A simulation study on shear thickening in wide-gap Couette geometry

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$$\rho \left\{ \frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} \right\} = -\nabla p + \eta_0 \nabla^2 \boldsymbol{u}, \quad \nabla \cdot \boldsymbol{u} = 0$$

$$\downarrow$$

$$\mathrm{Re} \equiv \frac{L_0 U_0}{\eta_0/\rho}$$

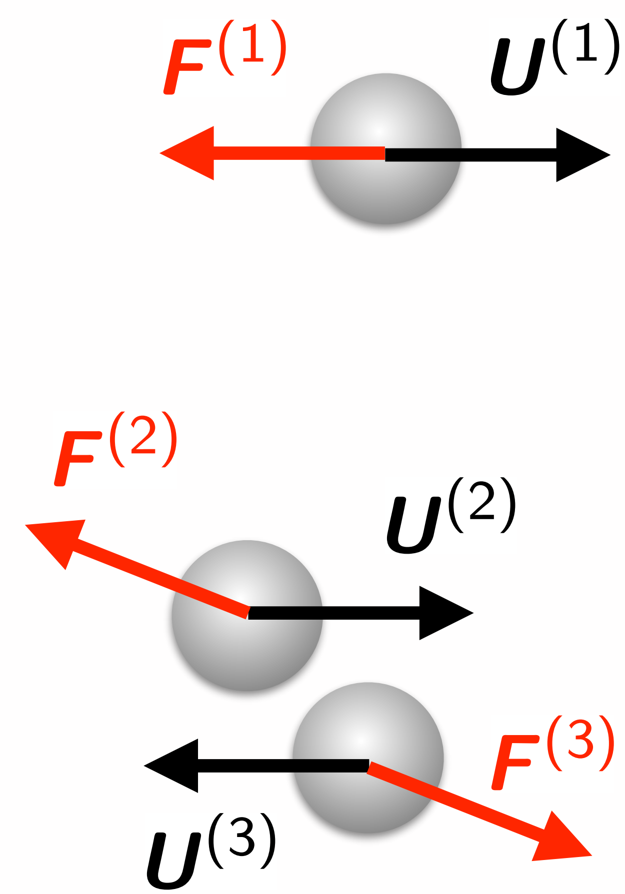
$$\mathrm{Re} \left\{ \frac{\partial \tilde{\boldsymbol{u}}}{\partial \tilde{t}} + (\tilde{\boldsymbol{u}} \cdot \tilde{\nabla})\tilde{\boldsymbol{u}} \right\} = -\tilde{\nabla}\tilde{p} + \tilde{\nabla}^2 \tilde{\boldsymbol{u}}$$

$$\downarrow \quad \mathrm{Re} \to 0$$

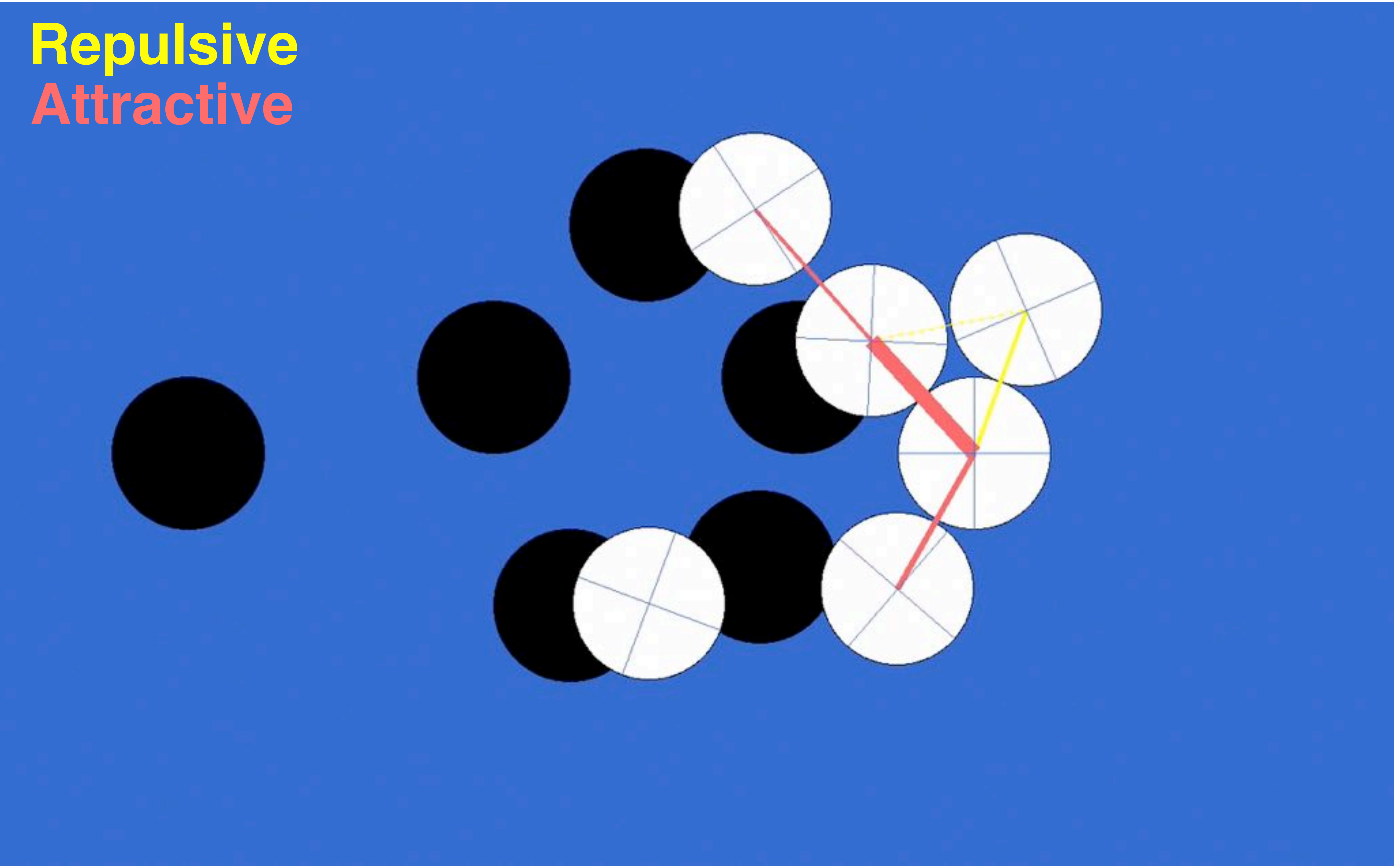
$$\mathbf{0} = -\tilde{\nabla}\tilde{p} + \tilde{\nabla}^2 \tilde{\boldsymbol{u}}$$

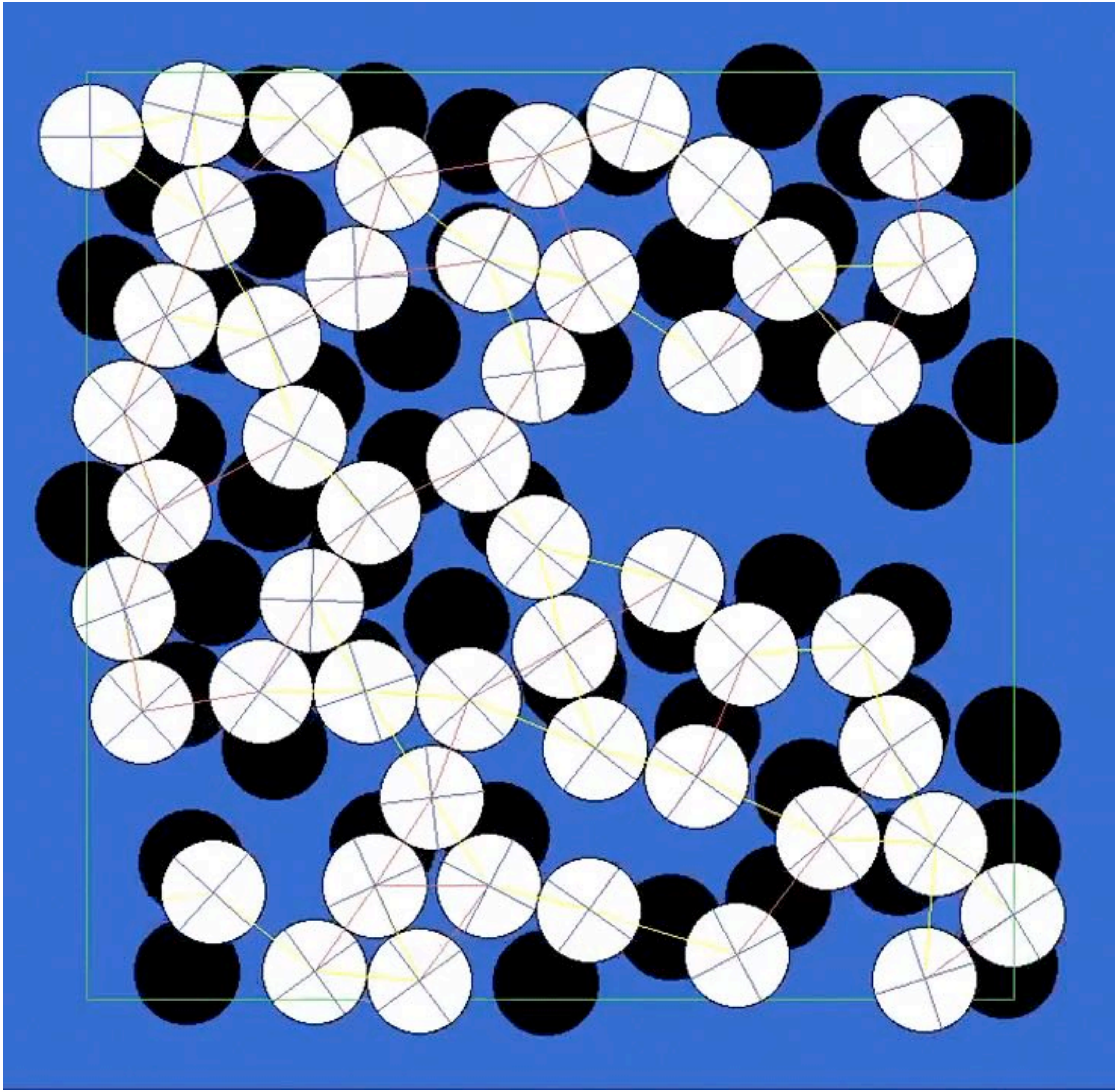
$$\downarrow$$

$$\begin{pmatrix} \boldsymbol{F}^{(1)} \\ \vdots \\ \boldsymbol{F}^{(n)} \\ \boldsymbol{T}^{(1)} \\ \vdots \\ \boldsymbol{T}^{(n)} \end{pmatrix} = -\boldsymbol{R}_{FU} \begin{pmatrix} \boldsymbol{U}^{(1)} \\ \vdots \\ \boldsymbol{U}^{(n)} \\ \boldsymbol{\Omega}^{(1)} \\ \vdots \\ \boldsymbol{\Omega}^{(n)} \end{pmatrix}$$

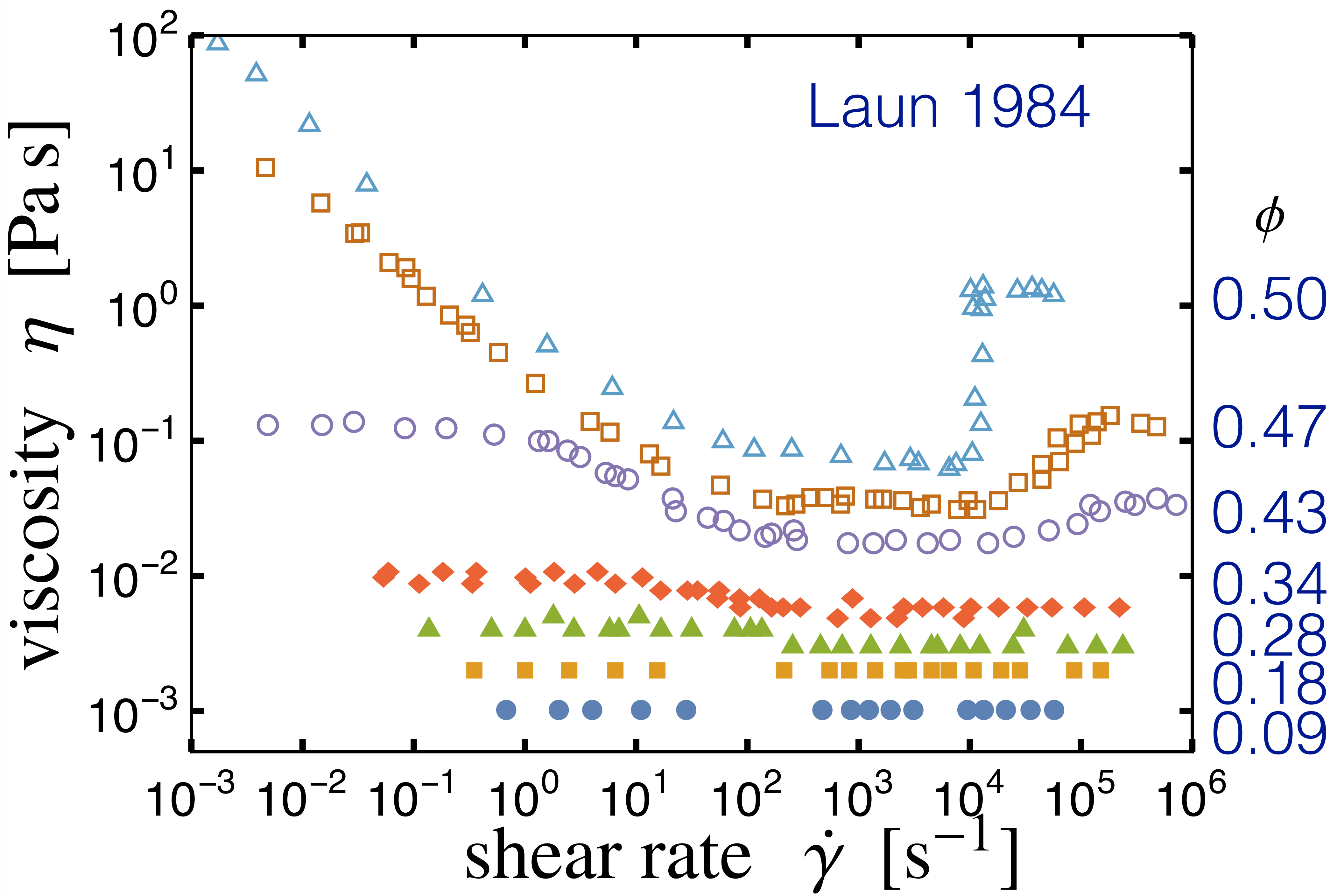


Stokes flow: Zero-Reynolds number fluid mechanics

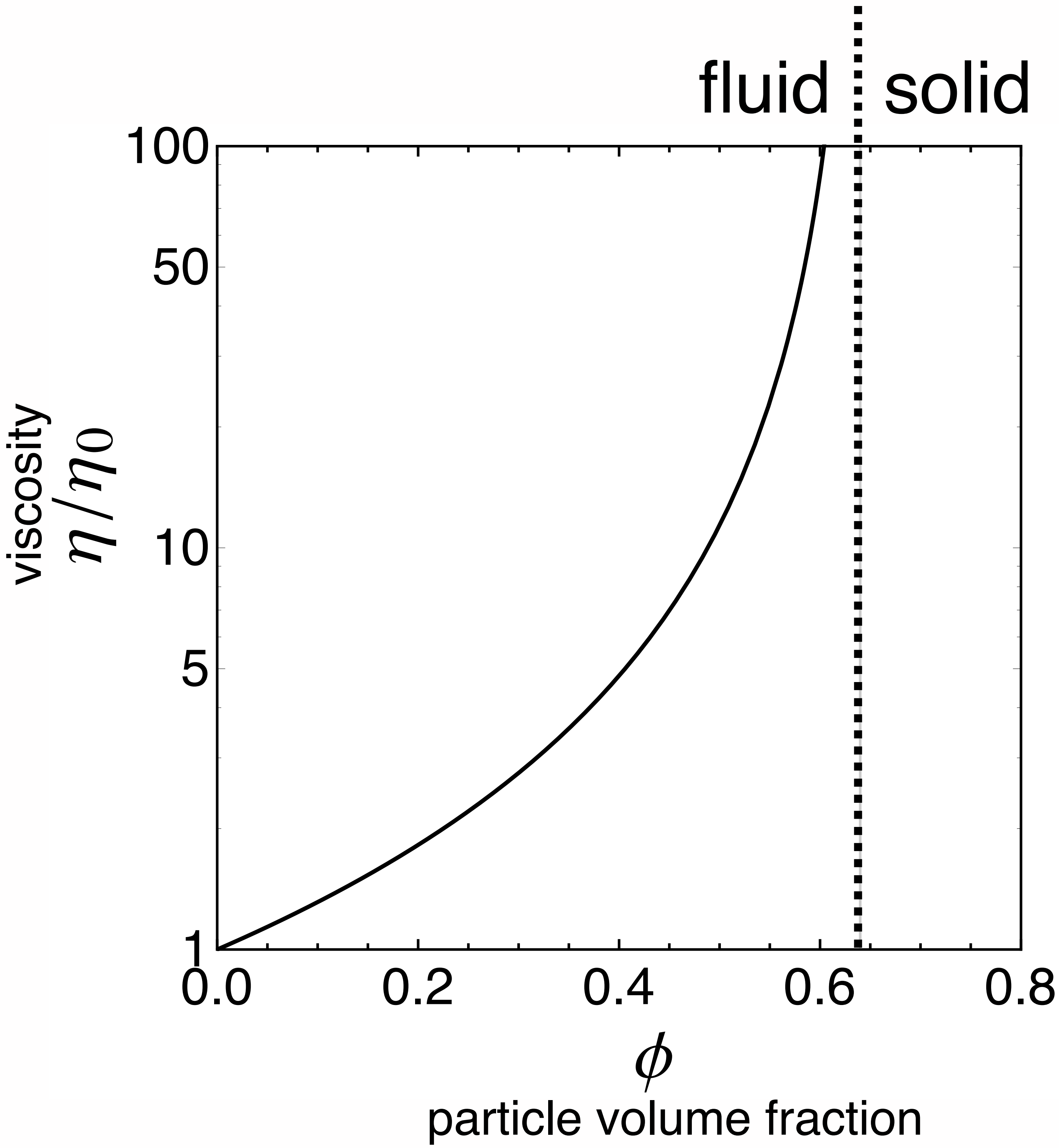




The effective shear viscosity η of a colloidal suspension of rigid spherical particles in a Newtonian fluid can vary by orders of magnitude depending on how rapidly it is sheared, as characterized by the applied shear rate $\dot{\gamma}$.



