

KITP program: Physics of Dense Suspensions

Extensional and shear flow material functions  
of dense suspensions—  
*microstructure, particle pressure, and  $N_1$*

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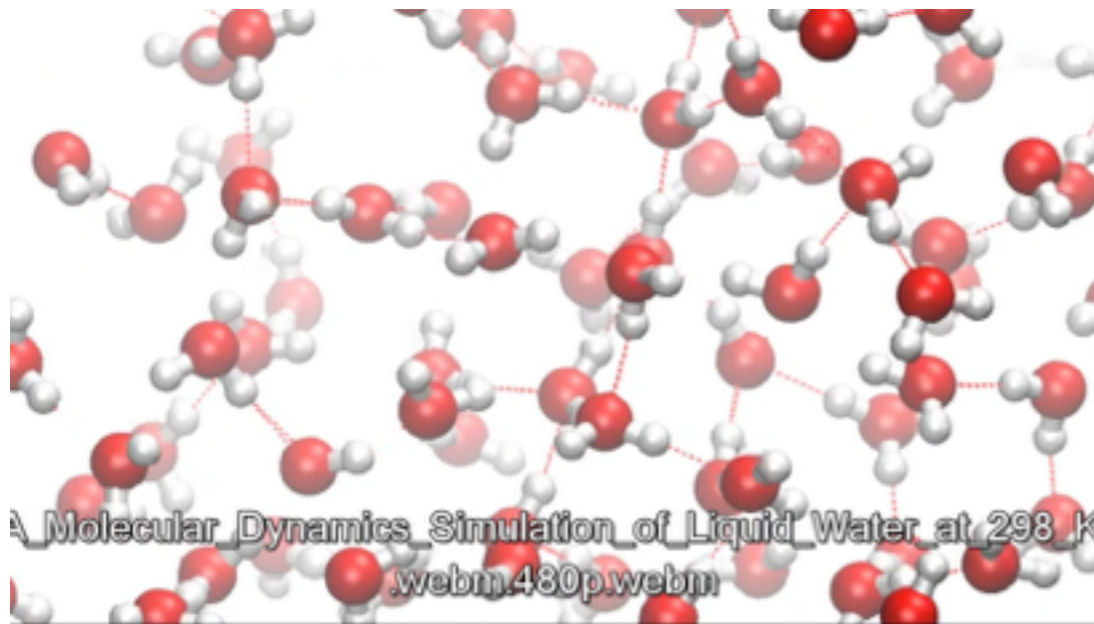
科研費  
KAKENHI

JSPS KAKENHI

JP17K05618



# MD simulation



Molecular dynamics

$$10^{-12} \text{ s}$$

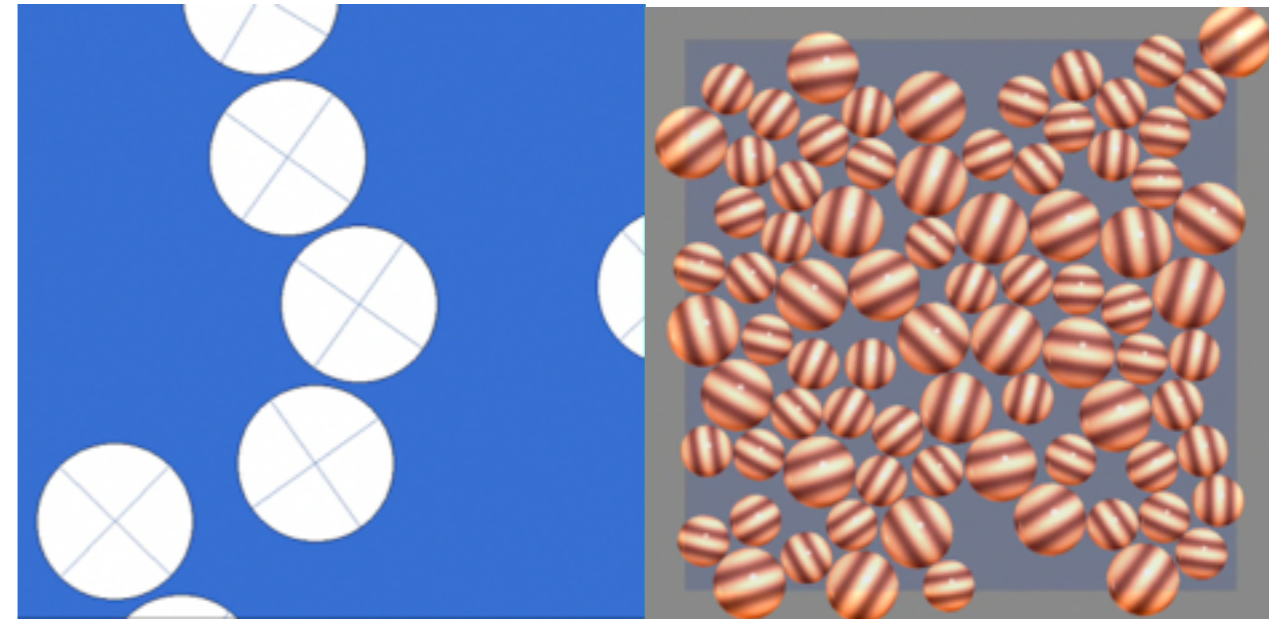


**Newtonian**

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta_0\mathbf{D}$$

Stokesian Dynamics

Discrete Element Method



Dynamics of solid particles  
in a viscous liquid

$$\frac{6\pi\eta_0 a^3}{k_B T} \sim 1 \text{ s}$$



**non-Newtonian**

$$\boldsymbol{\sigma} = ???$$

# Rheology

velocity gradient

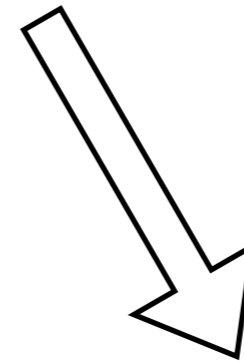
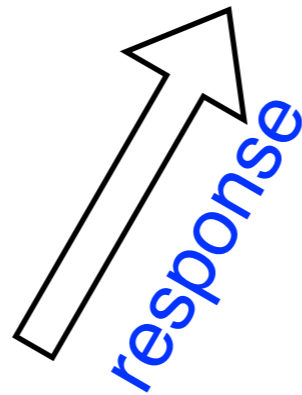
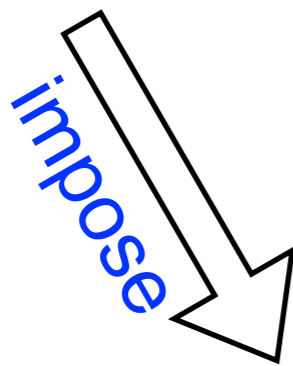
$$\begin{pmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_x}{\partial y} & \frac{\partial u_x}{\partial z} \\ \frac{\partial u_y}{\partial x} & \frac{\partial u_y}{\partial y} & \frac{\partial u_y}{\partial z} \\ \frac{\partial u_z}{\partial x} & \frac{\partial u_z}{\partial y} & \frac{\partial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

stress tensor

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

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

*Constitutive modeling*



**MD-like  
Particle simulation**

**material functions**

scalars

(*not* coordinate specific)  
physical interpretations

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

# Outline

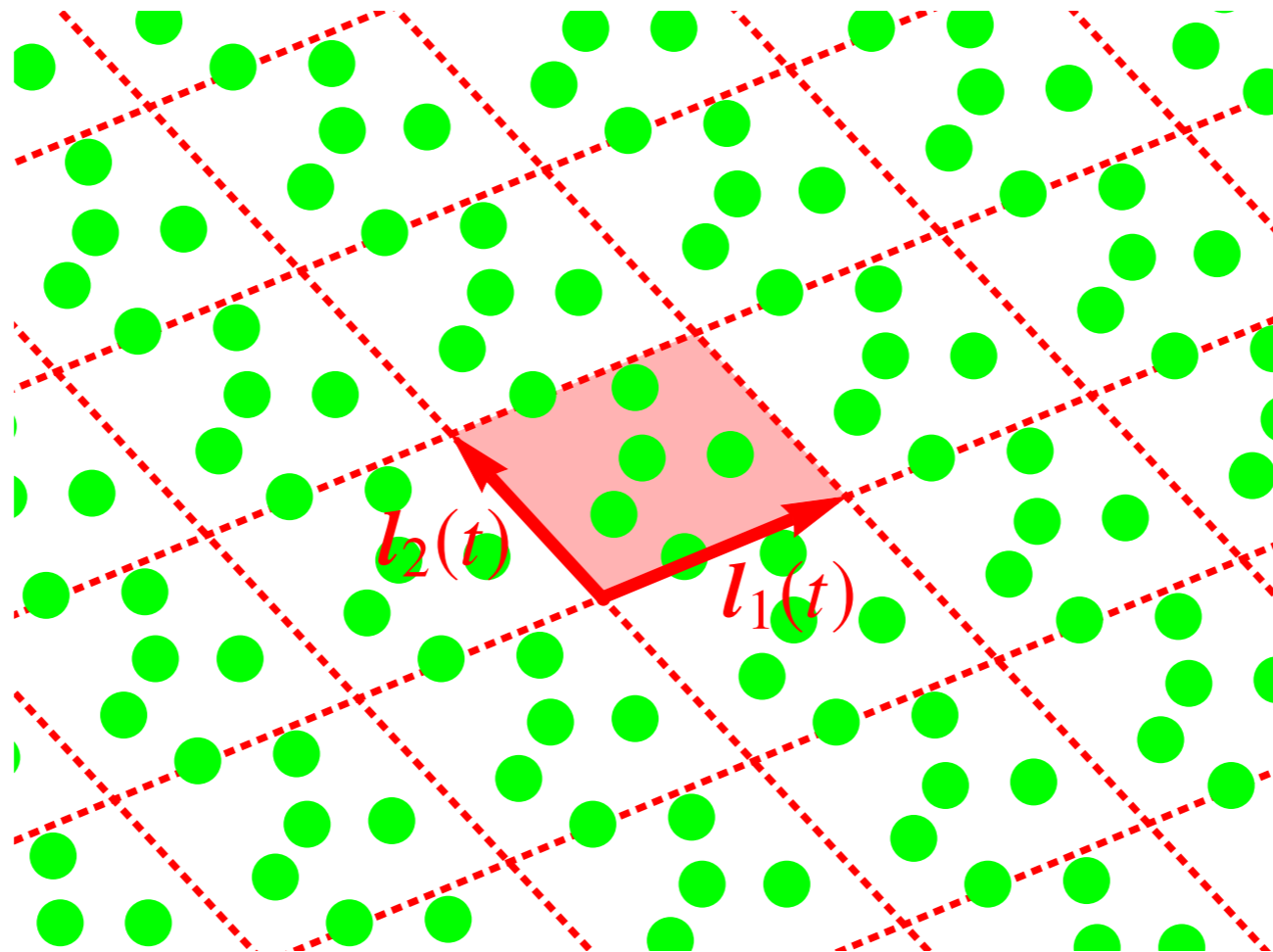
1. Periodic boundary conditions
2. Simulation model for particle dynamics
3. Material functions
4.  $N_1$  issue
5. Extensional rheology

# Time-dependent periodic boundary conditions

To impose  $\nabla u$  and to evaluate stress tensor  $\sigma$

$$\mathbf{r}' = \mathbf{r} + i\mathbf{l}_1(t) + j\mathbf{l}_2(t) \quad \begin{array}{l} i = \pm 1, \pm 2, \dots \\ j = \pm 1, \pm 2, \dots \end{array}$$

