Direct numerical simulation of breakup of rod-like nano-particle aggregates under simple shear

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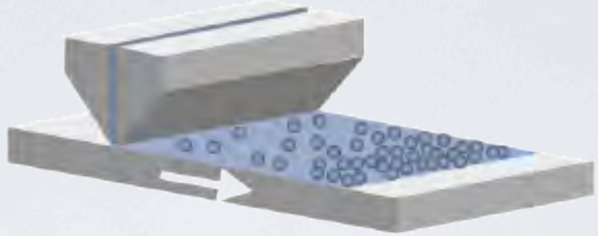
単純剪断場における 棒状ナノ粒子凝集体の解砕シミュレーション

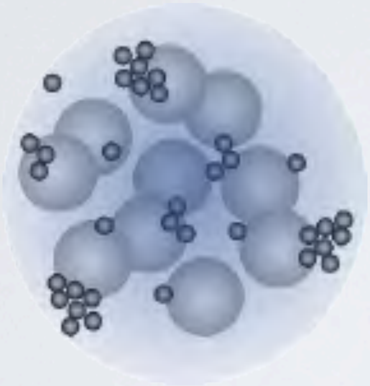
小池修＊・辰巳怜†・山口由岐夫＊

Colloidal Suspensions in Industrial Use



Coating

Kneading
Dispersing

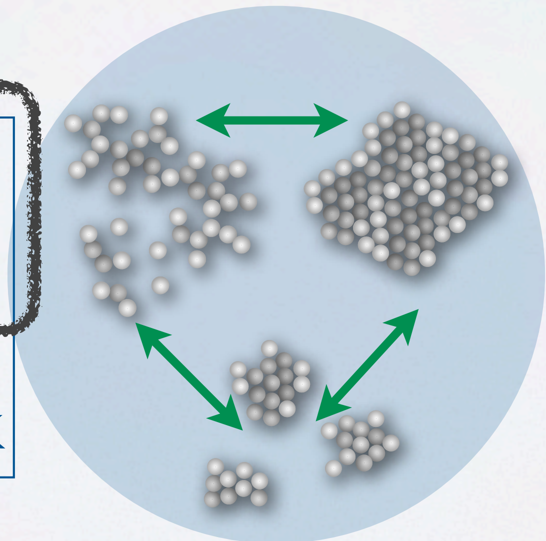


Chemical
Mechanical
Polishing

Flow field can induce athermal Particle structures

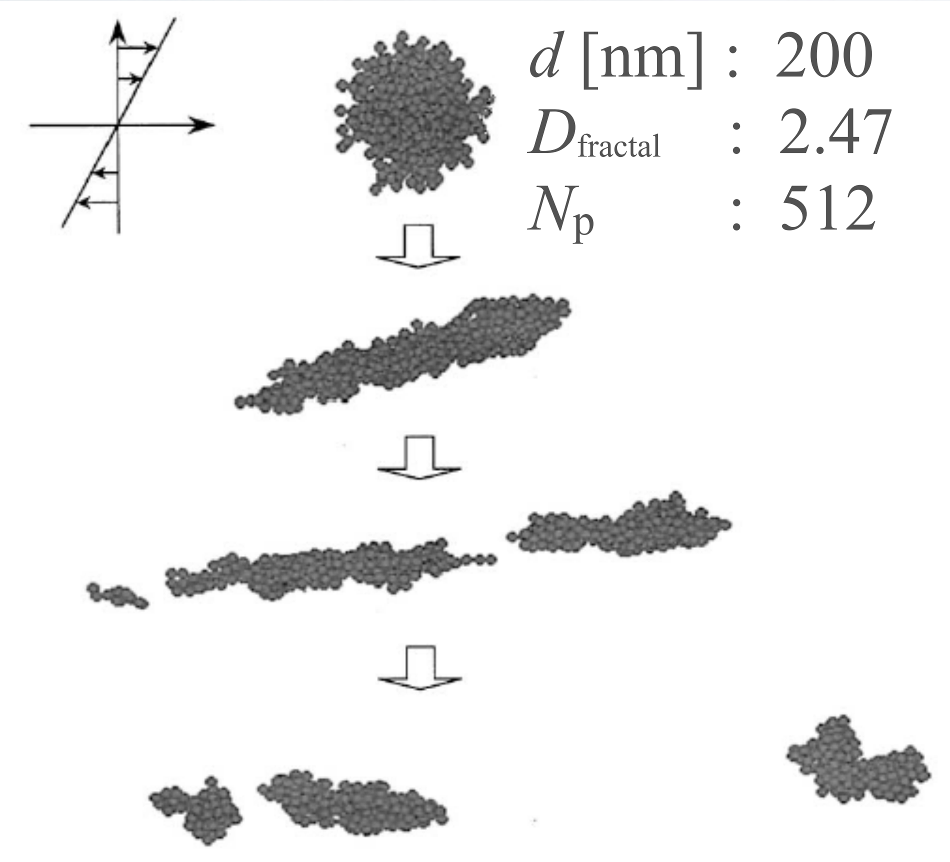
Size Distribution
Orietation

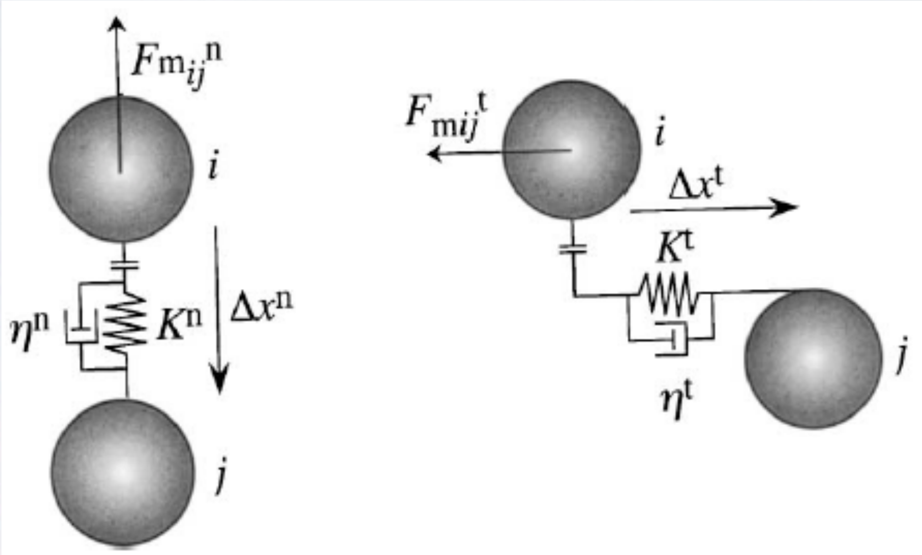
Contact Network



Viscosity
Thermal/Electrical
Conductivity
Optical Property
Mass Diffusivity

Existing Work I - spherical particle -





Flow : Stokes dynamics

Particle : DEM

van der Waals force
no friction rule

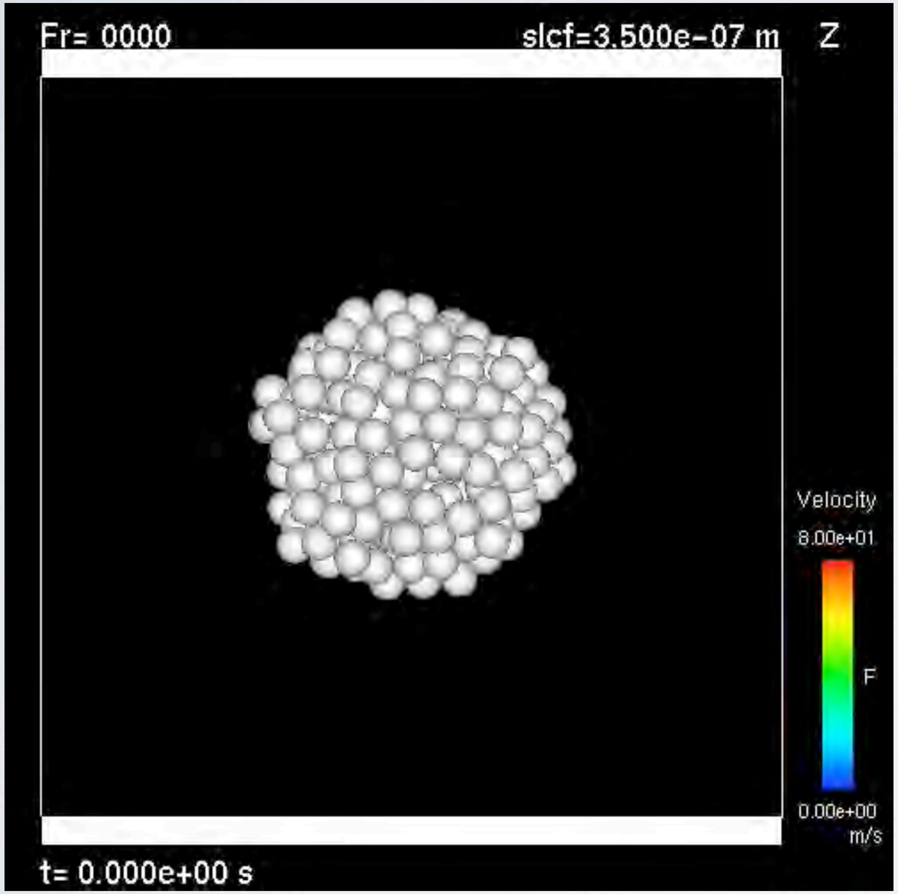
Efficiency of fragmentation :

