SIMULATION OF COHESIVE FINE POWDERS UNDER PLANE SHEAR

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  - properties of cohesive fine powders
  - previous works and goal of our studies
- Model & Setup of MD simulation
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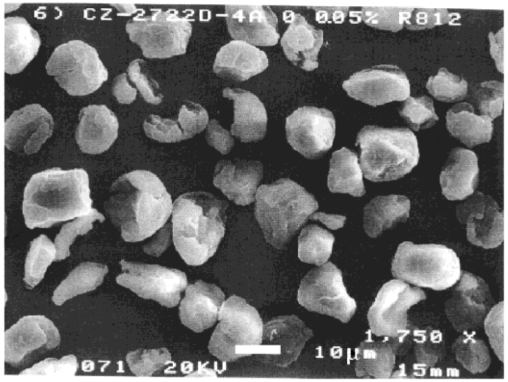
  - Cluster analysis
  - Velocity distribution function
- Summary & Future perspective

Cohesive fine powders

Particles whose size is nano order
(fine powder)

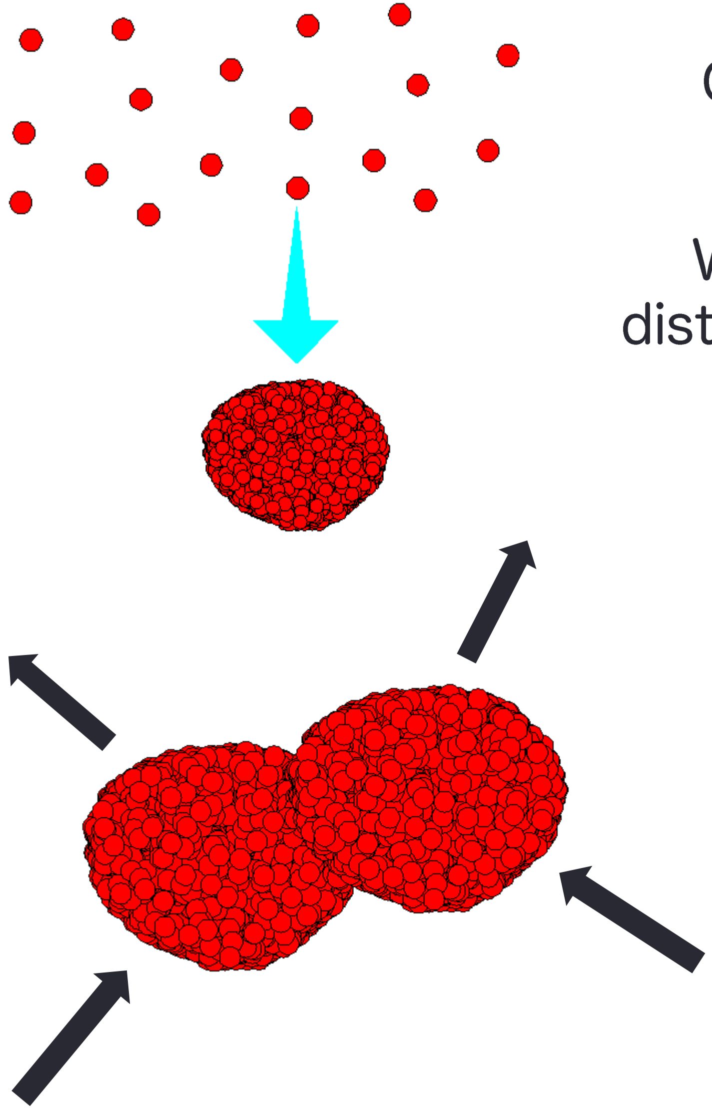


Toner particle[1]

PM2.5[3]

Intermolecular force
cannot be neglected.

[1] A. Castellanos, *Adv. Phys.* **54**, 263 (2005)
[2] Wikipedia " Particulates"



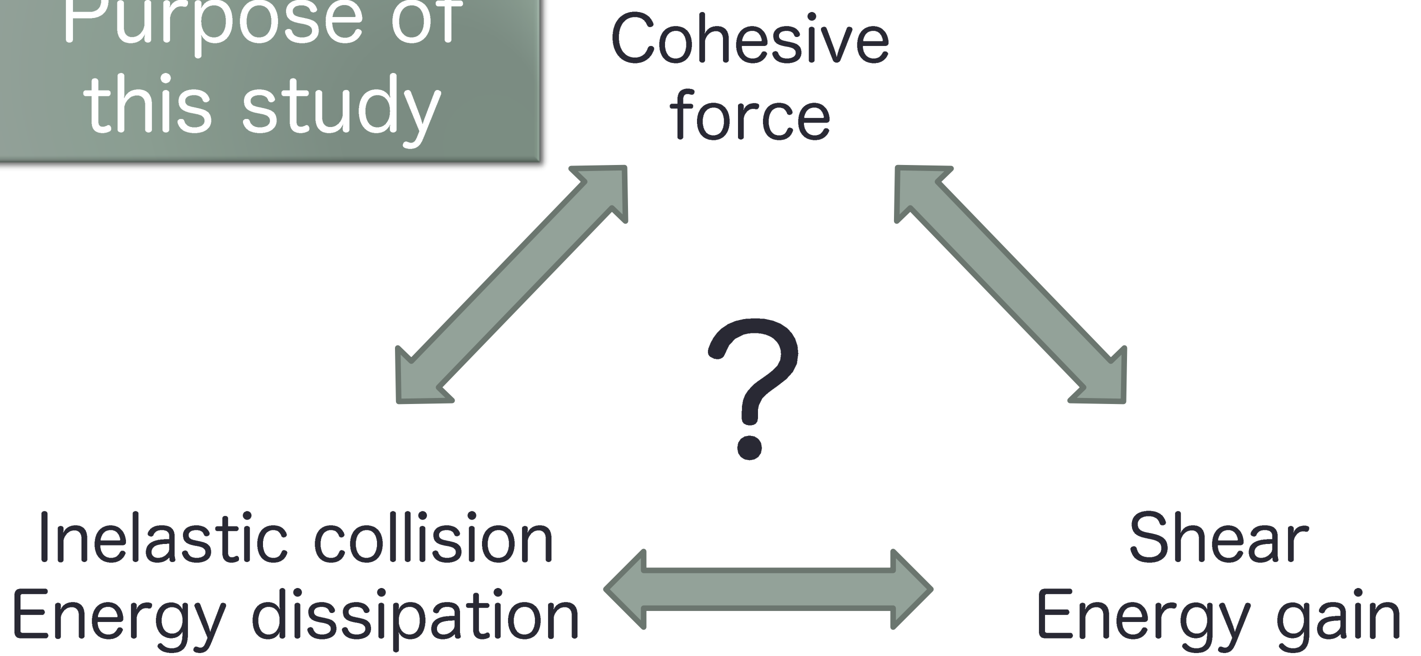
One particle has a lot of atoms.

When particles collide, energy is distributed into the internal degree of freedom.

Collisions become inelastic.

