

Classification of the reversible-irreversible transitions in particle trajectories near the jamming transition

Nagoya University

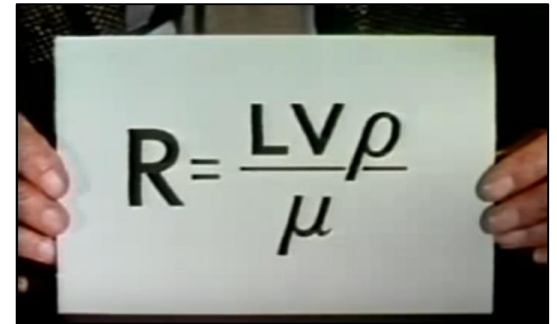
Takeshi Kawasaki

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Ludovic Berthier (Univ. Montpellier)

K. Nagasawa, K. Miyazaki, and T. Kawasaki , to be submitted.
T. Kawasaki and L. Berthier, Phys. Rev. E **94**, 022615 (2016).

Taylor's experiment

Low Reynolds number flow: a particle trajectory can be reversible!



$$(\nabla \cdot \mathbf{v}) = 0,$$

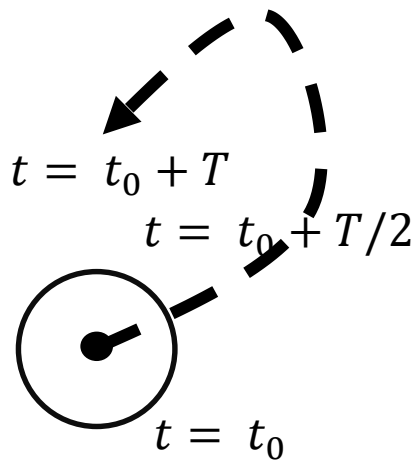
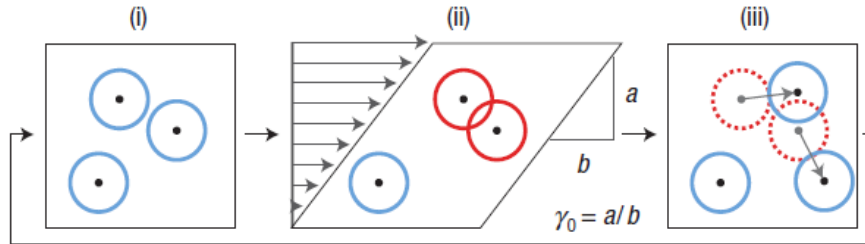
$$0 = -\nabla P + (\nabla \cdot \boldsymbol{\tau})$$

$$\boldsymbol{\tau} = \mu[\nabla \mathbf{v} + (\nabla \mathbf{v})^t].$$

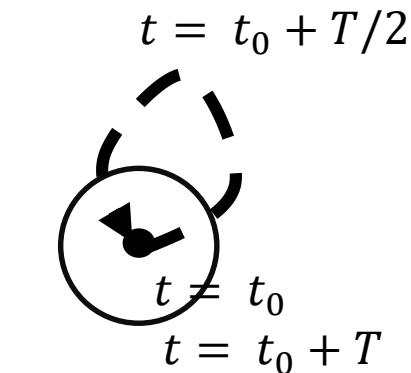
Taylor & Friedman (1966), Low Reynolds Number Flows
(National Committee on Fluid Mechanics Films, Encyclopedia Britannica Education Corp.,
United States)

Reversible-irreversible (RI) transition is a non-equilibrium phase transition!

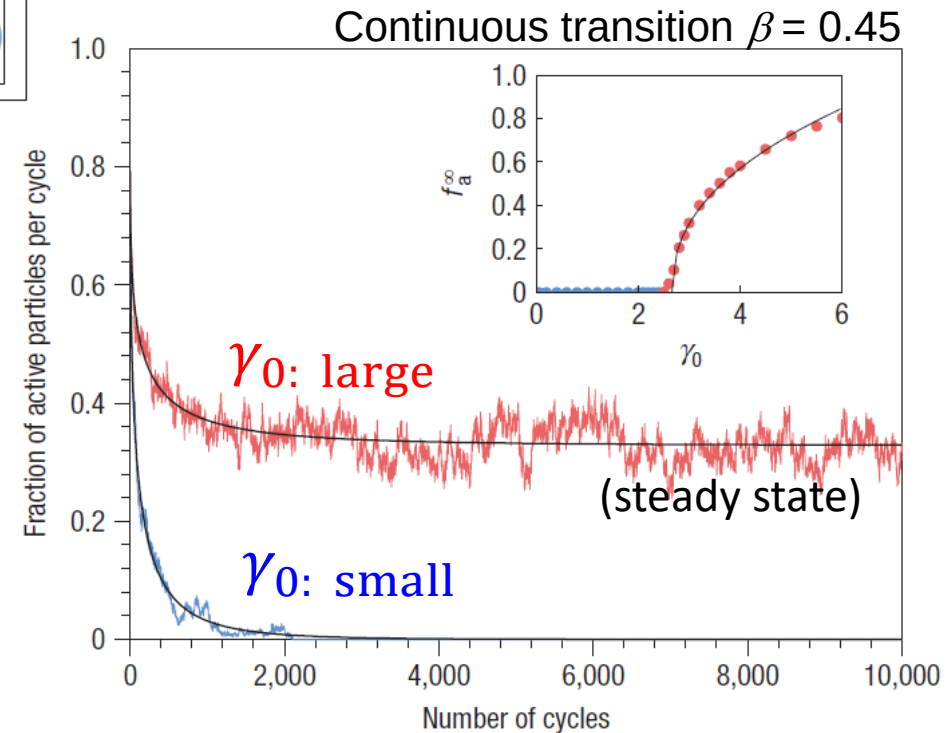
Oscillatory shear experiment and model of low density colloidal suspensions ($\phi = 0.20$)



Irreversible



Reversible
(Absorbing state)



This absorbing state transition shows Conserved Directed Percolation (CDP) ($\beta = 0.62$) like critical behavior.

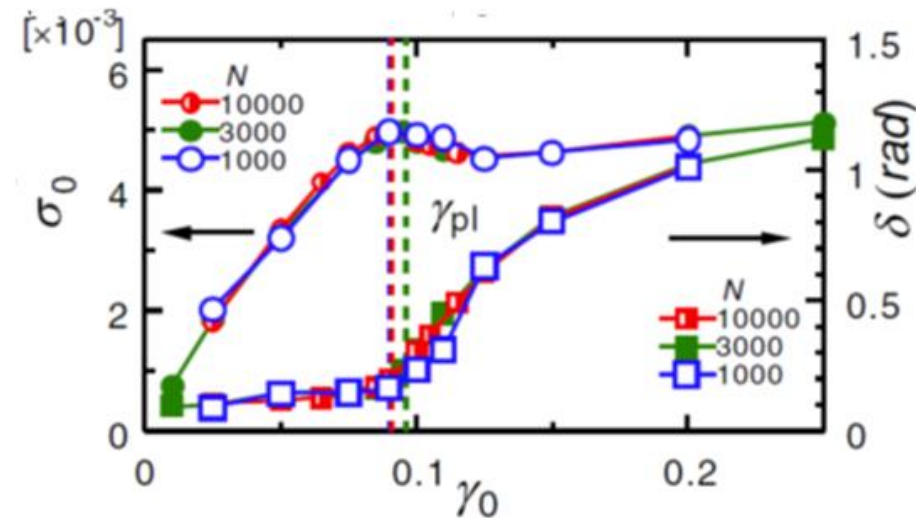
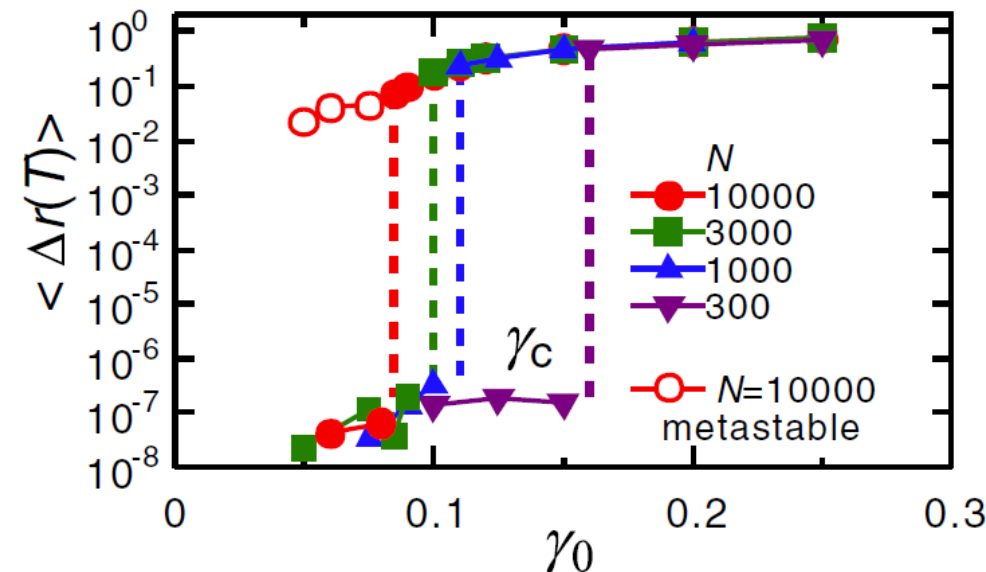
Even in very high density system, RI transition takes place -- behaving differently from low density suspensions

Oscillatory shear numerical experiment in highly dense suspensions in 3D

($\varphi = 0.80$ cf. $\varphi_J = 0.647$)

Time averaged one cycle displacement : $\langle \Delta r(T) \rangle$

Stress-strain curve:



“Discontinuous” RI transition

Yielding transition

$$\gamma_c \approx 0.0885$$

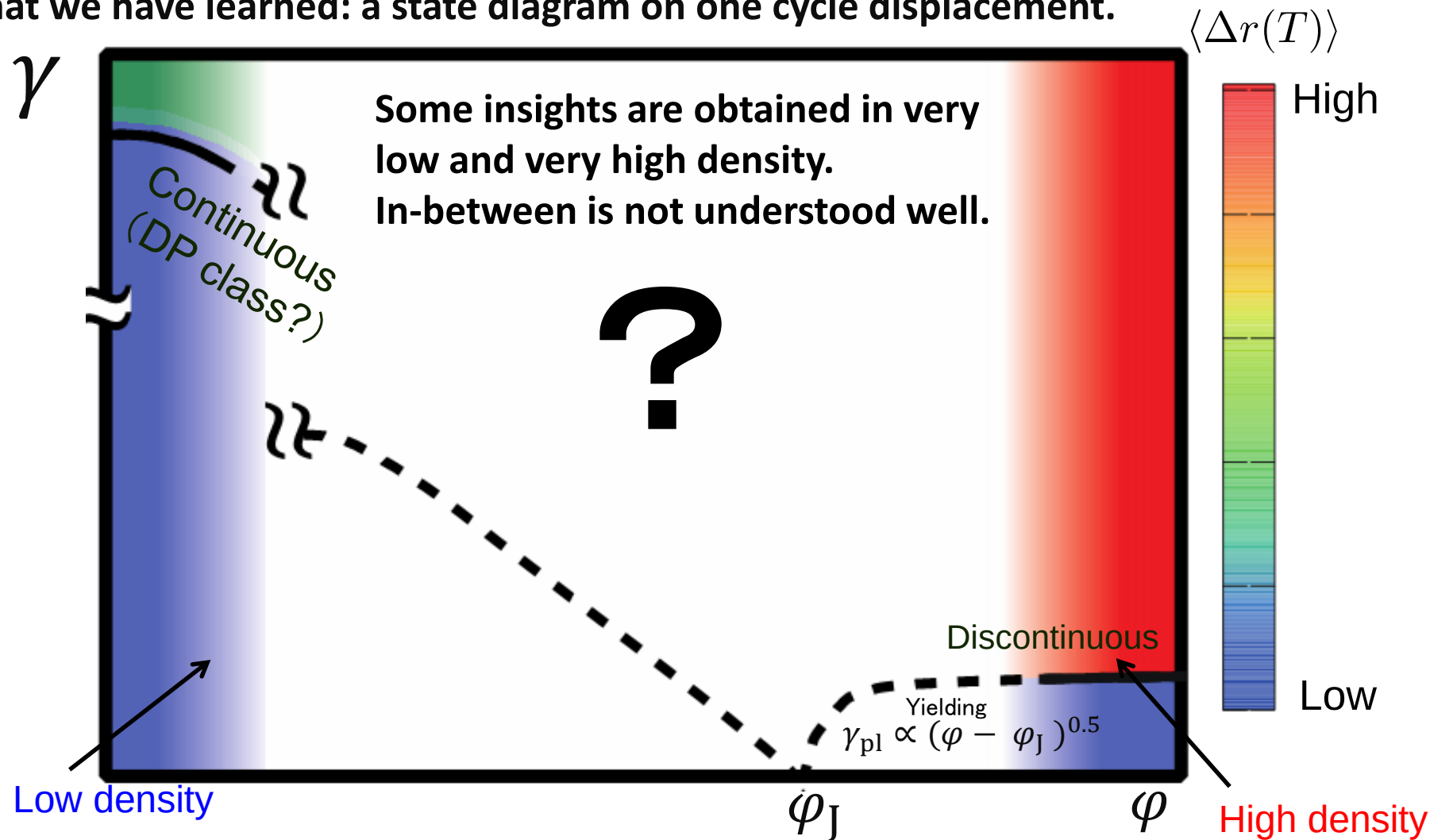
$$\gamma_{pl} \approx 0.09$$

close relation

Discontinuous RI transition is associated with yielding transition.

