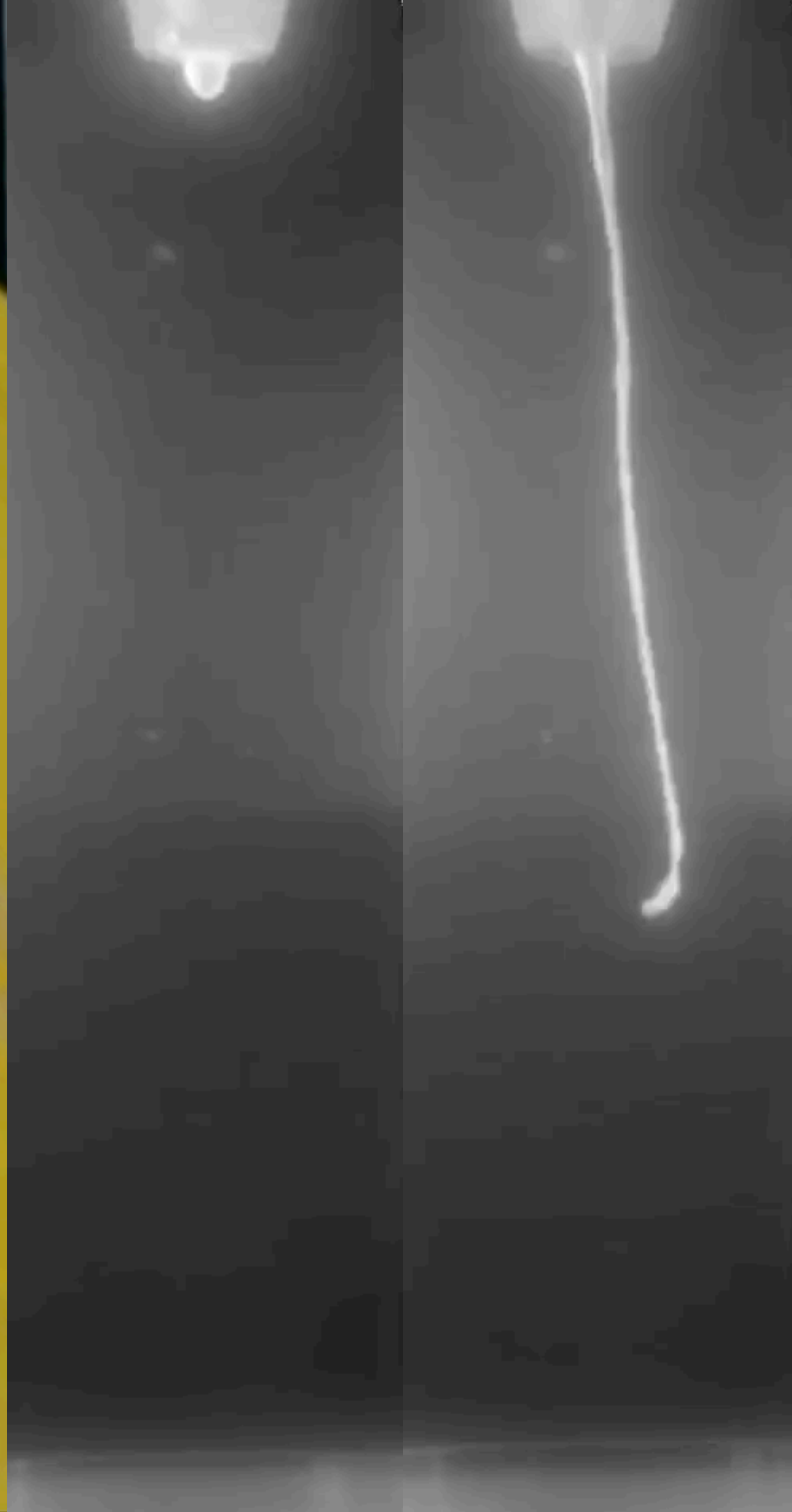
On constitutive models of dense suspensions

Issues that need to be tackled

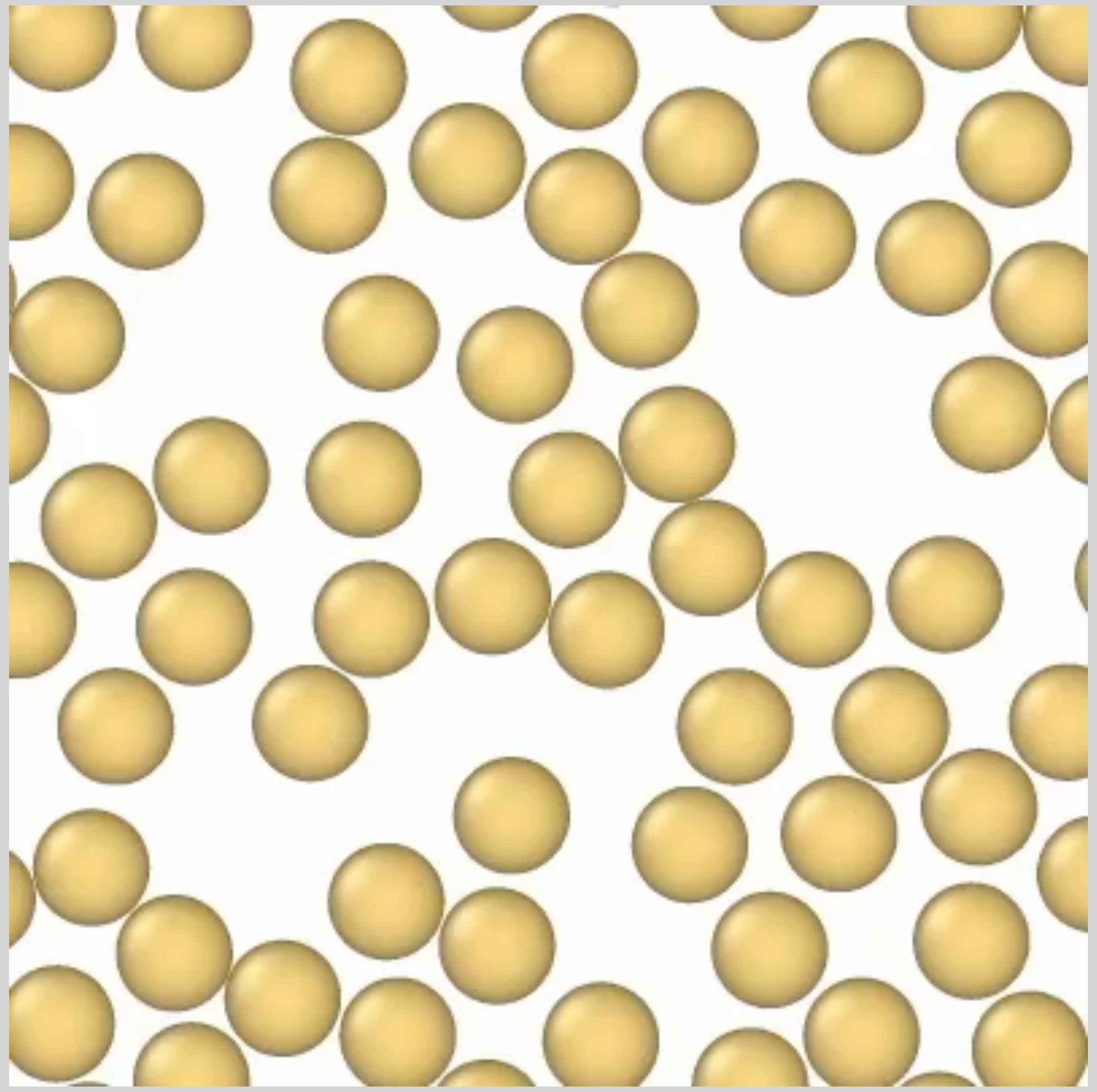
Ryohei Seto, Wenzhou Institute, UCAS

equilibrium $Pe = 0$

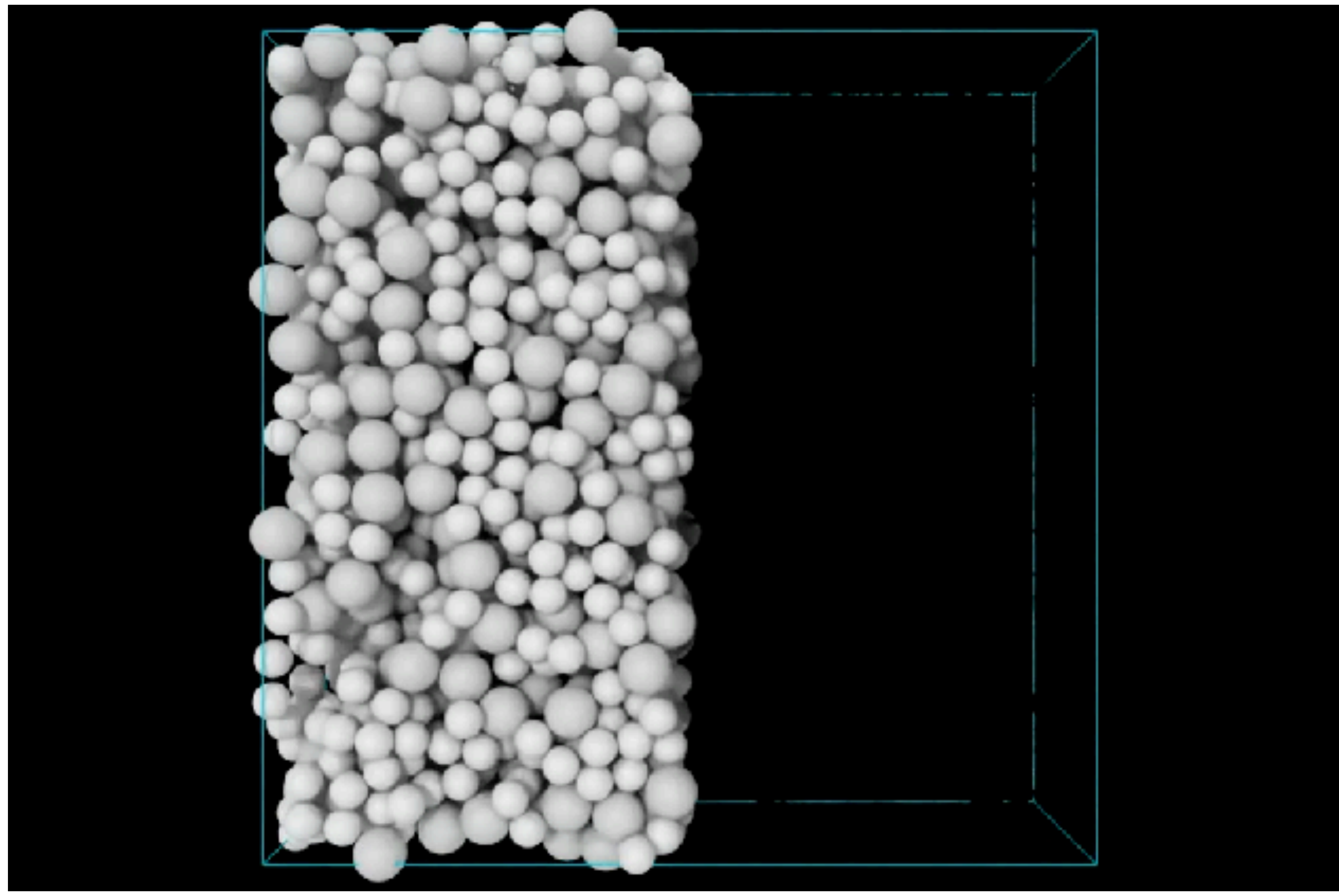
$Pe > 0$ *out-of-equilibrium*

slow → *fast*



Peclet number

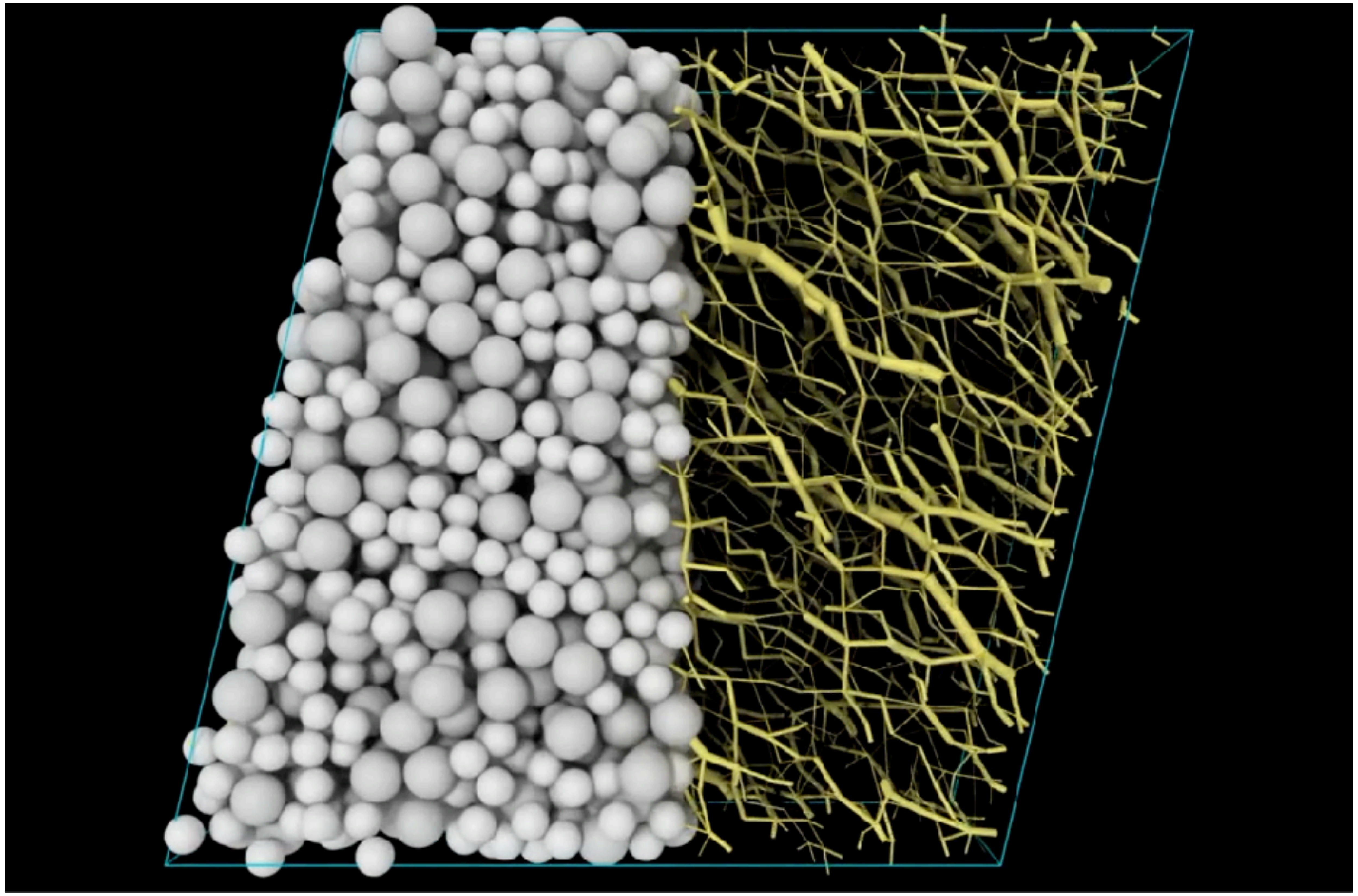
$$Pe = \left(\frac{\textit{time scale of shear}}{\textit{relaxation time}} \right)^{-1}$$



Brownian motion **potential force**	+ hydrodynamic forces **+ contact friction**
diffusion *self assembly*	*shear-induced diffusion* *shear-induced microstructure*
equilibrium phases	**Rheology** **Mechanics / migration**

What shear thickening study brought us?

Seto, Mari, Morris, and Denn
PRL, JOR, PRE, and PNAS (2013–2015)



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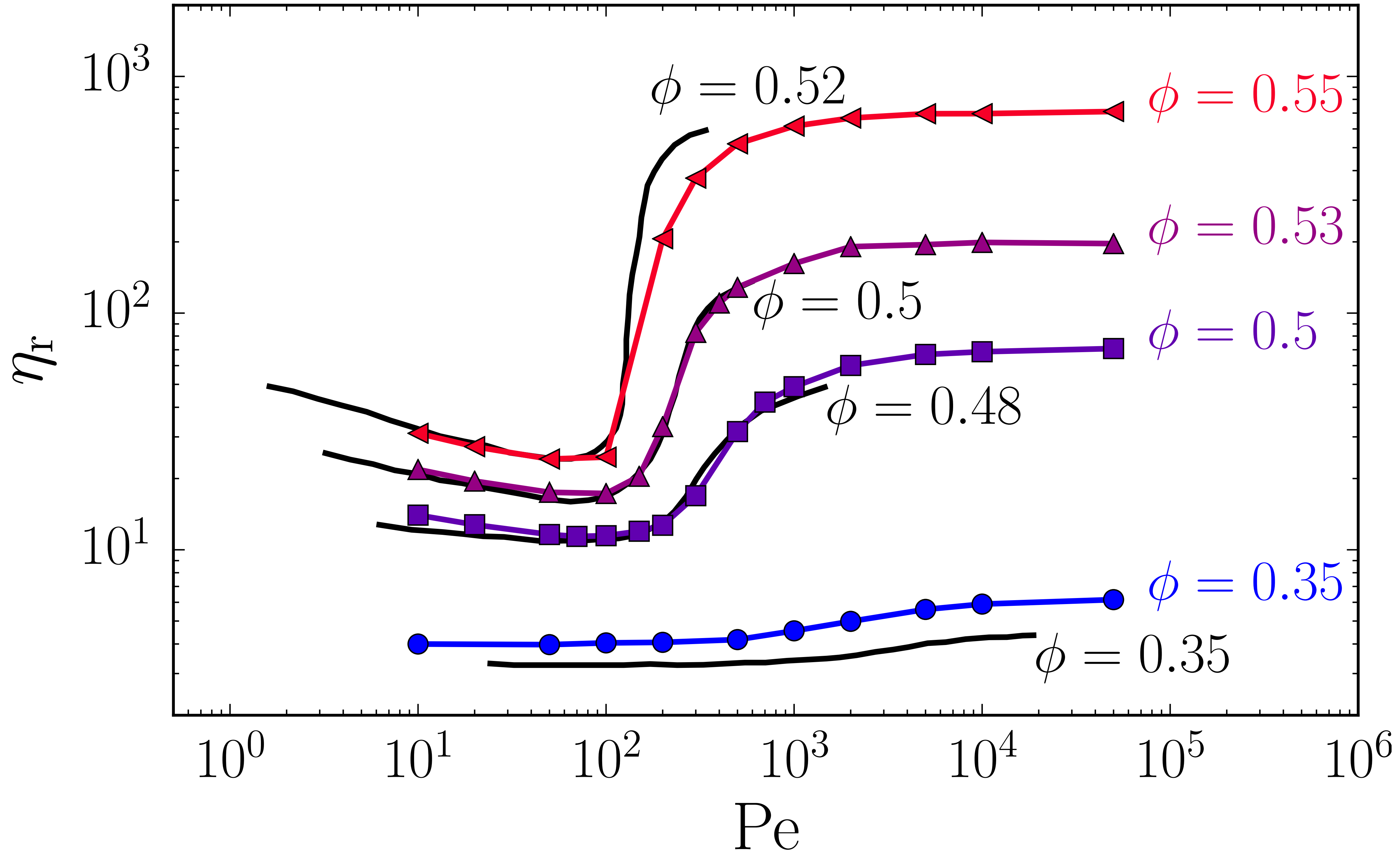
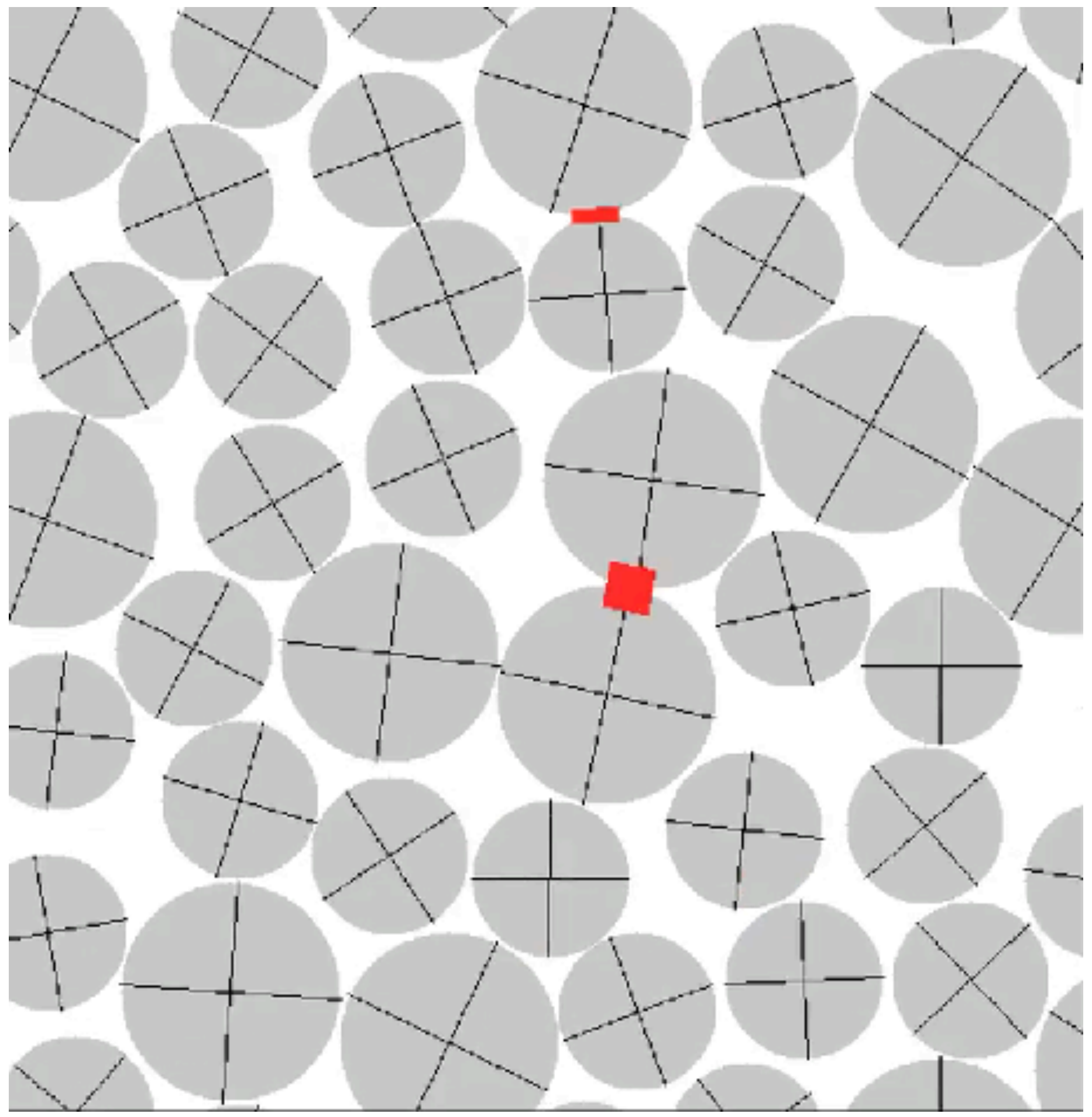