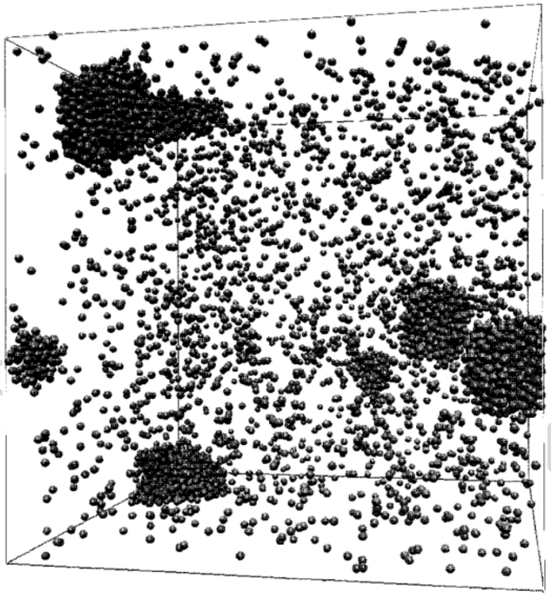
Fine powders = intermolecular force + inelastic collision

Purpose of this study



Previous study①

Cohesive force



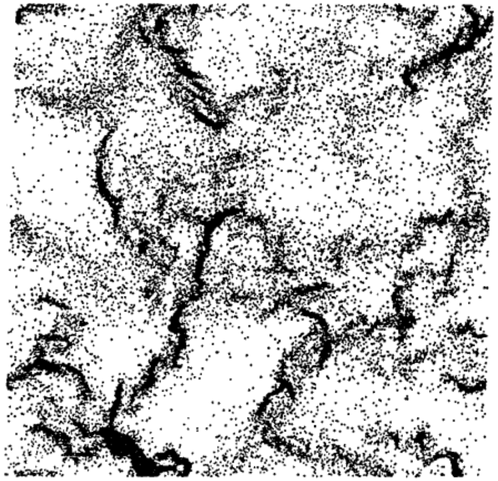
K. Yasuoka and M. Matsumoto, J. Chem. Phys., 109 (1998)

Inelastic collisio
Energy dissipat

Shear
Energy gain

Gas-liquid phase transition
=> nucleation

Previous study②



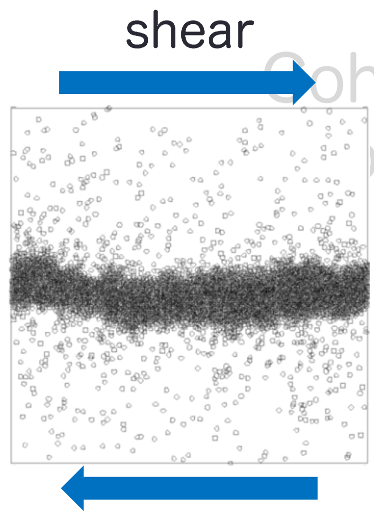
I. Goldhirsch and G. Zanetti, *Phys. Rev. Lett.*, **70** (1993)

Inelastic collision
Energy dissipation

Shear
Energy gain

Uniform state: unstable
=> Cluster formation

Previous study③



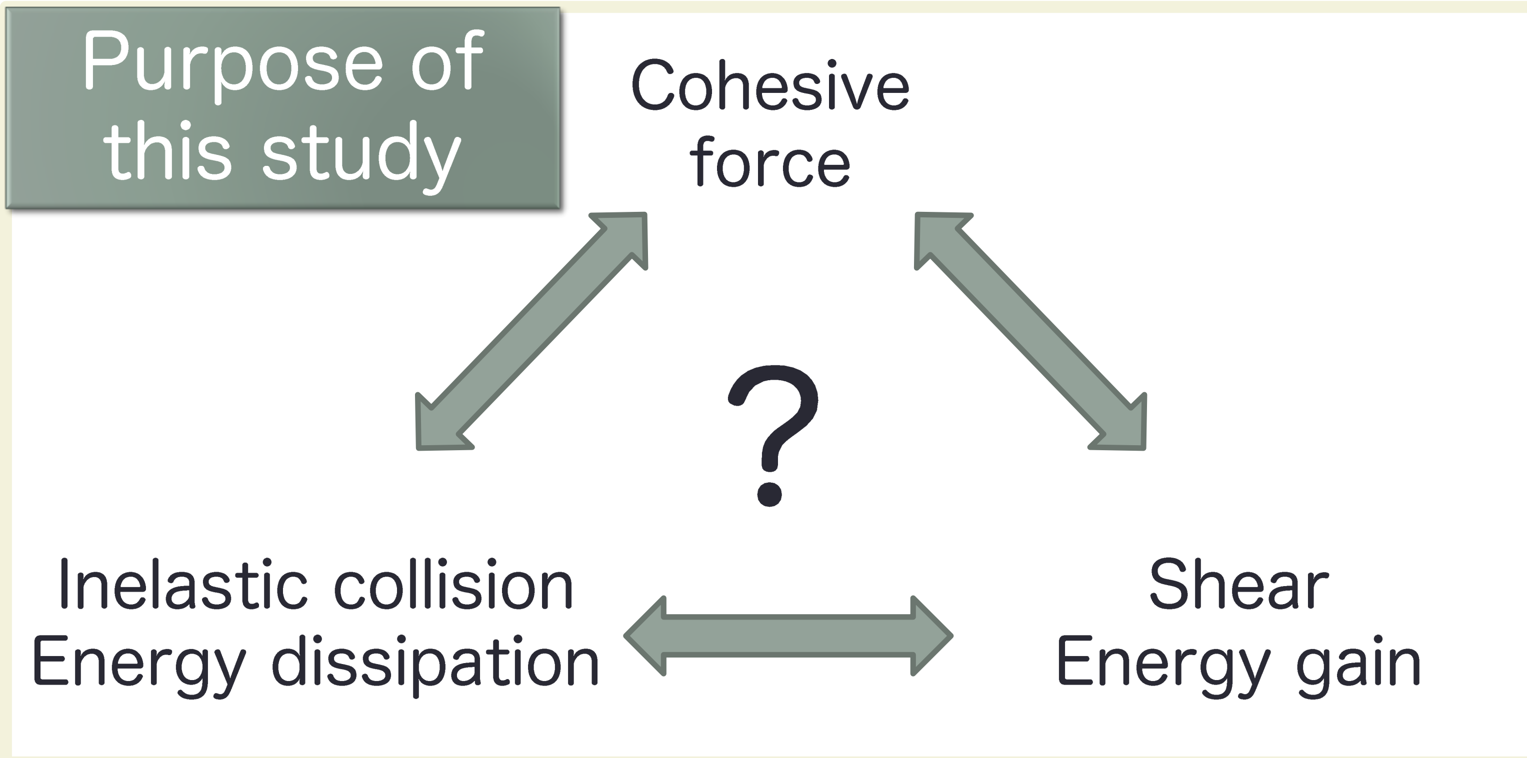
K. Saitoh and H. Hayakawa, *Phys. Rev. E,* 75 (2007)

→ Coexistence:
dense and dilute region

Inelastic collision Energy dissipation	⇔	Shear Energy gain

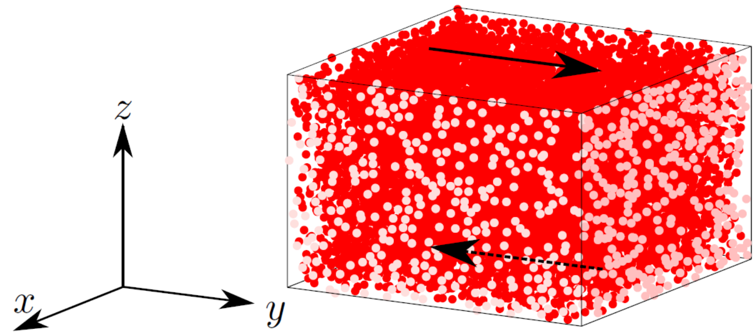
This phenomena can be reproduced by the hydrodynamic equations.