Shear flow < Elongation flow

K. Higashinani et al.,
Chem. Eng. Sci. 56 (2001) 2927

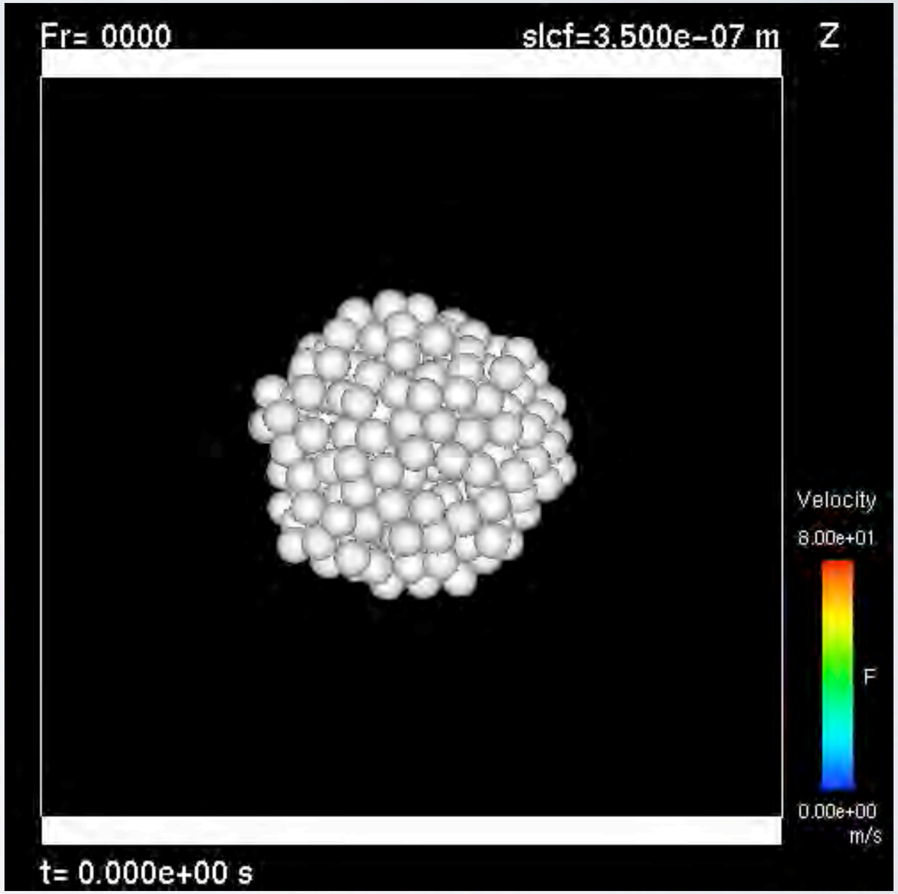
Existing Work II - spherical particle -

Frictionless



$\mu = 0$

Frictional

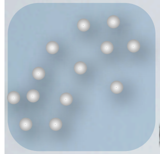


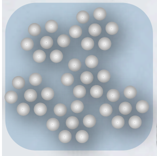
$\mu = 1$

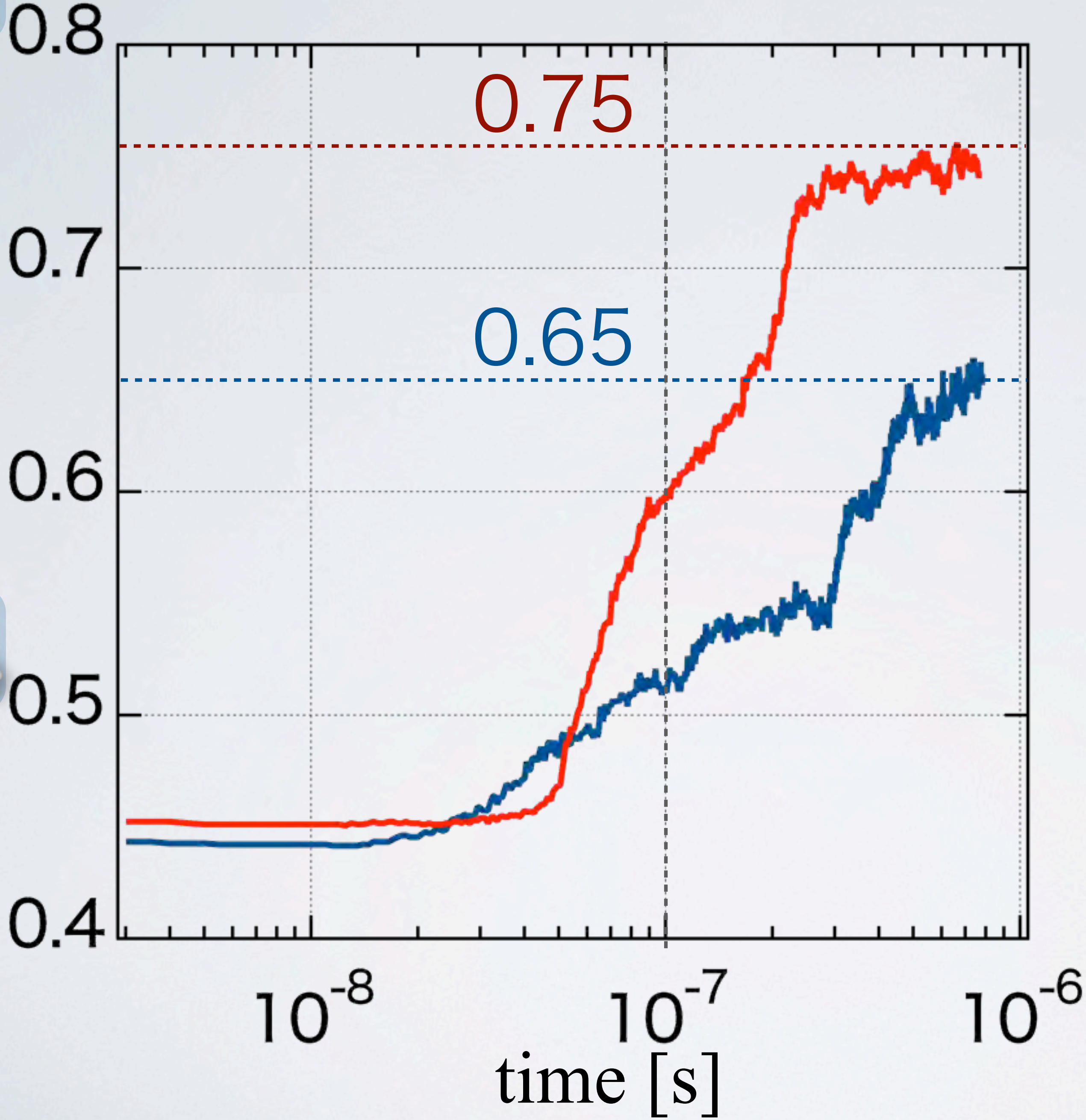
d [nm] : 50
D_{fractal} : 2.89
N_{p} : 297