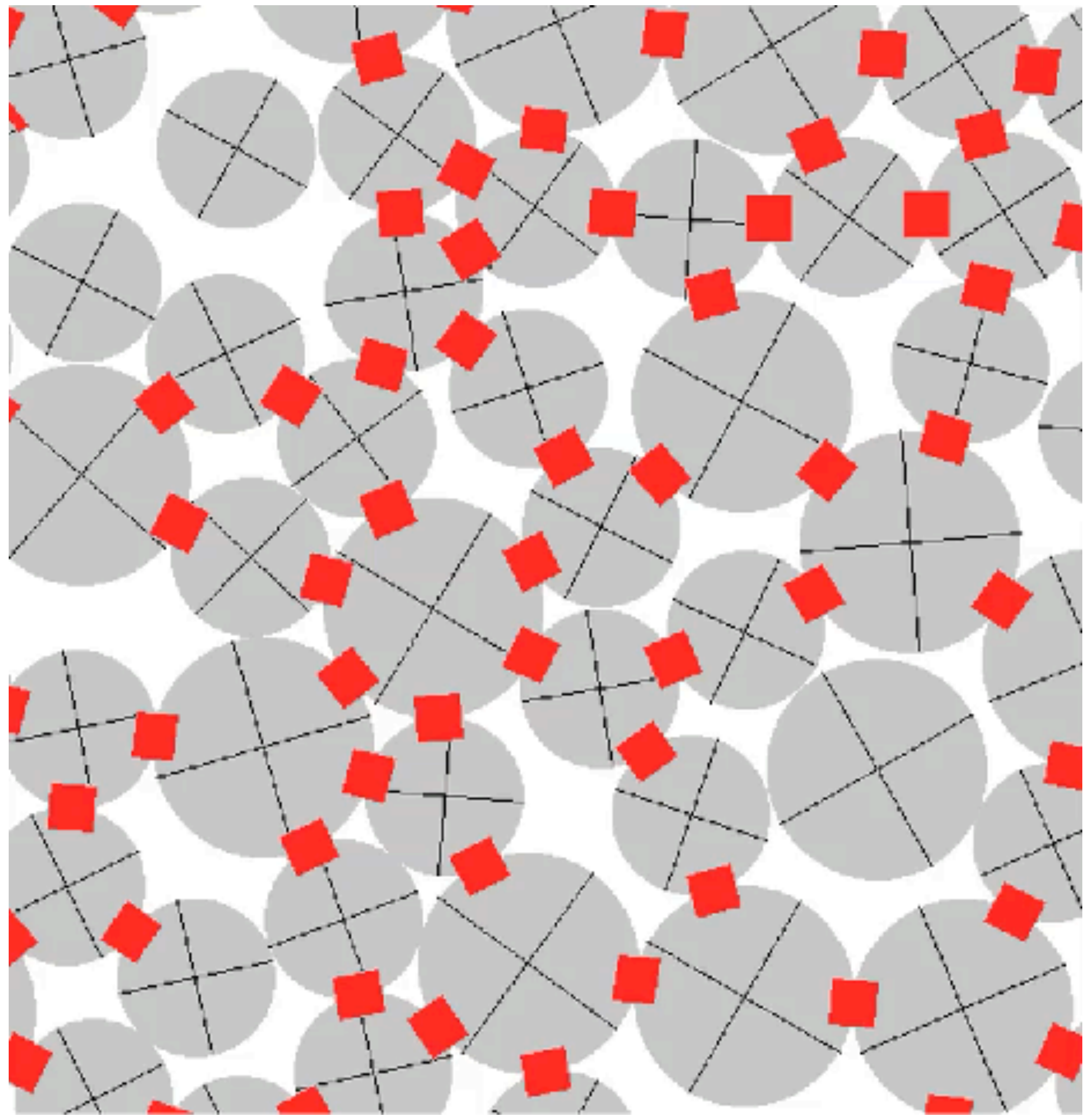
Experimental data: Cwalina & Wagner 2014

What shear thickening study brought us?

Weak shear



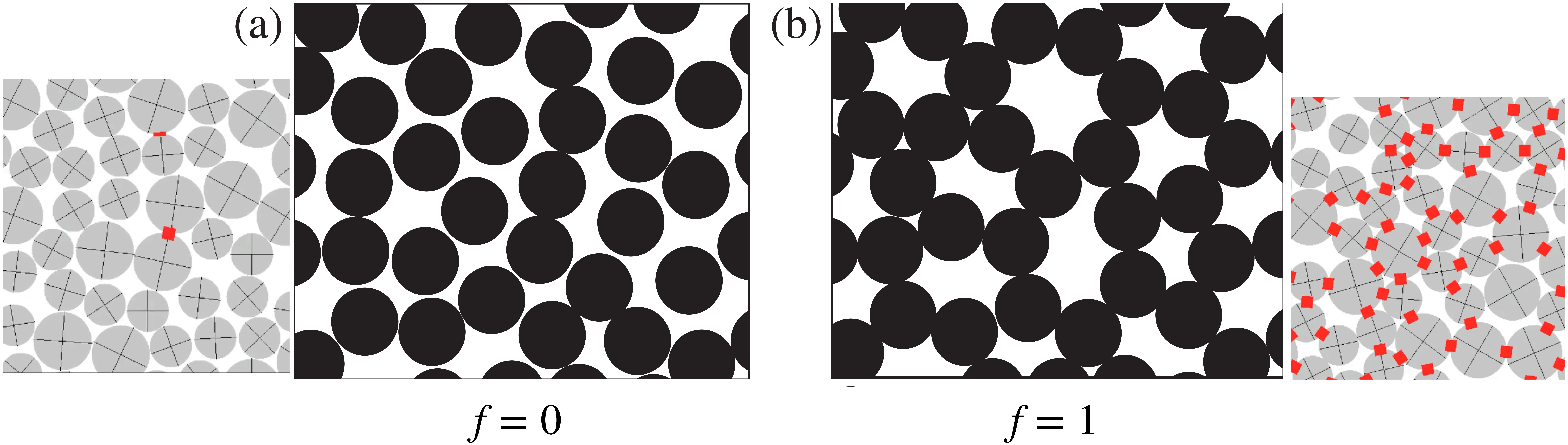
Strong shear



Red dotts indicate contact

contact is frictional

cf. Nakanishi et al. 2012



"The dilatant fluid contains dispersed granular particles, which provides the system with **an internal degree of freedom** for a macroscopic description. Figure shows a schematic illustration for a relaxed state (a) and that for a jammed state (b)"

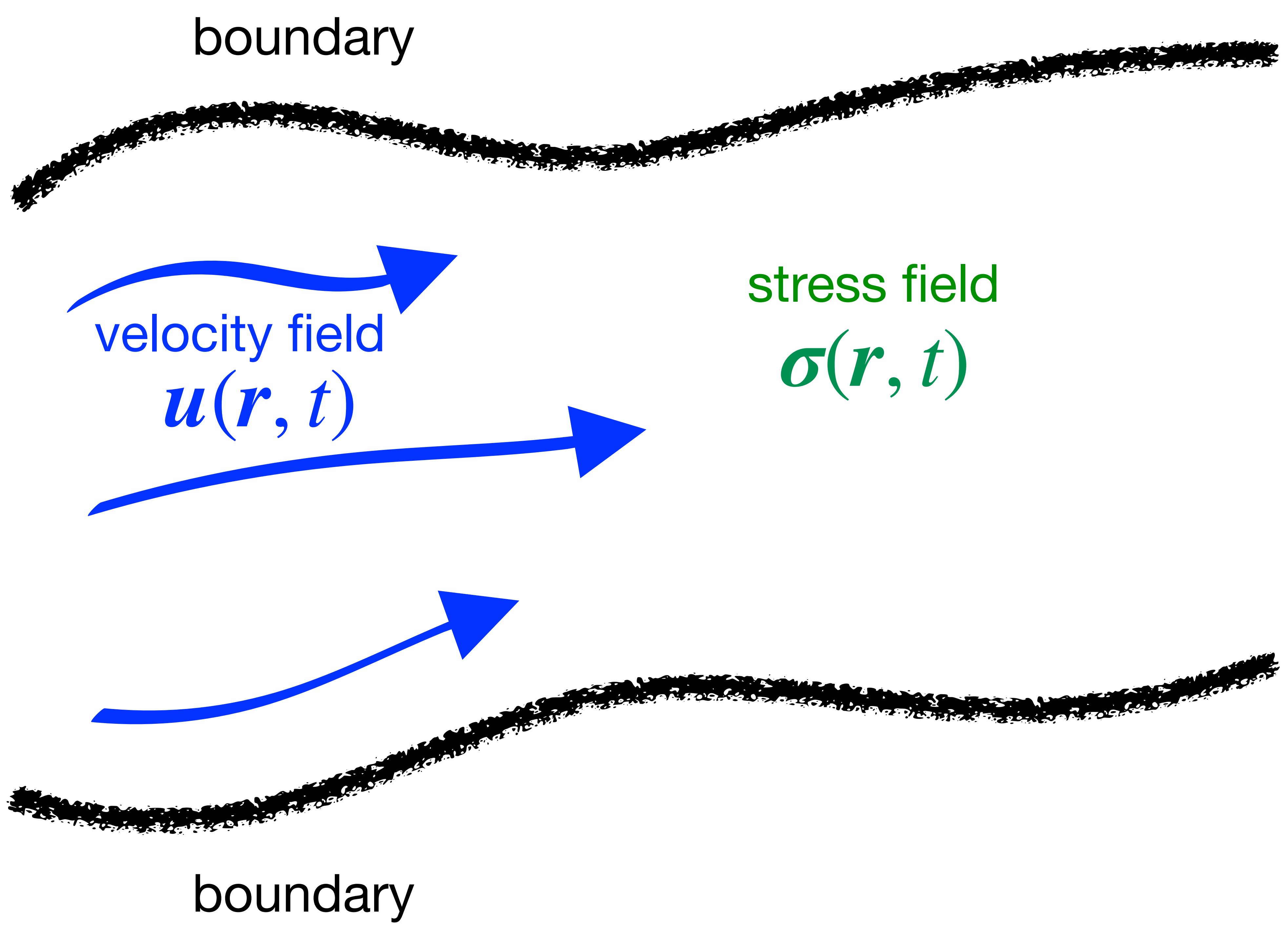
"the viscosity η is not constant but depends on the **internal state variable** f of the medium."

What shear thickening study brought us?

- *The purely hydrodynamic assumption* does not hold.
- (Granular) *solid mechanics* is embedded in incompressible fluids

We need to reflect them in constitutive models.

review for constitutive models for fluids



Constitutive model for the most common viscous fluid

Momentum balance $\rho \frac{D\boldsymbol{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma}$

Incompressibility $\nabla \cdot \boldsymbol{u} = 0$

$$\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + (\boldsymbol{u} \cdot \nabla)$$

Newtonian model “isotropic & no memory”

$$\boldsymbol{\sigma} = -p\mathbf{I} + \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}})$$

η: viscosity p: pressure

Constitutive models for very dilute suspensions

Very dilute suspensions $\phi < 0.05$

$$\boldsymbol{\sigma} = -p\mathbf{I} + \eta(\phi)(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}})$$

$$\eta(\phi) = \eta_0(1 + 2.5\phi)$$ (Einstein 1906)

Newtonian, i.e., no memory and isotropic

The presence of particles enhances viscosity in Newtonian model

Constitutive models for semi-dilute suspensions

$$\eta(\phi) = \eta_0(1 + 2.5\phi + C\phi^2)$$ **(Batchelor 1972)**

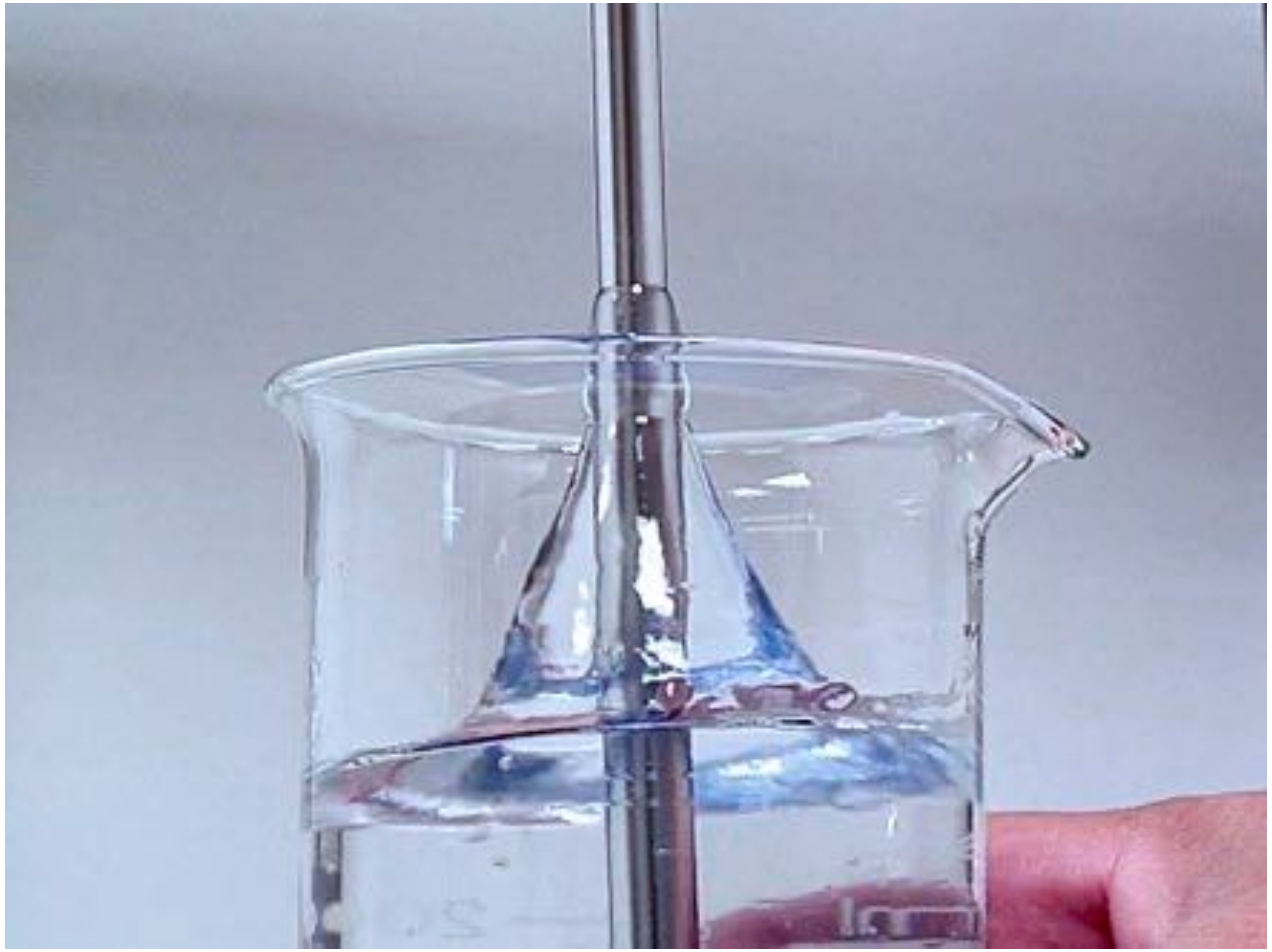
Some flow-rate and flow-type dependence can appear through C

However, only some steady state values were given.

$$C = \begin{cases} 6.95 & \text{radial symmetry etc.} \\ 5 & \text{randome structure} \end{cases}$$

C with general flow history is not given,
so this is not complete constitutive model.

viscoelastic fluids?

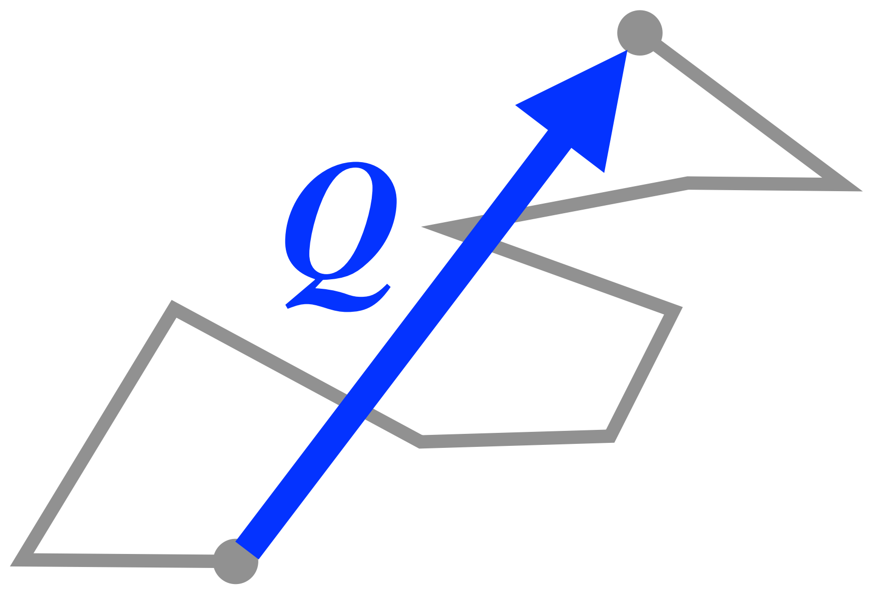


Constitutive models for viscoelastic fluids

Momentum balance $\rho \frac{D\boldsymbol{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma}$ Incompressibility $\nabla \cdot \boldsymbol{u} = 0$

stress tensor $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau}$ $\boldsymbol{\tau} = g(\mathbf{c} - \mathbf{I})$

conformation tensor $\mathbf{c} = \frac{1}{l_{\mathrm{eq}}^2}\langle \mathbf{Q}\mathbf{Q}^{\mathsf{T}} \rangle$



time evolution of $\mathbf{c}(\boldsymbol{r}, t)$ $\frac{D\mathbf{c}}{Dt} = (\mathbf{c} \cdot \nabla u + \nabla u^T \cdot \mathbf{c}) - \frac{1}{\lambda}(\mathbf{c} - \mathbf{I}) - \frac{\alpha}{\lambda}(\mathbf{c} - \mathbf{I})^2$

driving deformation by flow gradient — relaxation — nonlinear effect

λ: relaxation time

α: nonlinear parameter
- Linear ($\alpha = 0$) — Oldroyd-B model
- Nonlinear ($0 < \alpha \leq 1$) — Giesekus model