Purpose

What we have learned: a state diagram on one cycle displacement.



L. Corté, et al., Nat Physics **4**, 420 (2008)

T. Kawasaki and L. Berthier, Phys. Rev. E **94**, 022615 (2016).

E. Tjhung and L. Berthier, Phys. Rev. E **96**, 050601 (2017).

Purpose : To understand RI transition in wide range of density across jamming transition.

Method : Numerical simulations of athermal particles with oscillatory shear.

Numerical methods

- **2D overdamped athermal frictionless** particles with oscillatory shear, (Lees- Edward boundary condition)

$$\xi_s \left[\frac{\partial \mathbf{r}_i}{\partial t} - \dot{\gamma}(t) y_i \mathbf{e}_x \right] + \sum_j \frac{\partial U(r_{ij})}{\partial \mathbf{r}_i} = \mathbf{0}$$

- **Interaction potential (Harmonic sphere)**

$$U(r_{ij}) = \frac{\epsilon}{2} (1 - r_{ij}/a_{ij})^2 \Theta(a_{ij} - r_{ij}),$$

- **Strain evolution with oscillation**

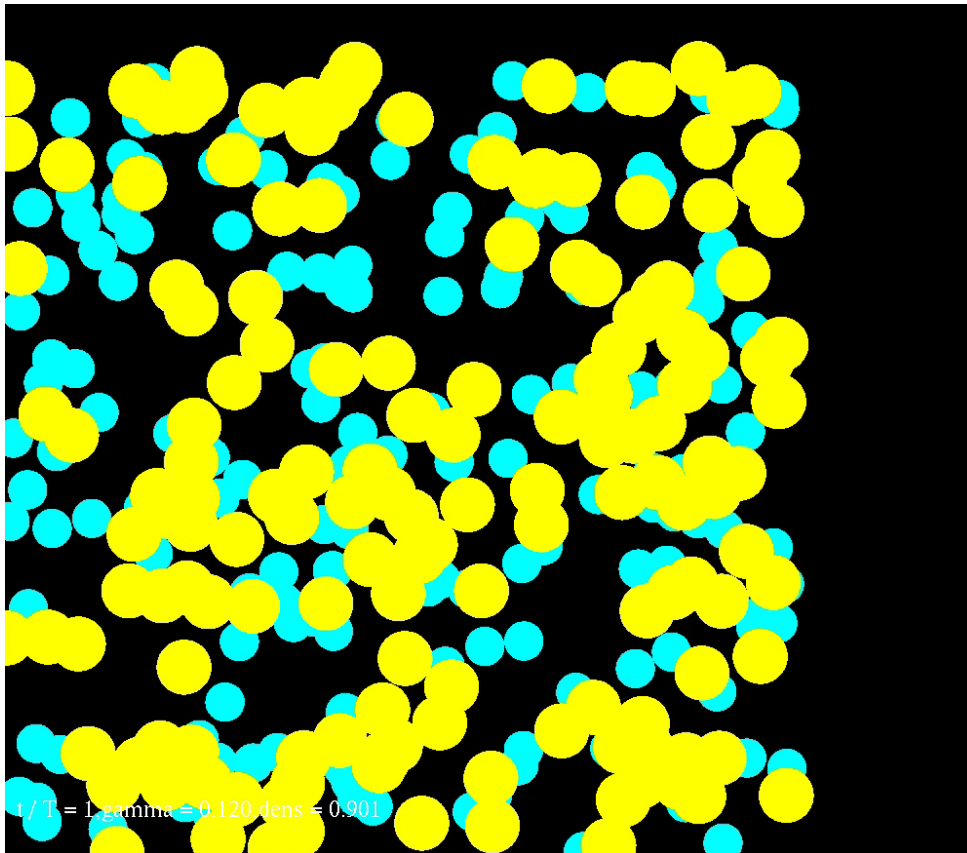
$$\begin{aligned} \dot{\gamma}(t) &= \gamma_0 \omega \sin(\omega t) \\ \gamma(t) &= \gamma_0 [1 - \cos(\omega t)], \end{aligned} \quad \omega = 2\pi/T$$

- **Oscillation period:** $T = 10^4 \tau$ ($\tau = \xi_s \sigma^2 / \epsilon$)
- **Simulation time:** $4000T$
- **System size:** $L = 20\sigma$ ($L = 40\sigma$: check of finite size effect)
- **Packing fraction:** $\varphi = 0.70 - 1.0$ cf: $\varphi_J(2D) = 0.843$

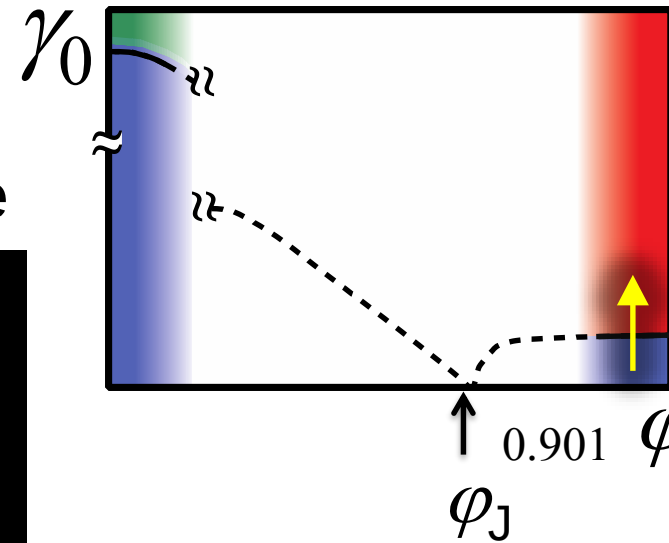
Particle trajectory (movie)

$$\varphi = 0.901, \gamma_0 = 0.10$$

yellow : large particle blue : small particle



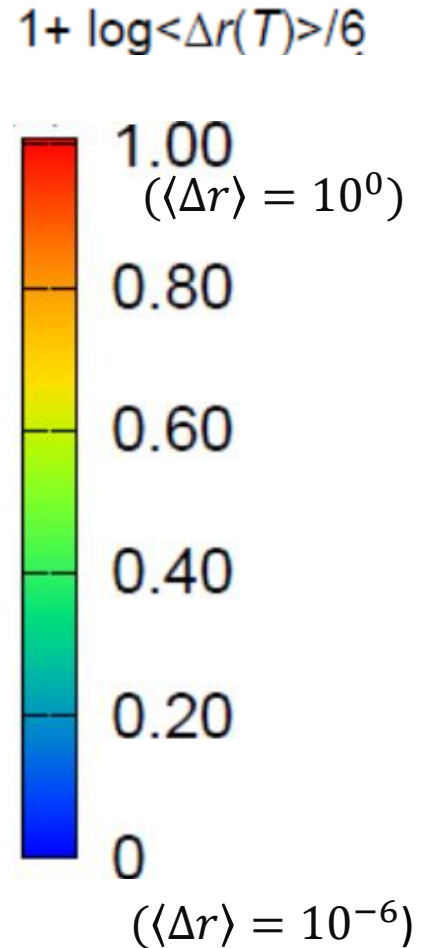
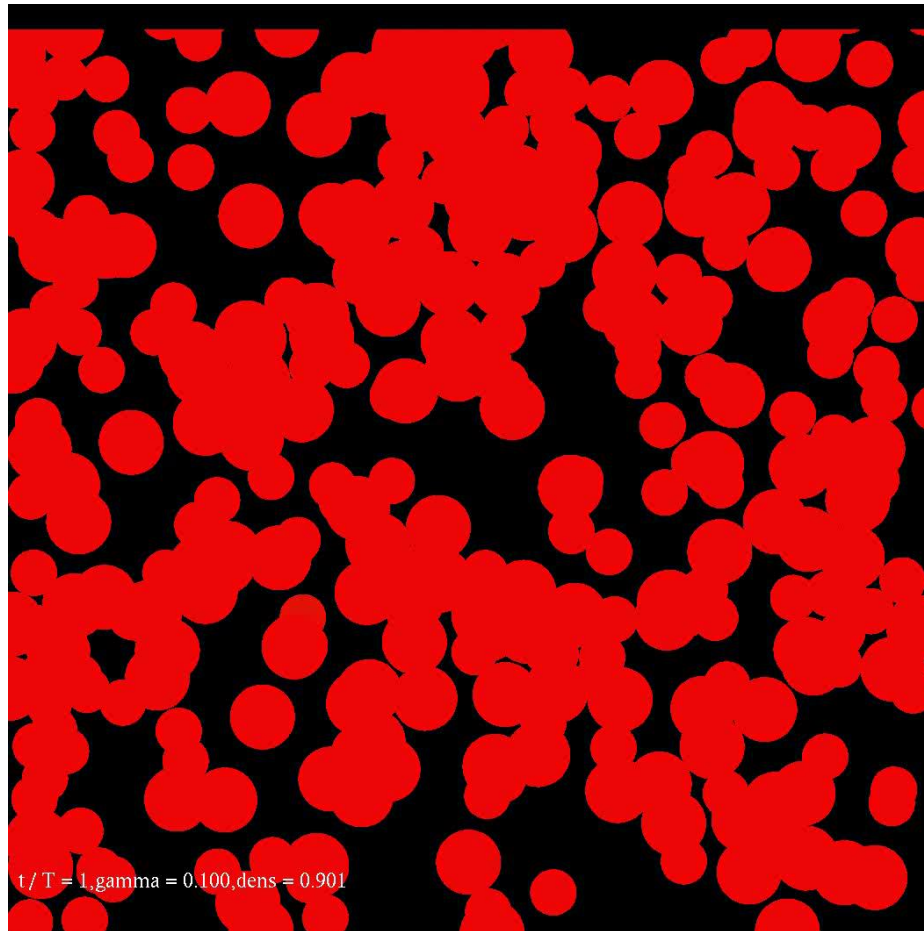
$$L = 20 \sigma$$



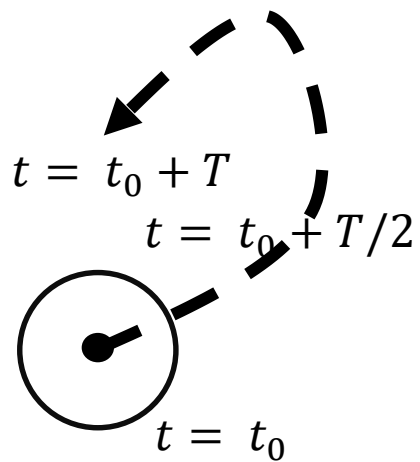
Particle trajectory (Stroboscopic: every one cycle)