Jamming transition



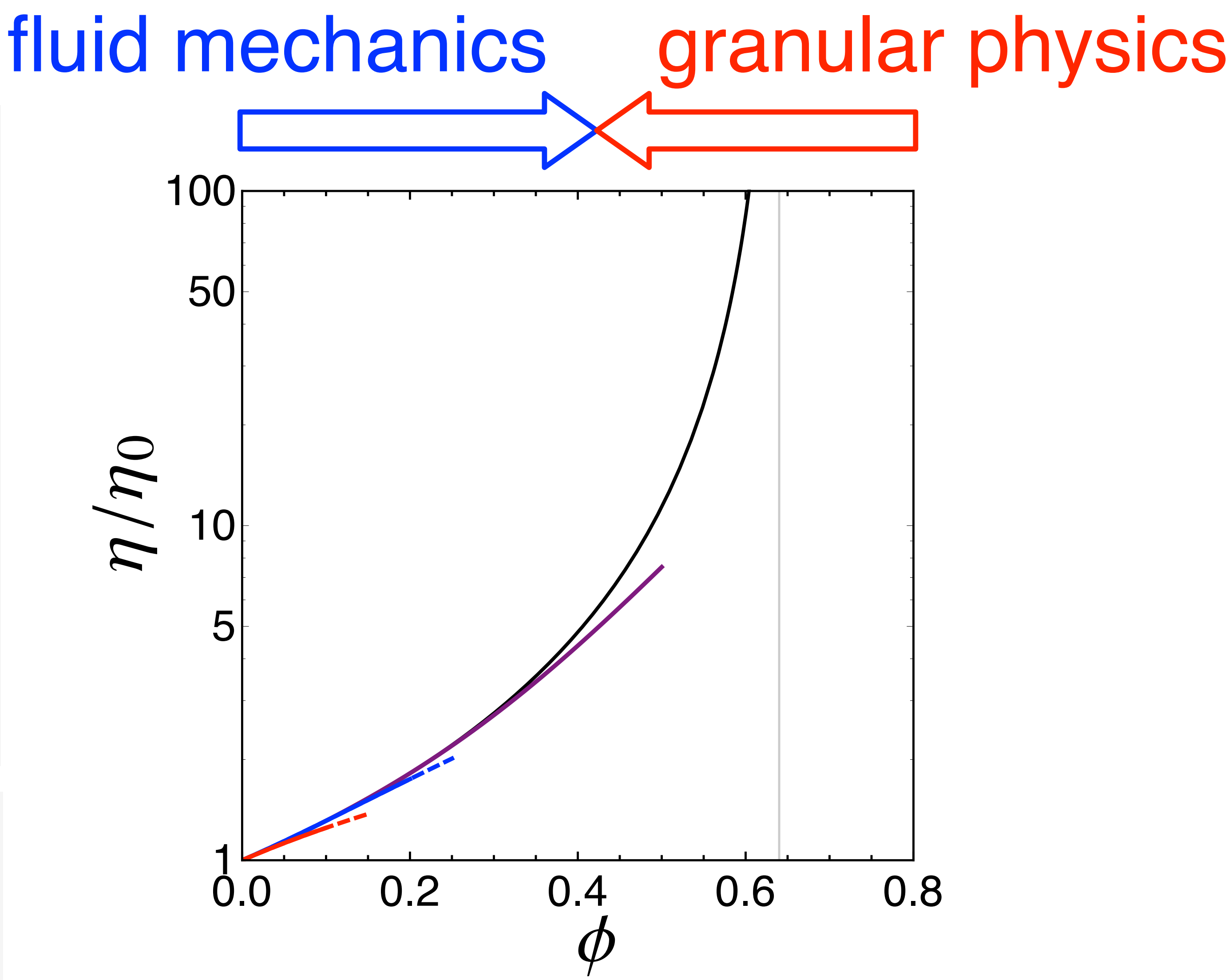
Coupled SD-DEM — Seto, Mari, Morris & Denn (2013) and Mari, Seto, Morris & Denn (2014, 2015)

Stokesian Dynamics

- Hydrodynamic interactions
  ~~far field~~ + lubrication
- Overdamped dynamics
- (Repulsive interparticle forces)
- (Brownian motion)

Discrete Element Method

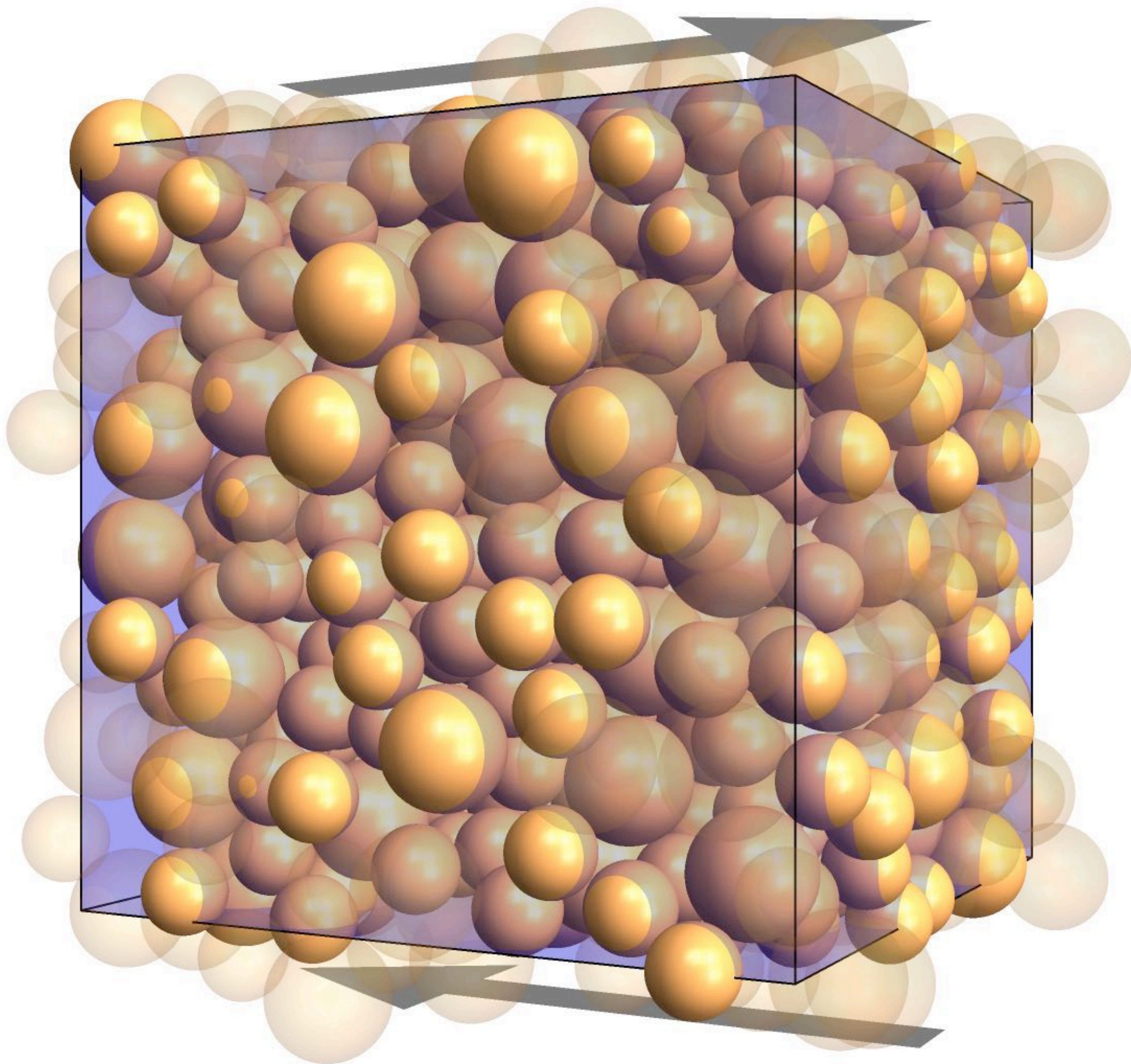
- Contact forces
  stiff sphere + friction
- ~~Inertia of particles~~

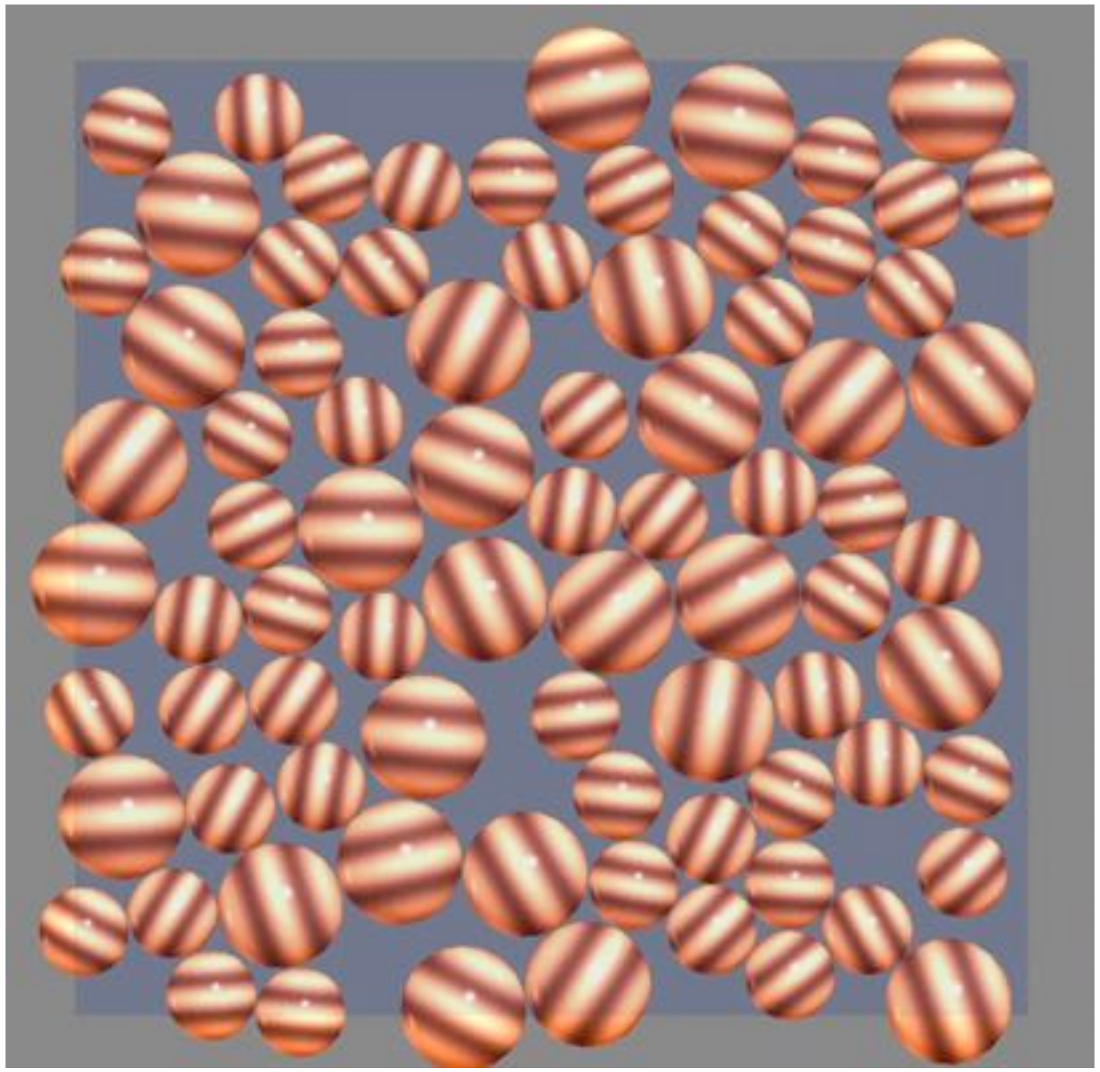


SD-DEM simulation

- 2-d and 3-d simulations
- $N = 500\text{–}3000$
- Bidisperse ($a_2/a_1 = 1.4$, $\phi_2 = \phi_1 = 0.5\phi$)
- Lees–Edwards periodic boundary conditions
- Rate-controlled and stress-controlled simulations

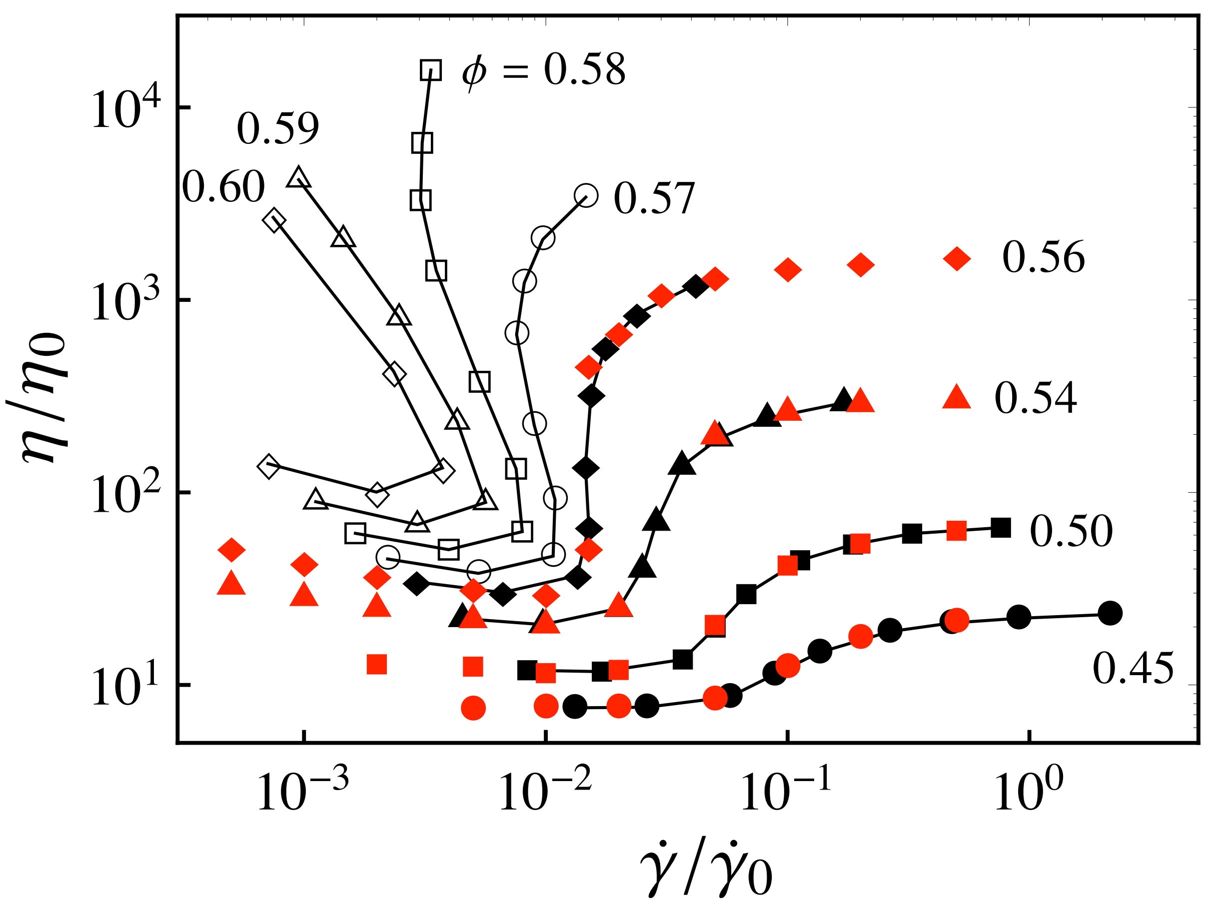
Friction!