Koike et al.,
2014 SCEJ 46th Fall Meeting

NBA



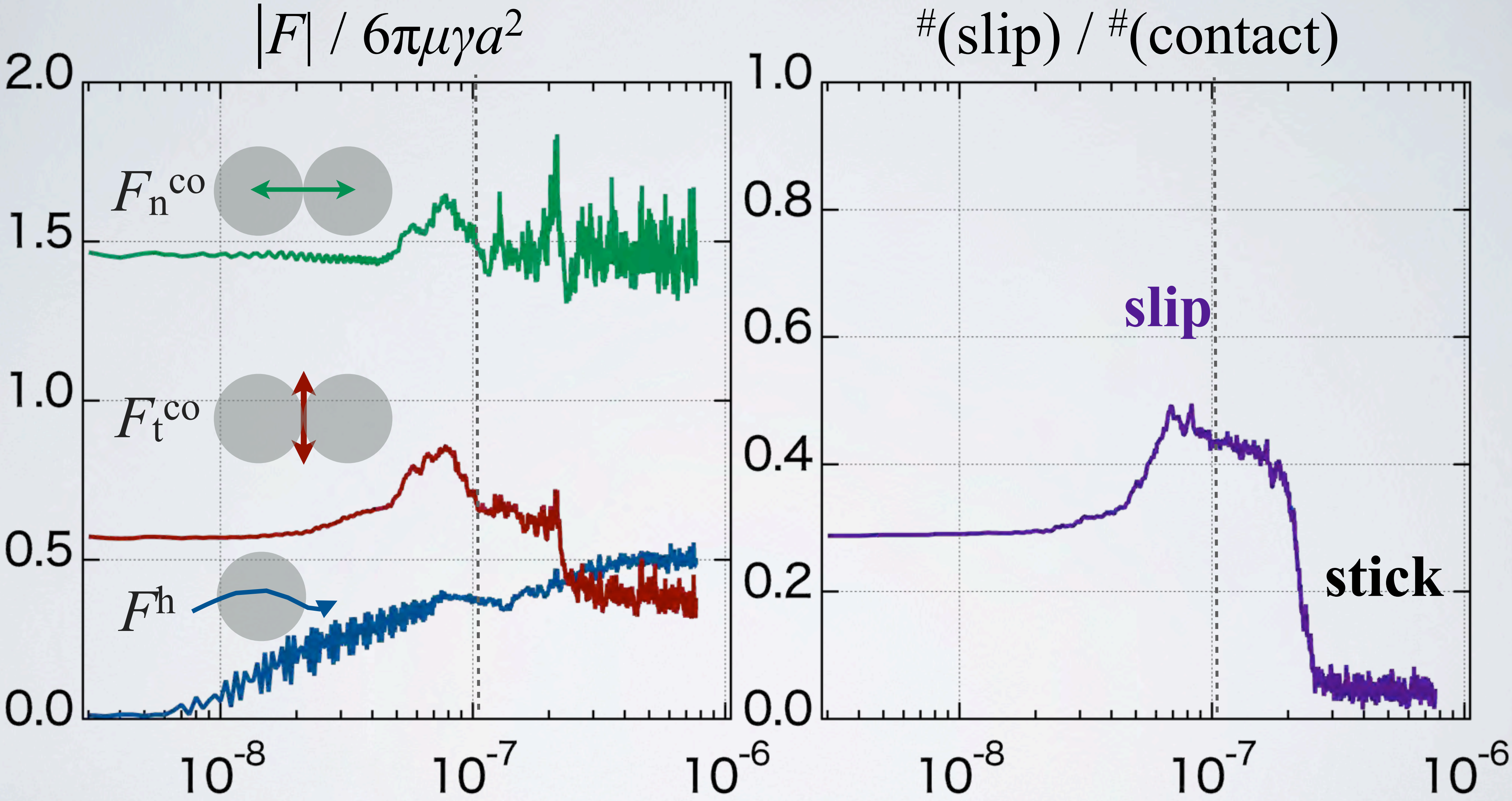




$\mu = 1$：
concave → convex

$\mu = 0$：
convex

Average forces & Slip



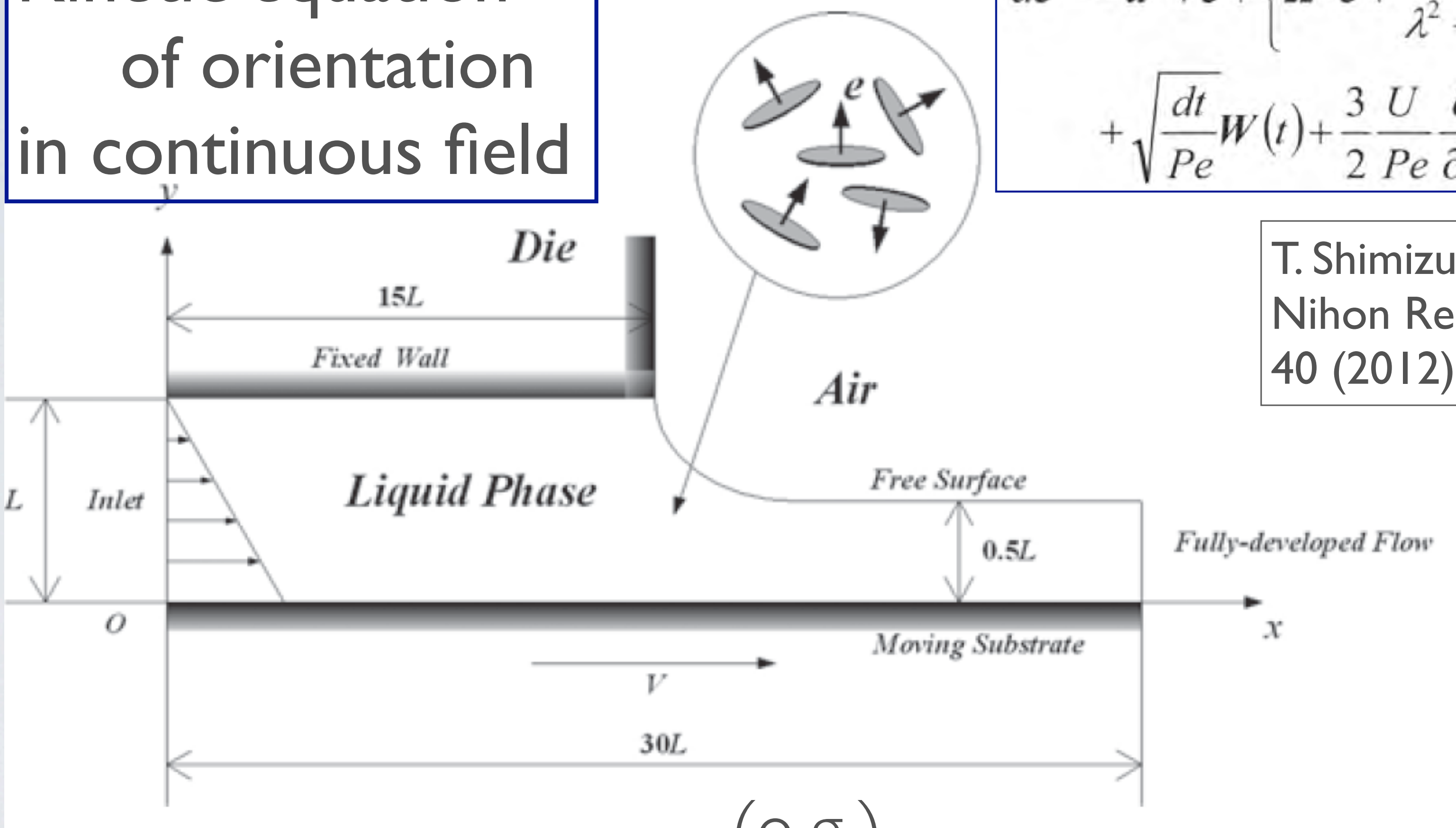
$\mu = 1$

Existing Work III - non-spherical particle -

Kinetic equation
of orientation
in continuous field

$$de = -\boldsymbol{u}\cdot\nabla \boldsymbol{e} + \left\{ \boldsymbol{\Omega}\cdot\boldsymbol{e} + \frac{\lambda^2-1}{\lambda^2+1}\left[\boldsymbol{D}\cdot\boldsymbol{e} - (\boldsymbol{D}:\boldsymbol{ee})\boldsymbol{e}\right] \right\} dt + \sqrt{\frac{dt}{Pe}}\boldsymbol{W}(t) + \frac{3}{2}\frac{U}{Pe}\frac{\partial}{\partial \boldsymbol{e}}(\boldsymbol{ee}:\boldsymbol{S})dt$$

T. Shimizu and T. Yamamoto,
Nihon Reoroji Gakkaishi
40 (2012) 111



(e.g.)