Above jamming transition

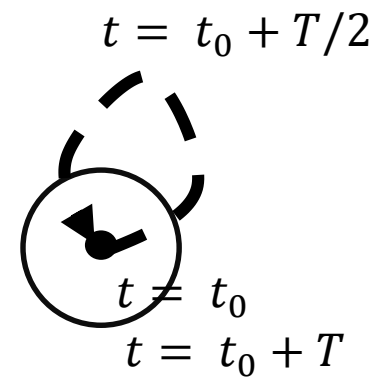
$$\varphi = 0.901, \gamma_0 = 0.10$$



$$L = 20 \sigma$$



Irreversible



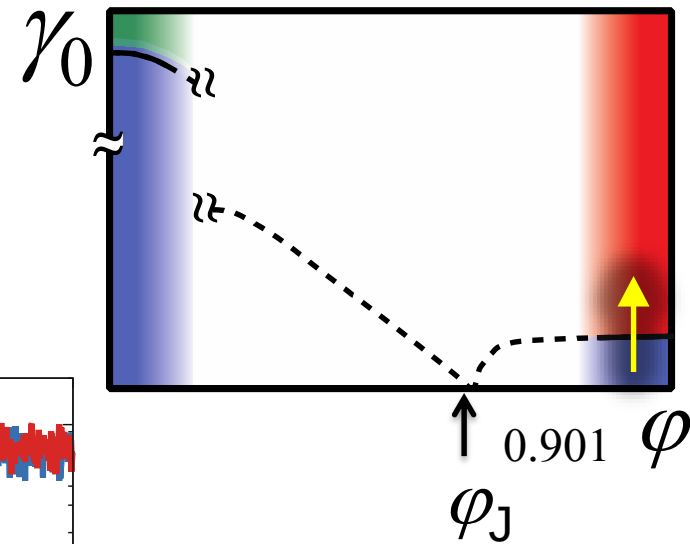
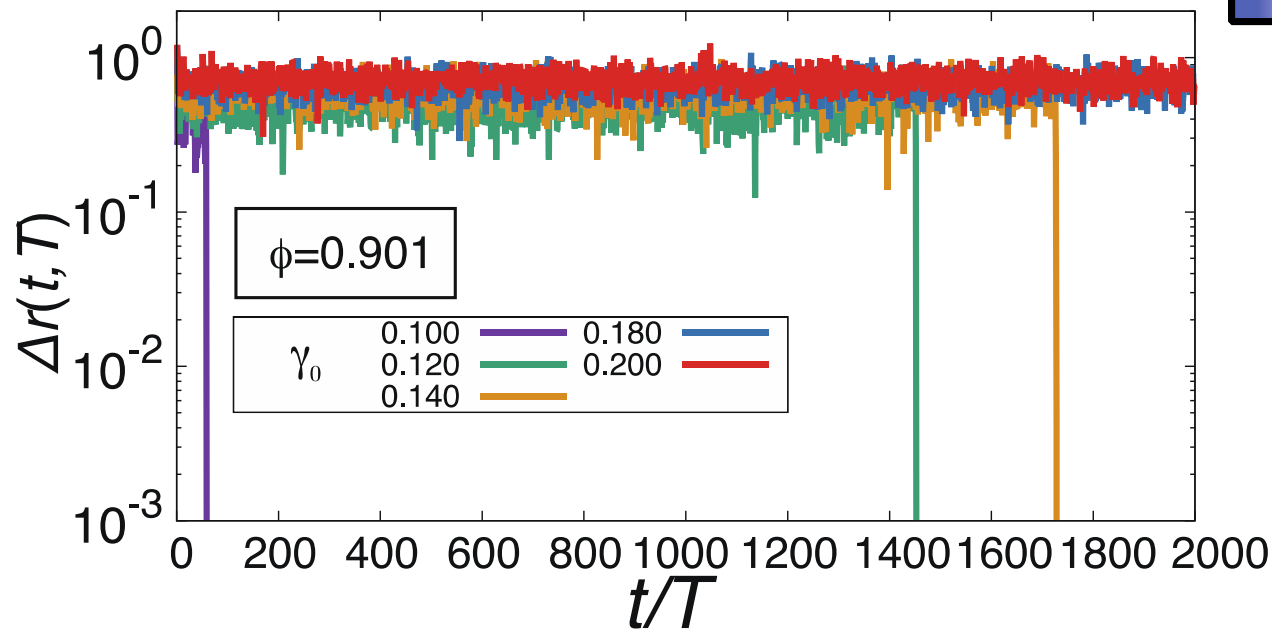
Reversible

(Absorbing state)

Results: One cycle trajectory above jamming transition density

Displacement per cycle

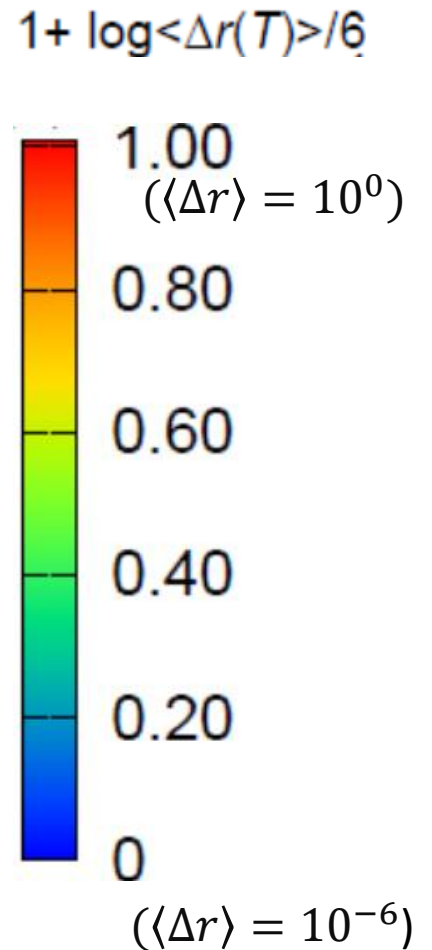
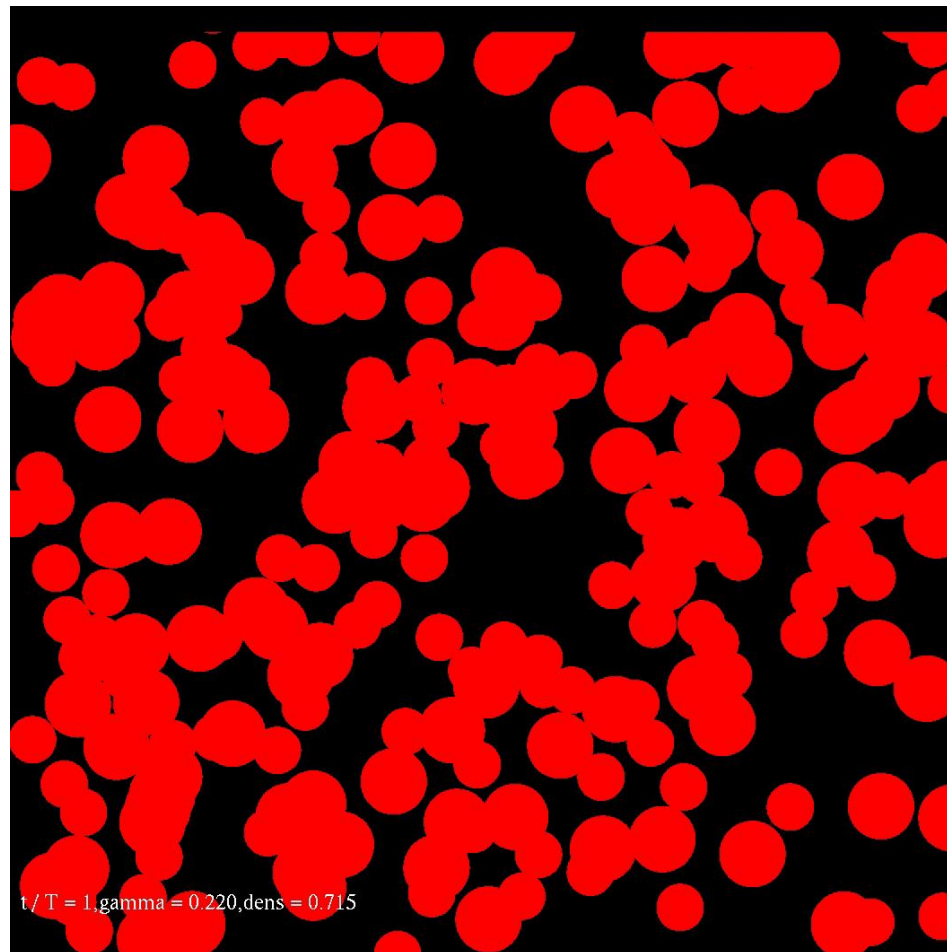
$$\Delta r(t, T) = \frac{1}{N} \sum_j |\vec{r}_j(t + T) - \vec{r}_j(t)|$$



Discontinuous transition

Stroboscopic particle displacements

Low density : $\phi = 0.715$

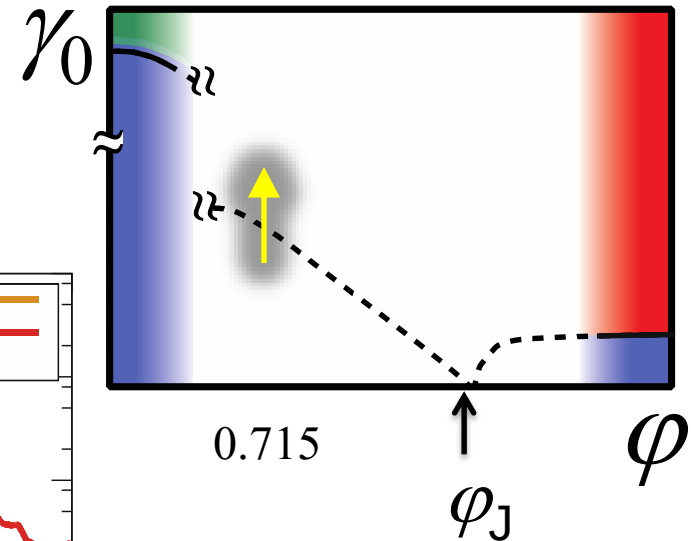
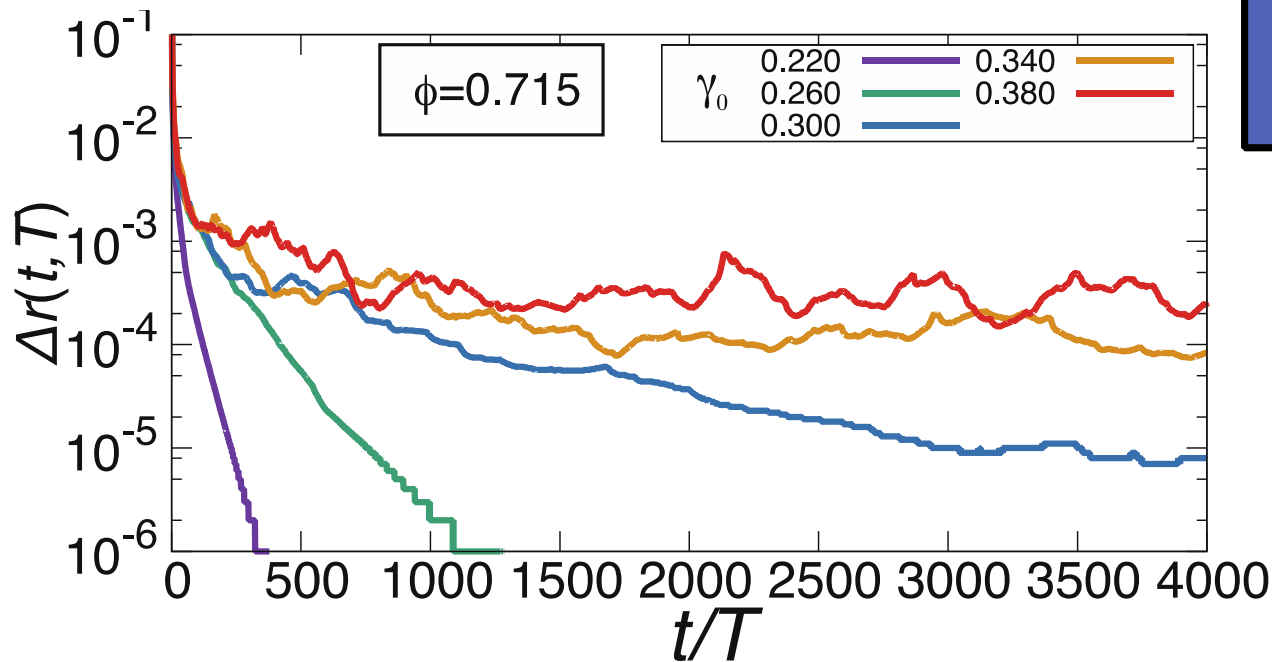


$\gamma_0 = 0.220$

Results: One cycle trajectory in low density

Displacement per cycle

$$\Delta r(t, T) = \frac{1}{N} \sum_j |\vec{r}_j(t + T) - \vec{r}_j(t)|$$

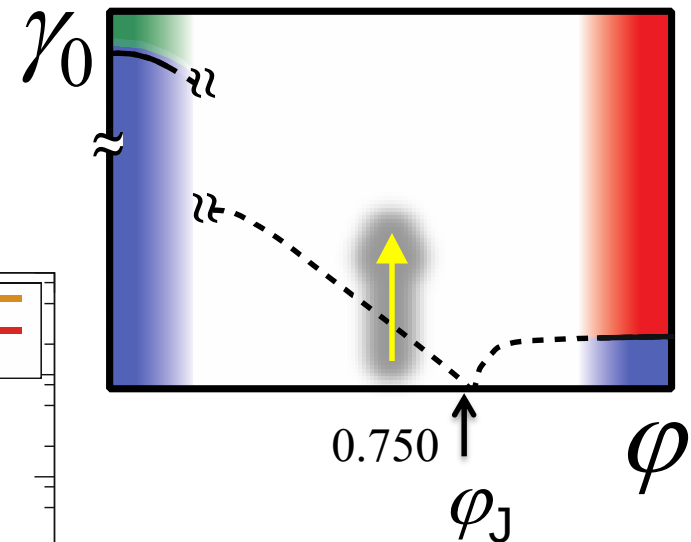
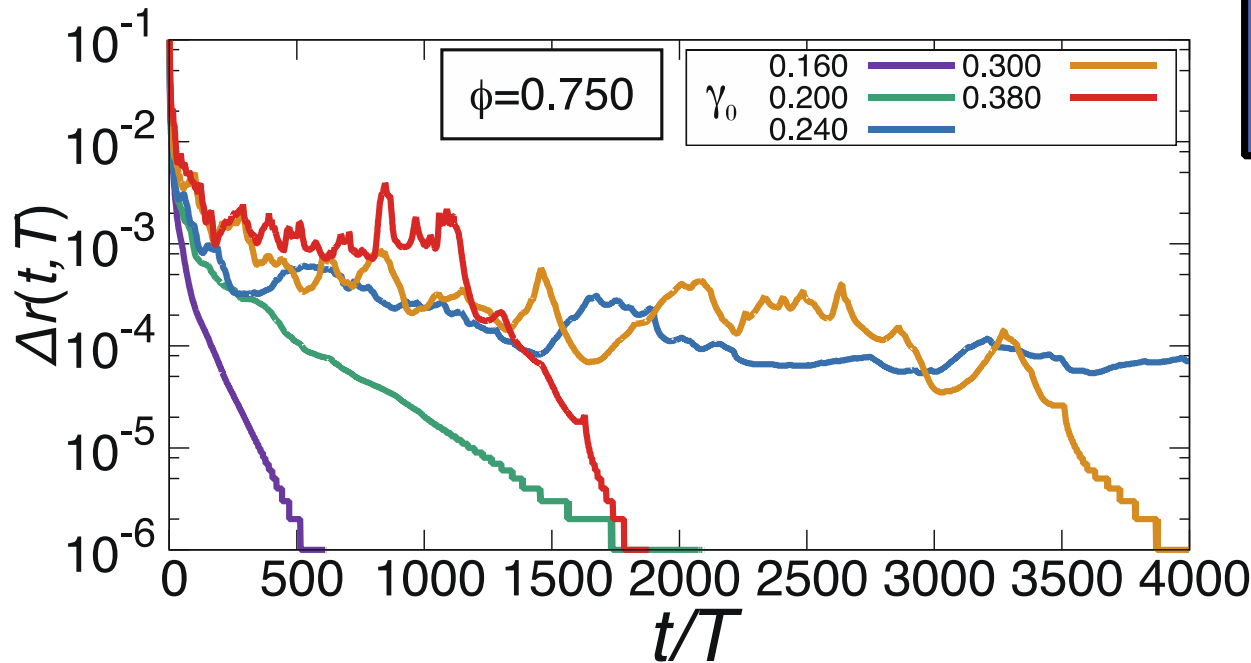