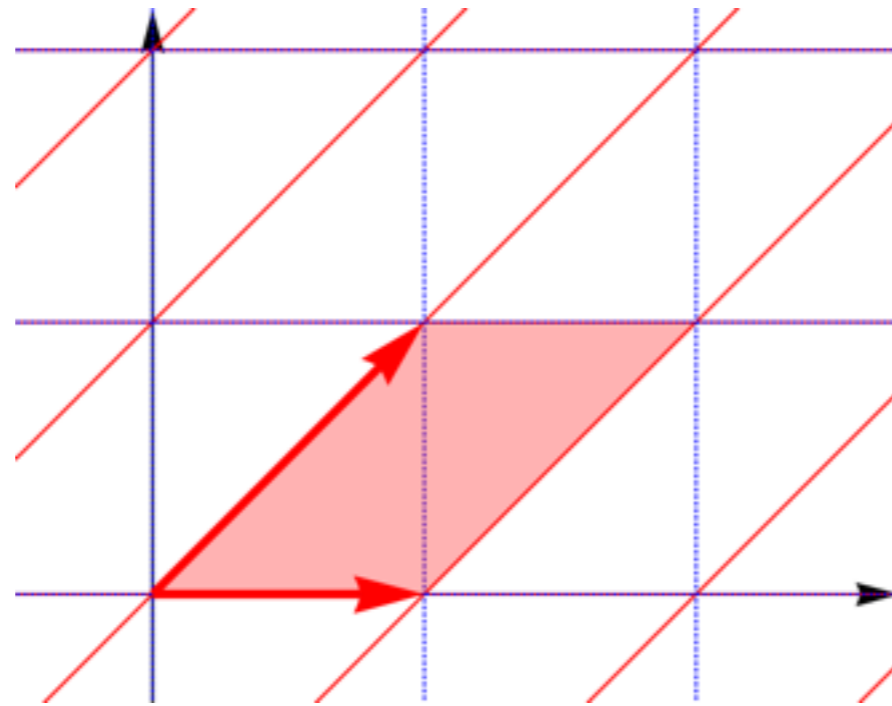
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# Time-dependent periodic boundary conditions

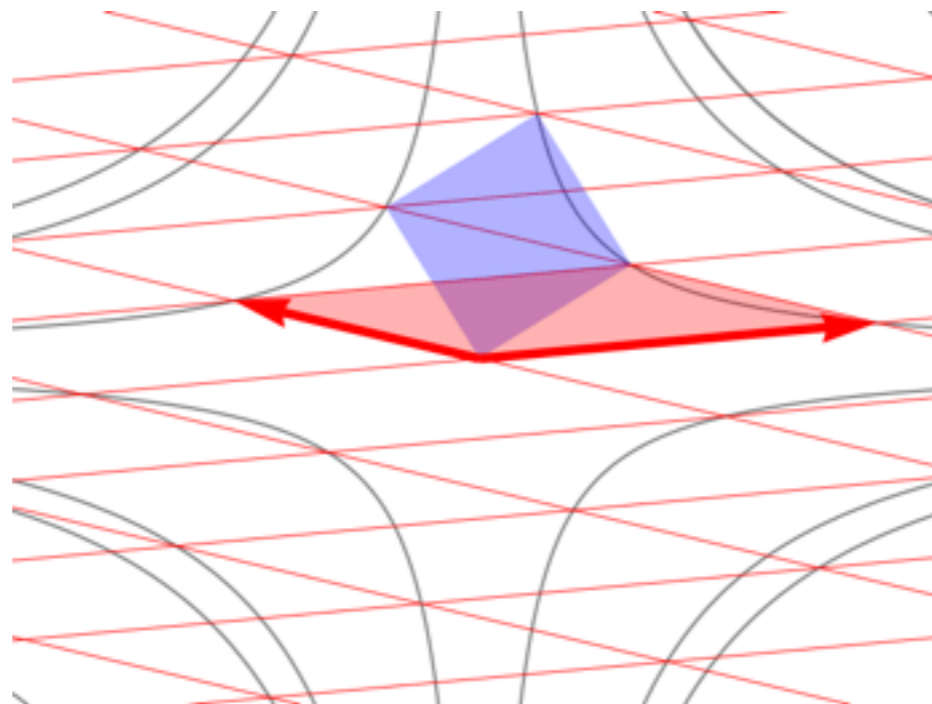
$$\mathbf{r}' = \mathbf{r} + i\mathbf{l}_1(t) + j\mathbf{l}_2(t) \quad \begin{array}{l} i = \pm 1, \pm 2, \dots \\ j = \pm 1, \pm 2, \dots \end{array}$$

$$\nabla \mathbf{u} = \begin{pmatrix} 0 & \dot{\gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



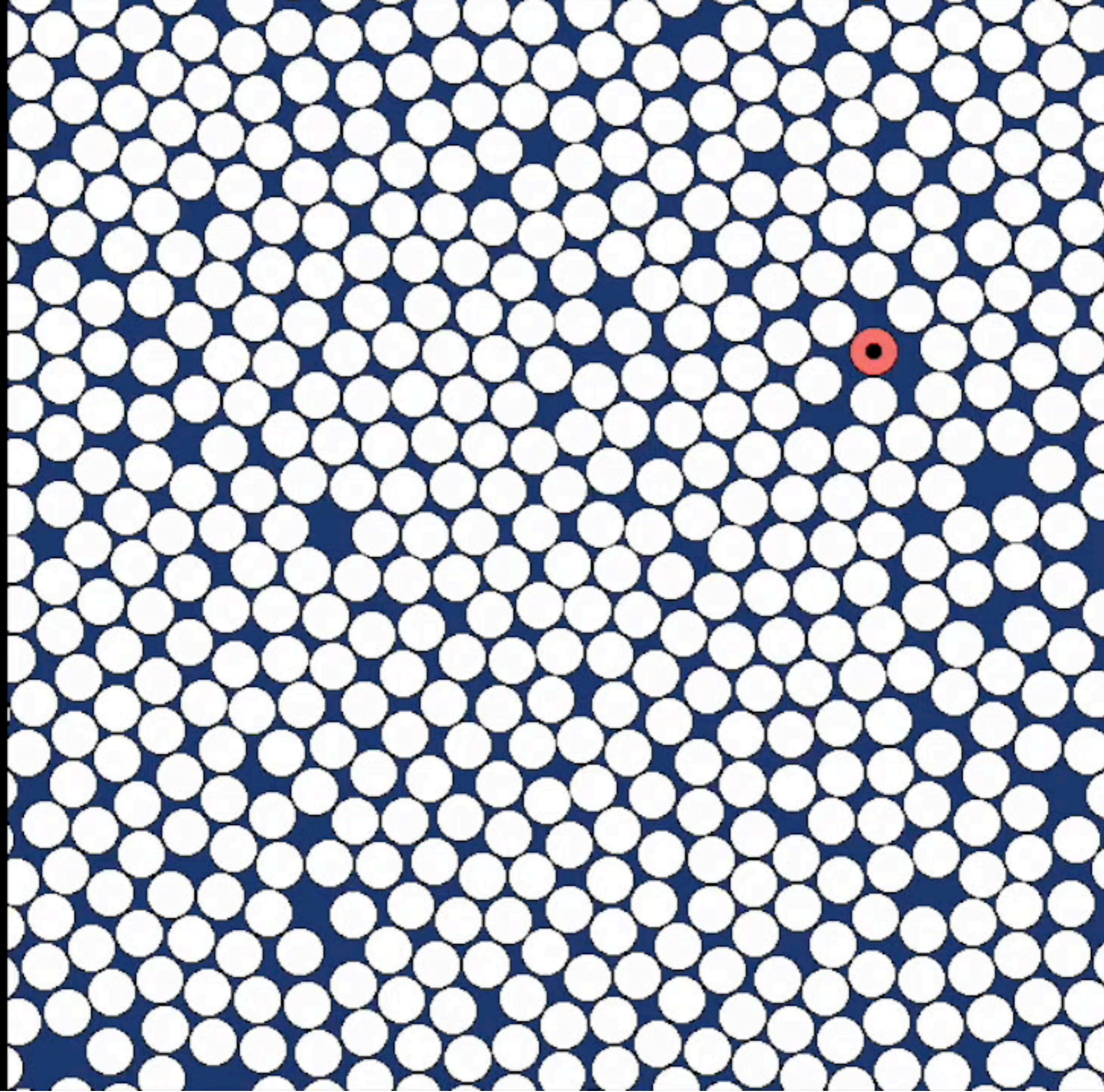
Lees-Edwards P.B.C.  
simple shear

$$\nabla \mathbf{u} = \begin{pmatrix} \dot{\epsilon} & 0 & 0 \\ 0 & -\dot{\epsilon} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



Kraynik-Reinelt P.B.C.  
**planar extensional  
(pure shear)**

Kraynik and Reinelt (1992)  
Sami, Master Thesis (1996)  
in Brady's group  
Todd and Daivis (1998)



