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Direct Numerical Simulation of the Dynamics of Colloidal Particles with Adsorptive Solute Transport

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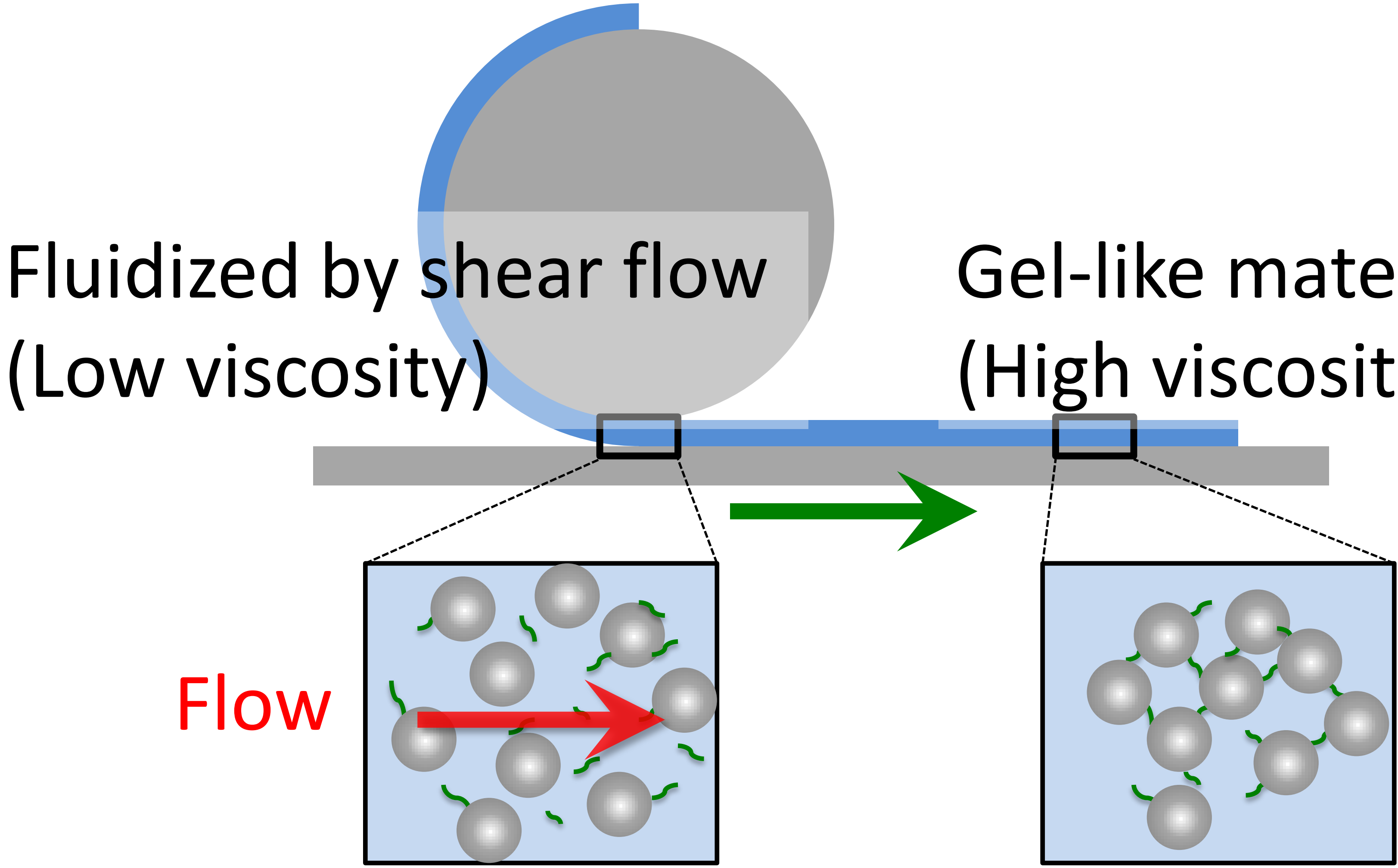
Purpose

- Coating of colloidal suspension with polymer additives

Colloidal particles are bridged by polymers to form weak floc (thixotropic paint).