$$\dot{\boldsymbol{e}} = \boldsymbol{\Omega}\cdot\boldsymbol{e} + \frac{\lambda^2-1}{\lambda^2+1}\left[\boldsymbol{D}\cdot\boldsymbol{e} - (\boldsymbol{D}:\boldsymbol{ee})\boldsymbol{e}\right]$$

Jeffery 1922

$$\dot{\boldsymbol{S}} = \boldsymbol{\Omega}\cdot\boldsymbol{S} - \boldsymbol{S}\cdot\boldsymbol{\Omega} + \frac{\lambda^2-1}{\lambda^2+1}\left[\boldsymbol{D}\cdot\boldsymbol{S} + \boldsymbol{S}\cdot\boldsymbol{D} - 2\hat{\boldsymbol{S}}:\boldsymbol{D}\right] + 2C\dot{\gamma}(\boldsymbol{I} - 3\boldsymbol{S})$$

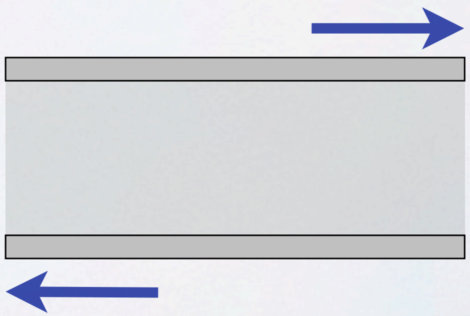
Folgar-Tucker 1984

Objective

- To investigate breakup process of rod-like nano-particle aggregates by DNS

Method

- Direct Numerical Simulation by IBM + DEM (SNAP-F)
- Simple shear flow inside a plane-parallel channel



