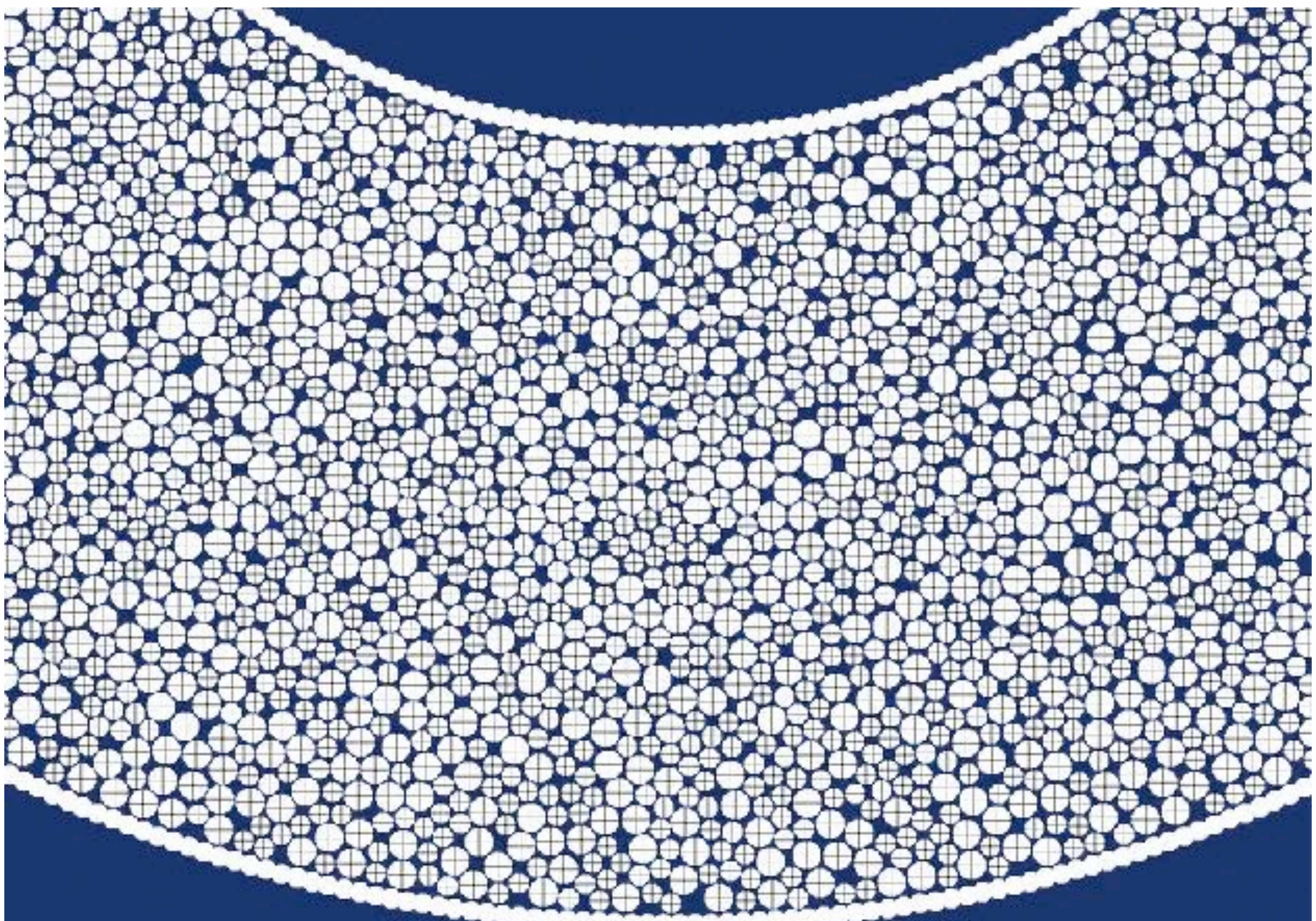
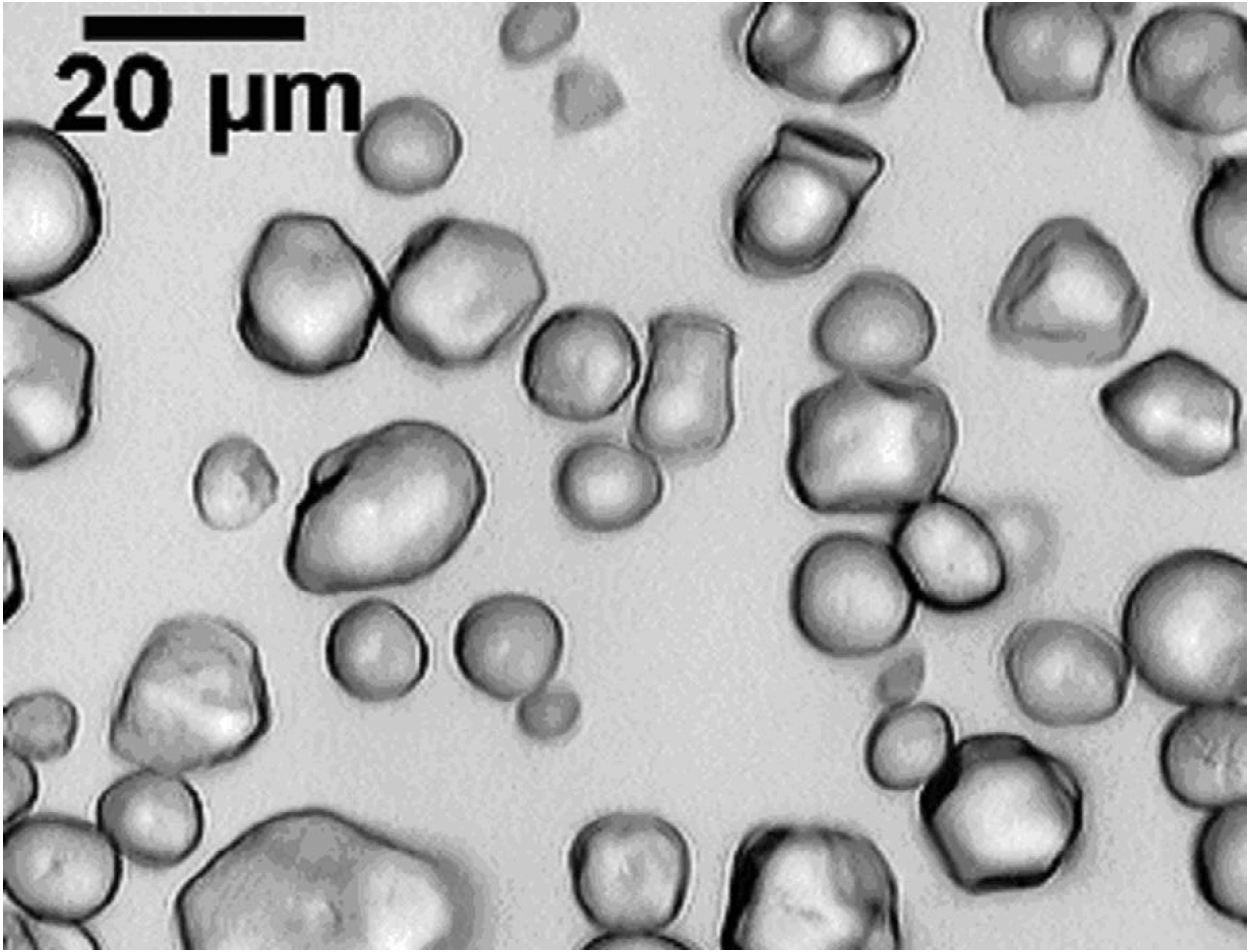
Migration and jamming in wide-gap Couette flows of dense suspensions

Ryohei Seto
Kyoto University, Dept. of Chemical Engineering

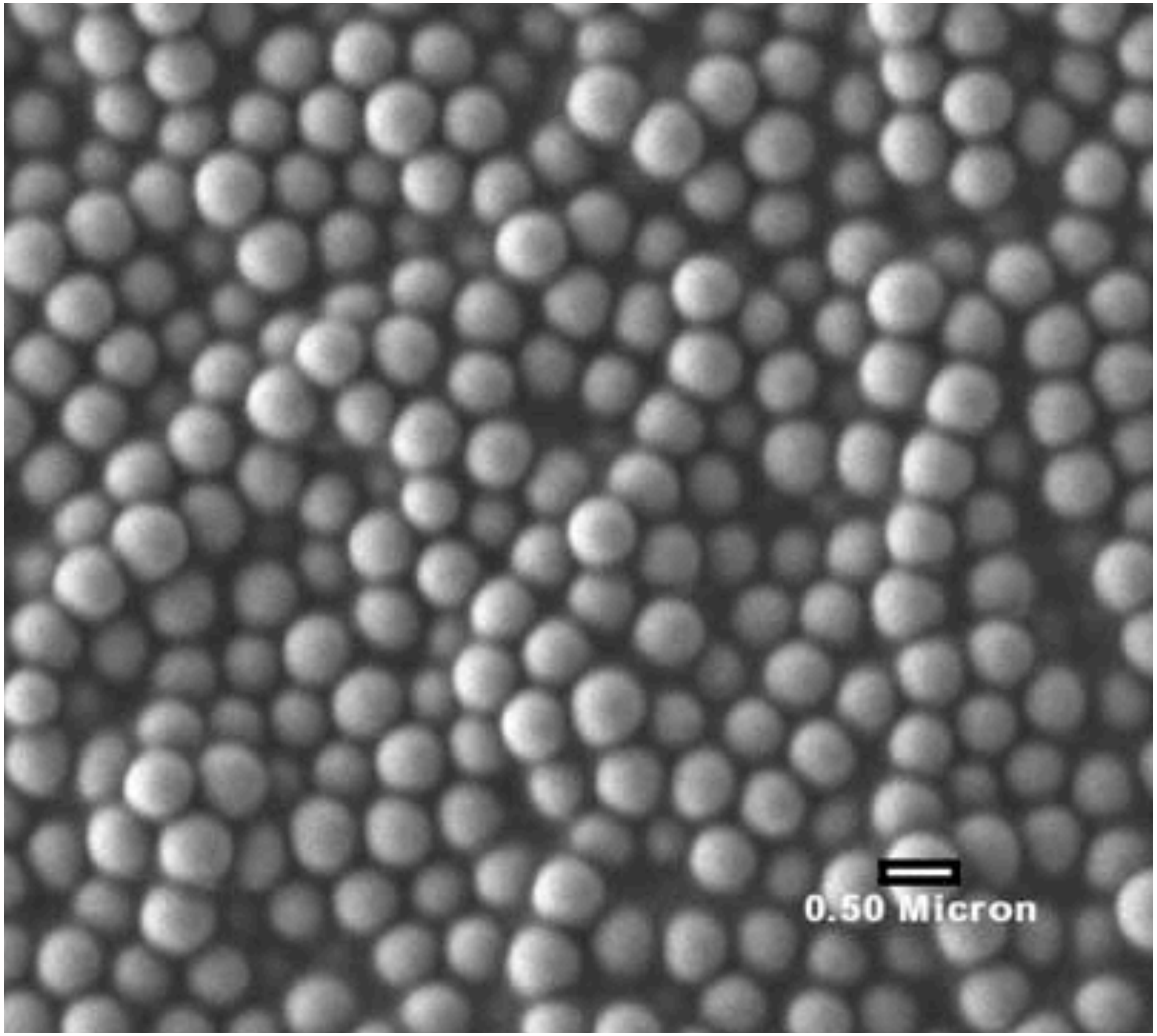


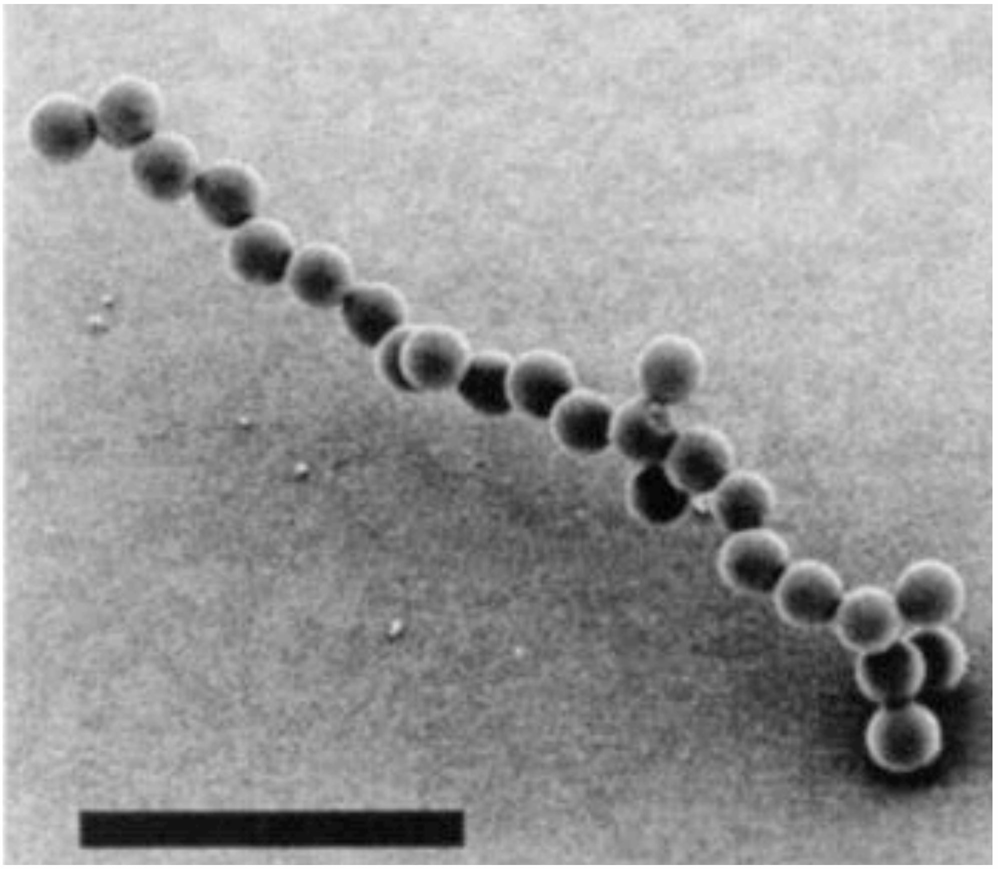
- Introduction—a bit of history
- Modeling strategy to capture dynamics of colloids (Modified Stokesian Dynamics)
- Flow in a Widegap Couette cell

Cornstarch



Silica





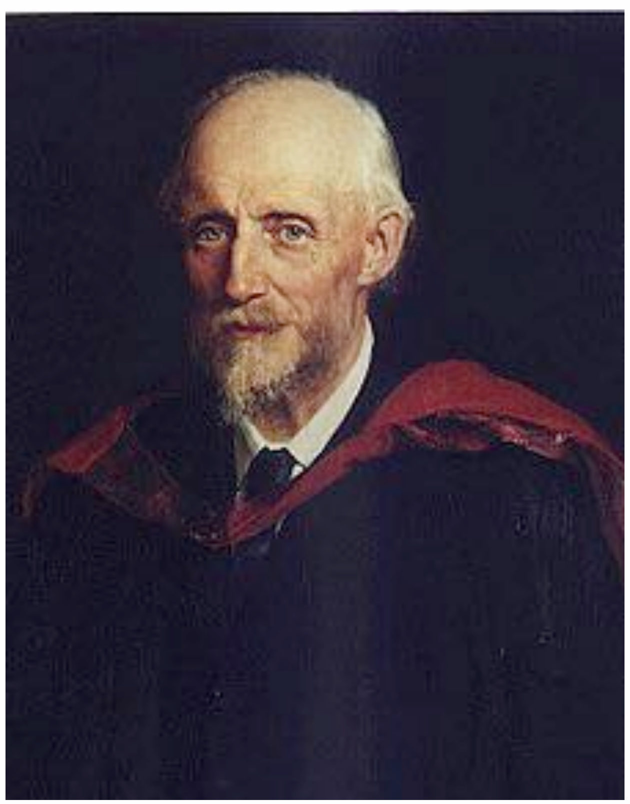
10 $[\mu m]$

0.5 $[\mu m]$

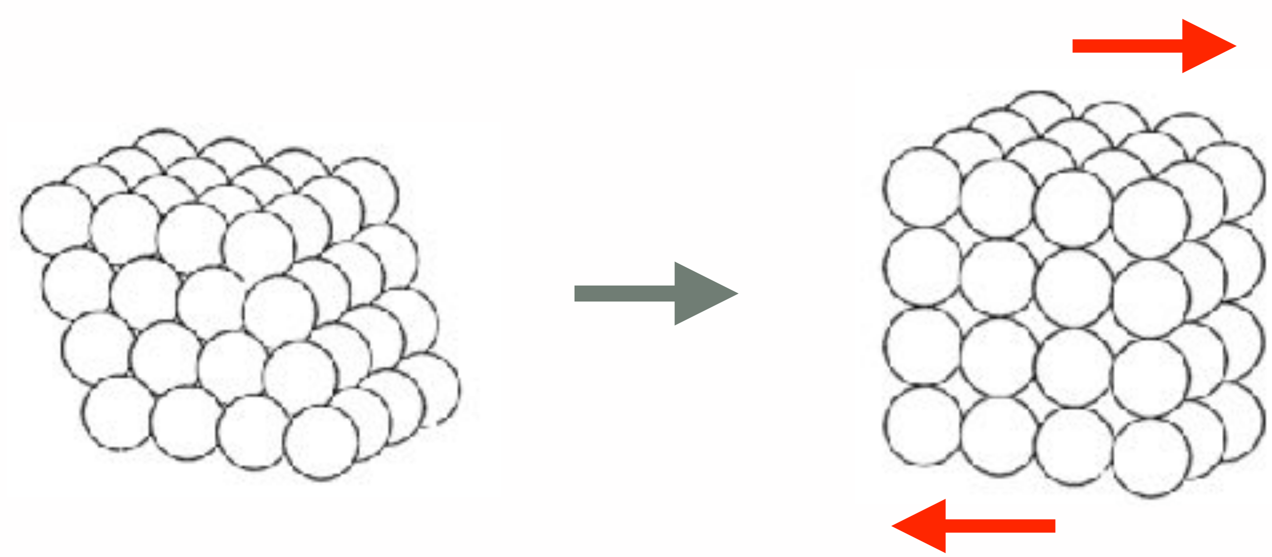
“On the dilatancy of media composed of rigid particles in contact”

Reynolds 1885

“If in any way the volume be fixed, then all change of shape is prevented.”



from wikipedia



“Experiments on a gravity-free dispersion of large solid spheres in a Newtonian fluid under shear”

Bagnold 1954

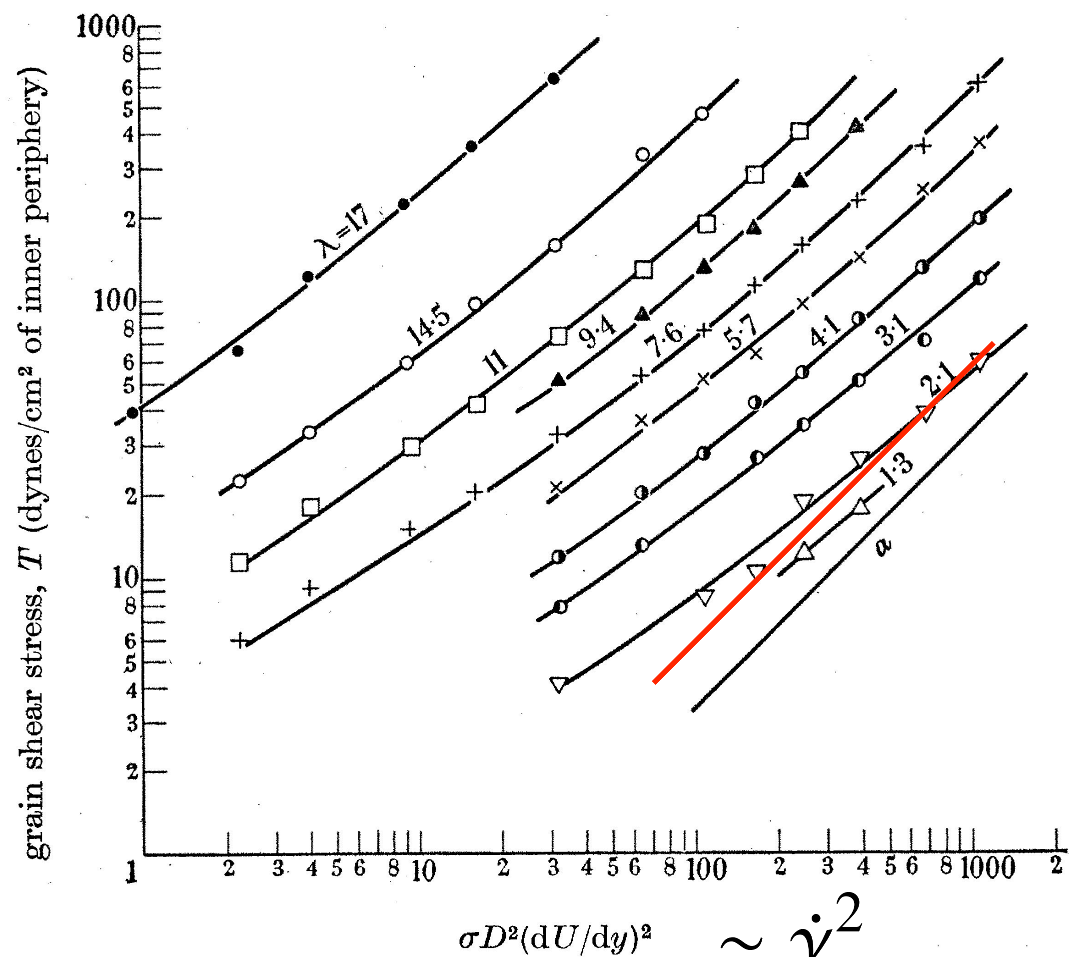
spherical droplets of mixture of paraffin wax and lead stearate ($\sim 1.32\,\mathrm{mm}$)

When shear rate $\dot{\gamma}$ is low, shear stress $\propto \dot{\gamma}$ viscous effect of solvent

When shear rate $\dot{\gamma}$ is high, shear stress $\propto \dot{\gamma}^2$ particle inertia

from wikipedia

Shear stress



$\sim \dot{\gamma}^2$

Hydrodynamic theory

Einstein 1906

$$\eta = \eta_0(1 + 2.5\phi) \text{ for } \phi \ll 1$$

from wikipedia

Batchelor & Green 1972

$$\eta \approx \eta_0(1 + 2.5\phi + 6.9\phi^2)$$

two-body problem

one-body problem

Hydrodynamic simulation

from http://www.che.caltech.edu

Stokesian Dynamics

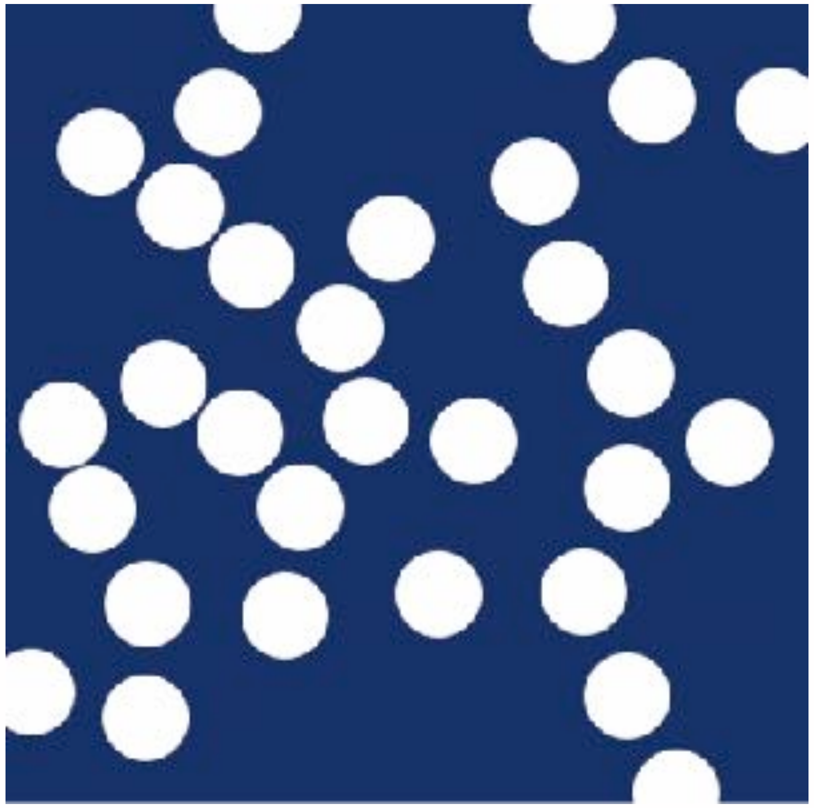
Brady & Bossis 1985

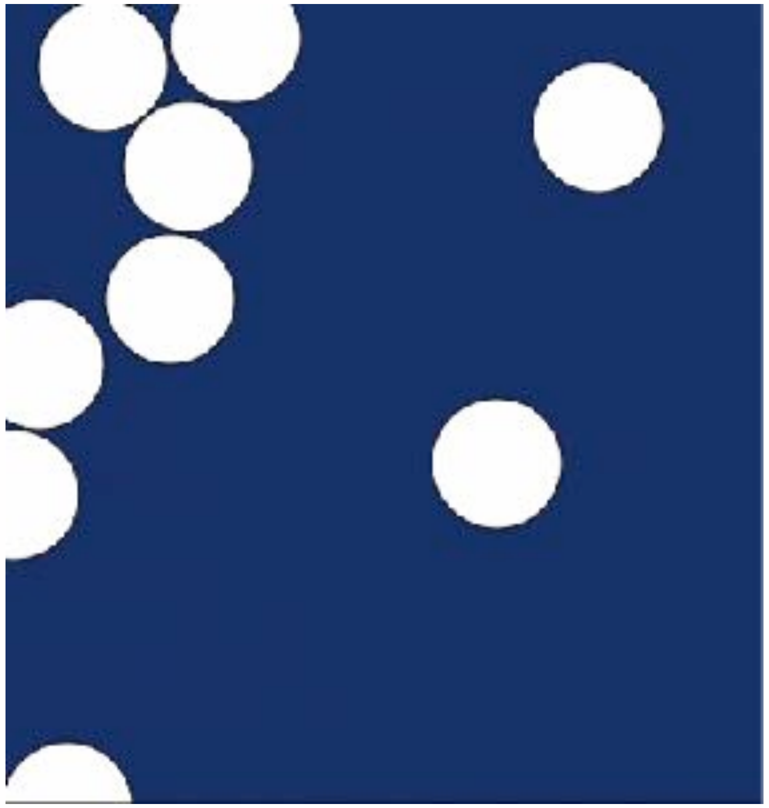
6*N*-dimensional overdamped Langevin eq.