- Construction of a direct simulation model for colloidal suspensions with adsorptive solutes
- Simulation of colloid-polymer suspension in a fluid flow

Coating of thixotropic paint



Fluidized by shear flow
(Low viscosity)

Gel-like material
(High viscosity)

Flow

Dispersion

Flocculation

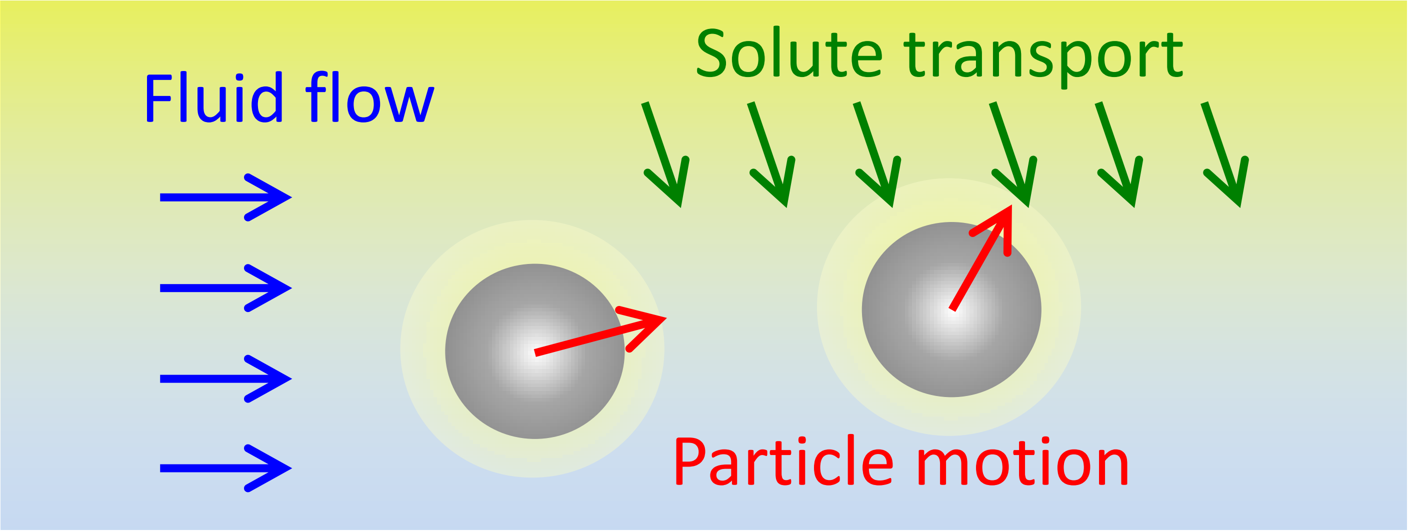
Modeling

Model Spherical particles in a Newtonian fluid containing a single solute species

Governing equations

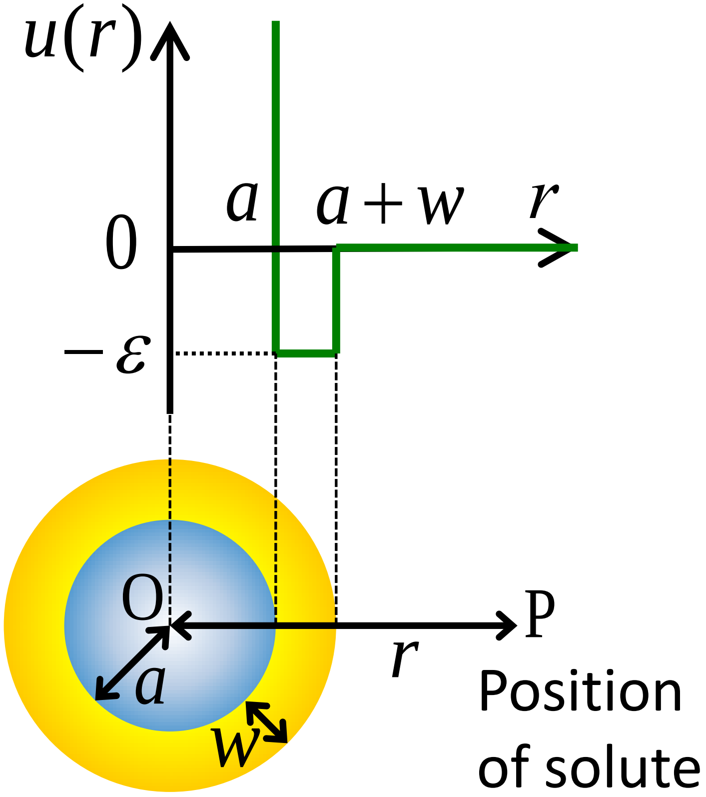
Temporal evolutions of

- Colloidal particles
- Fluid flow field
- Solute concentration field



Model of adsorption

Particle-solute interaction: Square-well potential



$$u(r)=\begin{cases}\infty & r<a\\ -\varepsilon & a\le r<a+w\\ 0 & r\ge a+w\end{cases}$$