Particle simulations for local rheology

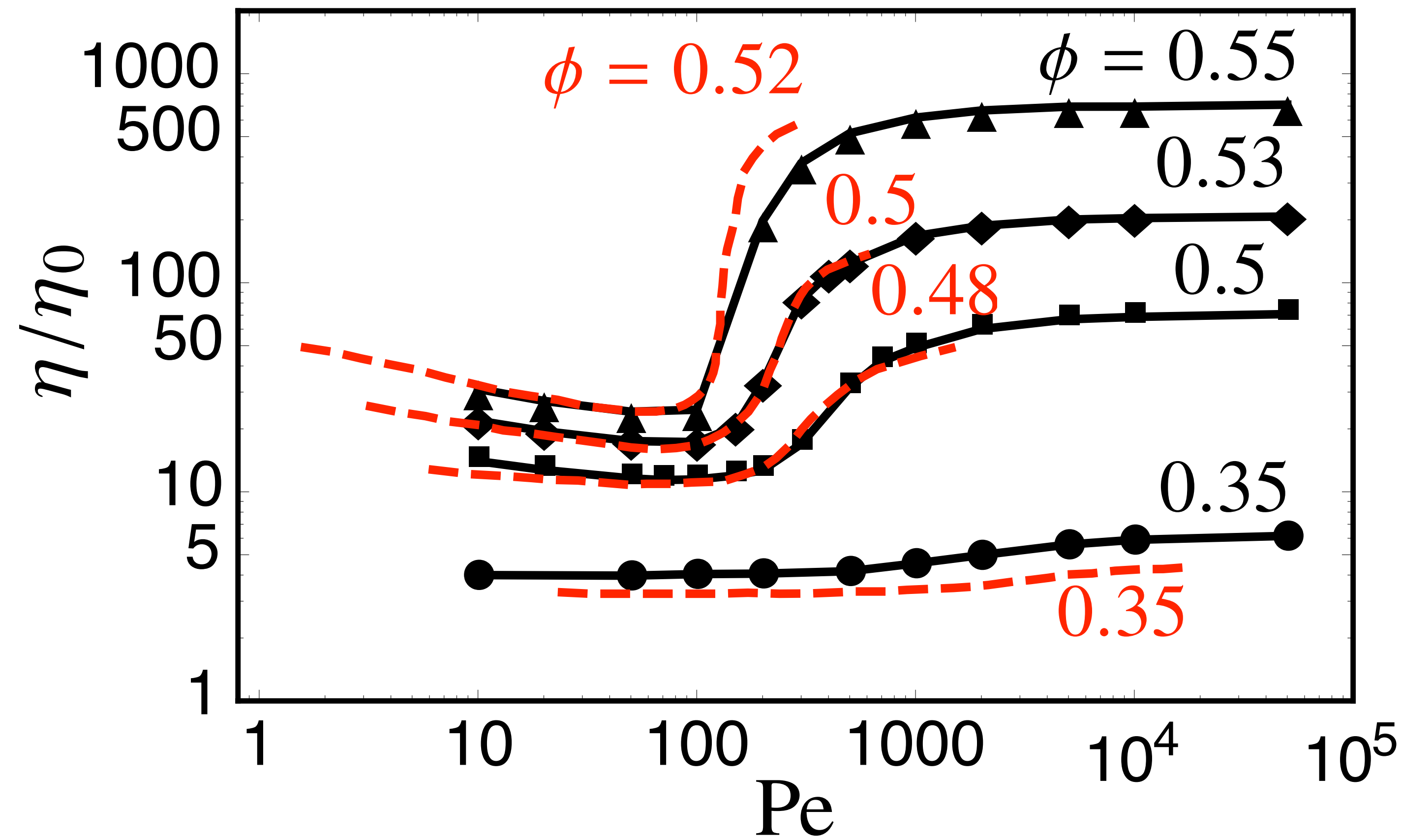
Stress controlled
vs rate controlled



PRE 2015

S-shaped rheology curves

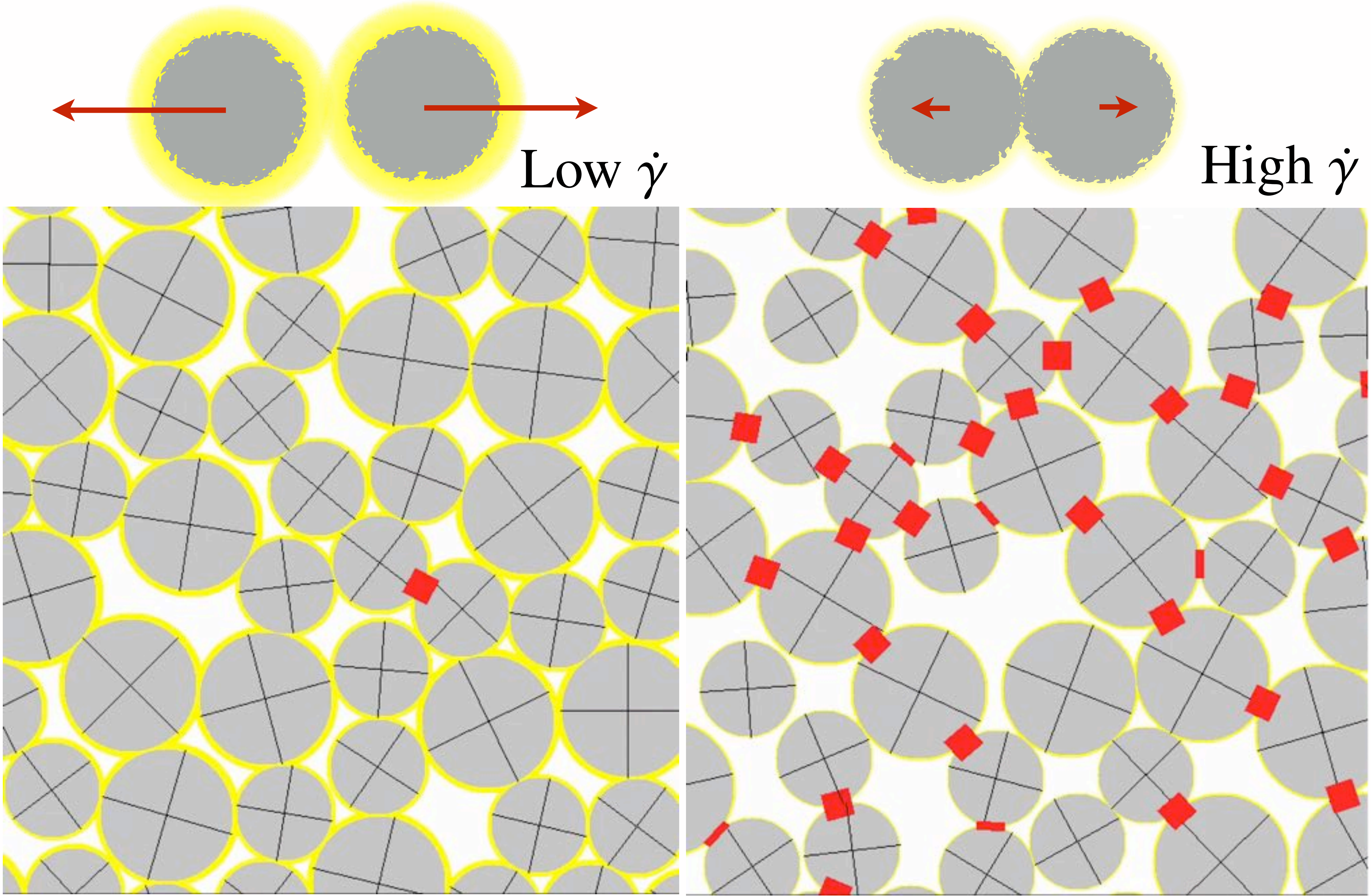
simulation
vs experiment

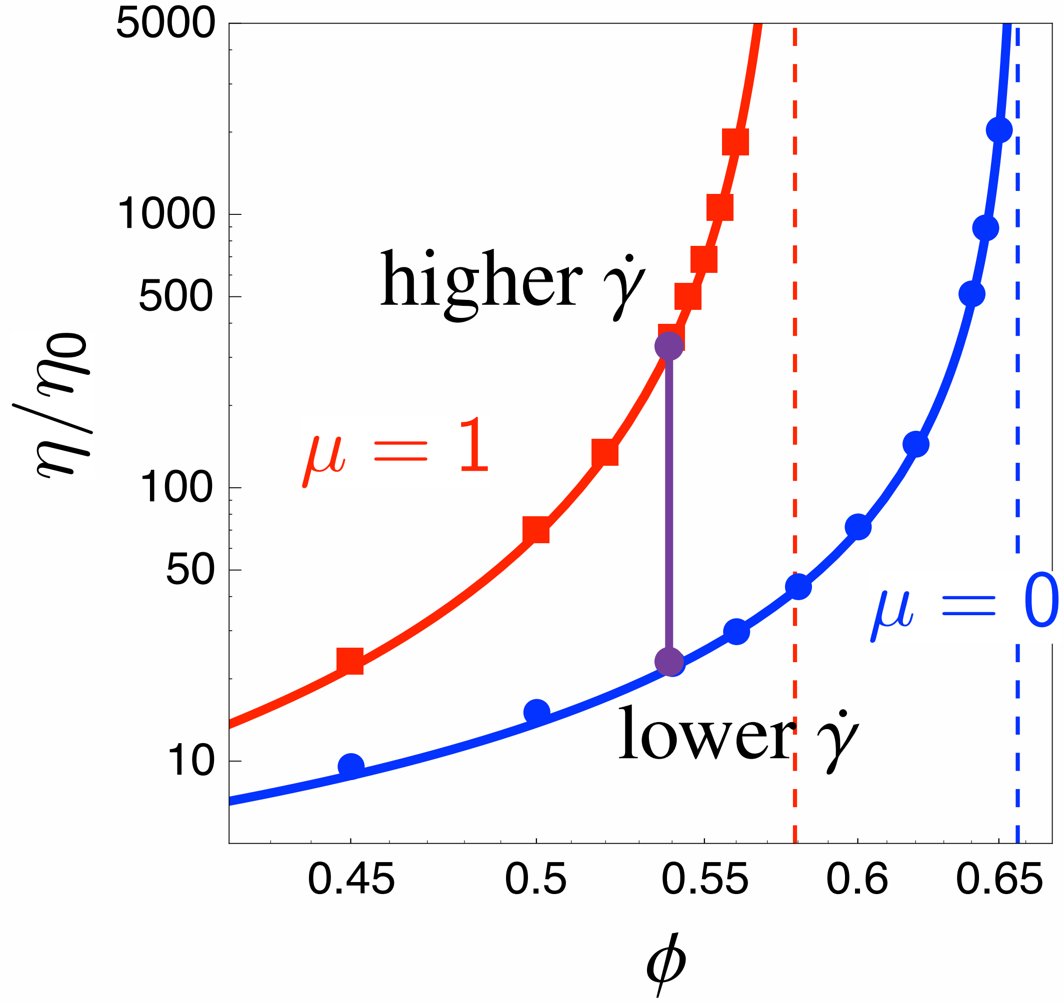


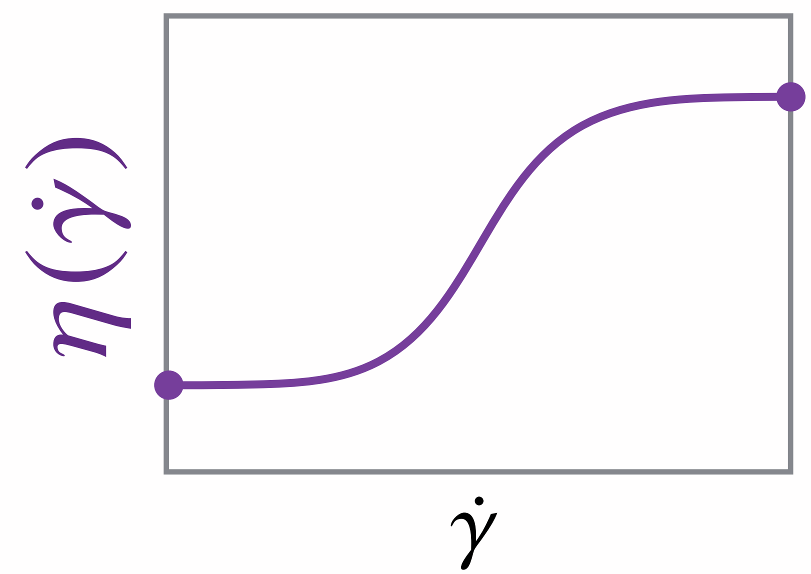
PNAS 2015

Brownian force
(+ repulsive force)

Where does the rate-dependence come from?





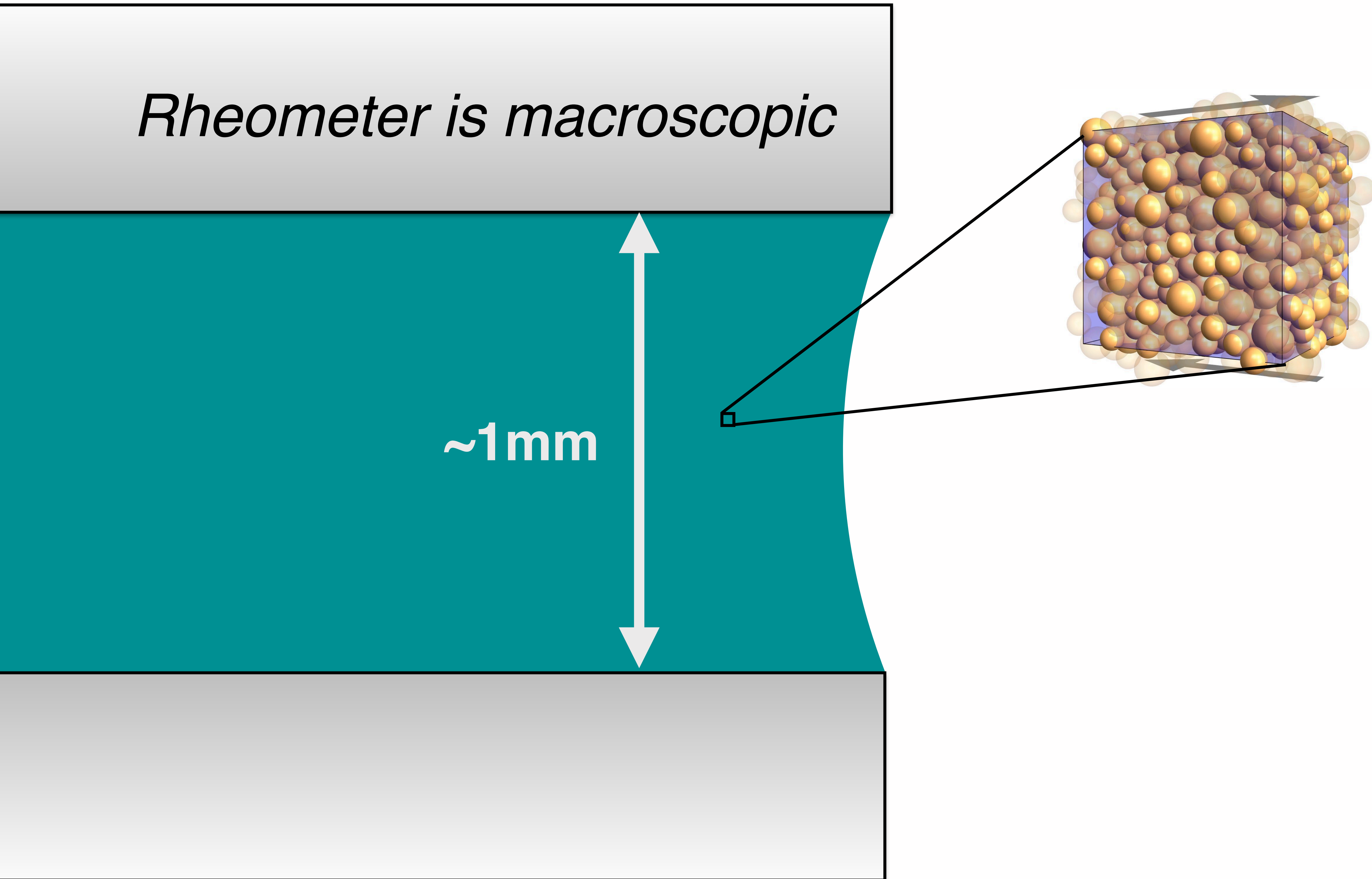


$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{C}} + \boldsymbol{F}_{\mathrm{R}} = \boldsymbol{0} \longrightarrow \tilde{\boldsymbol{F}}_{\mathrm{H}} + \tilde{\boldsymbol{F}}_{\mathrm{C}} + \frac{\dot{\gamma}_0}{\dot{\gamma}} \hat{\boldsymbol{F}}_{\mathrm{R}} = \boldsymbol{0}$$

hydrodyn. *repulsive*

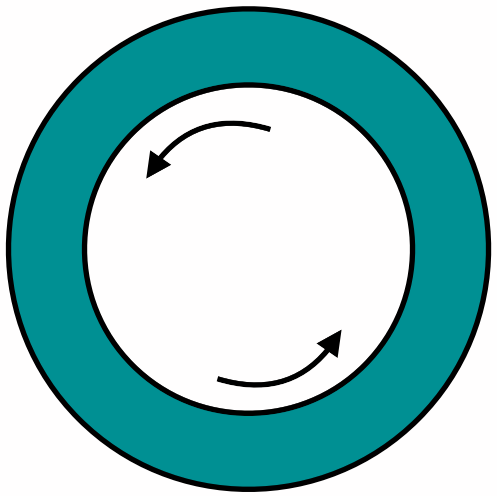
contact

If macroscopic rheology = local rheology,
our simulation can reproduce rheology measurements.



However, does macroscopic rheology = local rheology?

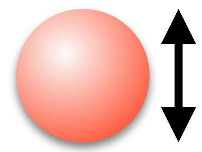
de Cagny 2015 (J. Rheol)