$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{B}} = 0$$

$$\boldsymbol{F}_{\mathrm{H}} = -\boldsymbol{R} \cdot (\boldsymbol{U} - \boldsymbol{u}) + \boldsymbol{R}' : \boldsymbol{D}$$

$$\boldsymbol{u}(\boldsymbol{r}) = \nabla \boldsymbol{u} \cdot \boldsymbol{r} = \boldsymbol{D} \cdot \boldsymbol{r} + (\boldsymbol{\omega}/2) \times \boldsymbol{r}$$





- Introduction—a bit of history
- Modeling strategy to capture dynamics of colloids (Modified Stokesian Dynamics)
- Flow in a Widegap Couette cell

Mechanical properties of fluid materials

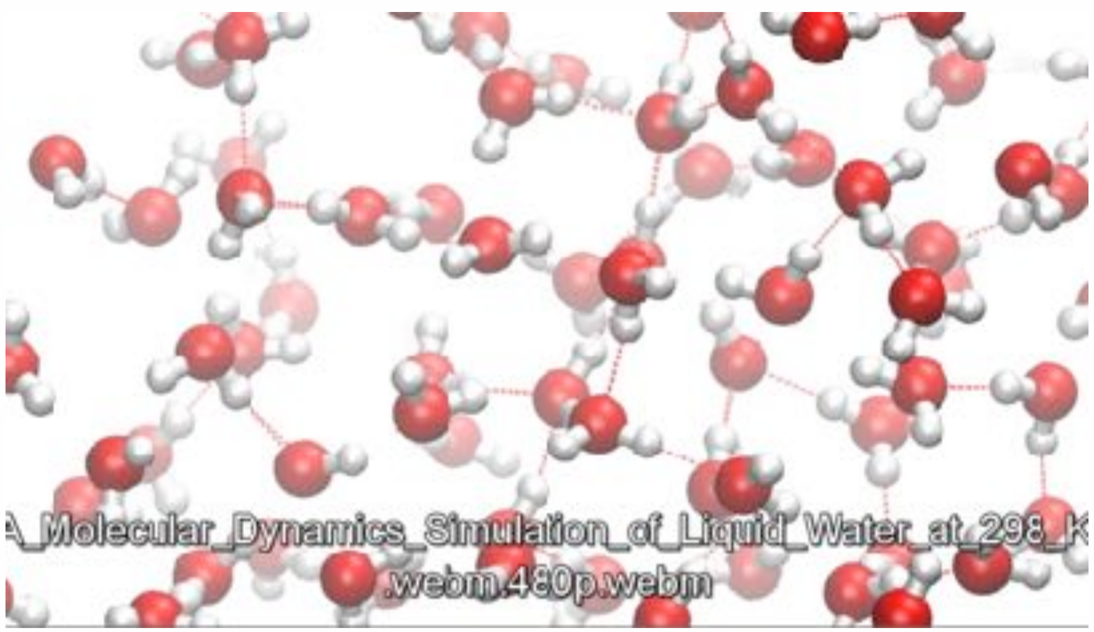
Liquid

Newtonian

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta\boldsymbol{D}$$

$$\boldsymbol{D} \equiv \frac{1}{2}\left(\nabla\boldsymbol{u}[\boldsymbol{r}(t), t] + \nabla\boldsymbol{u}^{\mathrm{T}}[\boldsymbol{r}(t), t]\right)$$

Molcular dynamics



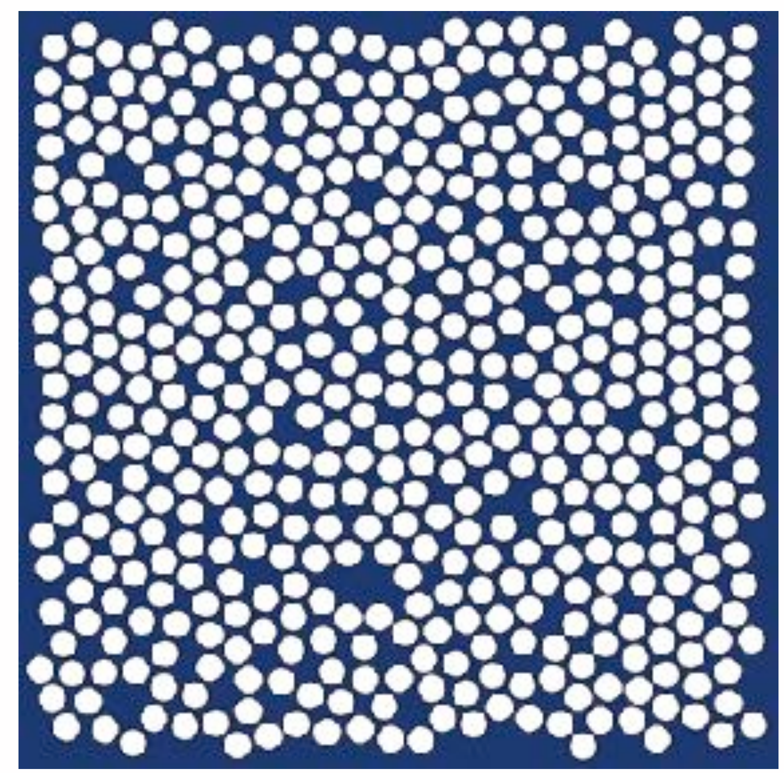
$$\frac{\textbf{mean free path}^2}{\textbf{velocity}} \sim 10^{-11}\ [\mathrm{s}]$$

Suspensions

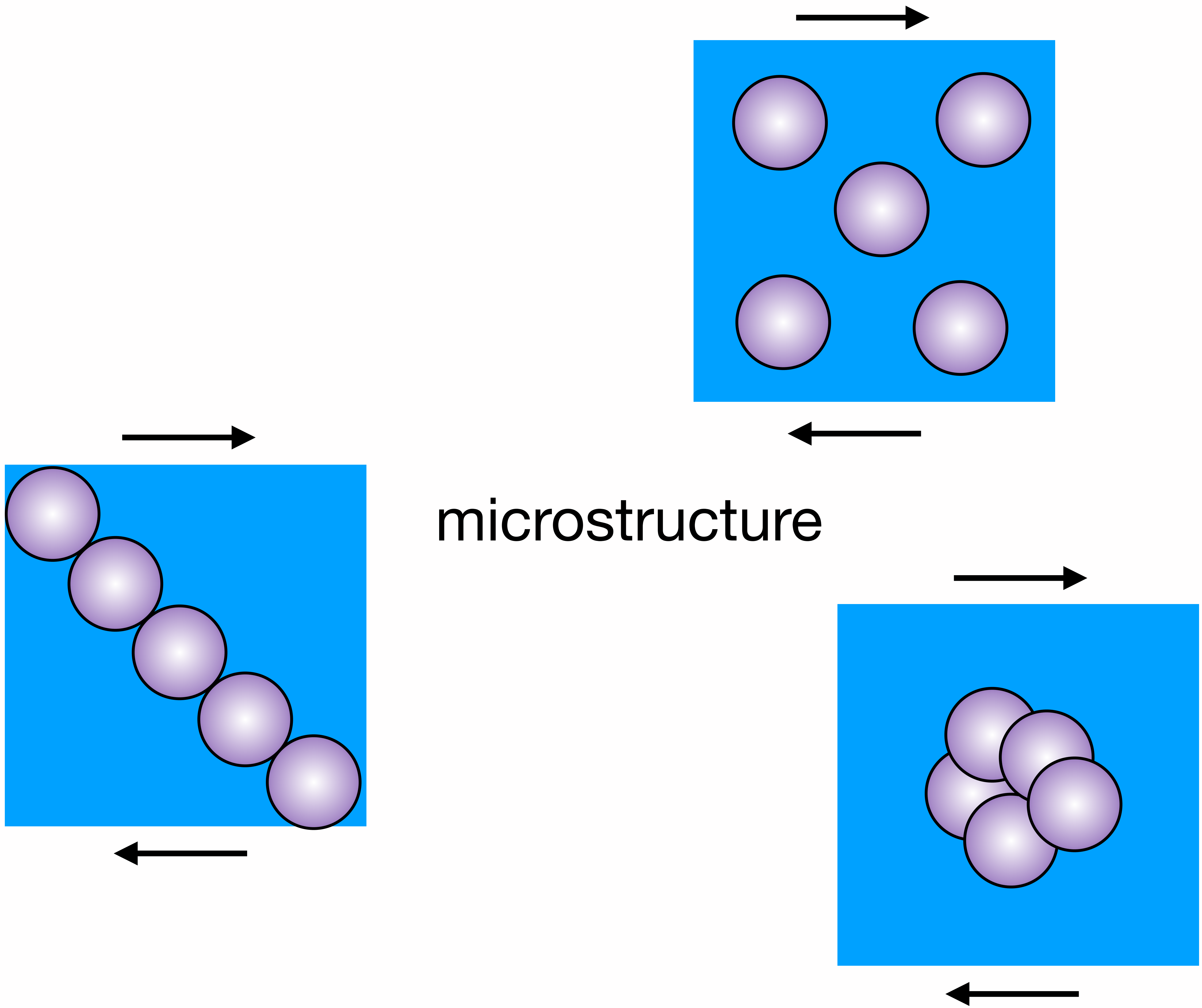
Non-Newtonian

?

Stokesian dynamics



$$\frac{\textbf{radius}^2}{\textbf{diffusion constant}} \sim 1\ [\mathrm{s}]$$


microstructure

Rheology

$$\rho\left\{\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right\} = \nabla\cdot\boldsymbol{\sigma}$$

Constitutive modeling

velocity gradient

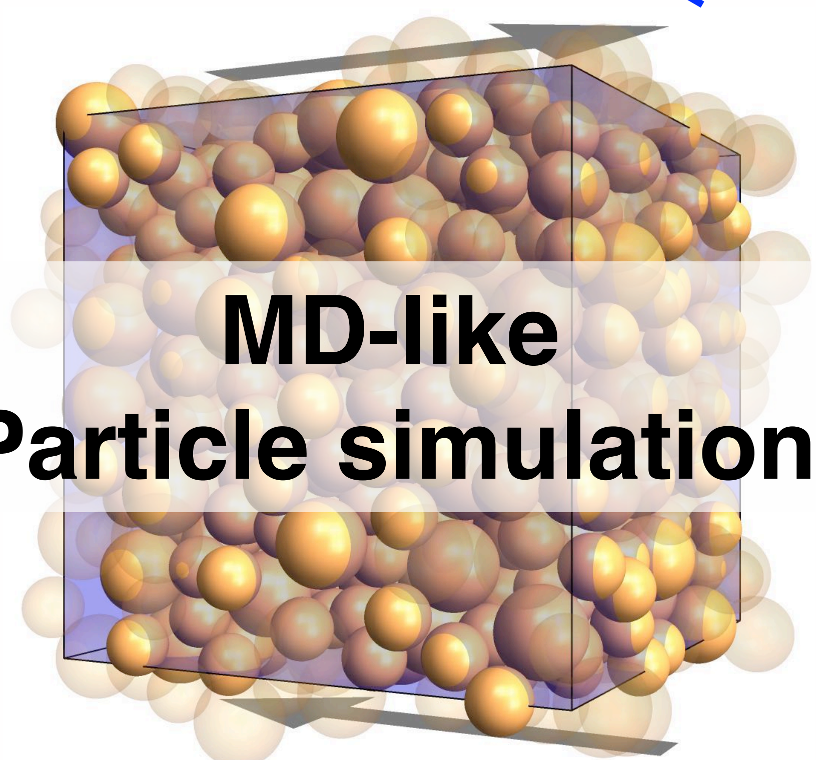
$$\begin{pmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_x}{\partial y} & \frac{\partial u_x}{\partial z} \\ \frac{\partial u_y}{\partial x} & \frac{\partial u_y}{\partial y} & \frac{\partial u_y}{\partial z} \\ \frac{\partial u_z}{\partial x} & \frac{\partial u_z}{\partial y} & \frac{\partial u_z}{\partial z} \end{pmatrix}$$

stress tensor

$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix}$$

impose

response



material functions

scalars

(*not* coordinate specific)

physical interpretations

$$\eta(\dot{\gamma}),\ N_1(\dot{\gamma}),\ N_2(\dot{\gamma})$$

Zero-Reynolds number hydrodynamics

Navier-Stokes equations (non-linear)

$$Re\left\{\frac{\partial \overrightarrow{u}}{\partial t} + (\overrightarrow{u}\cdot\nabla)\overrightarrow{u}\right\} = -\nabla p + \nabla^2\overrightarrow{u}$$

$$Re \equiv \frac{\rho_0 a^2 \dot{\gamma}}{\eta_0} \to 0$$

Stokes equations (linear)

$$\overrightarrow{0} = -\nabla p + \nabla^2\overrightarrow{u}$$

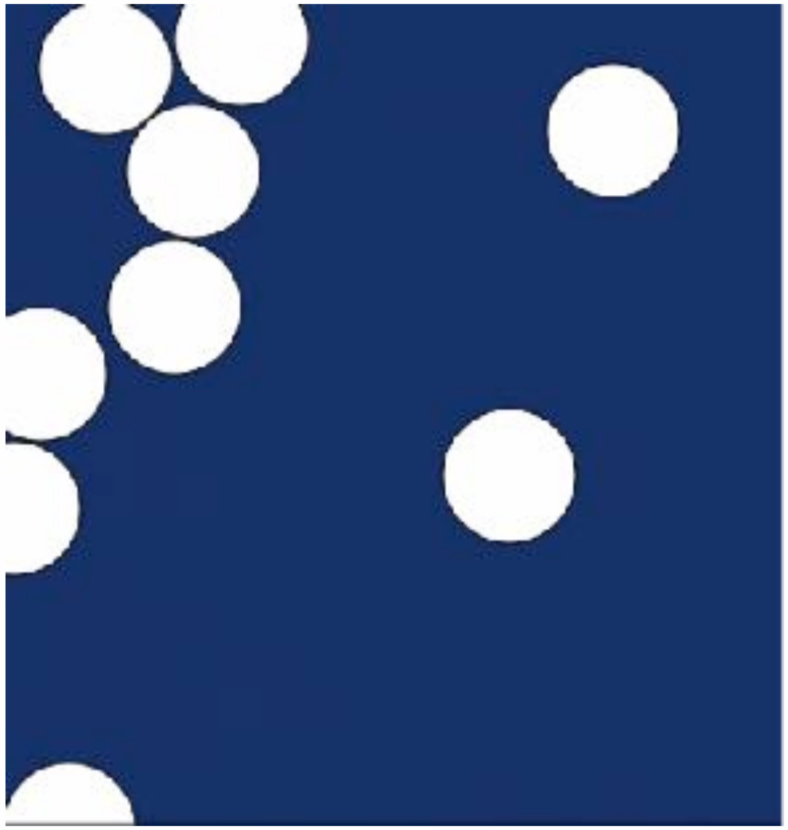
Hydrodynamic interactions

(6 *N* dimension)

$$\boldsymbol{F}_{\mathrm{H}} = -\boldsymbol{R}\cdot(\boldsymbol{U}-\boldsymbol{u}) + \boldsymbol{R}' : \boldsymbol{D}$$

$$\boldsymbol{u}(\boldsymbol{r}) = \nabla\boldsymbol{u}\cdot\boldsymbol{r} = \boldsymbol{D}\cdot\boldsymbol{r} + (\boldsymbol{\omega}/2)\times\boldsymbol{r}$$

cf. Stokes drag $\mathrm{R} = 6\pi\eta_0 a\mathrm{I}$



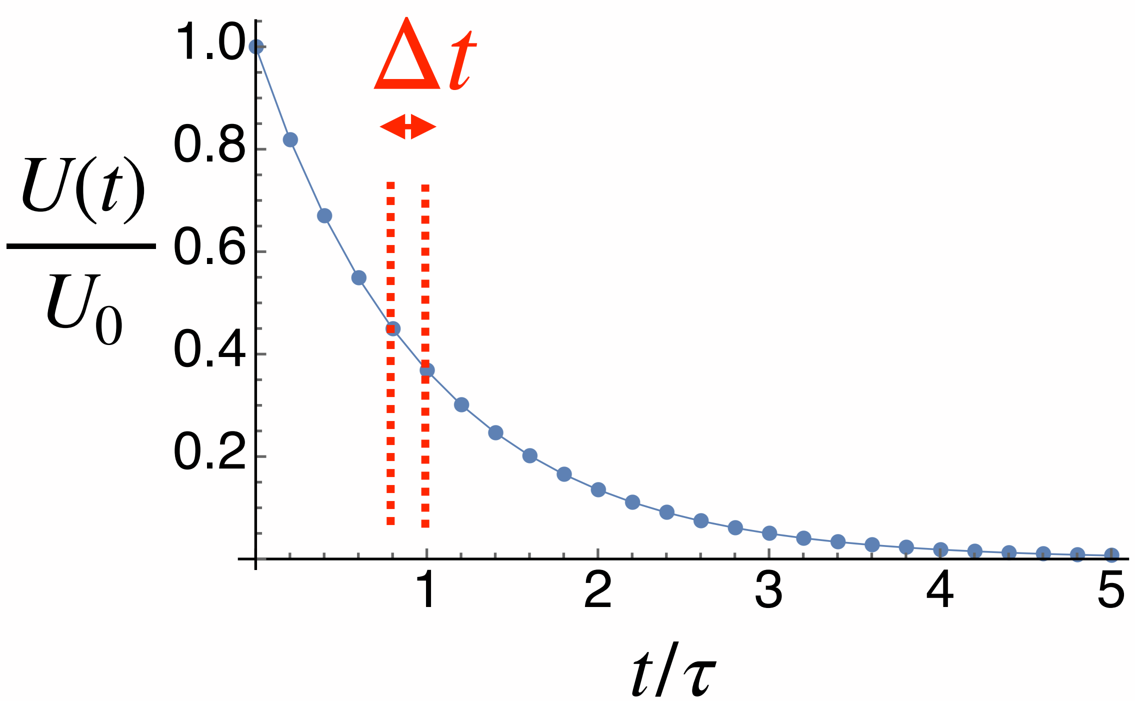
Newtonian dynamics vs. Overdamped dynamics

$$m\frac{dU}{dt} = -6\pi\eta_0 a U$$

$$U(t) = U_0 \exp(-t/\tau)$$

time step for numerical integration

$$\Delta t \ll \tau$$

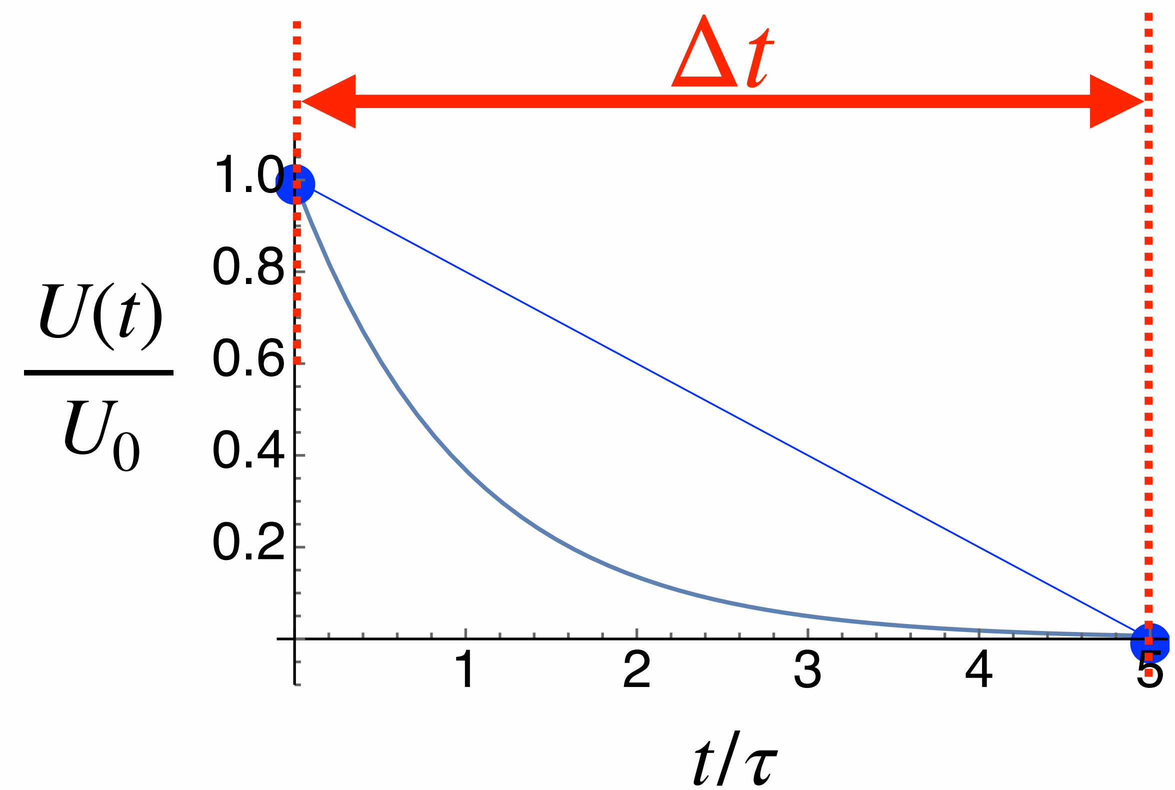


$$0 \rightarrow m\frac{dU}{dt} = -6\pi\eta_0 a U$$

$$U(0) = U_0$$

$$U(\Delta t) = 0$$

$$\Delta t \gg \tau$$



$\eta_0 = 0.001$ [Pa s]
$a = 1$ [μm]
$\rho = 1000$ [kg/m^3]

$$\rightarrow \tau = \frac{m}{6\pi\eta_0 a} \approx 2 \times 10^{-7} \text{ [s]}$$

cf. time-scale of shear flow

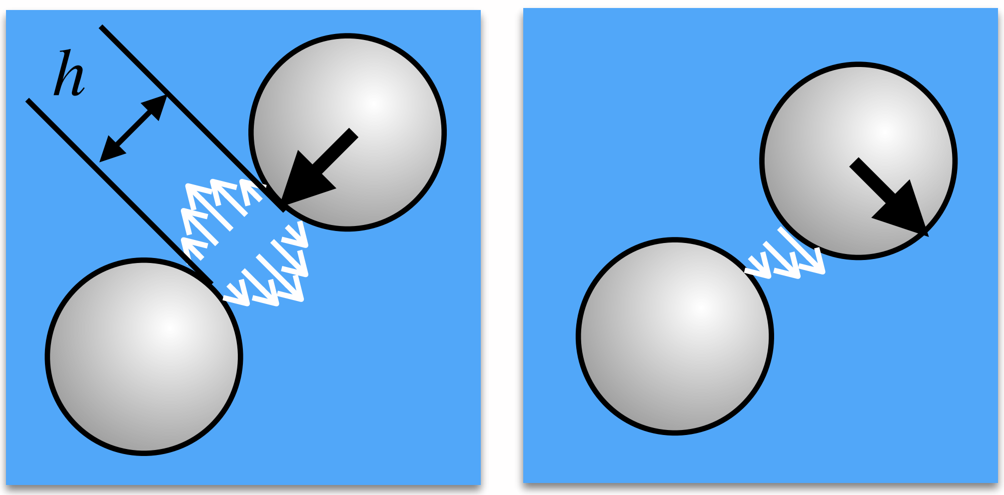
$$\tau_{\text{shear}} = 1/\dot{\gamma}$$