Microstructure tensors

conformation tensor

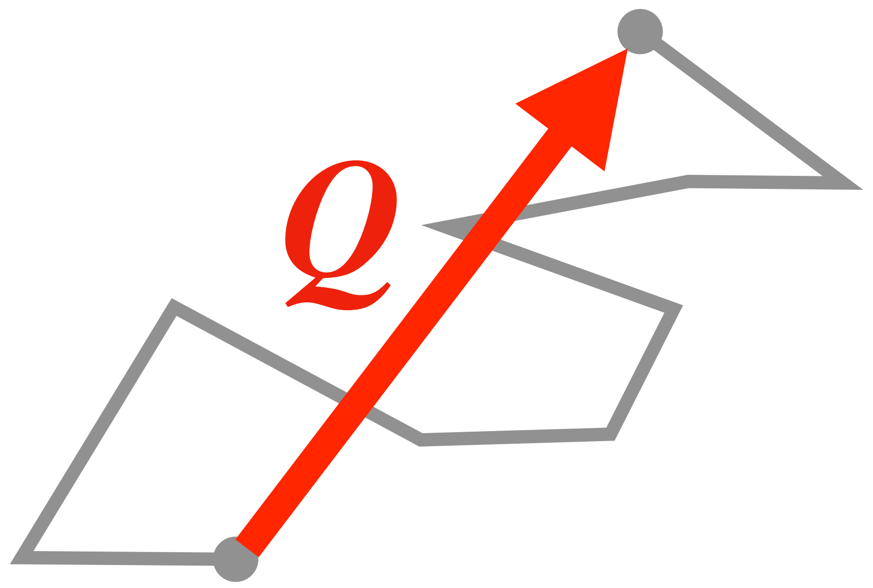
$$\mathbf{c} = \frac{1}{l_{\mathrm{eq}}^2}\langle \mathbf{QQ} \rangle$$

orientation distribution tensor

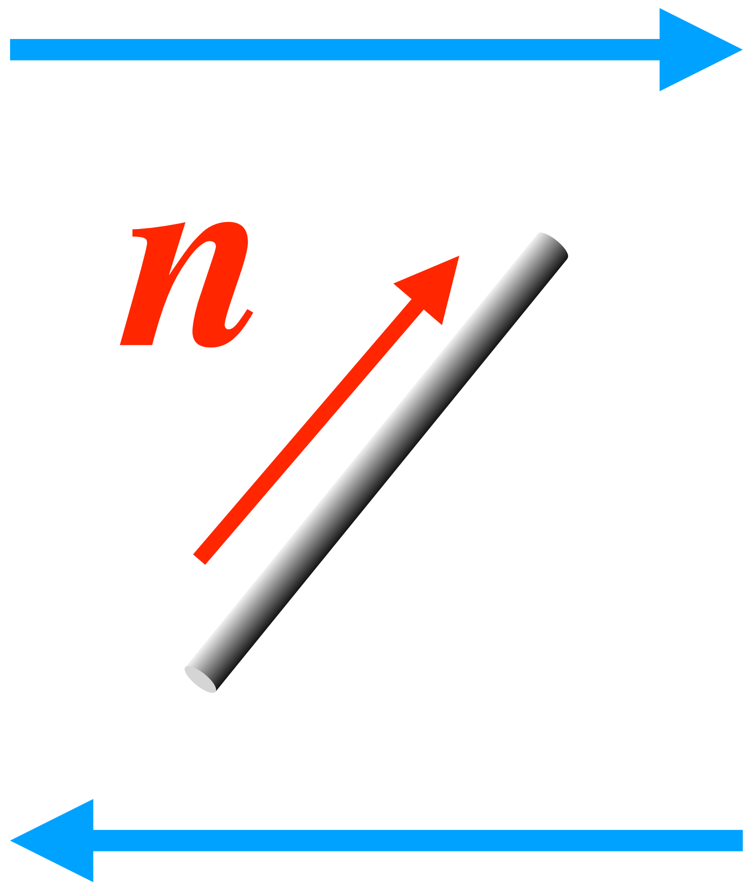
$$\mathbf{A} = \langle \boldsymbol{nn} \rangle$$

fabric tensor

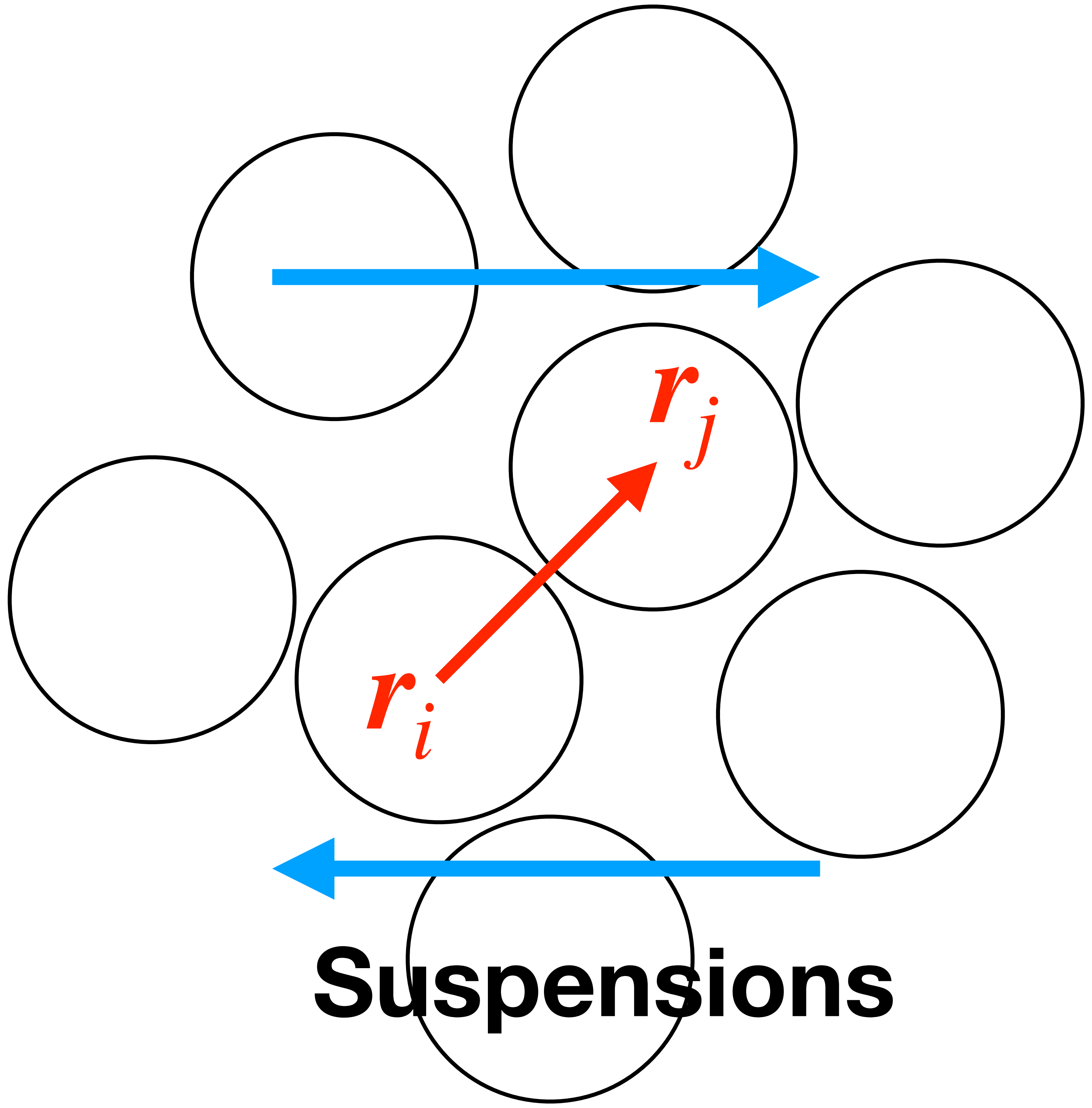
$$\mathbf{A} = \langle \boldsymbol{nn} \rangle$$



Polymer chains



Rods



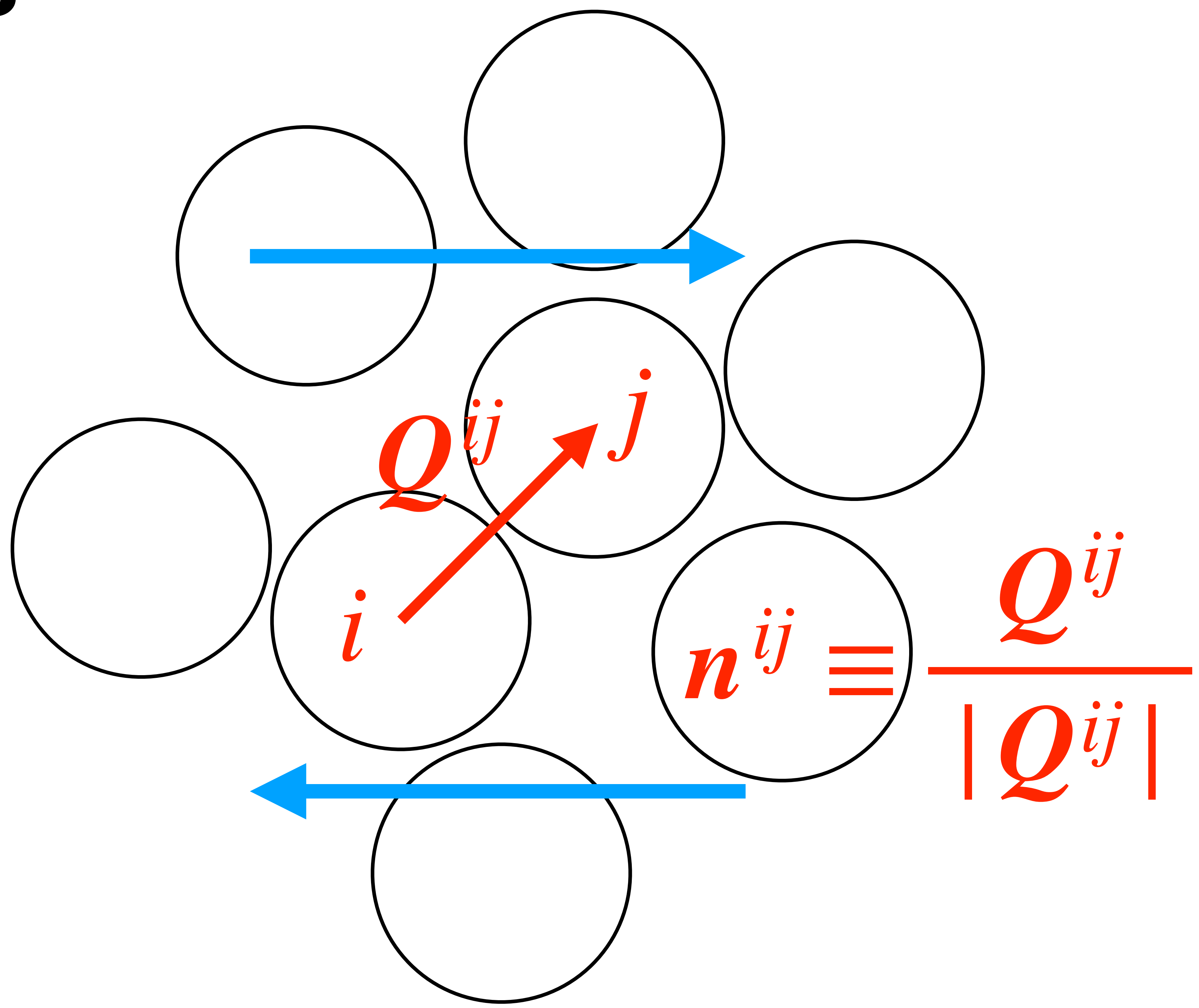
Suspensions

$$\boldsymbol{n}^{ij} = \frac{\boldsymbol{Q}^{ij}}{|\boldsymbol{Q}^{ij}|}$$

Constitutive models for particle suspensions

Phan-Thien's (1995)

$$\boldsymbol{\sigma} = -p\mathbf{I} + \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}}) + \boxed{\frac{N}{2V}\langle \boldsymbol{F}\boldsymbol{Q}\rangle}$$



Purely hydrodynamic force

$$\boldsymbol{F}^{pq} = \left(\zeta_{\mathrm{sq}}(h)\boldsymbol{n}\boldsymbol{n} + \zeta_{\mathrm{sh}}(\boldsymbol{I} - \boldsymbol{n}\boldsymbol{n})\right)\frac{d}{dt}|\boldsymbol{Q}^{pq}|$$

$$\zeta_{\mathrm{sh}} = 0$$

$$\langle\boldsymbol{\sigma}\rangle = -\langle p\rangle\boldsymbol{\delta} + \eta(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}}) + \boxed{\mu(\phi)\left(\boldsymbol{\kappa} : \langle \boldsymbol{n}\boldsymbol{n}\boldsymbol{n}\boldsymbol{n}\rangle + \frac{1}{2}\dot{\gamma}K\langle\boldsymbol{n}\boldsymbol{n}\rangle\right)}$$

$$\mu(\phi) = 2a^2N\zeta_{\mathrm{sq}}(h)/V$$

Constitutive models for particle suspensions

Time evolution

Phan-Thien's (1995)

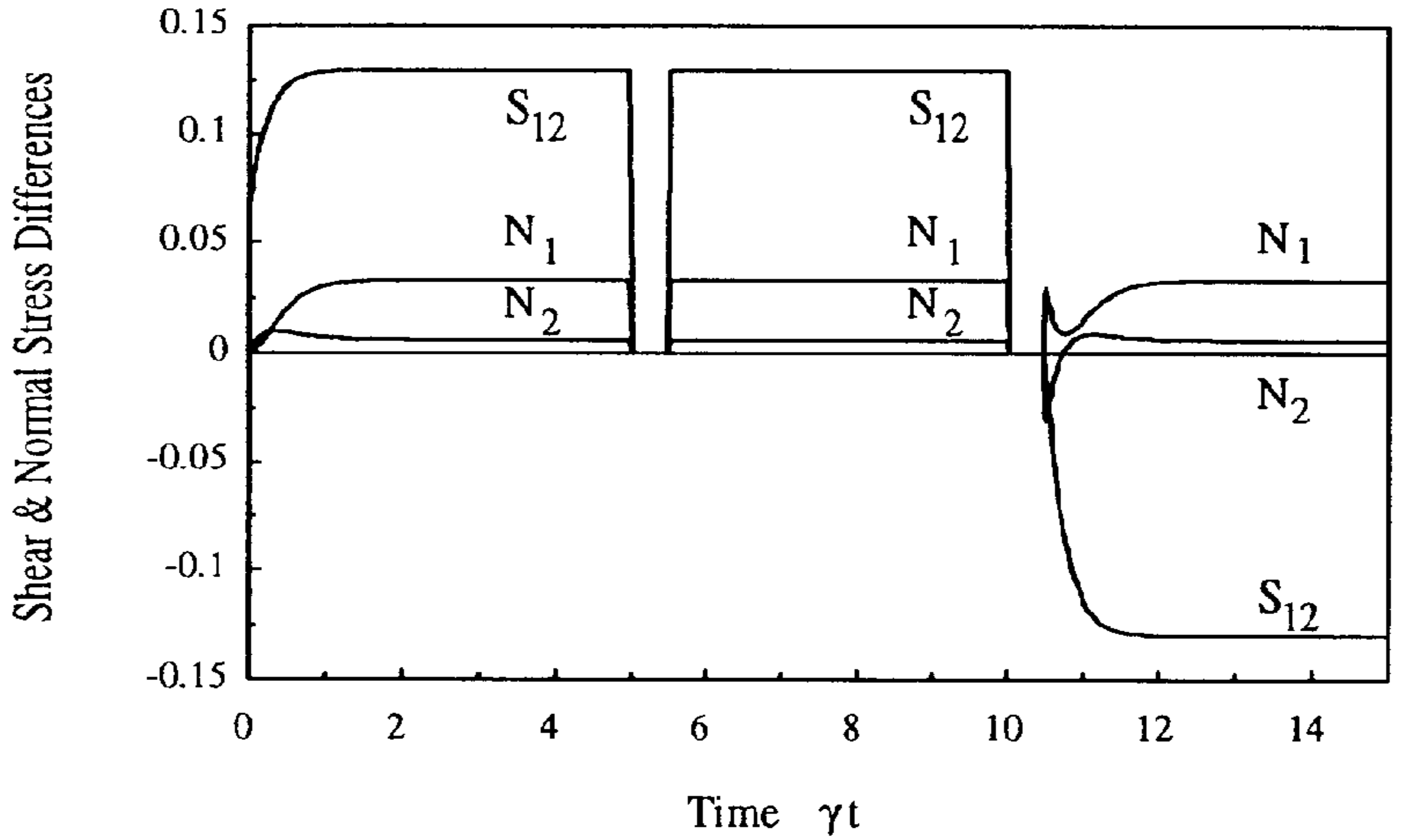
$$\frac{d}{dt}\boldsymbol{Q} = \nabla \boldsymbol{u} \cdot \boldsymbol{Q} + \boldsymbol{B}(t)$$

$$\langle \boldsymbol{B} \rangle = \mathbf{0},\ \langle \boldsymbol{B}(t+\Delta t)\boldsymbol{B}(t) \rangle = B \exp(-\Delta t/\tau_c)\boldsymbol{\delta}$$

$$\frac{D}{Dt}\langle \boldsymbol{nn} \rangle = \nabla \boldsymbol{u} \cdot \langle \boldsymbol{nn} \rangle + \langle \boldsymbol{nn} \rangle \cdot \nabla \boldsymbol{u}^{\mathsf{T}} - 2\mathbf{D} : \langle \boldsymbol{nnnn} \rangle - \frac{3}{2}\dot{\gamma}K\left(\langle \boldsymbol{nn} \rangle - \frac{1}{3}\mathbf{I}\right)$$

This time evolution is rather simple.

Stopping and starting shear flow

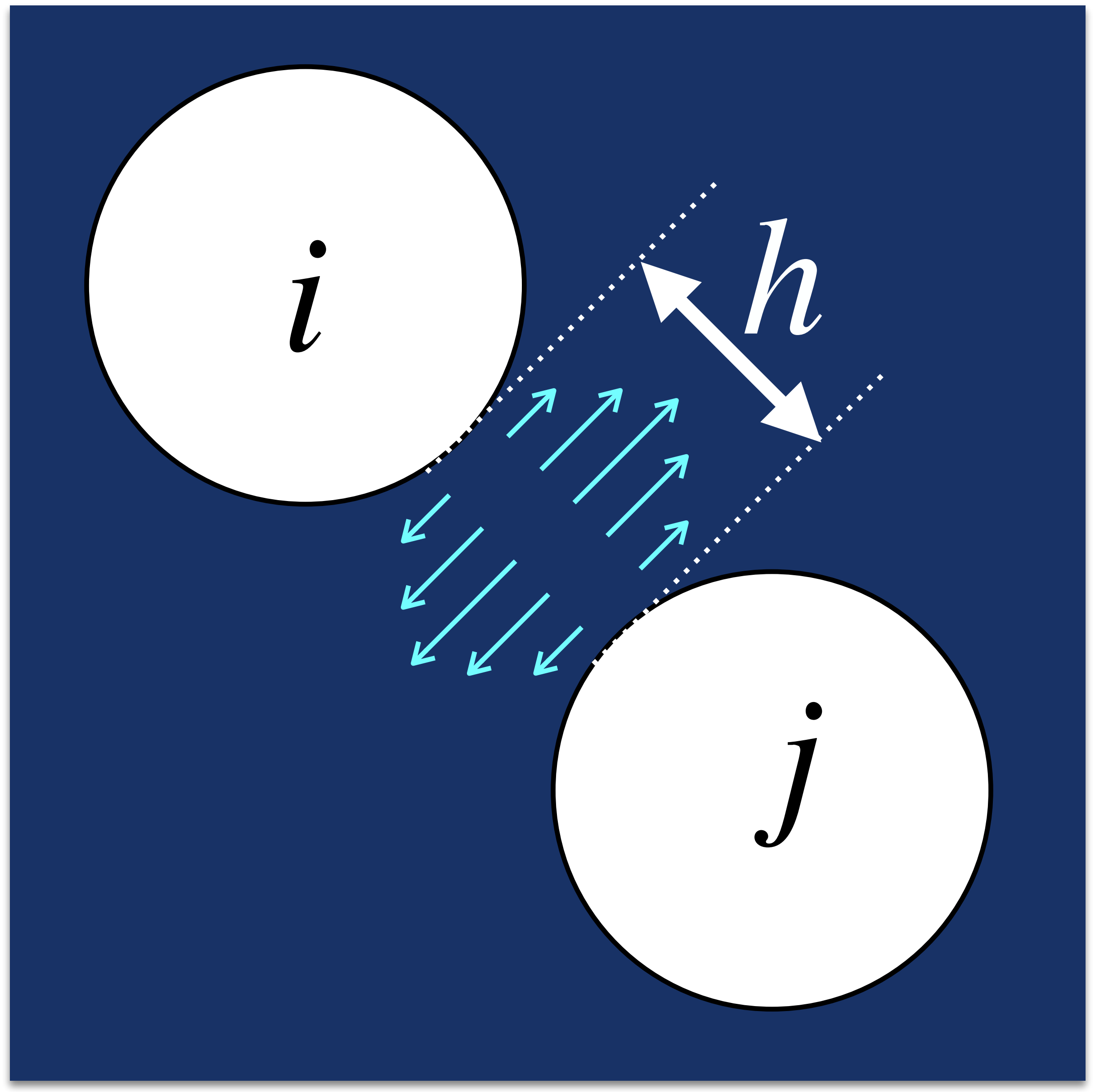


No direct contact

The hydrodynamic lubrication singularity is derived from the Stokes equation.

$$\boldsymbol{F}^{ij}_{\mathrm{lub}} \sim -\frac{1}{h}(\boldsymbol{U}^i - \boldsymbol{U}^j) \cdot \boldsymbol{n}\boldsymbol{n}$$