$R_{in} = 4.1\,\mathrm{cm}$

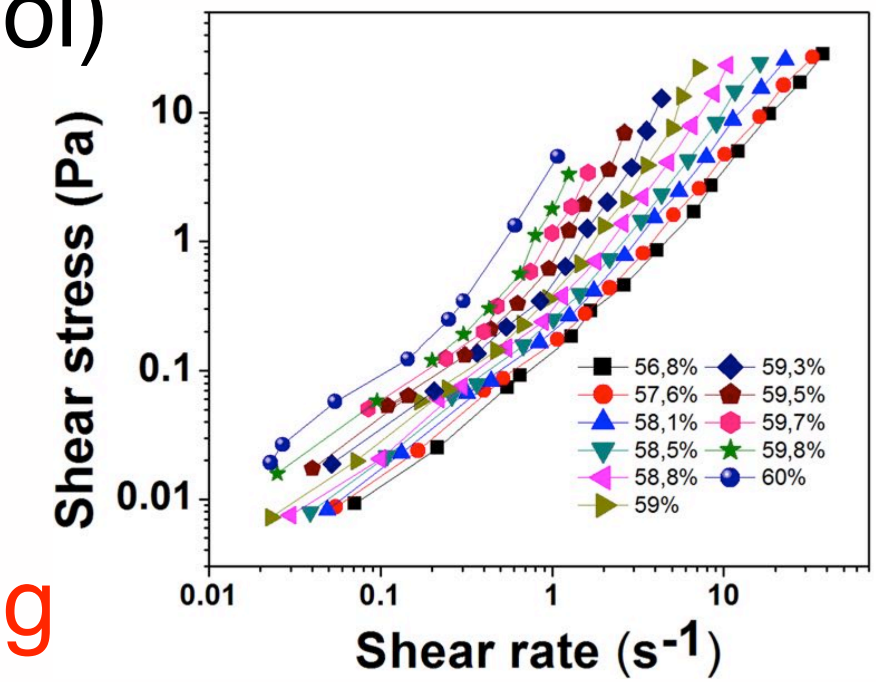
$R_{out} = 6\,\mathrm{cm}$

$R_{out} - R_{in} = 1.9\,\mathrm{cm}$

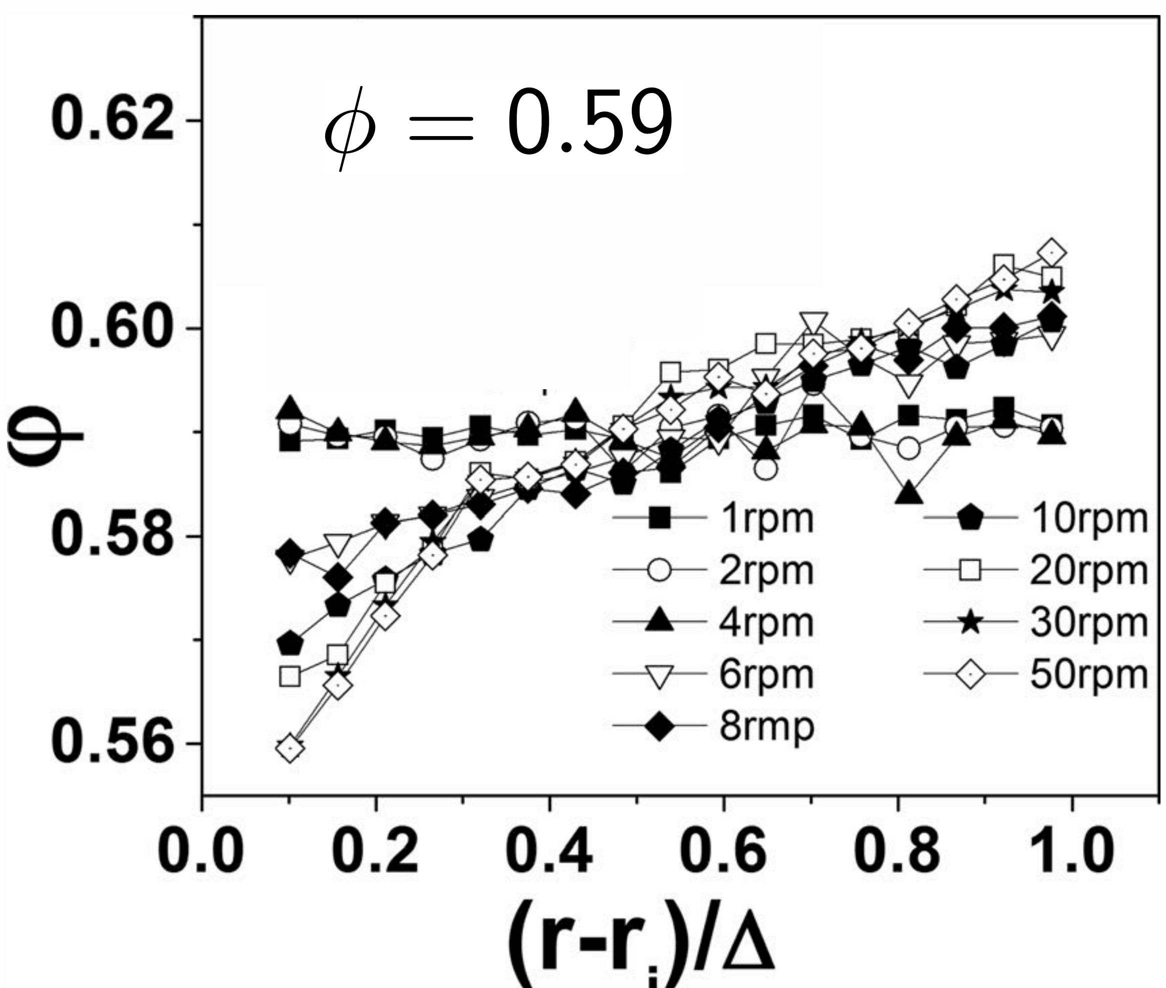


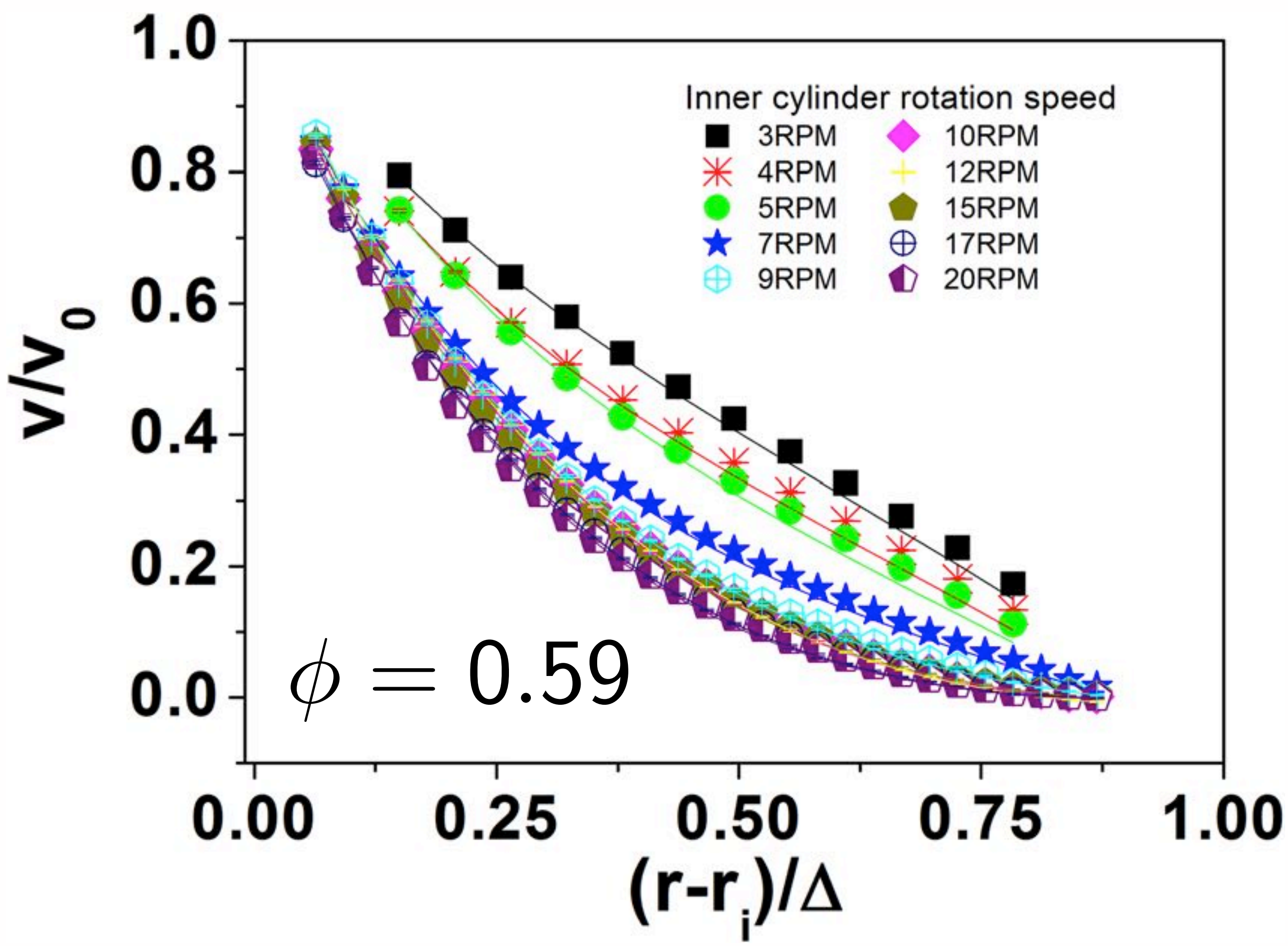
$d = 40\,\mu\mathrm{m}$

polystyrene beads



Magnetic Resonance Imaging

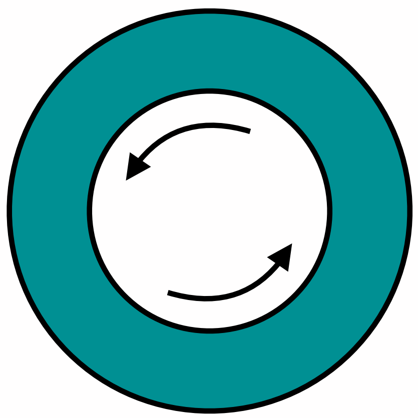




Macroscopic Discontinuous Shear Thickening

Fall 2015 (PRL)

"DST is observed only when the flow separates into a low-density flowing and a high-density jammed region"

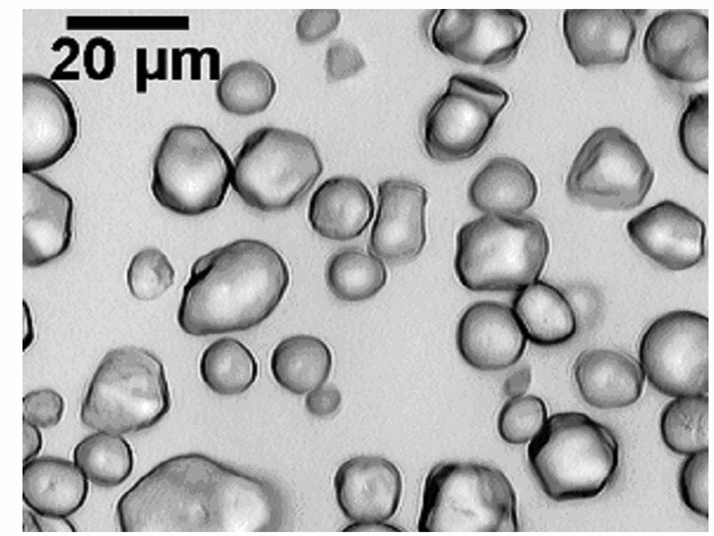


$R_{in} = 3\,\mathrm{cm}$

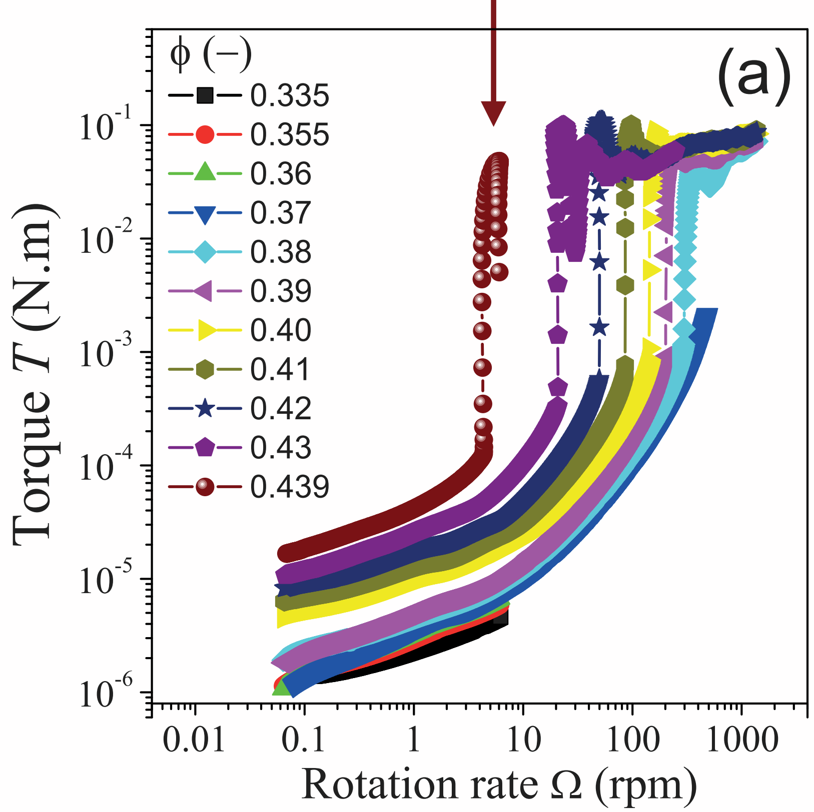
$R_{out} = 5\,\mathrm{cm}$

$R_{out} - R_{in} = 2\,\mathrm{cm}$

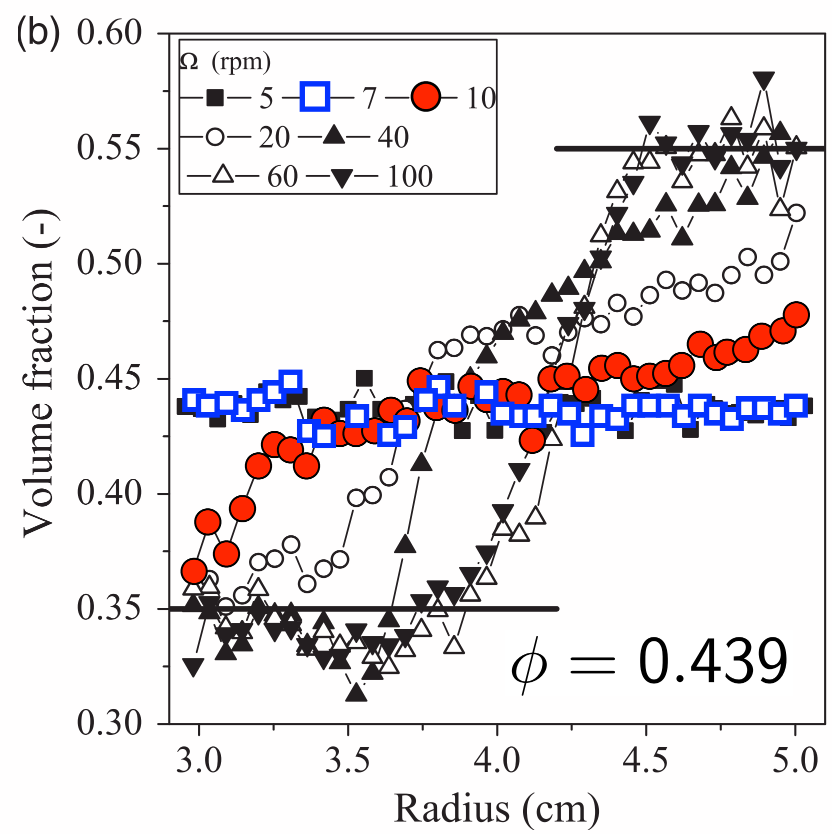
cornstarch suspension

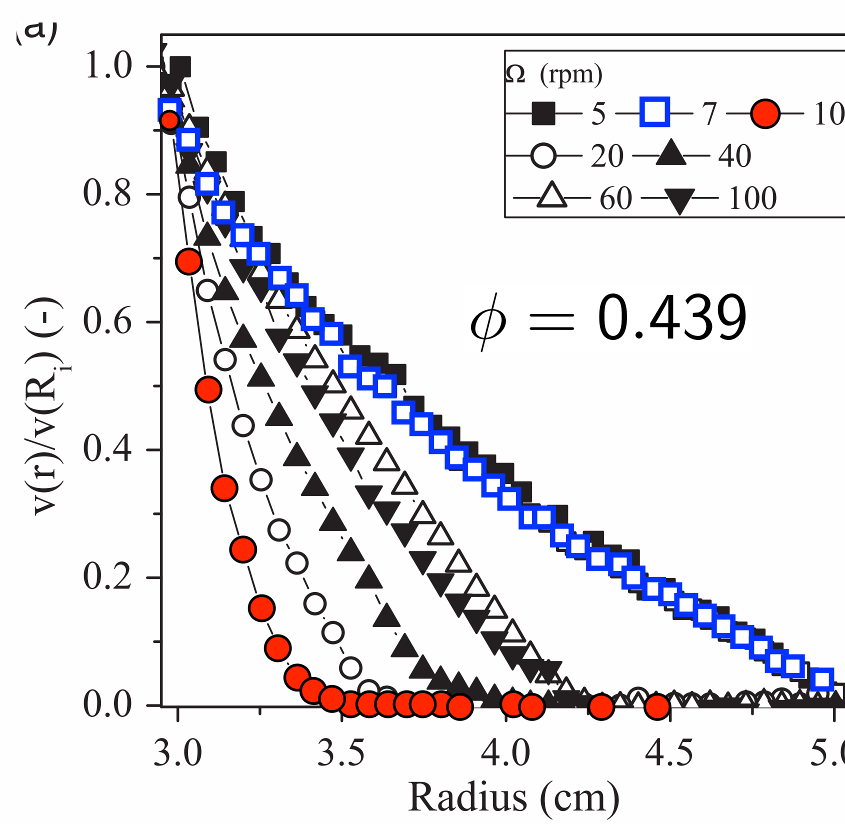


$\phi = 0.439$



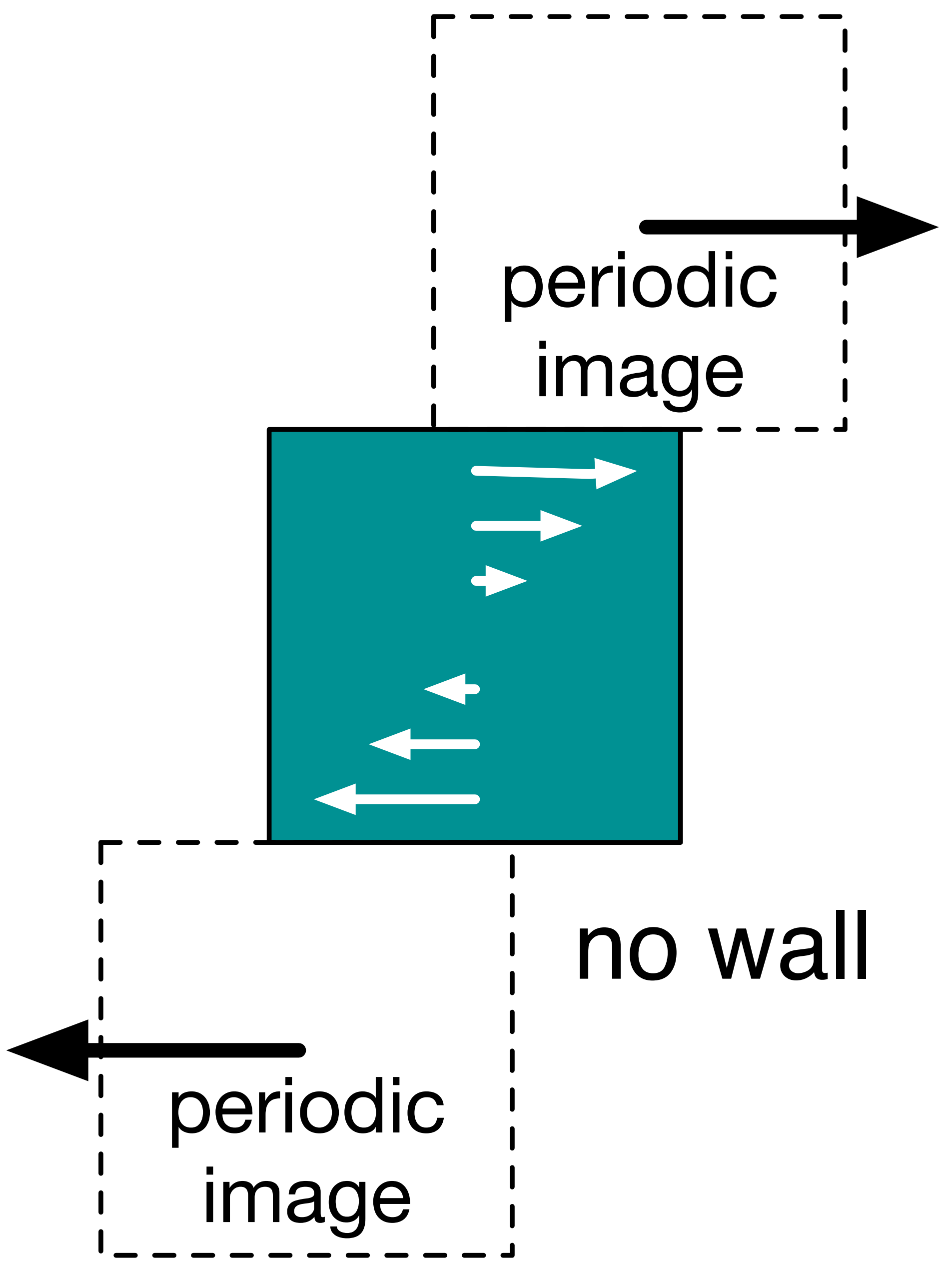
Magnetic Resonance Imaging





Our original simulation

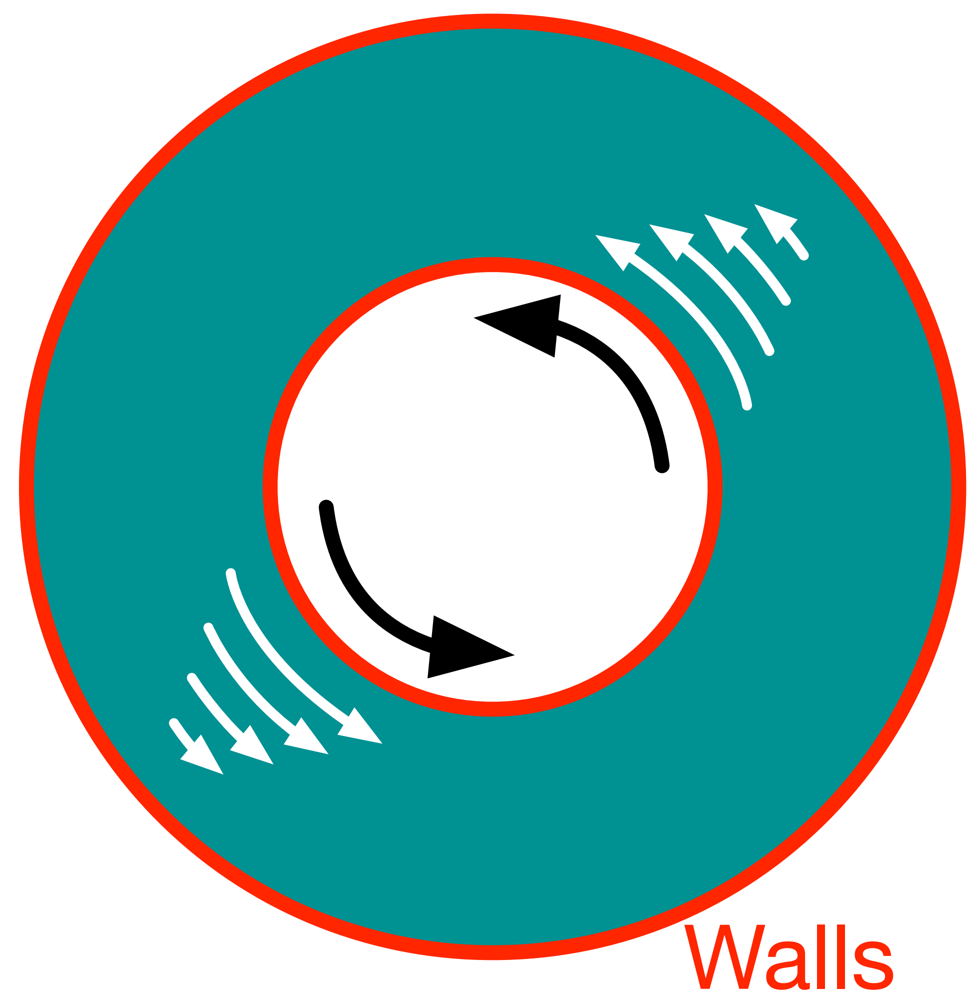
Lees-Edwards periodic b.c.
(mainly 3D)
To reproduce bulk rheology



imposing simple shear flow

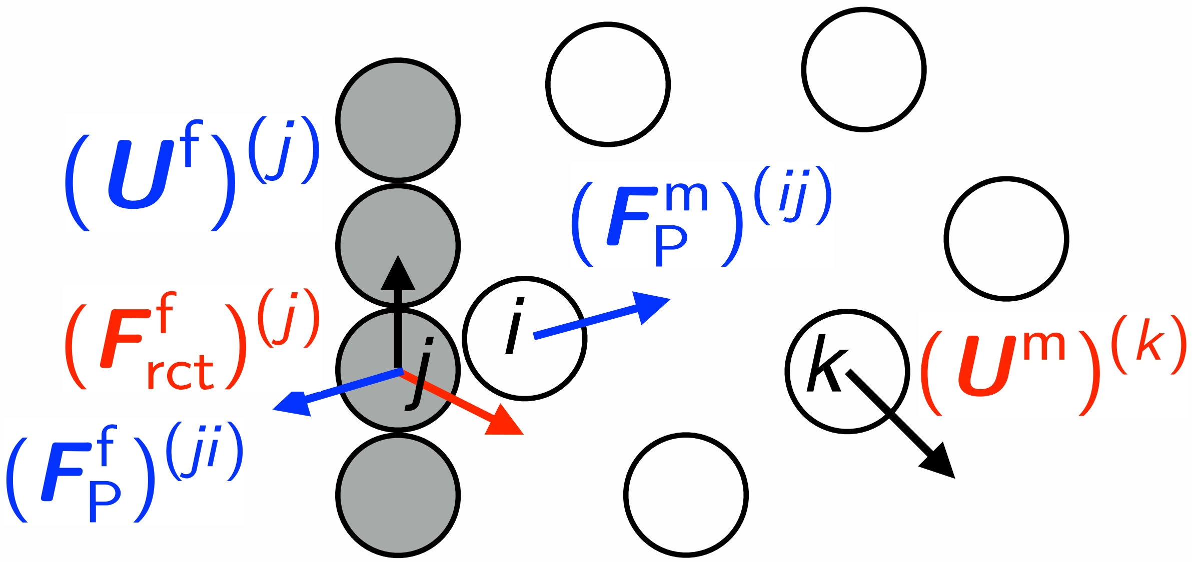
New simulation

Wide-gap rotary Couette cell
(2D)
To mimic a non-uniform
macroscopic b.c.