Purely hydrodynamic suspensions

force balance eq. $\boldsymbol{F}_{\mathrm{H}} = \boldsymbol{0}$

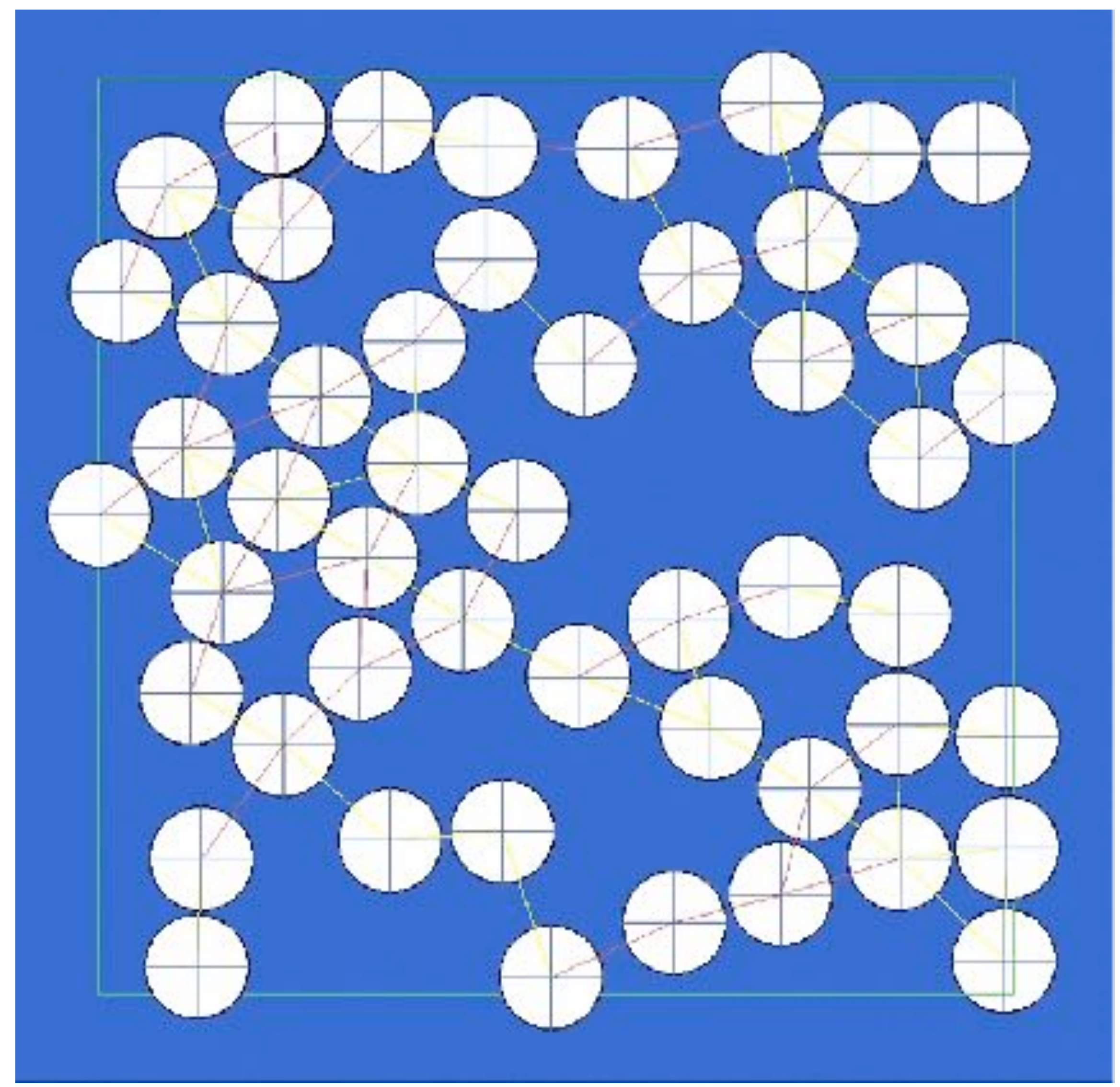
hydrodynamic interaction $\boldsymbol{F}_{\mathrm{H}} = -\mathsf{R} \cdot (\boldsymbol{U} - \boldsymbol{u}) + \mathsf{R}' : \mathsf{D}$

Perfect reversibility, if lubrication layers can remain.

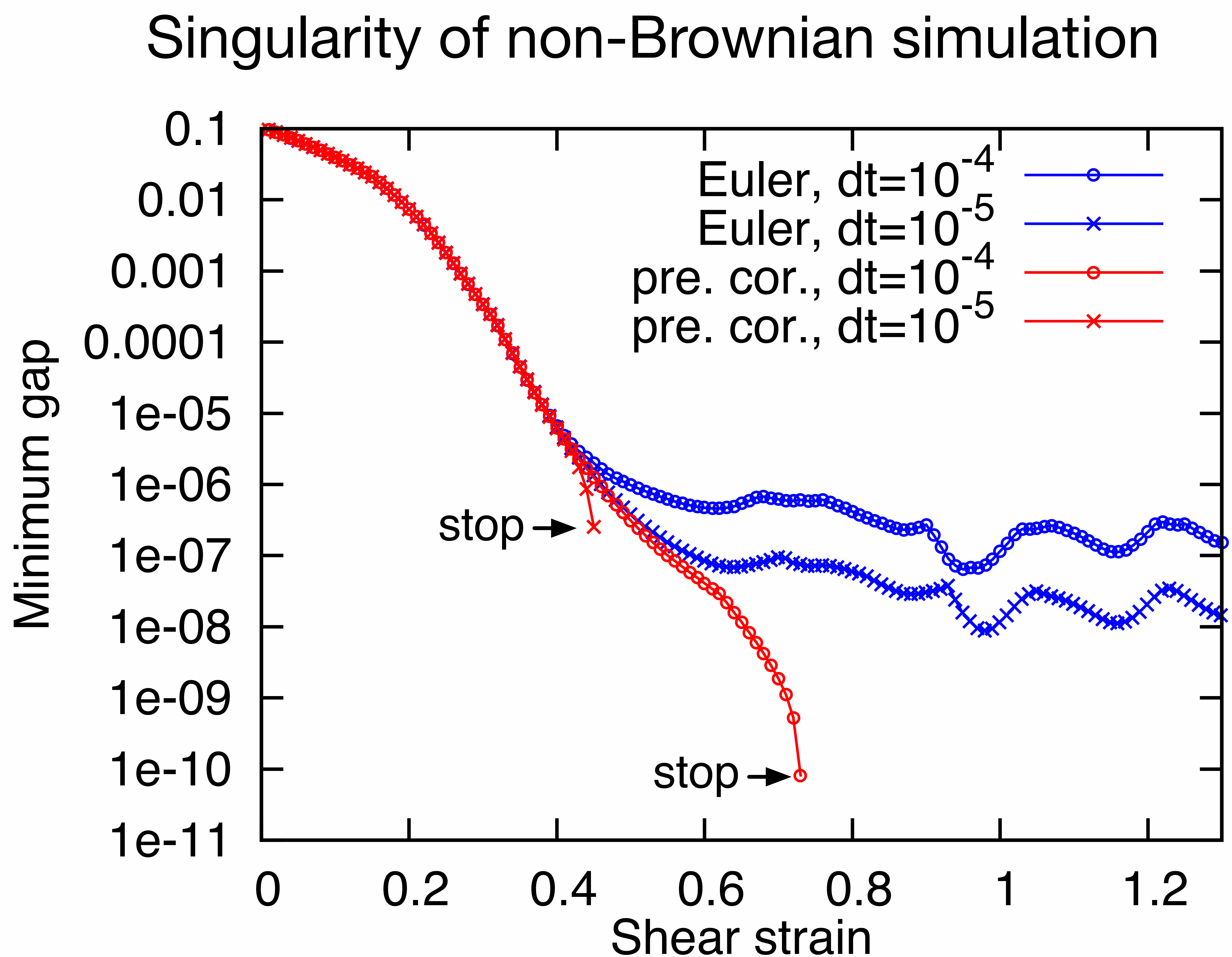


$$F_{\mathrm{Lub}}^{(\mathrm{nor})} \sim -\frac{1}{h} \Delta U^{(\mathrm{nor})}$$

$$F_{\mathrm{Lub}}^{(\mathrm{tan})} \sim -\log\left(\frac{1}{h}\right) \Delta U^{(\mathrm{tan})}$$



shear reversal demo

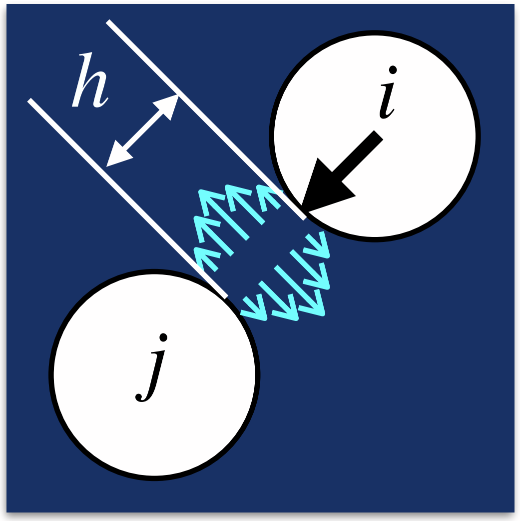


Singularity of non-Brownian simulation
Euler, dt=10^-4
Euler, dt=10^-5
pre. cor., dt=10^-4
pre. cor., dt=10^-5
stop
stop
Minimum gap
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
1e-09
1e-10
1e-11
0
0.2
0.4
0.6
0.8
1
1.2
Shear strain

Regularize the singularity

lubrication force

$$\boldsymbol{F}_{\mathrm{lub}} = -\frac{3\pi\eta_0 a^2}{2h}(\boldsymbol{U}^i - \boldsymbol{U}^j)\cdot\boldsymbol{nn}$$



$$\frac{1}{h} \to \begin{cases} \frac{1}{h+\delta} & h > 0 \\ \frac{1}{\delta} & h \le 0 \end{cases}$$

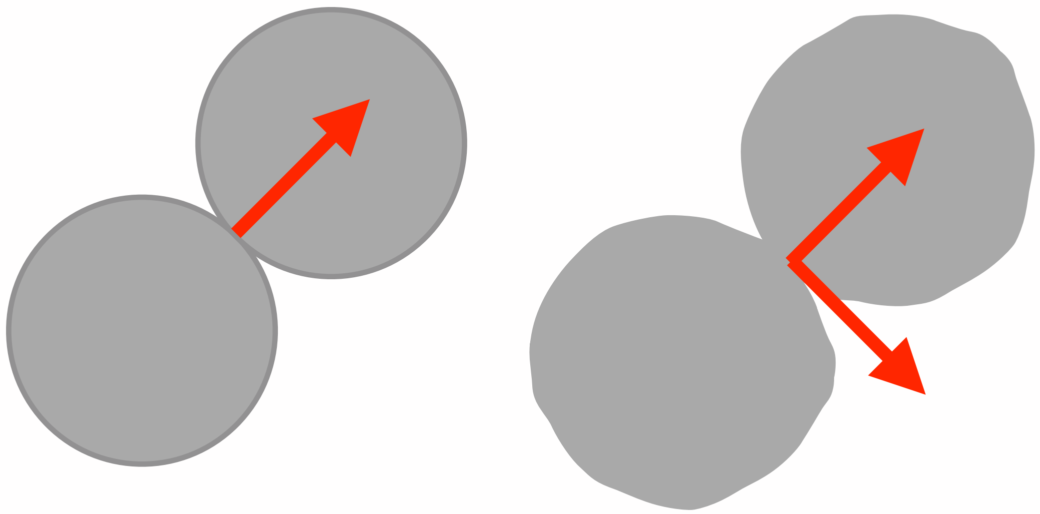
$$\delta = 10^{-3}a$$

Particle contacts are no longer forbidden!!

We need a contact force model because particle contacts are no longer forbidden

$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{C}} = \boldsymbol{0}$$

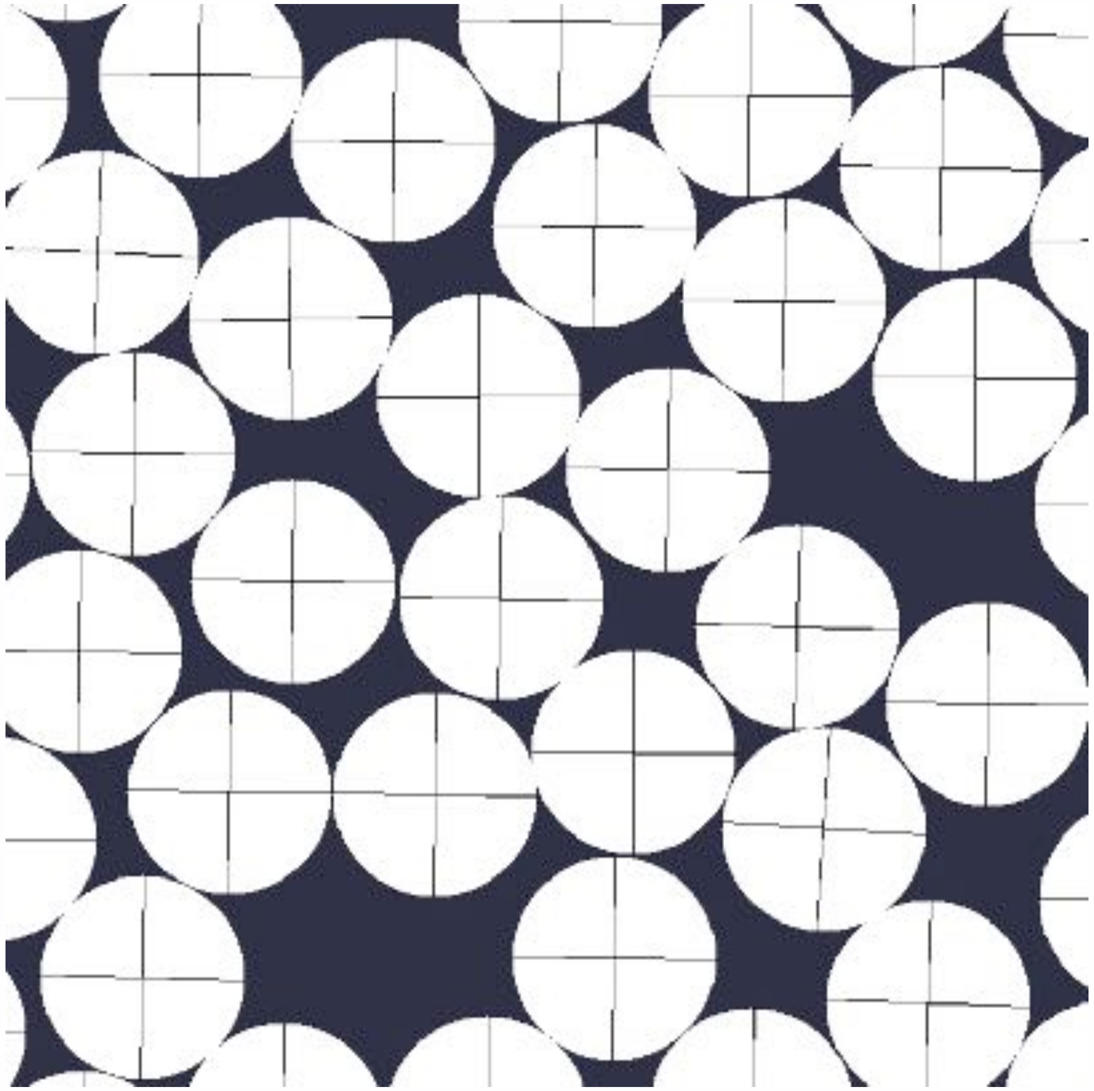
$$\boldsymbol{F}_{\mathrm{H}} = -\,\mathsf{R} \cdot (\boldsymbol{U} - \boldsymbol{u}) + \mathsf{R}' : \mathsf{D}$$



$$|\boldsymbol{F}_{\mathrm{C}}^{tan}| < \mu |\boldsymbol{F}_{\mathrm{C}}^{nor}|$$

$$\left(\boldsymbol{F}_{\mathrm{C}}^{ij}\right)^{nor} = k_{\mathrm{n}}(r_{ij} - 2a)\boldsymbol{n}^{ij}$$

$$\left(\boldsymbol{F}_{\mathrm{C}}^{ij}\right)^{tan} = -\,k_{\mathrm{t}}\boldsymbol{\xi}^{ij}$$

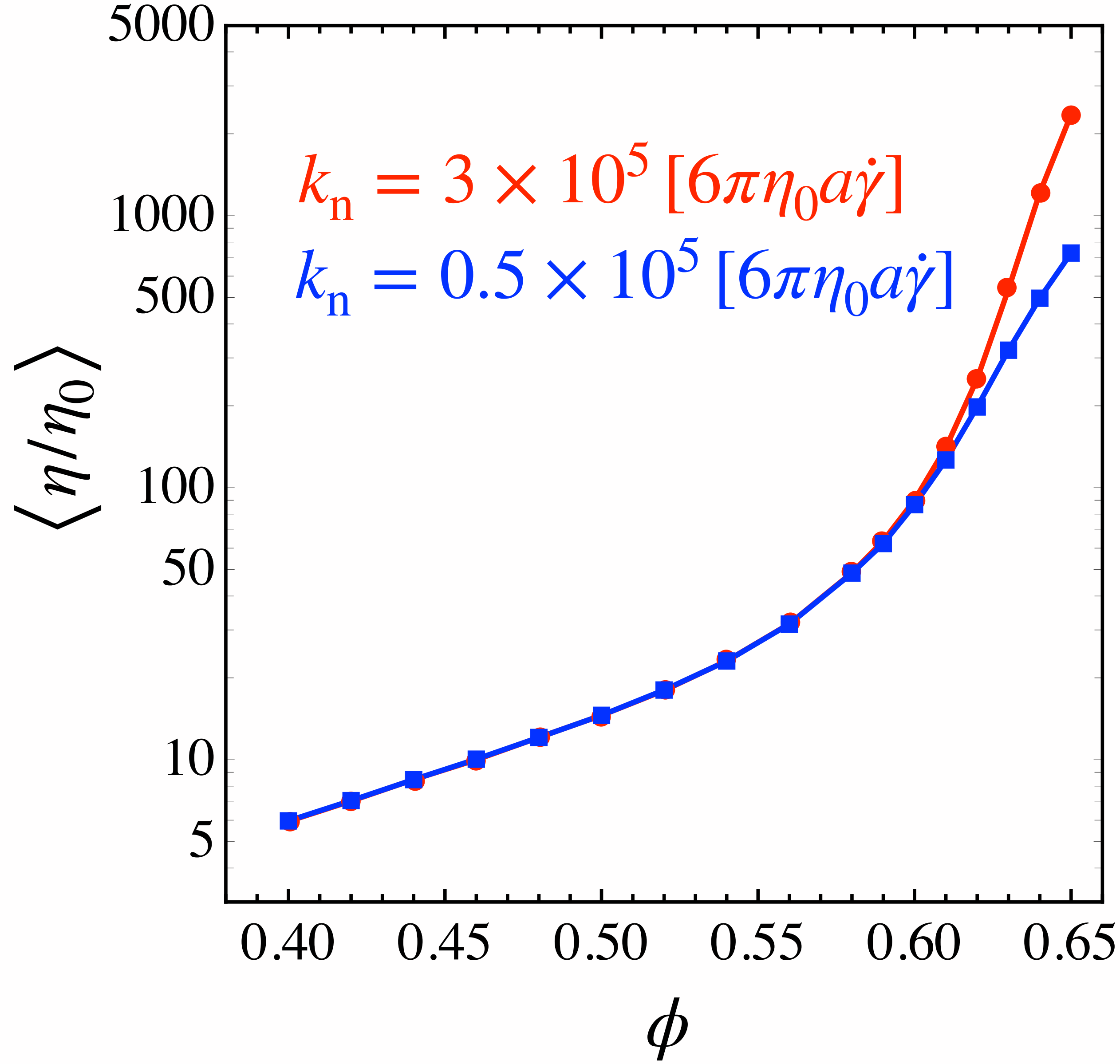


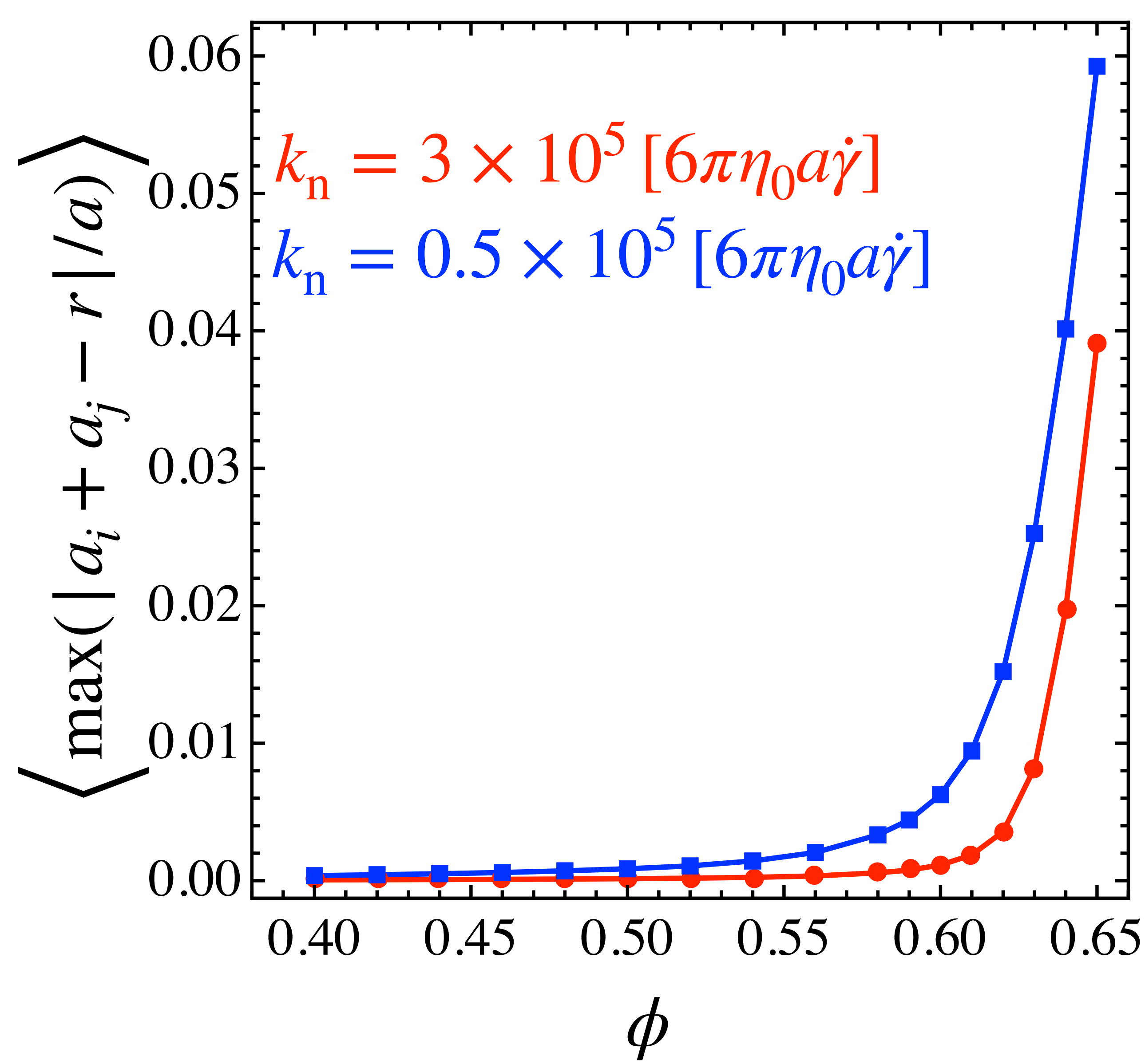
Effect of particle softness

$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{C}} = \boldsymbol{0}$$

$$\boldsymbol{F}_{\mathrm{C}}^{n} = k_{\mathrm{n}}(r - 2a)\boldsymbol{n}$$ **frictionless** $\mu = 0$