Purpose of this study



Competition of
gas-liquid phase transition
and
dissipative structure

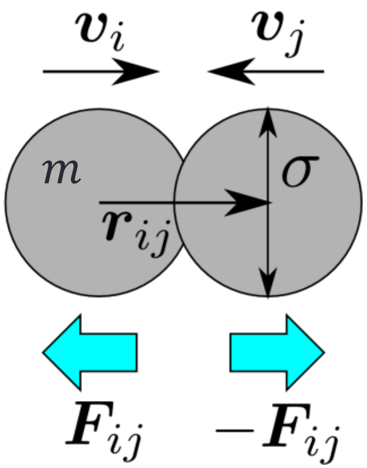
Model & Setup



Molecular dynamics simulation

- $N = 10{,}000$ molecules (diameter σ, mass m)
- system size : $L \times L \times L$
- interaction model
  - intermolecular force = Lennard-Jones potential

$$U^{\mathrm{LJ}}(r_{ij}) = \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] & (r_{ij} \le 3\sigma) \\ 0 & (r_{ij} > 3\sigma) \end{cases}$$

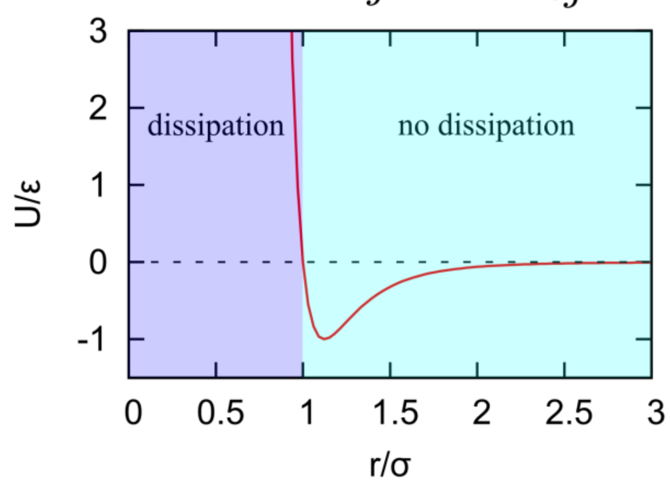


  - inelastic collision = dashpot (ζ : dissipation rate)

$$\boldsymbol{F}^{\mathrm{vis}}(\boldsymbol{r}_{ij}, \boldsymbol{v}_{ij}) = \begin{cases} -\zeta(\boldsymbol{v}_{ij}\cdot\hat{\boldsymbol{r}}_{ij})\hat{\boldsymbol{r}}_{ij} & (r_{ij} \le \sigma) \\ 0 & (r_{ij} > \sigma) \end{cases}$$

force to "i"-th particle

$$\boldsymbol{F}_i = -\sum_{j\neq i} \nabla_i U^{\mathrm{LJ}}(\boldsymbol{r}_{ij}) + \sum_{j\neq i} \boldsymbol{F}^{\mathrm{vis}}(\boldsymbol{r}_{ij}, \boldsymbol{v}_{ij})$$



- shear
  - SLLOD algorithm

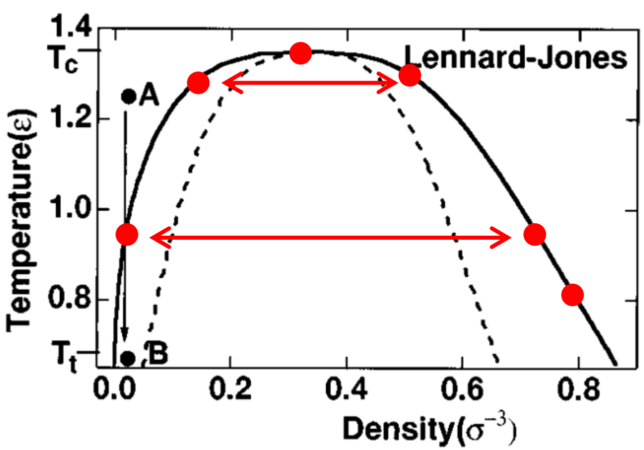
D. J. Evans & G. P. Morriss, *Phys. Rev. A* **30**, 1528 (1984)

「momentum」 = 「Couette flow」 + 「deviation」
(uniform shear)

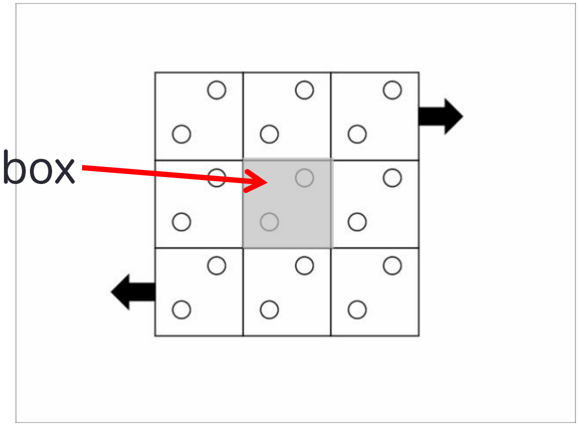
  - Lees-Edwards periodic boundary

A. W. Lees & S. F. Edwards, *J. Phys. C: Solid State Phys.* **5**, 1921 (1972)

- density



Simulation box

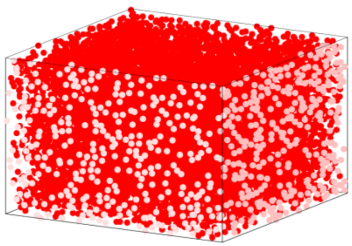


Lees-Edwards boundary condition

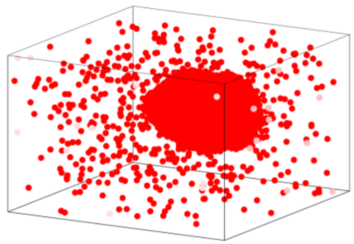
K. Yasuoka and M. Matsumoto, J. Chem. Phys., 109 (1998)