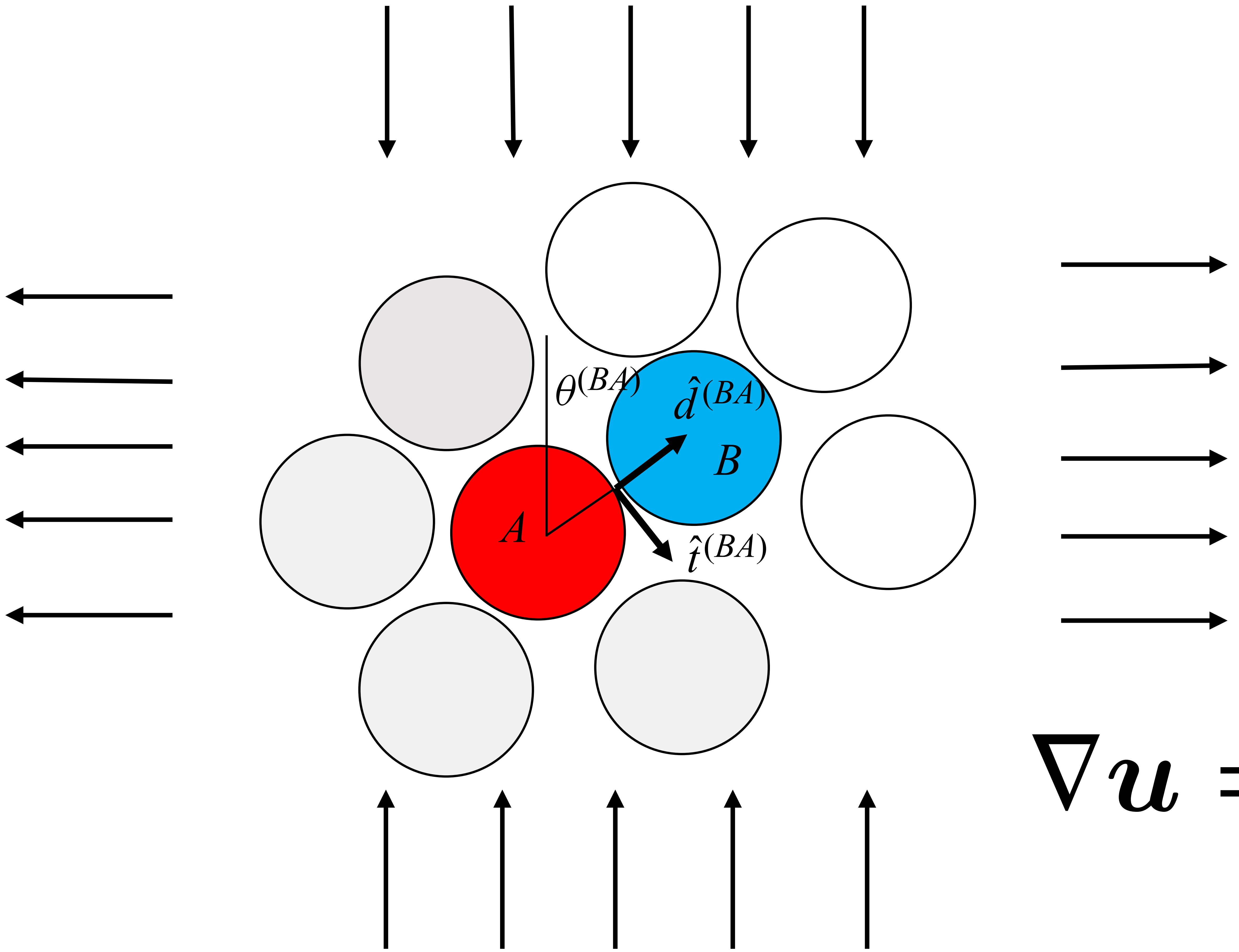
Jeffrey and Onishi (1984)



Force blance equation to predict trajectories and microstructure

Jenkins, Seto, and La Ragione. JFM 2021

Hydrodynamic force + repulsive force (no contact force)



$$\nabla \boldsymbol{u} = \begin{pmatrix} \dot{\varepsilon} & 0 & 0 \\ 0 & -\dot{\varepsilon} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Force blance equation to predict trajectories and microstructure

Jenkins, Seto, and La Ragione. JFM 2021

F_0 : **repulsive strength**

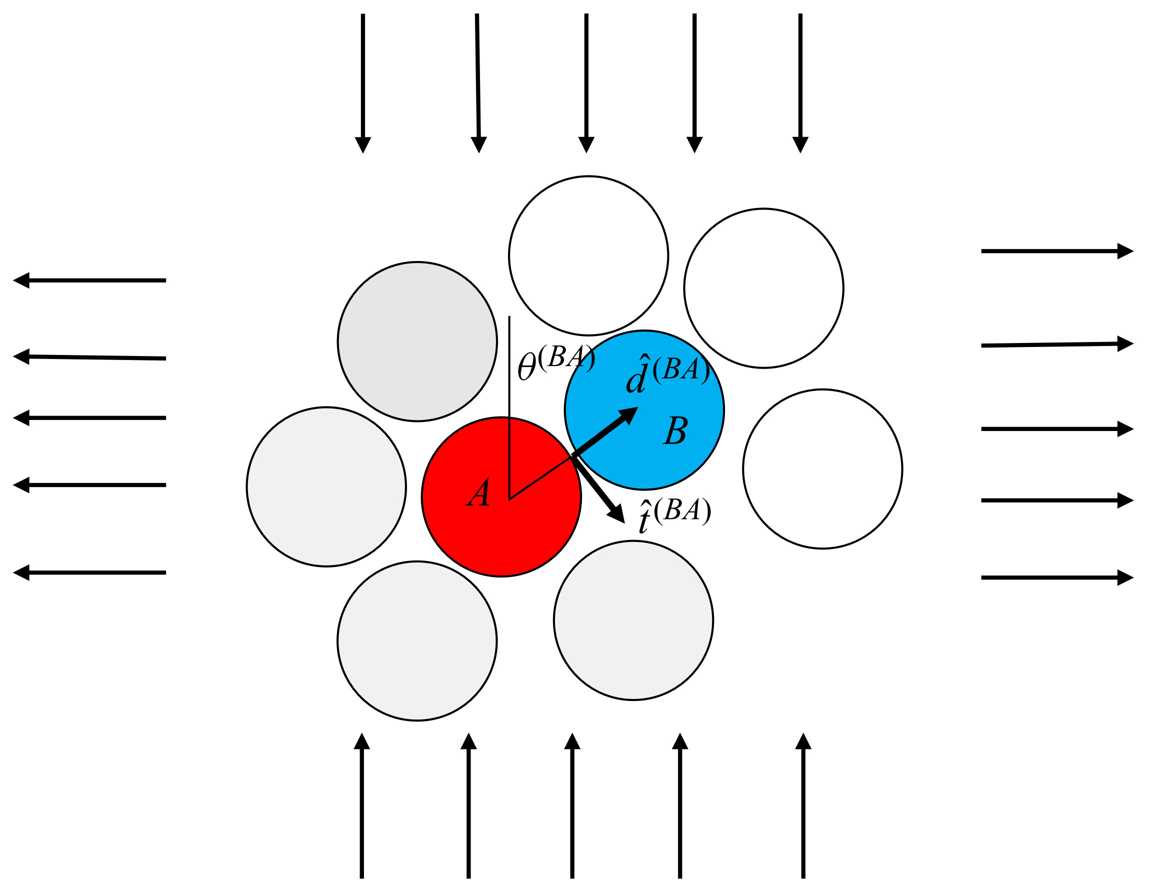
$$F_\alpha^{(BA)} = 6\pi\mu a K_{\alpha\beta}^{(BA)} v_\beta^{(BA)} - \frac{F_0}{s^{(BA)}}\hat{d}_\alpha^{(BA)} - 9.54\pi\mu a^2(\hat{t}_\beta D_{\beta\xi}\hat{d}_\xi)\hat{t}_\alpha^{(BA)} + \pi\mu a^2\left[\ln\left(\frac{a}{s^{(BA)}}\right) - 0.96\right]\omega^{(A)}\hat{t}_\alpha^{(BA)} + \pi\mu a^2 \ln\left(\frac{a}{s^{(BA)}}\right)\omega^{(B)}\hat{t}_\alpha^{(BA)}, \quad (2.7)$$

where

$$K_{\alpha\beta}^{(BA)} = \frac{1}{4}\frac{a}{s^{(BA)}}\hat{d}_\alpha^{(BA)}\hat{d}_\beta^{(BA)} + \left[\frac{1}{6}\ln\left(\frac{a}{s^{(BA)}}\right) + 0.64\right]\hat{t}_a^{(BA)}\hat{t}_\beta^{(BA)} \quad (2.8)$$

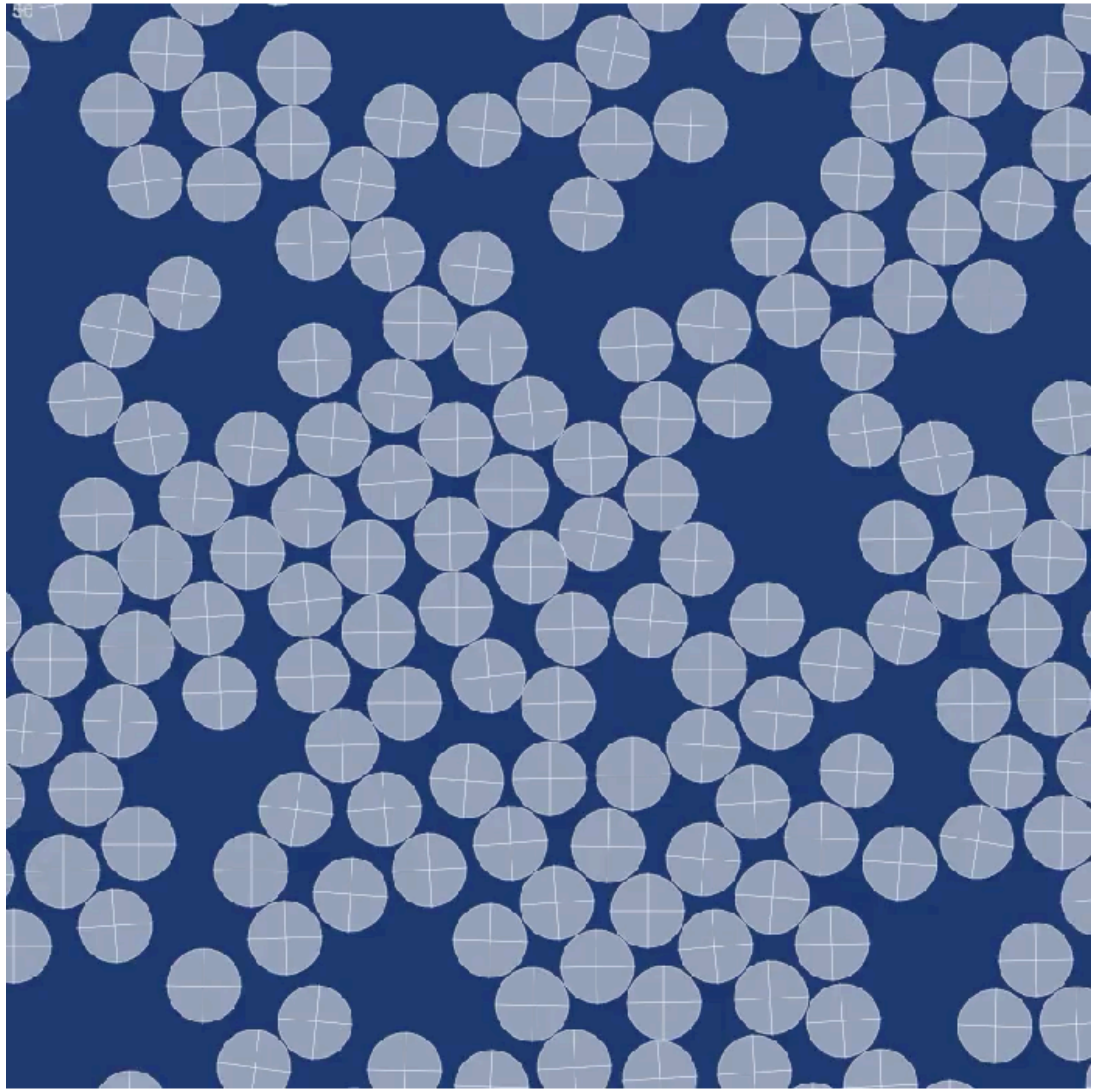
Force and torque balance to calculate trajectory

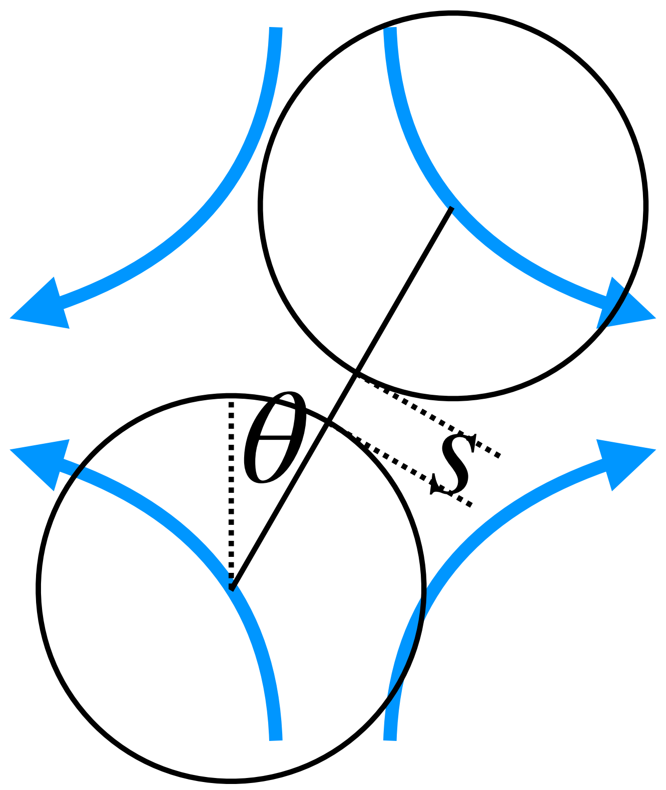
$$F_\alpha^{(BA)} + \sum_{m\neq B}^{N^{(A)}} F_\alpha^{(mA)} = 0; \qquad F_\alpha^{(AB)} + \sum_{m\neq A}^{N^{(B)}} F_\alpha^{(mB)} = 0,$$