Equation of Fluid Motion

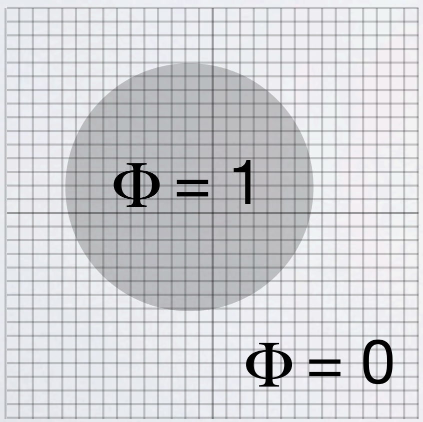
Immersed Boundary Method

Mass : $\nabla \cdot \boldsymbol{v} = 0$

Random force

Momentum: $\dfrac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} = -\nabla p + \nu \nabla^2 \boldsymbol{v} + \dfrac{1}{\rho_\mathrm{f}} \nabla \cdot \boldsymbol{S} + \Phi \boldsymbol{\alpha}$

Coupling term of fluid with solid : $\alpha = \dfrac{\boldsymbol{v}_\mathrm{p} - \boldsymbol{v}}{\Delta t} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} - \nu \nabla^2 \boldsymbol{v} - \dfrac{1}{\rho_\mathrm{f}} \nabla \cdot \boldsymbol{S}$



$$\boldsymbol{F}^\mathrm{h} = -\int_V \rho_\mathrm{f} \phi_\mathrm{p}(\boldsymbol{x}) \alpha(\boldsymbol{x}) dV$$

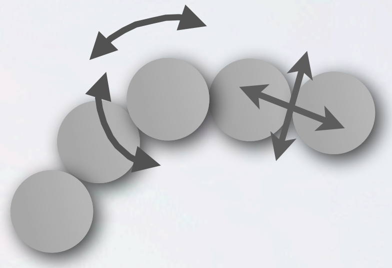
$$\boldsymbol{T}^\mathrm{h} = -\int_V \left\{ \boldsymbol{r}_\mathrm{p}(\boldsymbol{x}) \times \rho_\mathrm{f} \phi_\mathrm{p}(\boldsymbol{x}) \alpha(\boldsymbol{x}) \right\} dV$$

Equation of Bead Motion

DLVO

$$m\frac{d\boldsymbol{v}_{\mathrm{p}}}{dt} = \boldsymbol{F}^{\mathrm{co}} + \boldsymbol{F}^{\mathrm{bead}} + \boldsymbol{F}^{\mathrm{D}} + \boldsymbol{F}^{\mathrm{h}}$$

$$I\frac{d\boldsymbol{\omega}_{\mathrm{p}}}{dt} = \boldsymbol{T}^{\mathrm{co}} + \boldsymbol{T}^{\mathrm{bead}} + \boldsymbol{T}^{\mathrm{h}}$$



- DEM ＋ Coulomb's friction

$$\left|\boldsymbol{F}_{\mathrm{t}}^{\mathrm{co}}\right| = \min\left(\left|\boldsymbol{F}_{\mathrm{t}}^{\mathrm{co}}\right|, \mu\left|\boldsymbol{F}_{n}^{\mathrm{co}}\right|\right)$$

- Non-slip condition between beads

$$\boldsymbol{v}_i + a\boldsymbol{\omega}_i \times \boldsymbol{n}_{ij} = \boldsymbol{v}_j + a\boldsymbol{\omega}_j \times \boldsymbol{n}_{ji}$$

- Non-fracture inside rod

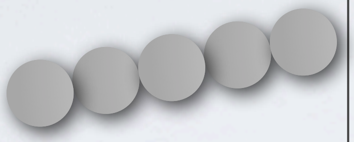
, but its fracture can directly be modeled

Simulation Condition

Particle

d [nm] : 50

r_p : 5



A [J] : $(1, 3.5)\times 10^{-20}$

59 rods (295 beads)

Fluid

η_s [Pa s] : 10^{-3}

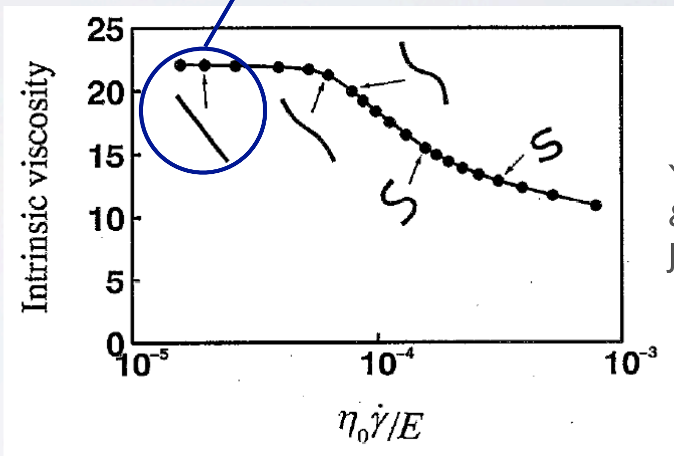
T [K] : 293.15

Field strength

/ rod strength :