# Time-dependent periodic boundary conditions

{ no worry for wall slips and migration  
{ little worry for shear banding

*All good for local rheology!*

*We need reliable **simulation models**  
for particle dynamics...*



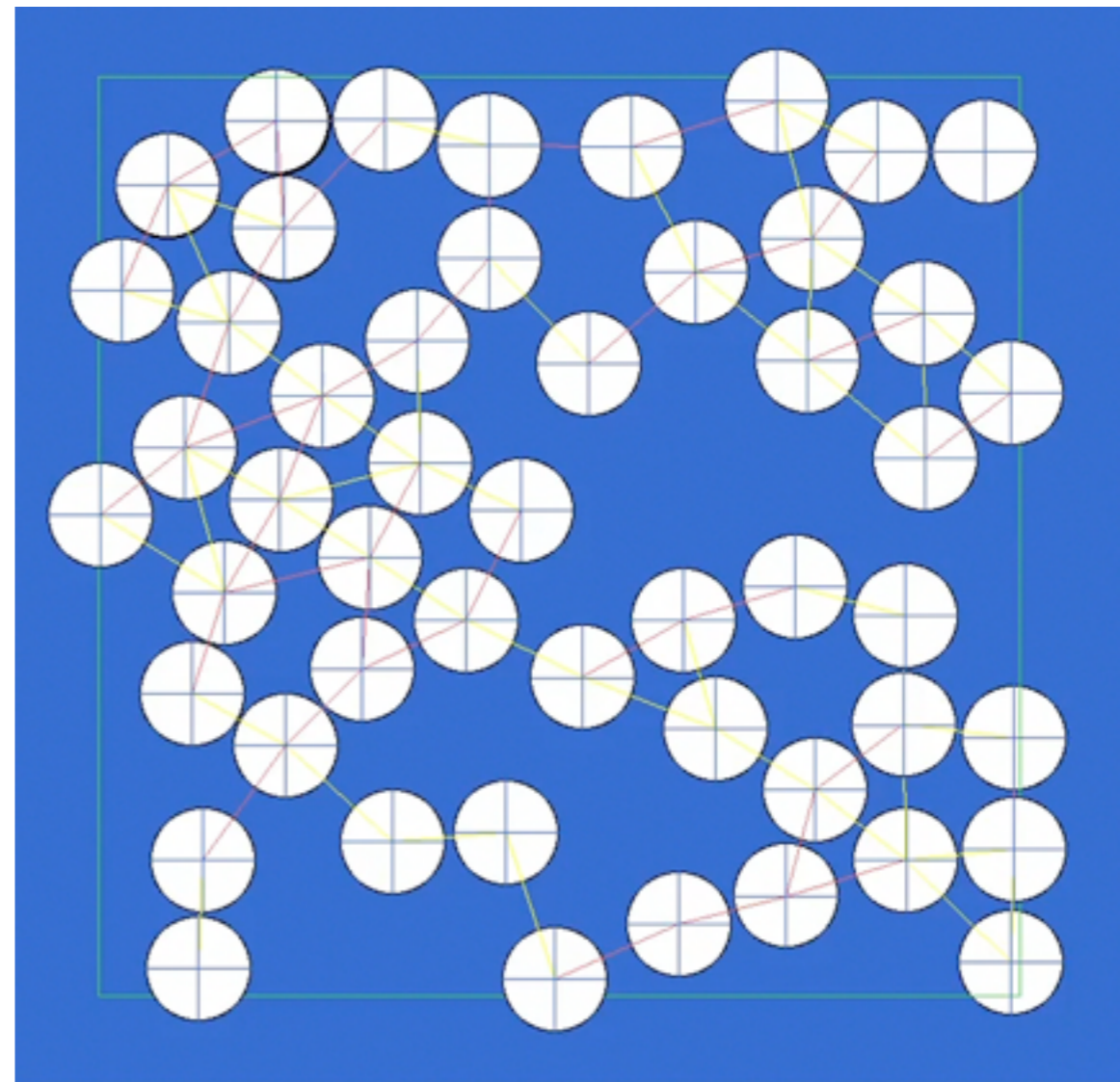
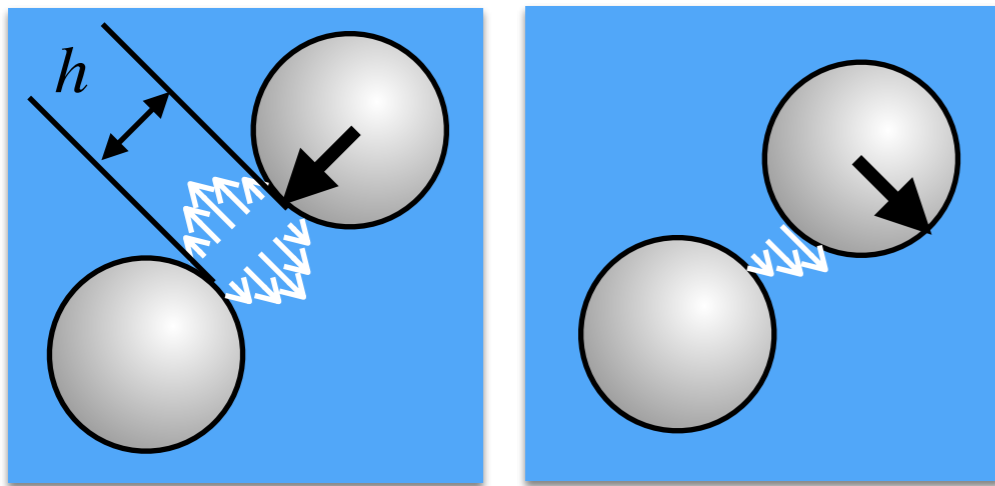
# Outline

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# *Purely* hydrodynamic suspensions

$$\vec{0} = -\nabla p + \nabla^2 \vec{u} \quad \text{Zero Reynolds number}$$

Perfect reversibility (*memory*),  
if lubrication layers can remain.

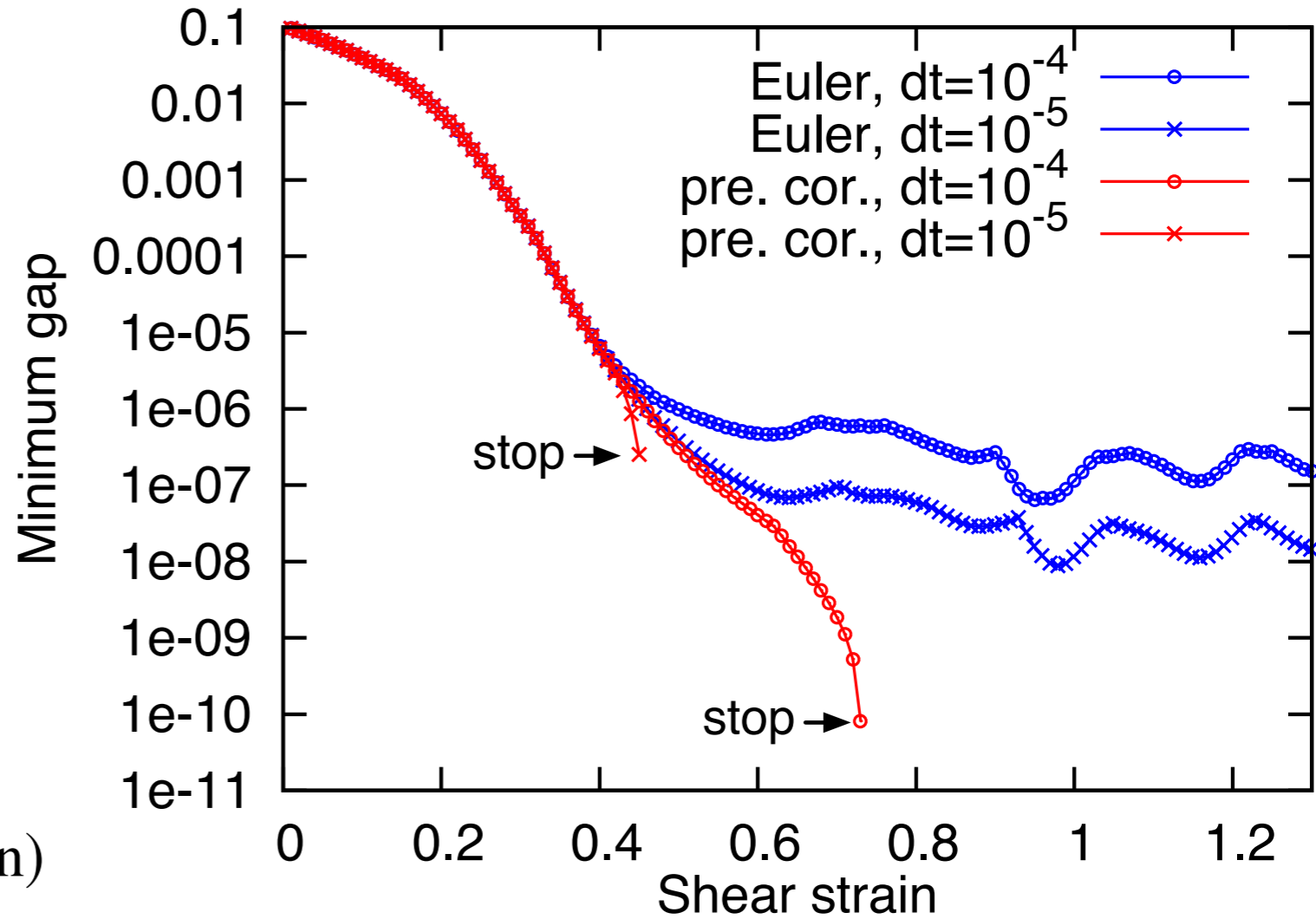
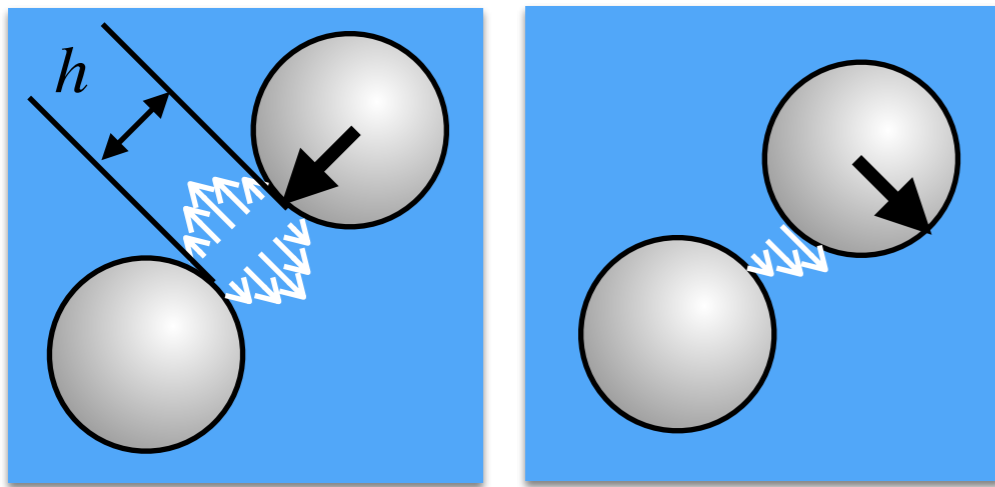


$$F_{\text{Lub}}^{(\text{nor})} \sim -\frac{1}{h} \Delta U^{(\text{nor})}$$
$$F_{\text{Lub}}^{(\text{tan})} \sim -\log \left( \frac{1}{h} \right) \Delta U^{(\text{tan})}$$

shear reversal demo

# *Purely* hydrodynamic suspensions

However, infinitesimal resolution is required!!