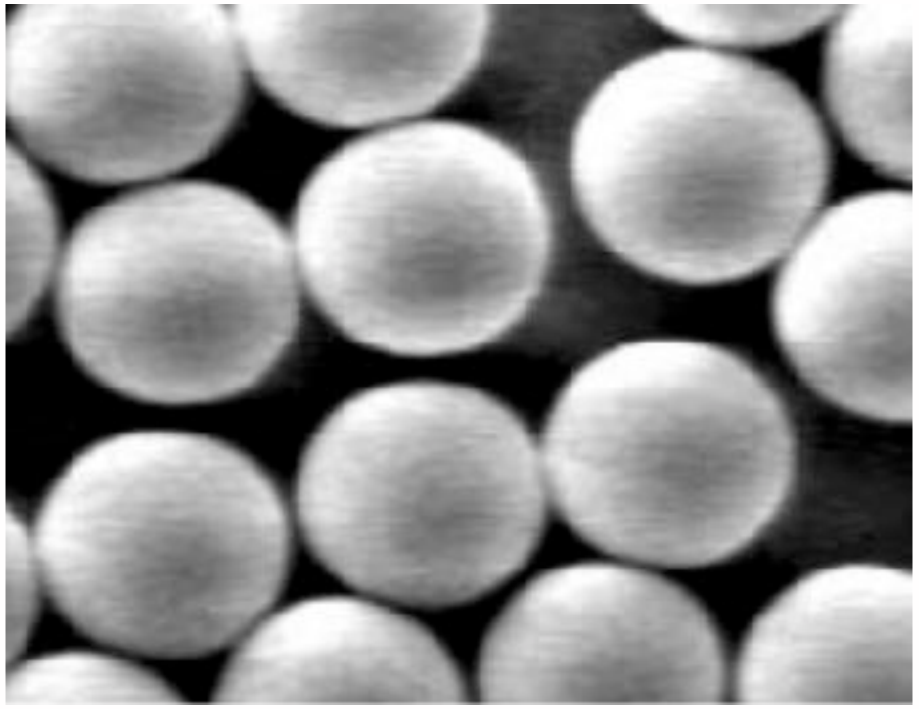
$$\boldsymbol{F}_{\mathrm{H}} = -\mathsf{R} \cdot (\boldsymbol{U} - \boldsymbol{u}) + \mathsf{R}' : \mathsf{D}$$





Contact deformation of Silica

$$F_n = k_n(2a - r)^{3/2}$$
$$k_n = \frac{4}{3}E\sqrt{a}$$



Young's Modulus of Silica (SiO2) $E = 65 \sim 75$ [GPa]

particle size $a = 10^{-6}$ [m]

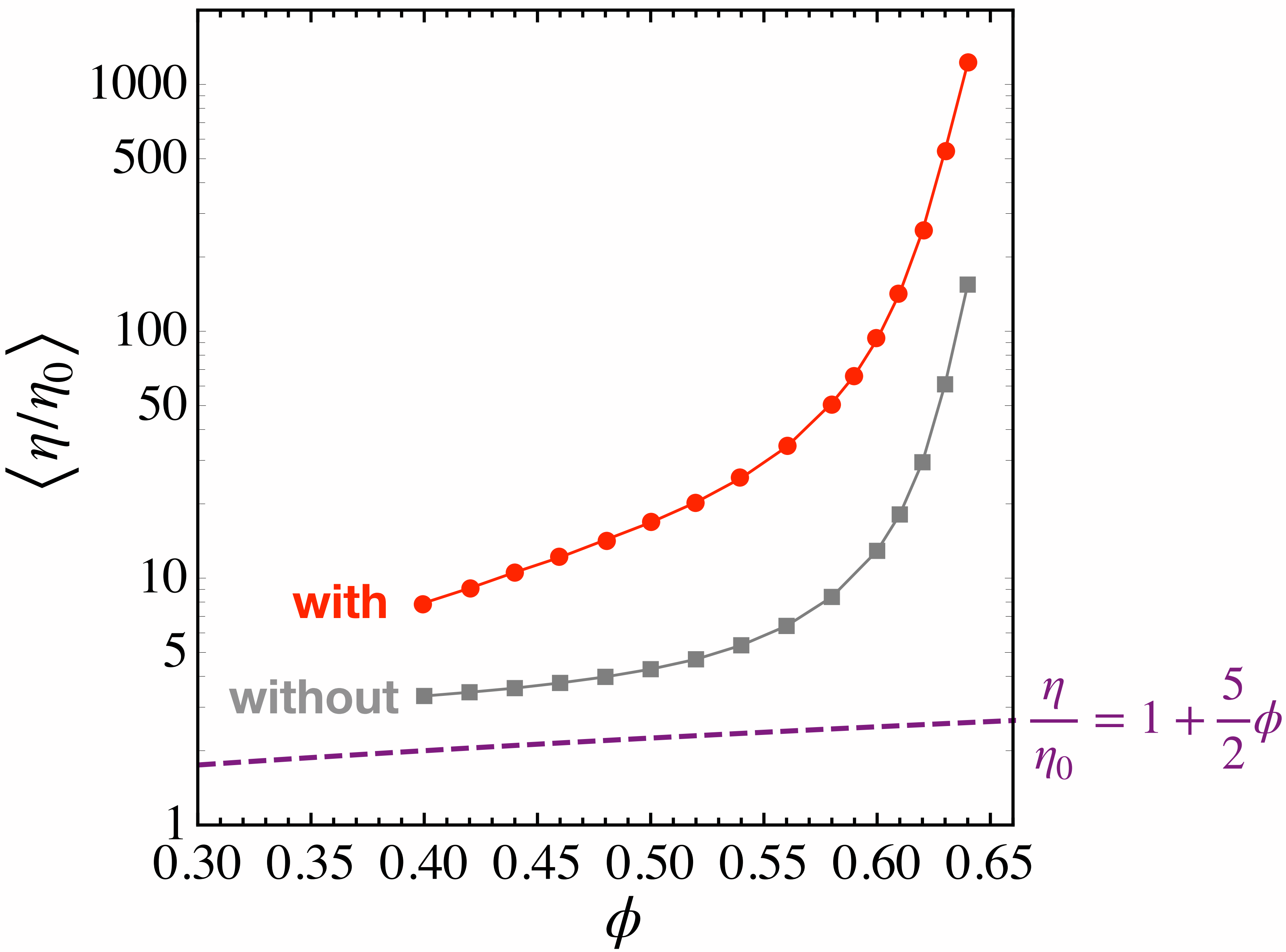
a large shear stress $\sigma_{xy} = 10^3$ [Pa]

typical force $F_n \sim \sigma_{xy} \times (2a)^2 = 4 \times 10^{-9}$ [N]

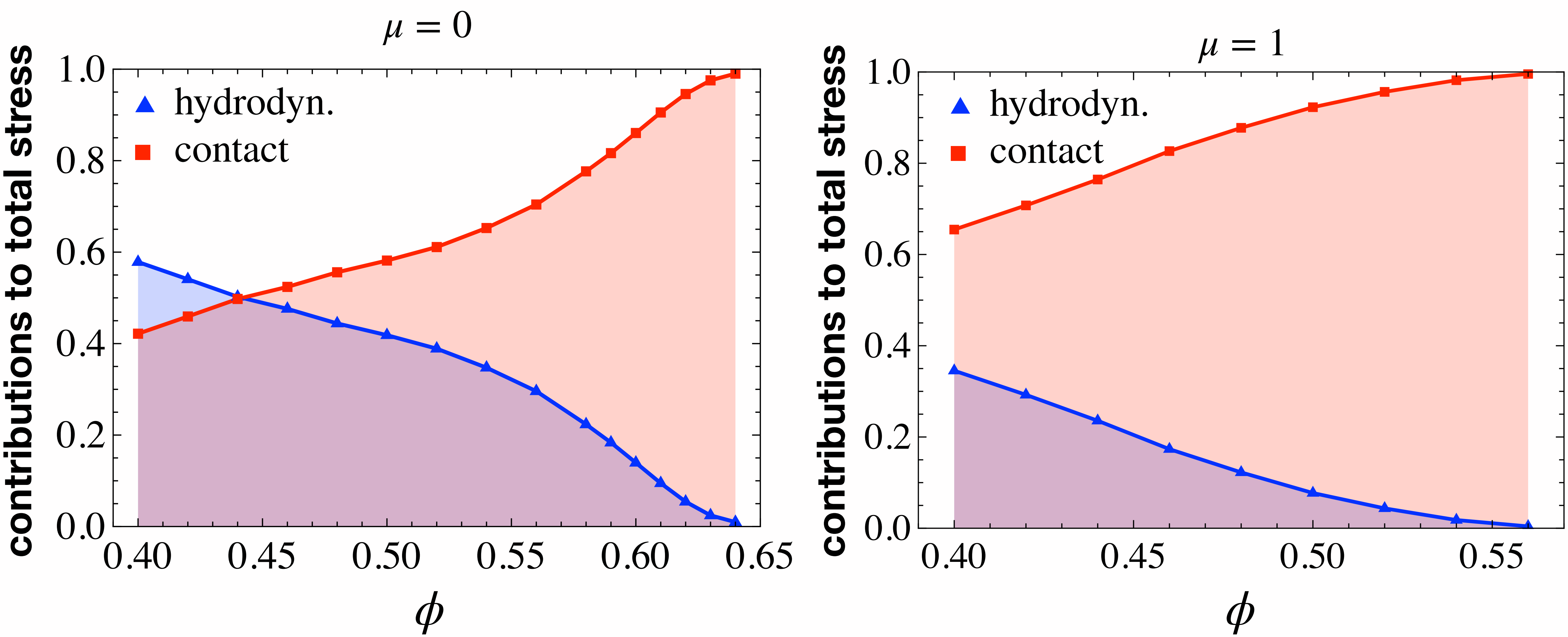
overlap $$\frac{2a - r}{a} \approx 10^{-5}$$

This level of stiffness is very difficult in simulation!!

With and without hydrodynamic lubrication



Hydrodynamic vs contact force contributions

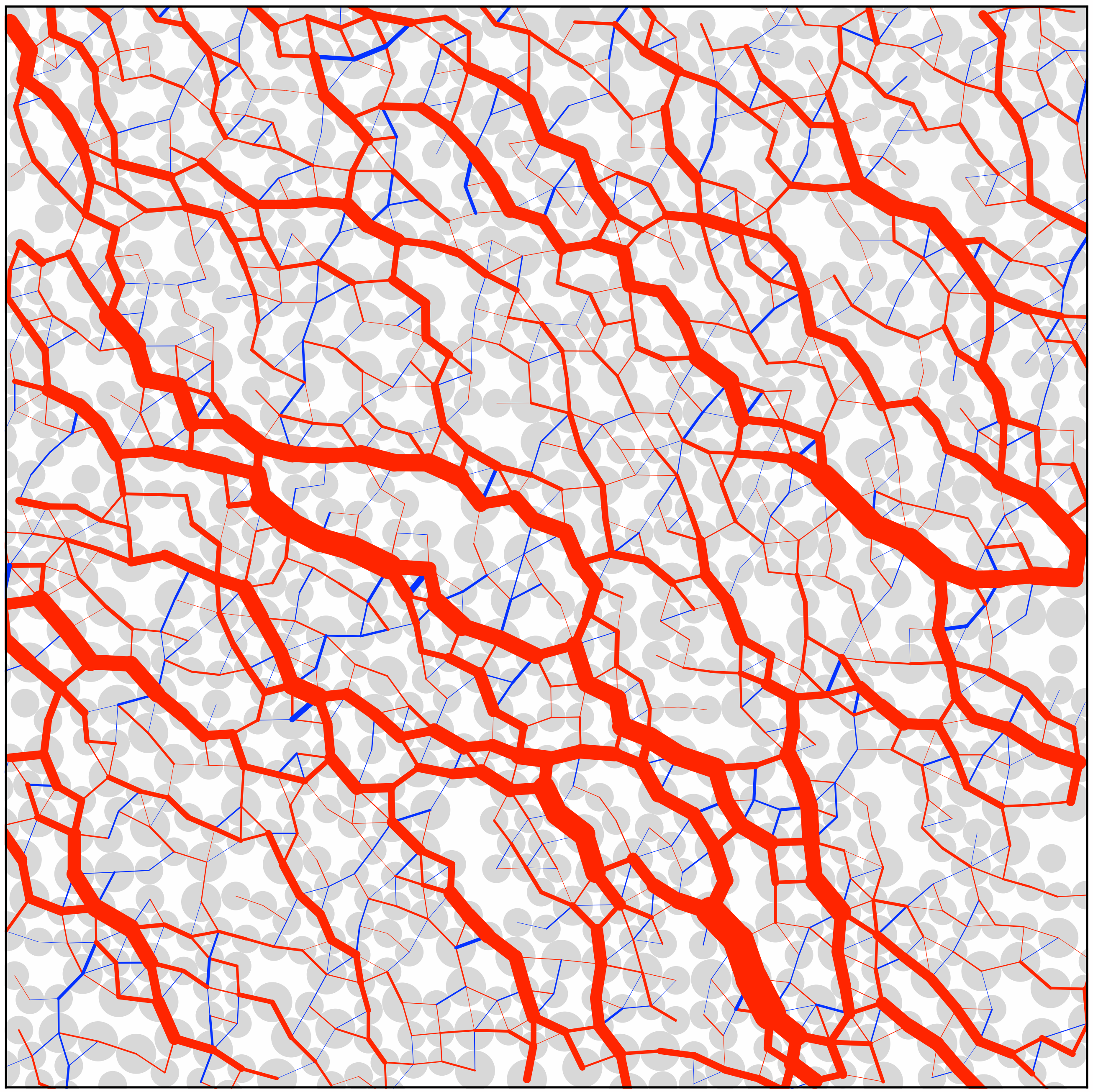


Force-chain network in 2D simulation

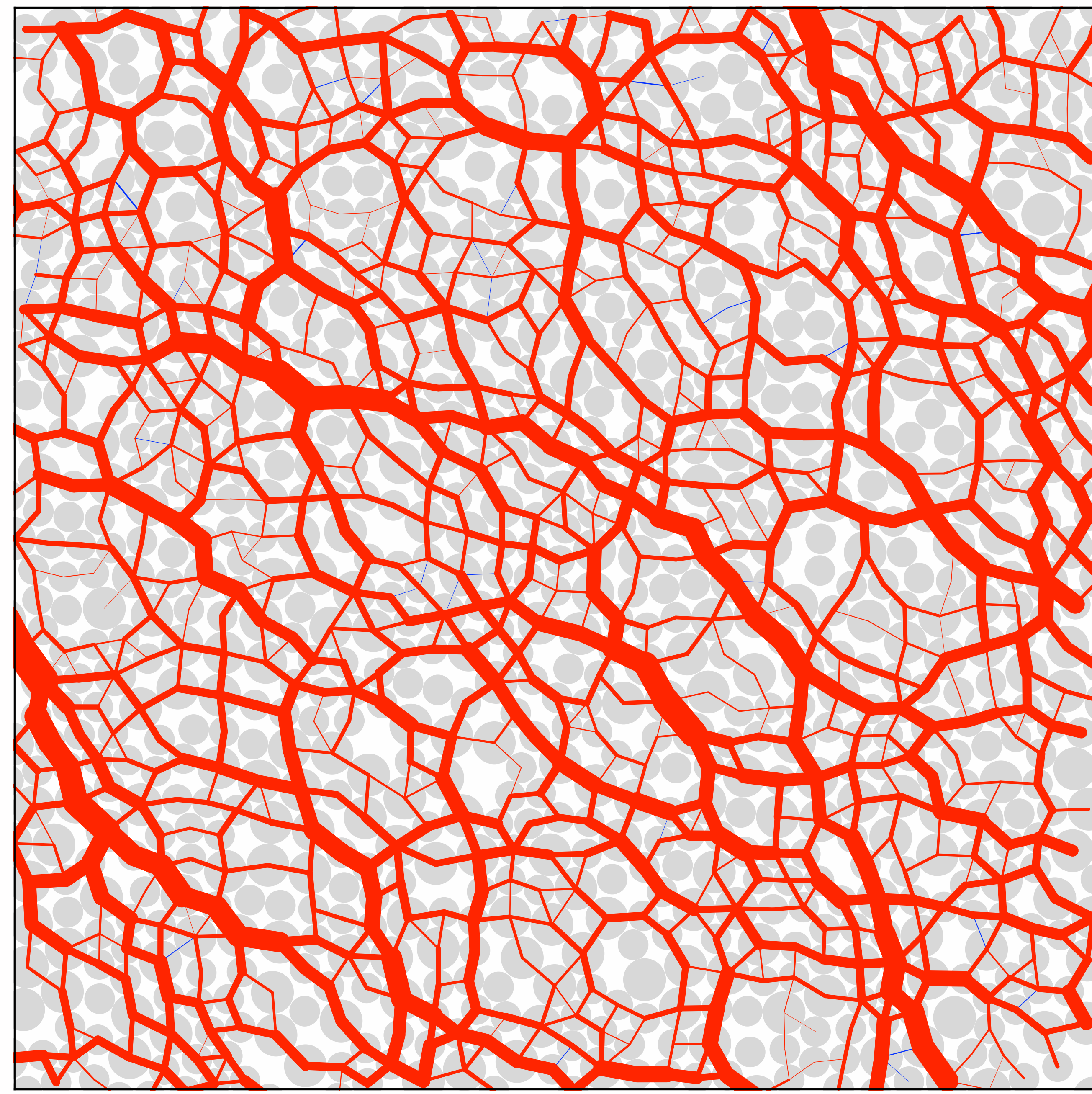
$$\bar{F}_{ij} \equiv -\overrightarrow{F}^{(ij)} \cdot \overrightarrow{n}_{ij}$$

repulsive
attractive

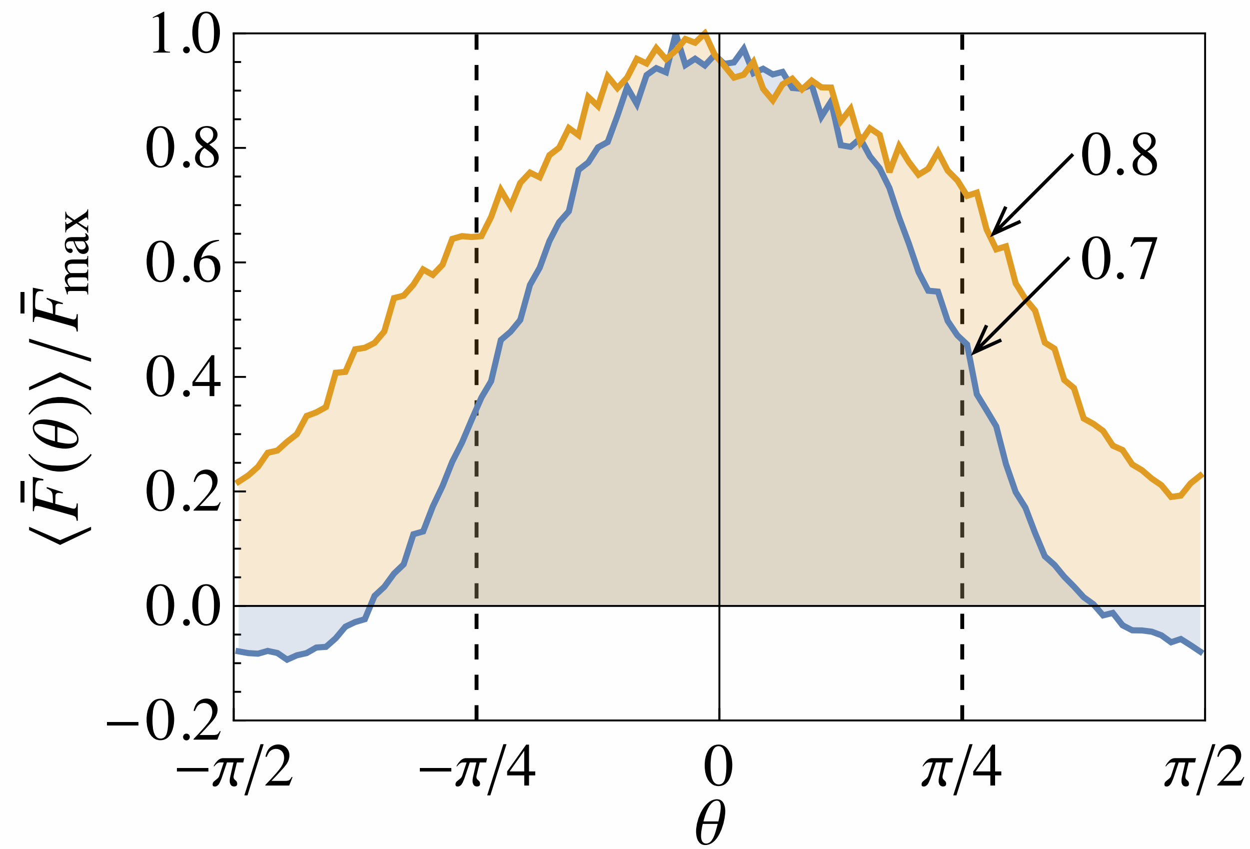
$\phi_{\text{area}} = 0.7 \quad \mu = 0.5$