Overdamped dynamics with constrained particles

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



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)

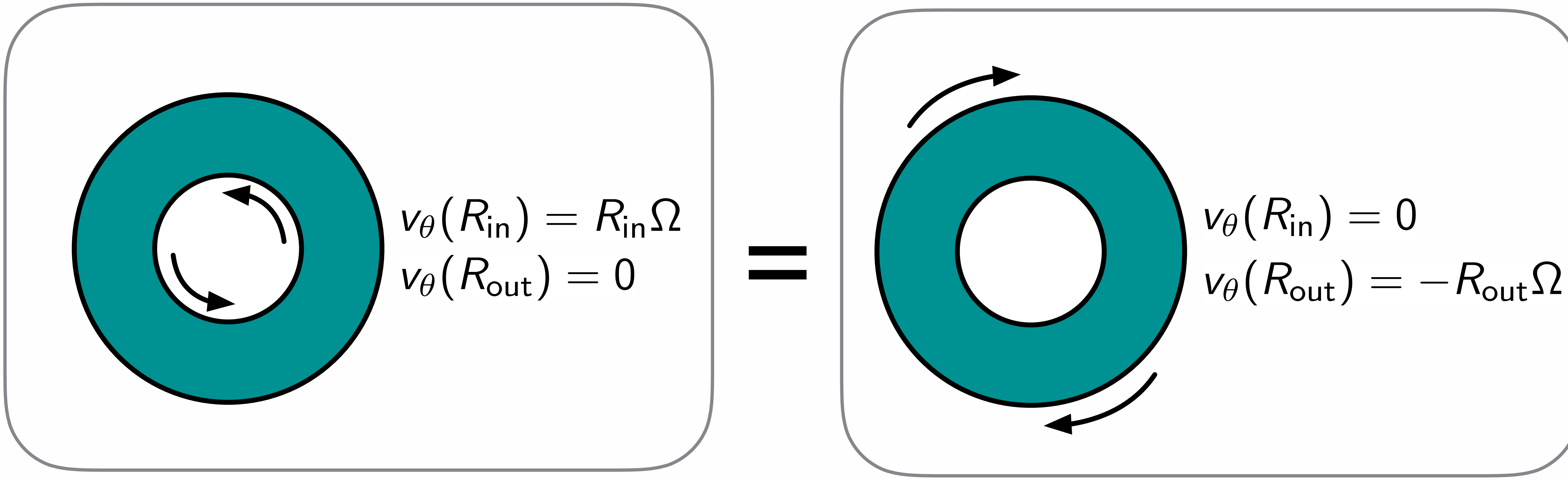
force balance equations

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

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*

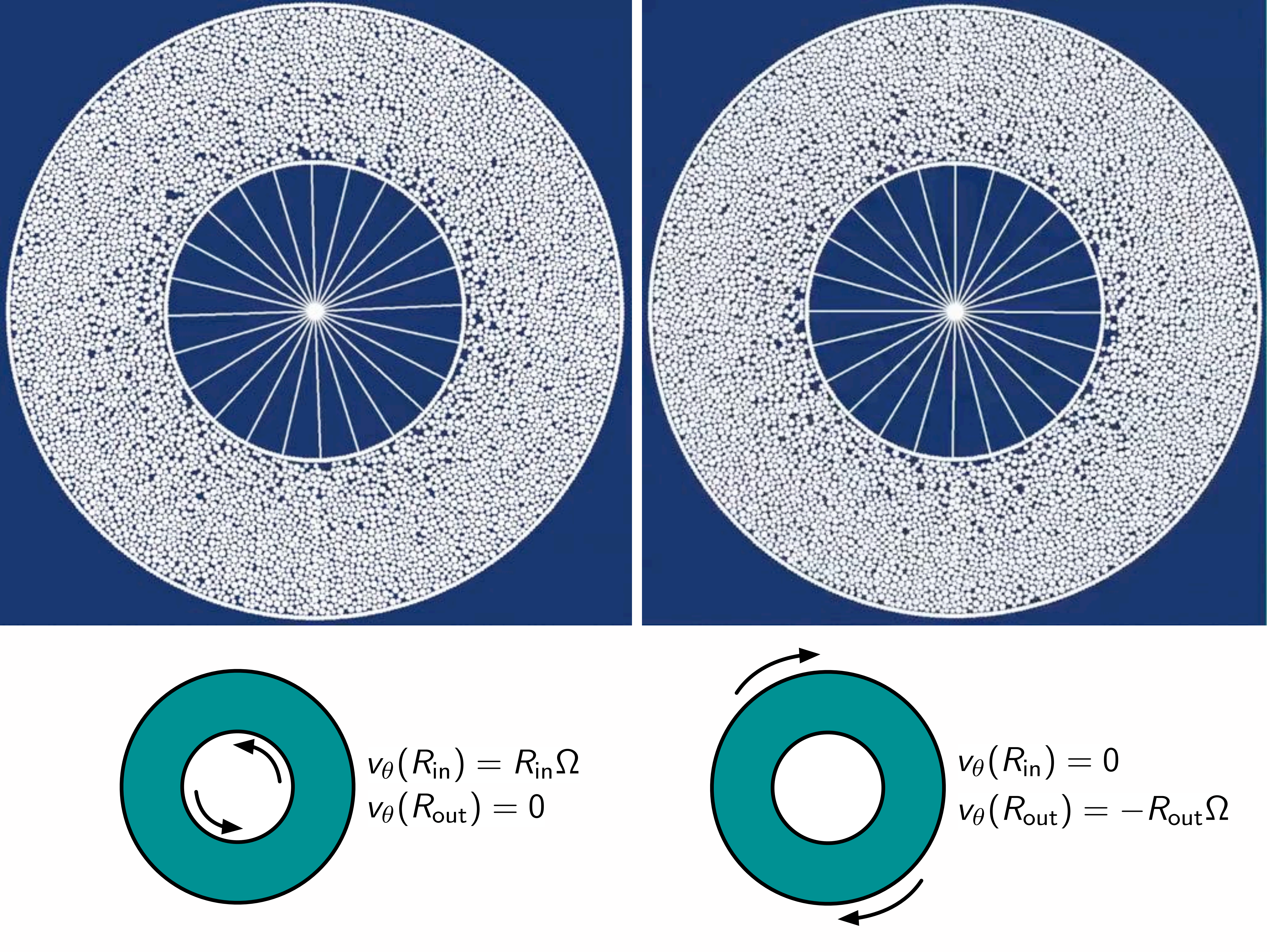
Frame invariant model



- Density matched suspension: $\rho_{\text{particle}} = \rho_{\text{liquid}}$
- Overdamped dynamics, i.e., no inertia (no centrifugal force)
- Hydrodynamics interaction is only lubrication: $\boldsymbol{F}_{\text{H}} \approx \boldsymbol{R}_{\text{Lub}}\boldsymbol{U}$
- No background flow is imposed ~~$\boldsymbol{U}^\infty$~~

cf. previous model

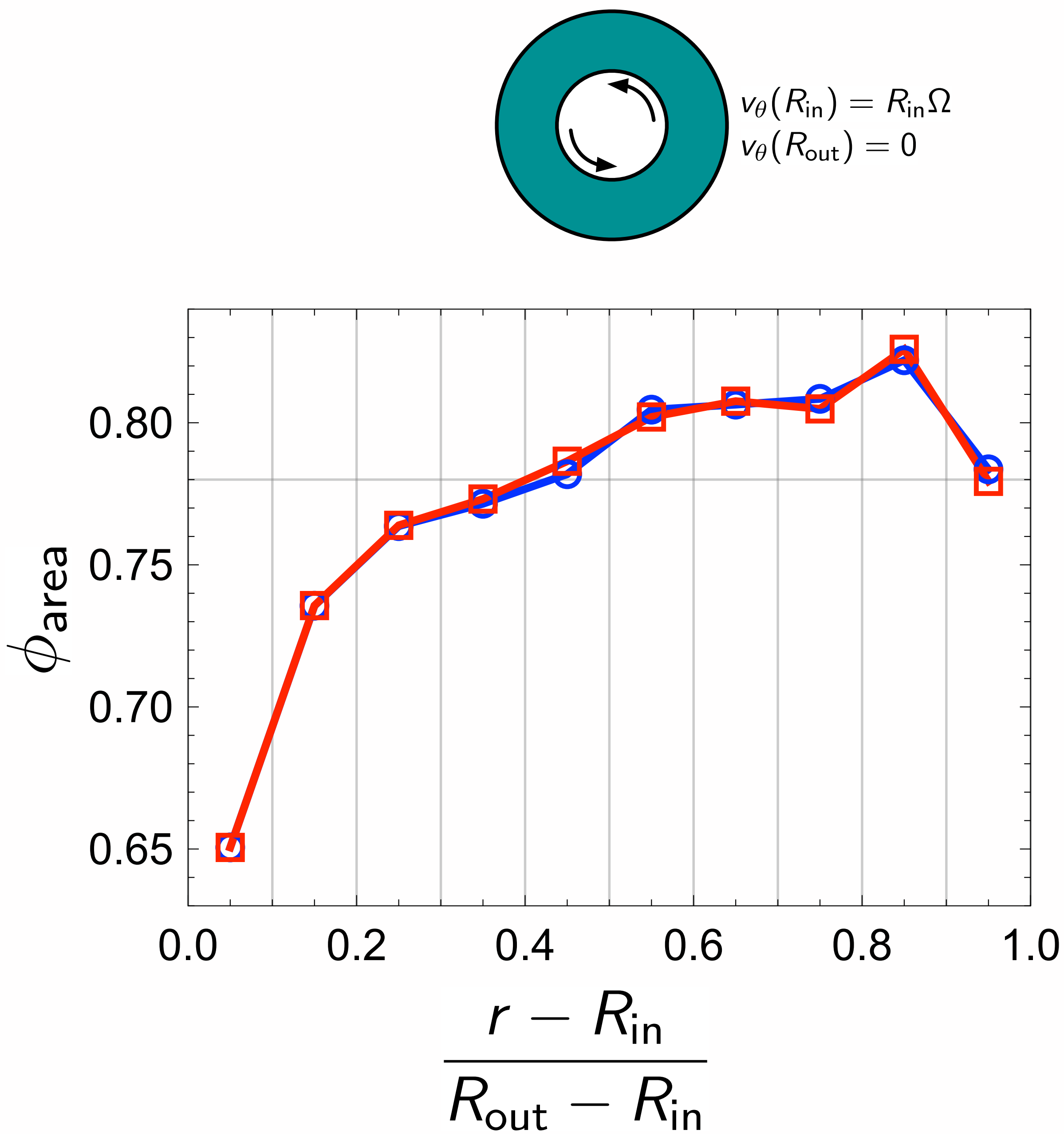
$$\boldsymbol{F}_{\text{H}} \approx -(\boldsymbol{R}_{\text{Stokes}} + \boldsymbol{R}_{\text{Lub}})(\boldsymbol{U} - \boldsymbol{U}^\infty) + \boldsymbol{R}'_{\text{Lub}} : \boldsymbol{E}^\infty$$



$v_\theta(R_{\mathrm{in}}) = R_{\mathrm{in}}\Omega$
$v_\theta(R_{\mathrm{out}}) = 0$
$v_\theta(R_{\mathrm{in}}) = 0$
$v_\theta(R_{\mathrm{out}}) = -R_{\mathrm{out}}\Omega$