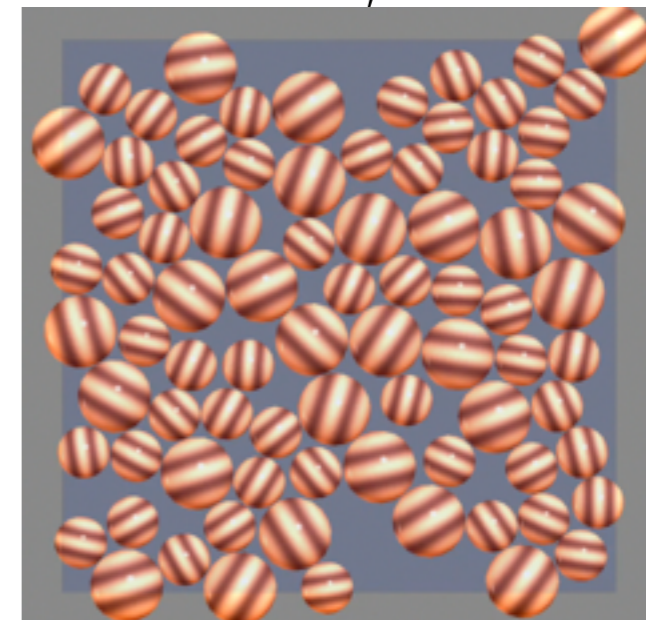
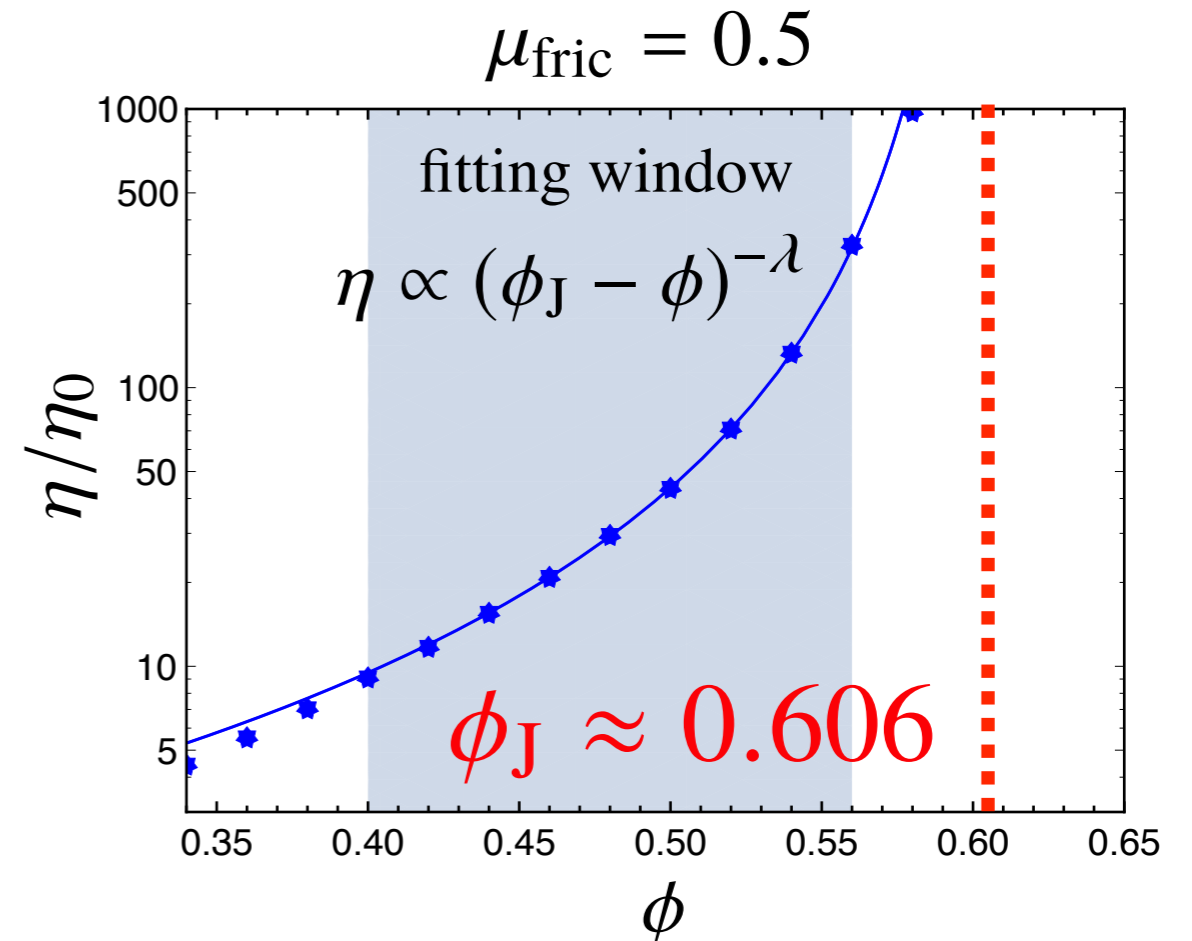
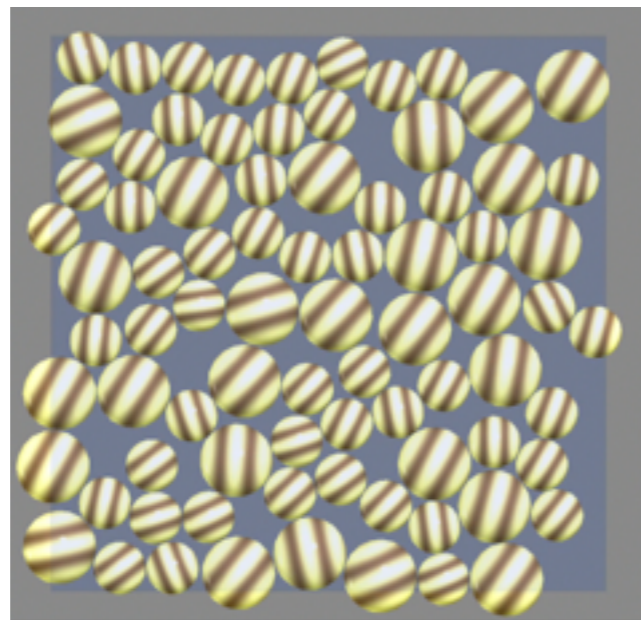
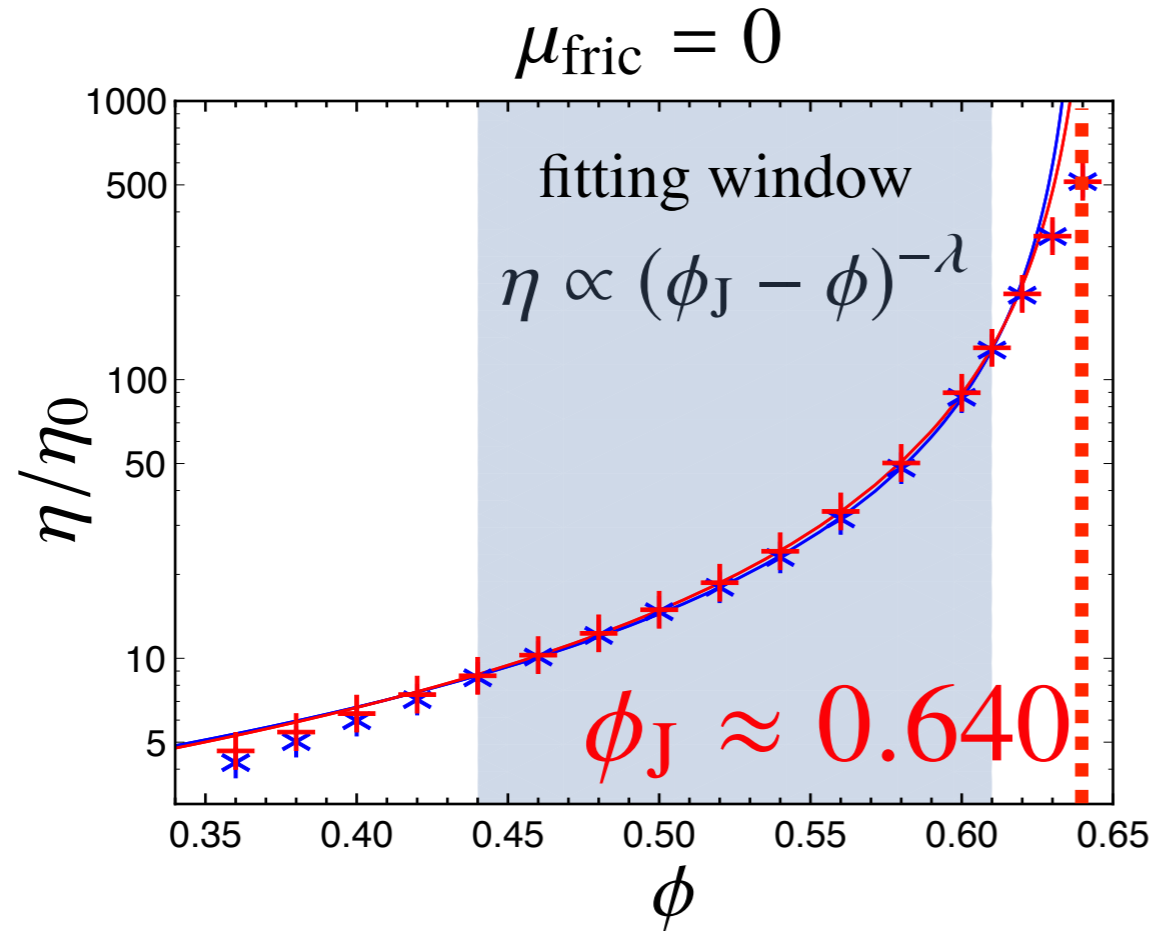


$$F_{\text{Lub}}^{(\text{nor})} \sim -\frac{1}{h} \Delta U^{(\text{nor})}$$

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

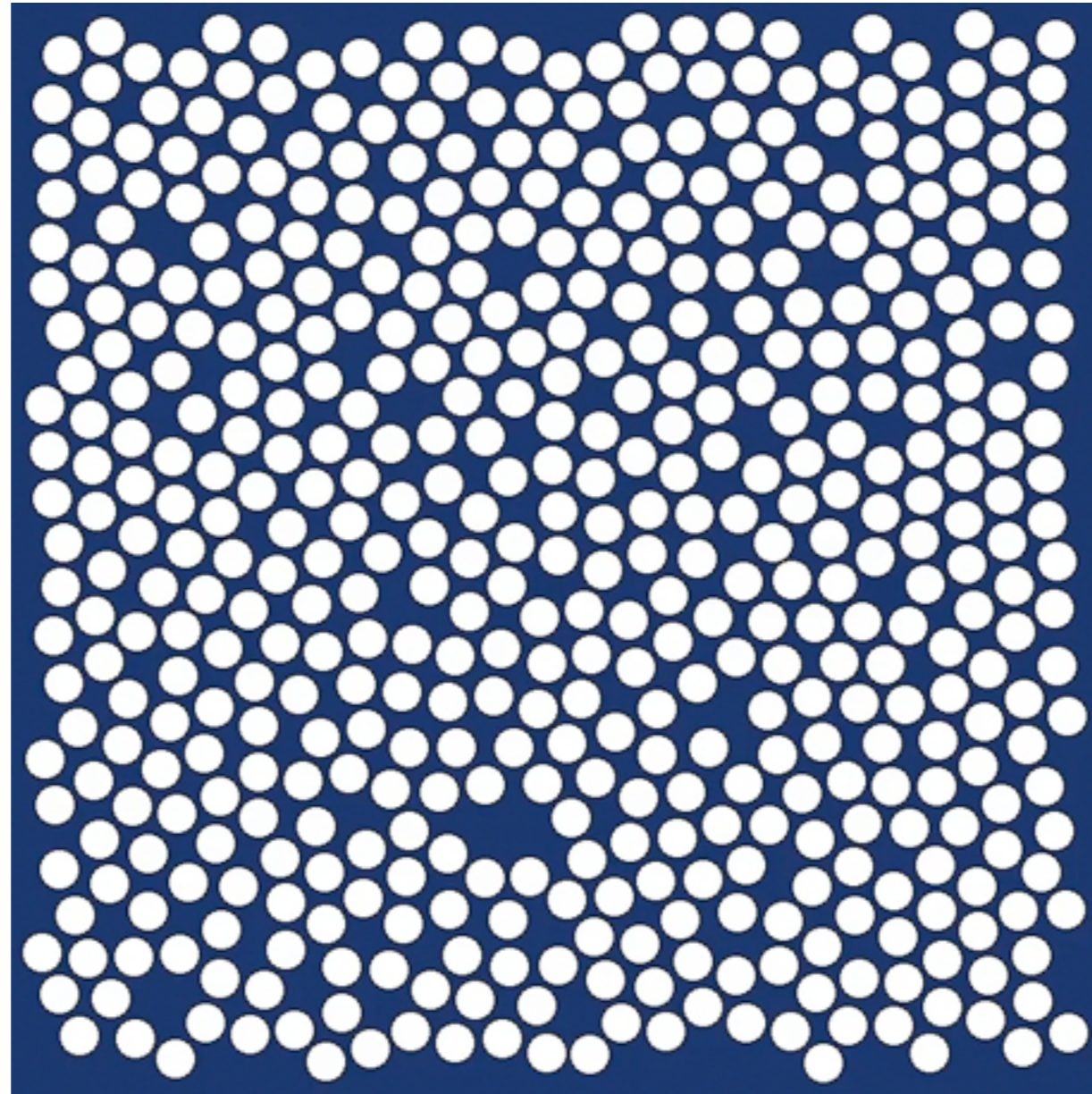
**Purely hydrodynamic suspensions**  $F_{\text{Lub}} \sim -\frac{1}{h + \delta} \Delta U$

**+ contact force (with some sliding constraint)**



# H.I. + Con. + **Brownian force or/and repulsive force**

*shear-induced* microstructure  $\Leftrightarrow$  *relaxed* microstructure  
**non-equilibrium** **equilibrium**