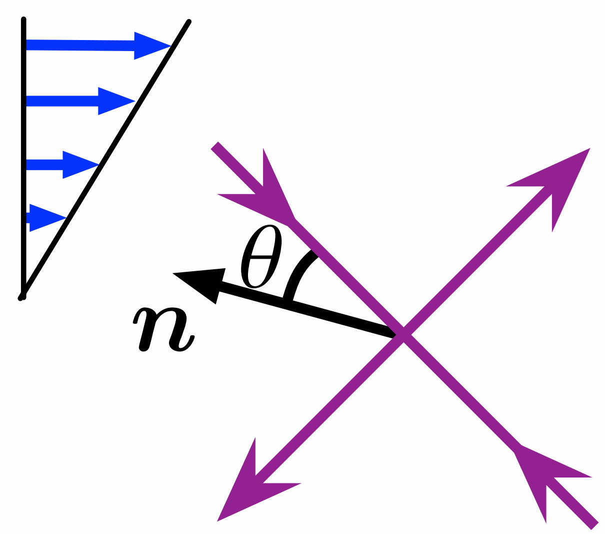


$\phi_{\text{area}} = 0.8 \quad \mu = 0.5$



Angular dependence of normal force

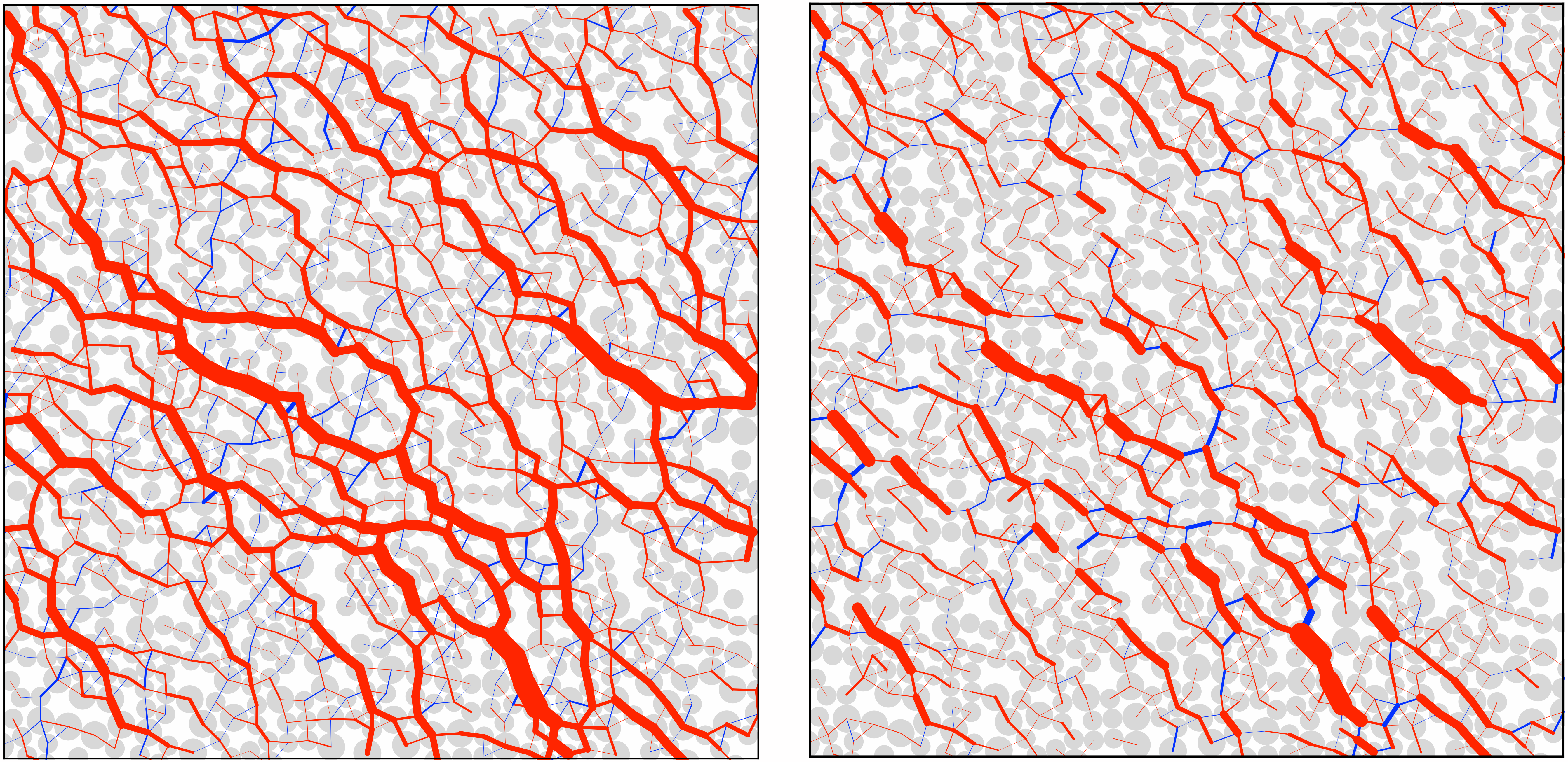




Only hydrodynamics forces are able to be attractive

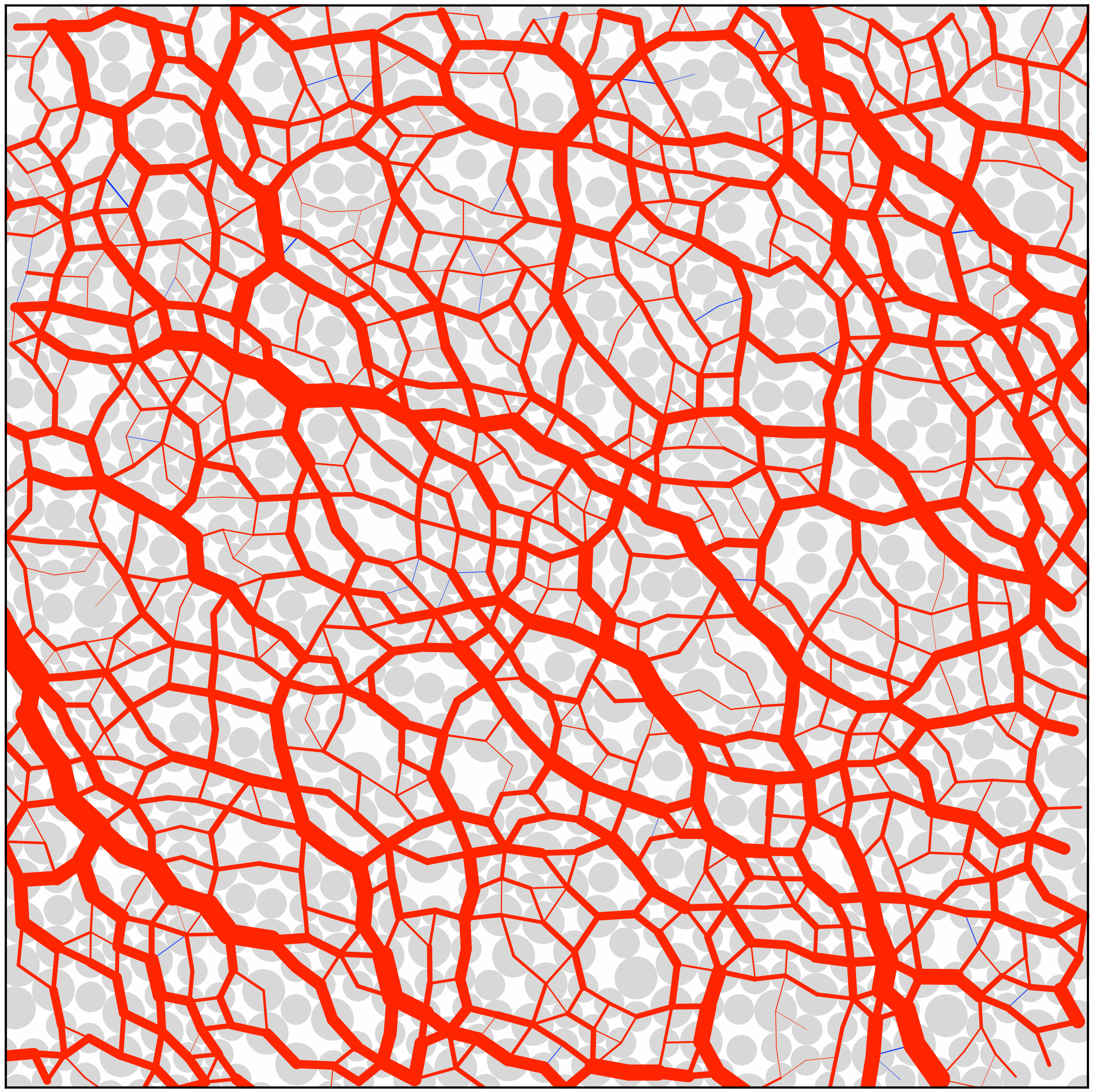
$\phi_{\text{area}} = 0.7 \quad \mu = 0.5$

normal force $\bar{F}_{ij} \equiv -\overrightarrow{F}^{(ij)} \cdot \overrightarrow{n}_{ij}$ **contribution to shear stress** σ_{xy}

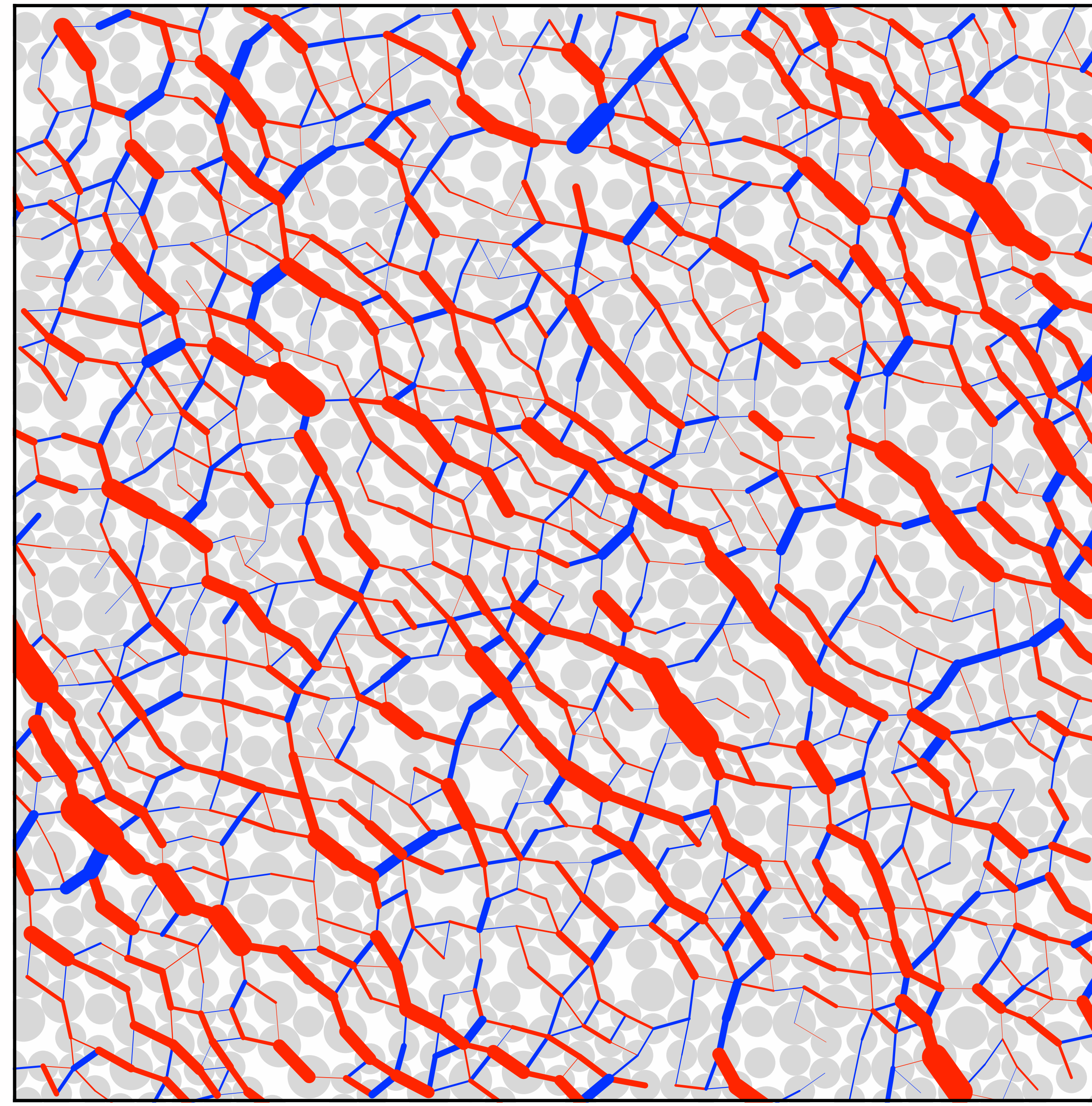


$\phi_{\text{area}} = 0.8 \quad \mu = 0.5$

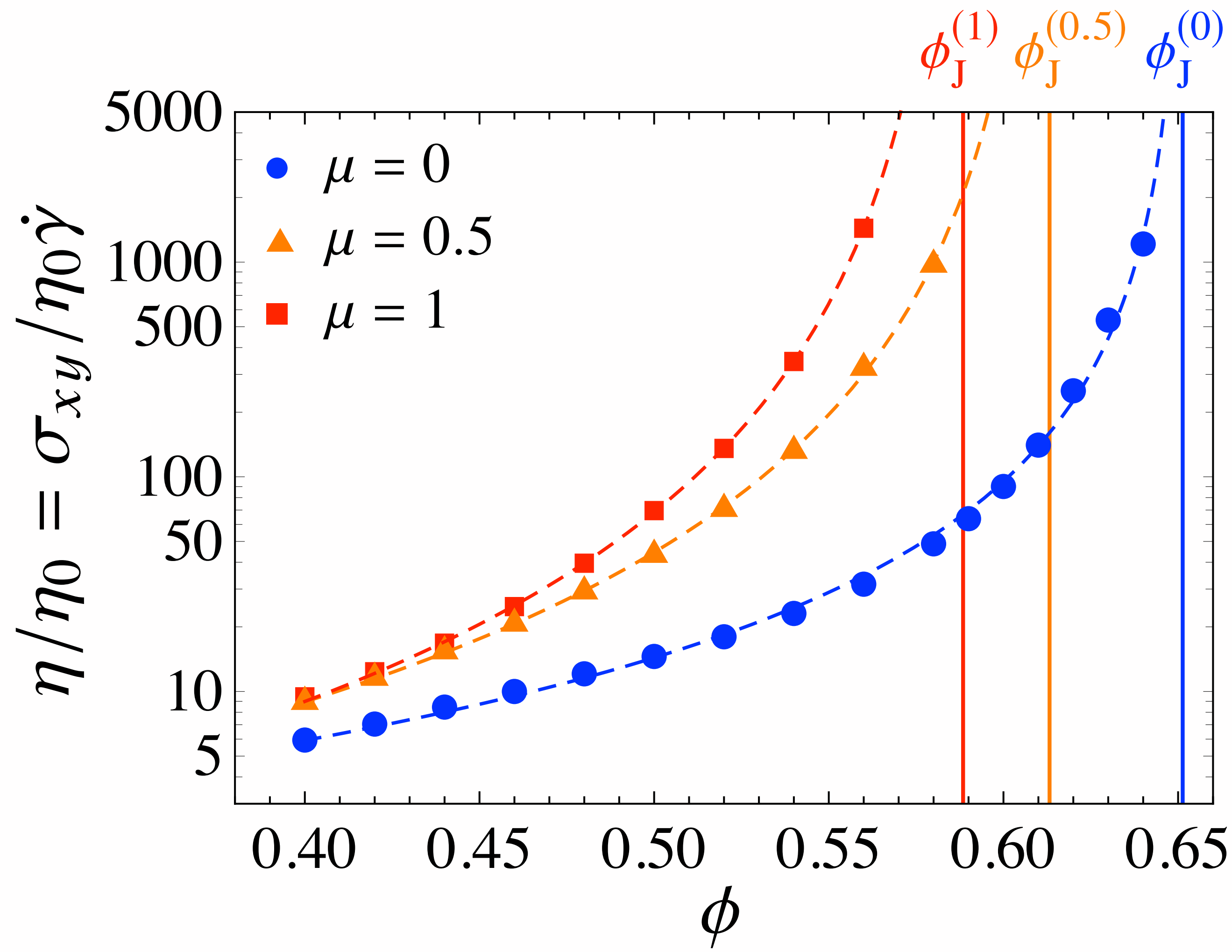
normal force $\bar{F}_{ij} \equiv -\overrightarrow{F}^{(ij)} \cdot \overrightarrow{n}_{ij}$



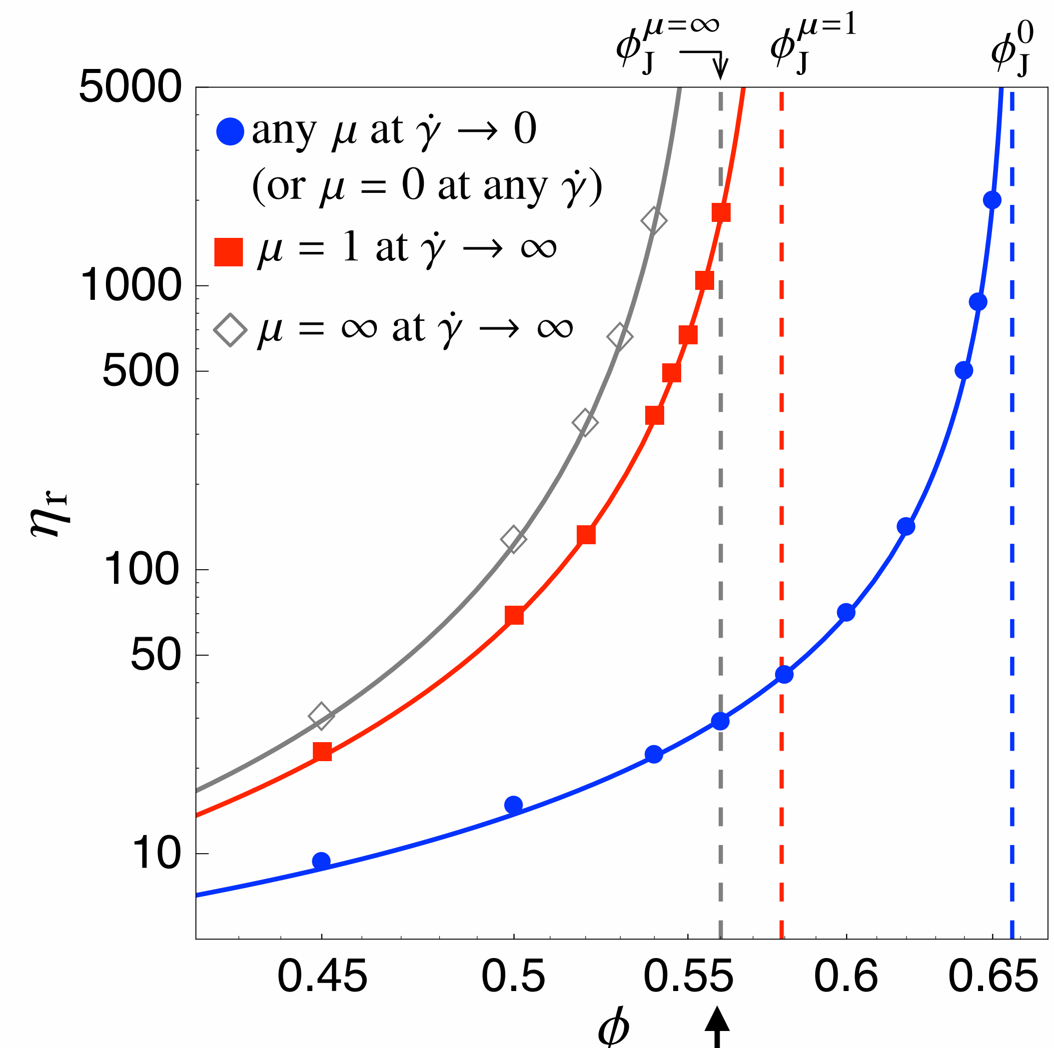
contribution to shear stress σ_{xy}



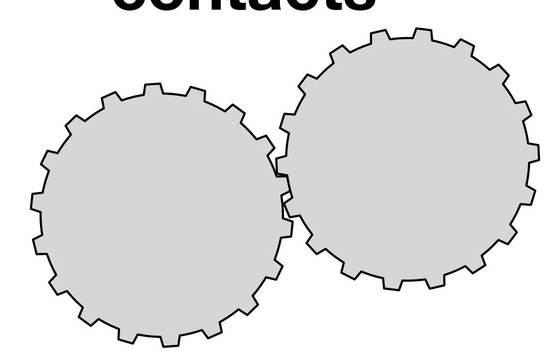
With and without contact friction



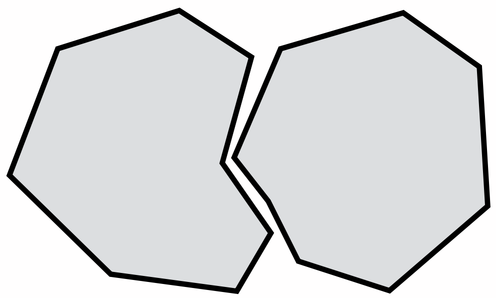
$$\eta/\eta_0 = c\left(\phi_J^{(\mu)} - \phi\right)^{-\lambda}$$