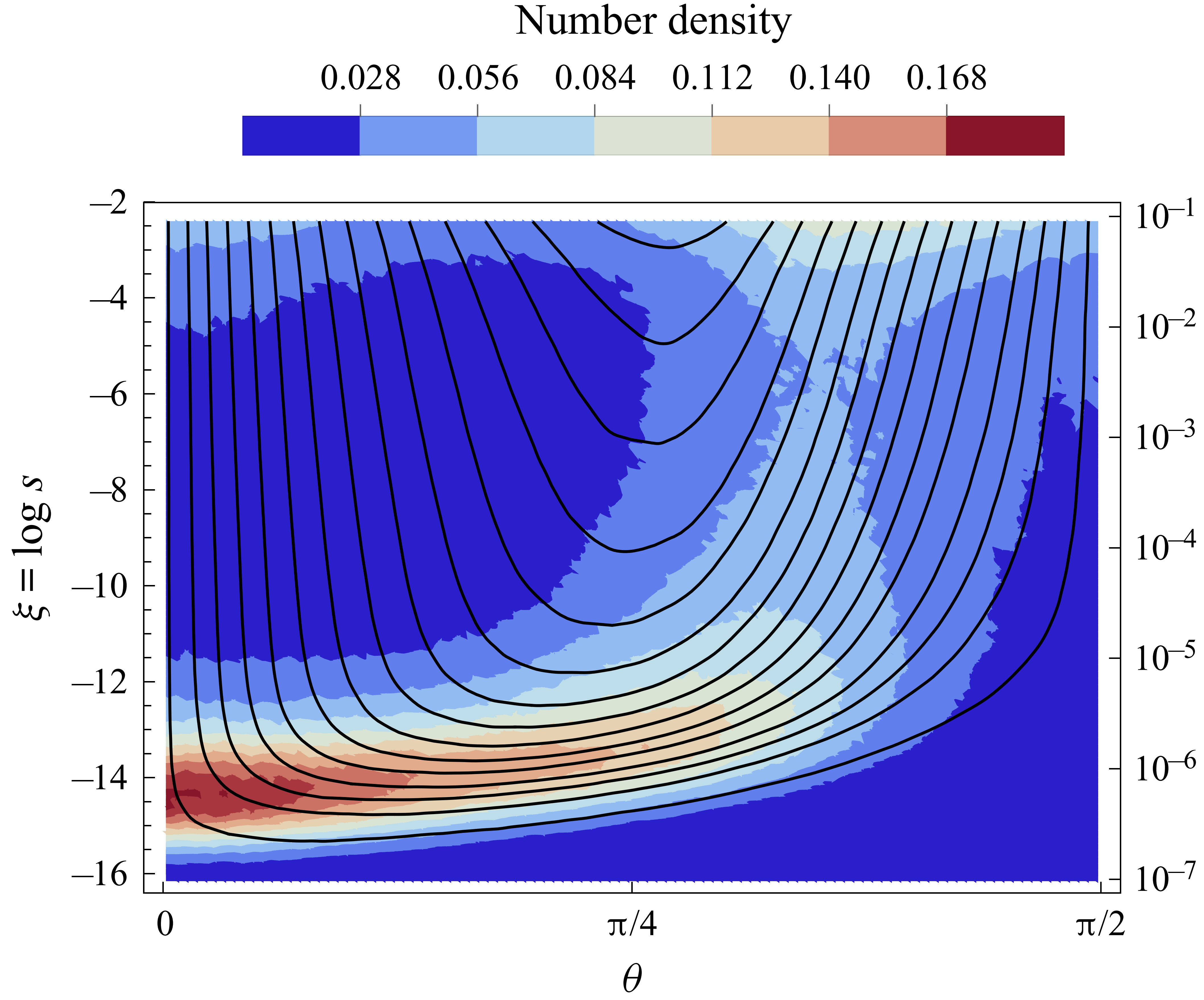


Particle simulation for extentional flows to compare with theory

Jenkins, Seto, and La Ragione. JFM 2021



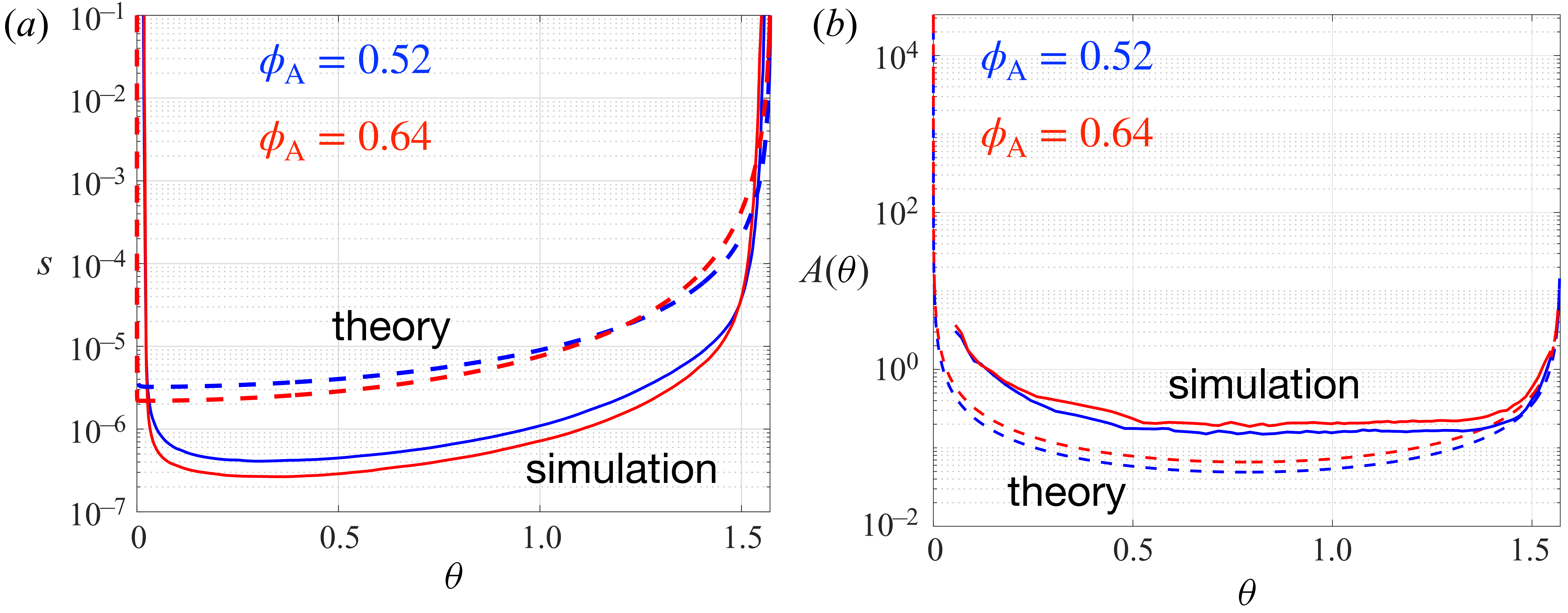




Reconstructuted trajectories from the averaged velocity field

Not very good agreement between simulation and theory…

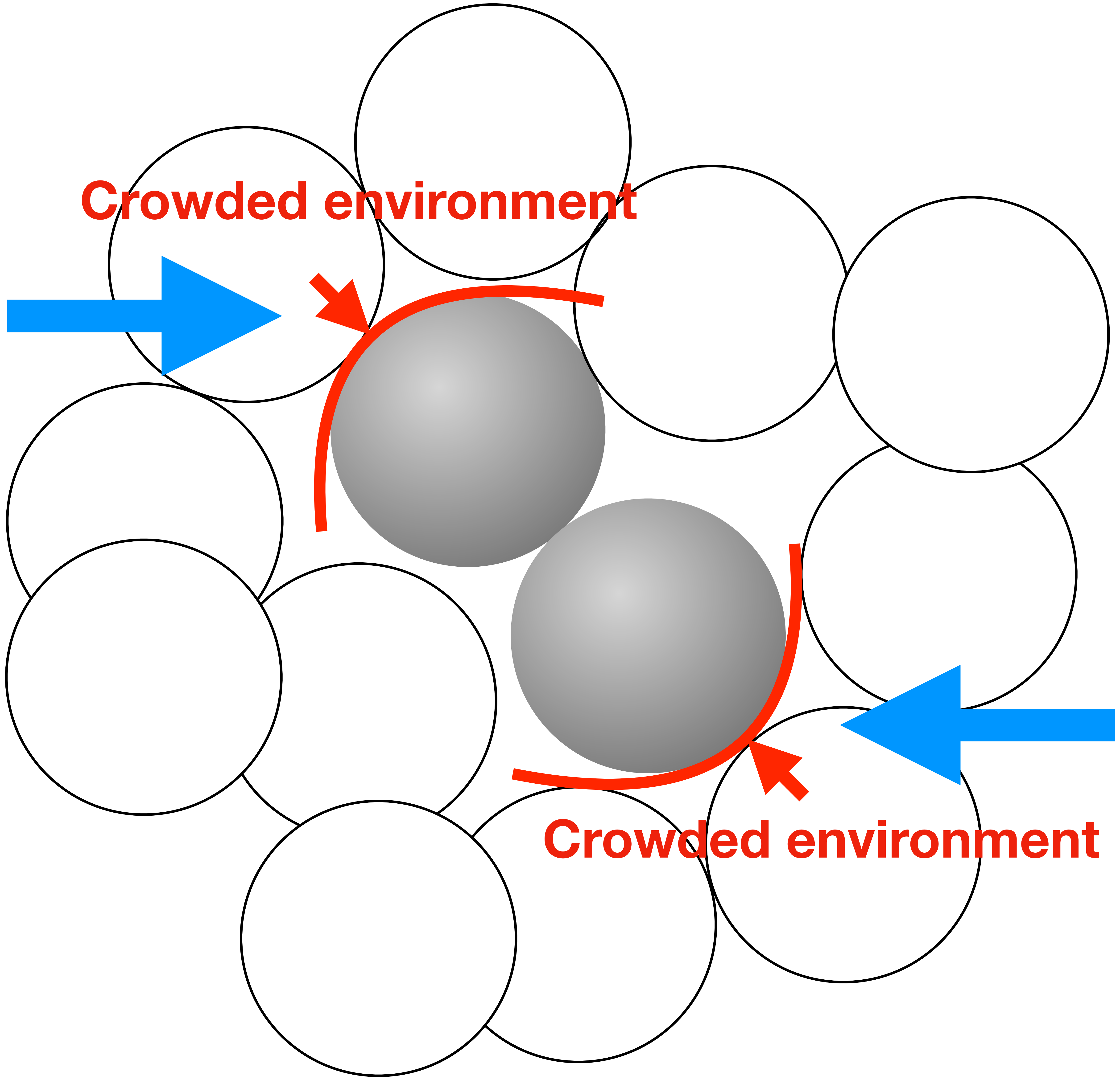
Jenkins, Seto, and La Ragione. JFM 2021

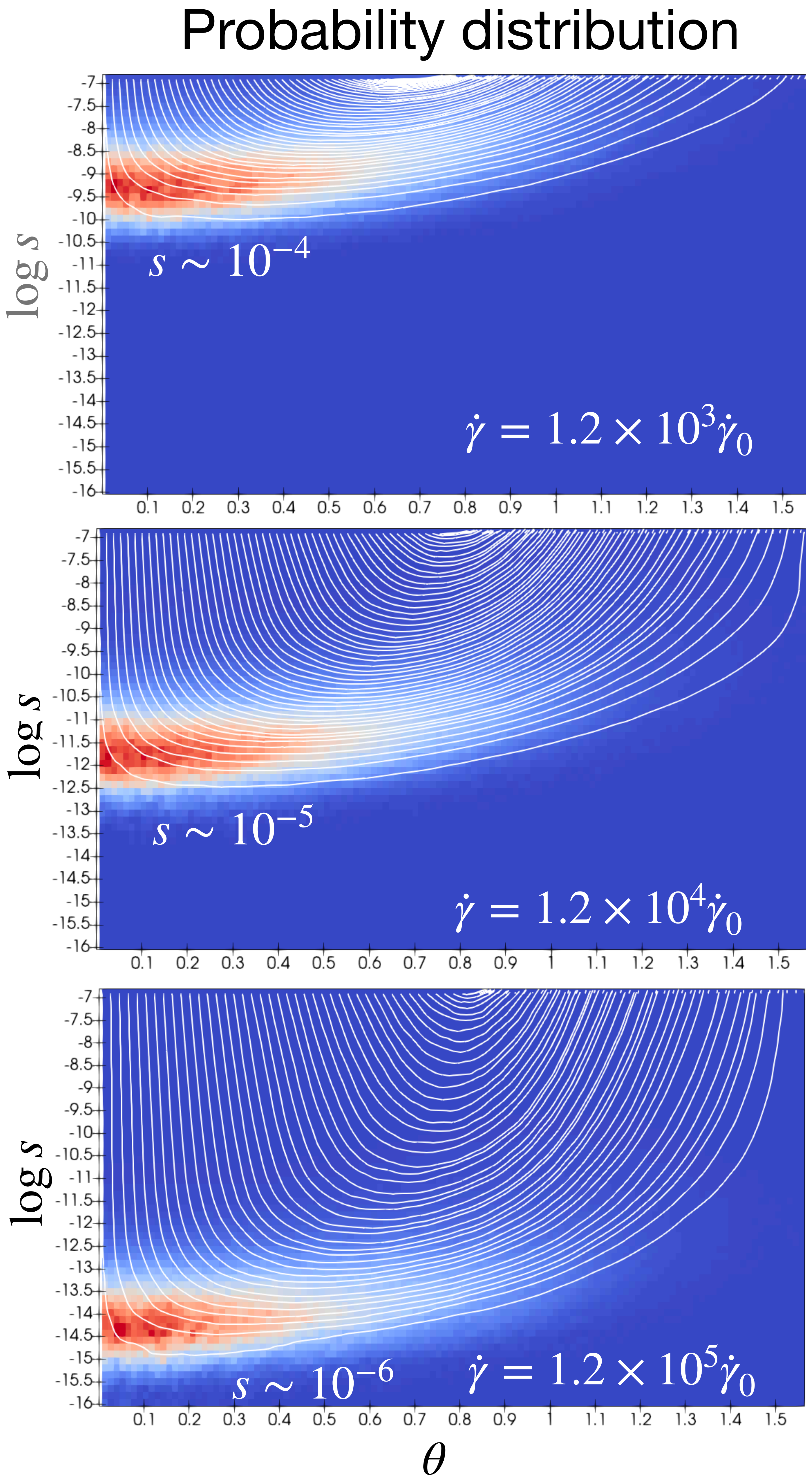


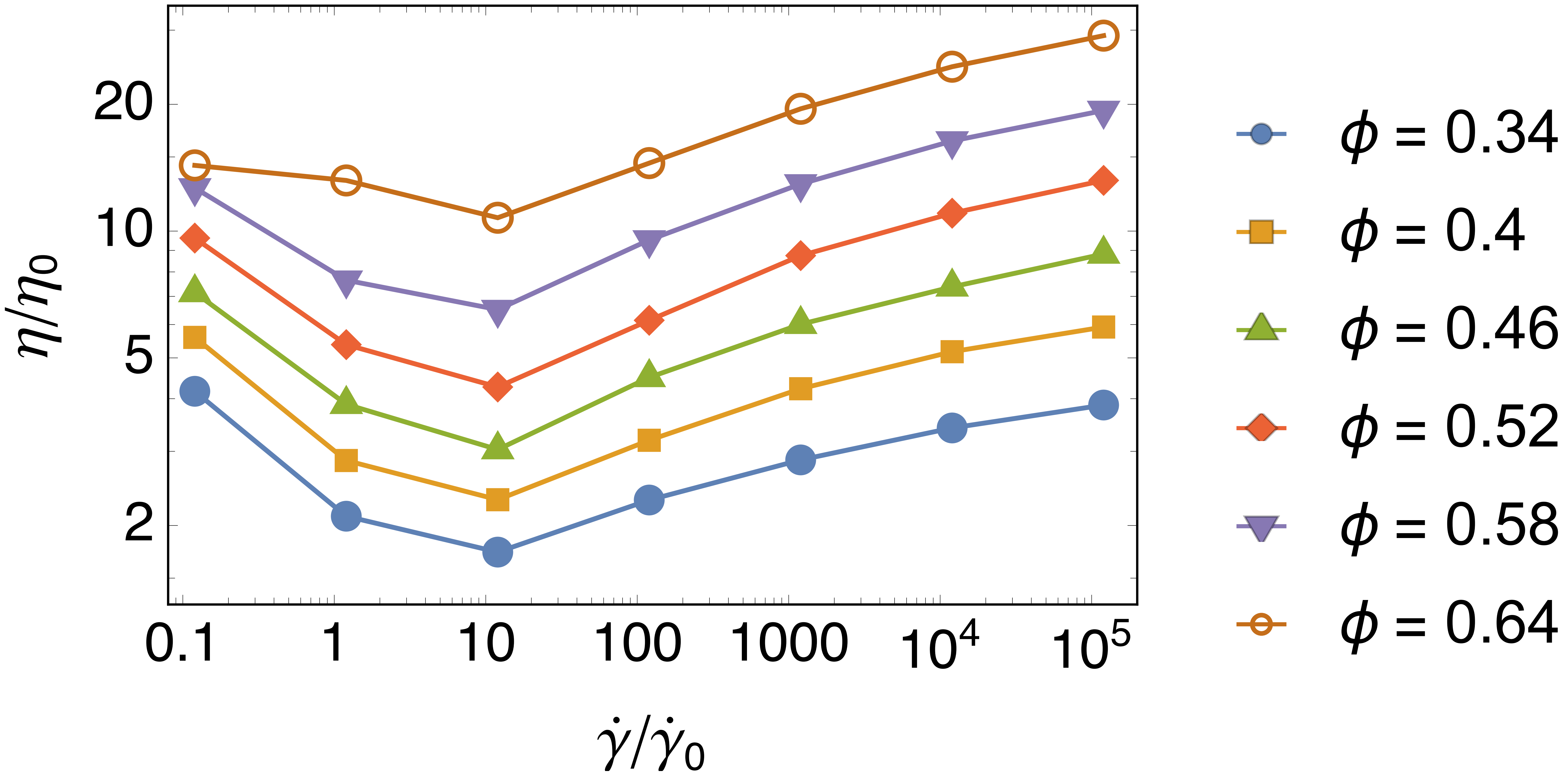
Not good agreement indicating we need more effects from background neighobrs

more effects from background neighobrs

(beynod mean field? Force chains?)




Probability distribution
log s
$s \sim 10^{-4}$
$\dot\gamma = 1.2 \times 10^3 \dot\gamma_0$
$s \sim 10^{-5}$
$\dot\gamma = 1.2 \times 10^4 \dot\gamma_0$
$s \sim 10^{-6}$
$\dot\gamma = 1.2 \times 10^5 \dot\gamma_0$
θ

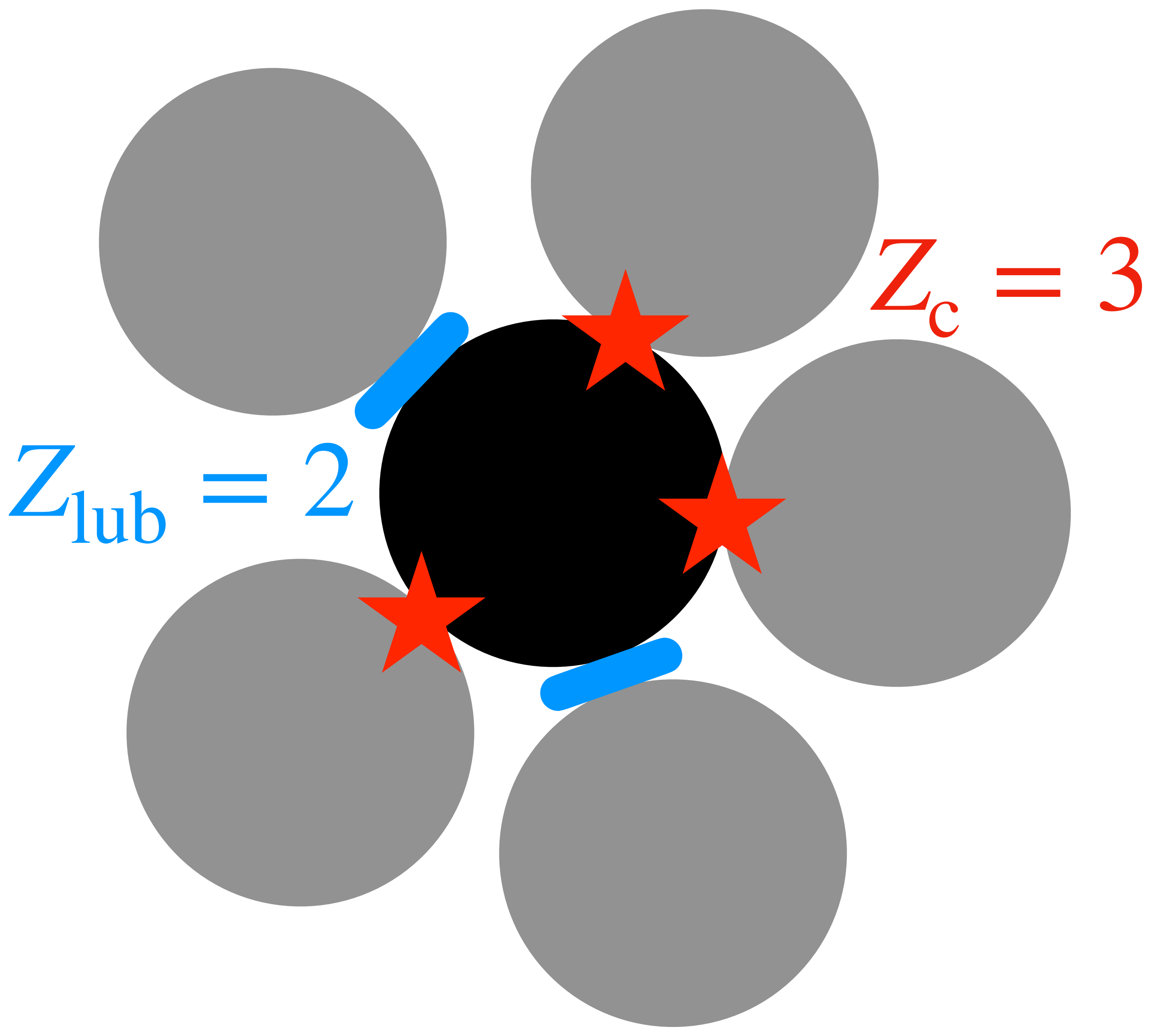

η/η_0
$\dot\gamma/\dot\gamma_0$
$\phi = 0.34$
$\phi = 0.4$
$\phi = 0.46$
$\phi = 0.52$
$\phi = 0.58$
$\phi = 0.64$

Some efforts after knowing the importance of frictional contacts

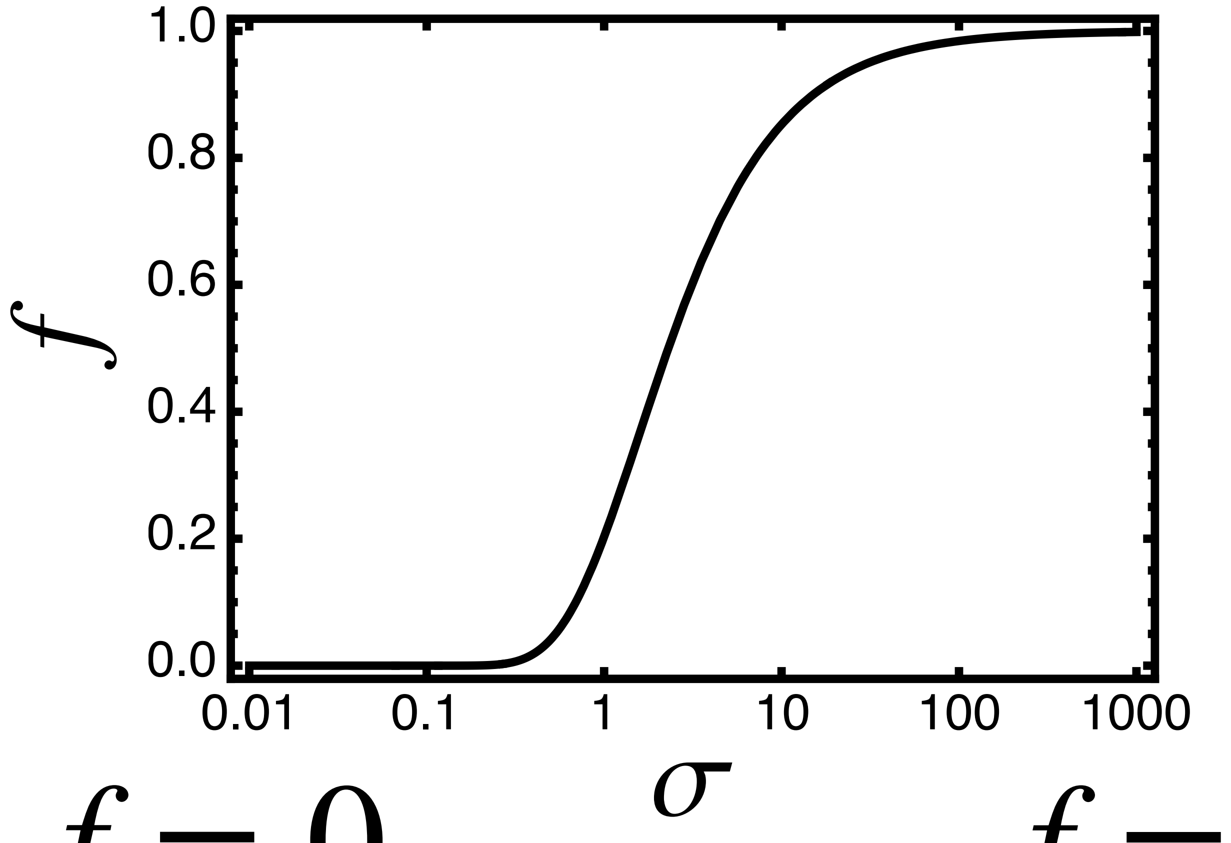
DST model for steady states (WC model)

Wyart and Cates. Phys. Rev. Lett. (2014)
cf. Nakanishi, Nagahiro, and Mitarai. Phys. Rev. E, (2012)

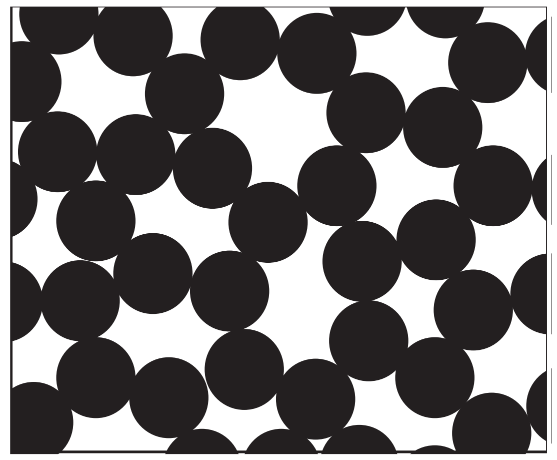
state variable $f \equiv \dfrac{Z_c}{Z_c + Z_{lub}}$