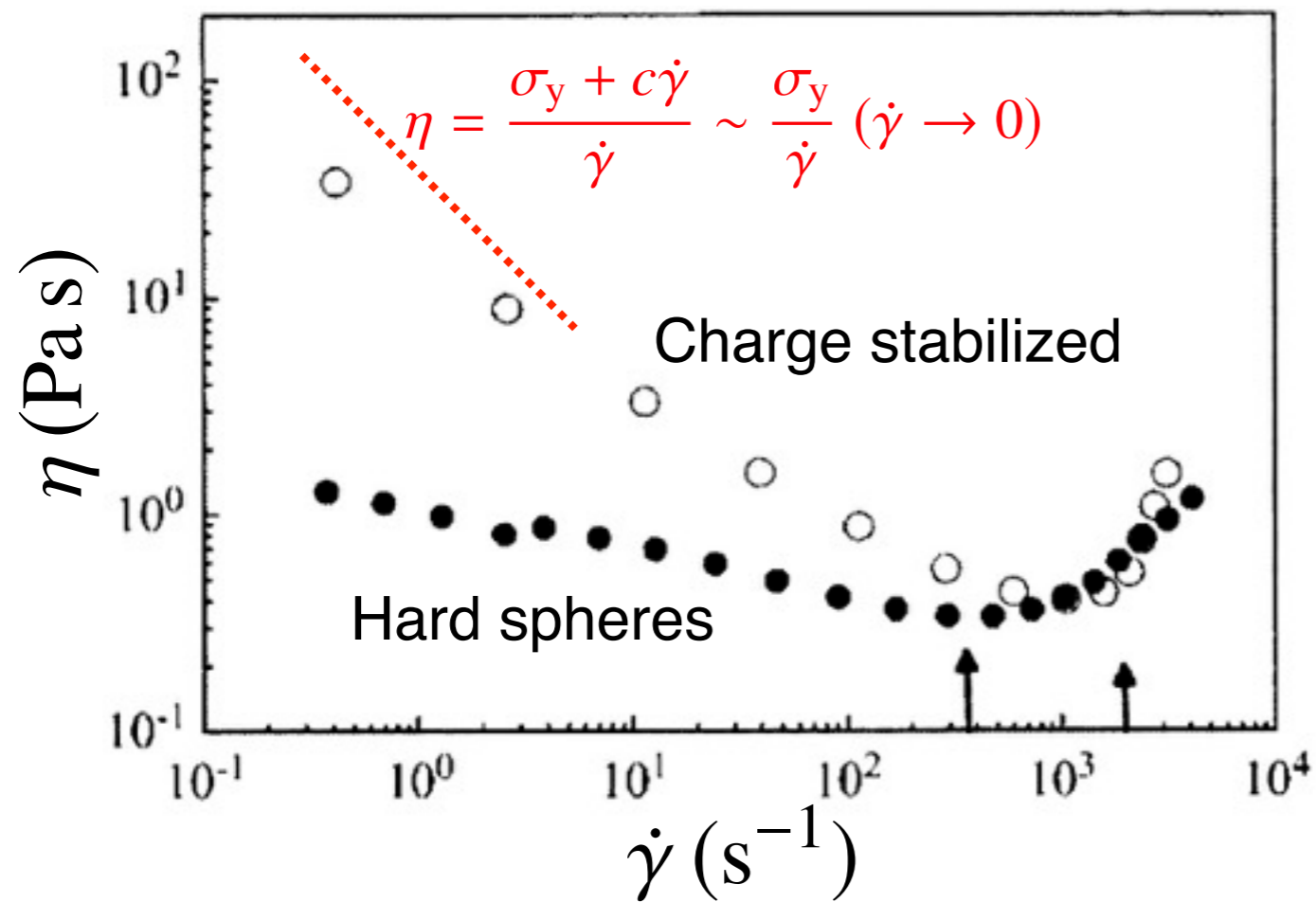


Demo for “flow–stop–flow–stop–...”

# H.I. + Con. + **Brownian force or/and repulsive force**

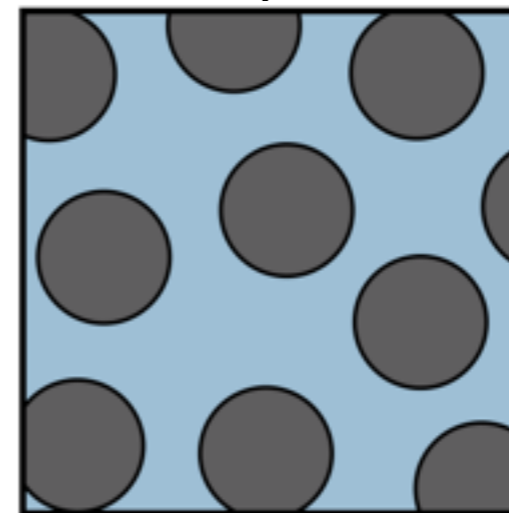
If volume fraction of particles with **extended radii** in the low shear rate exceeds jamming, the viscosity is infinity.

→ **Yield stress**

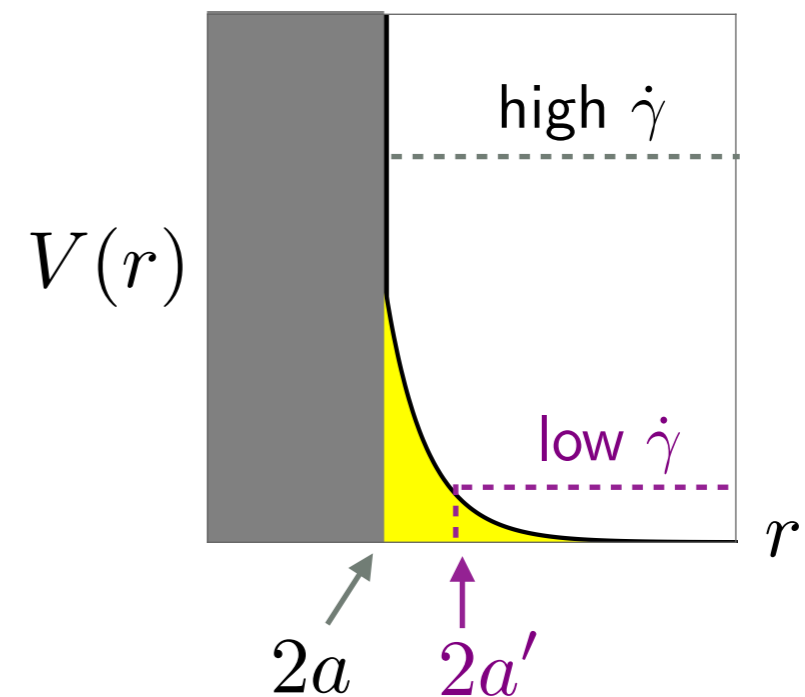
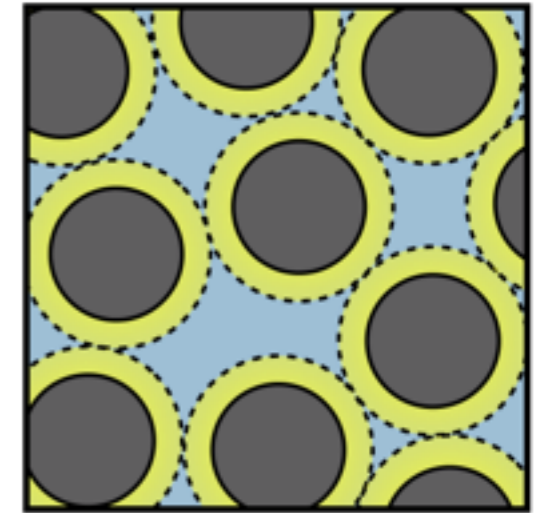