$$\frac{\eta_s \dot{\gamma}}{E} \sim 10^{-5} : \text{rigid}$$

Pe : 4.6×10^4

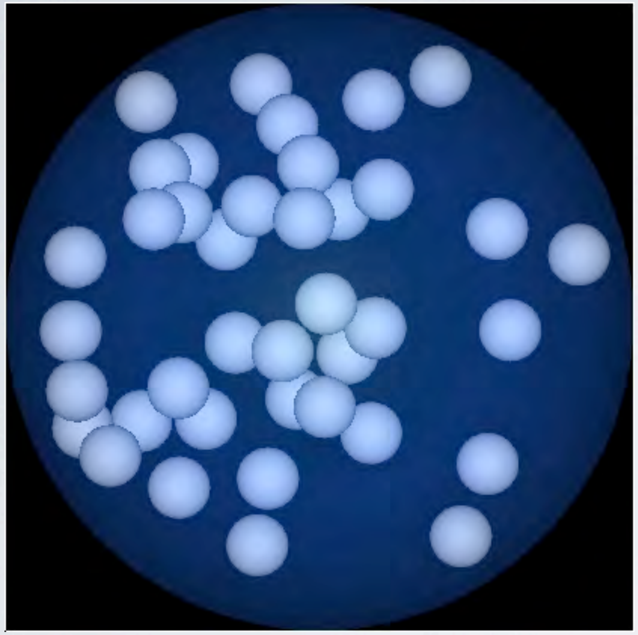


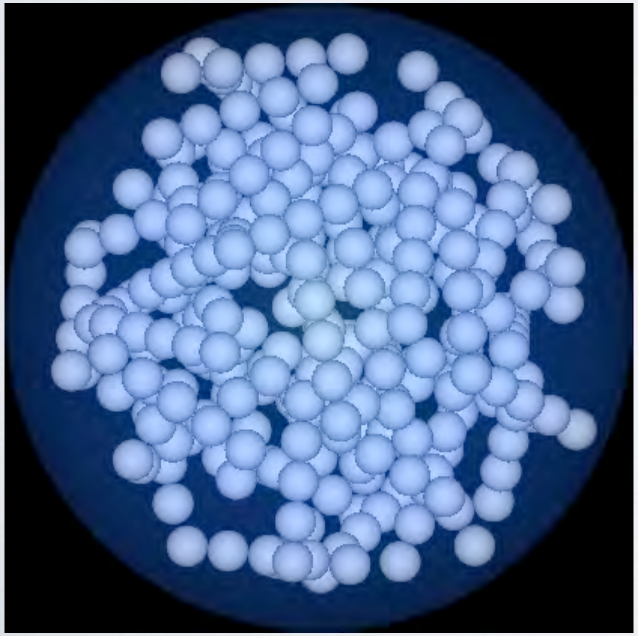
Yamamoto & Matsuoka J. Chem. Phys. , 100 (1994) 3317

Domain size

15d ×15d × 15d

How to Make Single Aggregate





- Confine particles in a droplet
- Shrink the droplet during drying
- Push particles into the center of droplet by capillary force

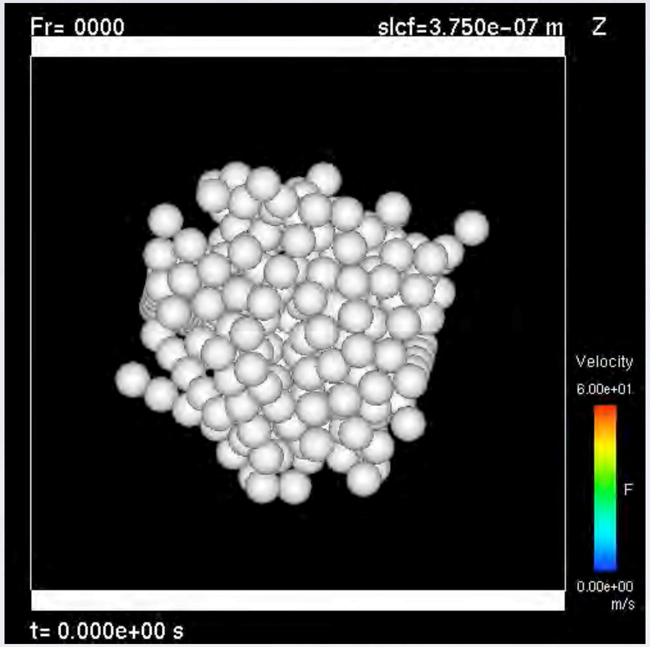
- Simple and efficient method
- It is hard to control the fractal dimension as in DLCA