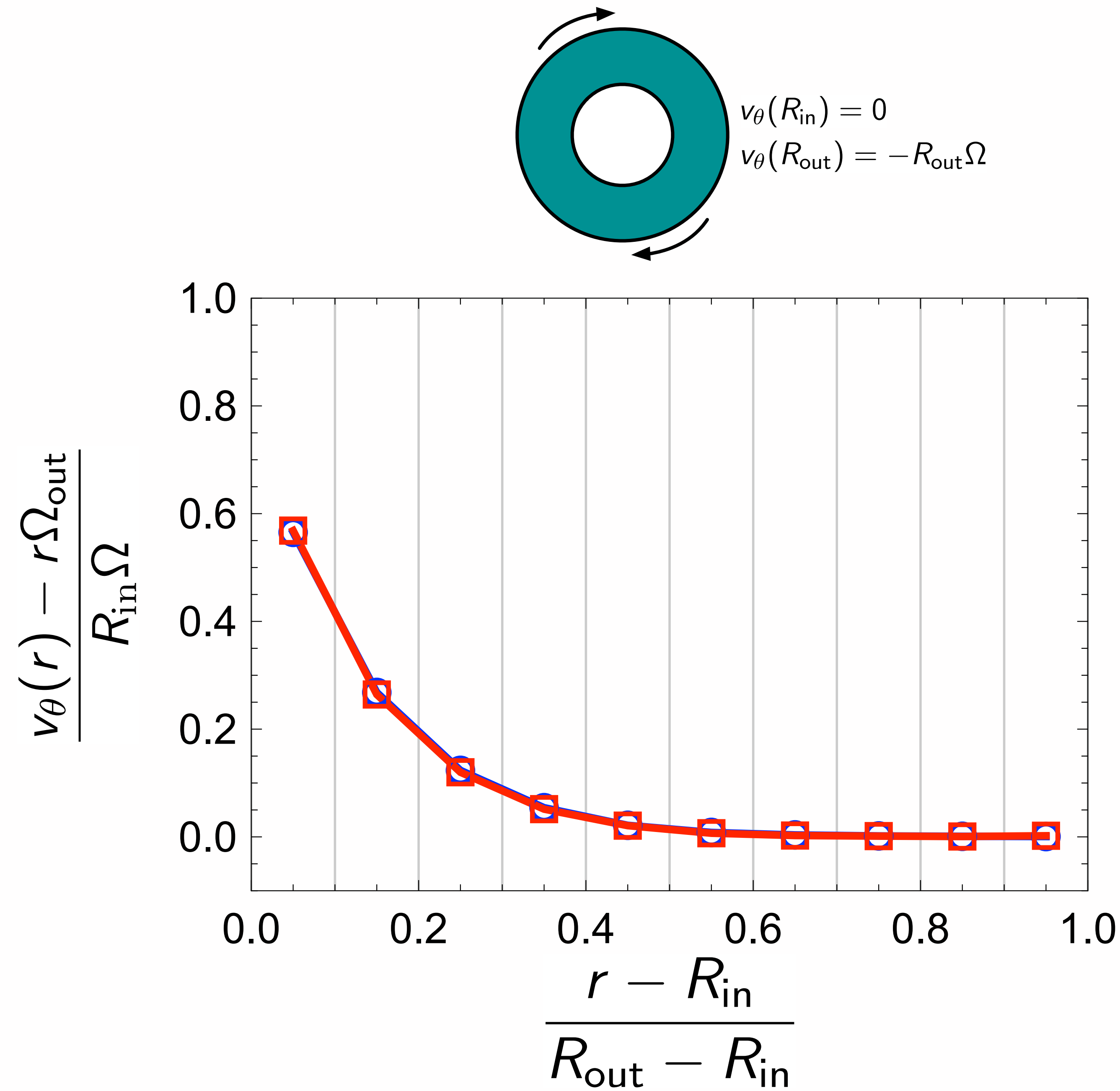
The present model is frame invariant

○ Rotating inner wheel



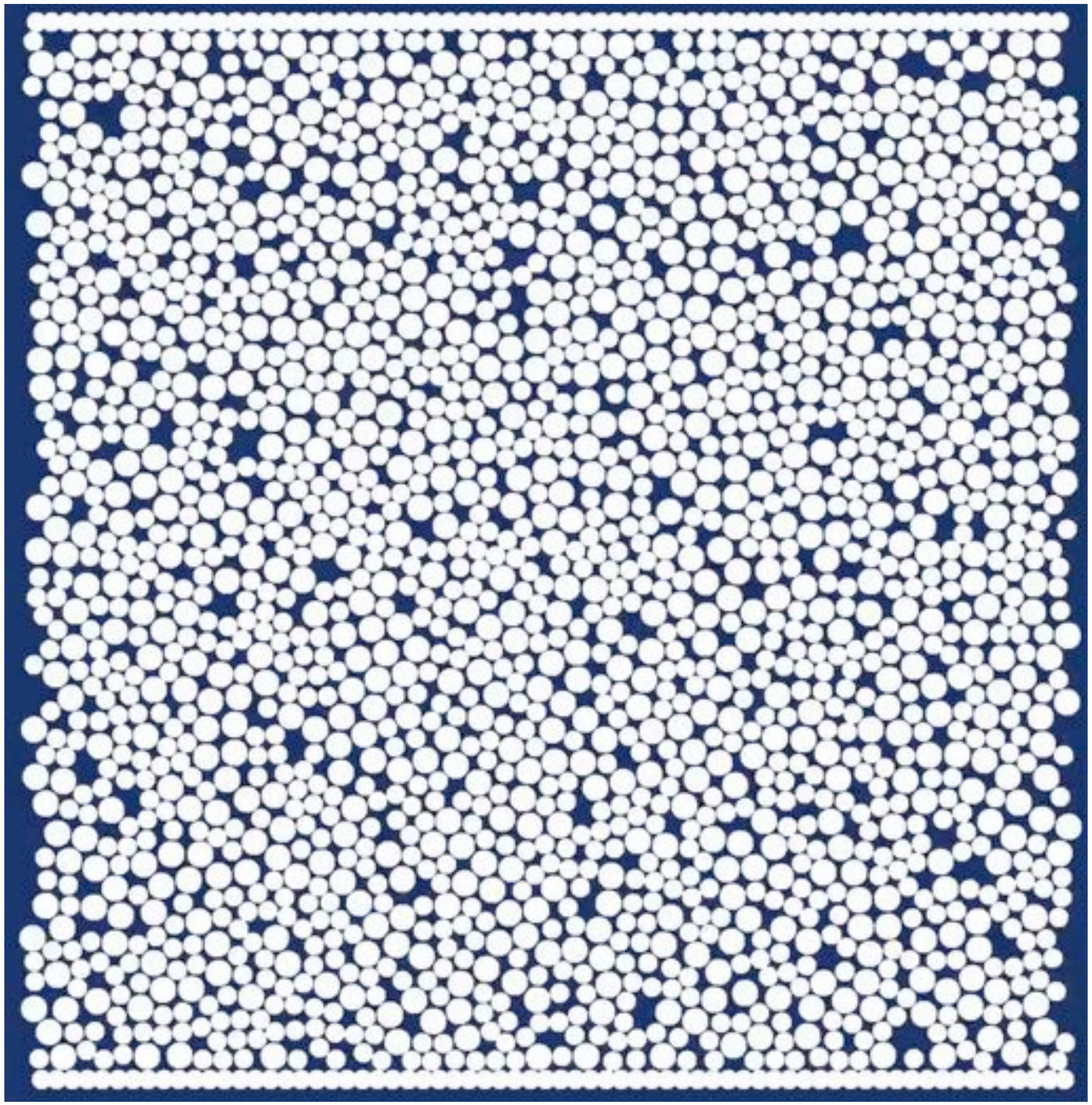
Area fraction profile

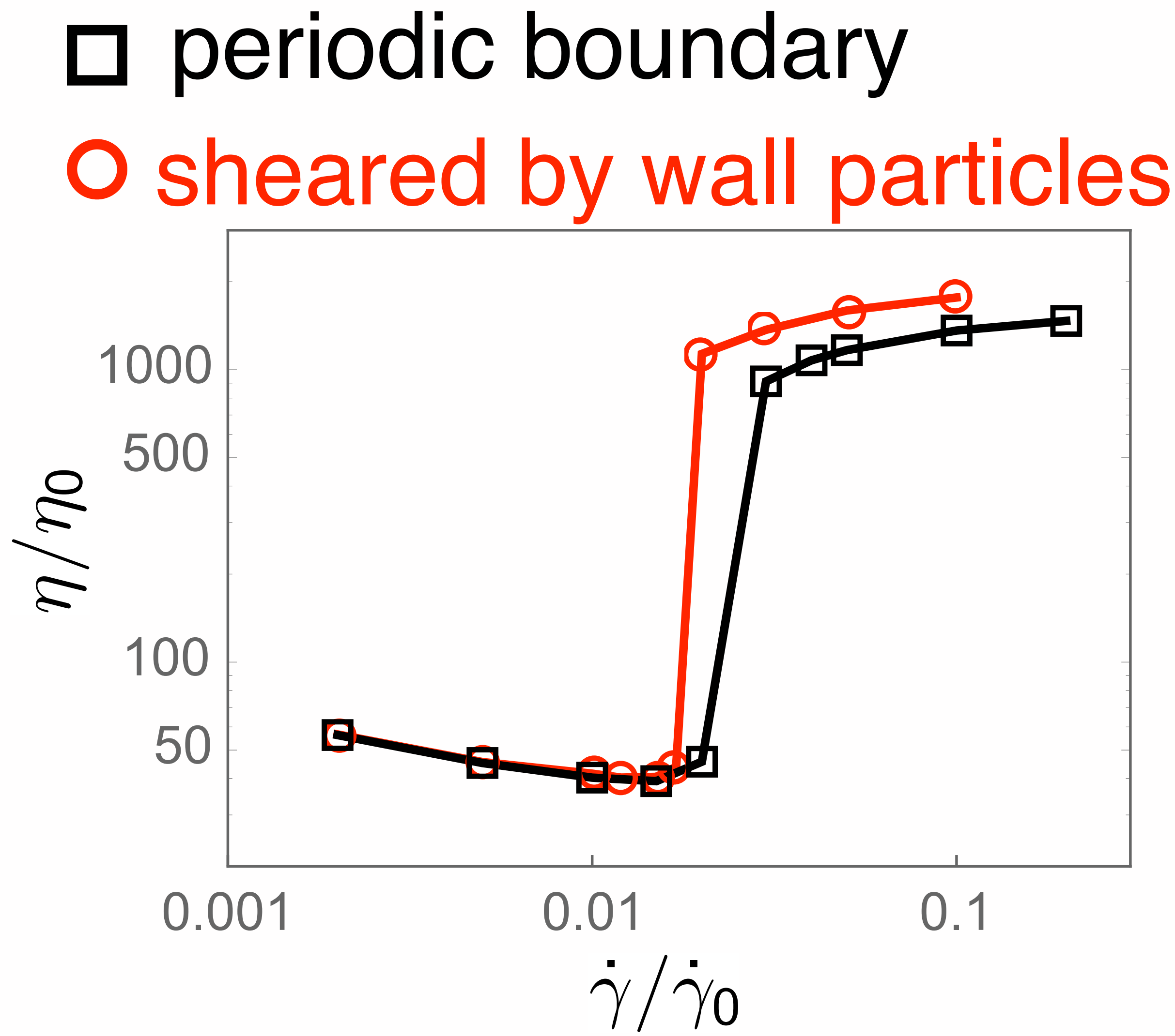
□ Rotating outer wheel



Velocity profile

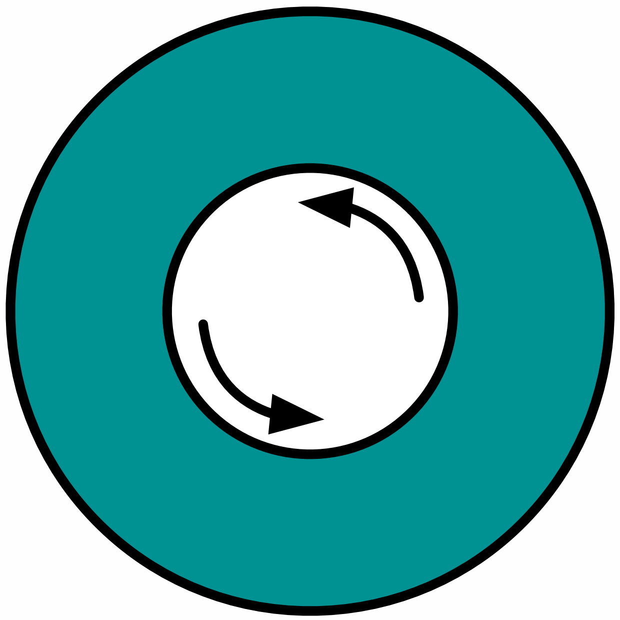
The present model can reproduce DST in simple shear both by Lees-Edwards and by walls





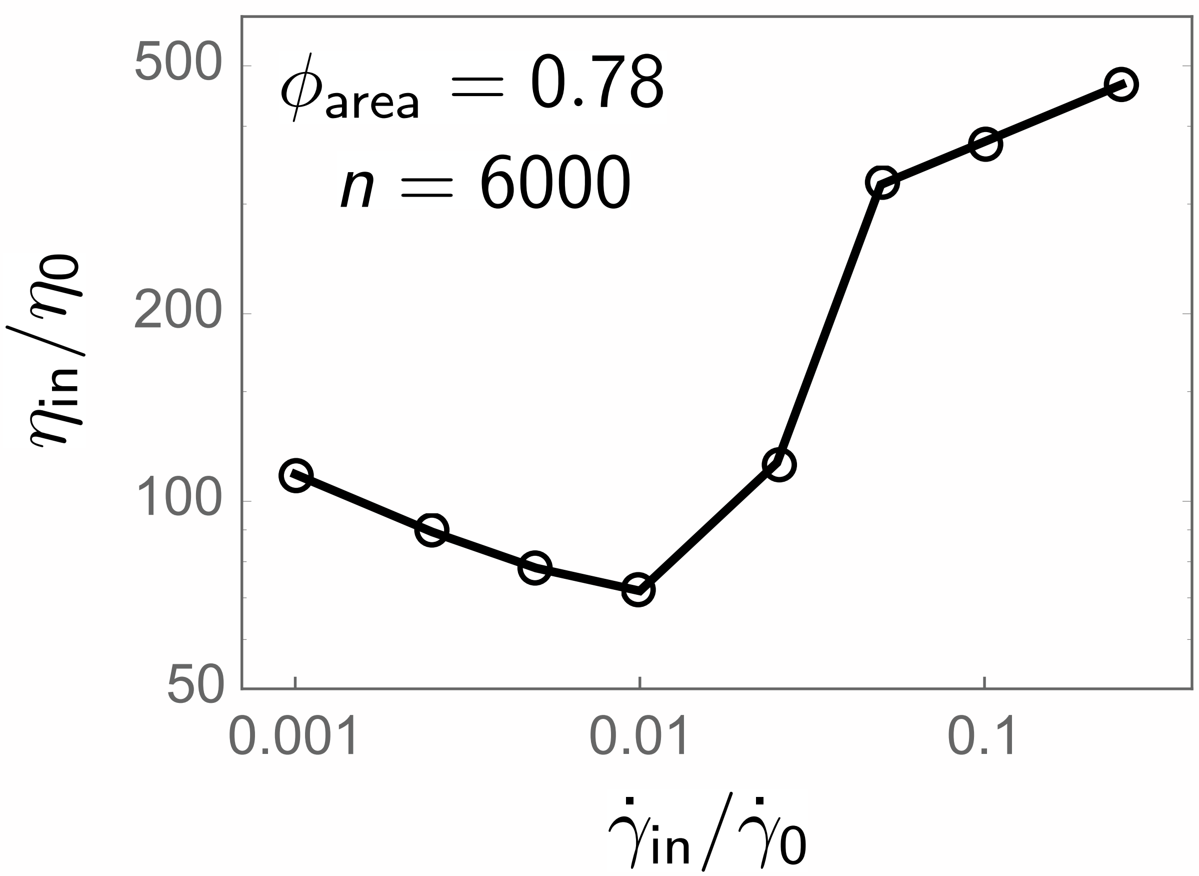
Macroscopic apparent rheology

torque $\boldsymbol{T}_{\text{in}} = \sum_{i \in \text{inner wheel}} \left\{ (\boldsymbol{r}^{(i)} - \boldsymbol{r}_0) \times (\boldsymbol{F}^{\text{f}}_{\text{act}})^{(i)} + (\boldsymbol{T}^{\text{f}}_{\text{act}})^{(i)} \right\}$



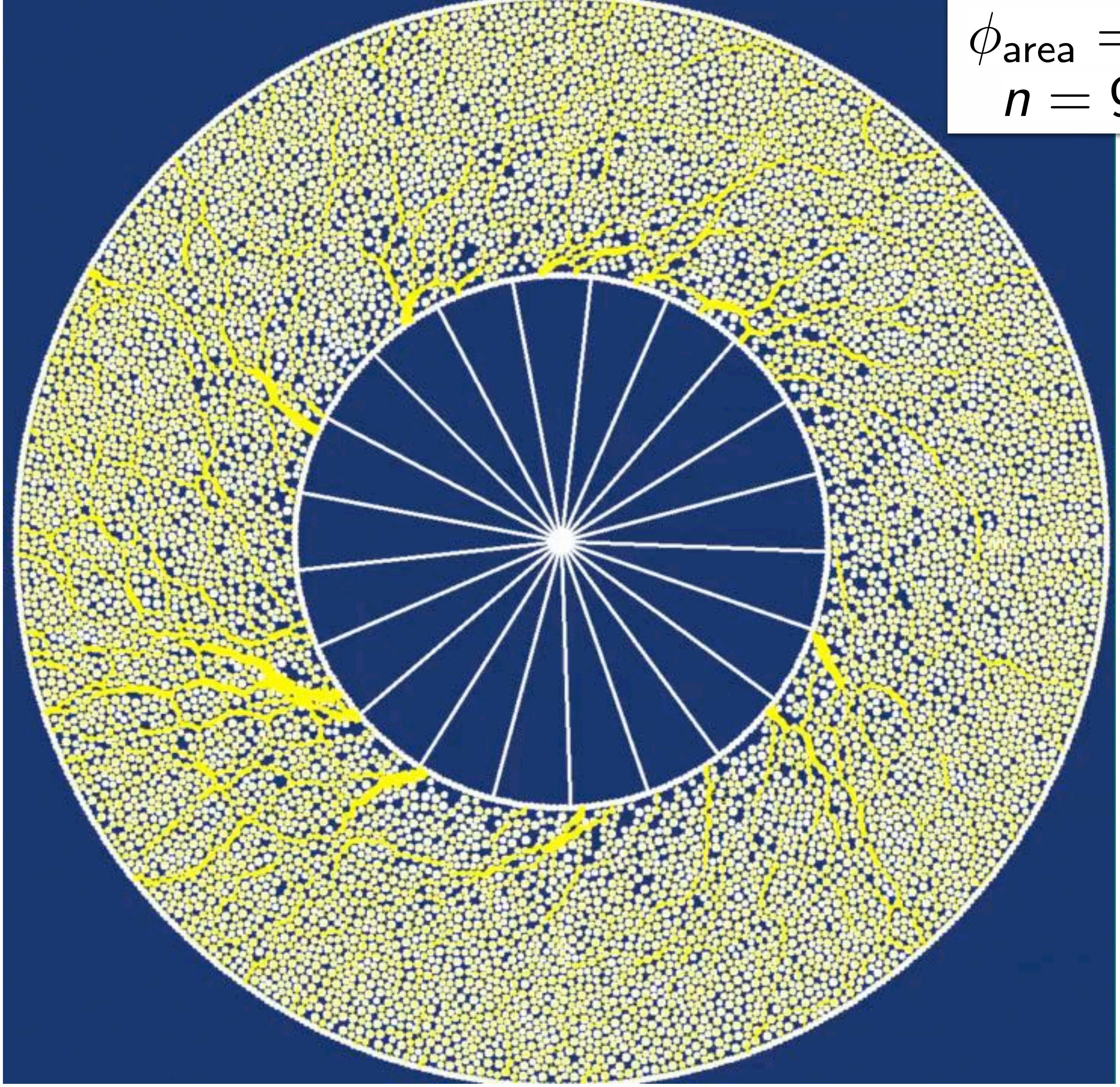
shear stress $\sigma^{\text{in}}_{\theta r} \equiv \dfrac{\boldsymbol{T}_{\text{in}} \cdot \boldsymbol{e}_z}{2\pi R^2_{\text{in}}}$ rate $\dot{\gamma}_{\text{in}} \equiv \dfrac{\Omega R_{\text{in}}}{R_{\text{out}} - R_{\text{in}}}$

apparent viscosity by the inner wheel $\eta_{\text{in}} \equiv \dfrac{\sigma^{\text{in}}_{\theta r}}{\dot{\gamma}_{\text{in}}}$



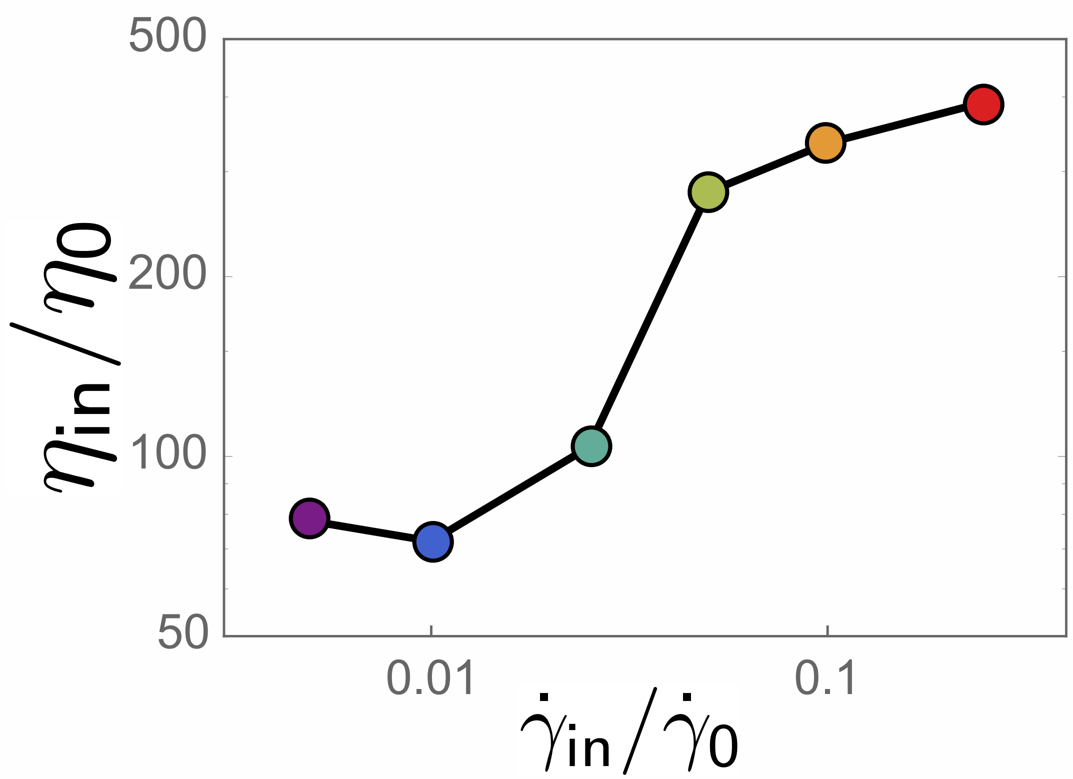
rate dependence due to repulsive force

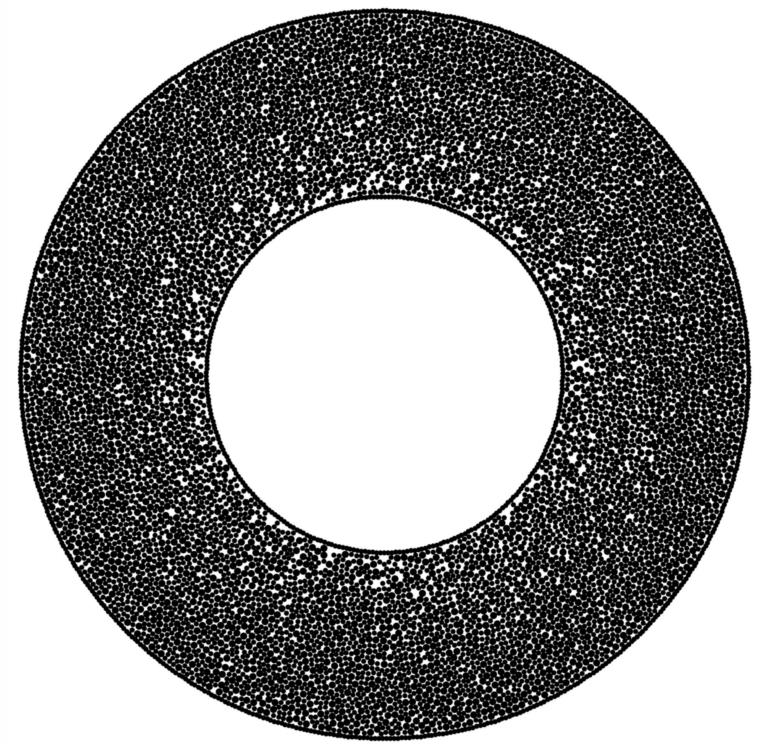
$\dot{\gamma}_0 = 6\pi\eta_0 a^2 / F^*_{\text{R}}$