Maranzano & Wagner 2001

Hard spheres

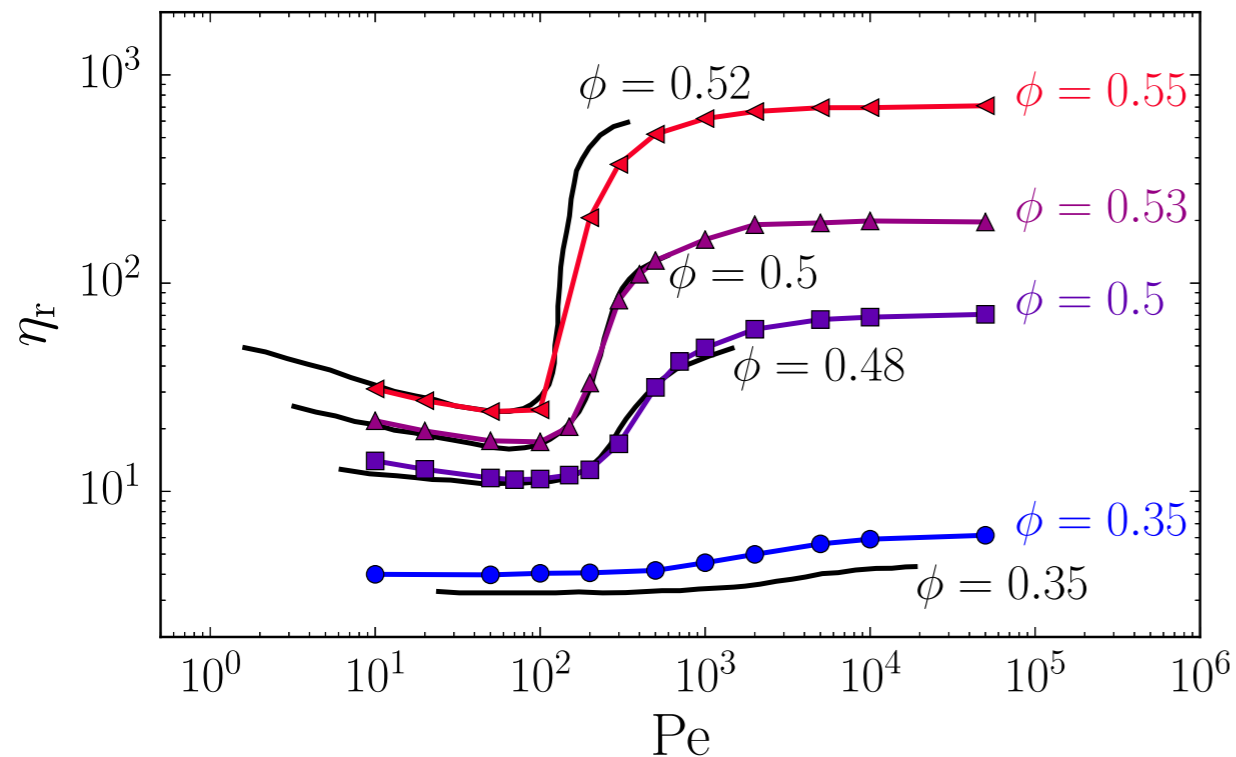


Charge stabilized



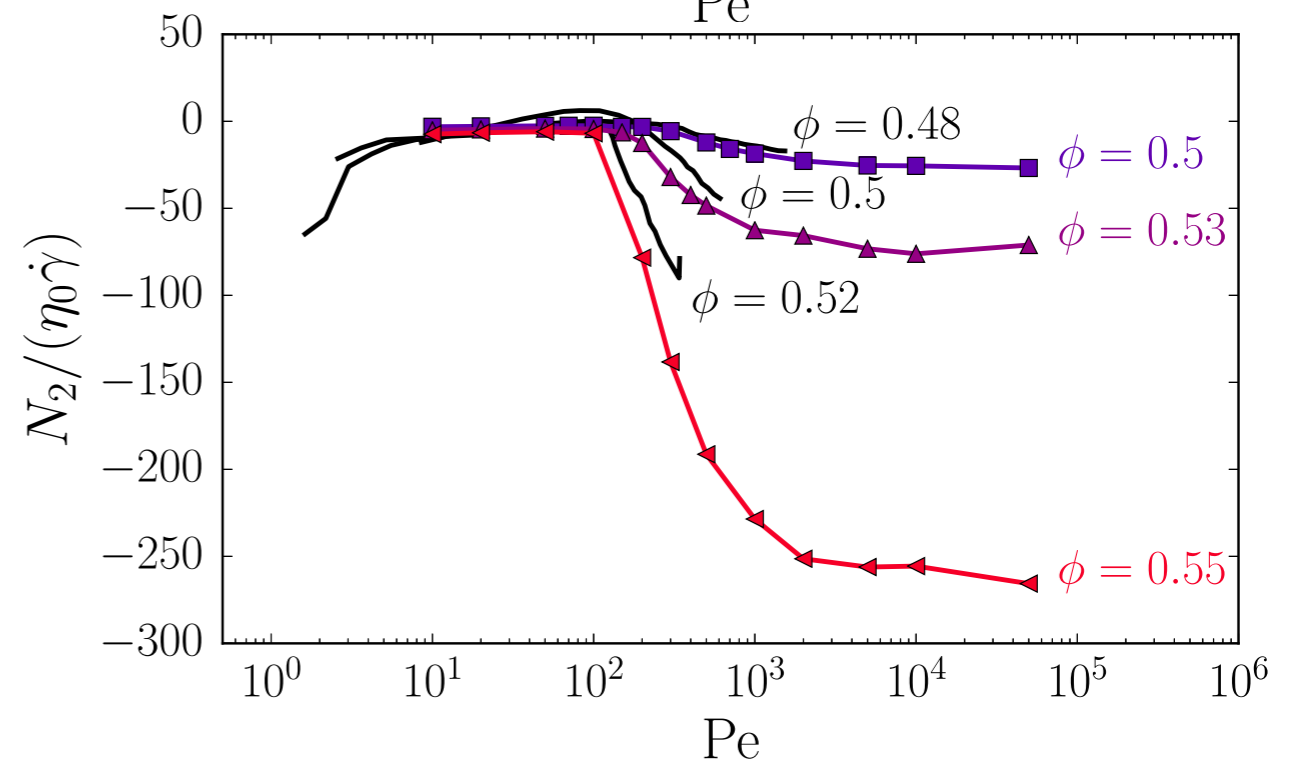
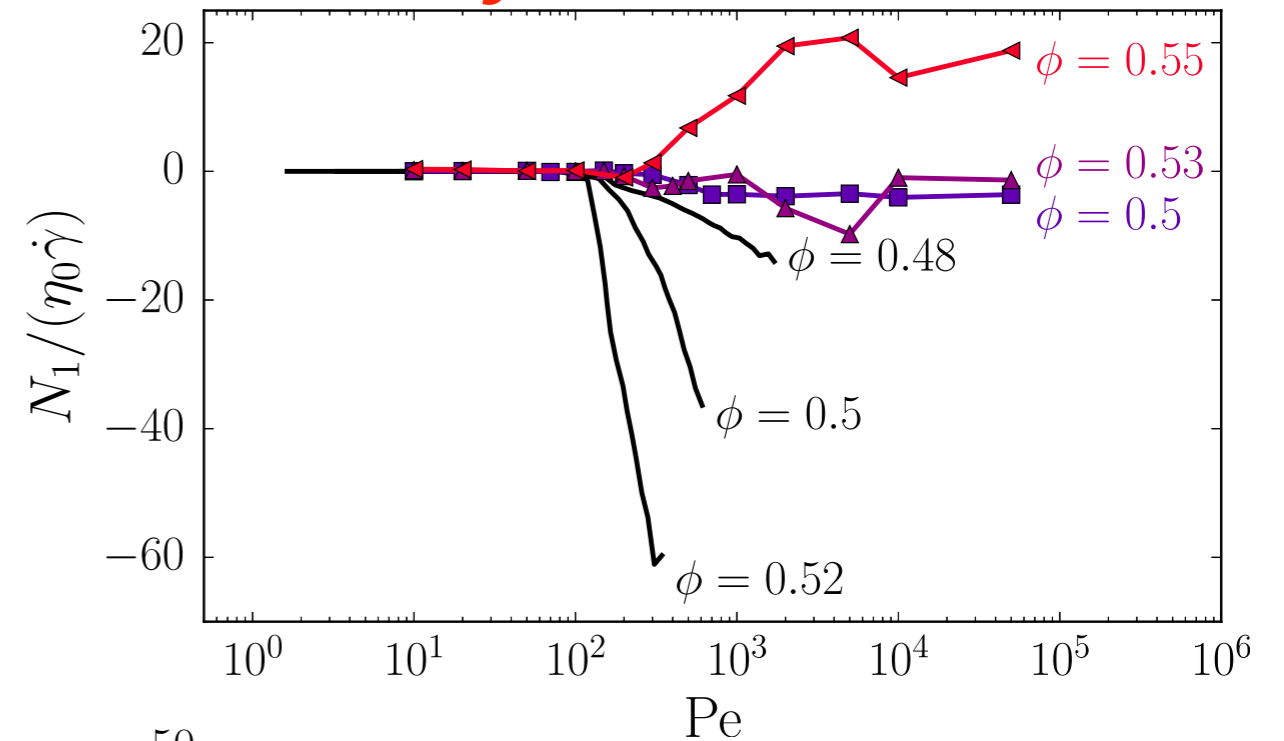
# Hydrodynamic interaction + **contact force** + **Brownian force or/and repulsive force**

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



**Experimental data**  
black-solid lines  
Cwalina and Wagner 2014

*very different!?*



# Outline

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5. Extensional rheology



# Rheology

velocity gradient

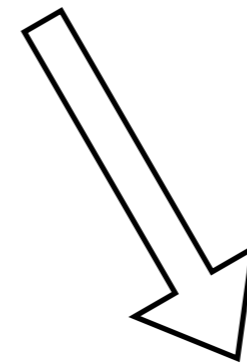
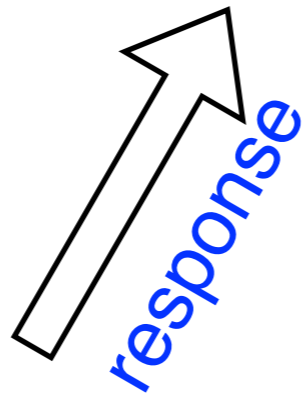
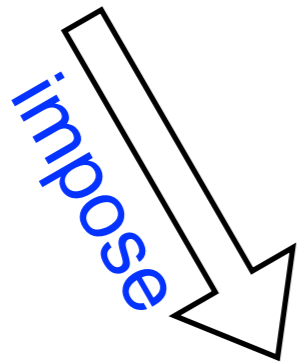
$$\begin{pmatrix} \frac{\partial u_x}{\partial x} & \frac{\partial u_x}{\partial y} & \frac{\partial u_x}{\partial z} \\ \frac{\partial u_y}{\partial x} & \frac{\partial u_y}{\partial y} & \frac{\partial u_y}{\partial z} \\ \frac{\partial u_z}{\partial x} & \frac{\partial u_z}{\partial y} & \frac{\partial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

stress tensor

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

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

*Constitutive modeling*



**MD-like  
Particle simulation**

**material functions**

scalars

(*not* coordinate specific)  
physical interpretations

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

# Conventional material functions

simple shear flow



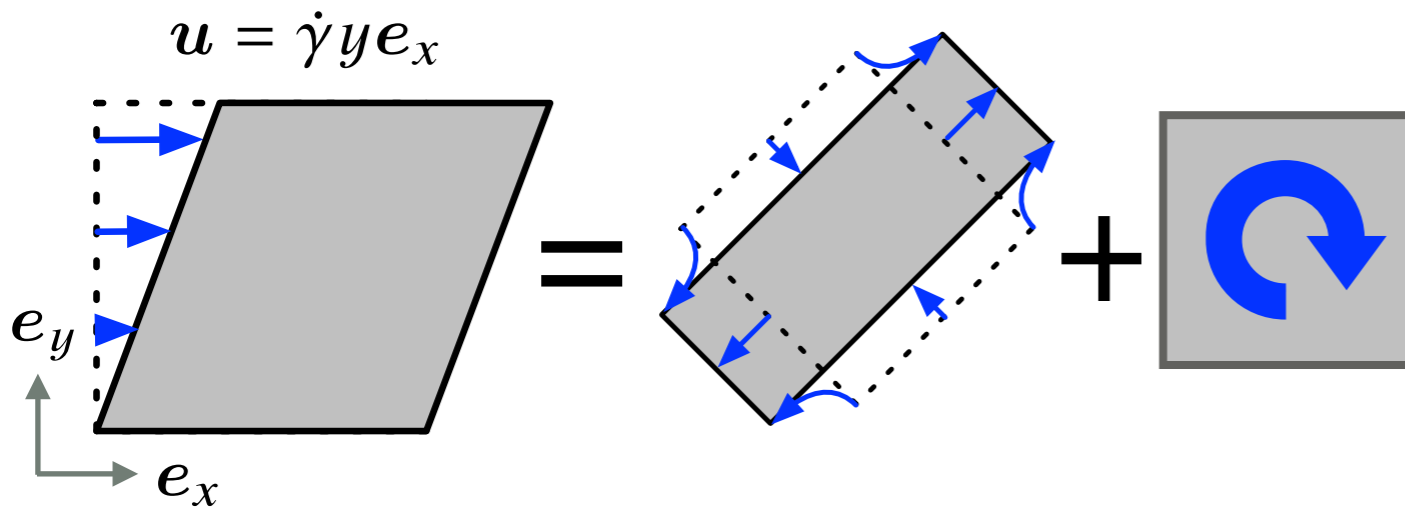
stress tensor

$$\nabla \mathbf{u} = \begin{pmatrix} 0 & \dot{\gamma} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \mathbf{D} + \mathbf{W}$$

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & 0 \\ \sigma_{xy} & \sigma_{yy} & 0 \\ 0 & 0 & \sigma_{zz} \end{pmatrix}$$

$$= -p\mathbf{I} + 2\eta(\dot{\gamma})\mathbf{D}$$

$$+ \frac{1}{3} \begin{pmatrix} 2N_1 + N_2 & 0 & 0 \\ 0 & -N_1 + N_2 & 0 \\ 0 & 0 & N_1 - 2N_2 \end{pmatrix}$$



$$\mathbf{D} = \begin{pmatrix} 0 & \dot{\gamma}/2 & 0 \\ \dot{\gamma}/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \mathbf{W} = \begin{pmatrix} 0 & \dot{\gamma}/2 & 0 \\ -\dot{\gamma}/2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

viscometric functions

$$\begin{cases} \eta \equiv \sigma_{xy} / \dot{\gamma} \\ N_1 \equiv \sigma_{xx} - \sigma_{yy} \\ N_2 \equiv \sigma_{yy} - \sigma_{zz} \end{cases}$$

# Generalized material functions

(Only planar flows in this talk)

$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix} \longrightarrow \sigma = -p\mathbf{I} + 2\eta\mathbf{D} + 2\lambda_0\mathbf{E} + 2\lambda_3\mathbf{G}_3$$