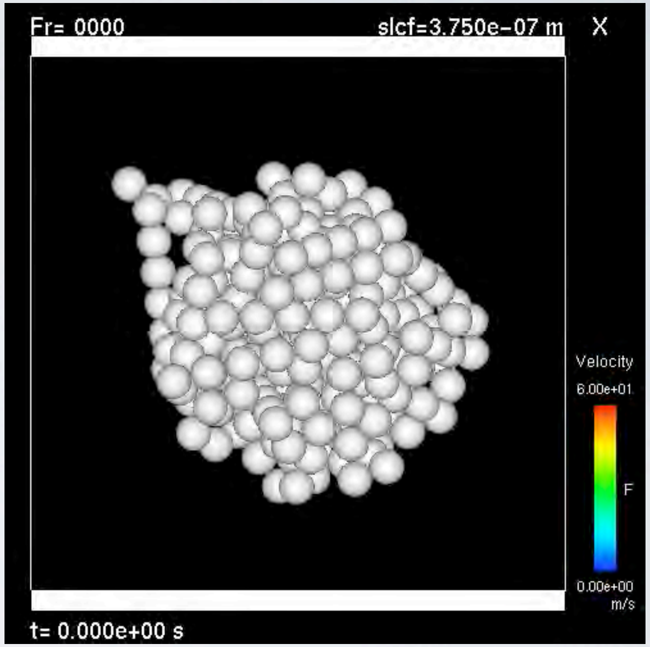
Breakup Process of Aggregate

$A = 3.5\times10^{-20}$

Frictionless

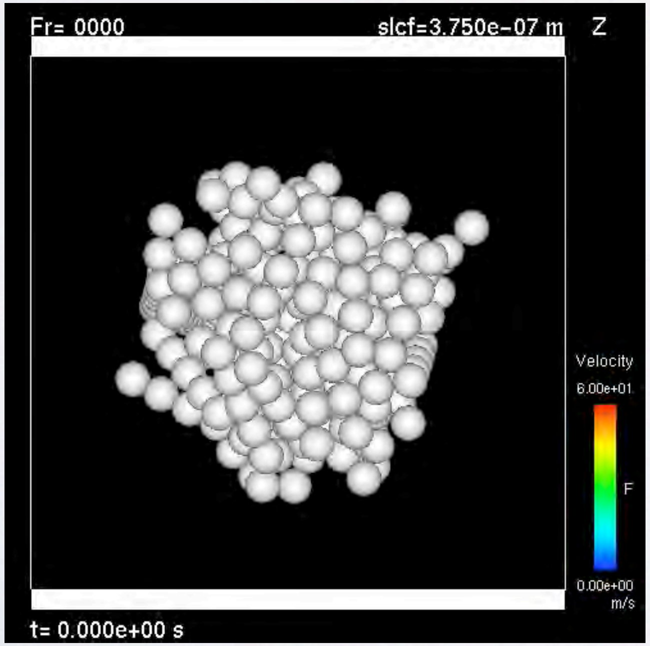
$\mu = 0$

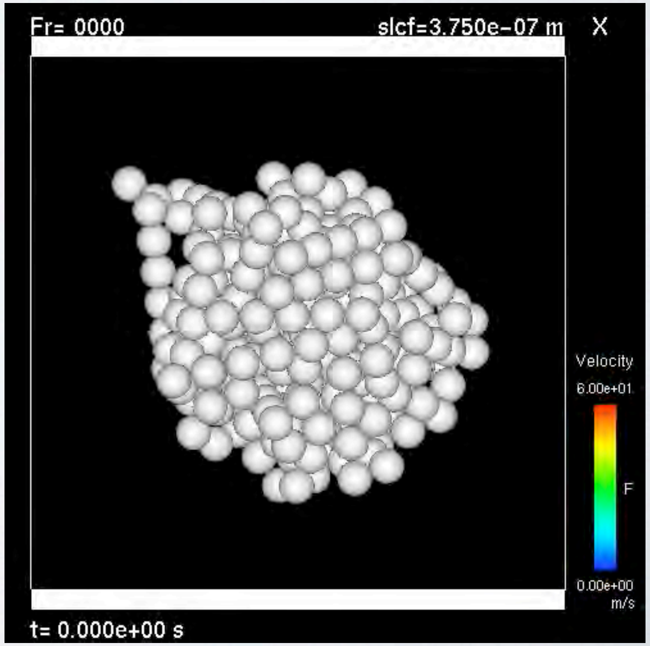




Frictional

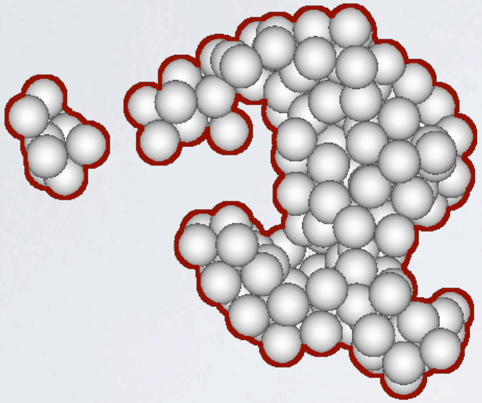
$\mu = 1$





Nondimensional Boundary Area

NBA



$$\text{NBA} = \frac{\text{surface area of aggregates}}{\text{total surface area of paticles}}$$

Definition of NBA

$$\text{NBA} = \frac{1}{N}\left[\frac{1}{12}\sum_{c=0}^{12}(12-c)n(c)\right]$$

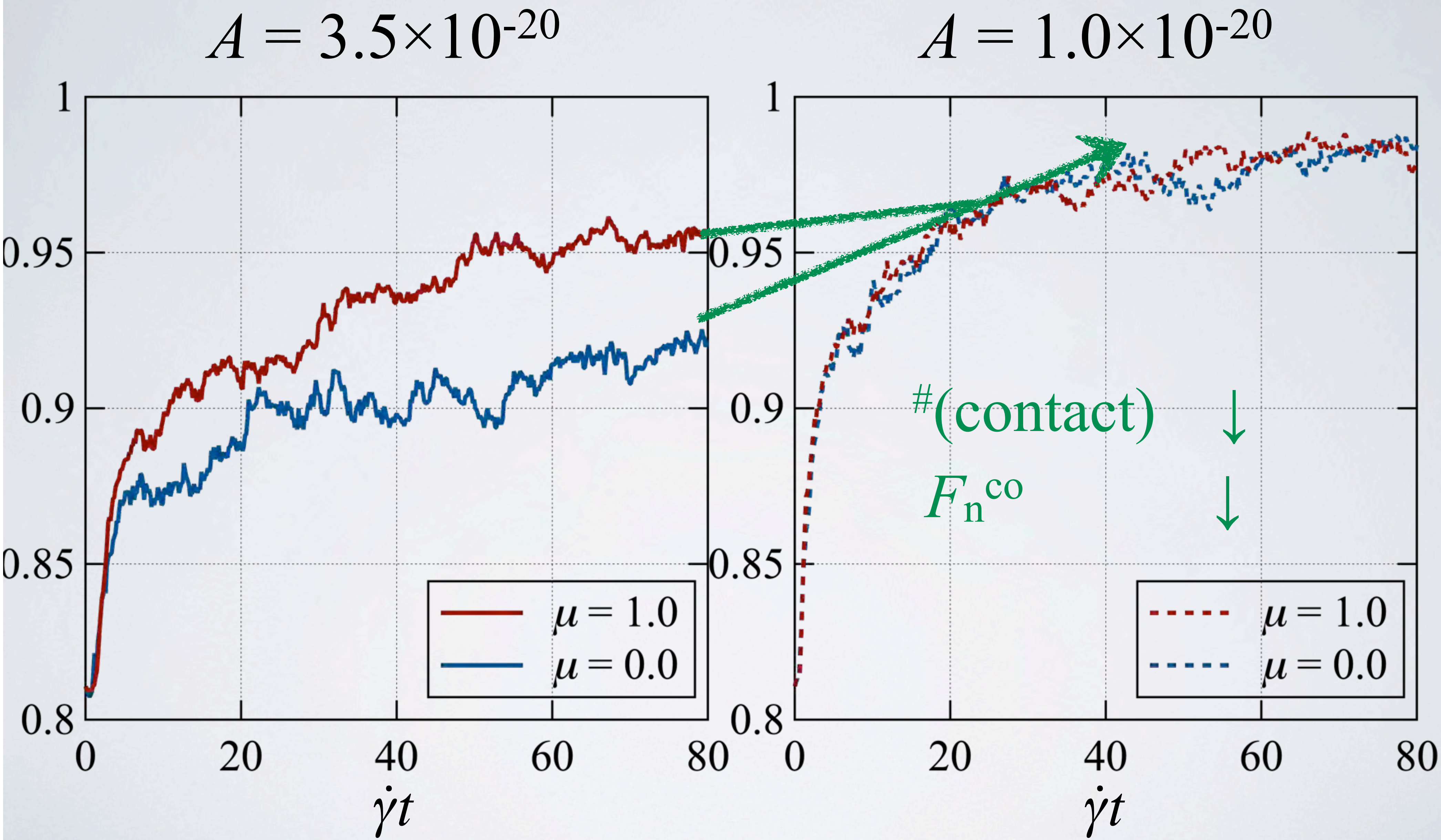
$n(c)$: number of particles with coordination number of c