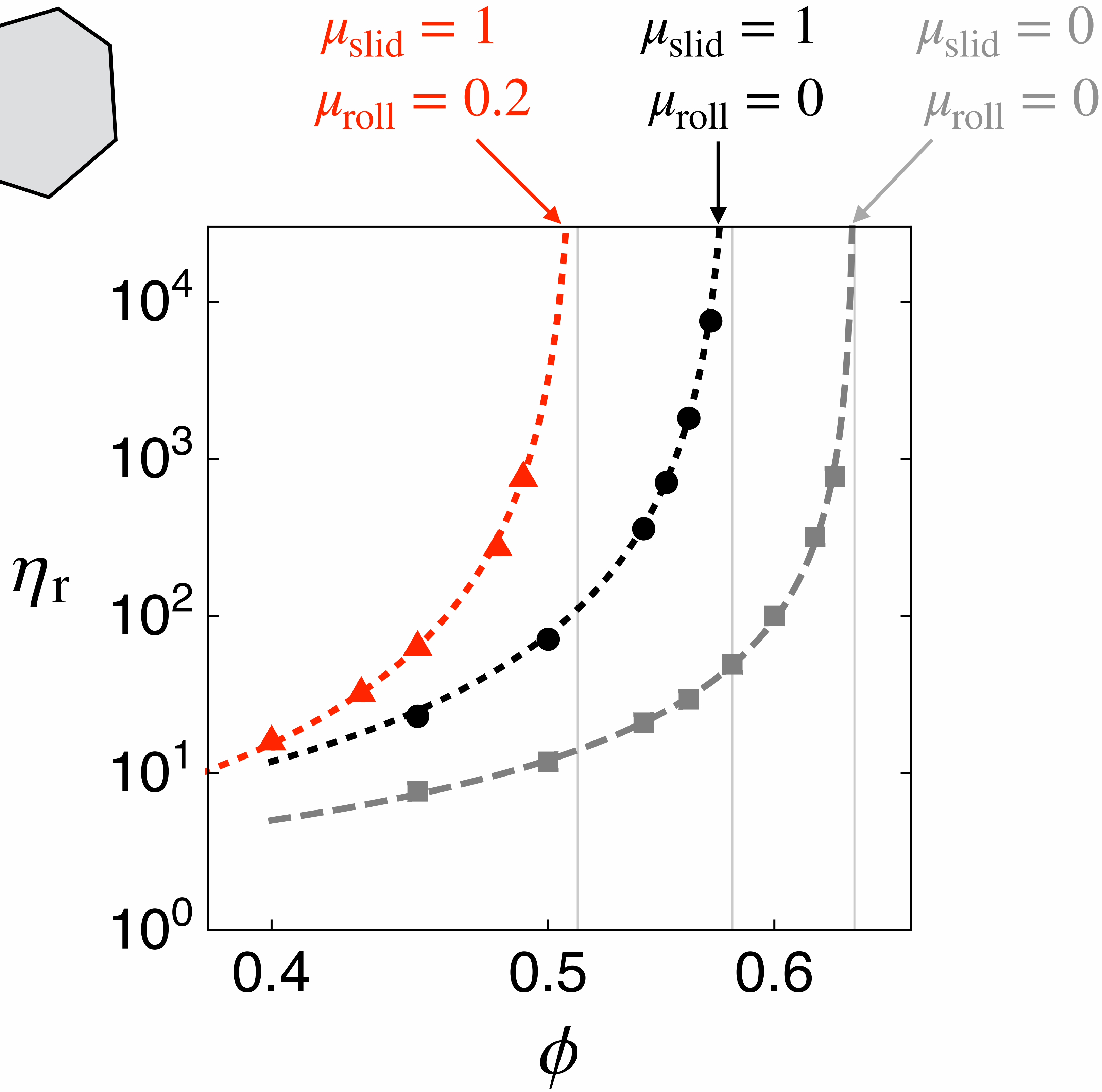


Jamming with gear-like contacts



with rolling friction

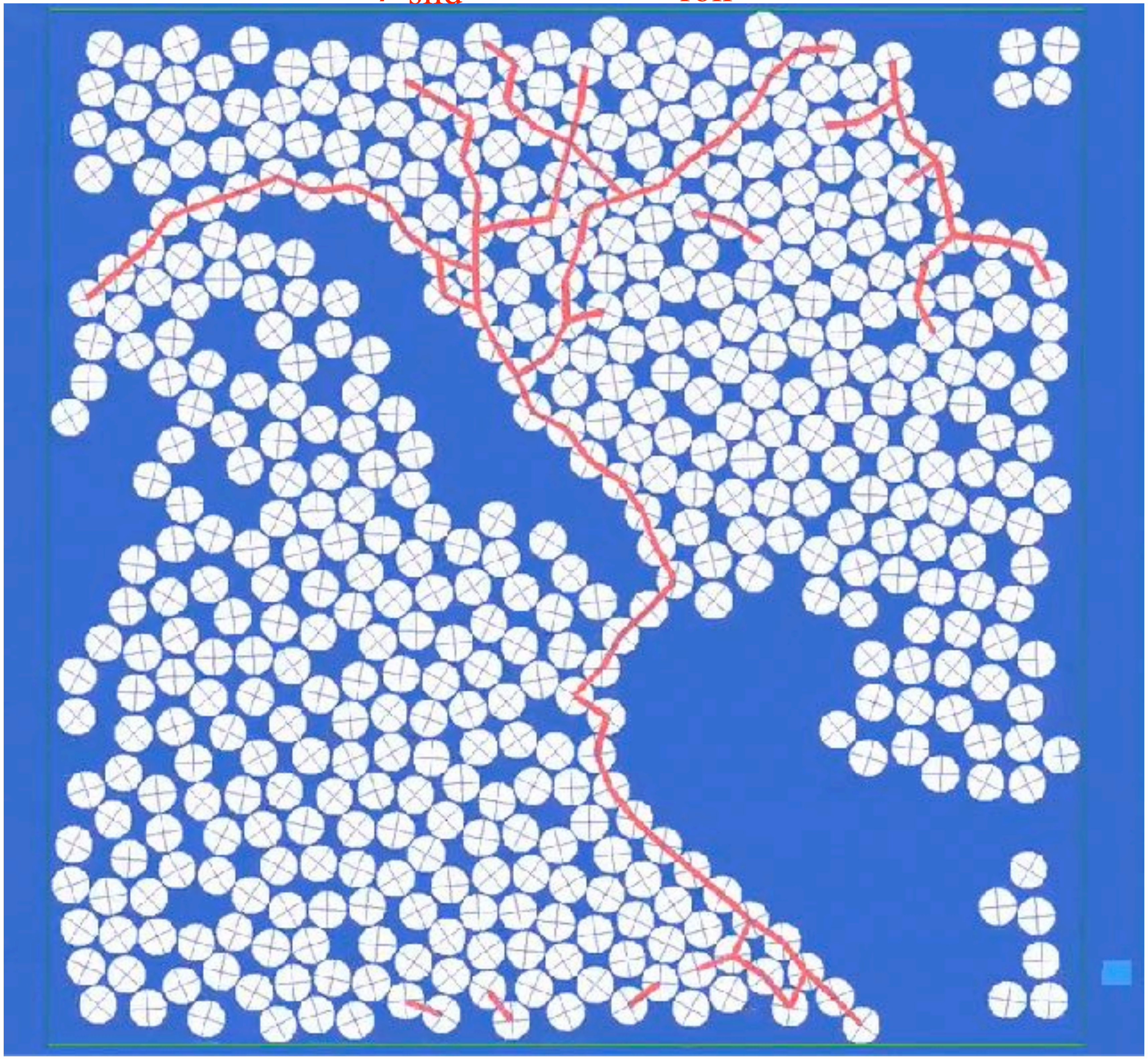




2D demo for an extreme contact model

no slide and rolling as long as pushing

$\mu_{\mathrm{slid}} = \infty \qquad \mu_{\mathrm{roll}} = \infty$

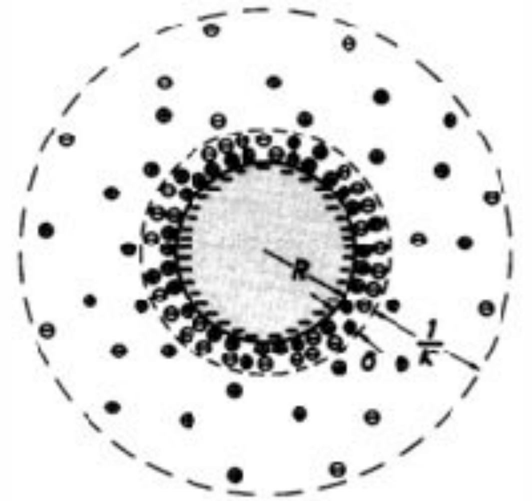


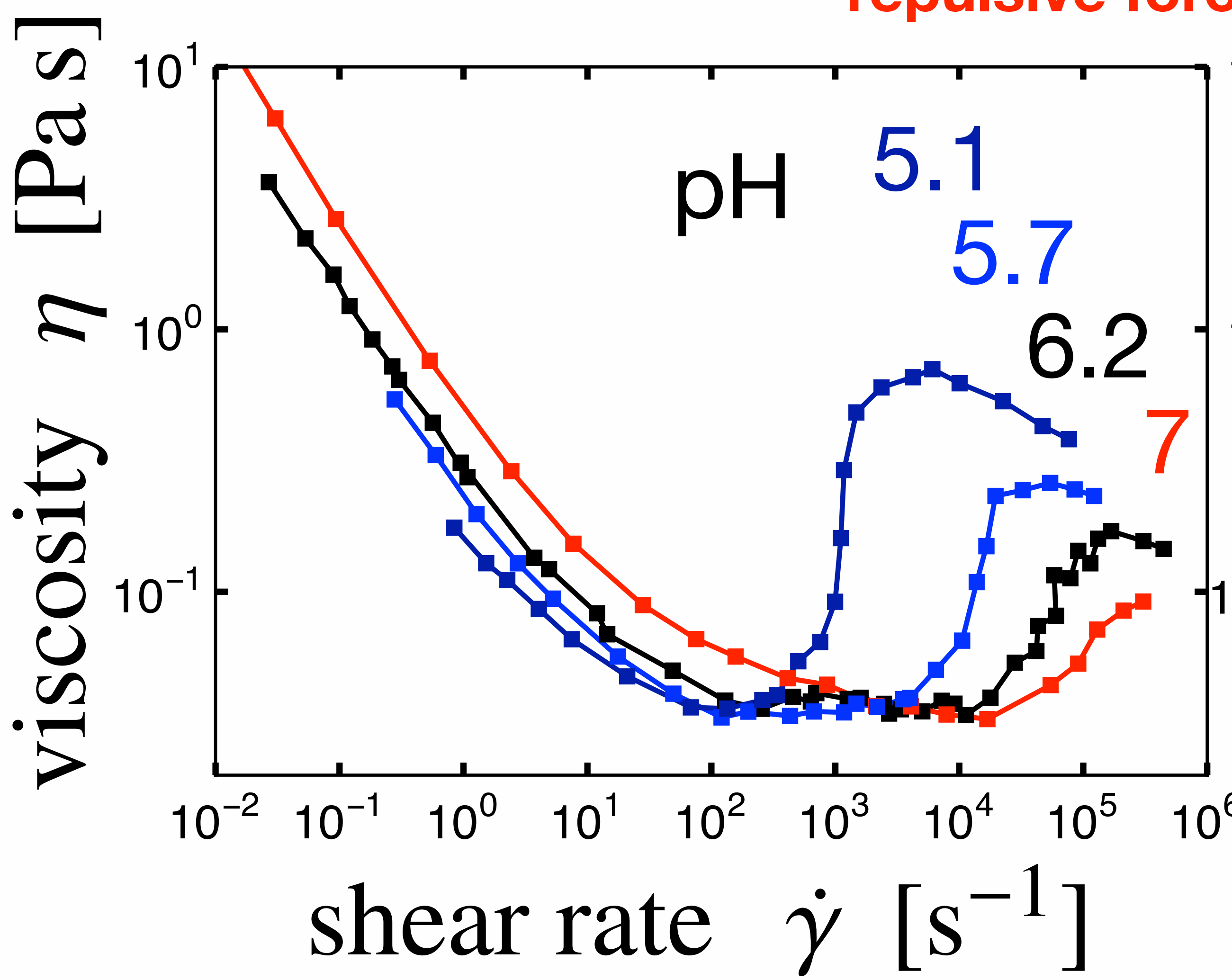
Origin of rate-dependence

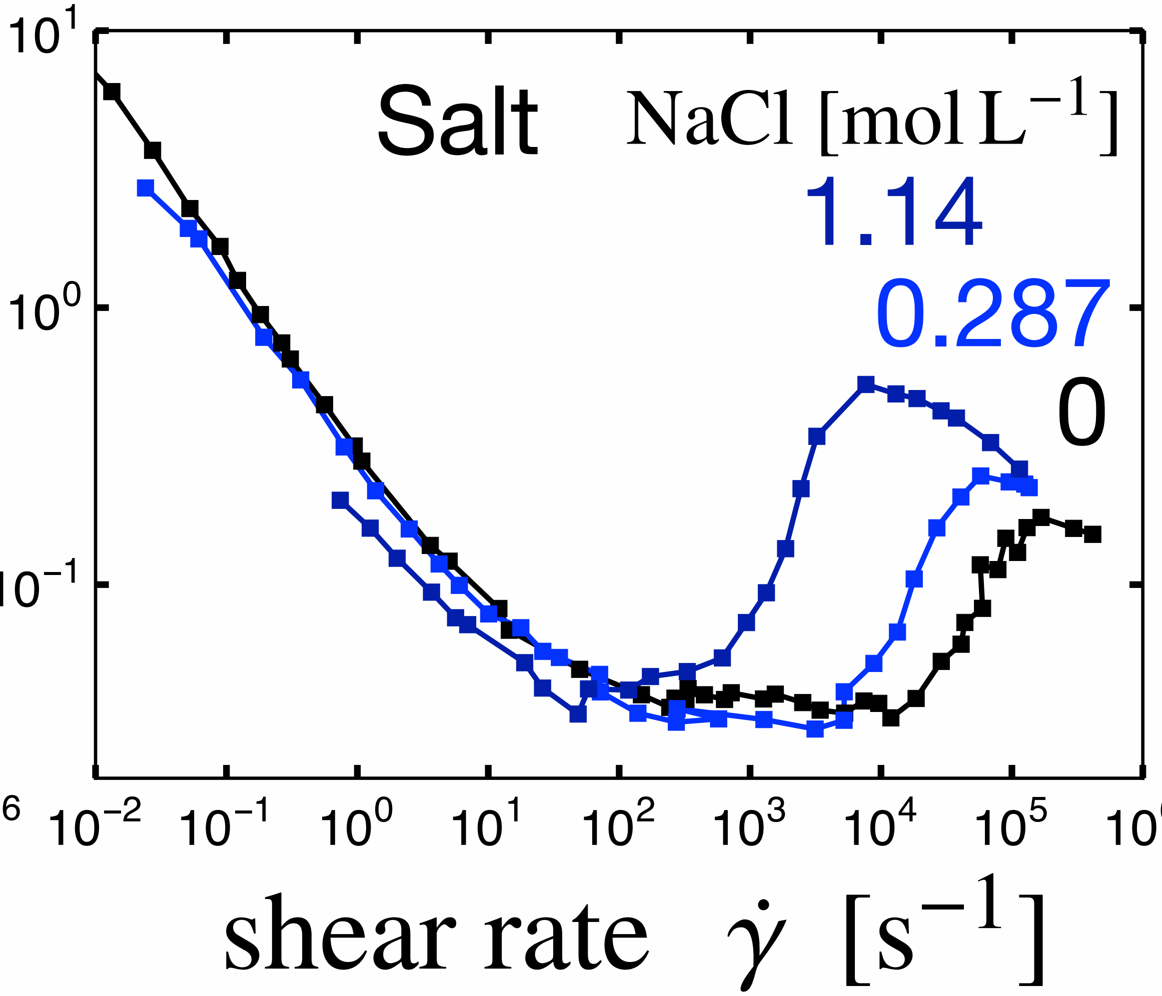
$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{C}} = \boldsymbol{0}$ **rate independent**

$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{C}} + \boldsymbol{F}_{\mathrm{R}} = \boldsymbol{0}$ **rate-dependent**

repulsive force

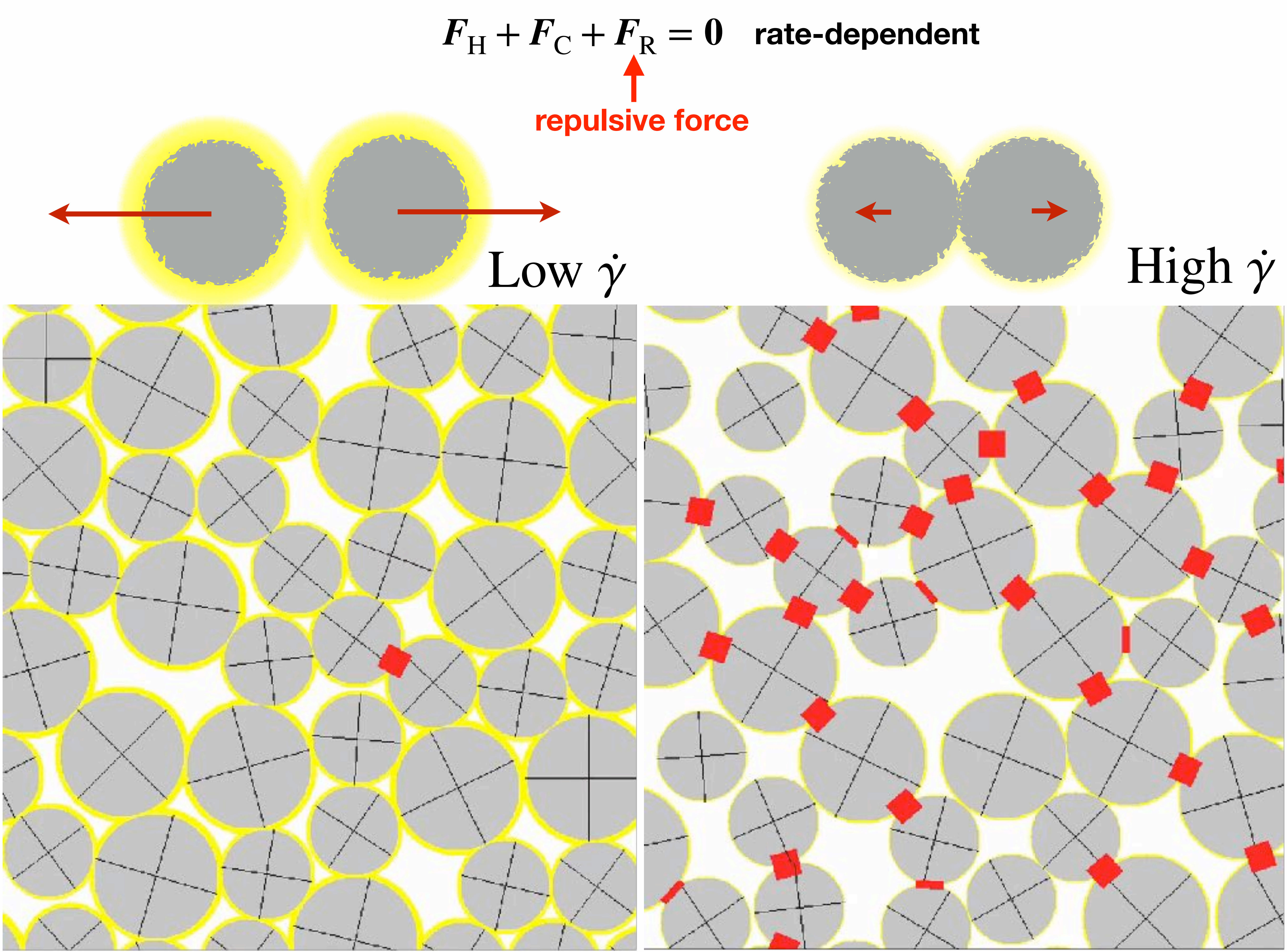




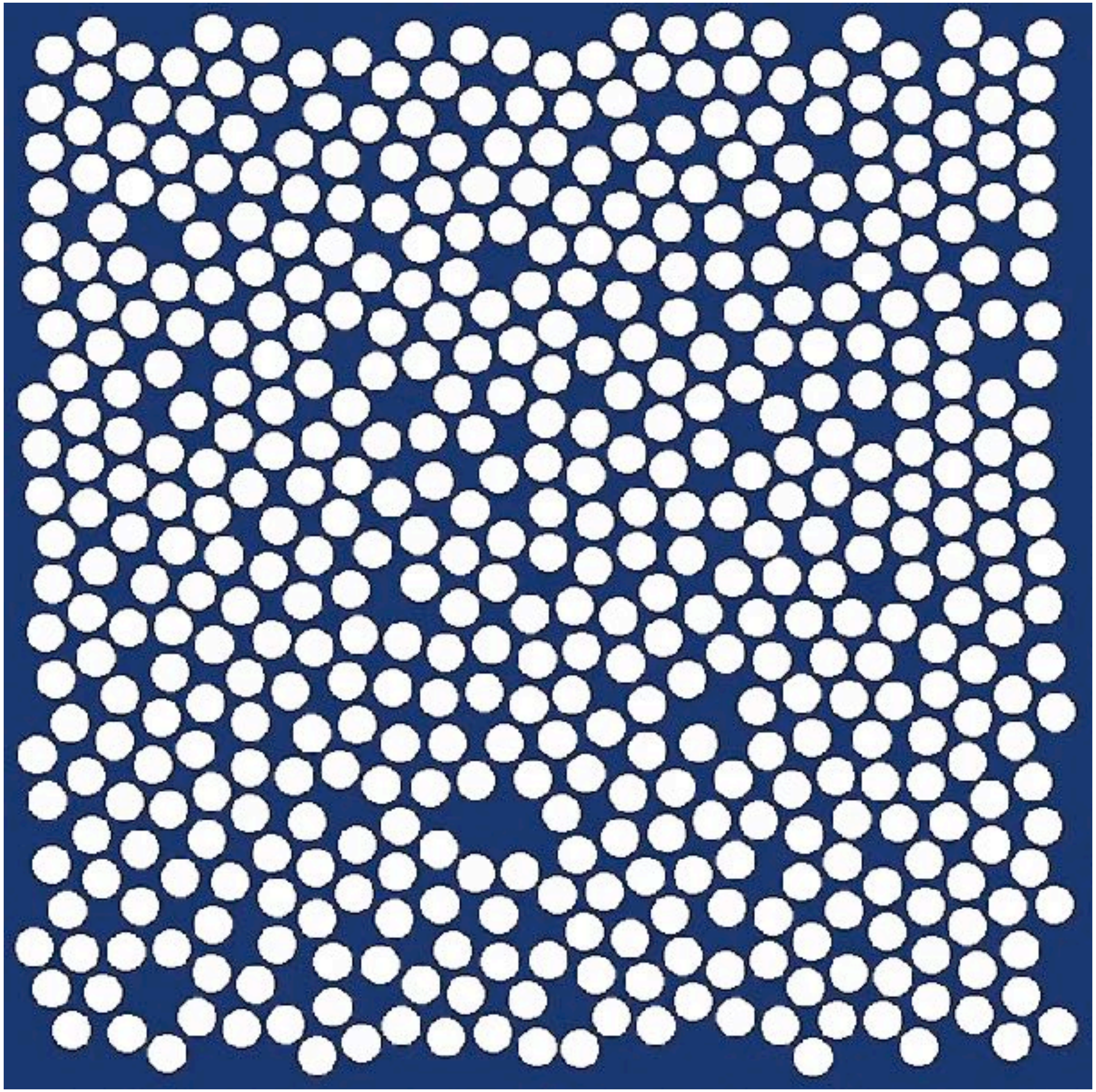


Laun 1984

Latex particles in water



$F_H + F_C + F_R = 0$ rate-dependent
repulsive force
Low $\dot{\gamma}$
High $\dot{\gamma}$



How do shear flows bring Brownian hard spheres to non-equilibrium states?

Stokesian Dynamics was introduced to tackle this problem

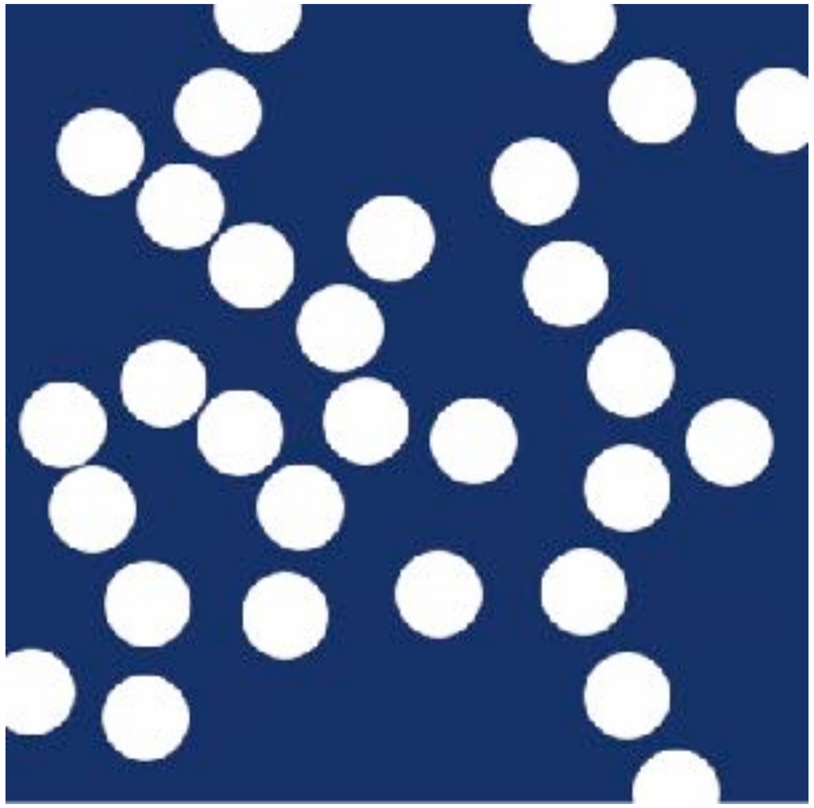
6*N*-dimensional overdamped Langevin eq.