Adsorption energy: $\beta\varepsilon=\varepsilon/RT$

Thickness of adsorption layer: w

Governing equations

Concentration

$$\frac{\partial c}{\partial t}+\nabla\cdot(c\boldsymbol{v})=-\nabla\cdot\boldsymbol{J}$$

Diffusion flux

B.C. on diffusion flux

- Impermeability
- Adsorption

to particles

Flow

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

$$\rho\left(\frac{\partial\boldsymbol{v}}{\partial t}+\boldsymbol{v}\cdot\nabla\boldsymbol{v}\right)=-\nabla p+\eta\nabla^2\boldsymbol{v}+\underline{\rho\Phi\boldsymbol{a}}-\underline{c\nabla U_{\mathrm{ad}}}-\nabla\pi$$

Constraint of particle velocities

Particle-solute interaction

Osmotic pressure

Total momentum conserved

Particles

$$M_i\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{V}_i=\underline{\boldsymbol{F}_i^H}+\underline{\boldsymbol{F}_i^S}$$

$$\boldsymbol{I}_i\cdot\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Omega}_i=\underline{\boldsymbol{N}_i^H}$$

Hydrodynamic force/torque

$$\boldsymbol{F}_i^H=-\int\rho\Phi\boldsymbol{a}\mathrm{d}\boldsymbol{r}\quad\boldsymbol{N}_i^H=-\int(\boldsymbol{r}-\boldsymbol{R}_i)\times\rho\Phi\boldsymbol{a}\mathrm{d}\boldsymbol{r}$$

Particle-solute interaction

$$\boldsymbol{F}_i^S=\int c\nabla U_{\mathrm{ad}}\mathrm{d}\boldsymbol{r}$$

Equation (Concentration)

Concentration

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\boldsymbol{v}) = -\nabla \cdot \boldsymbol{J}$$