N : total number of particles

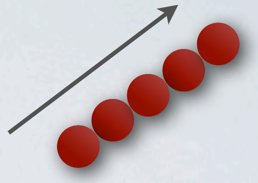
NBA = 1 : completely dispersed

NBA = 0 : close-packed

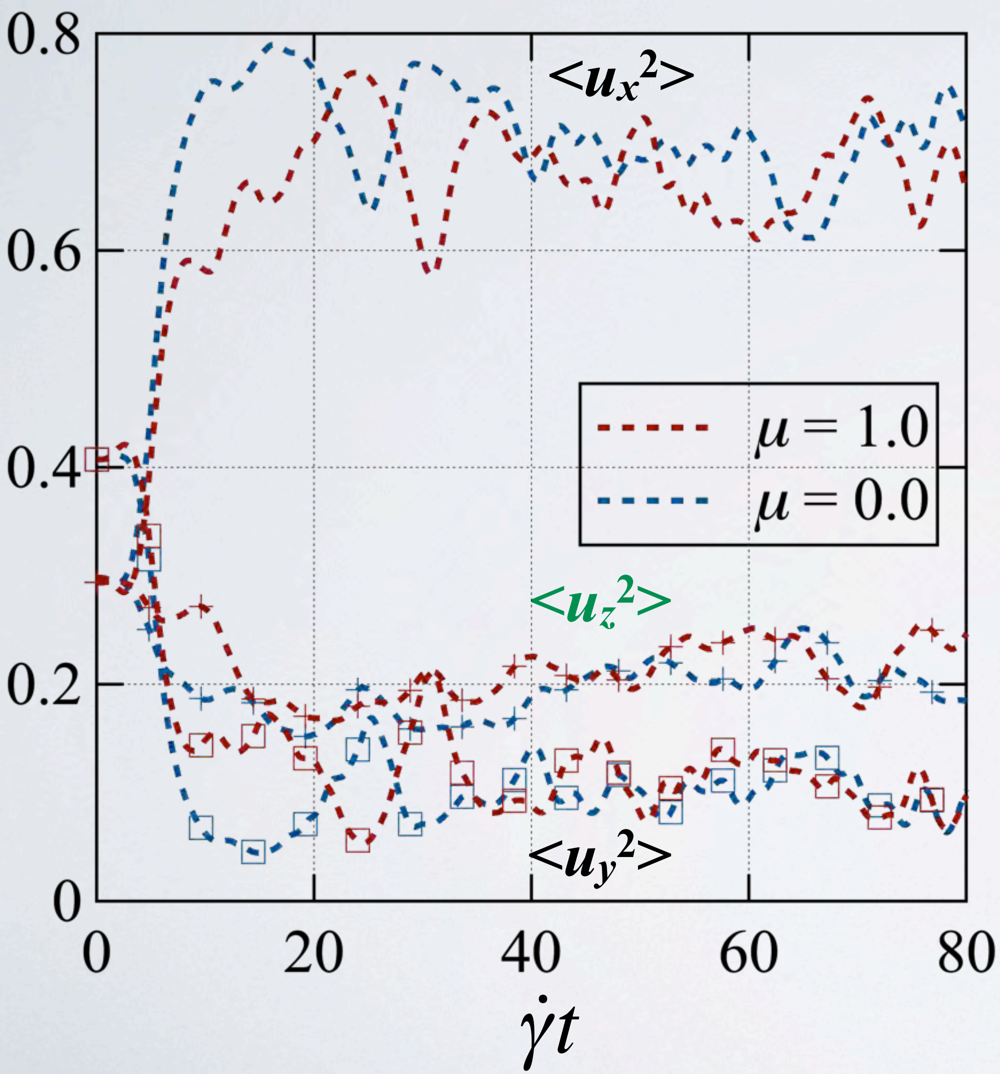
NBA


$A = 3.5\times10^{-20}$
$A = 1.0\times10^{-20}$
1
0.95
0.9
0.85
0.8
0
20
40
60
80
$\dot{\gamma}t$
$\mu = 1.0$
$\mu = 0.0$
#(contact) ↓
F_n^{co} ↓

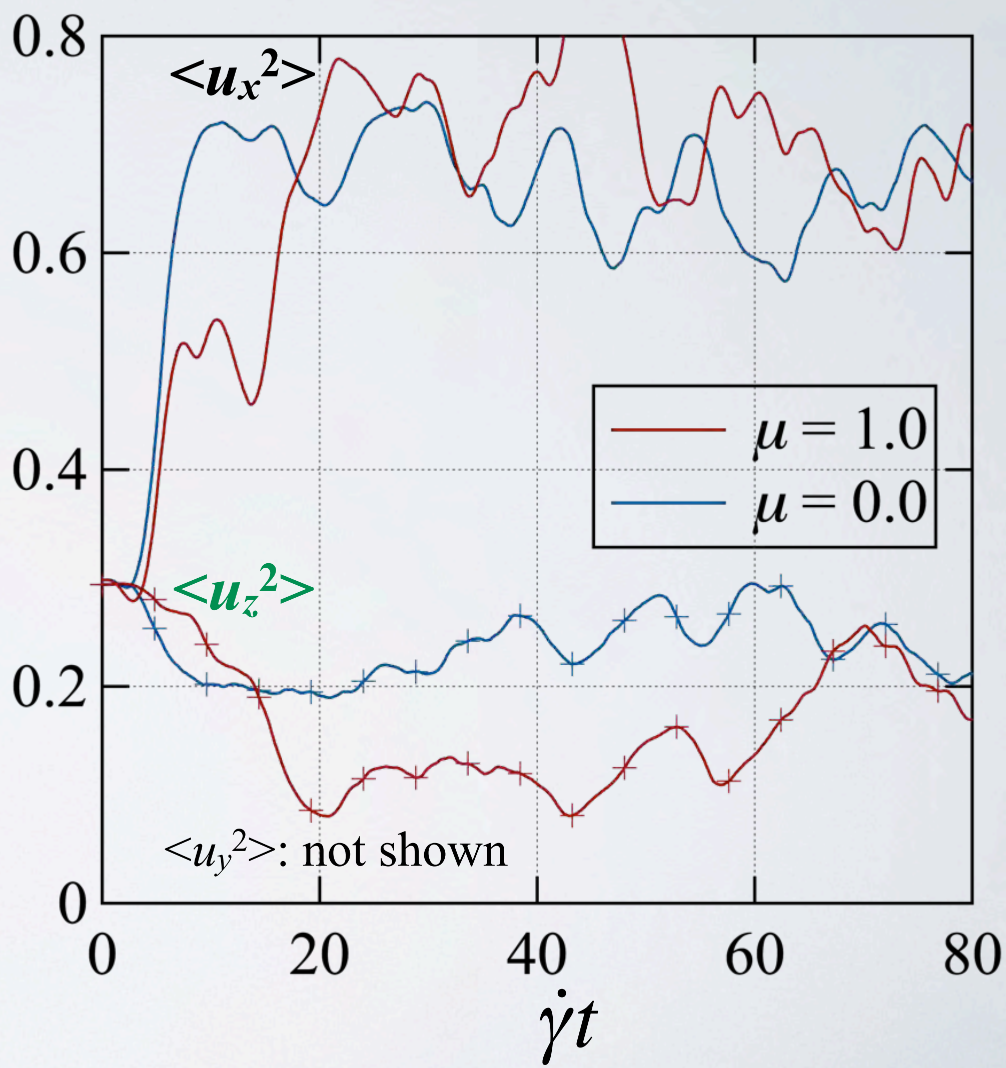
Orientation



$A = 1.0\times10^{-20}$



$A = 3.5\times10^{-20}$



Concluding Remarks

- DNS enable us to observe the detailed breakup process of the aggregate
- Friction should not be neglected for a relatively strong attractive system
- Friction acts nonlinearly on dispersion & orientation of rods
- Future work (i) : fracture of rods inside aggregate
- Future work (ii): its fracture mechanism of rods