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

shear thickening + shear banding

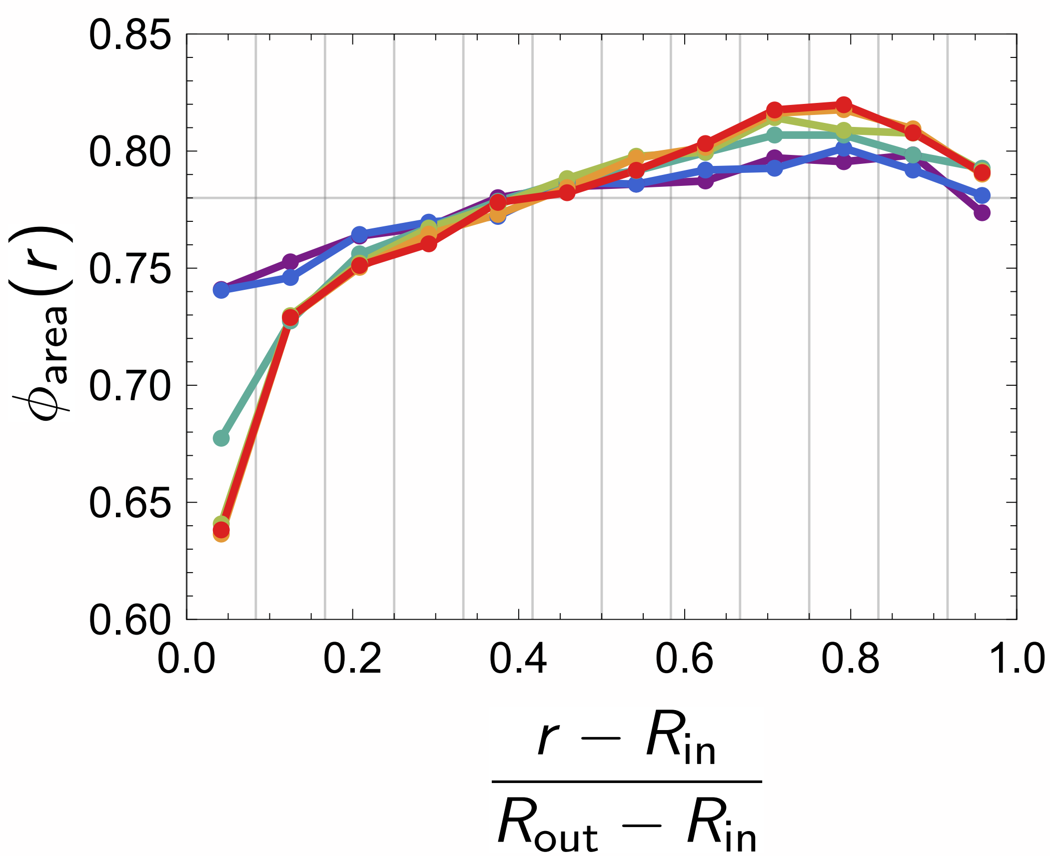


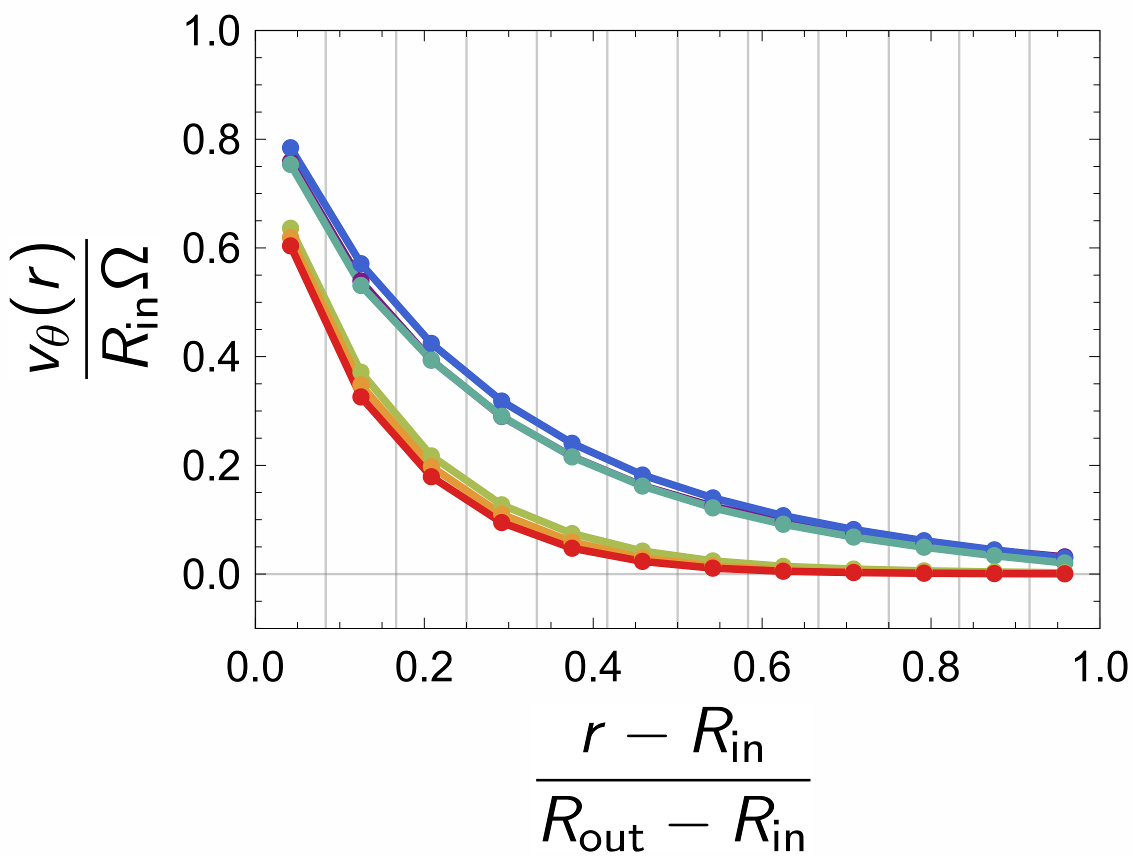


$$\phi_{area} = 0.78$$

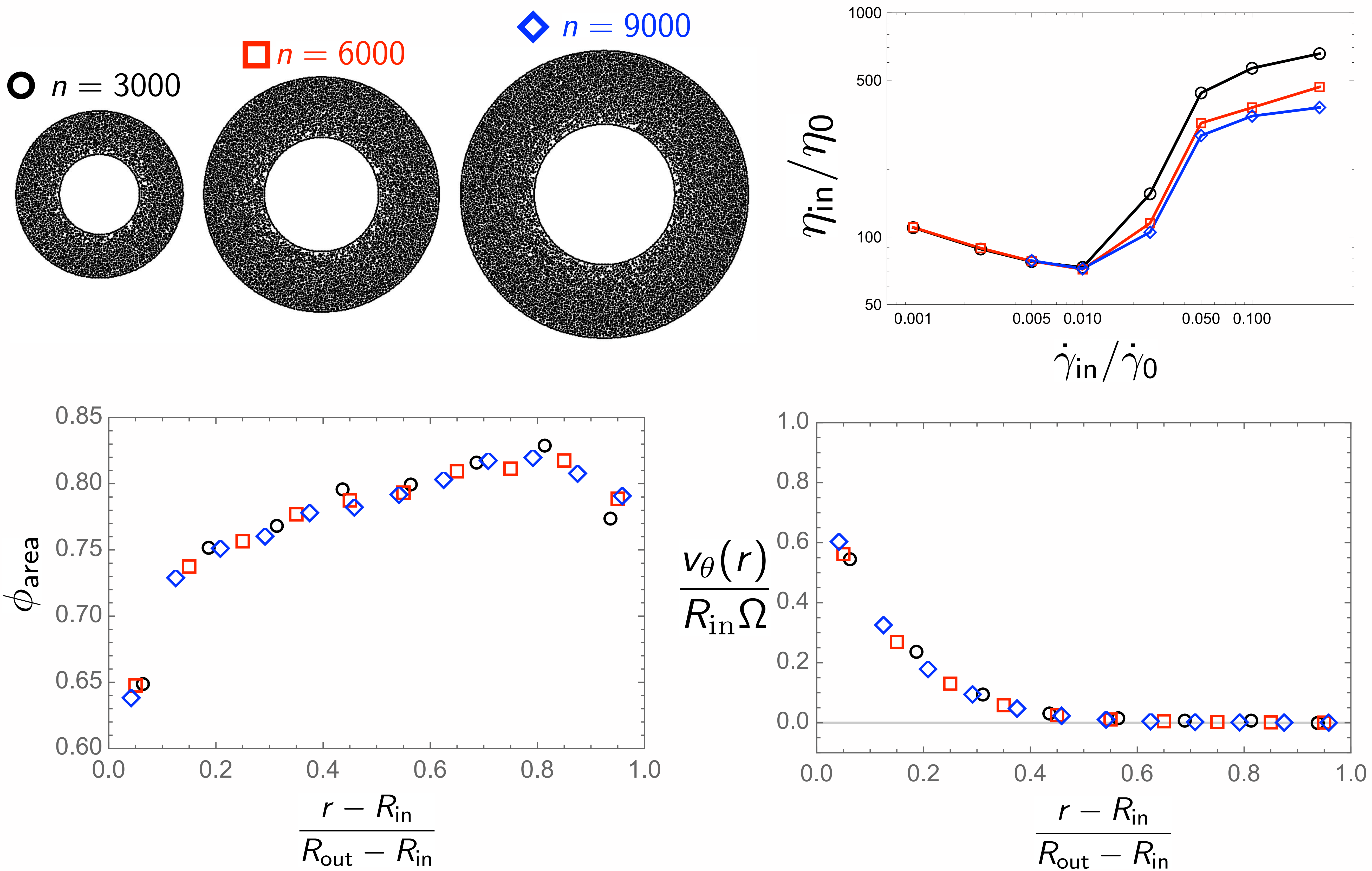
$$n = 9000$$

$$\frac{R_{out} - R_{in}}{2a} \approx 30$$



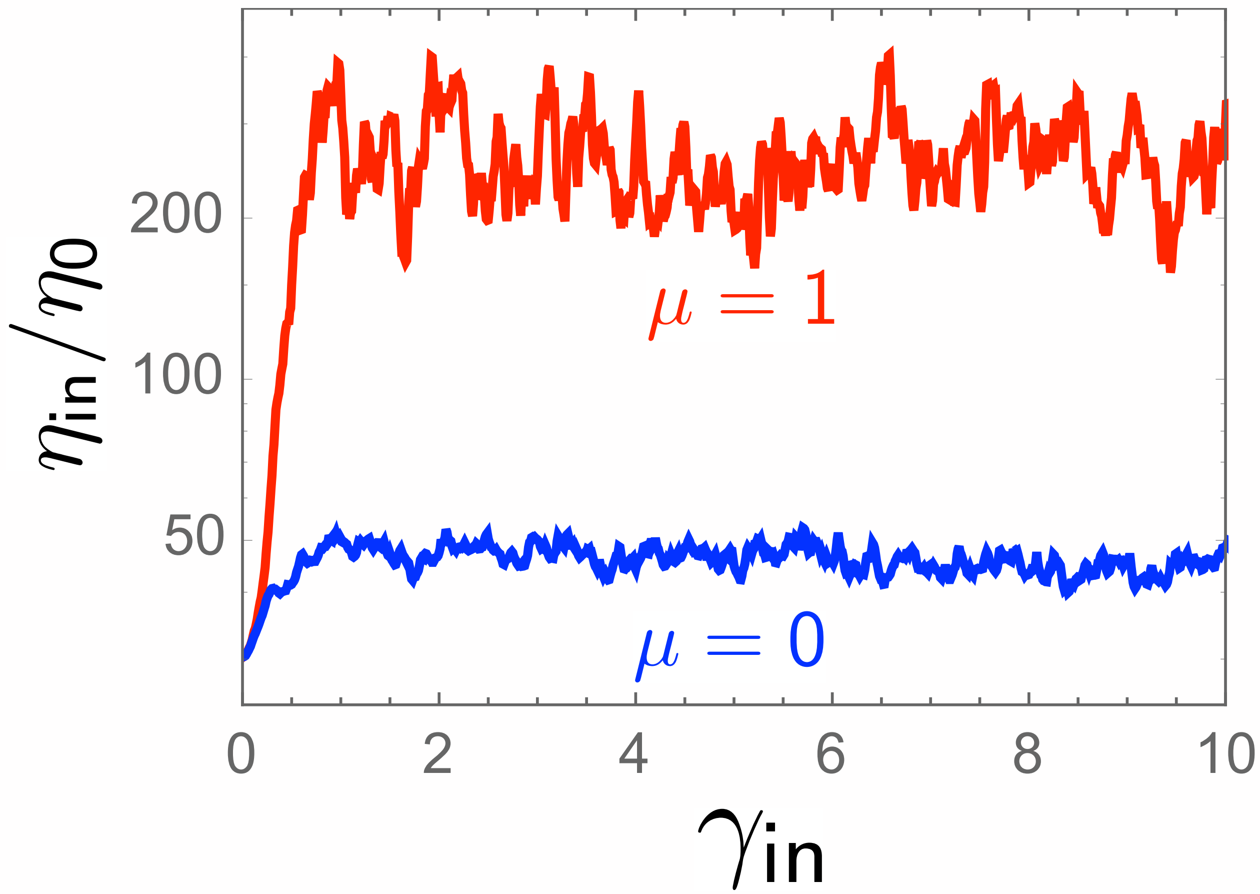


system size

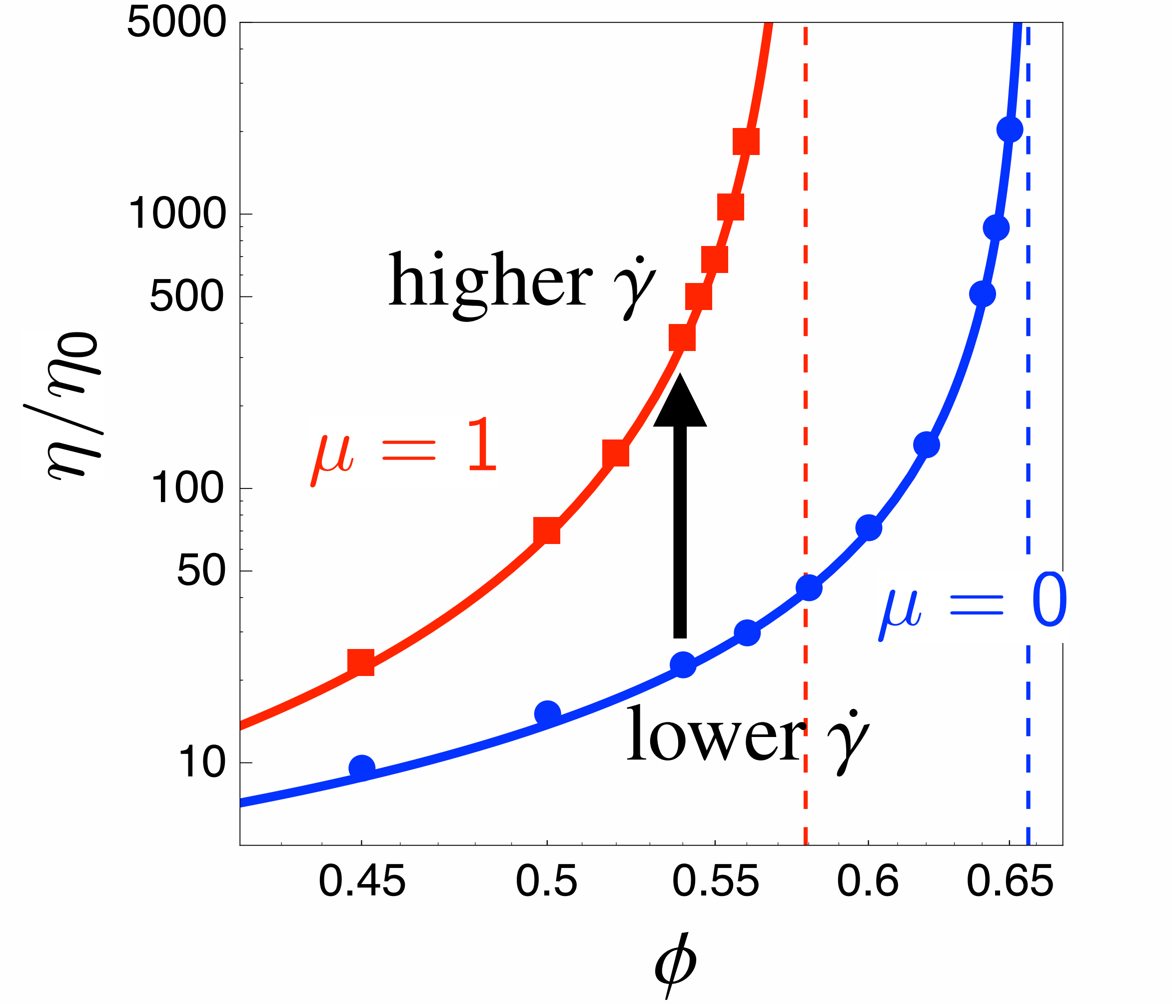


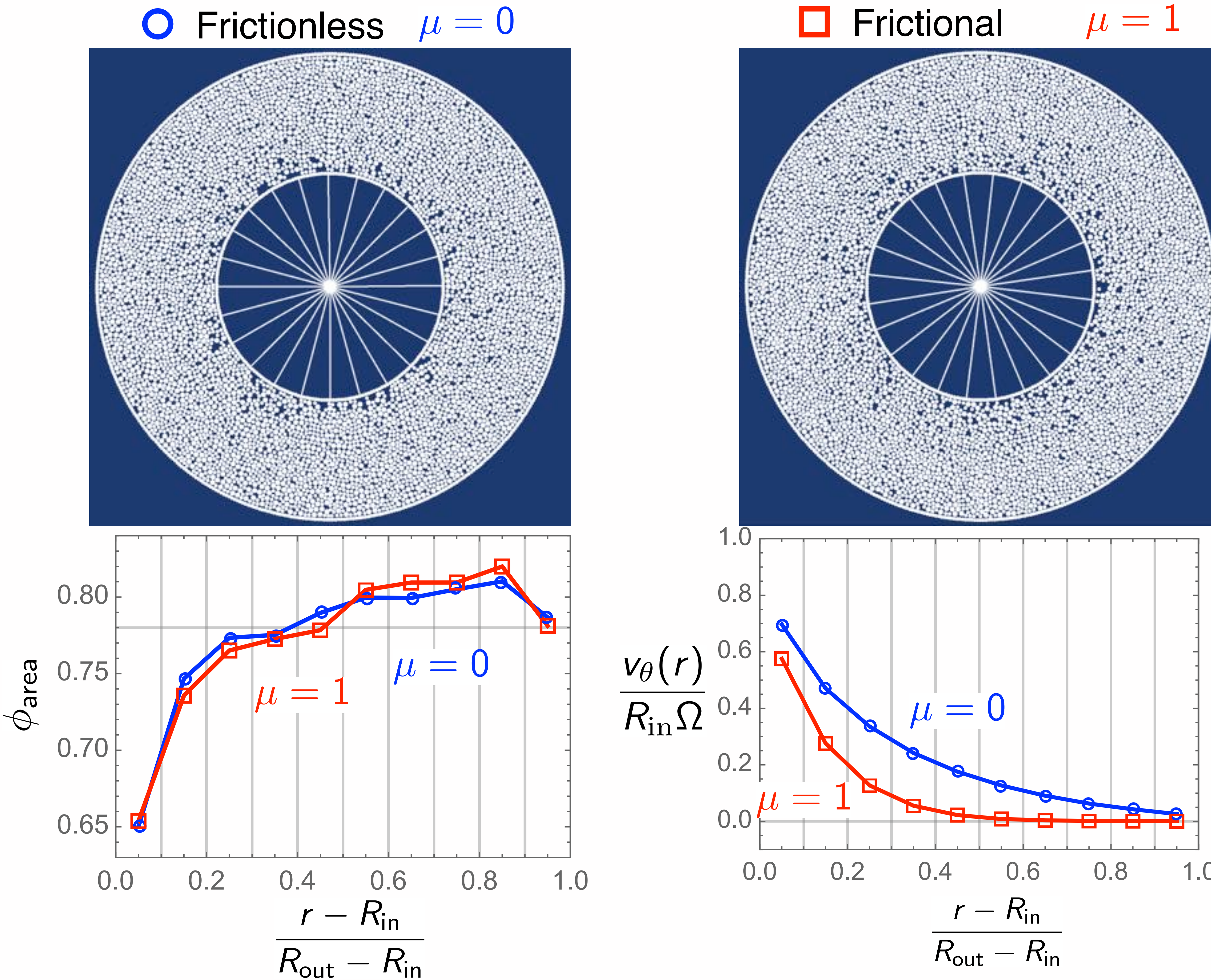
n = 3000
n = 6000
n = 9000
1000
500
100
50
0.001
0.005
0.010
0.050
0.100
η_{in}/η_0
$\dot{\gamma}_{in}/\dot{\gamma}_0$
0.85
0.80
0.75
0.70
0.65
0.60
ϕ_{area}
0.0
0.2
0.4
0.6
0.8
1.0
$\frac{r - R_{in}}{R_{out} - R_{in}}$
$\frac{v_\theta(r)}{R_{in}\Omega}$