Osmotic pressure

$$\pi = RT(\Xi - 1)c^*$$

Diffusion flux

$$\boldsymbol{J} = -D\underline{(1-\Phi)\Xi}\nabla \underline{c^*}$$

Indicator functions

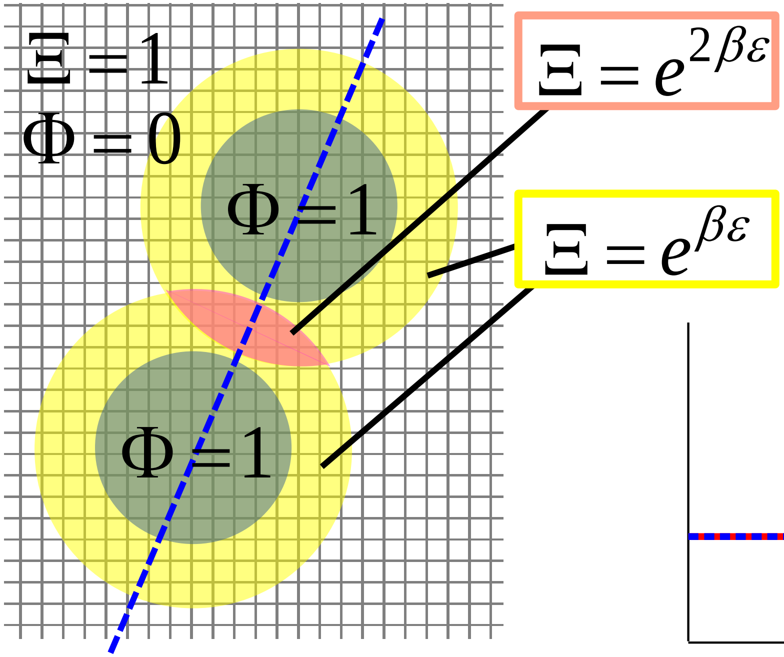
Φ : Particle domain

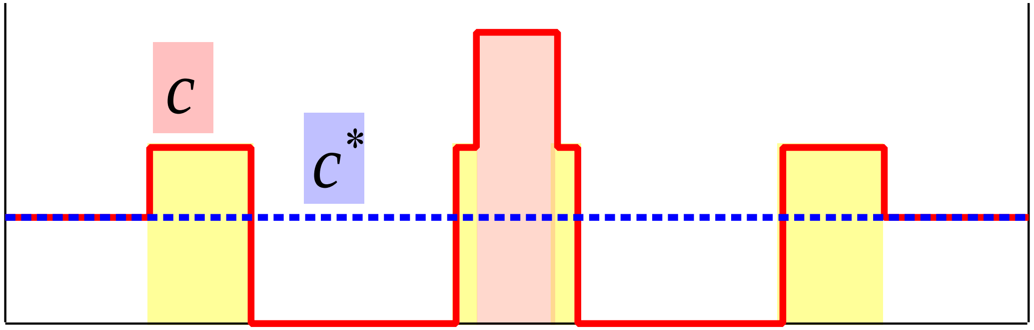
$\Xi = \exp(n\beta\varepsilon)$: Adsorption layer