Continuous transition

Results: One cycle trajectory below jamming transition density

Displacement per cycle

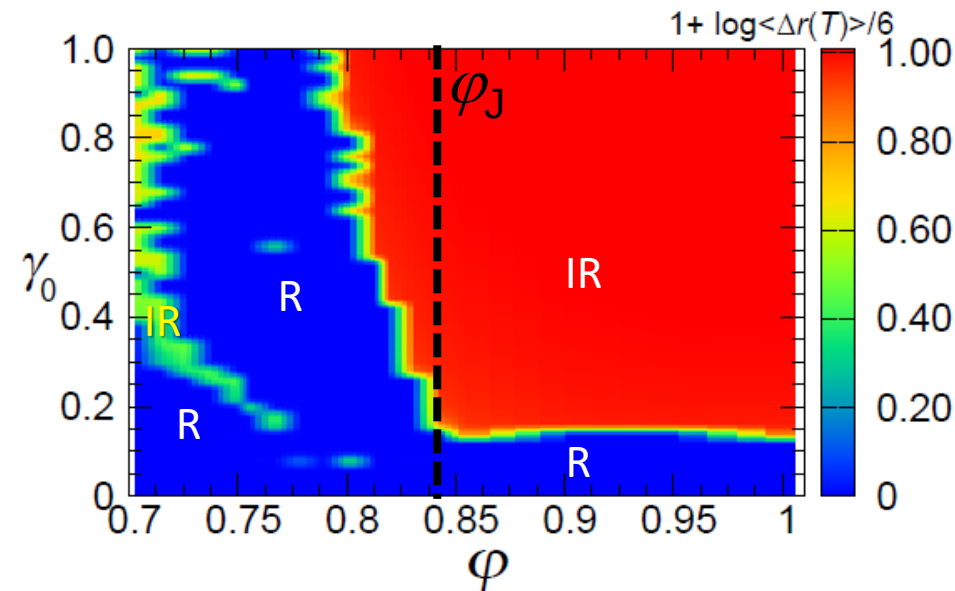
$$\Delta r(t, T) = \frac{1}{N} \sum_j |\vec{r}_j(t + T) - \vec{r}_j(t)|$$



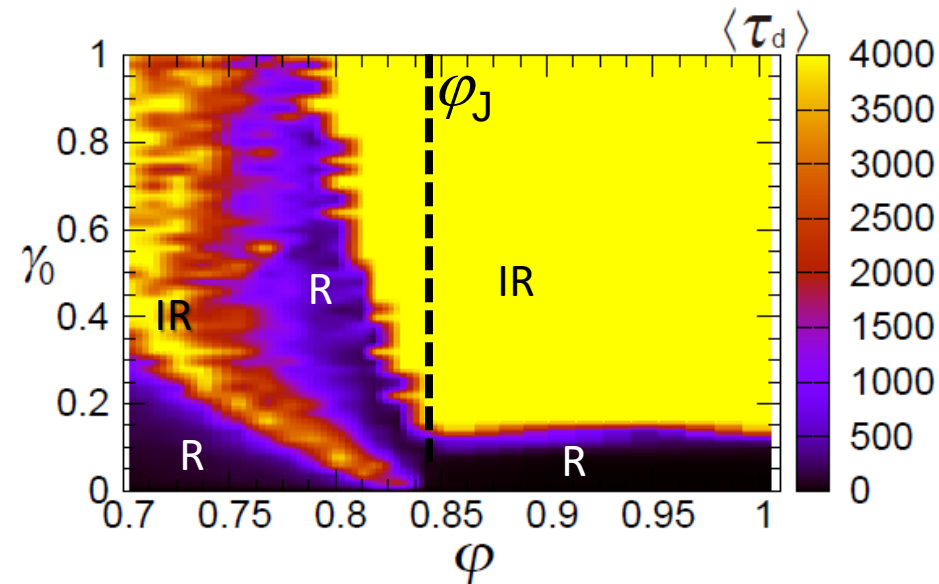
Reentrant transition

Results: State diagram for RI transitions

One cycle displacement



Life time of the irreversible state



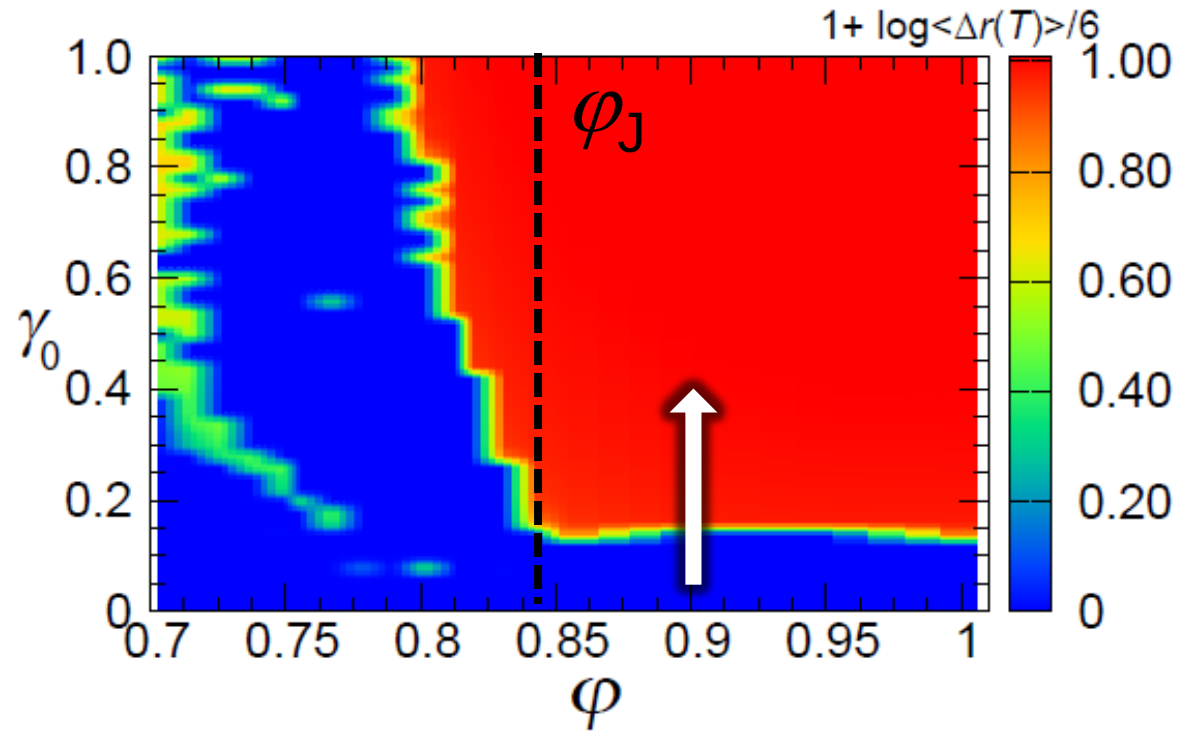
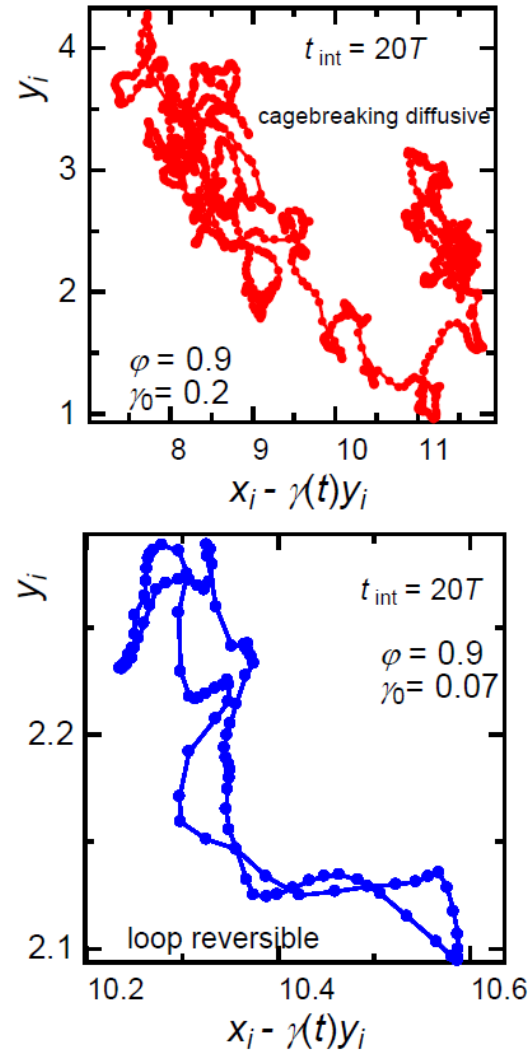
R: reversible, IR: irreversible

➡ To clarify the details of R-I states, we investigate single-particle trajectory, diffusivity, geometry of the particles, and mechanical property.

Results: Classifications of the particle trajectories above jamming

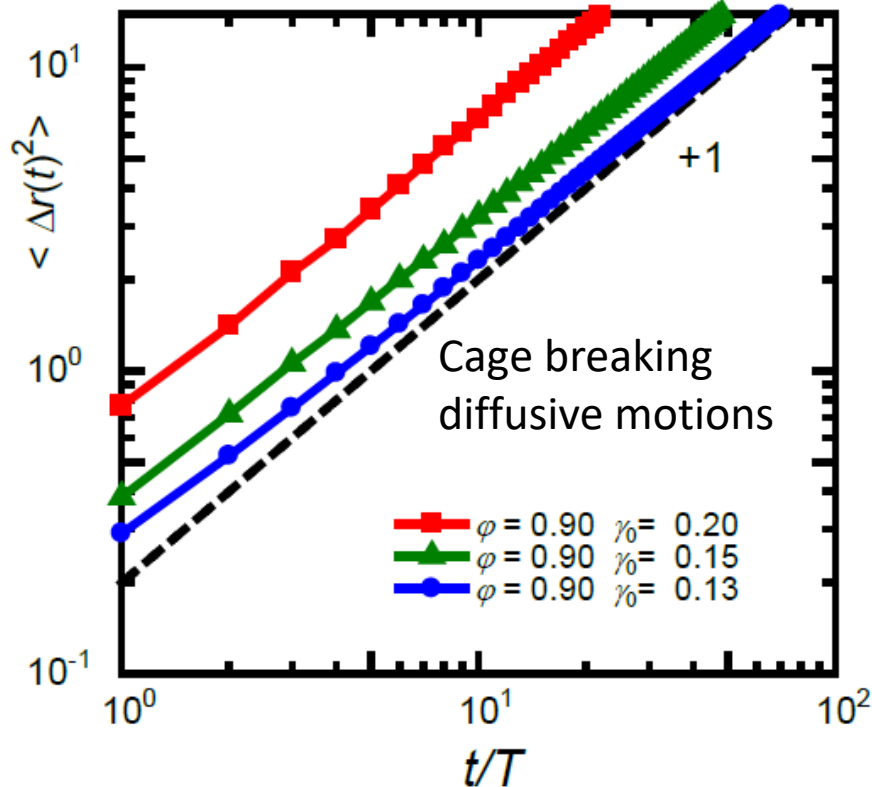
Non-affine single particle trajectory

i.e., a trajectory whose affine deformation is removed ($\varphi = 0.90$, 20 cycles)