Result: Typical shapes of steady phases

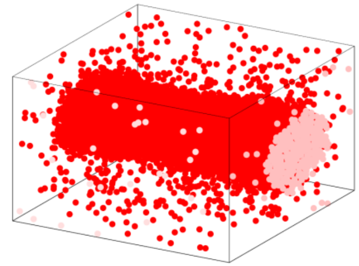
1. Uniform phase



2. Coexistence phase



droplet + gas



plug+ gas

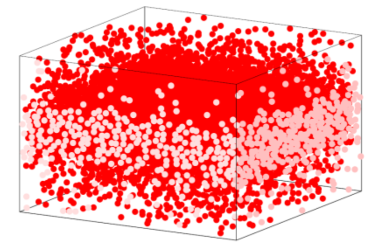
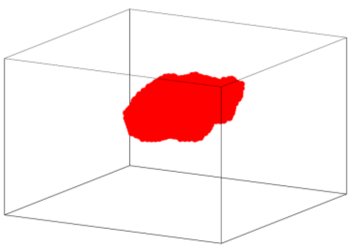
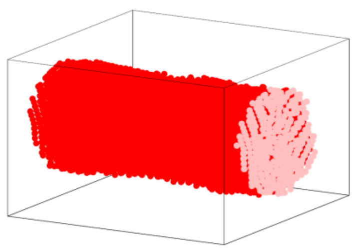


plate + gas

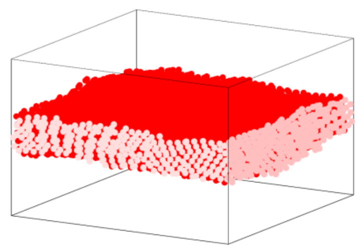
3. Cluster phase



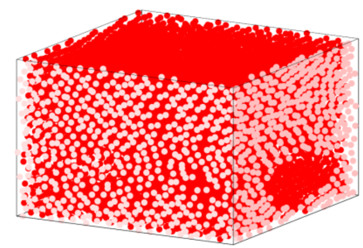
droplet



plug

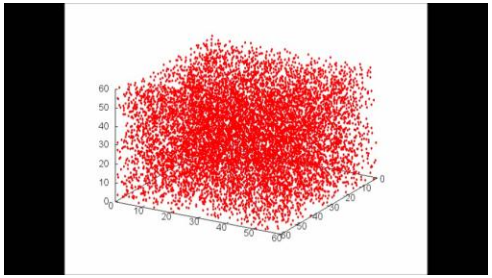


plate

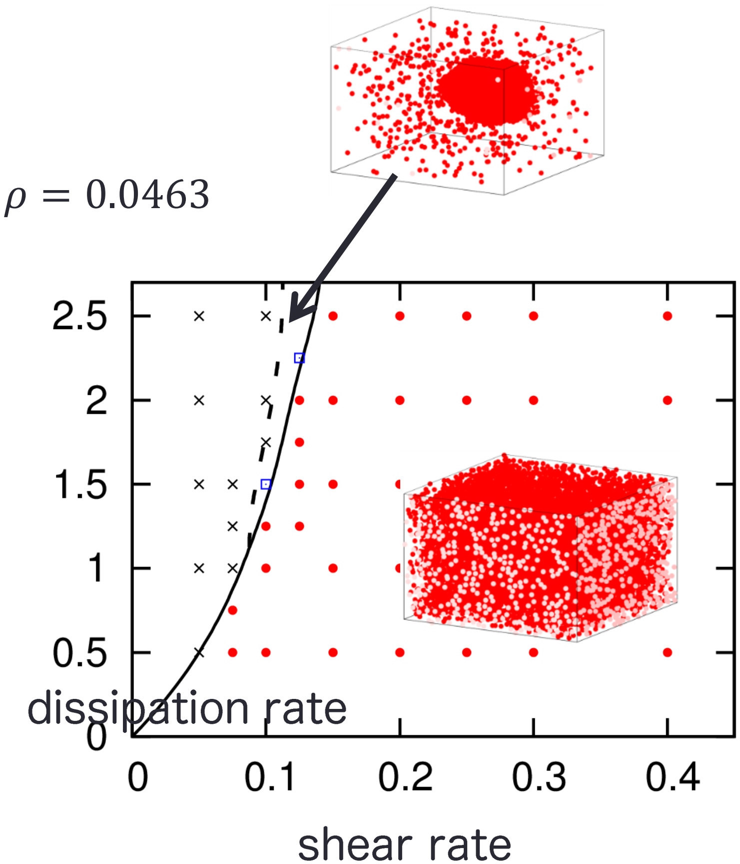


inverse plug

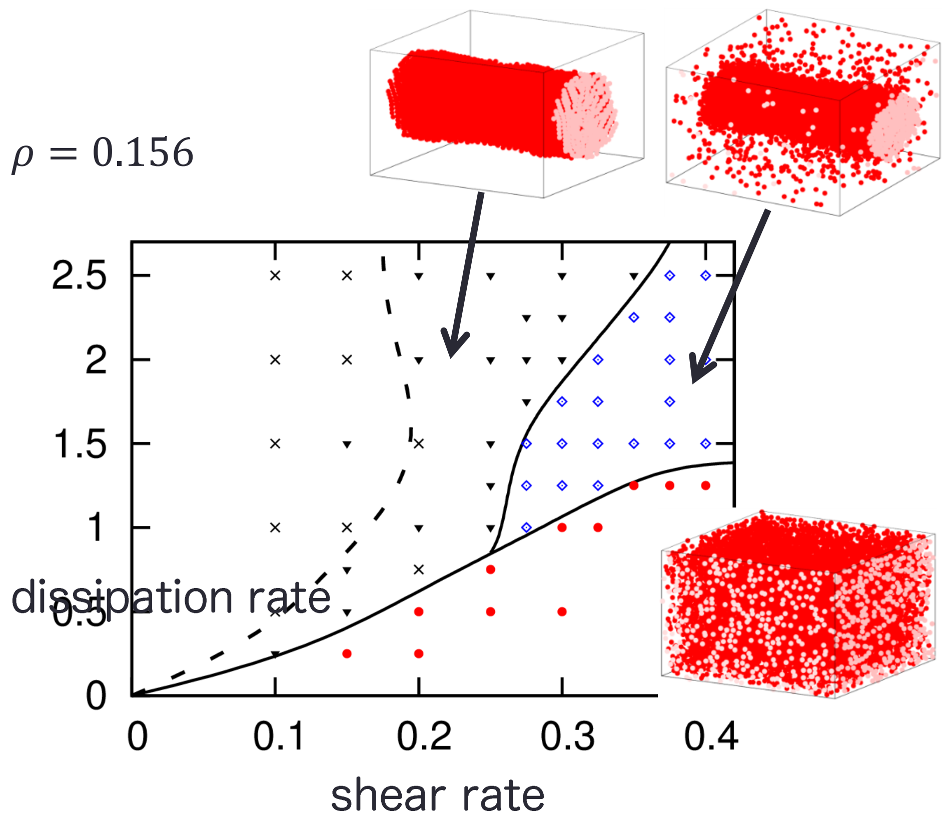
Typical time evolution
(cluster phase)