n : Overlapping number

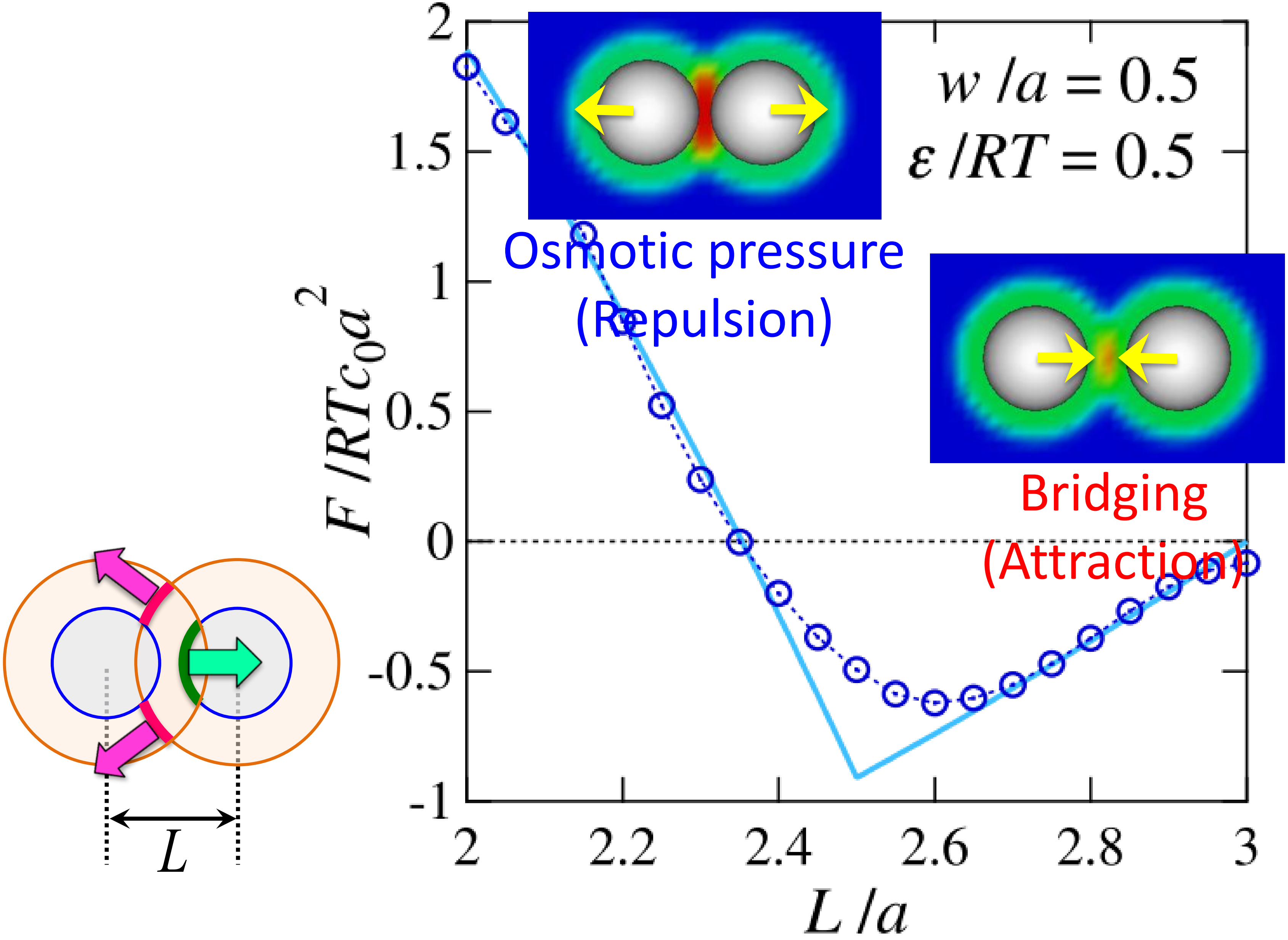
$$c = (1-\Phi)\Xi\underline{c^*}$$

Virtual concentration field





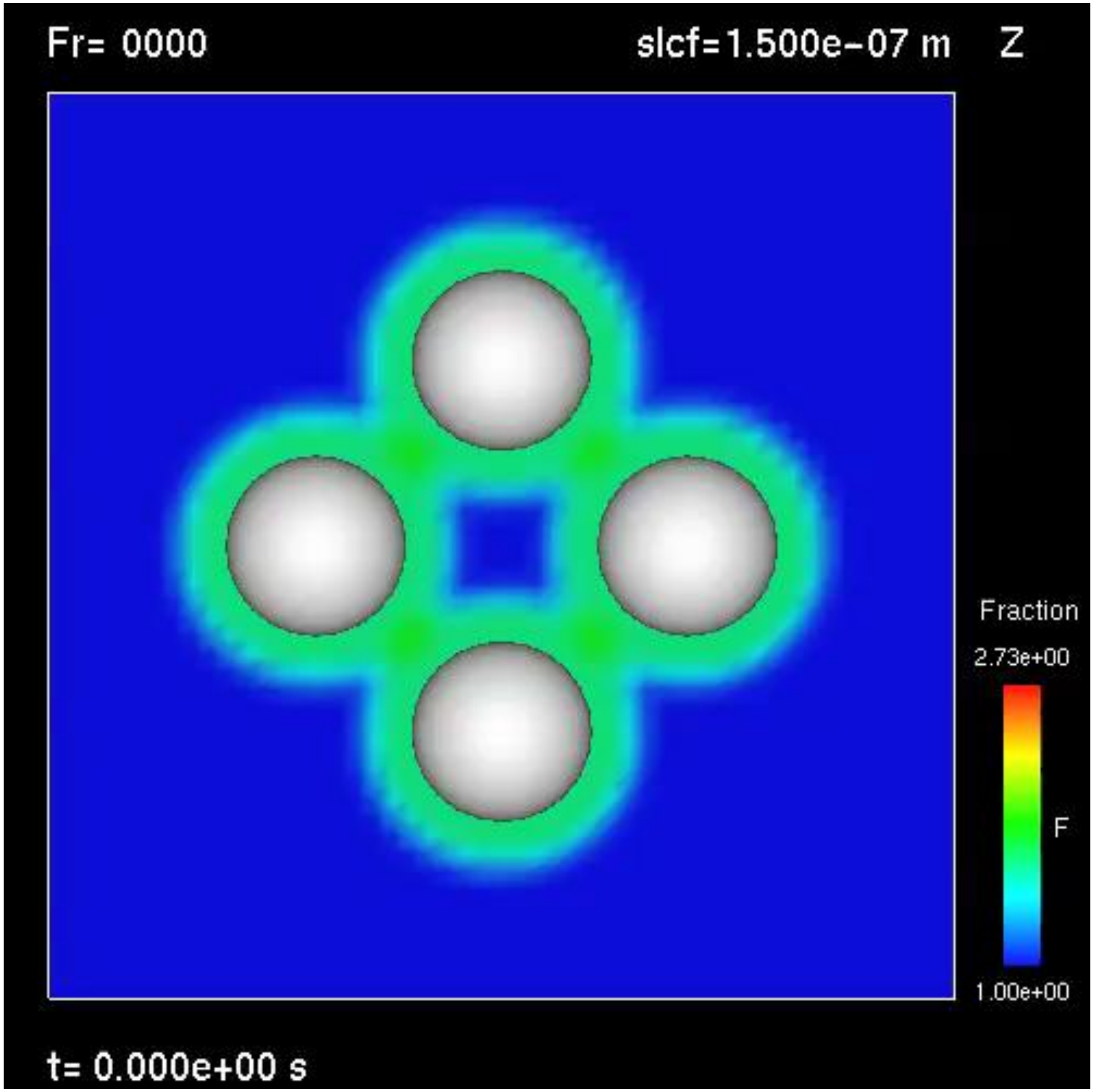
Interparticle Force



Osmotic pressure
(Repulsion)