**any (planar) uniform flows**

$$\mathcal{B} = (\mathbf{I}, \mathbf{D}, \mathbf{E}, \mathbf{G}_3)$$

Cf. Conventional material functions

$$\begin{cases} \eta \equiv \sigma_{xy} / \dot{\gamma} \\ N_1 \equiv \sigma_{xx} - \sigma_{yy} \\ N_2 \equiv \sigma_{yy} - \sigma_{zz} \end{cases}$$

simple shear flows

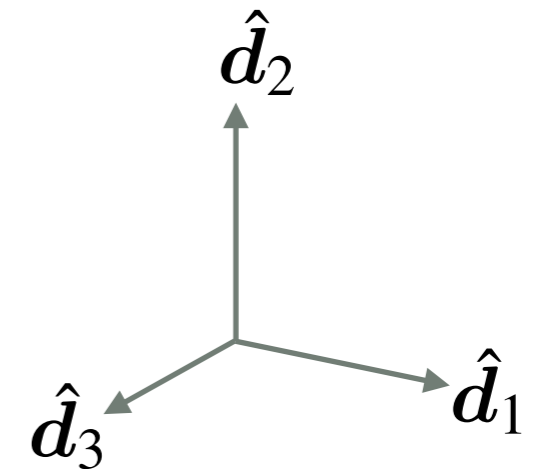
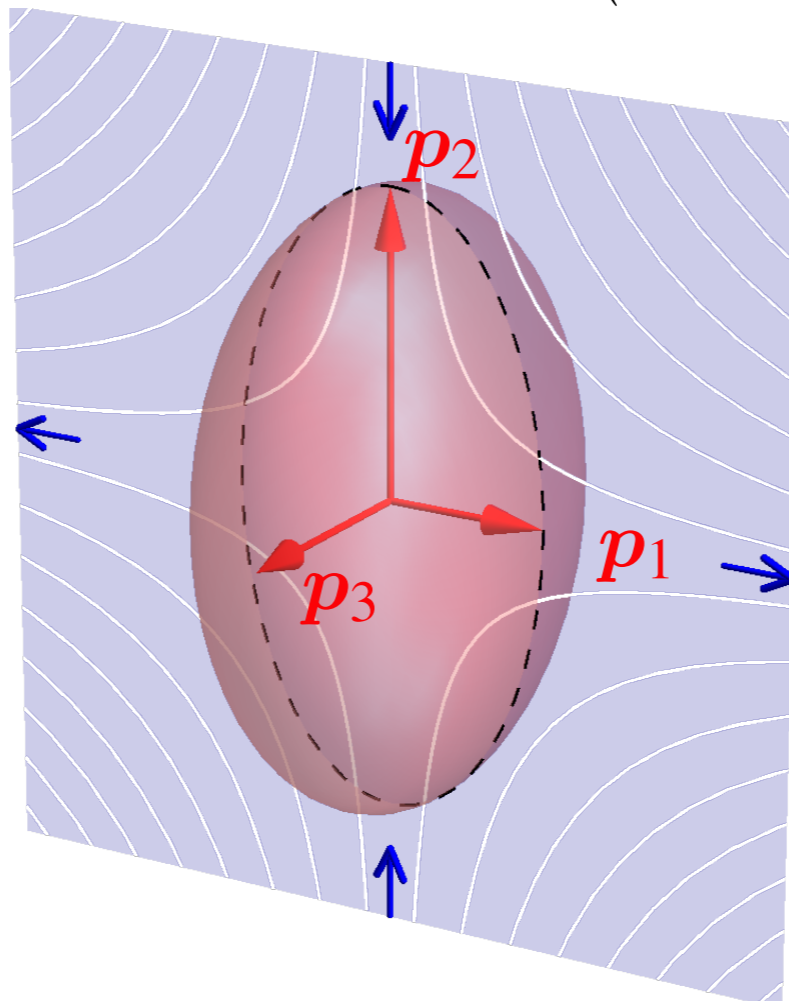
$$\begin{cases} p = -\frac{\sigma : \mathbf{I}}{\mathbf{I} : \mathbf{I}} = -\frac{\text{Tr } \sigma}{3} \\ \eta = \frac{\sigma : \mathbf{D}}{2\mathbf{D} : \mathbf{D}} \\ \lambda_0 = \frac{\sigma : \mathbf{E}}{2\mathbf{E} : \mathbf{E}} \\ \lambda_3 = \frac{\sigma : \mathbf{G}_3}{2\mathbf{G}_3 : \mathbf{G}_3} \end{cases}$$

Giulio G. Giusteri & Seto 2017 arXiv:1702.02745

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

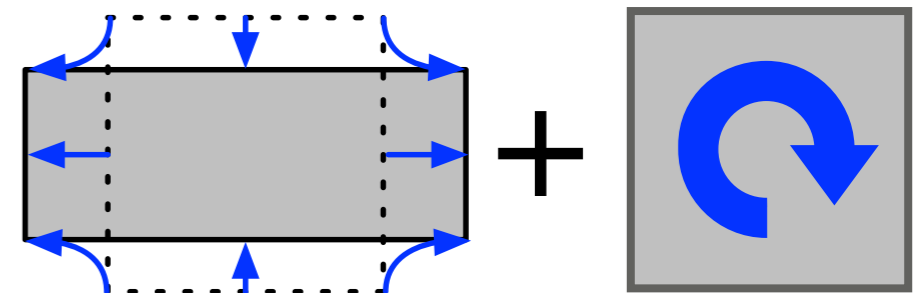
$$\mathbf{D} = \dot{\varepsilon}(\hat{\mathbf{d}}_1\hat{\mathbf{d}}_1 - \hat{\mathbf{d}}_2\hat{\mathbf{d}}_2) = \begin{pmatrix} \dot{\varepsilon} & 0 & 0 \\ 0 & -\dot{\varepsilon} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

*stress  
to keep flowing*



Eigenvectors of  $\mathbf{D}$

any uniform planar flows

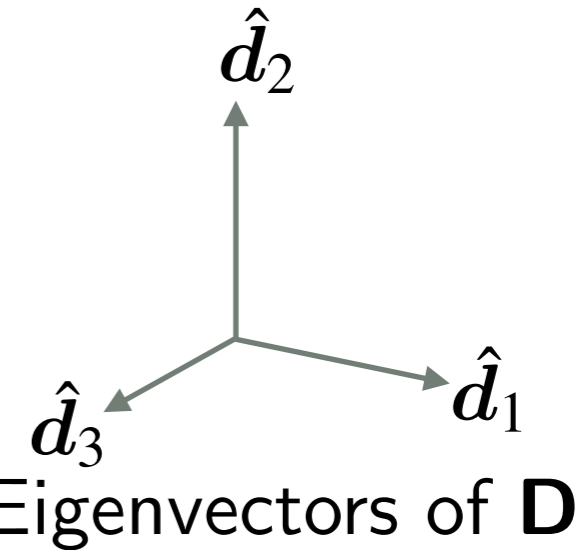
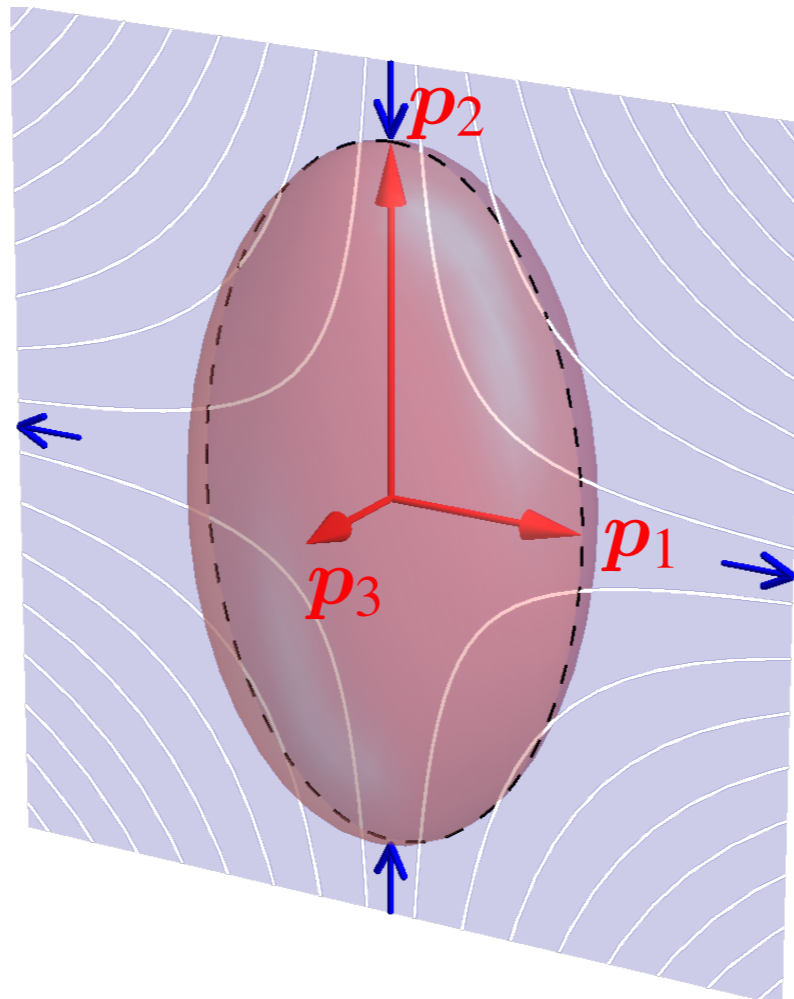


(Eigenvectors and eigenvalues of  $\mathbf{P} = -\boldsymbol{\sigma}$ )

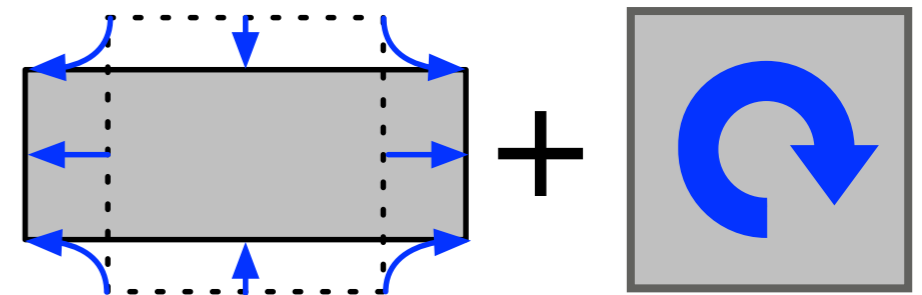
$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\mathbf{D} + 2\lambda_0\mathbf{E}$$

$$\mathbf{E} = \dot{\varepsilon} \left( -\frac{1}{2}\hat{\mathbf{d}}_1\hat{\mathbf{d}}_1 - \frac{1}{2}\hat{\mathbf{d}}_2\hat{\mathbf{d}}_2 + \hat{\mathbf{d}}_3\hat{\mathbf{d}}_3 \right) = \begin{pmatrix} -\dot{\varepsilon}/2 & 0 & 0 \\ 0 & -\dot{\varepsilon}/2 & 0 \\ 0 & 0 & \dot{\varepsilon} \end{pmatrix}$$