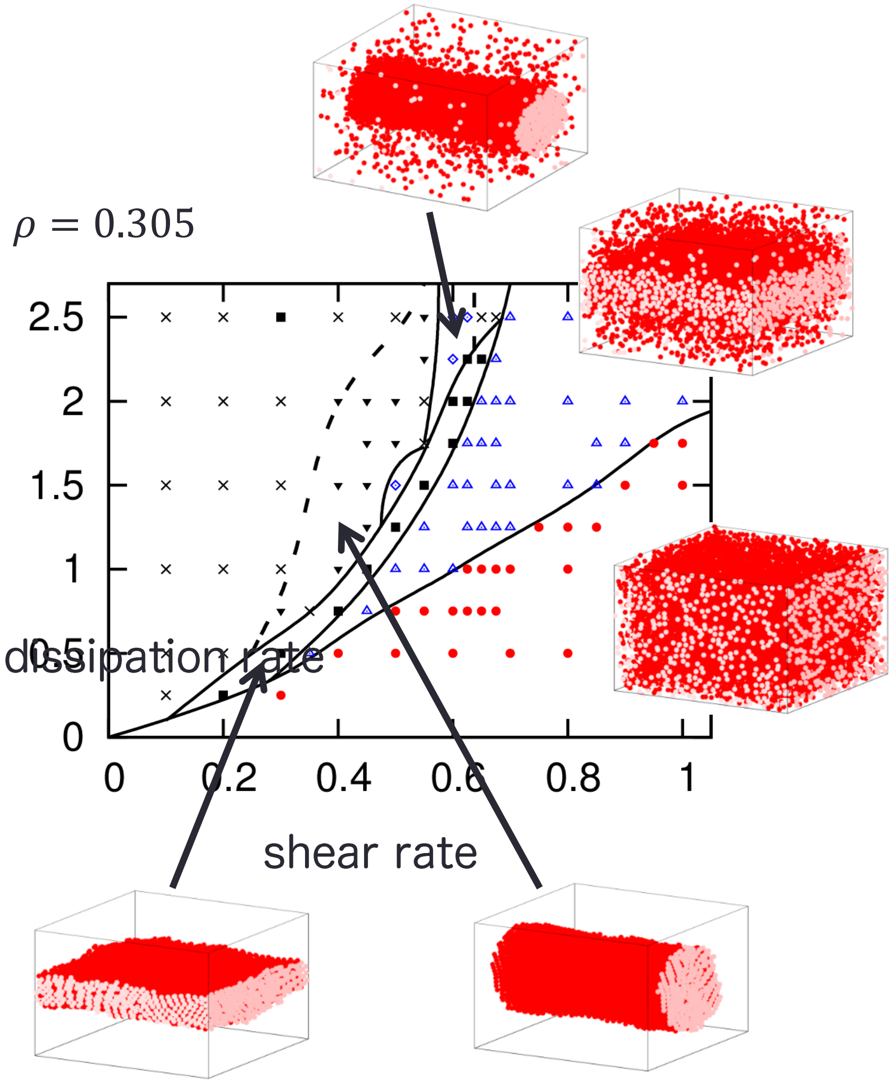


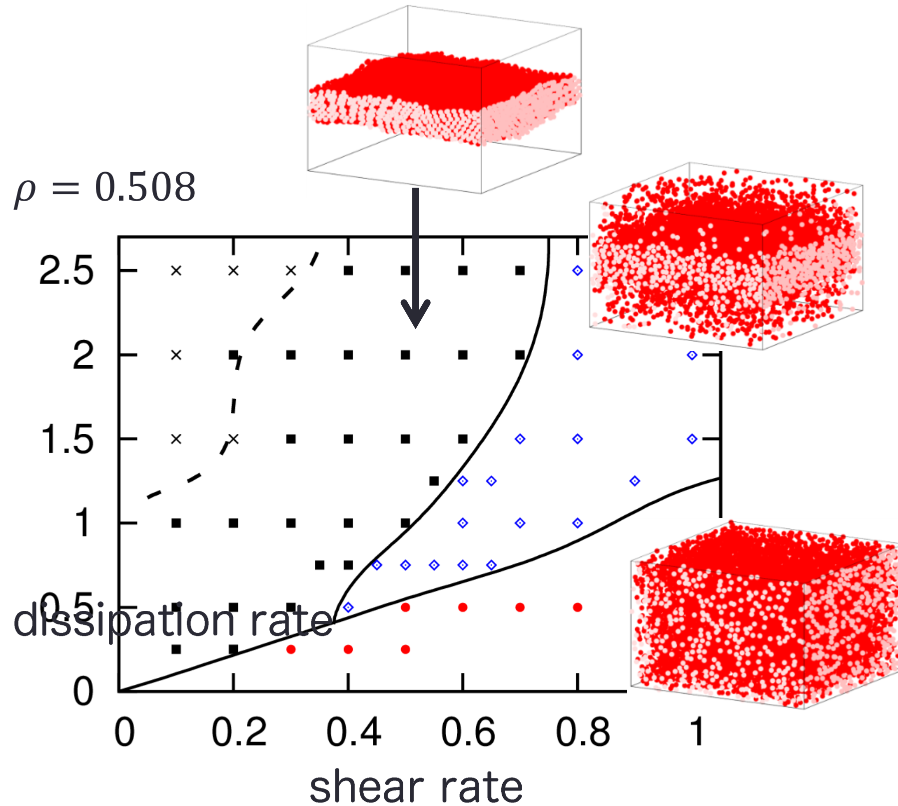
$\rho = 0.0463$

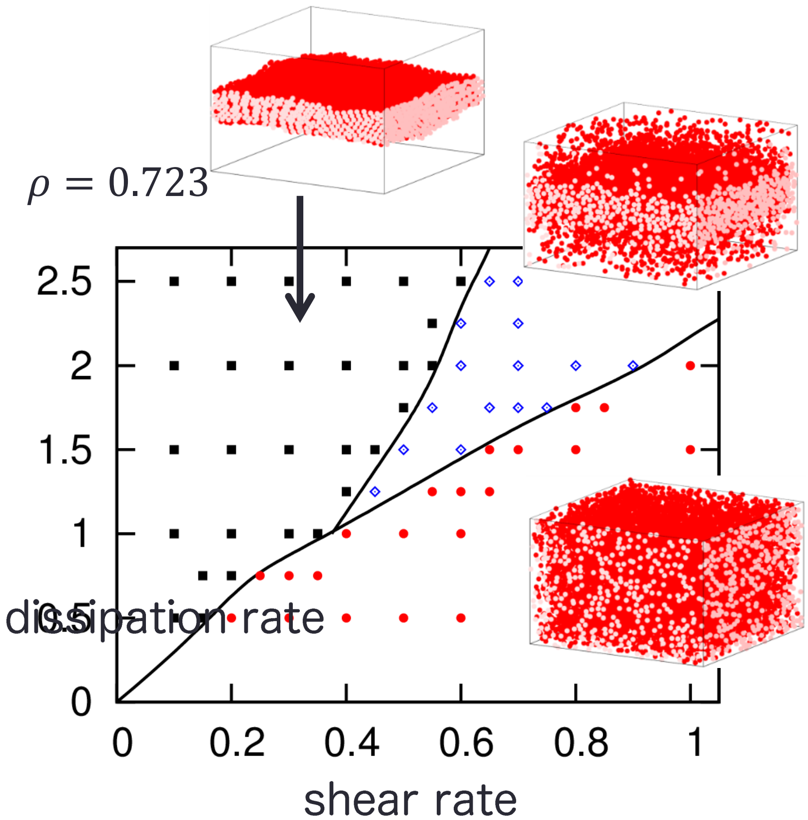


$\rho = 0.156$

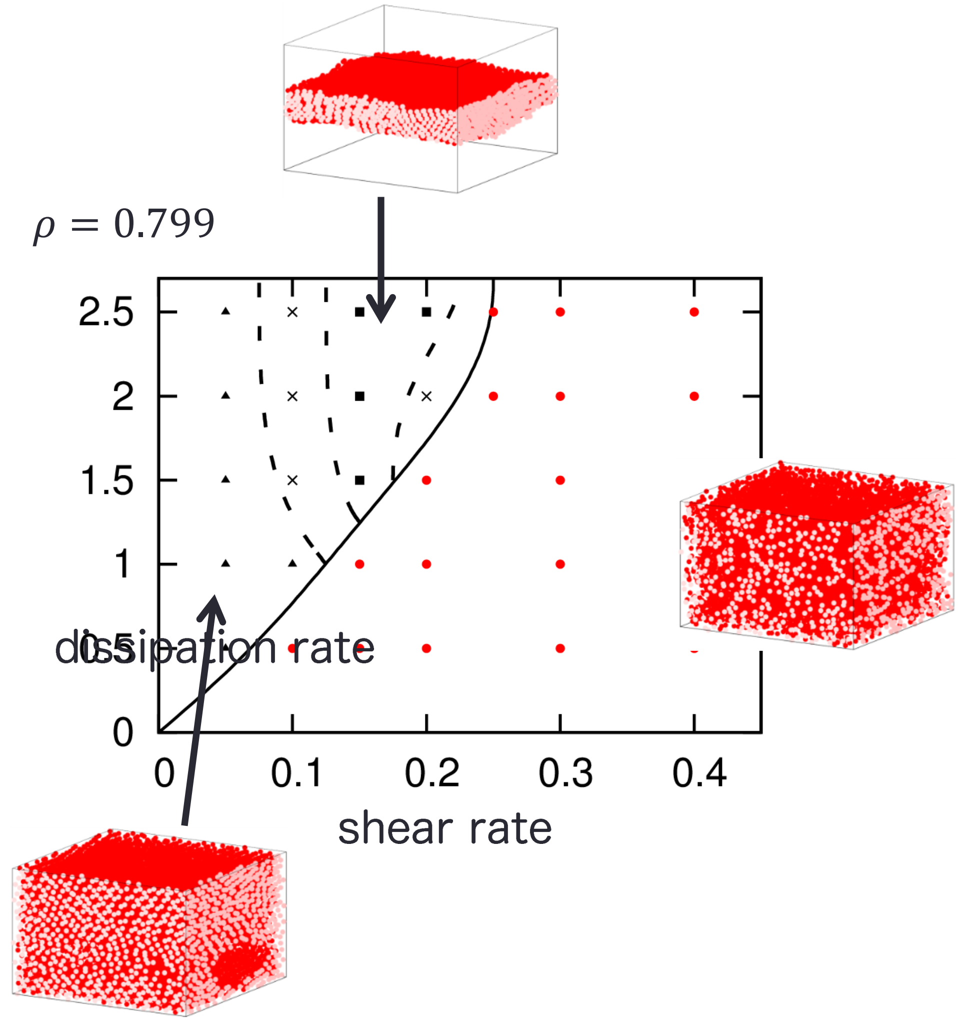



$\rho = 0.305$
2.5
2
1.5
1
0.5
0
0
0.2
0.4
0.6
0.8
1
dissipation rate
shear rate


$\rho = 0.508$
2.5
2
1.5
1
0.5
0
0
0.2
0.4
0.6
0.8
1
dissipation rate
shear rate



$\rho = 0.723$
2.5
2
1.5
1
0.5
0
dissipation rate
0
0.2
0.4
0.6
0.8
1
shear rate

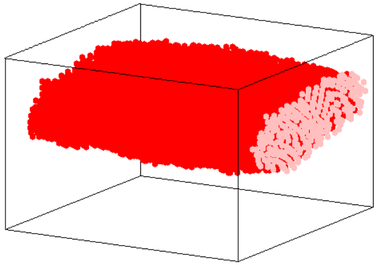


$\rho = 0.799$