Bridging
(Attraction)

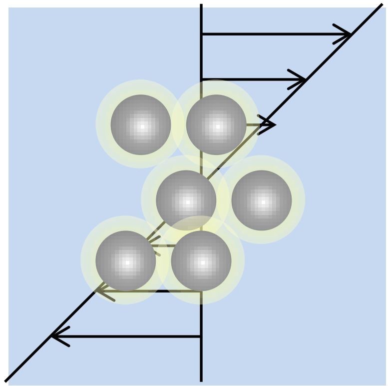
Weak Flocculation



Weak flocculation in shear flow

Stresses acting on a particle

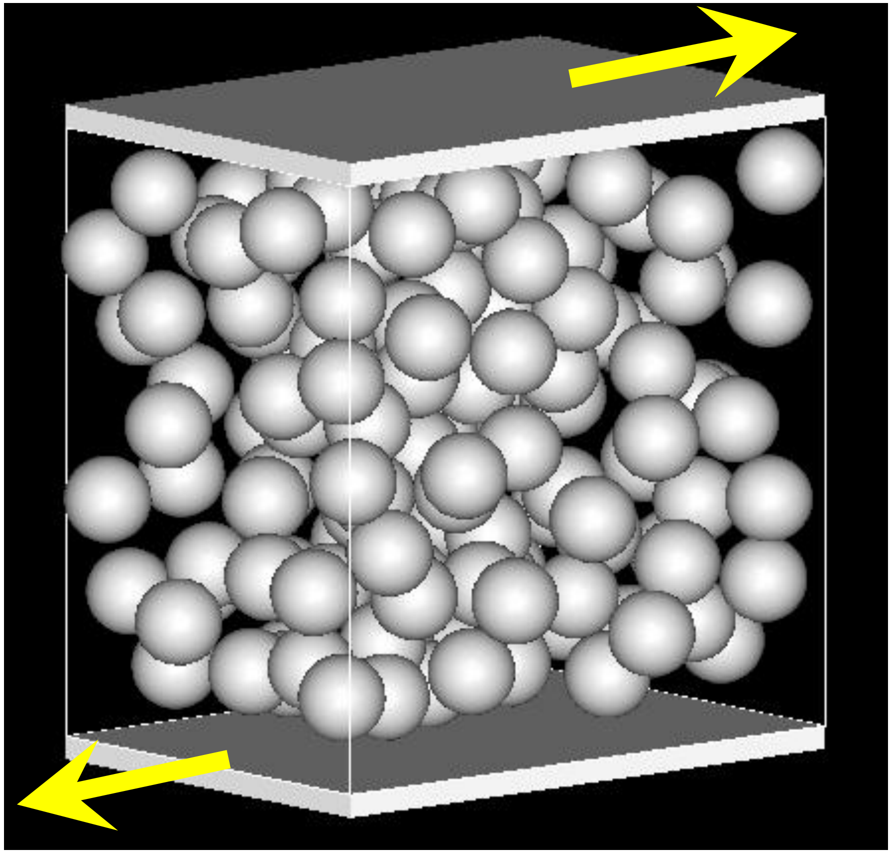
- Fluid shear flow : $\sigma_H \sim \eta\dot{\gamma}$
- Solute adsorption : $\sigma_S \sim c_0 RT$