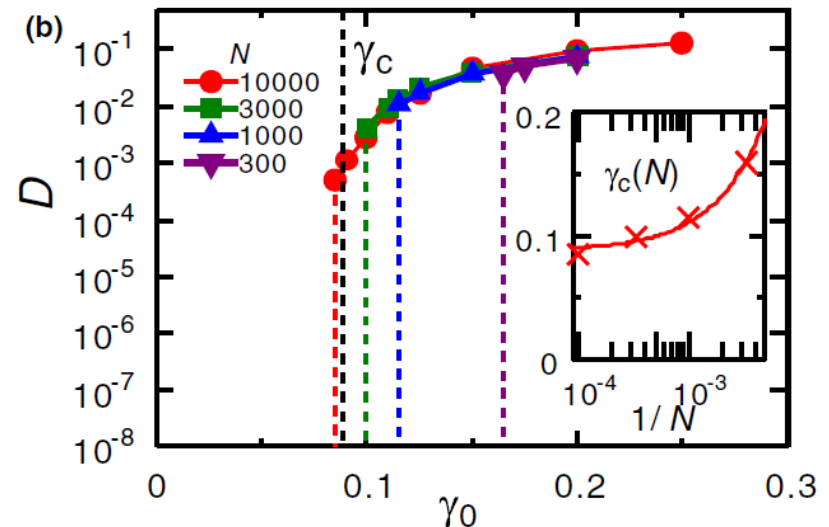
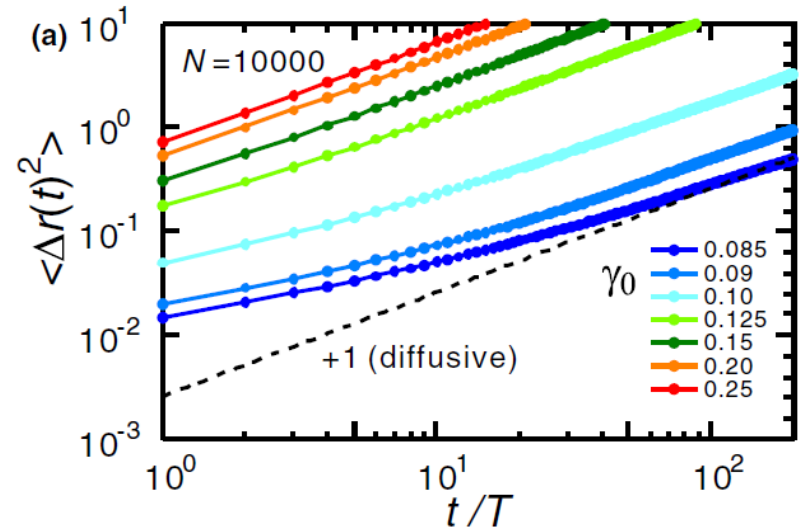


Results: Mean squared displacements

Mean squared displacements ($\varphi=0.90$)



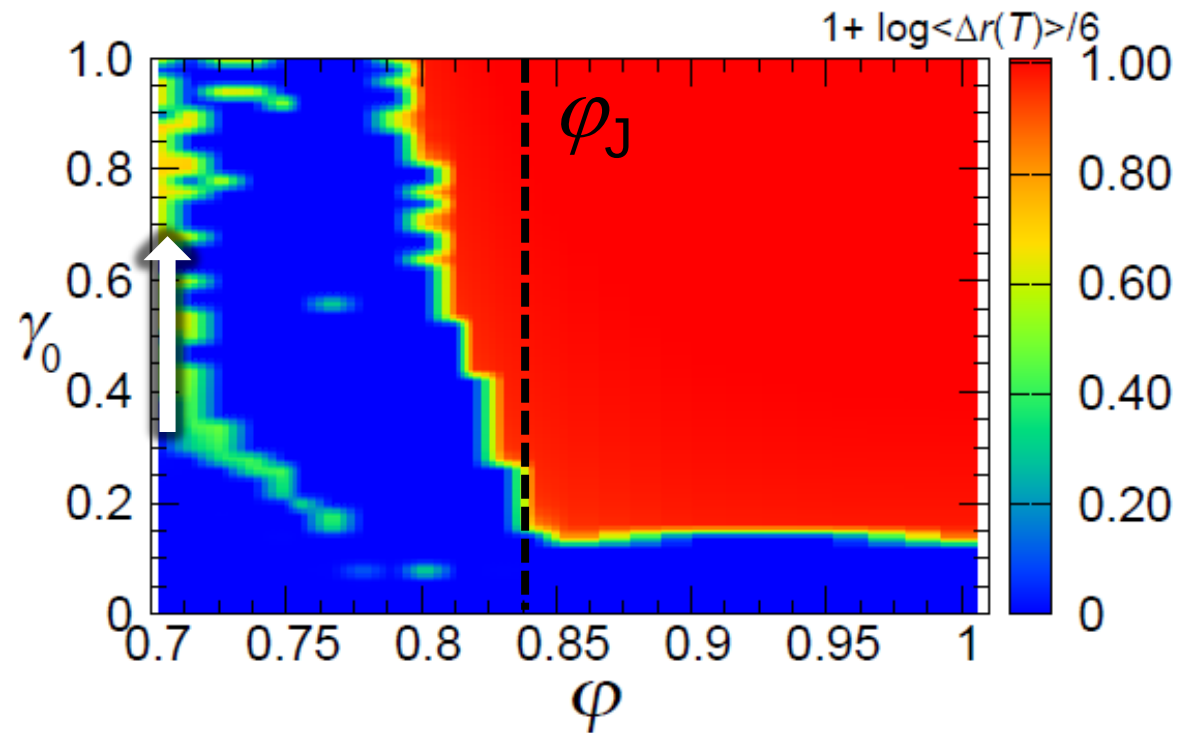
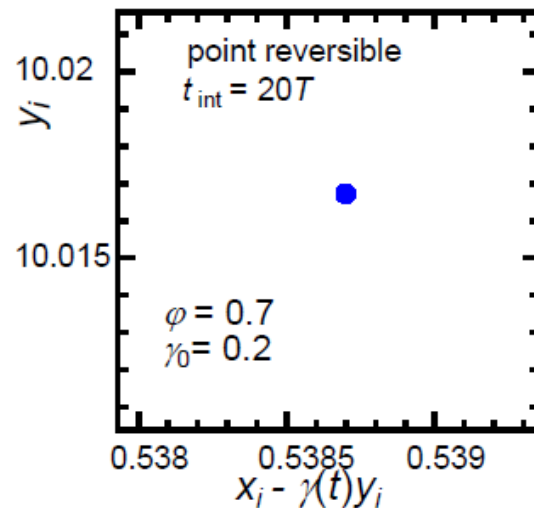
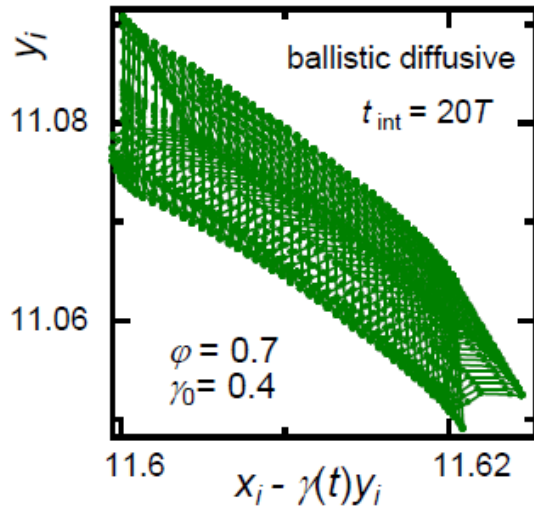
(Previous study) 3 dimensional system: $\varphi > \varphi_J$



T. Kawasaki and L. Berthier, Phys. Rev. E **94**, 022615 (2016).

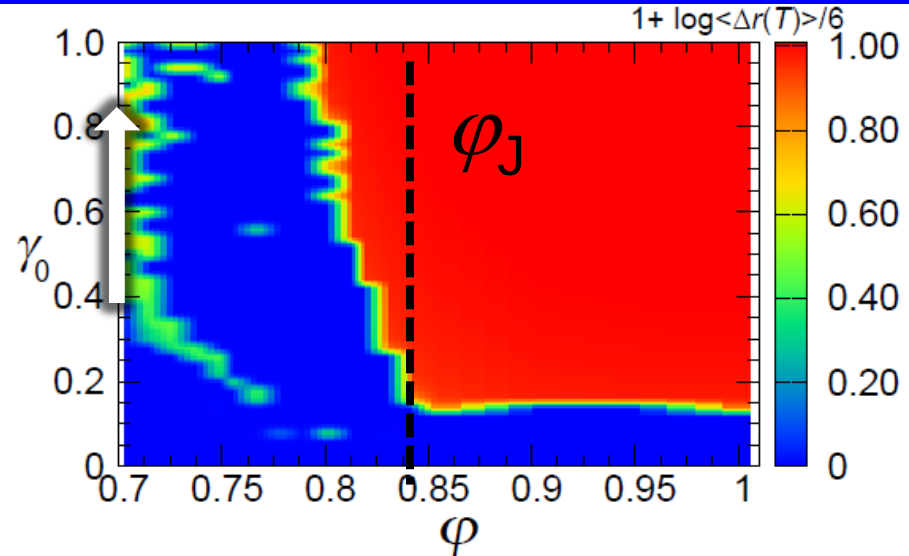
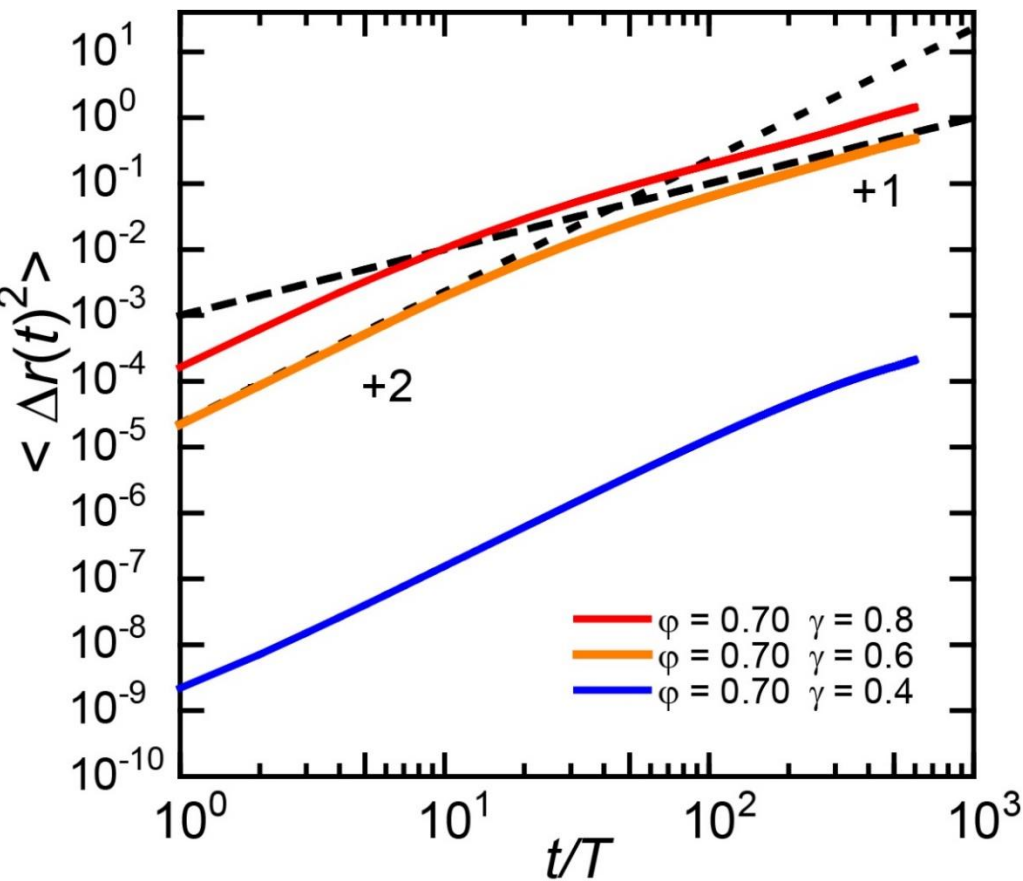
Classifications of the particle trajectories below jamming

Non-affine single particle trajectory ($\phi = 0.70$, 20 cycles)