2.5
2
1.5
1
0.5
0
dissipation rate
0
0.1
0.2
0.3
0.4
shear rate

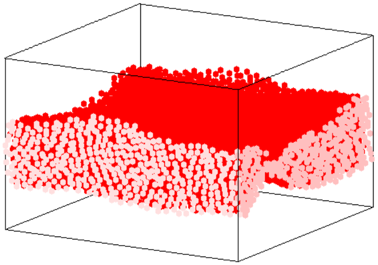
Initial configuration dependence

Effect of dissipation :

Same parameter => different shapes



plug



plate

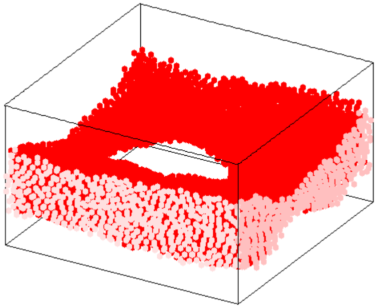
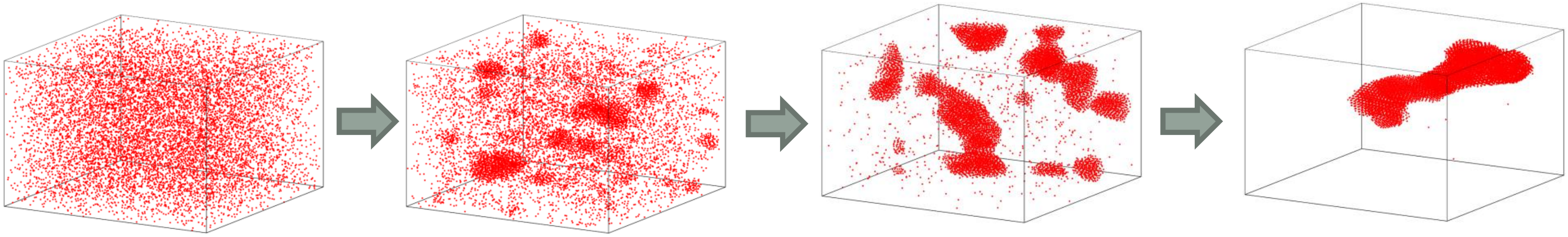


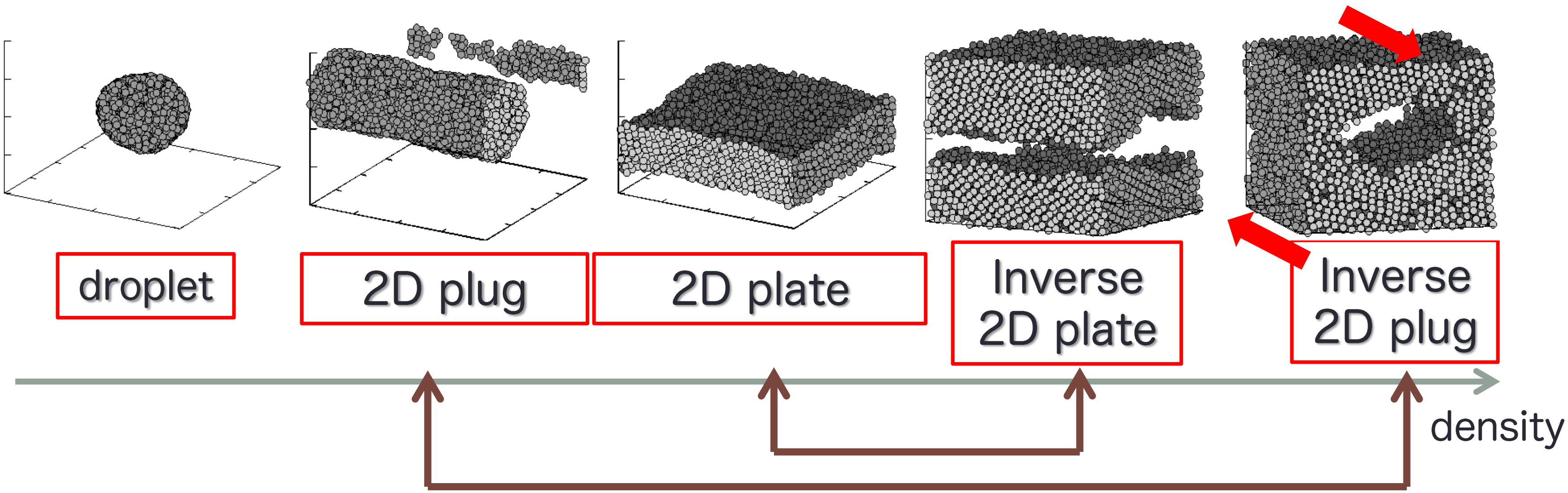
Plate with a hole

mechanism

There appear a lot of small clusters.
⇒ Clusters collide and there become big clusters.
⇒ Distorted shape of clusters become steady.