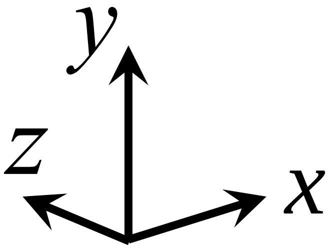


$$\Theta \equiv \frac{\eta\dot{\gamma}}{c_0 RT} \sim \frac{\sigma_H}{\sigma_S}$$

Ratio of stresses

Simulation domain





- System size

$$7d \times 7d \times 5d$$

d : Particle diameter

Periodic boundary on x, z directions

Simulation conditions

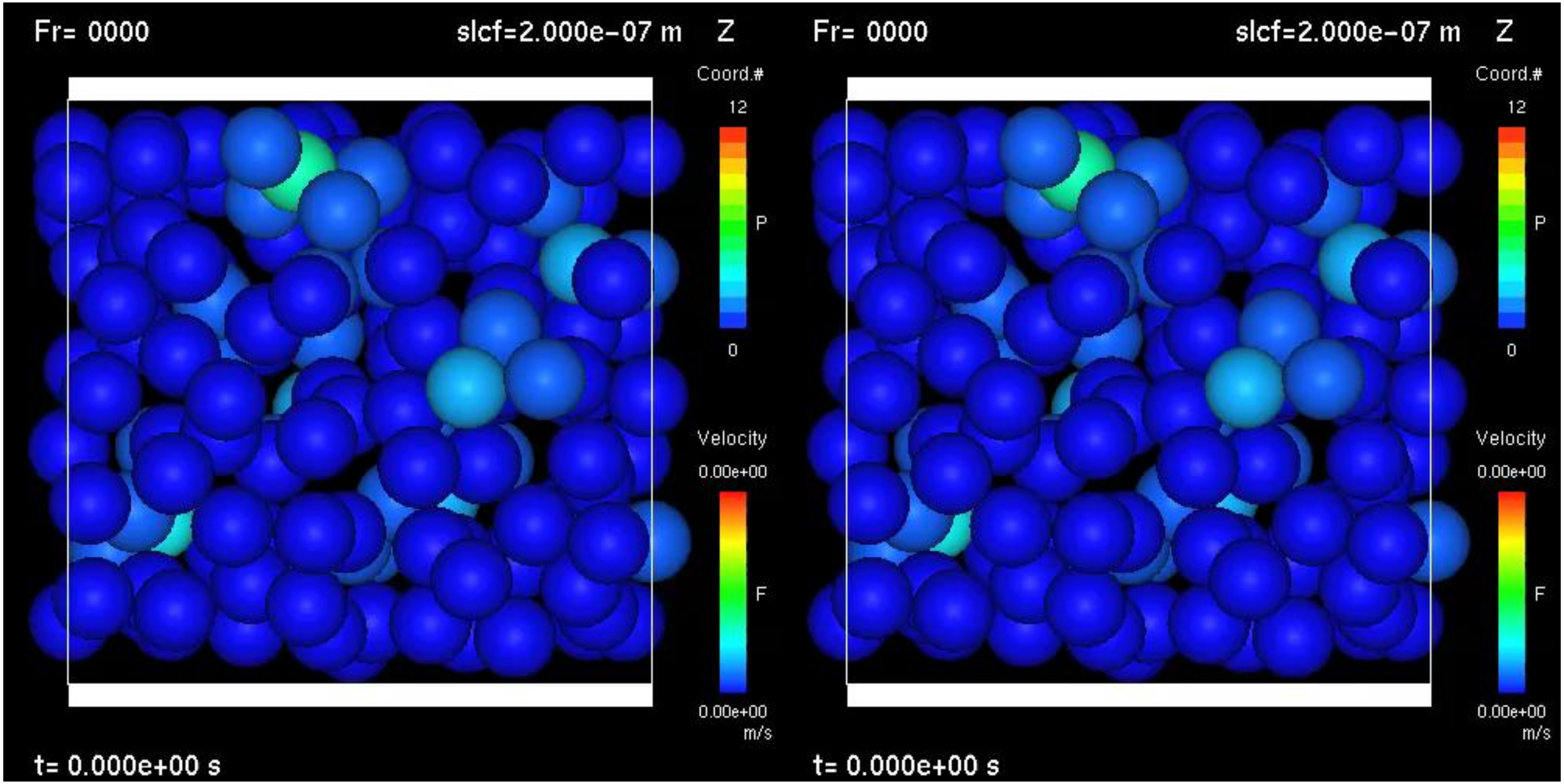
Particle

- Volume fraction $\phi = 30\ \mathrm{vol.\%}$
- Adsorption layer thickness $w/d = 0.25$
- Adsorption energy $\beta\varepsilon = 0.5$