$f(\sigma) = \exp(-A/\sigma)$



$f = 0$ $f = 1$



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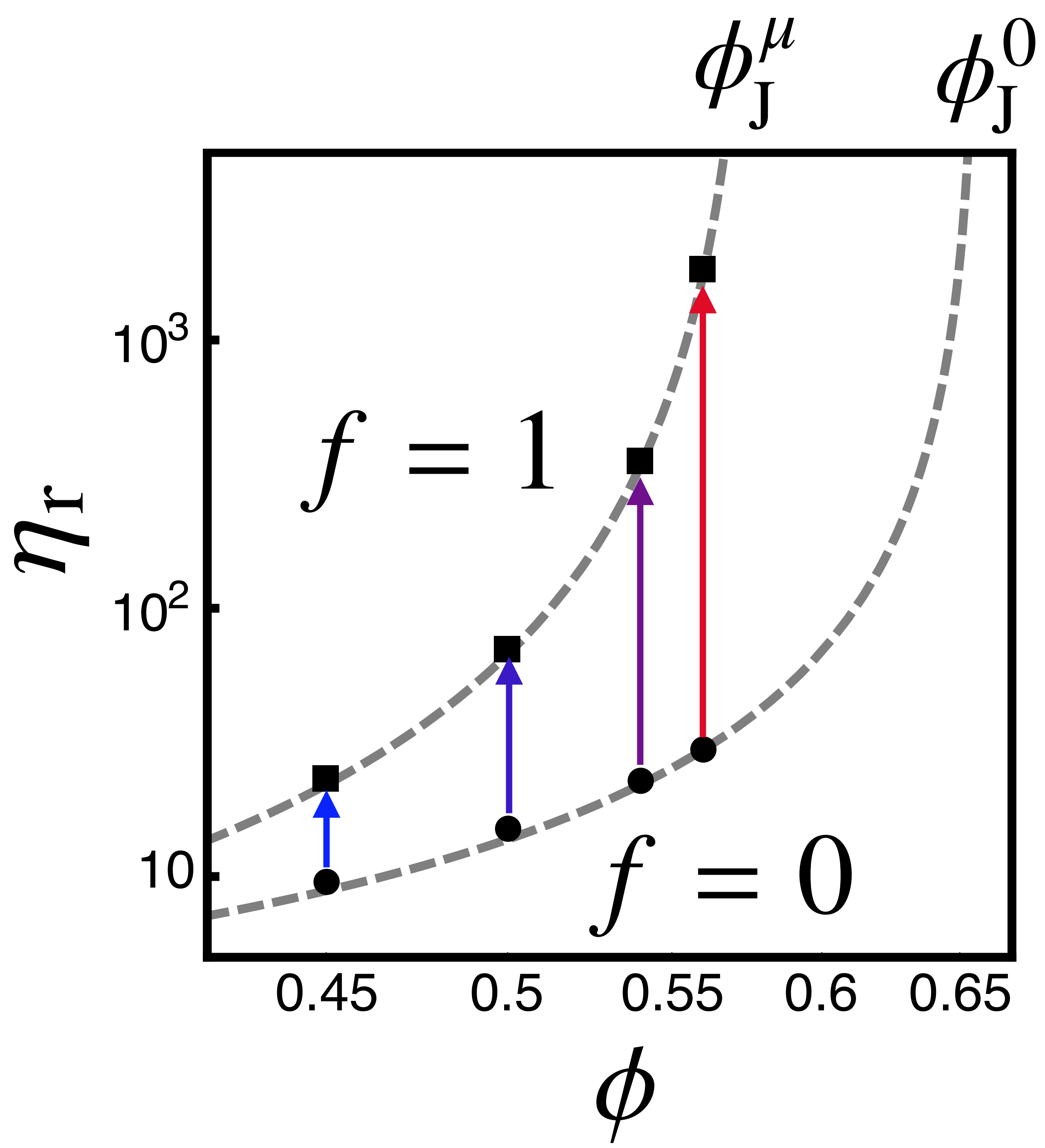
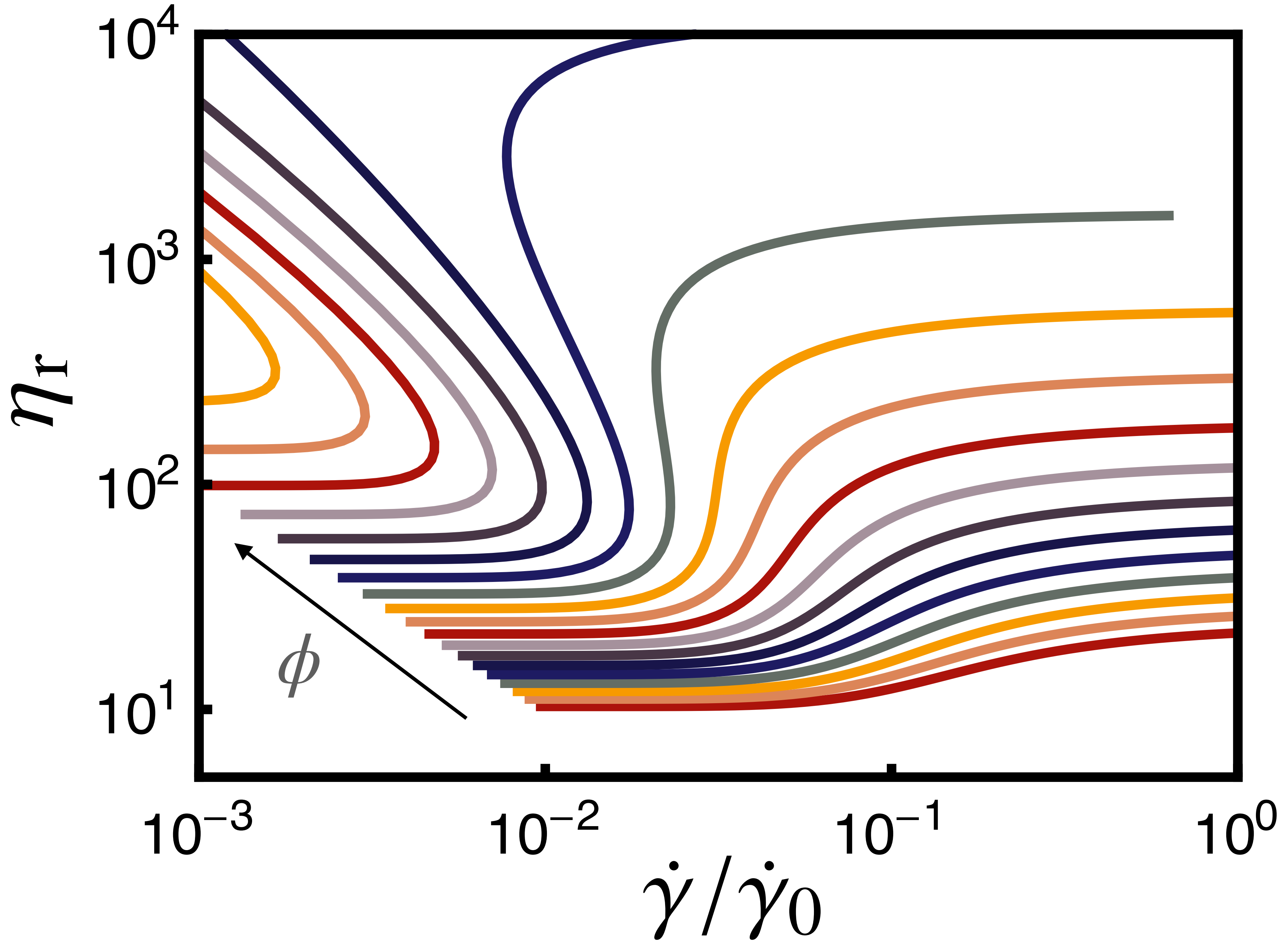
cf. Nakanishi, Nagahiro, and Mitarai. Phys. Rev. E, (2012)

state variable $f \equiv \dfrac{Z_c}{Z_c + Z_{lub}}$

$$\phi_J(f) = (1-f)\phi_J^0 + f\phi_J^\mu$$

$$\eta = \frac{\sigma}{\dot\gamma} = \left(1 - \frac{\phi}{\phi_J(f)}\right)^{-\lambda}$$





SPH implementation for the scalar model based on WC model

Angerman, Seto, Sandnes, and Ellero. Phys. Fluids, 2024 + draft in preparation

Also Baumgarten and Kamrin, PNAS 2019

Microstructure evolution $$\frac{Df(\boldsymbol{r},t)}{Dt} = k_{\mathrm{f}}\dot{\gamma}(\hat{f}(\sigma(\boldsymbol{r})) - f(\boldsymbol{r},t)) + \alpha\nabla^2 f(\boldsymbol{r},t)$$

α : microstructure diffusivity parameter

$\dot{\gamma}(\boldsymbol{r},t) \equiv \sqrt{\mathbf{D}:\mathbf{D}/2}$: local shear rate

$\hat{f}(\sigma)$: steady state value under shear stress σ

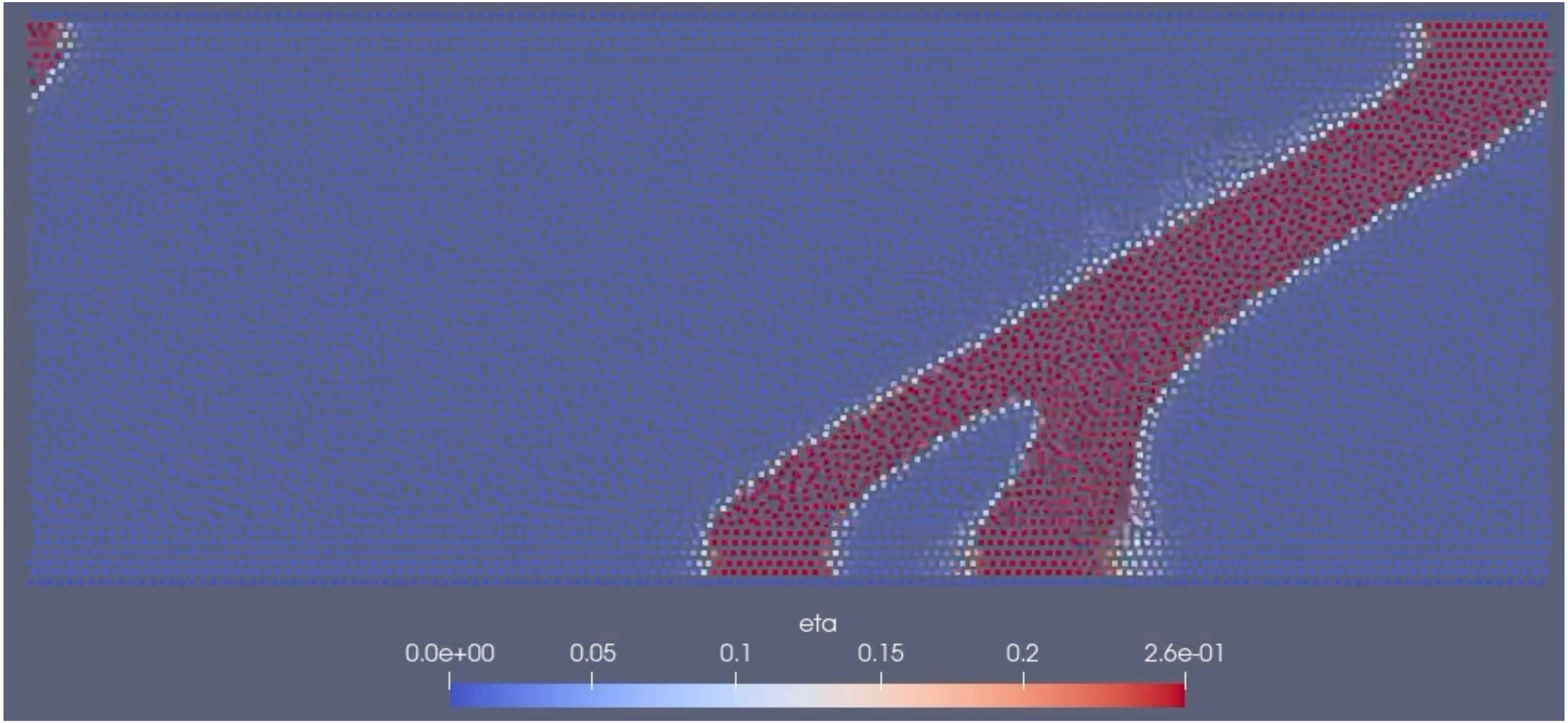
$f(\boldsymbol{r},t) \longrightarrow$

local jamming point and local viscosity

$$\phi_{\mathrm{J}}(f) = (1-f)\phi_{\mathrm{J}}^{0} + f\phi_{\mathrm{J}}^{\mu}$$

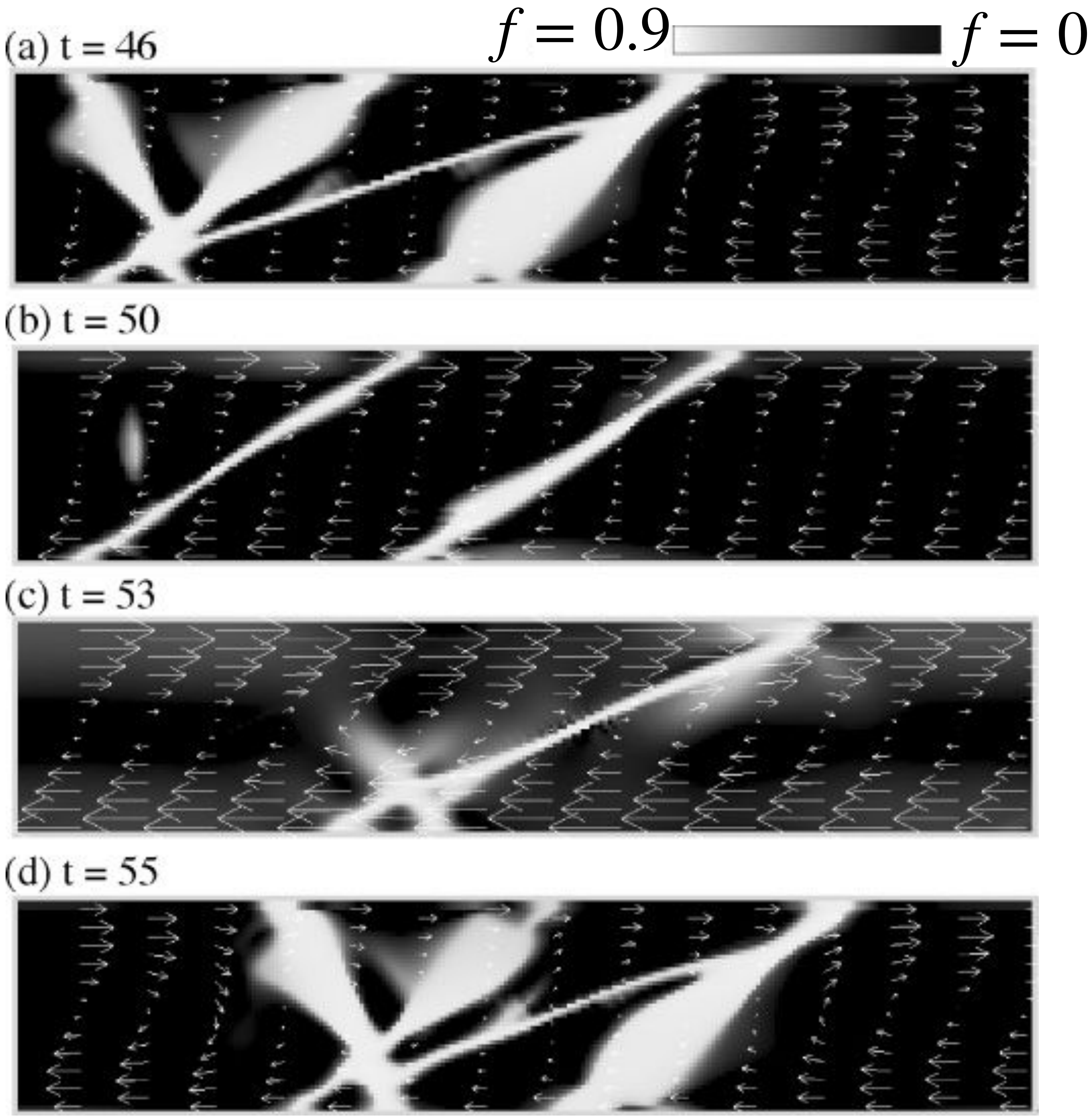
$$\eta = \frac{\sigma}{\dot{\gamma}} = \left(1 - \frac{\phi}{\phi_{\mathrm{J}}(f)}\right)^{-\lambda}$$

SPH demo for simple shear



viscosity

cf. Nakanishi et al. 2012



Tensorial constitutive models for dense suspensions

Gillissen, Ness, Peterson, Wilson, and Cates, Phys. Rev. Lett. (2019)

evolution of fabric tensor $\boldsymbol{A} = \langle \boldsymbol{nn} \rangle$

$$\partial_t \boldsymbol{A} = \underbrace{\nabla \boldsymbol{u} \cdot \boldsymbol{A} + \boldsymbol{A} \cdot \nabla \boldsymbol{u}^{\mathsf{T}} - 2 \nabla \boldsymbol{u} : \langle \boldsymbol{nnnn} \rangle}_{\text{convection}} - \beta \left(\boldsymbol{D}_{\mathrm{e}} : \langle \boldsymbol{nnnn} \rangle + \frac{\phi}{15} [2\boldsymbol{D}_{\mathrm{c}} + \mathrm{Tr}(\boldsymbol{D}_{\mathrm{c}}) \boldsymbol{\delta}] \right)$$

convection — buildup rate (β) — death — birth

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0 \boldsymbol{D} + \eta_0 \left(\frac{\alpha_0 \boldsymbol{D} : \langle \boldsymbol{nnnn} \rangle}{(1 - \phi/\phi_{\mathrm{RCP}})^2} + \frac{\chi_0 \boldsymbol{D}_{\mathrm{c}} : \langle \boldsymbol{nnnn} \rangle}{(1 - \xi/\xi_{\mathrm{J}})^2} \right)$$

jamming coordinate $\xi \equiv \langle \boldsymbol{nn} \rangle : \boldsymbol{D}_{\mathrm{c}} / |\boldsymbol{D}_{\mathrm{c}}|$

jamming point $\xi^{\mathrm{J}}(f) = (1-f)\xi_1^{\mathrm{J}} + f\xi_2^{\mathrm{J}}$ $\qquad$ $f(\Pi) = \exp(-\Pi^*/\Pi)$

$$\boldsymbol{D} \equiv (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathsf{T}})/2 = \boldsymbol{D}_{\mathrm{c}} + \boldsymbol{D}_{\mathrm{e}}$$

(I still don't understand this decomposition and their effects in the model)

Do we really need $\langle nn \rangle$?

Constitutive model for shear jamming and fragility

Giusteri and Seto, Phys. Rev. Lett (2021)

Evolution of the deformation gradient tensor

$$\frac{\partial \mathbf{F}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\mathbf{F} = (\nabla \boldsymbol{u})\mathbf{F}$$

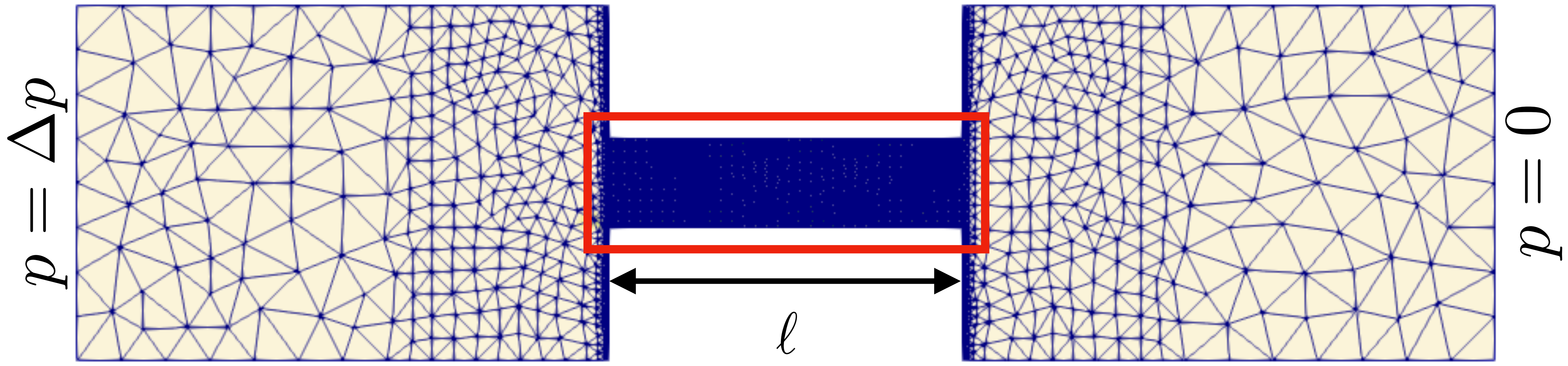
define $\mathbf{B} \equiv \mathbf{F}\mathbf{F}^{\mathsf{T}}$ and $\mathbf{L} \equiv \frac{1}{2}\log \mathbf{B}$