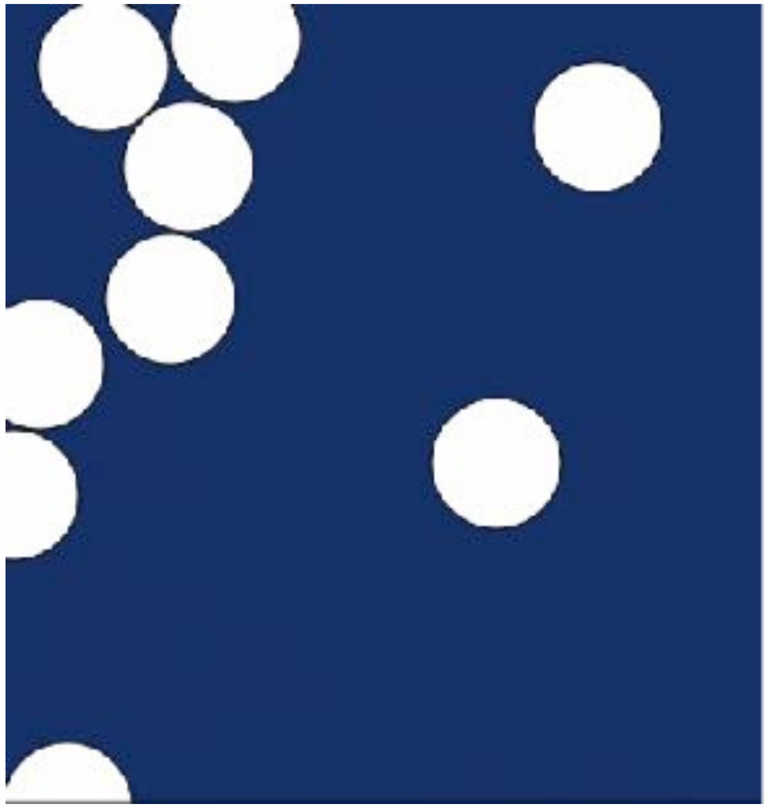
$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{B}} = \boldsymbol{0}$$

$$\boldsymbol{u}(\boldsymbol{r}) = \nabla \boldsymbol{u} \cdot \boldsymbol{r} = \mathsf{D} \cdot \boldsymbol{r} + (\boldsymbol{\omega}/2) \times \boldsymbol{r}$$

hydrodynamic force $\boldsymbol{F}_{\mathrm{H}} = -\,\mathsf{R} \cdot (\boldsymbol{U} - \boldsymbol{u}) + \mathsf{R}' : \mathsf{D}$

Brownian force $\langle \boldsymbol{F}_{\mathrm{B}} \rangle = 0, \quad \langle \boldsymbol{F}_{\mathrm{B}}(t_1) \boldsymbol{F}_{\mathrm{B}}(t_2) \rangle = 2 k_{\mathrm{B}} T \mathsf{R} \delta(t_1 - t_2)$





Modified Stokesian Dynamics

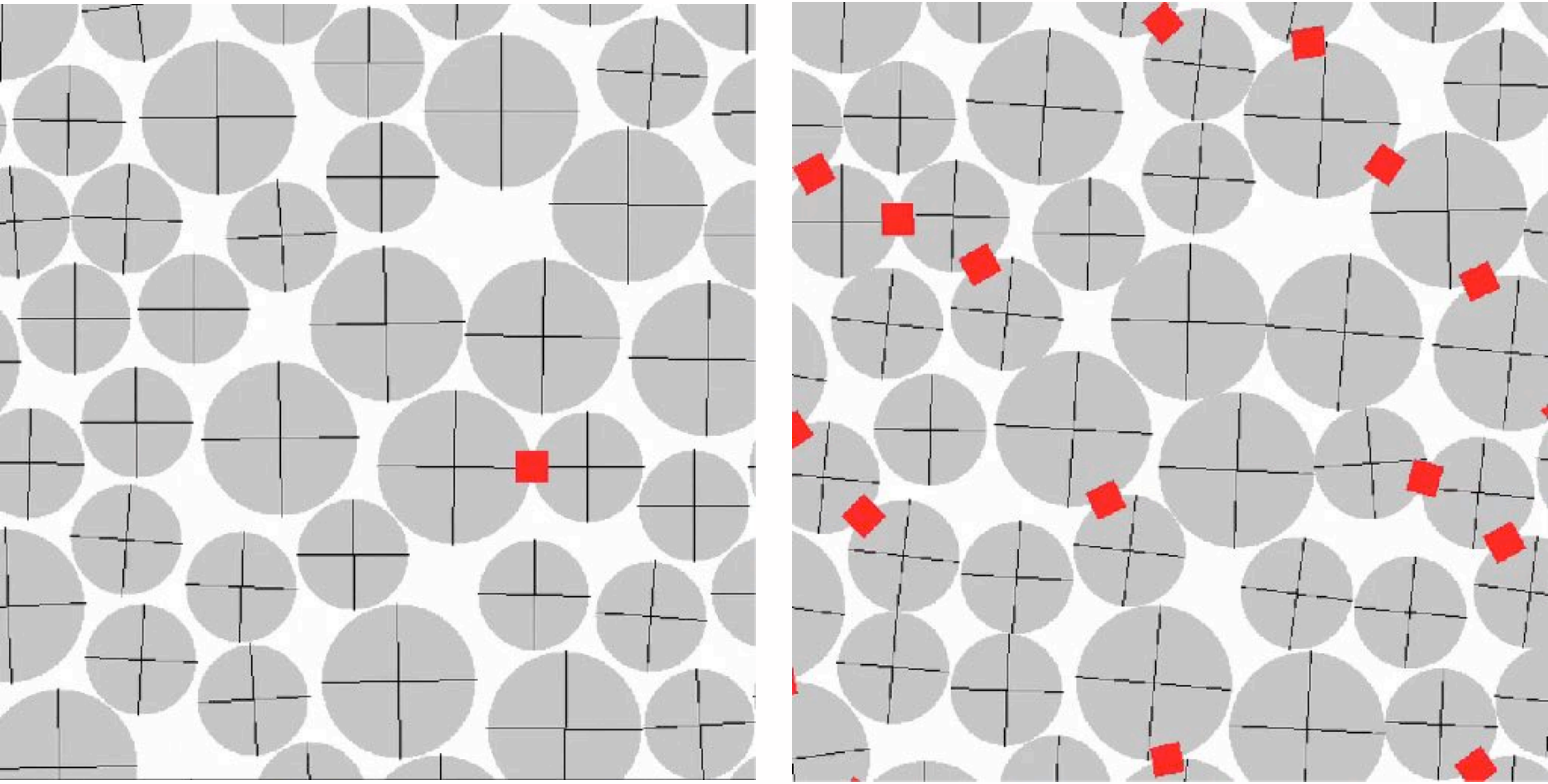
Step 1: Remove lubrication singularity

$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{B}} + \boldsymbol{F}_{\mathrm{C}} = \boldsymbol{0}$$

Step 2: Introduce a contact-force model

Contacts in sheared Brownian motions

Pe = 1 Pe = 100



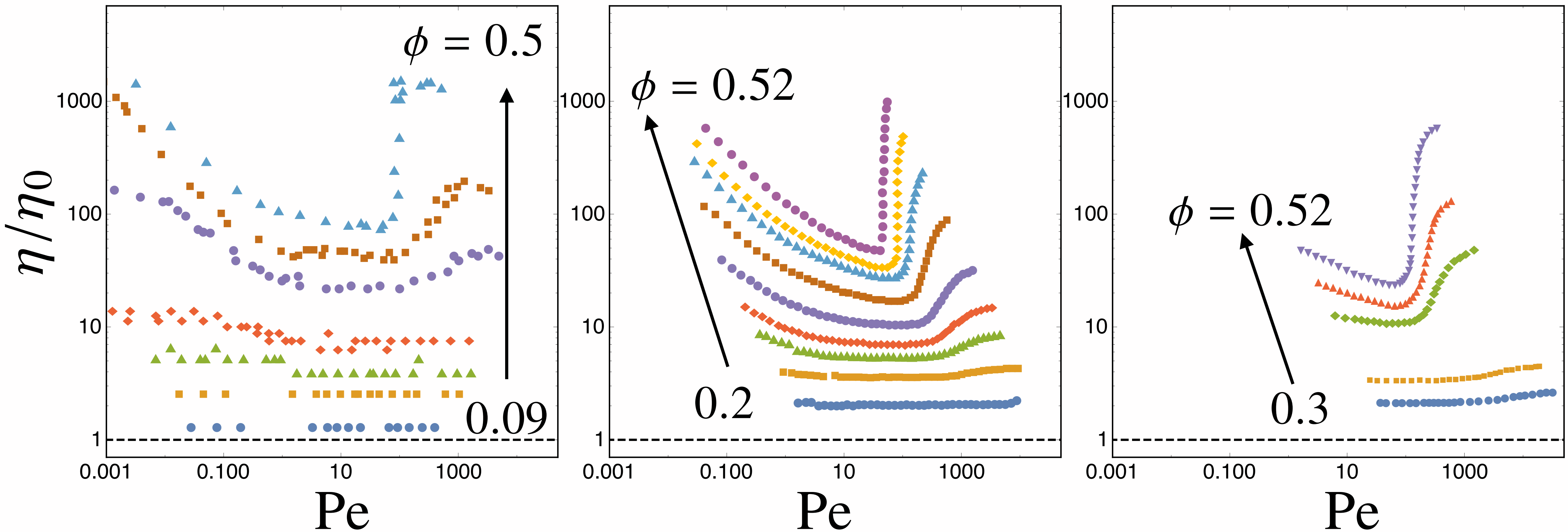
Péclet number: $\mathrm{Pe} \equiv \dfrac{6\pi\eta_0 a^3 \dot{\gamma}}{k_\mathrm{B}T}$

Experimental data

$a = 125\,\mathrm{nm}$ | $\eta_0 = 0.001\,\mathrm{Pa\,s}$

$a = 225\,\mathrm{nm}$ | $\eta_0 = 0.049\,\mathrm{Pa\,s}$

$a = 260\,\mathrm{nm}$ | $\eta_0 = 0.05\,\mathrm{Pa\,s}$

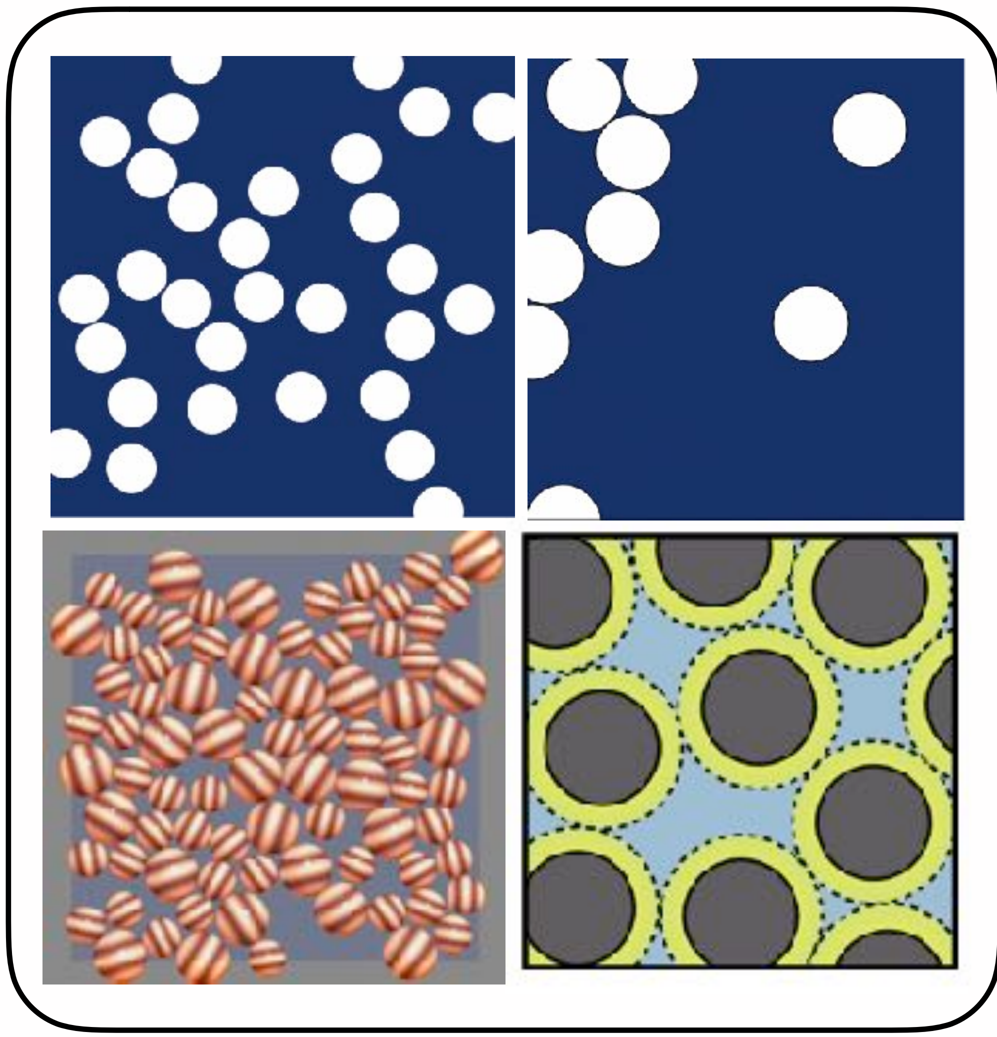


Laun 1984 | Egres 2005 | Cwalina 2014

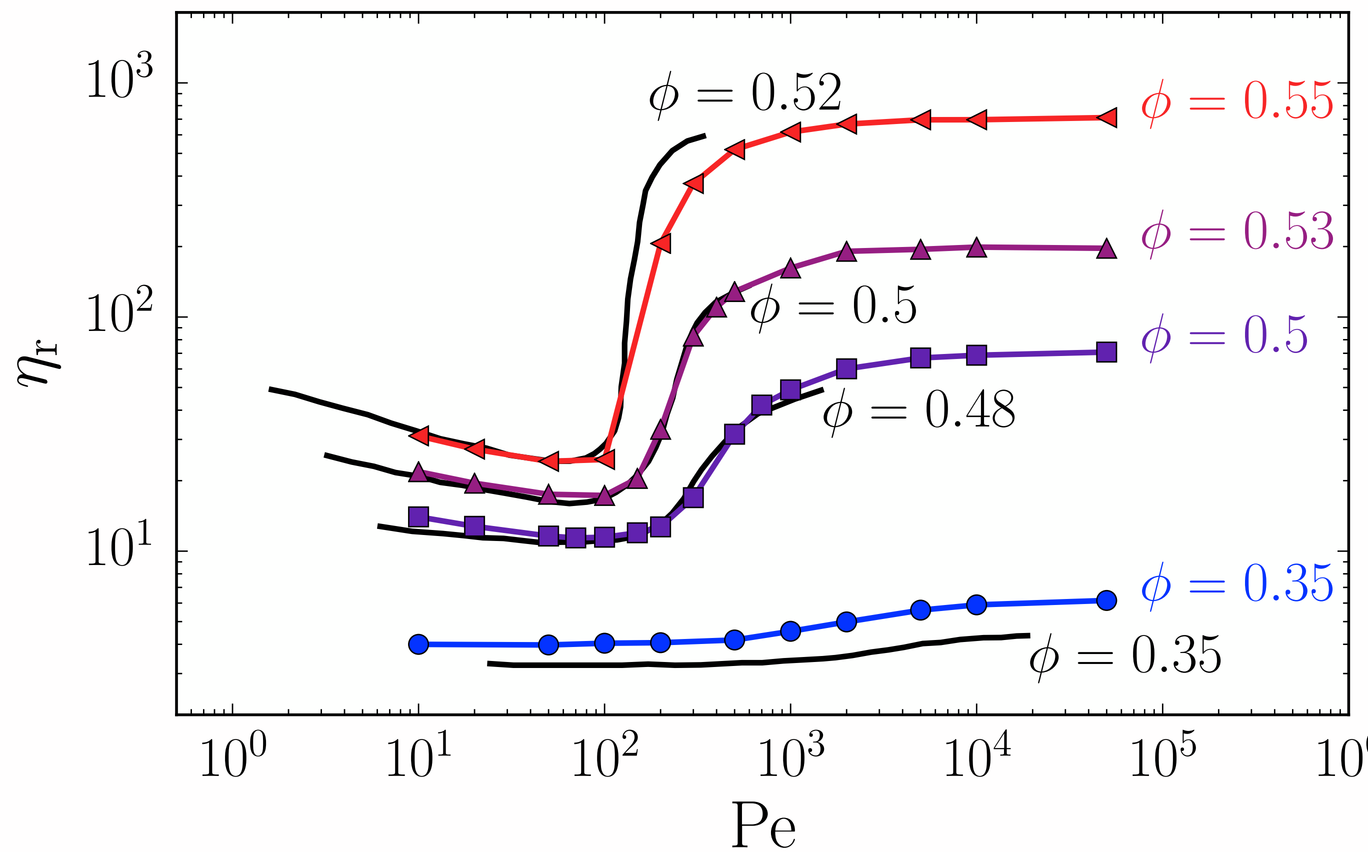
Prof. Wagner's group

To match experimental data

Stokesian Dynamic + DEM



$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{B}} + \boldsymbol{F}_{\mathrm{C}} + \boldsymbol{F}_{\mathrm{R}} = \boldsymbol{0}$$



Experimental data
black-solid lines

Cwalina and Wagner, JOR (2014)

- Introduction—a bit of history
- Modeling strategy to capture dynamics of colloids (Modified Stokesian Dynamics)
- Flow in a Widegap Couette cell

Mechanical properties of fluid materials

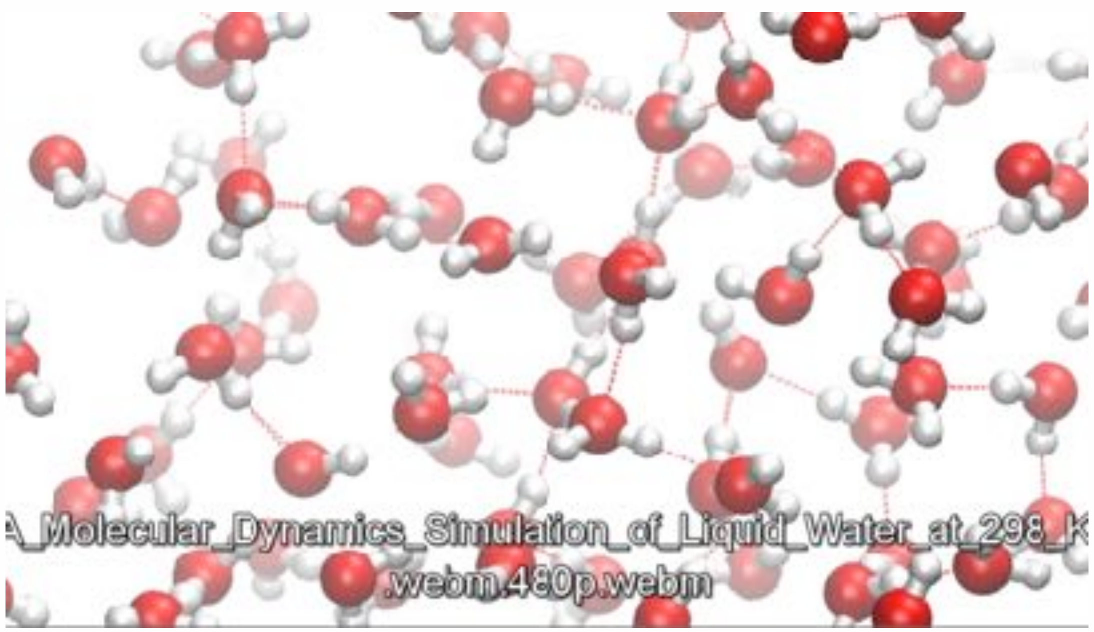
Liquid

Newtonian

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta\boldsymbol{D}$$

$$\boldsymbol{D} \equiv \frac{1}{2}\left(\nabla \boldsymbol{u}[\boldsymbol{r}(t), t] + \nabla \boldsymbol{u}^{\mathrm{T}}[\boldsymbol{r}(t), t]\right)$$

Molcular dynamics



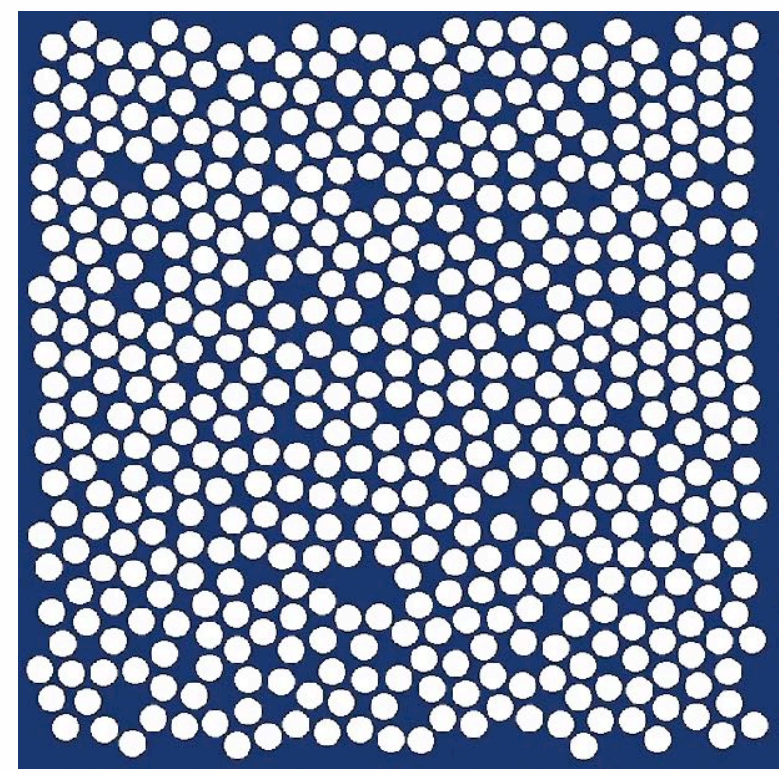
$$\frac{\textbf{mean free path}^2}{\textbf{velocity}} \sim 10^{-11}\,[\mathrm{s}]$$

Suspensions

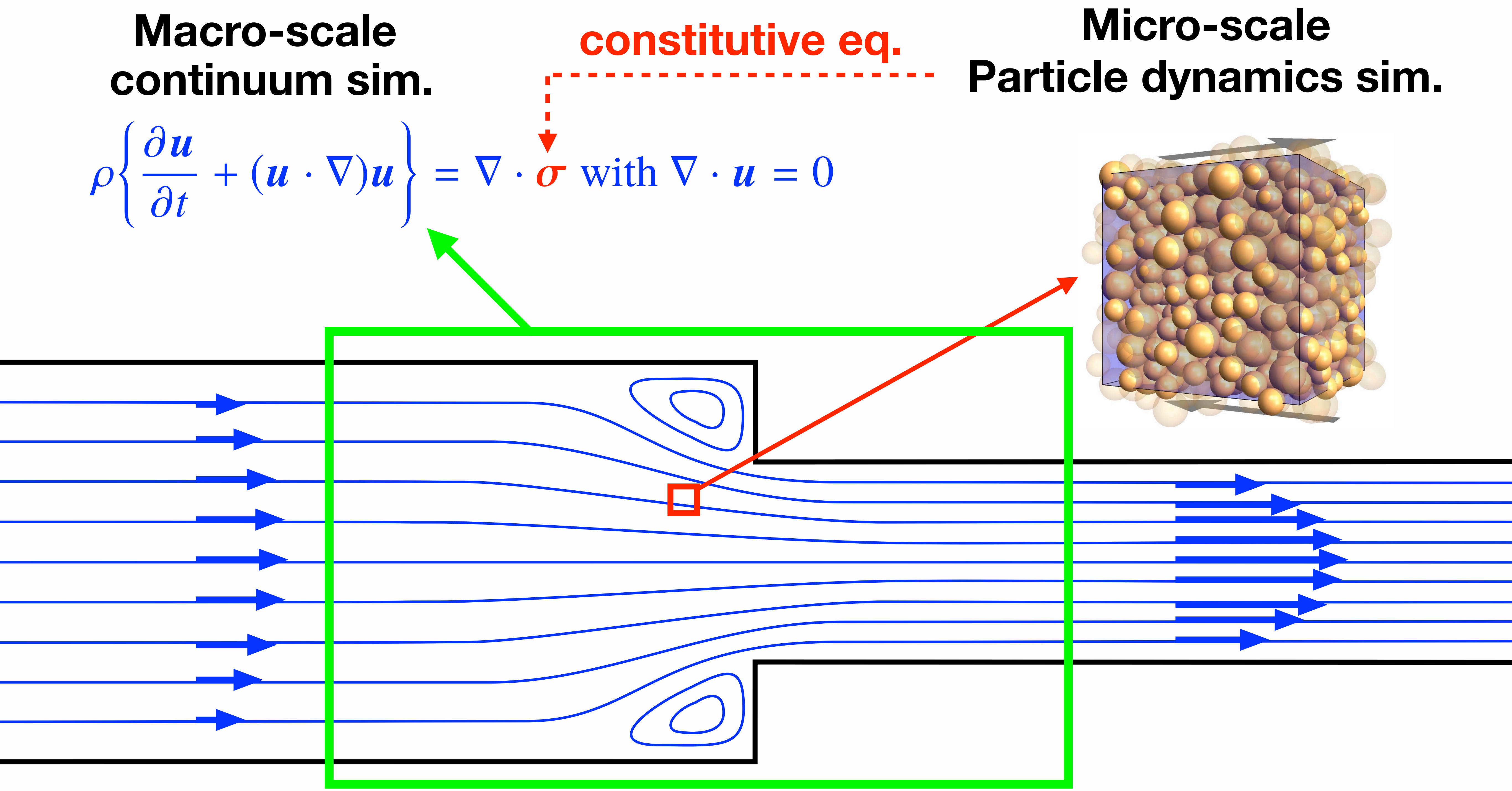
Non-Newtonian

?