Results: Mean squared displacements below jamming

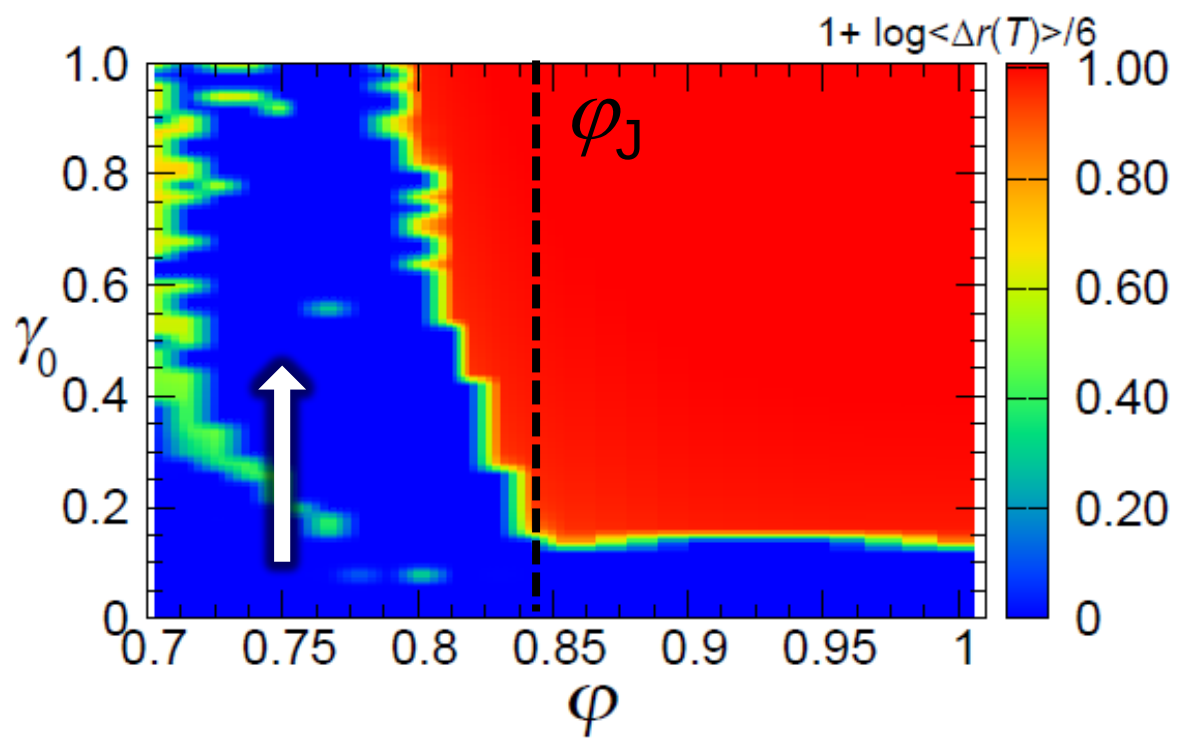
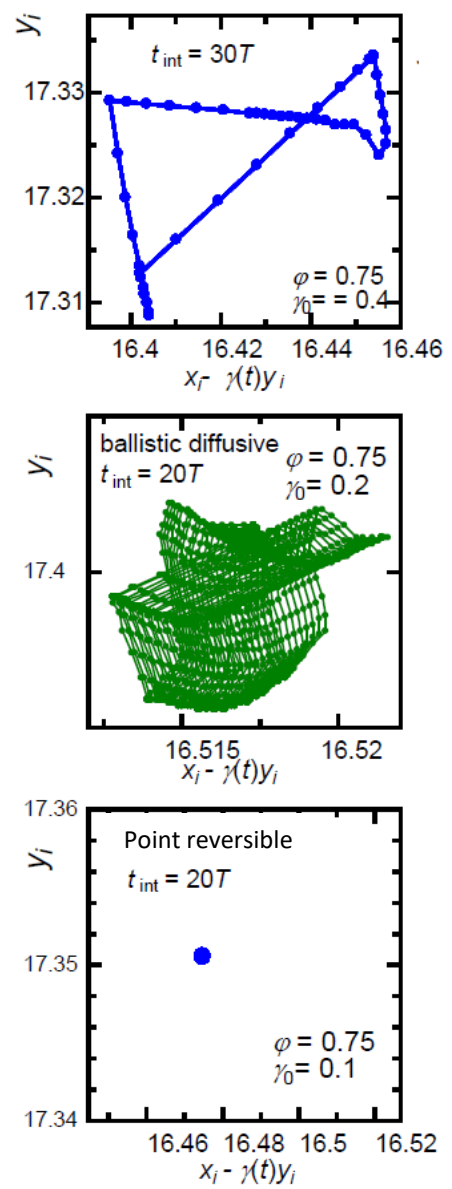
Mean squared displacements ($\phi = 0.70$)



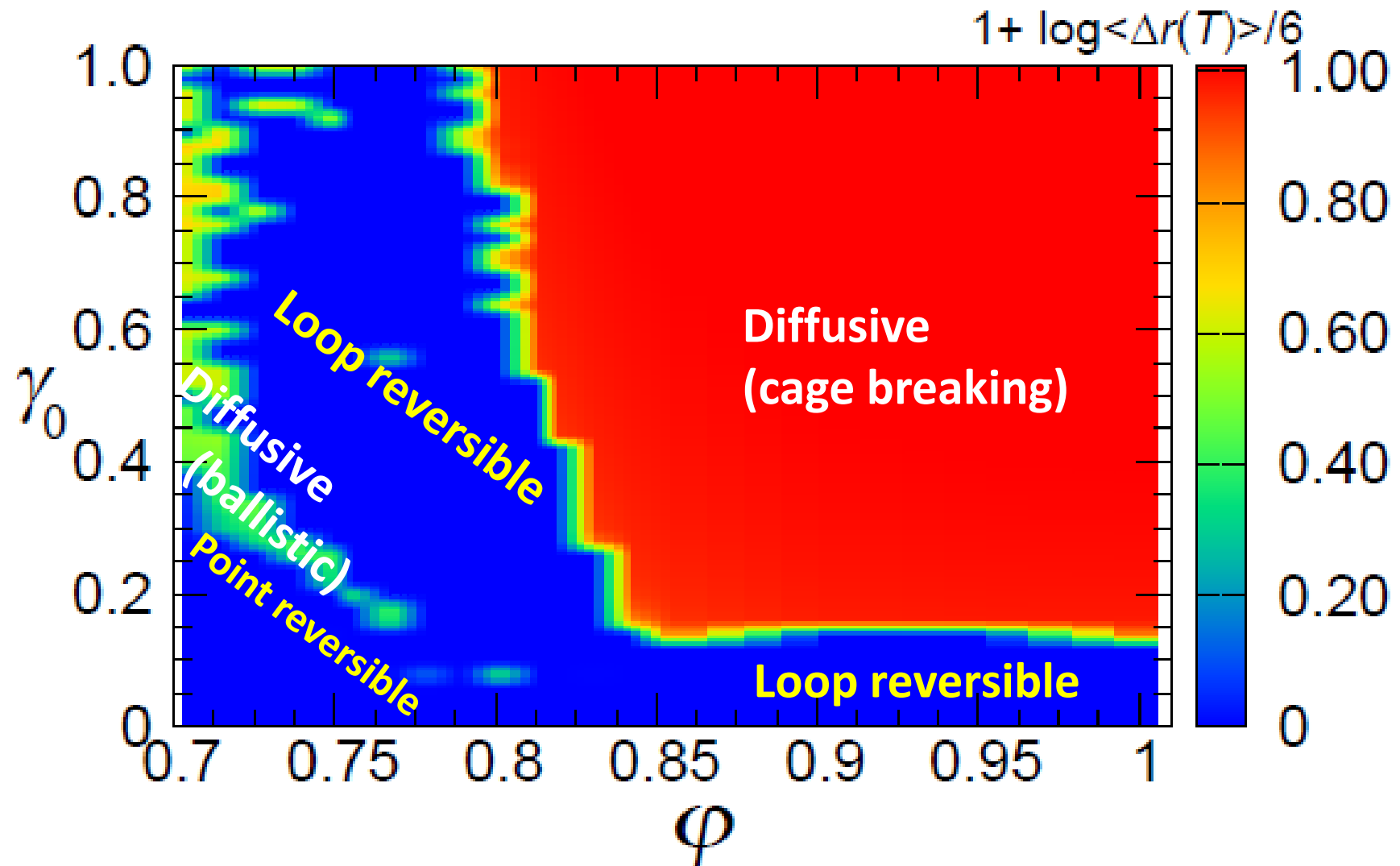
- In short time regime, particles move ballistically.
- The lasting time of the ballistic motion becomes critically long close to RI transition point.

Classifications of the particle trajectories at reentrant regime

Non-affine single particle trajectory ($\varphi = 0.75$, 20 cycles)

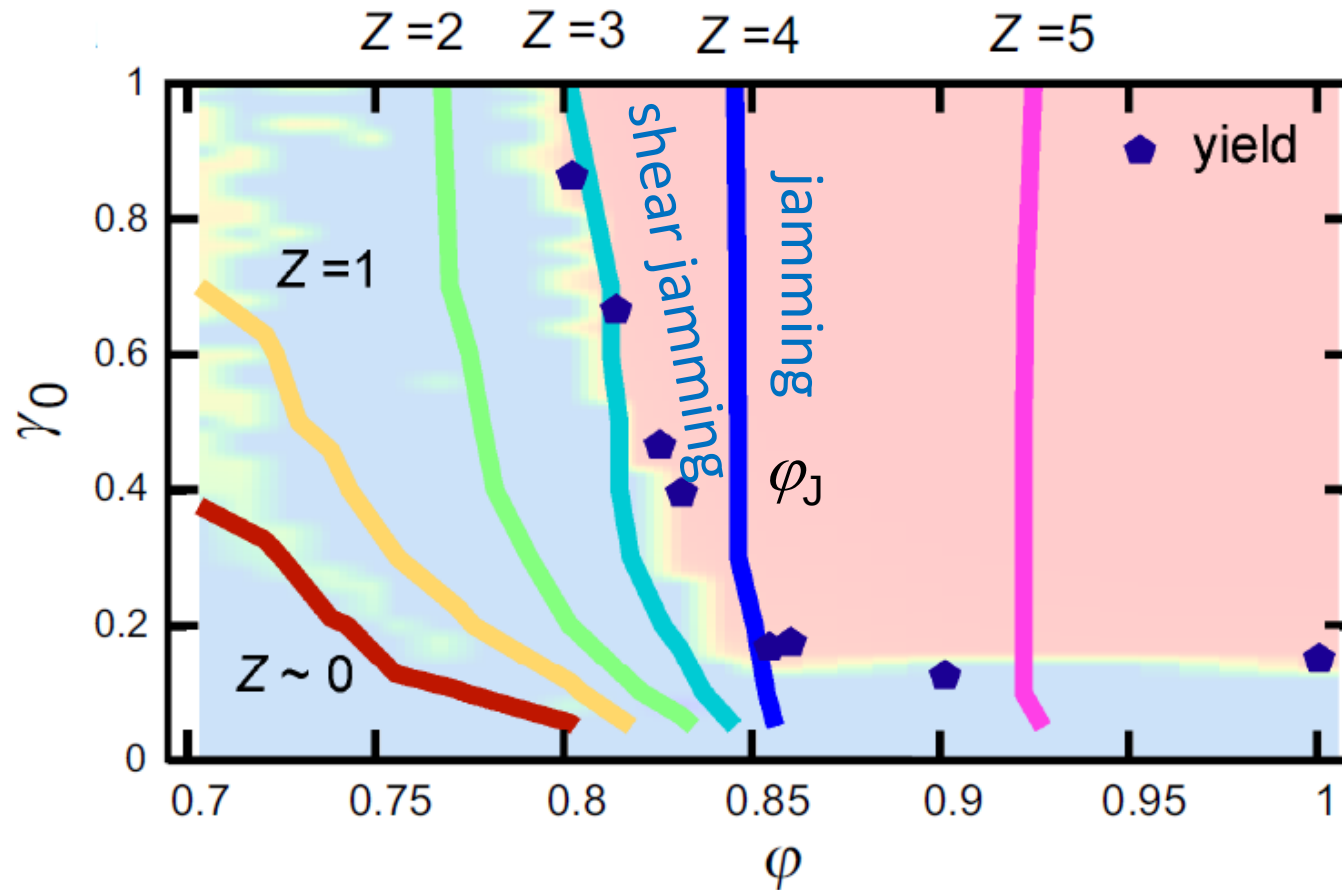


Classifications of the particle trajectories: summary



Relationship among the geometry of the particles, mechanical property and RI transition

Condition for a stable packing: $Z \geq 4$ ($= 2d$: *isostatic*)



(1) $Z = 3$ in unjam regime: discontinuous transition ➡ Related to shear jamming. [H. A. Vinutha and S. Sastry, Nat Phys **12**, 578 (2016)]

(2) $Z \sim \delta(> 0)$: Continuous transition (3) $Z = 1$: Reentrant transition

➡ Finding the correlation among the RI transitions, coordination number, and mechanical property.

Summary

We investigated RI transitions for wide-range of density across the jamming transition.

(1) Found various types of RI transitions around jamming density.

(2) Classified RI transitions on the single particle trajectories.