Typical cluster shapes and density

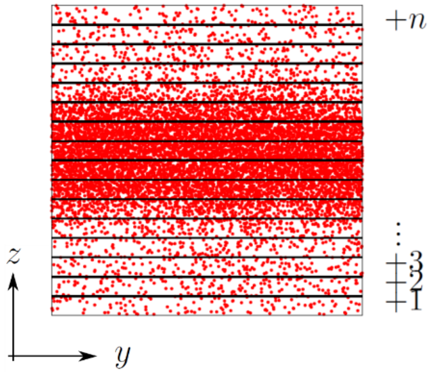


⇨ The system has particle-hole symmetry with respect to the density.

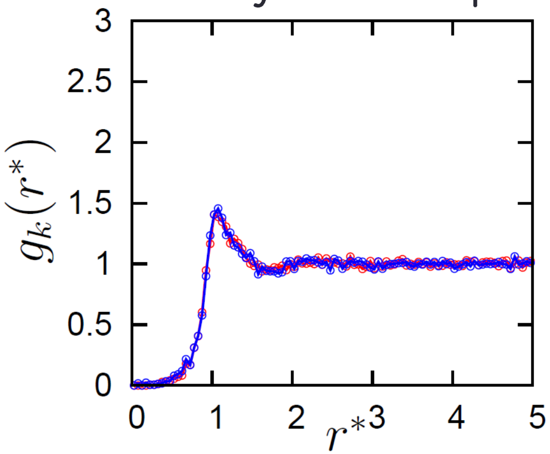
Result 2. Pair correlation function

System is anisotropic.

=> We use bins, whose width (z-direction) is σ.

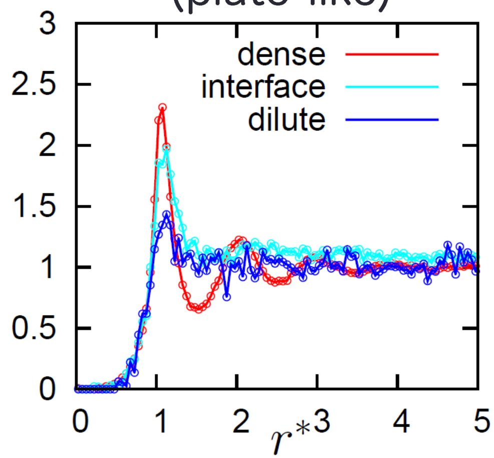


Uniformly sheared phase



All region => gas-like

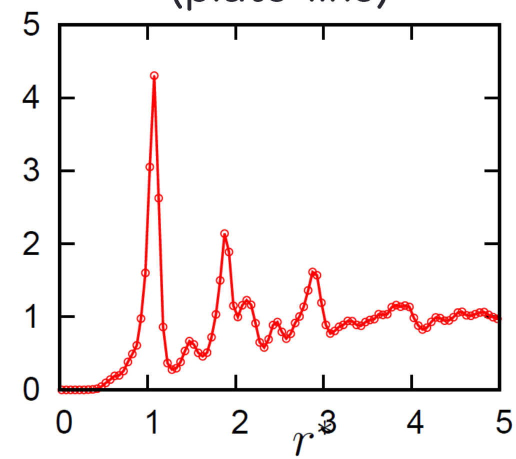
Coexistence phase (plate-like)



Dense => liquid-like

Dilute => gas-like

Cluster phase (plate-like)



Cluster => crystal

Cluster analysis

Size distribution $\phi(n)$

- Definition of a "cluster"
  = Whether the distance of two particles r_0 is less than 1.3σ.

- Cluster phases
  => All particles coagulate and
  become one big cluster as time goes on.
  => $\phi(n) = 1\ (\mathrm{n = N}),\ 0\ (\mathrm{n < N})$

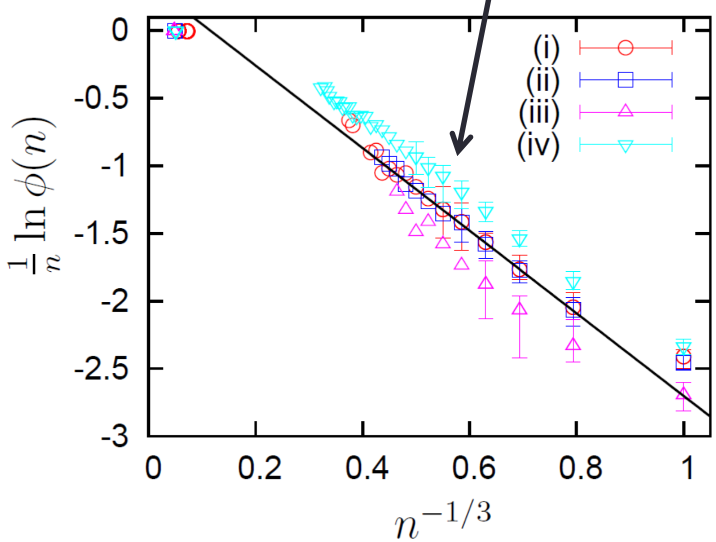
- Coexistence phases
  From classical nucleation theory,

$$\frac{1}{n}\ln\phi(n) = \ln S - K\sigma_s n^{-1/3},$$

S: supersaturation ratio

$$K = \frac{(4\pi)^{1/3}(3/\rho_l)^{2/3}}{k_\mathrm{B}T}$$

slope $K\sigma_S \cong 3.0$



Estimation of K and σ_S

We regard the liquid region as a cluster.

- Surface tension for planar surface

$$\sigma_s = \frac{1}{2L_x L_y} \left\langle \sum_{i<j} \frac{r_{ij}^2 - 3z_{ij}^2}{r_{ij}} \frac{\partial U^{\mathrm{LJ}}(r_{ij})}{\partial r_{ij}} \right\rangle,$$

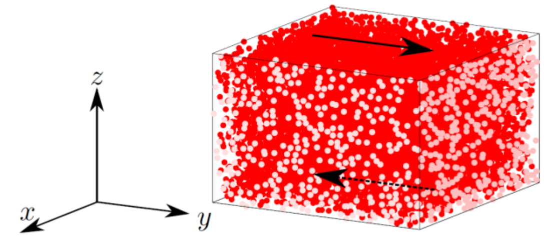
in the case of $\rho = 0.305,\ \dot{\gamma} = 0.6,\ \zeta = 1.5,$

$K \cong 7.0,\ \sigma_S \cong 0.74$

=> $K\sigma_S \cong 5.2$

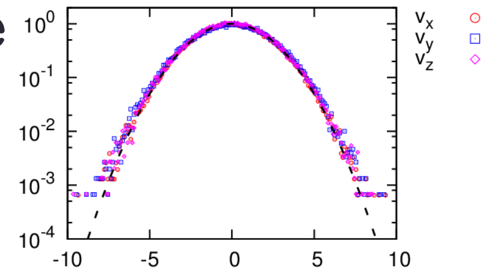
=> $K\sigma_S$ is different from the simulation results ($K\sigma_S \cong 3.0$).