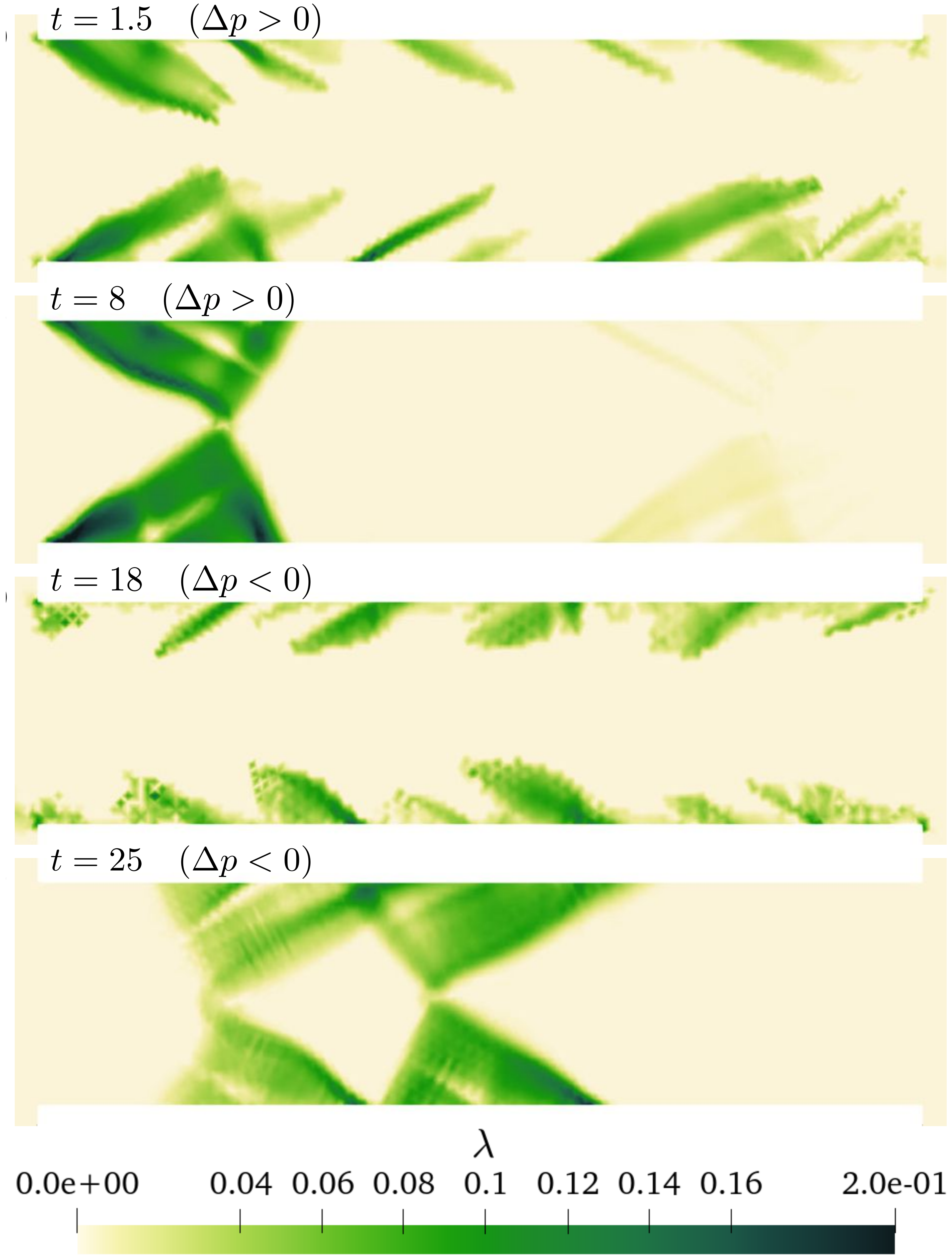
Projection to the edge of neutral zone

$$\Pi(\mathbf{M}) \equiv \begin{cases} \mathbf{M} & \text{if } \|\mathbf{M}\| \leq r, \\ r\mathbf{M}/\|\mathbf{M}\| & \text{if } \|\mathbf{M}\| > r. \end{cases}$$

Emergence of elastic stress

$$\mathbf{S} = 2\eta\mathbf{D} + 2\kappa(\mathbf{L} - \Pi(\mathbf{L})),$$





Free surface flows

Roll-wave instability due to DST negative slope

Darbois Texier, Lhuissier, Forterre, and B. Metzger, Comm. Phys., 2020.

free-surface perturbation h_1:

$$\tilde{h} = 1 + h_1$$

$$\frac{\partial h_1}{\partial \tilde{t}} + \tilde{c}\,\frac{\partial h_1}{\partial \tilde{x}} = \frac{A}{\tan\theta}\,\frac{\partial^2 h_1}{\partial \tilde{x}^2}$$

$$A = \mathrm{d}\tilde{\dot{\gamma}}/\mathrm{d}\tilde{\tau}_b|_{\tilde{\tau}_b=1}$$

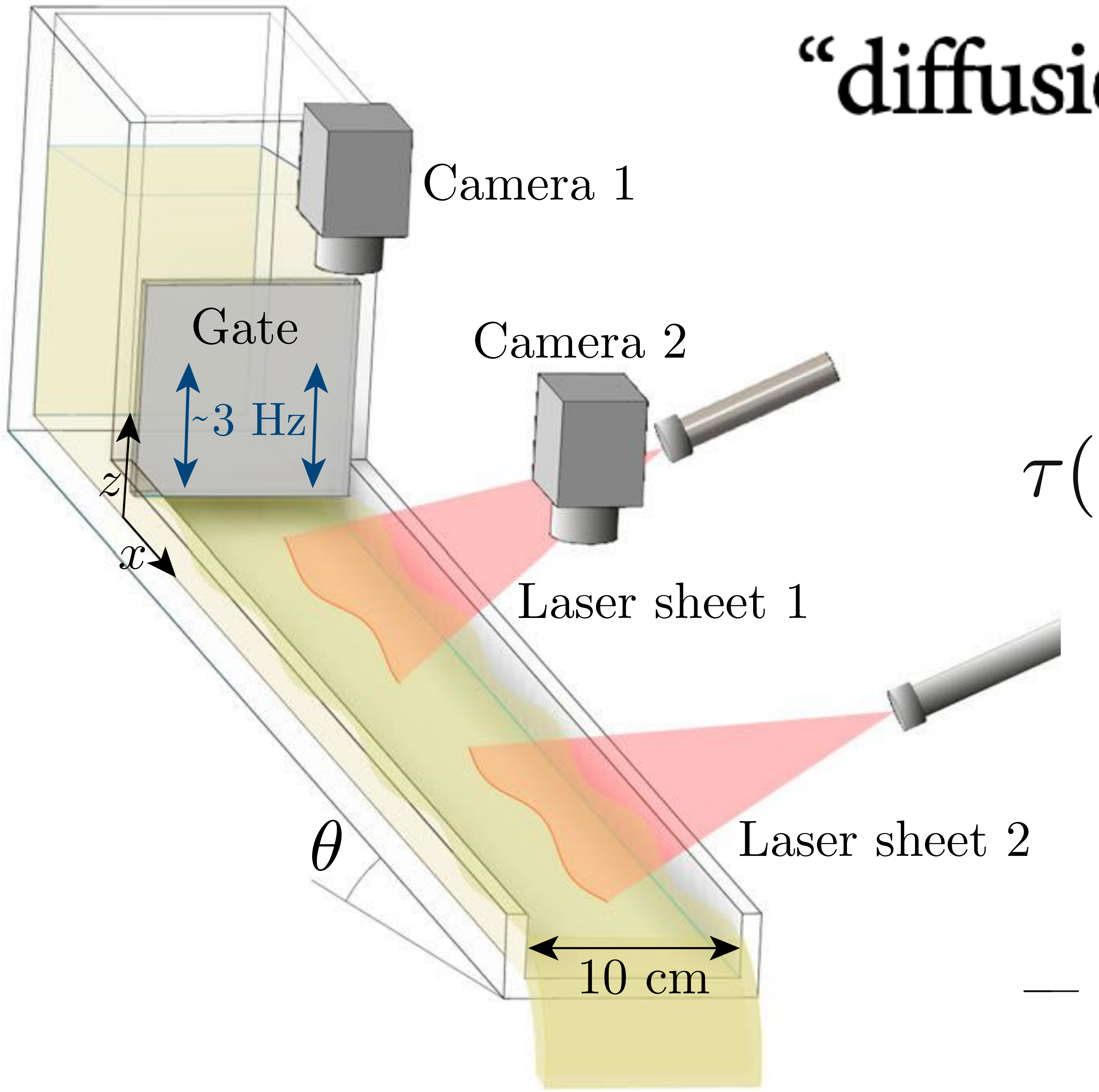
"diffusion coefficient"

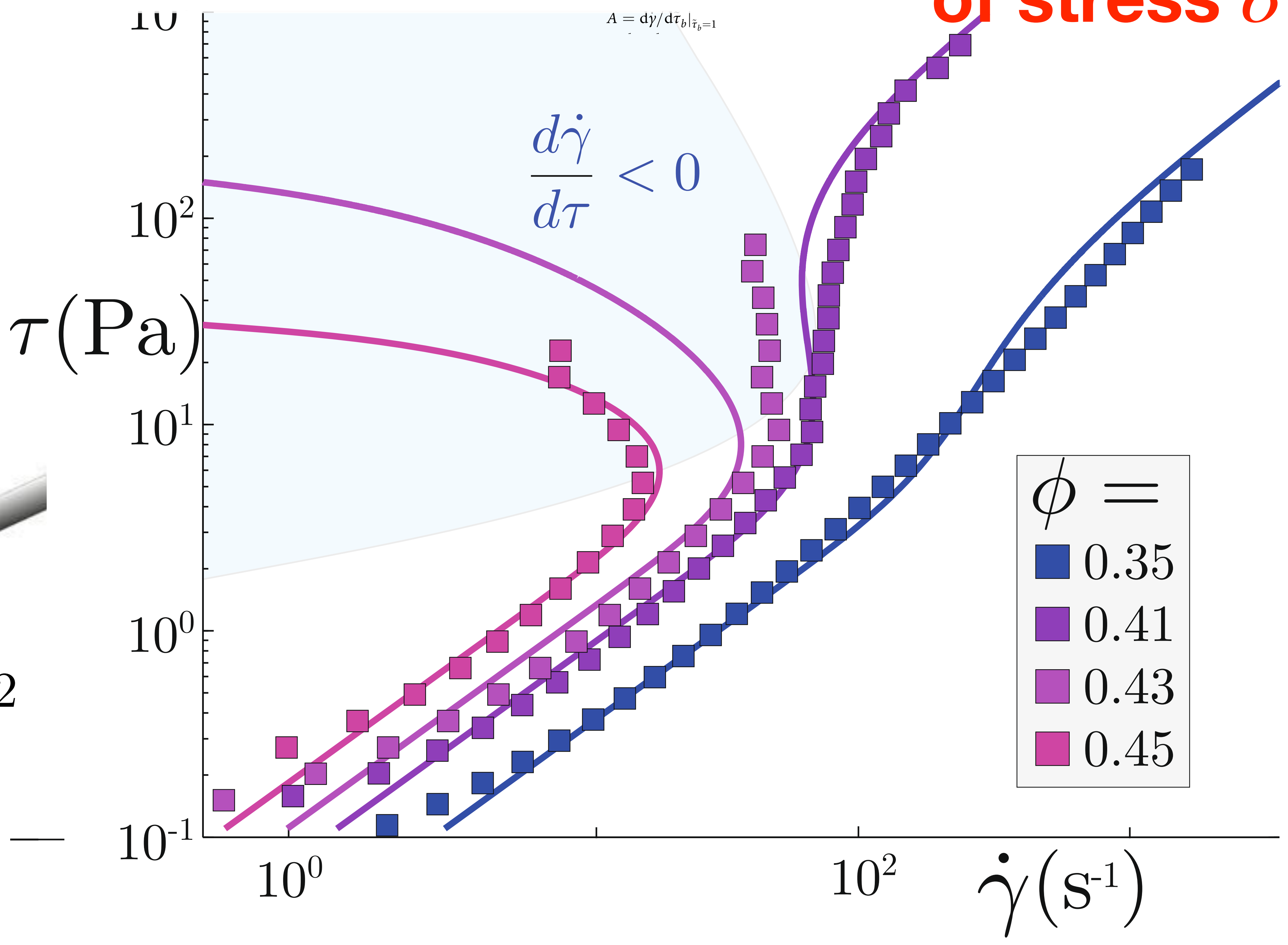
$\eta(\tau)$ **model**

viscosity is function of stress σ

(a)

(b)

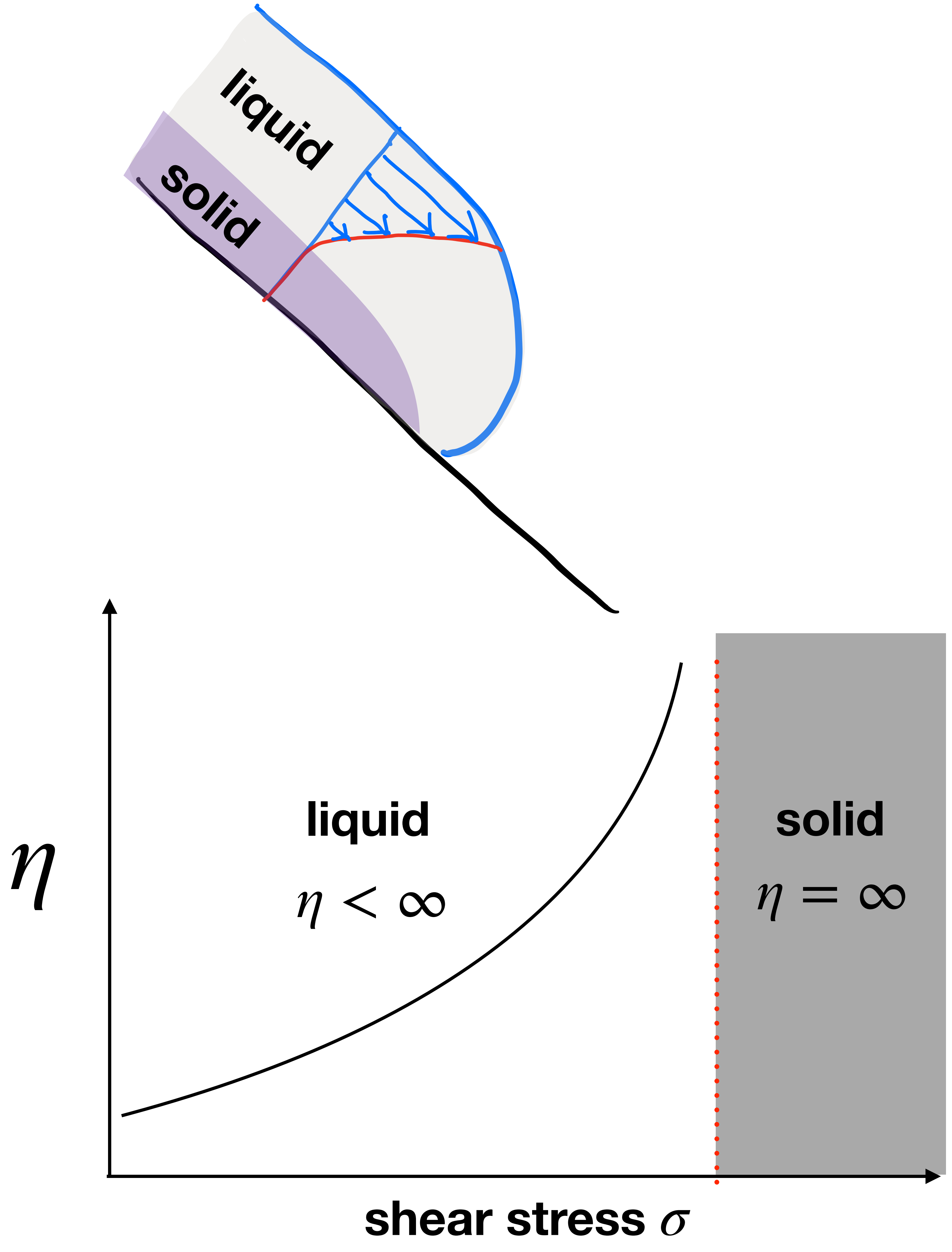


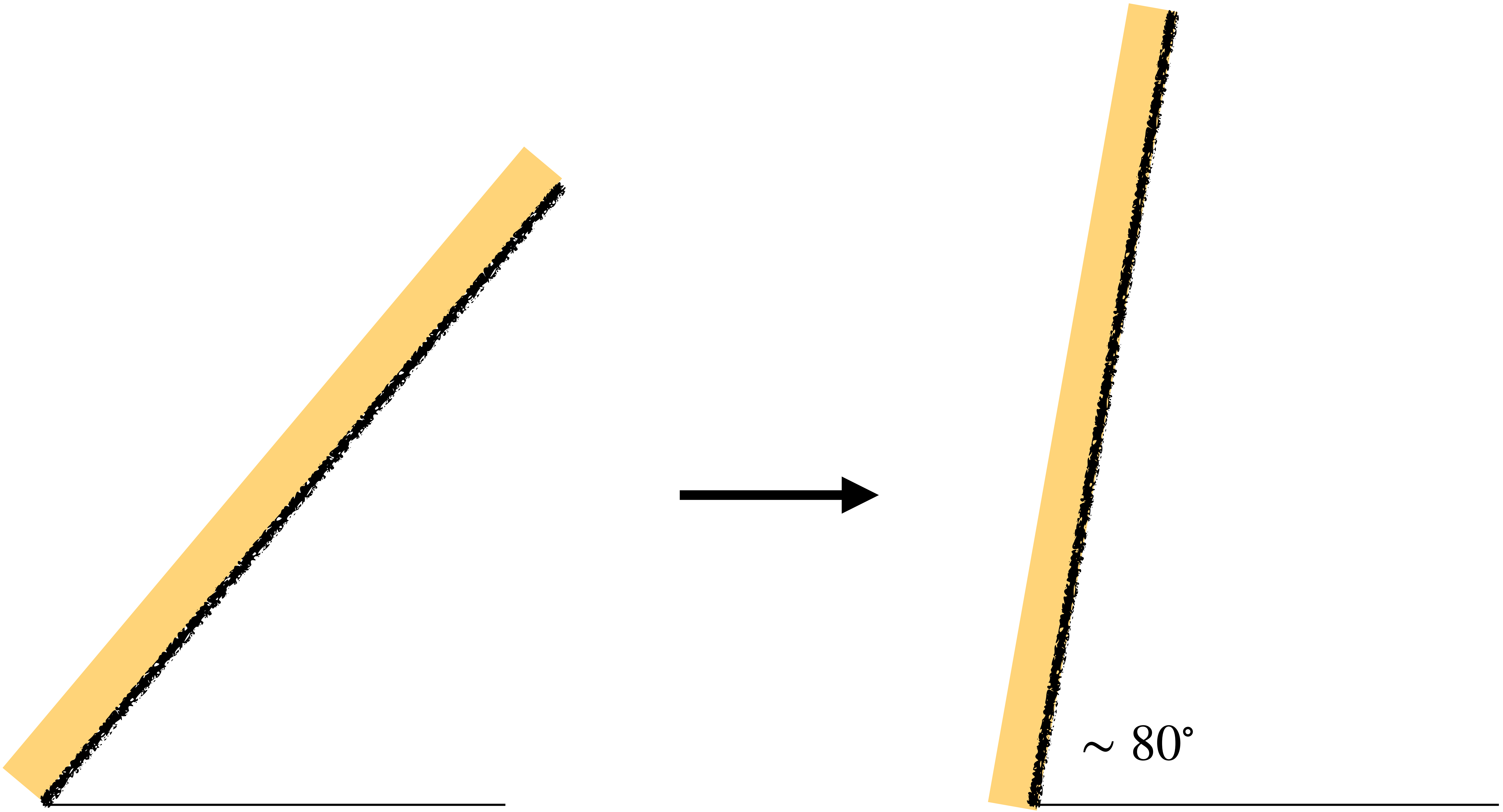


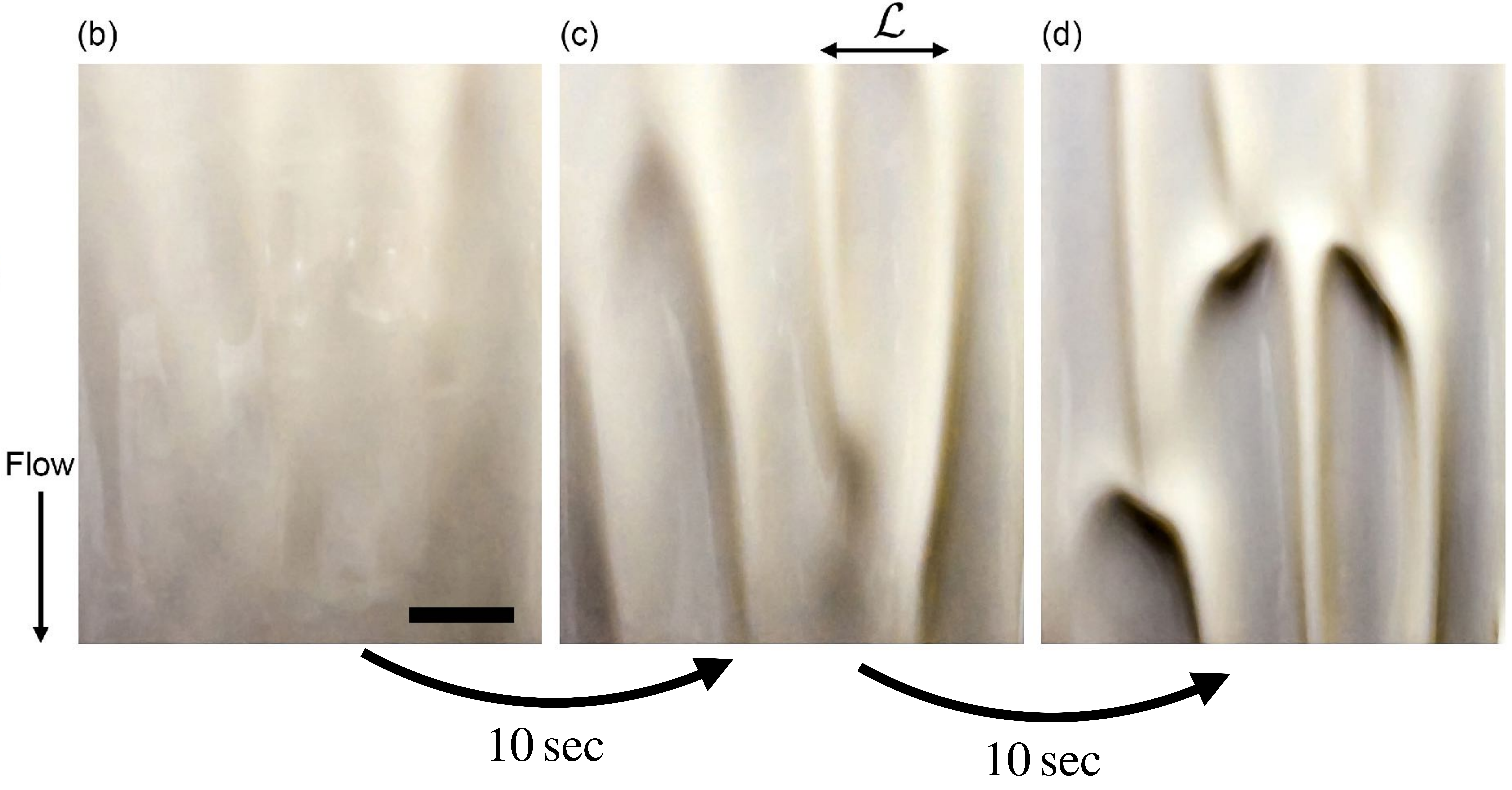
10.1038/s42005-020-00500-4

Beyond linear stability analysis?