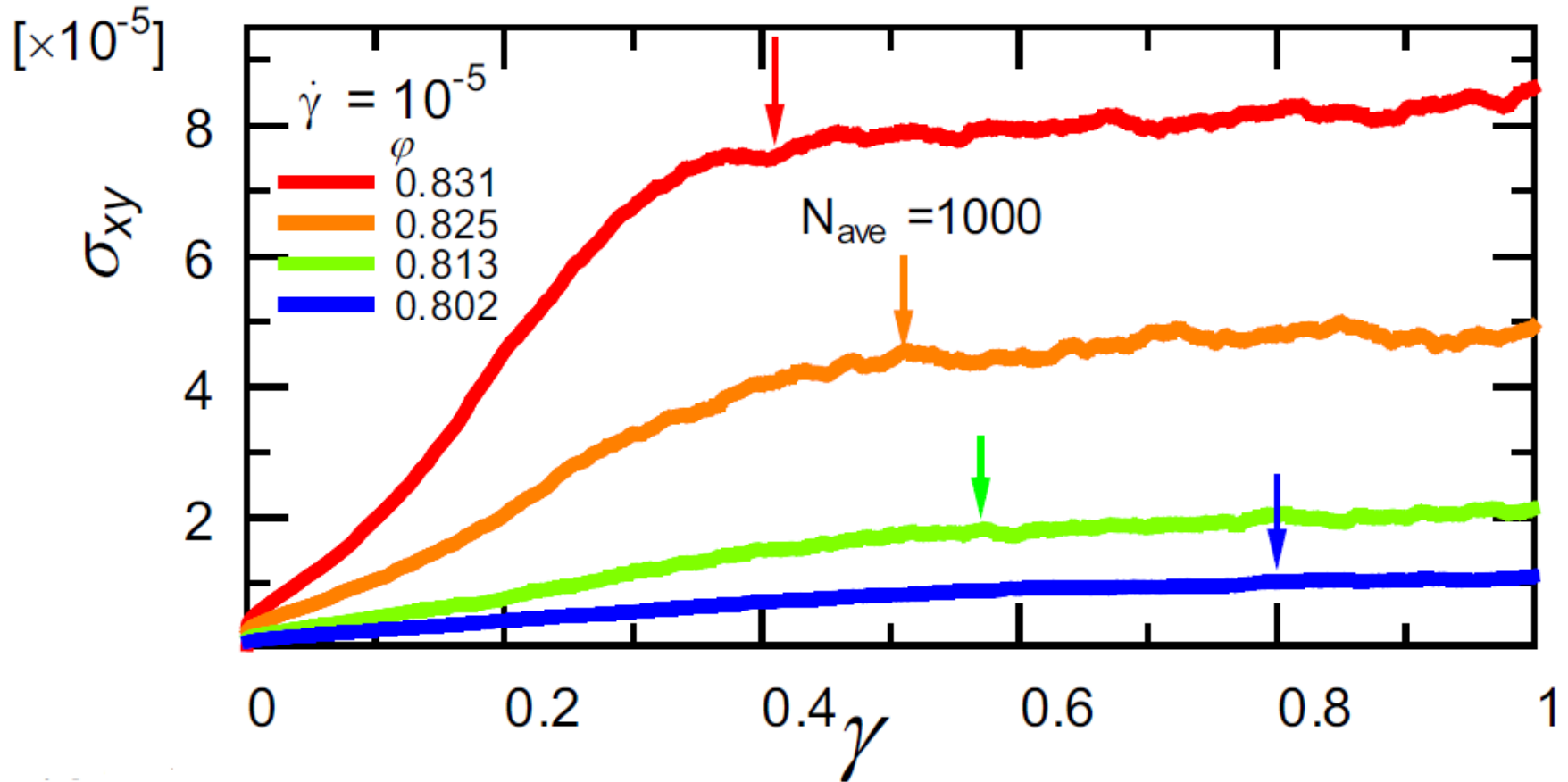
(3) Found correlations among RI transitions, particle geometry, and mechanical property.

Future work :

Relation between RI transition and yielding transition very close to jamming transition which is expected to be critical but not confirmed in the present study.

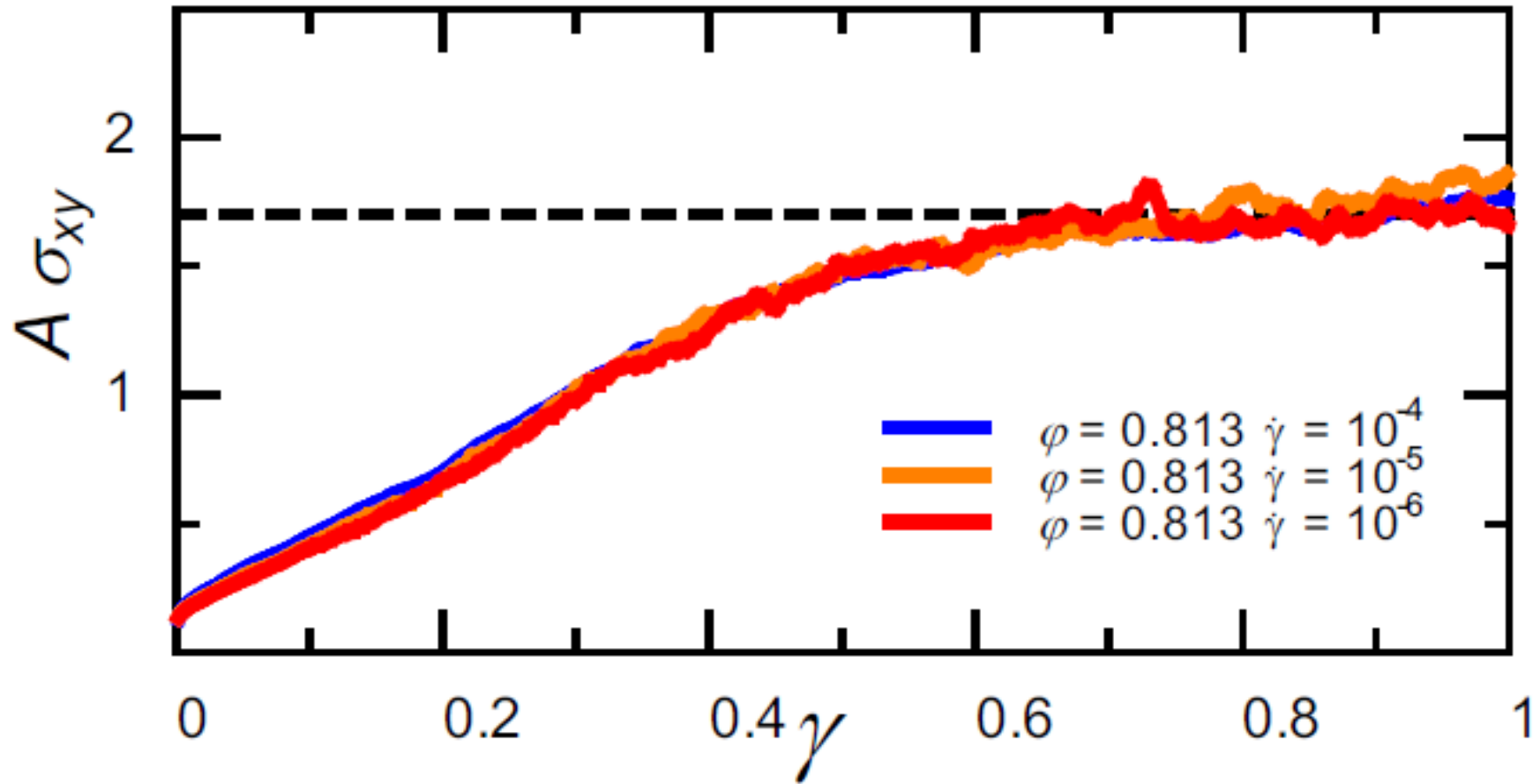
Stress strain curves below jamming

Packing fraction dependence



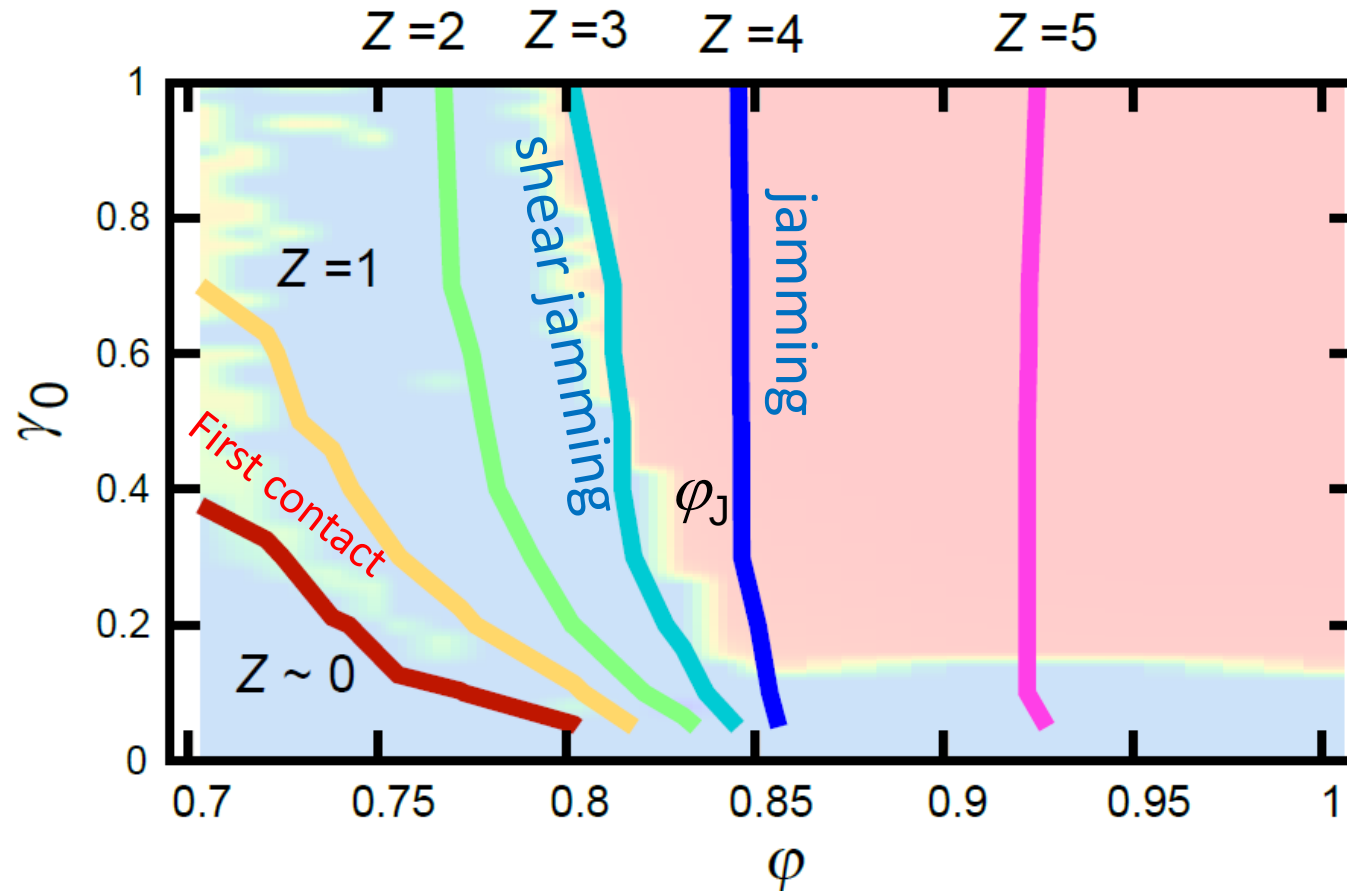
Stress strain curve below jamming

Shear rate dependence



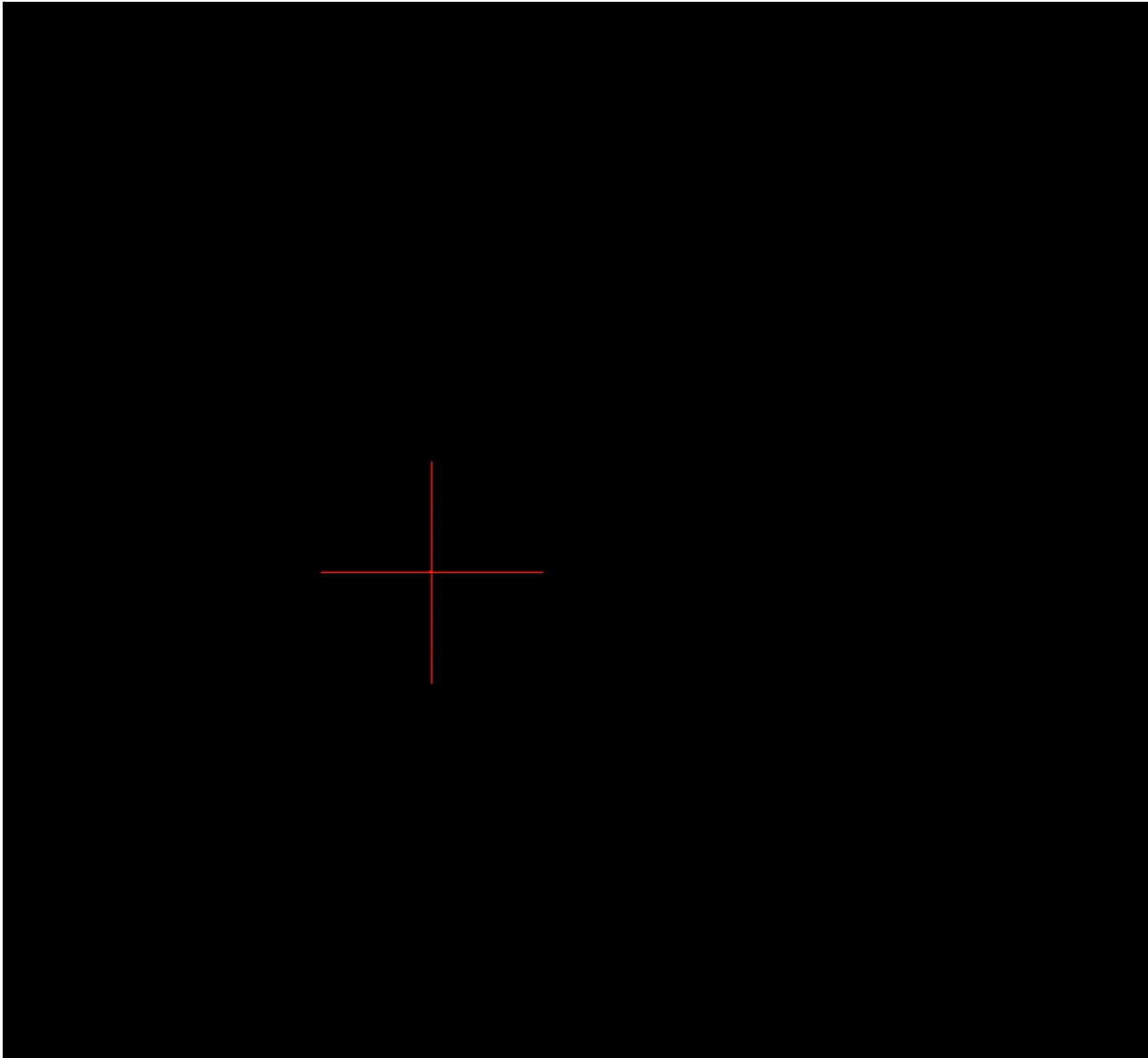
Relation between RI transition and coordination number