Stokesian dynamics

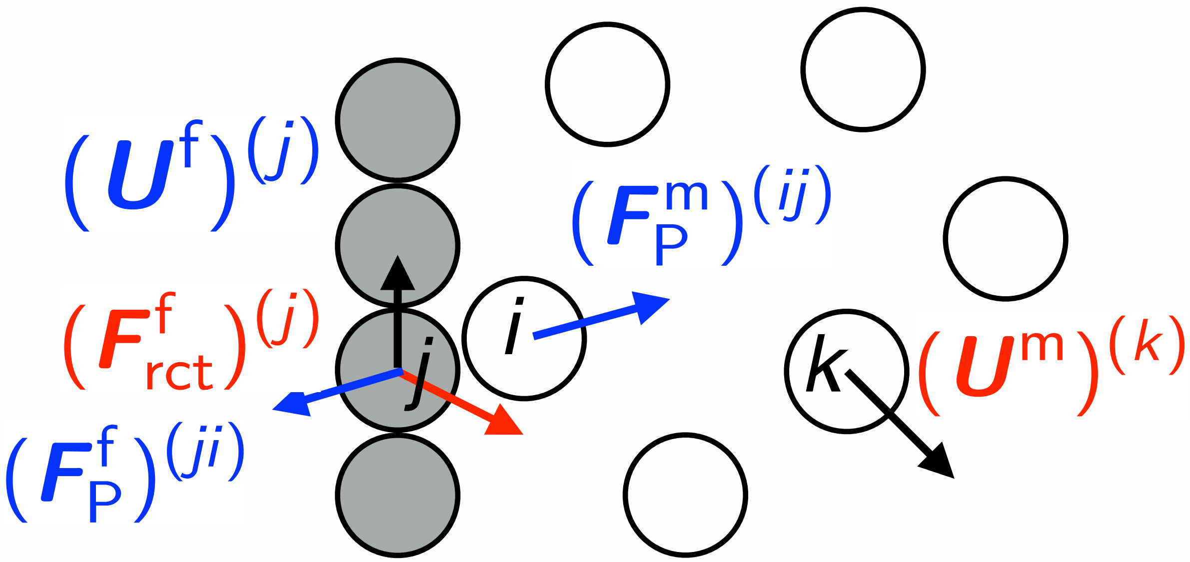


$$\frac{\textbf{radius}^2}{\textbf{diffusion constant}} \sim 1\,[\mathrm{s}]$$


Macro-scale
continuum sim.
constitutive eq.
Micro-scale
Particle dynamics sim.
$\rho\left\{\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right\} = \nabla\cdot\boldsymbol{\sigma}$ with $\nabla\cdot\boldsymbol{u} = 0$

Force-balance dynamics with fixed particles

- ○ Velocities of mobile particles to be solved: $\boldsymbol{U}^{\mathrm{m}} = (\boldsymbol{U}^{(1)}, \dots, \boldsymbol{U}^{(n)})$
- ● Velocities of fixed particles: $\boldsymbol{U}^{\mathrm{f}} = (\boldsymbol{U}^{(n+1)}, \dots, \boldsymbol{F}^{(n+m)})$



known $(\boldsymbol{U}^{\mathrm{f}}, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{m}}, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{f}})$

to find $(\boldsymbol{U}^{\mathrm{m}}, \boldsymbol{F}_{\mathrm{rct}}^{\mathrm{f}})$

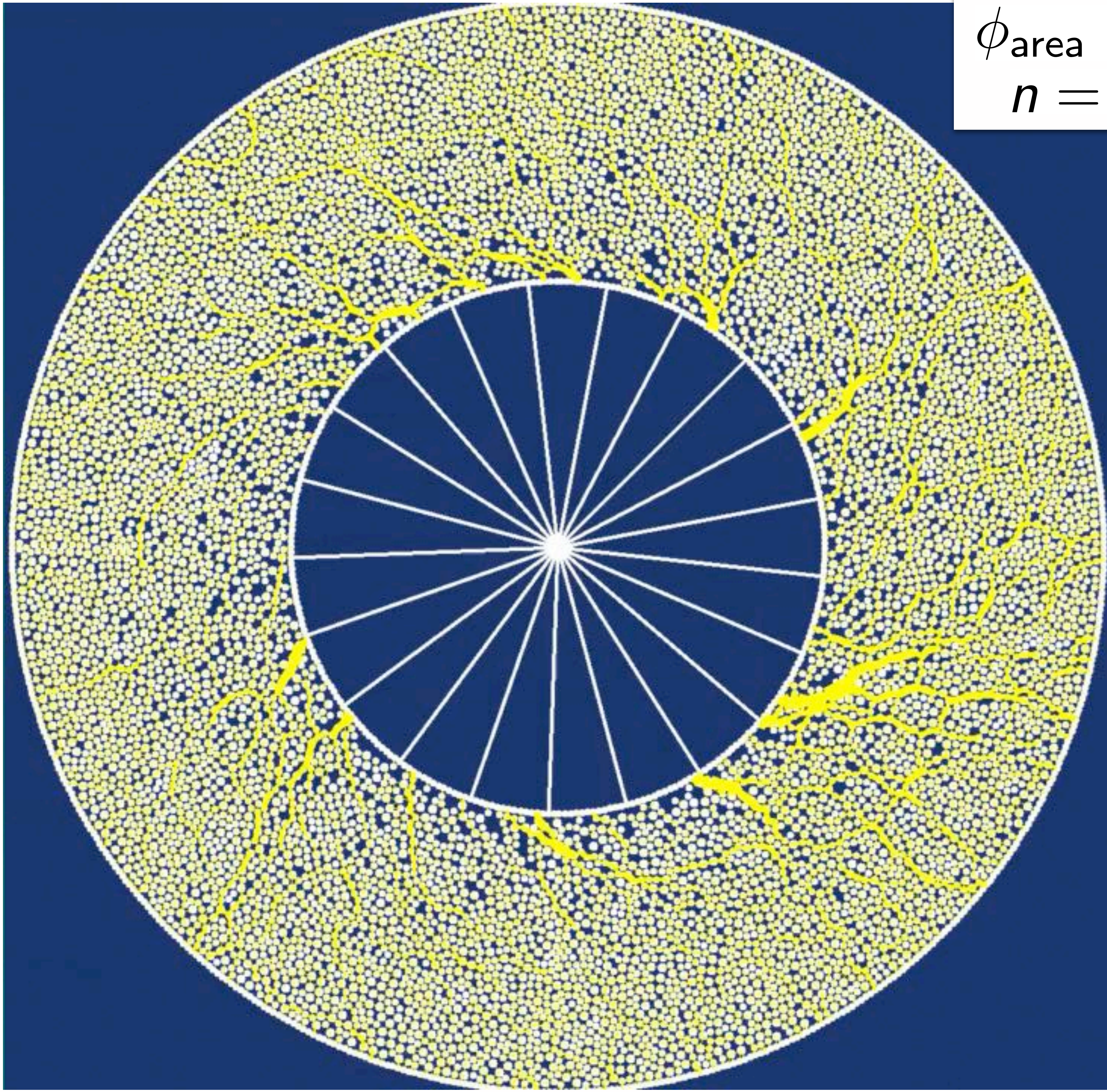
$\boldsymbol{F}_{\mathrm{P}}$: interparticle forces (and torques)

force balance equations

$$\begin{cases} \begin{pmatrix} \boldsymbol{F}_{\mathrm{H}}^{\mathrm{m}} \\ \boldsymbol{F}_{\mathrm{H}}^{\mathrm{f}} \end{pmatrix} + \begin{pmatrix} \boldsymbol{F}_{\mathrm{P}}^{\mathrm{m}} \\ \boldsymbol{F}_{\mathrm{P}}^{\mathrm{f}} \end{pmatrix} + \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{F}_{\mathrm{rct}}^{\mathrm{f}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{0} \end{pmatrix} \\ \begin{pmatrix} \boldsymbol{F}_{\mathrm{H}}^{\mathrm{m}} \\ \boldsymbol{F}_{\mathrm{H}}^{\mathrm{f}} \end{pmatrix} = - \begin{pmatrix} \boldsymbol{R}_{FU}^{\mathrm{mm}} & \boldsymbol{R}_{FU}^{\mathrm{mf}} \\ \boldsymbol{R}_{FU}^{\mathrm{fm}} & \boldsymbol{R}_{FU}^{\mathrm{ff}} \end{pmatrix} \begin{pmatrix} \boldsymbol{U}^{\mathrm{m}} \\ \boldsymbol{U}^{\mathrm{f}} \end{pmatrix} \end{cases}$$

step1 $\boldsymbol{U}^{\mathrm{m}} = (\boldsymbol{R}_{FU}^{\mathrm{mm}})^{-1} \left(\boldsymbol{F}_{\mathrm{P}}^{\mathrm{m}} - \boldsymbol{R}_{FU}^{\mathrm{mf}} \boldsymbol{U}^{\mathrm{f}} \right)$ *dynamics*

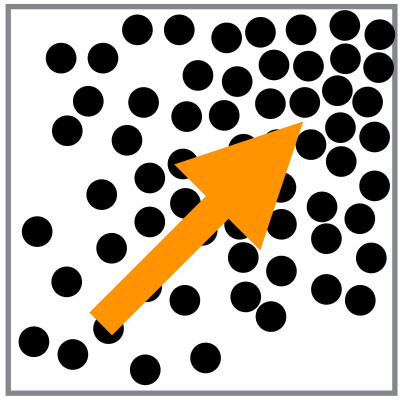
step2 $\boldsymbol{F}_{\mathrm{rct}}^{\mathrm{f}} = \boldsymbol{R}_{FU}^{\mathrm{fm}} \boldsymbol{U}^{\mathrm{m}} + \boldsymbol{R}_{FU}^{\mathrm{ff}} \boldsymbol{U}^{\mathrm{f}} - \boldsymbol{F}_{\mathrm{P}}^{\mathrm{f}}$ *used in rheology*

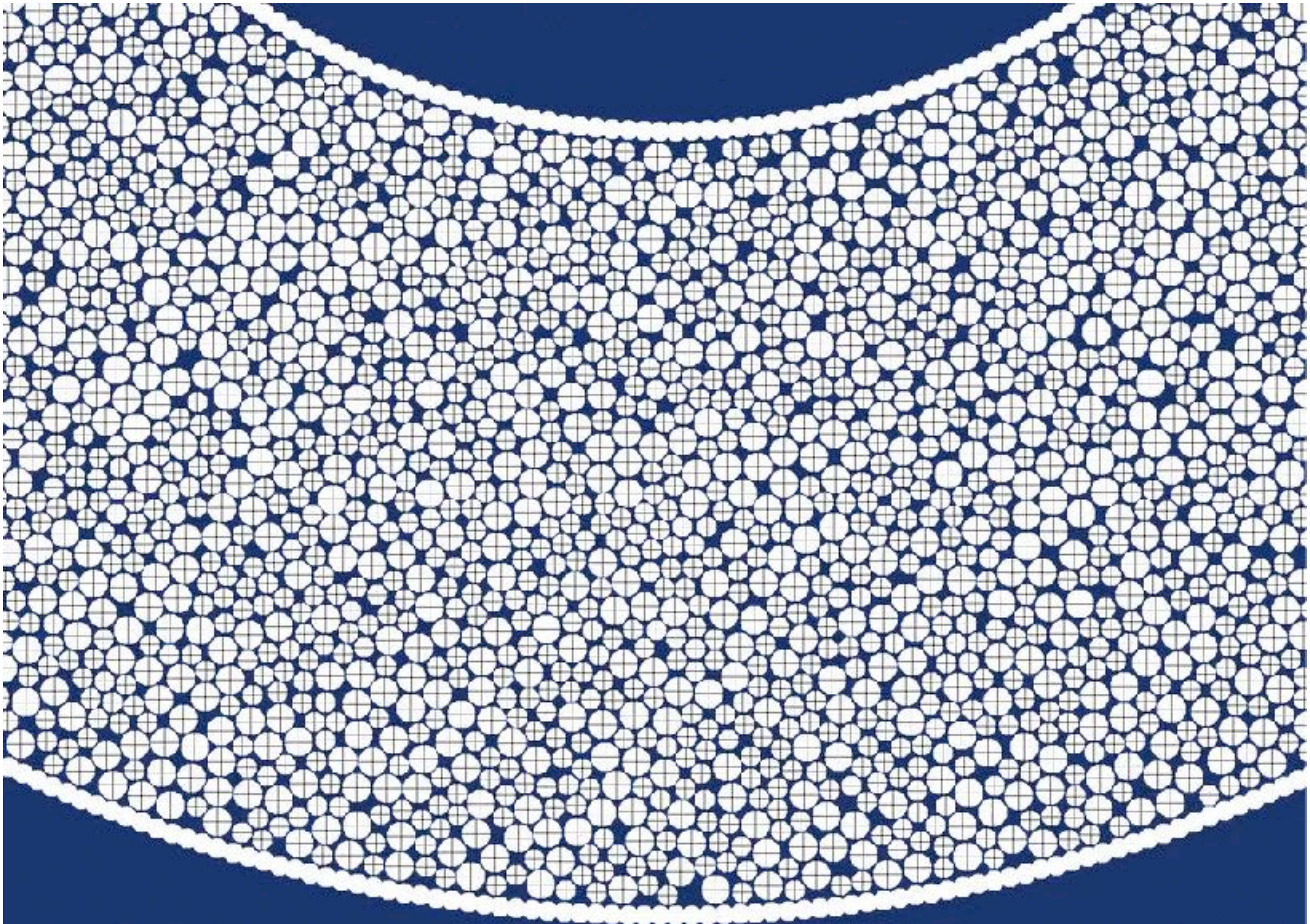


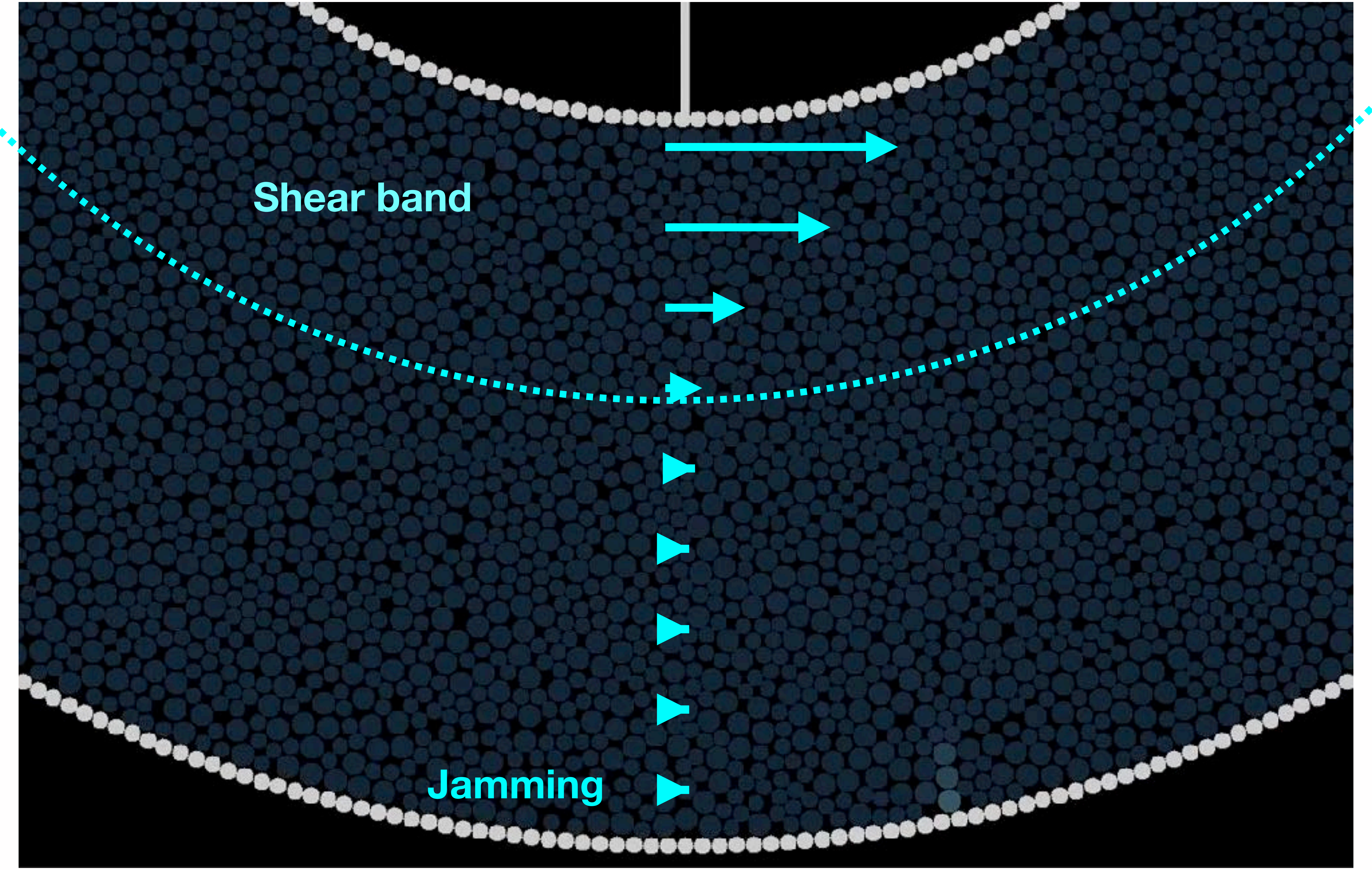
$\phi_{\text{area}} = 0.78$
$n = 9000$

Migration

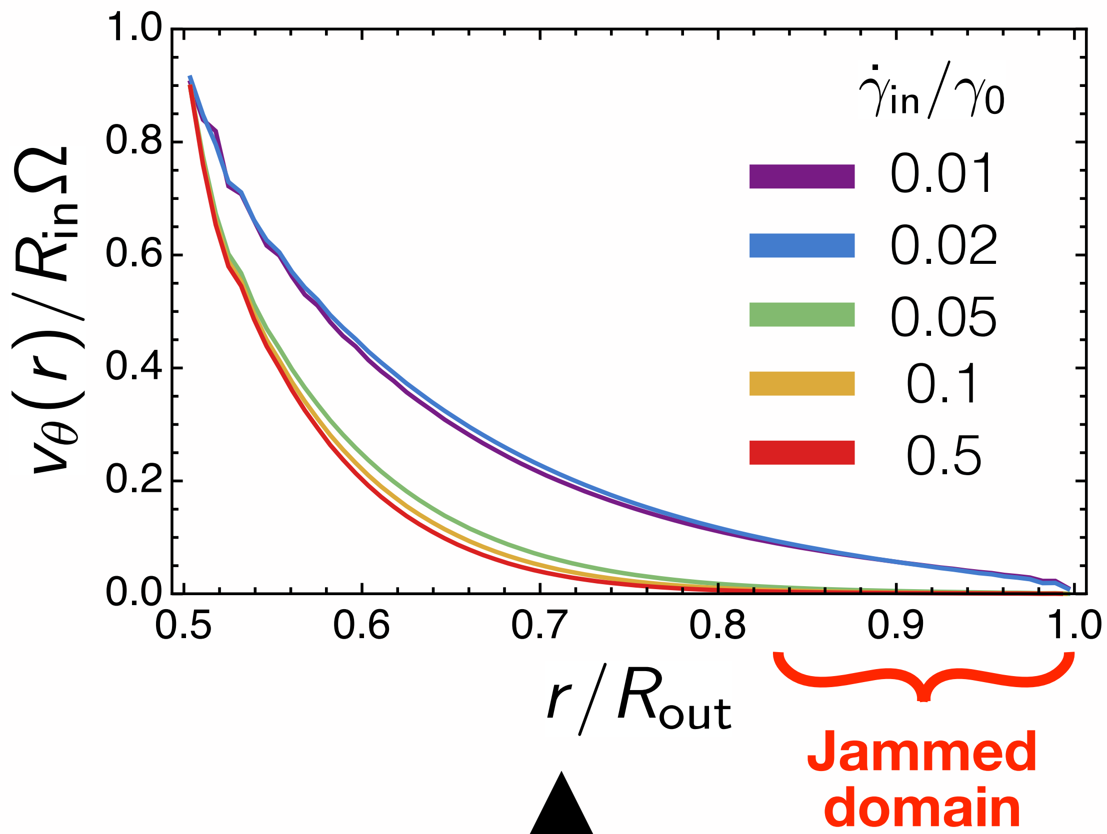
$$j_{\text{radial}} = \frac{2a^2}{9\eta_0} f(\phi)\, \nabla \cdot \boldsymbol{\sigma}$$

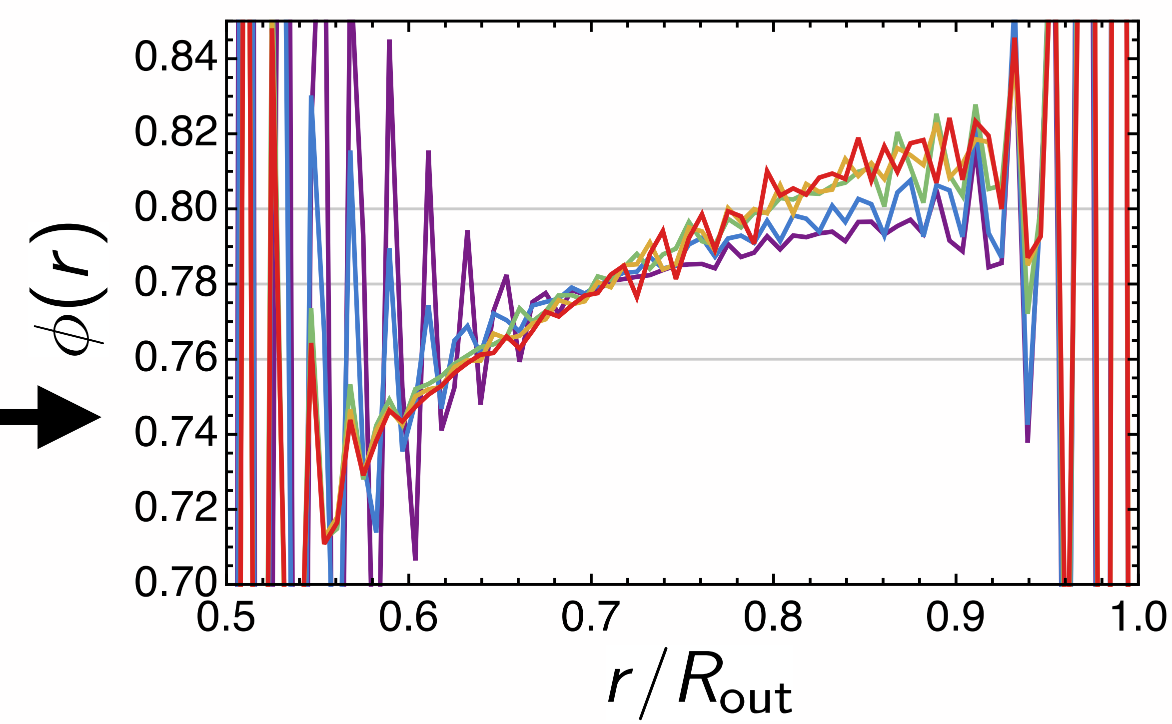


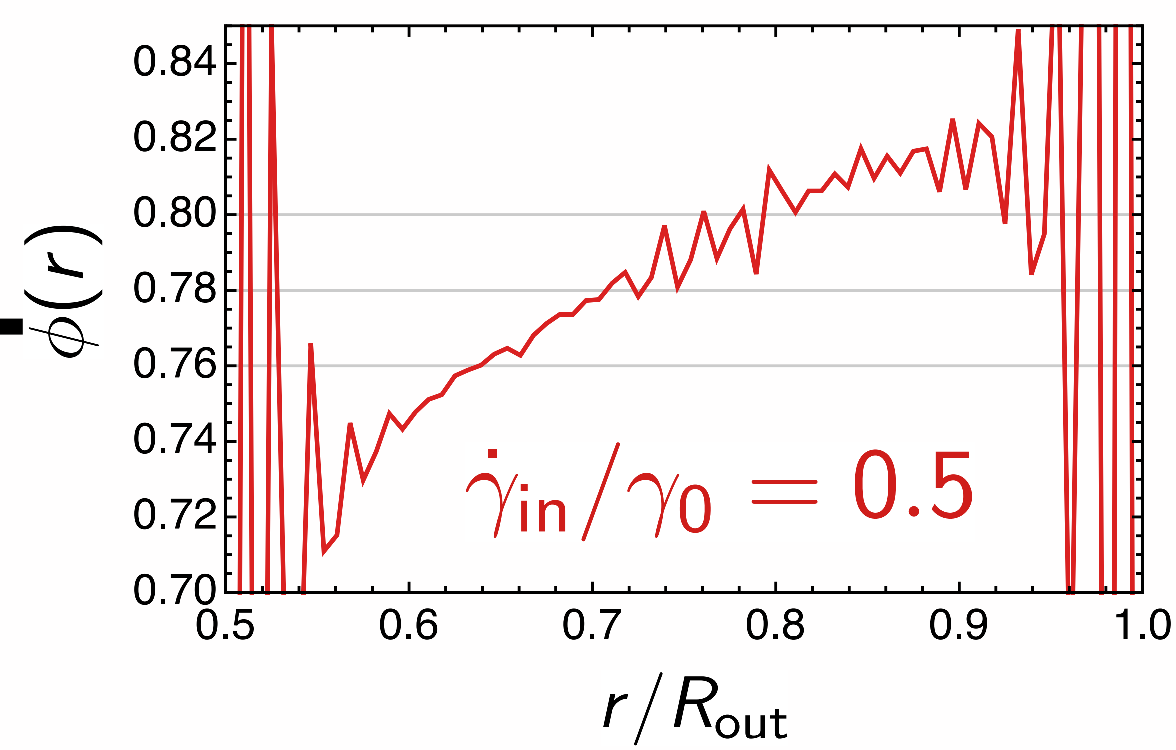



Shear band
Jamming

Monolayer simulation for wide-gap Couette cells







$$\eta(r) = \eta(\phi(r))$$

local viscosity

Summary

Simulation models for colloidal suspensions
are very different from MD simulations. (Particles are not points)

We introduced a Modified Stokesian Dynamics simulation.
- A realistic choice to avoid lubrication singularity
- Various possibilities for contact interaction between colloids
- Additional force is essential for rate-dependence

Although we now know rheology of dense suspensions well,
we know little about fluid mechanics of dense suspensions