Fluid

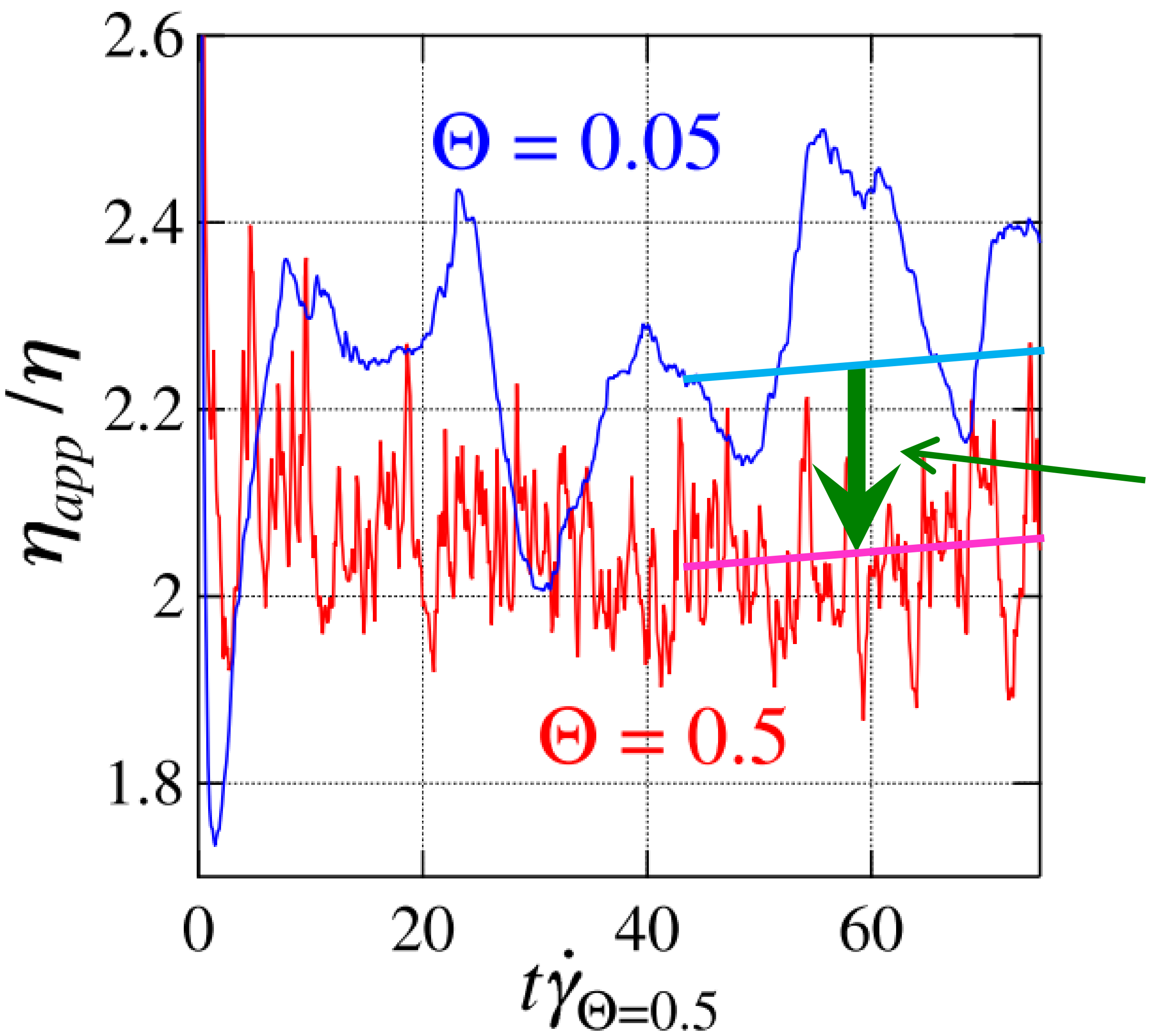
- Schmidt number $\mathrm{Sc} = \eta/\rho D = 10$
- Ratio of stresses $\Theta = 0.05,\ 0.5$

Simulation results



$\Theta = 0.05$ $\Theta = 0.5$

Viscosity



$$\frac{\eta_{app}}{\eta} = \frac{1}{\dot{\gamma}} \left| \frac{\partial v_x}{\partial y} \right|_{wall}$$

Breakup of floc

Time variation ← Particle structure change

Summery

- Direct simulation model of colloidal suspensions with adsorptive solute is constructed.

- By the present model of solute adsorption, weak flocculation in flow field is described.

- As shear stress is increased, floc is broken to decrease viscosity.

Outlook for Application

- Drying and concentration process of colloid-polymer suspensions