Velocity distribution function (VDF)

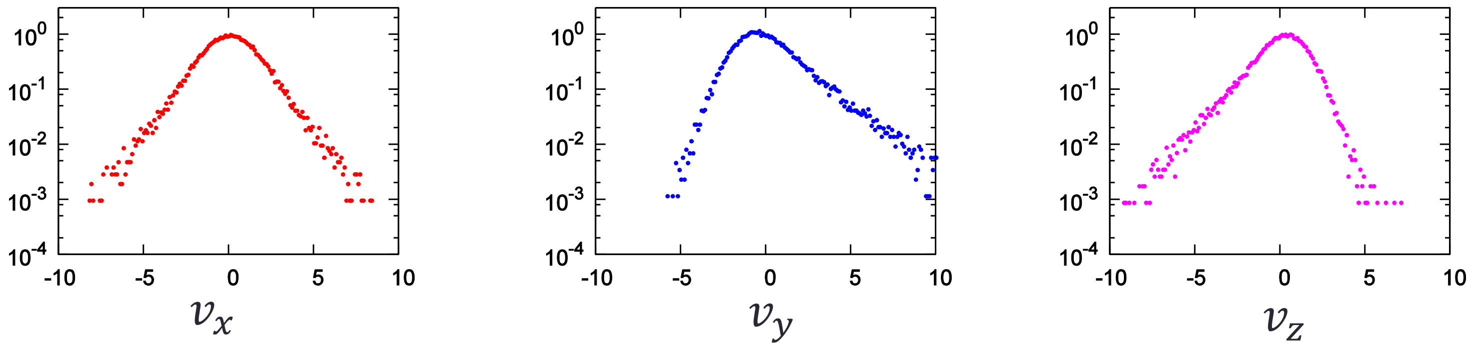


- We calculated VDF for each bin.

1. Uniformly sheared phase
   => VDF is Gaussian



2. Cluster phases
   => The granular temperature becomes zero as time goes on because of inelastic collisions.
3. Coexistence phase
   - $\begin{cases} \text{dense region} \\ \text{dilute region} \end{cases}$ => VDF is Gaussian.
   - Interface region => VDF has an exponential tail.



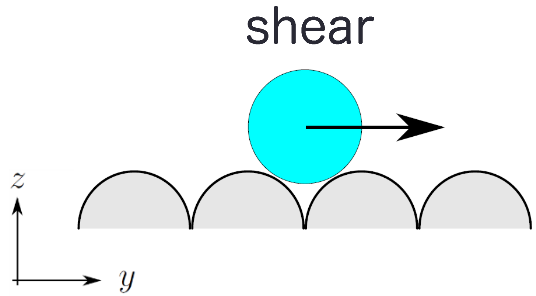
Discussion: Reason for the deviation from Gaussian

We regard the dense region as a rough wall.
Particles in the dilute region move along this wall.

Langevin equation for the Coulomb friction

$$\frac{d\boldsymbol{v}}{dt} = -\mu\frac{\boldsymbol{v}}{|\boldsymbol{v}|} + \boldsymbol{\xi},$$

$$\langle\xi_\alpha(t)\xi_\beta(t')\rangle = 2D\delta_{\alpha\beta}\delta(t-t'),$$



Fokker-Planck equation

$$\frac{\partial P(\boldsymbol{v},t)}{\partial t} = \frac{\partial}{\partial \boldsymbol{v}}\cdot\left(\mu\frac{\boldsymbol{v}}{|\boldsymbol{v}|}P(\boldsymbol{v},t) + D\frac{\partial}{\partial \boldsymbol{v}}P(\boldsymbol{v},t)\right),$$

If the system is steady, we obtain

$$P(v) \propto \exp\left(-\frac{\mu}{D}|v|\right),$$

Summary

- 8 different phases (3 types)
  (Uniform…1, Coexistence…3, Cluster…4)
  dissipation >> shear … initial configuration dependence
  cluster shapes … particle-hole symmetry

- Binwise pair correlation function

- Cluster analysis
  Size distribution (coexistence phase) is consistent with CNT.

- Velocity distribution function
  VDF in the interface deviates from Gaussian (=>exponential tail).

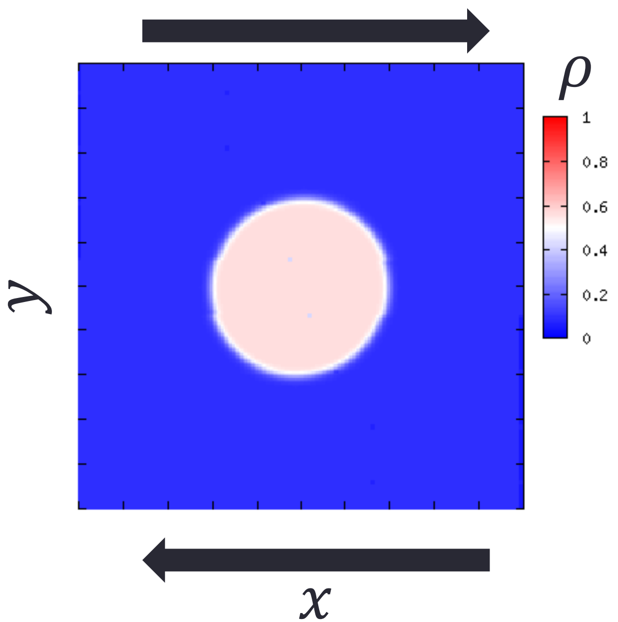
Hydrodynamic approach

Can we reproduce various phases by using hydrodynamic equations?

Dynamic van der Waals theory + Dissipation term under plane shear

$$\frac{\partial n}{\partial t^*} = -\nabla_i^*(n v_i) ,$$
$$\frac{\partial}{\partial t^*}\rho v_i = -\nabla_j^*(\rho v_i v_j) + \nabla_j^* \sigma_{ij}^* ,$$
$$\frac{\partial}{\partial t^*} e_T^* = -\nabla_i^* \left(e_T^* v_i - \sigma_{ij}^* v_j\right) + \nabla_i^*(\lambda \nabla_i^* T) ,$$

$$p = \phi\Theta/(1-\phi) - \phi^2$$
$$p_1 = -\Theta|\nabla\phi|^2 - 2\phi\Theta\nabla^2\phi$$
$$\tau_{ij} = \phi(\nabla_i u_j + \nabla_j u_i) + \delta_{ij}(1-2/d)\phi\nabla_k u_k$$
$$\pi_{ij} = (p+p_1)\delta_{ij} + 2\Theta(\nabla_i\phi)(\nabla_j\phi)$$
$$\sigma_{ij} = \alpha\tau_{ij} - \pi_{ij}$$



Numerically solved under plane shear condition