Frictional particles vs. Frictionless particles



cf. simple shear simulation



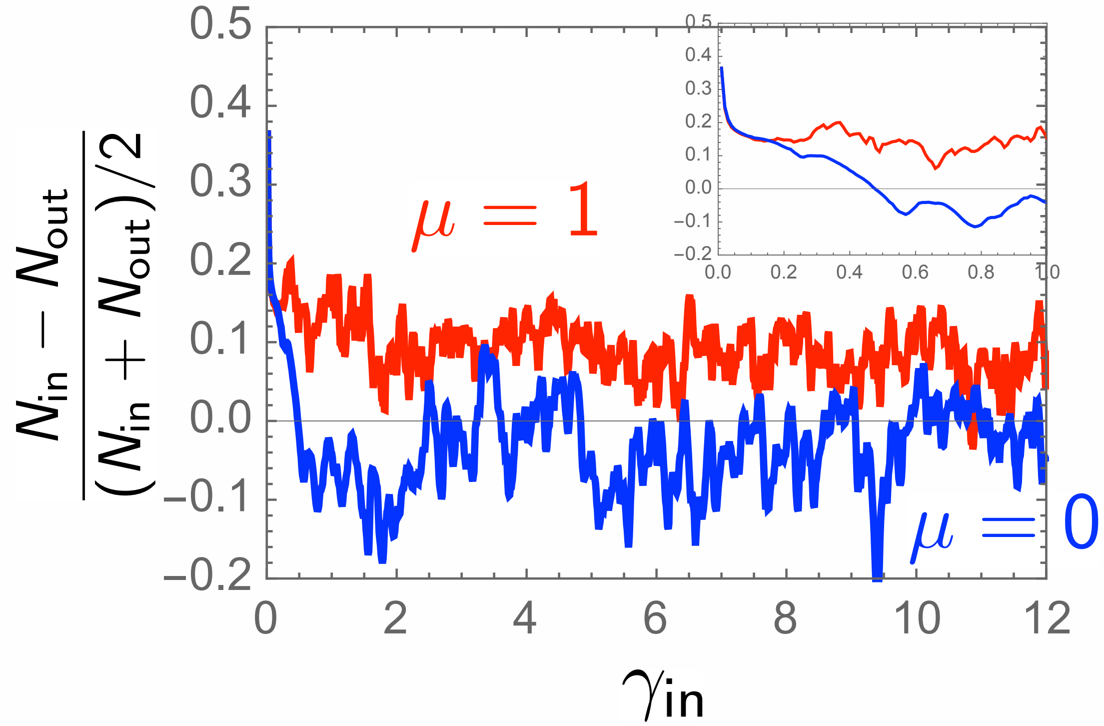


Frictionless $\mu = 0$
Frictional $\mu = 1$
ϕ_{area}
0.65
0.70
0.75
0.80
$\mu = 1$
$\mu = 0$
0.0
0.2
0.4
0.6
0.8
1.0
$\frac{r - R_{\text{in}}}{R_{\text{out}} - R_{\text{in}}}$
$\frac{v_\theta(r)}{R_{\text{in}}\Omega}$
0.0
0.2
0.4
0.6
0.8
1.0
$\mu = 0$
$\mu = 1$
0.0
0.2
0.4
0.6
0.8
1.0
$\frac{r - R_{\text{in}}}{R_{\text{out}} - R_{\text{in}}}$

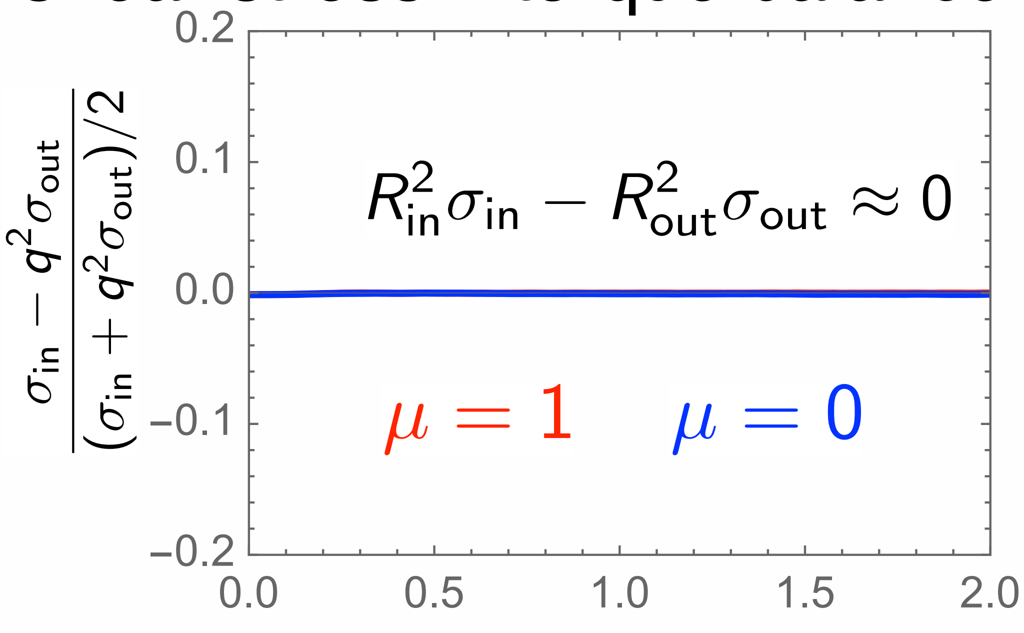
Migration by particle pressure gradient
(Morris and Boulay 1999)

$\boldsymbol{j} \propto \nabla \cdot \boldsymbol{\Sigma}^{\mathrm{P}}$ ($\boldsymbol{\Sigma}^{\mathrm{P}}$: particle pressure)

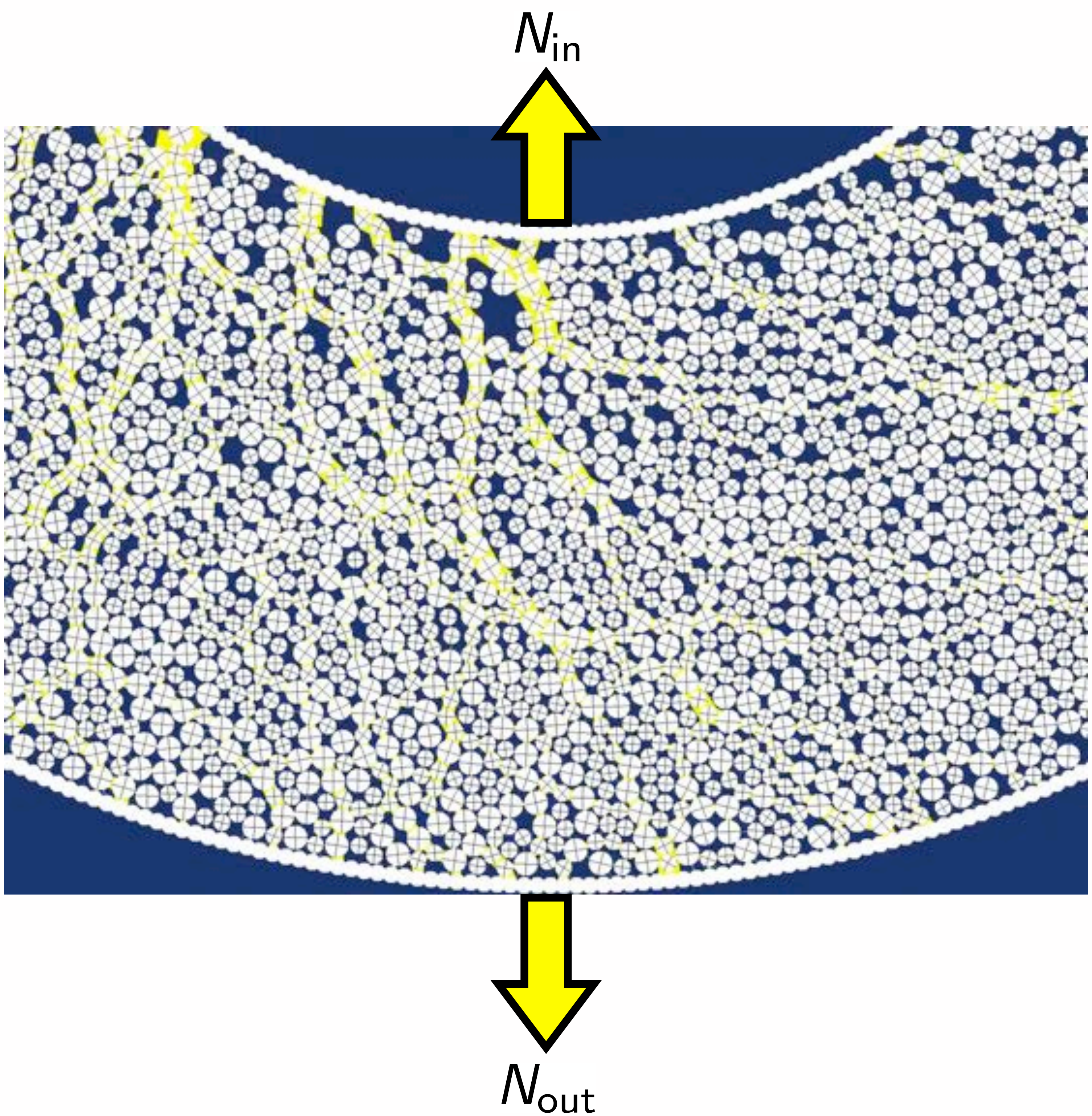
normal stresses



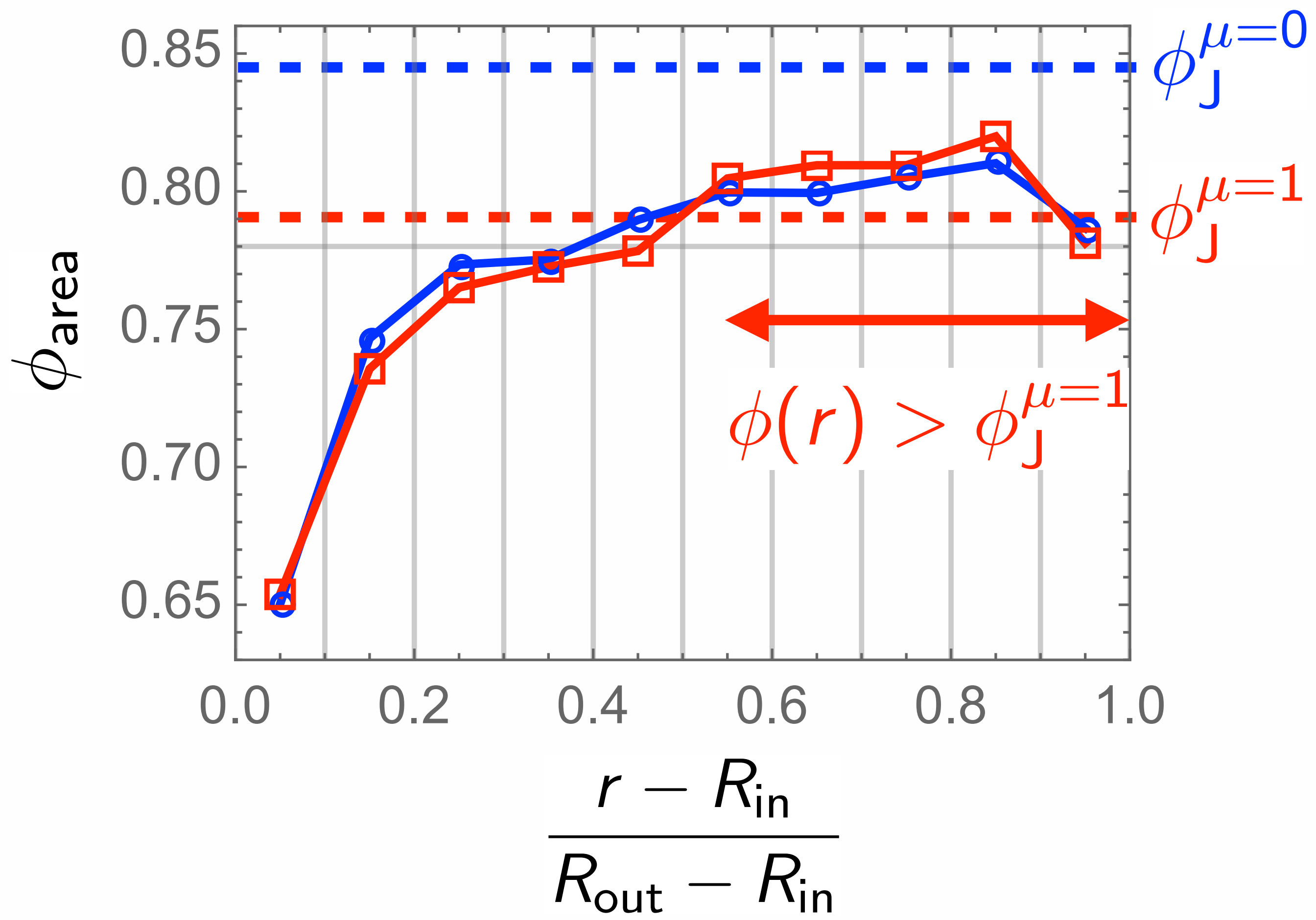
shear stress ~ torque balance

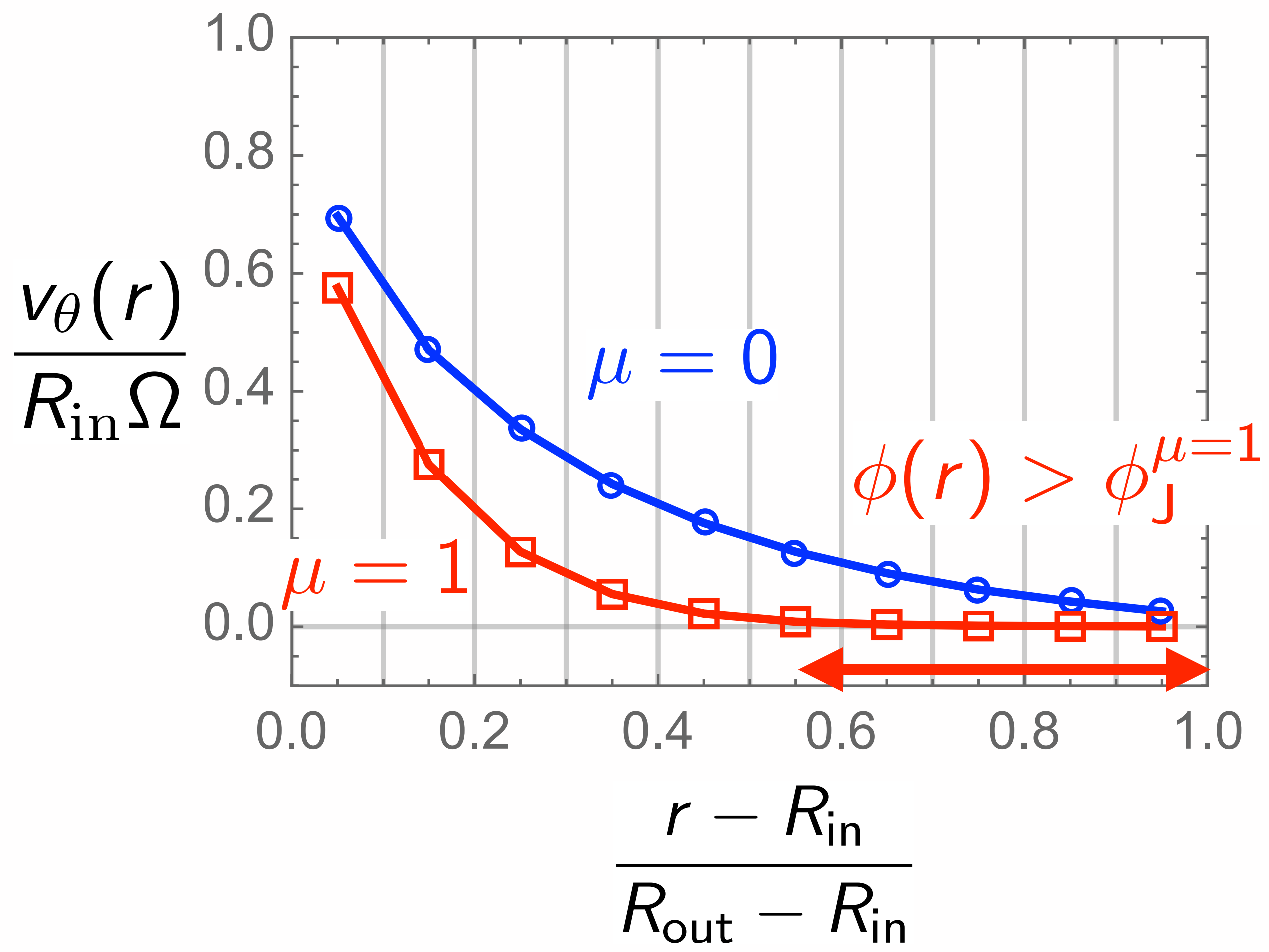


$q \equiv R_{out}/R_{in}$



Frictional jamming achieved by migration





Conclusion

We usually assume uniform simple shear flows
in our DST simulation.

Some experimentalists reported macroscopic DST.
Macroscopic rheology ≠ local rheology?

We extended our DST simulation
for a wide-gap Couette geometry,
and we also obtained similar macroscopic behavior…

Migration + Shear banding + Jamming + Shear thickening

This work may provide some insights
for macroscopic description of DST suspension flows.