Condition for a stable packing: $Z \geq 4$ ($= 2d$ isostatic)



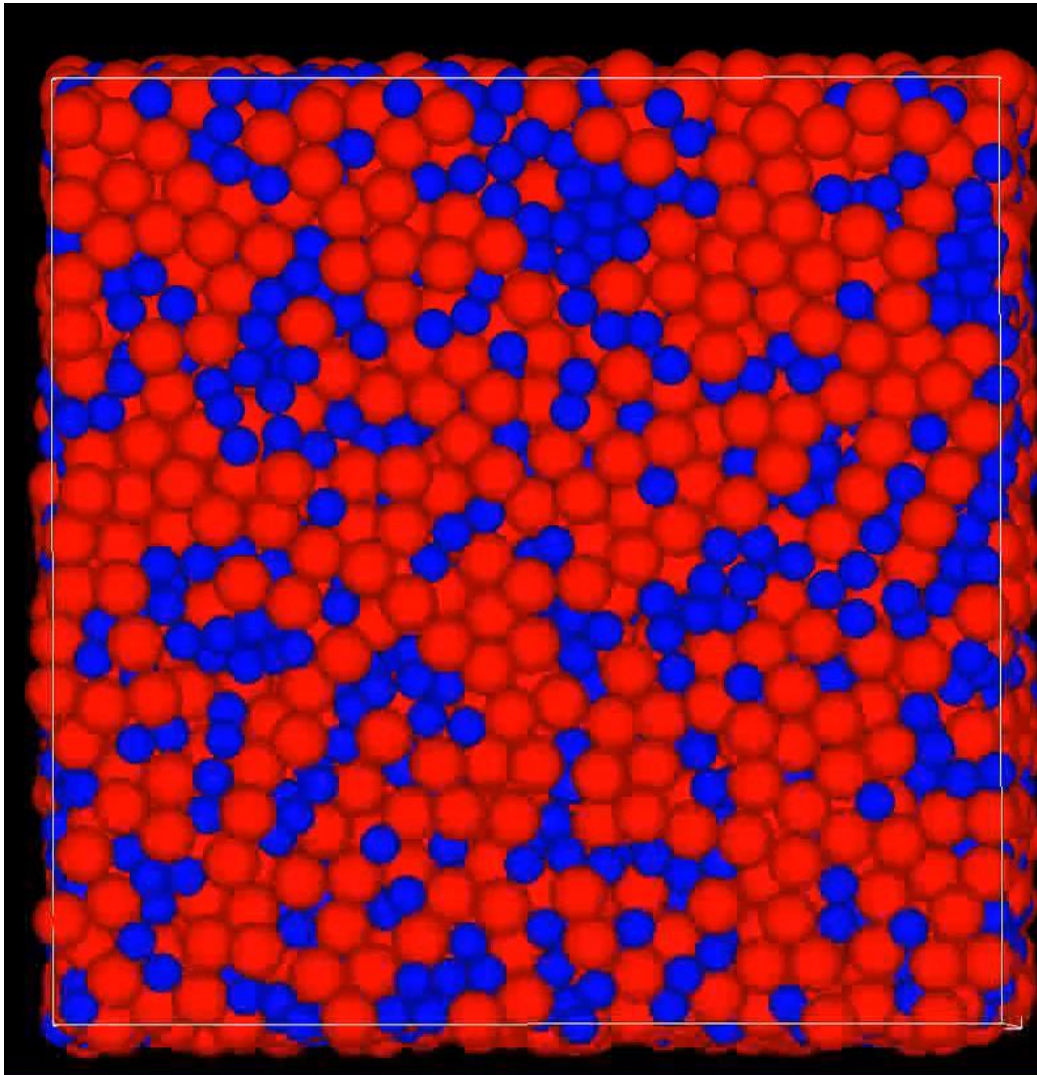
(1) $Z = 3$ in unjam regime: discontinuous transition ➡ Related to shear jamming. [H. A. Vinutha and S. Sastry, Nat Phys **12**, 578 (2016).]

(2) $Z \sim \delta(> 0)$: Continuous transition (3) $Z = 1$: Reentrant transition



高密度分散系における粒子軌道の可逆・不可逆転移

高密度粒子分散系 ($\varphi = 0.80$ cf. $\varphi_f = 0.647$) の周期剪断数値実験



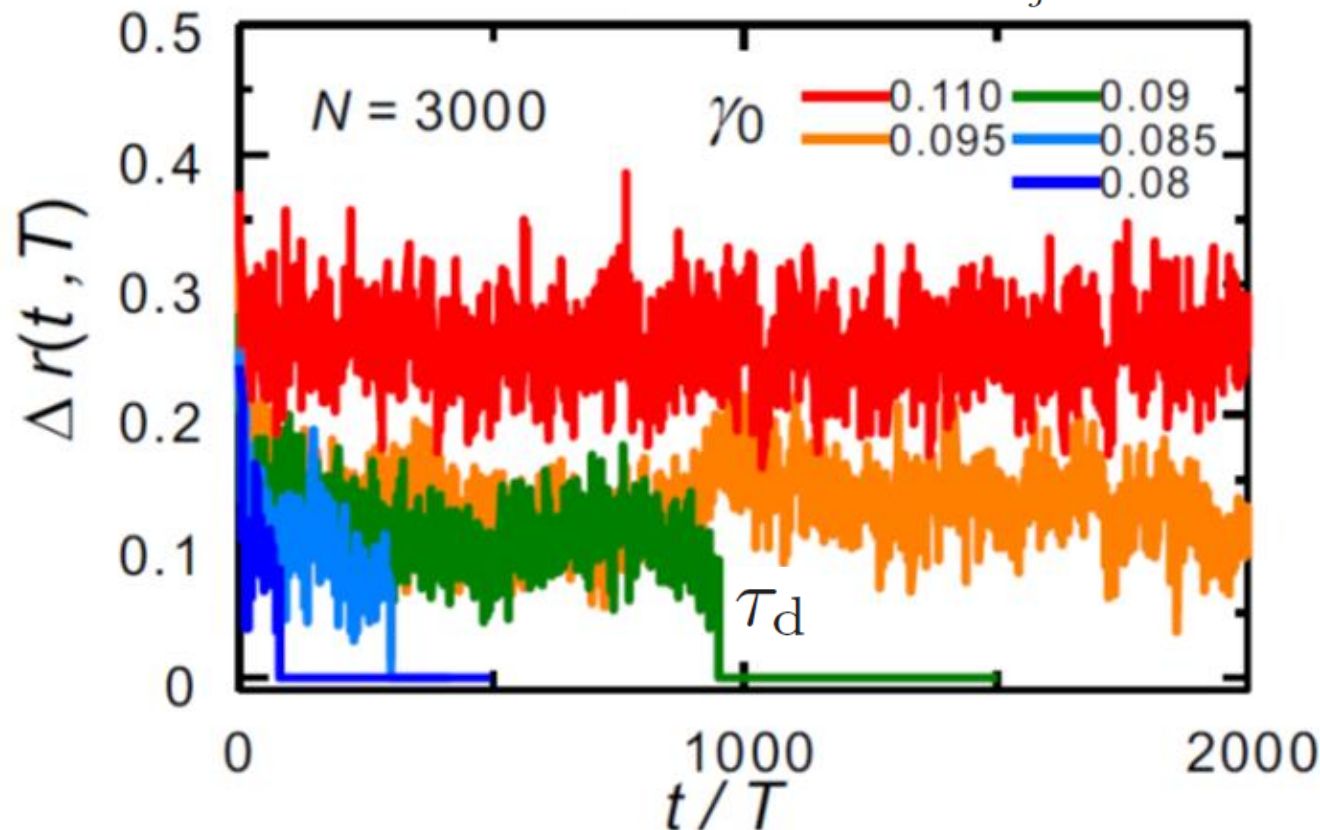
$$N = 10000$$
$$\gamma_0 = 0.05$$

T. Kawasaki and L. Berthier, Phys. Rev. E **94**, 022615 (2016).²⁷

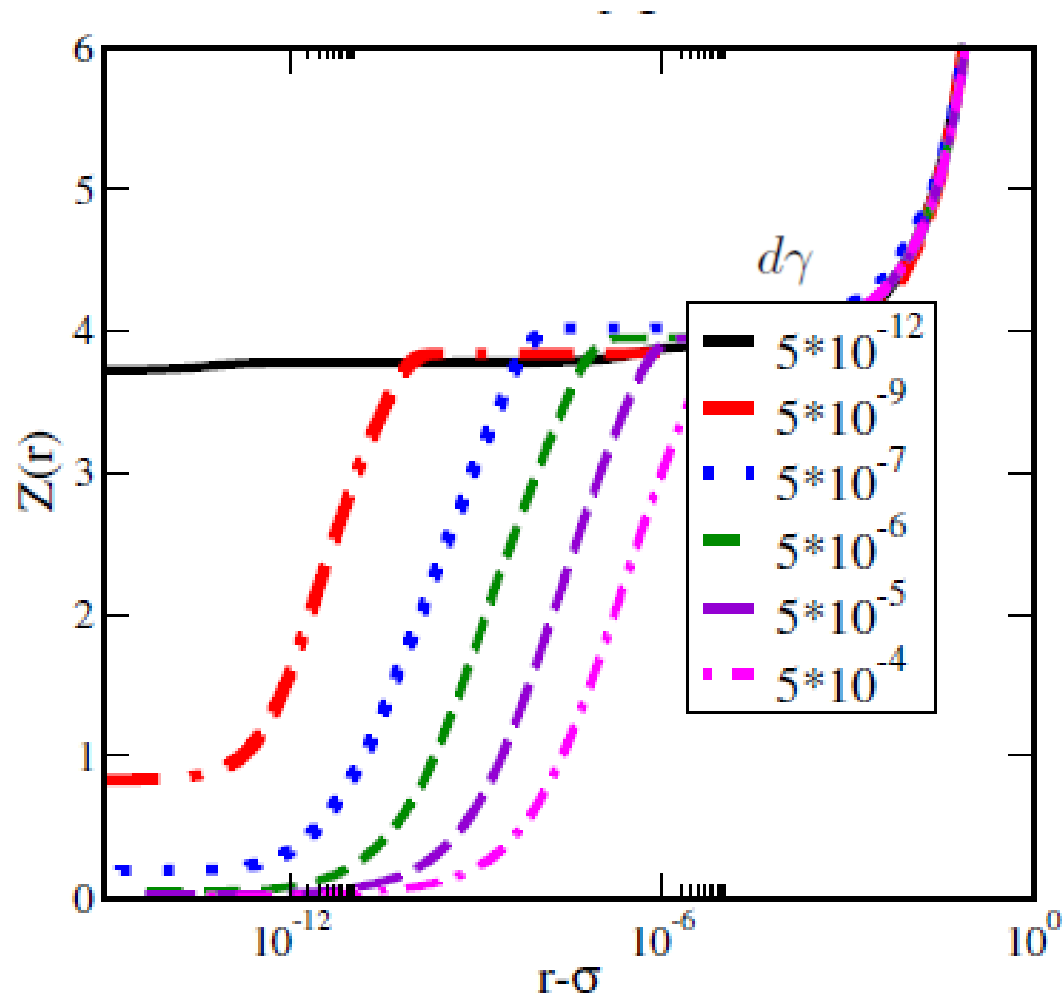
RI transition takes place also in very high density system

Oscillatory shear numerical experiment in highly dense suspensions ($\varphi = 0.80$
cf. $\varphi_J = 0.647$)

One cycle displacement:
$$\Delta r(t, T) = \frac{1}{N} \sum_j |\vec{r}_j(t + T) - \vec{r}_j(t)|$$



Contact number below jamming



r : Threshold distance for determining the nearest neighbors.