} \approx \dot{\gamma}^{-0.664}$



Long-time tails above jamming

- **The power-law decay**
  - Velocity auto-correlation functions for $\dot{\gamma} t_0 \ll 1$ and $\phi > \phi_c$ are described as

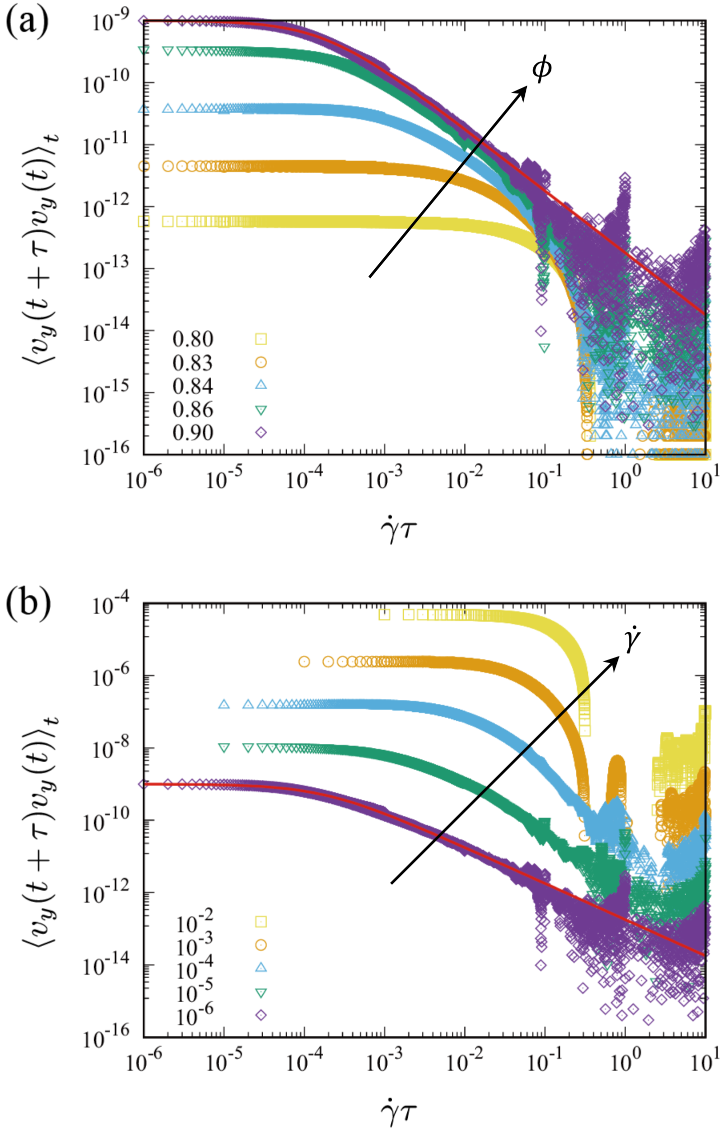
$$C(\tau) = \frac{1}{1 + c_0 \dot{\gamma} \tau}$$

  - If $\dot{\gamma}\tau \gg 1$, $C(\tau) \sim (\dot{\gamma}\tau)^{-1}$ and the GK formula diverges as

$$D = \langle {v_y}^2 \rangle \int_0^\infty C(\tau)\, d\tau \to \infty$$

- **cf.) A. Lemaitre and C. Caroli (2009)**

$$D \sim d_0 L \dot{\gamma} \ \to\ \infty \text{ for } L \ \to\ \infty.$$



Scaling relation

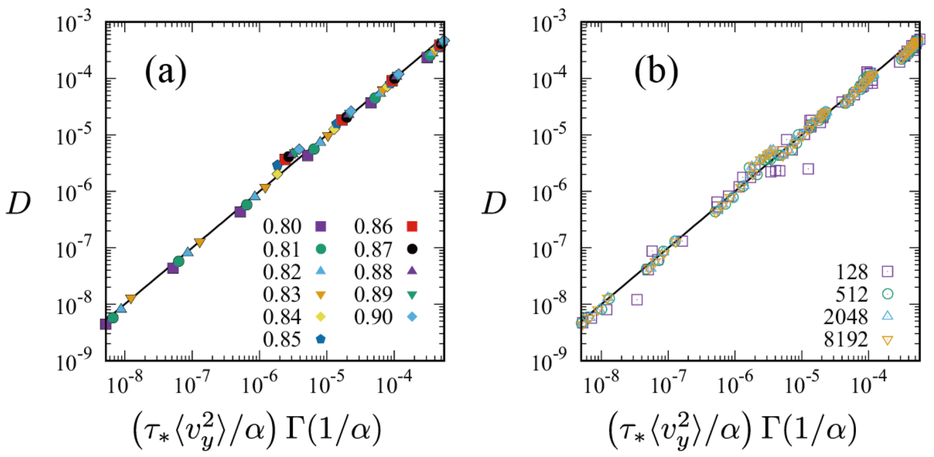
The reduced GK formula

- If $C(\tau)$ is replaced with the stretched exponential,

$$\int_0^\infty \exp\left[-\left(\frac{\tau}{\tau_*}\right)^\alpha\right] d\tau = \frac{\tau_*}{\alpha}\Gamma\left(\frac{1}{\alpha}\right)$$

$$\therefore D = \frac{\tau_* \langle {v_y}^2 \rangle}{\alpha}\Gamma\left(\frac{1}{\alpha}\right)$$

ϕ-dependence N-dependence



- Substituting the critical scaling of D, τ_*, and $\langle {v_y}^2 \rangle$, we suggest the following relation.

ν ⋯ diffusion, ψ ⋯ squared velocity, ϵ ⋯ relaxation time, ➡ $\nu + \psi - \epsilon = \lambda$

K.S. and T. Kawasaki, *Phys. Rev. Research* (2026) in press.

- We have investigated shear-induced diffusion of soft particles in two dimensions by MD simulations.
- If the system is below jamming, the velocity auto-correlation functions are well described by stretched exponential function, $C(\tau) = \exp[-(\tau/\tau_*)^\alpha]$.
- Both the mean squared velocities $\langle {v_y}^2 \rangle$ and relaxation time τ_* exhibit critical scaling near jamming, where we estimated their critical exponents quantitatively.
- According to the reduced GK formula, we suggest a scaling relation between the critical exponents of D, $\langle {v_y}^2 \rangle$, and τ_*.
- If the system is above jamming and sheared quasi-statically, i.e., $\phi > \phi_c$ and $\dot{\gamma} t_0 \ll 1$, the velocity auto-correlation function exhibits a long-time tail, $C(\tau) \sim (\dot{\gamma}\tau)^{-1}$, so that the GK formula for shear-induced diffusion coefficient D diverges.

Outlook

- Shear-induced diffusion of frictional systems, etc.