from youtube




~ 80°


(b)
(c)
$\mathcal{L}$
(d)
Flow
10 sec
10 sec

Ridge instability due to normal-stress dilatancy

Xiong, Angerman, Ellero, Sandnes, and Seto, 2024

second normal stress difference

$$N_2 = \sigma_{zz} - \sigma_{yy} = -\alpha\sigma_{xz}$$

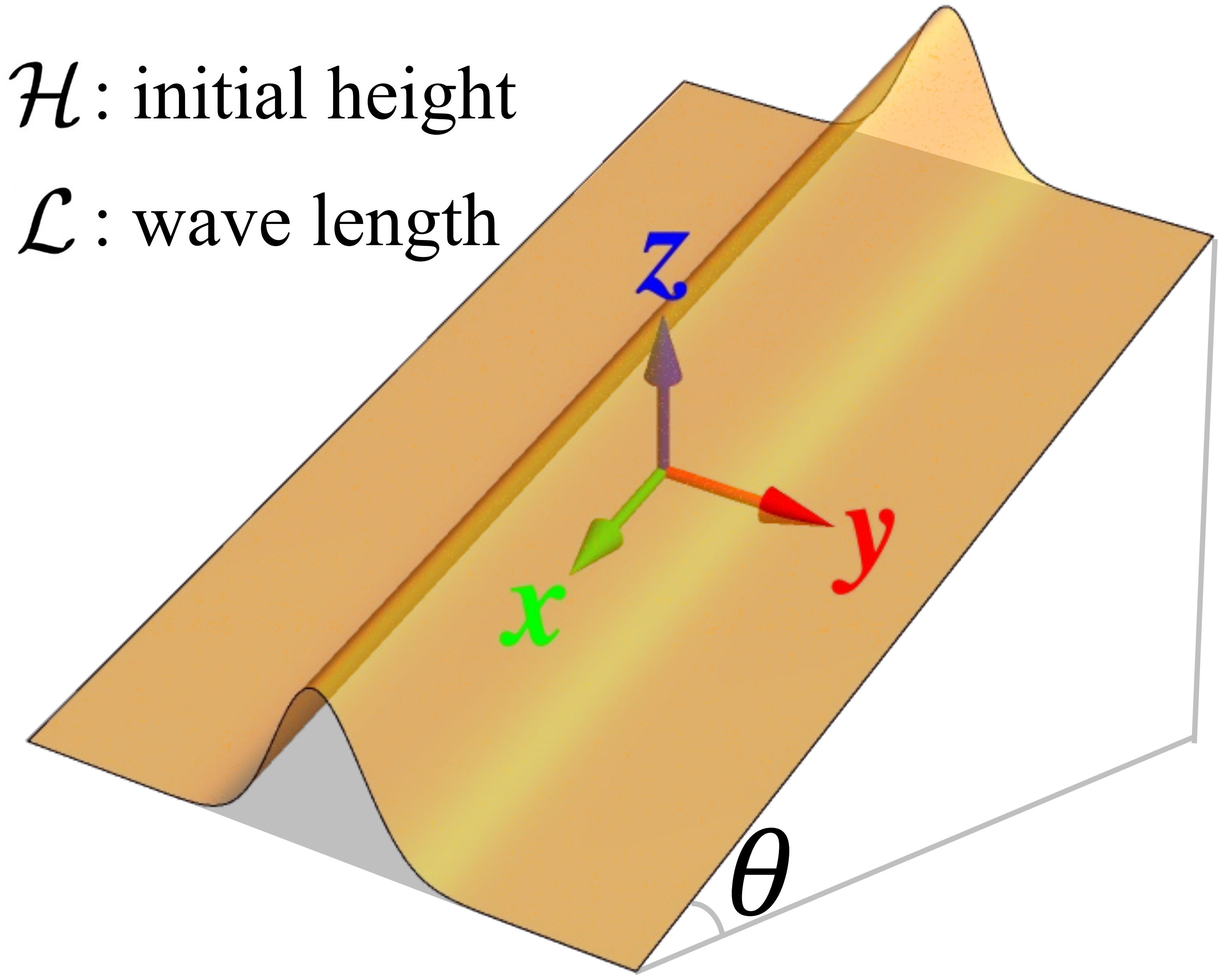
More surface push and less horizontal push

Free surface function:

$h(y,t)$

$\mathcal{H}$: initial height

$\mathcal{L}$: wave length



linear stability analysis

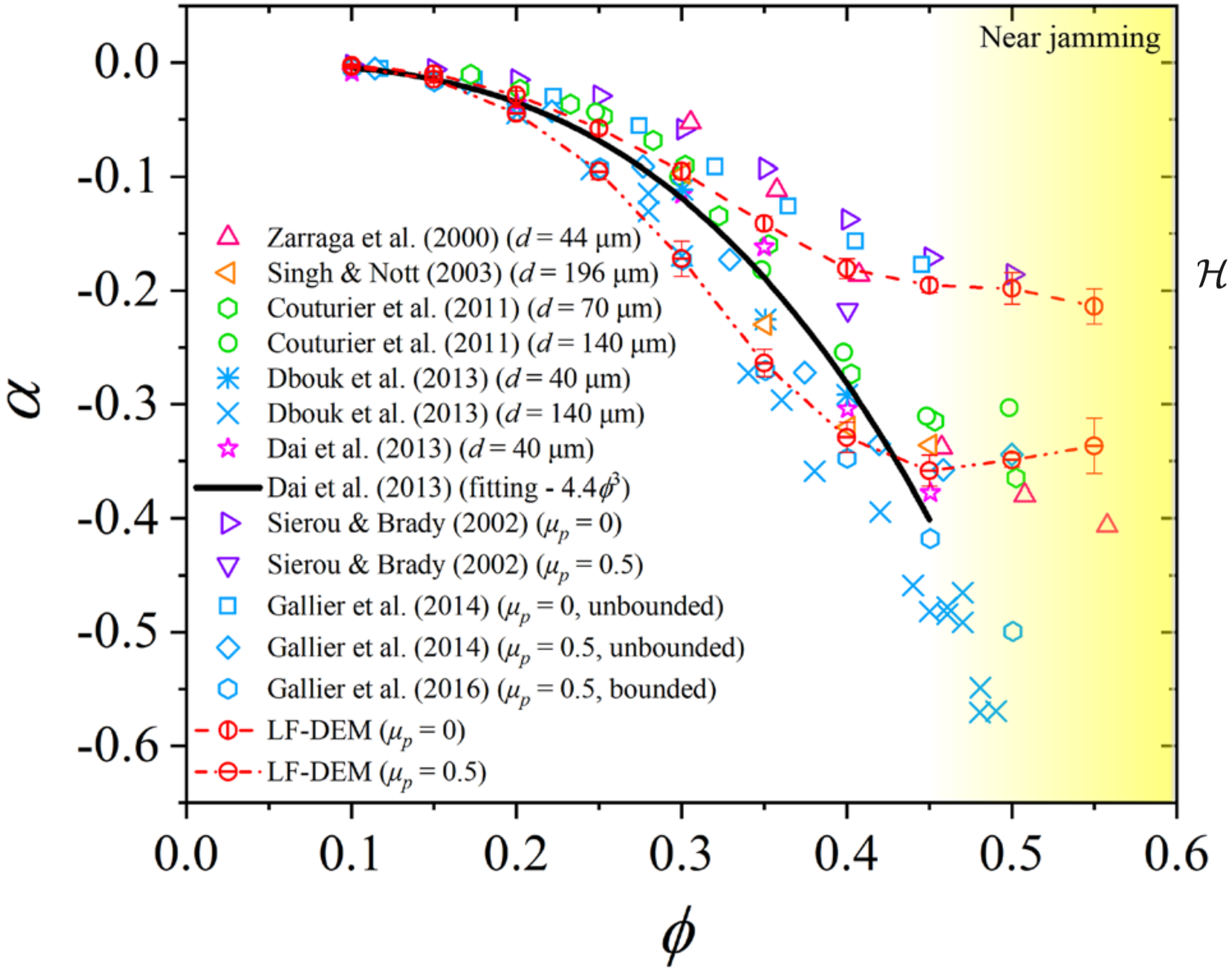
$$\tilde{h} = 1 + \tilde{h}'$$

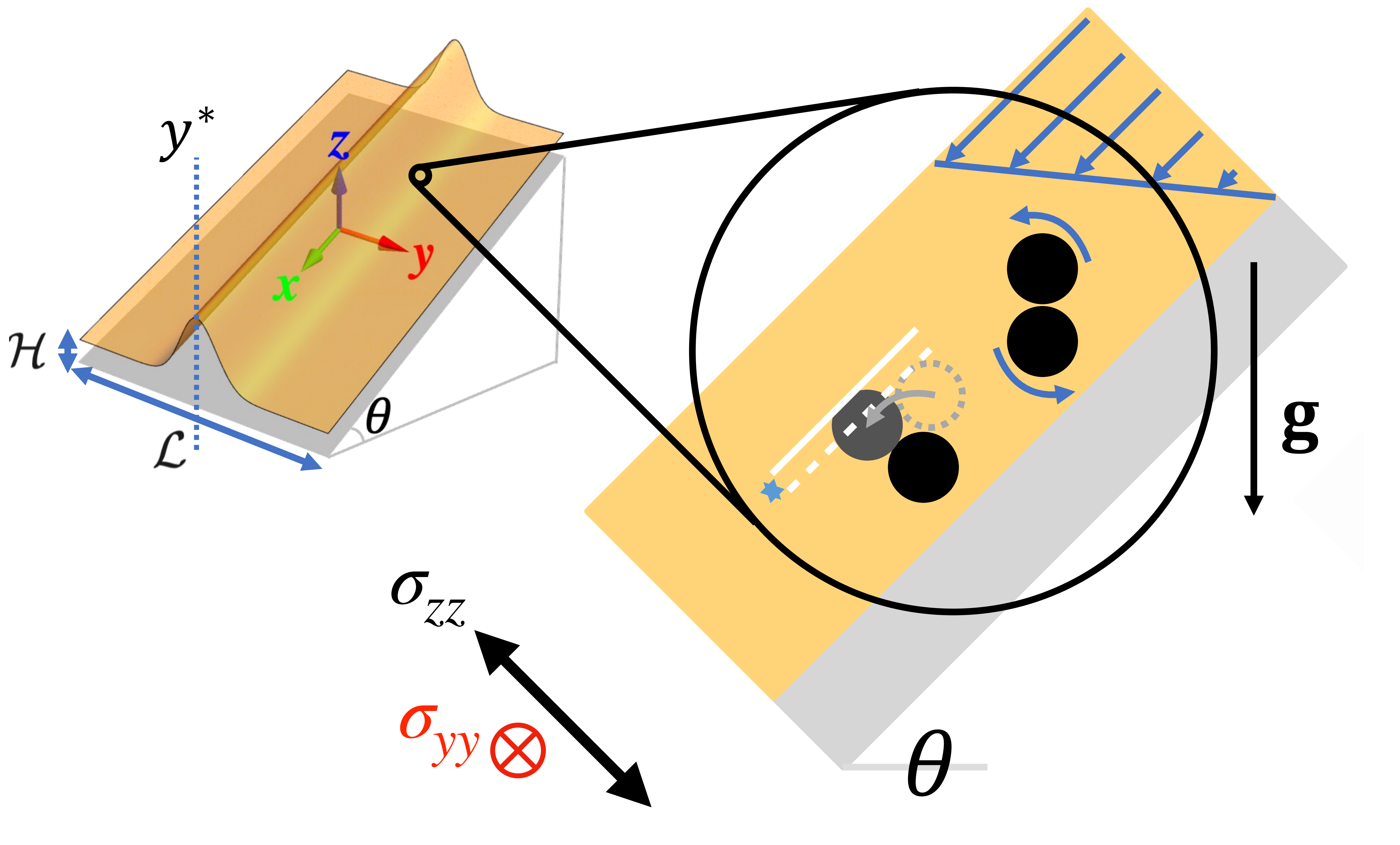
$$\frac{\partial \tilde{h}'}{\partial \tilde{t}} = \frac{\epsilon}{3\tilde{\eta}(0)}\left(\frac{1}{\tan(\theta)} + \alpha\right)\frac{\partial^2 \tilde{h}'}{\partial \tilde{y}^2}$$

"diffusion coefficient"

Ridge instability due to normal-stress dilatancy

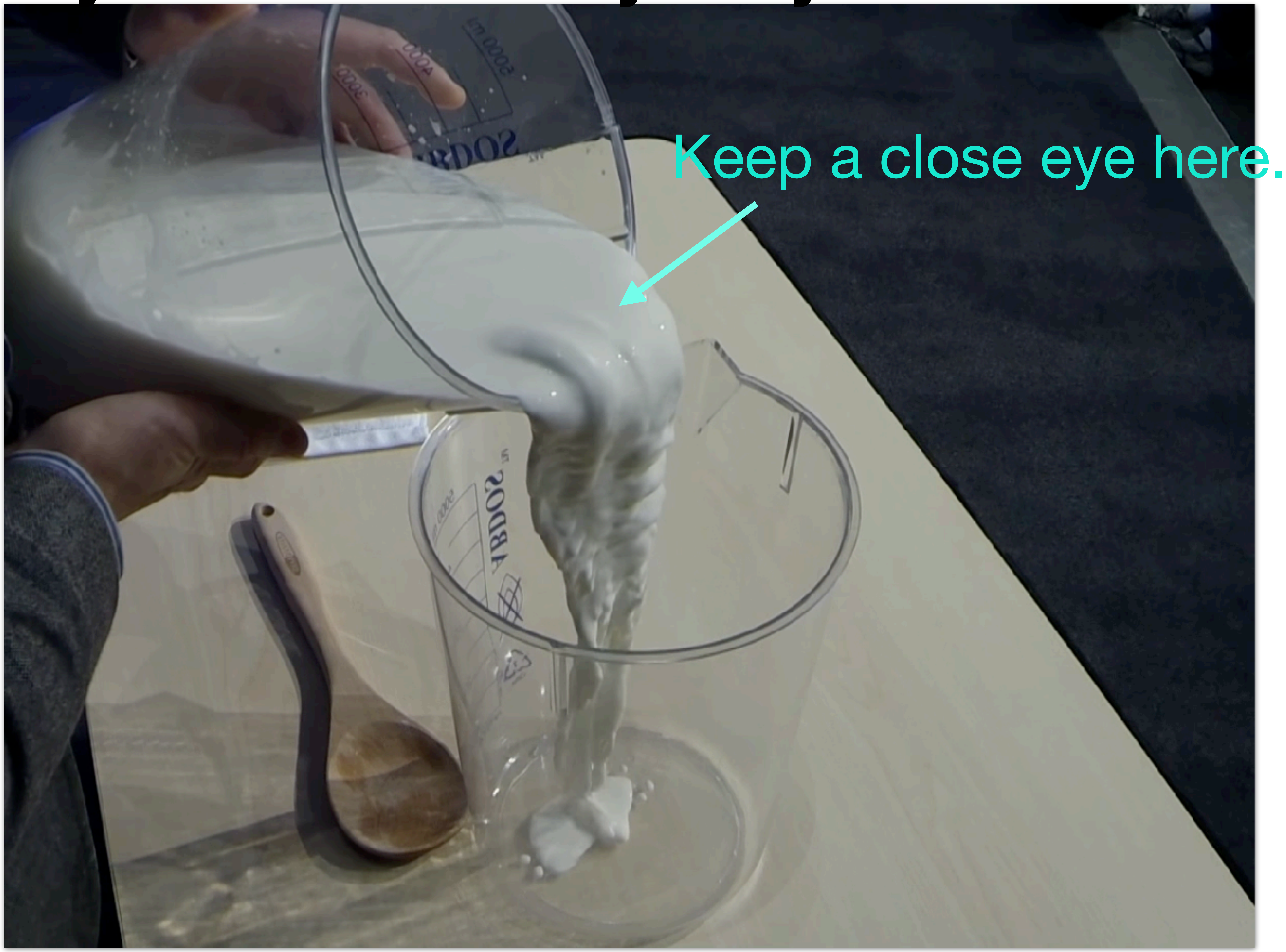
Xiong, Angerman, Ellero, Sandnes, and Seto, 2024





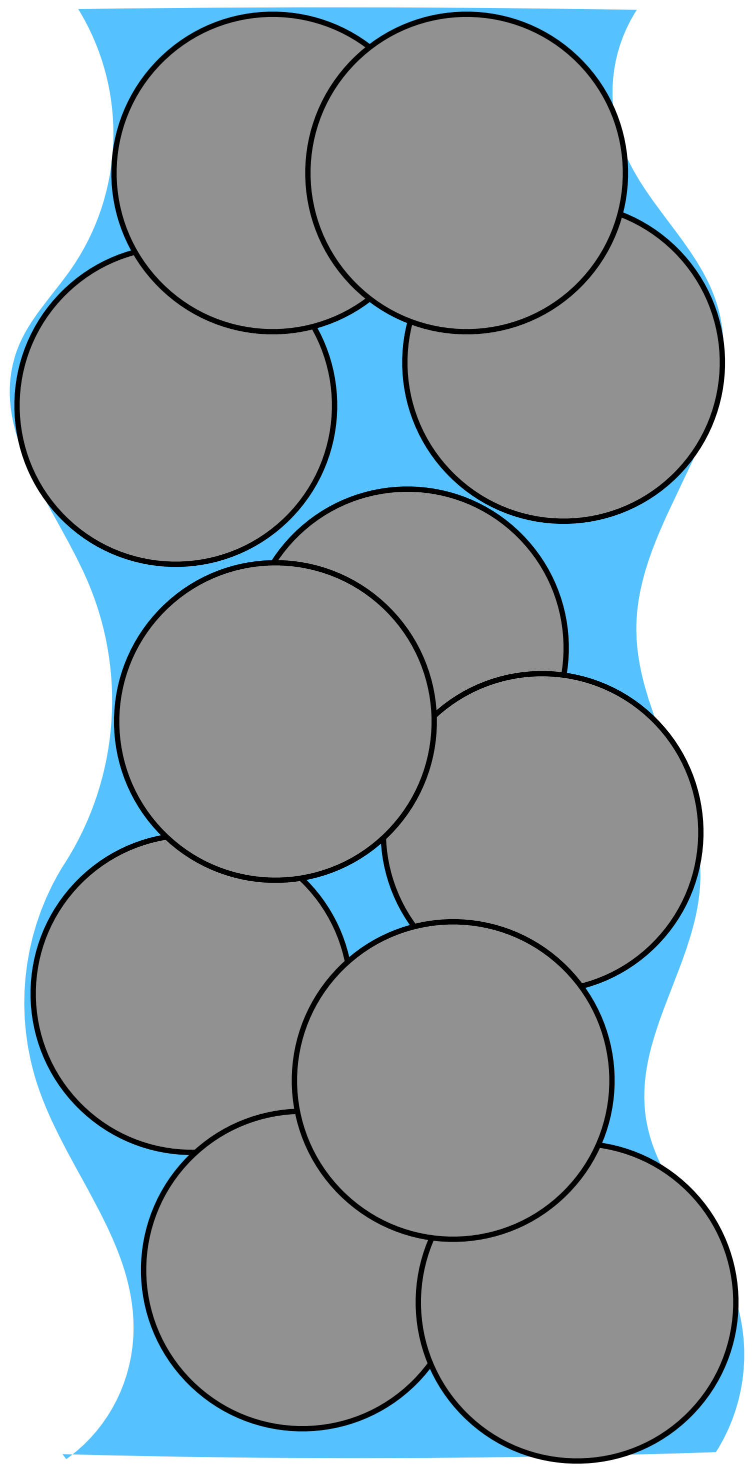
$$N_2 = \sigma_{zz} - \sigma_{yy} = -\alpha\sigma_{xz}$$

Beyond linear stability analysis?



Public lecture by Mike Cates from youtube

Stretching induced jamming?



Summary

We are still trying to figure out how to describe dense suspensions macroscopically correct.

Previously, we considered suspensions as viscous fluids with viscosity depending on shear induced microstructure.

It is still a challenge to incorporate the emerging solid structure due to stresses and constraints in continuum models.