*in-plane*  
*out-of-plane*  
*anisotropy*



any uniform planar flows



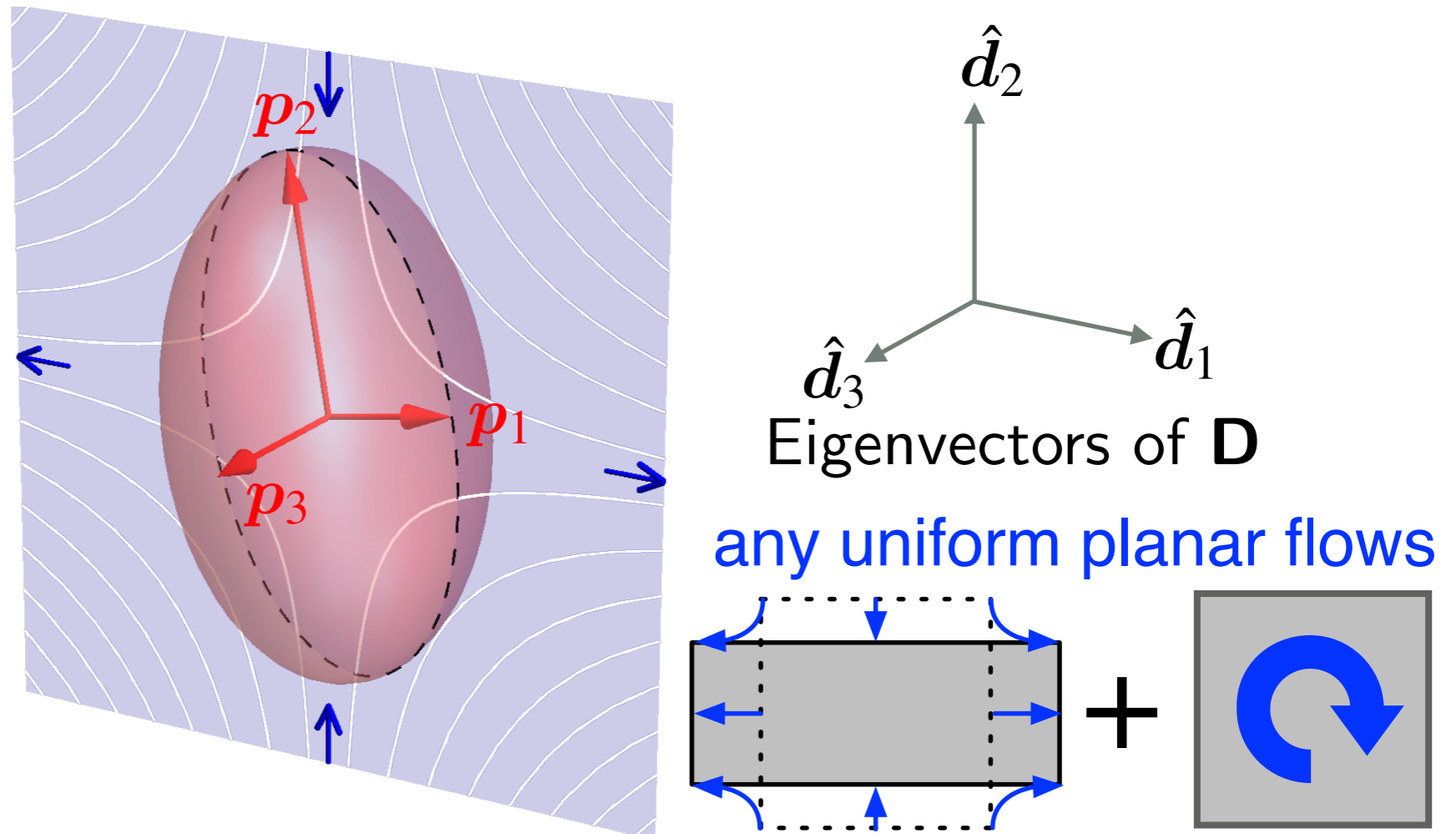
(Eigenvectors and eigenvalues of  $\mathbf{P} = -\boldsymbol{\sigma}$ )

**Giulio G. Giusteri & Seto 2017 arXiv:1702.02745**

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\mathbf{D} + 2\lambda_3\mathbf{G}_3$$

$$\mathbf{G}_3 = \dot{\varepsilon}(\hat{\mathbf{d}}_1\hat{\mathbf{d}}_2 + \hat{\mathbf{d}}_2\hat{\mathbf{d}}_1) = \begin{pmatrix} 0 & \dot{\varepsilon} & 0 \\ \dot{\varepsilon} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

*reorientation  
of principal  
directions*



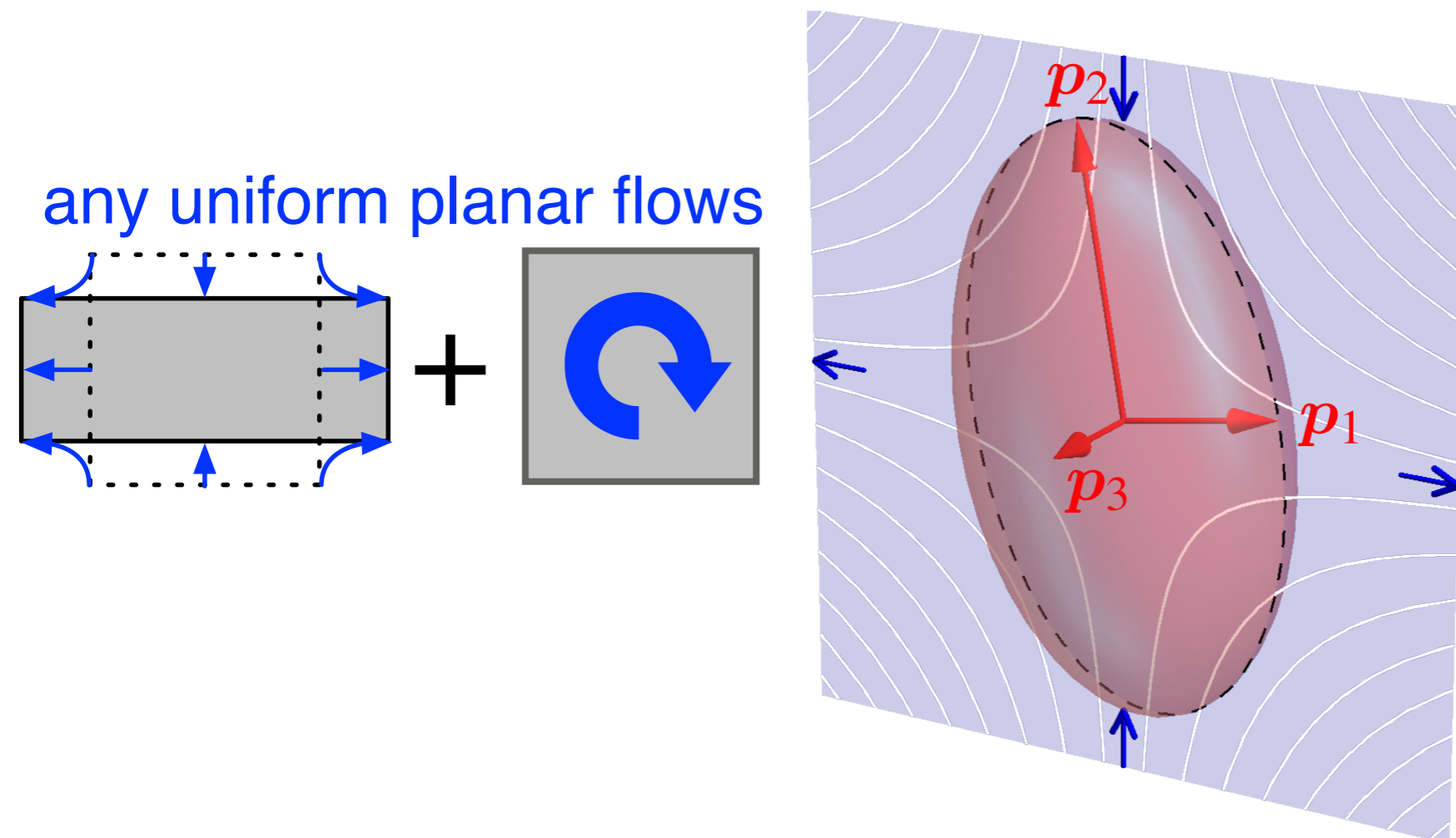
(Eigenvectors and eigenvalues of  $\mathbf{P} = -\boldsymbol{\sigma}$ )

# Generalized material functions

(Only planar flows in this talk.)

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\mathbf{D} + 2\lambda_0\mathbf{E} + 2\lambda_3\mathbf{G}_3$$

$\mathcal{B} = (\mathbf{I}, \mathbf{D}, \mathbf{E}, \mathbf{G}_3)$  orthogonal tensorial basis



$$p = -\frac{\boldsymbol{\sigma} : \mathbf{I}}{\mathbf{I} : \mathbf{I}} = -\frac{\text{Tr } \boldsymbol{\sigma}}{3}$$

$$\eta = \frac{\boldsymbol{\sigma} : \mathbf{D}}{2\mathbf{D} : \mathbf{D}}$$

$$\lambda_0 = \frac{\boldsymbol{\sigma} : \mathbf{E}}{2\mathbf{E} : \mathbf{E}}$$

$$\lambda_3 = \frac{\boldsymbol{\sigma} : \mathbf{G}_3}{2\mathbf{G}_3 : \mathbf{G}_3}$$

(Eigenvectors and eigenvalues of  $\mathbf{P} = -\boldsymbol{\sigma}$ )

Giulio G. Giusteri & Seto 2017 arXiv:1702.02745

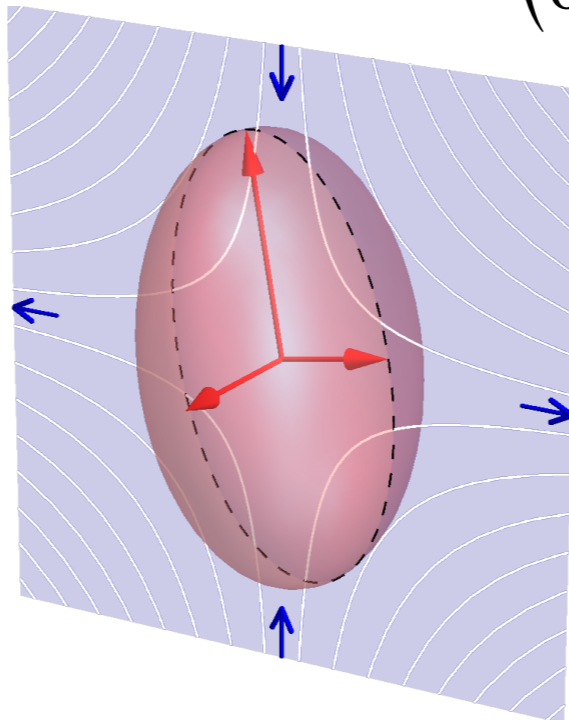
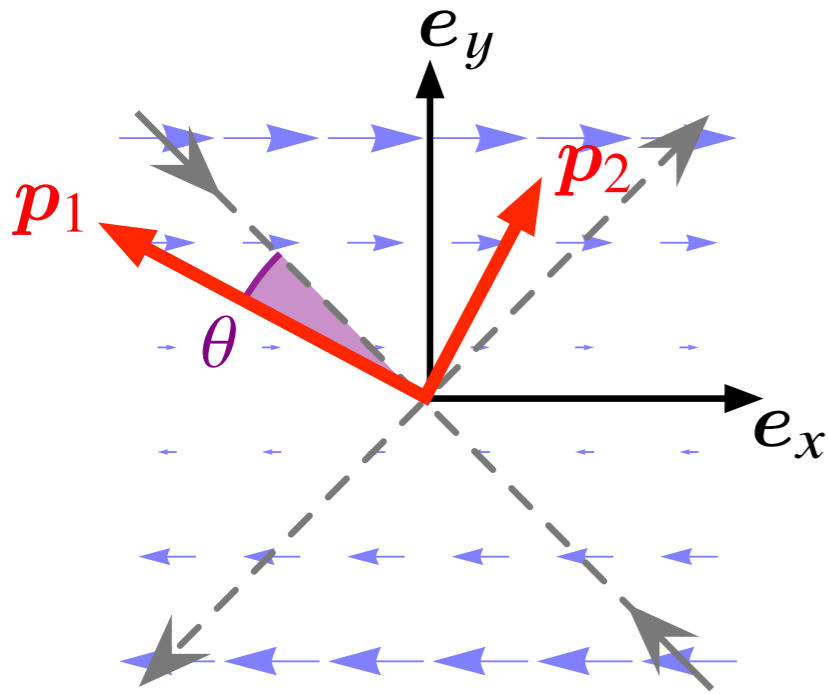
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$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\eta\mathbf{D} + 2\lambda_3\mathbf{G}_3$$

$$\mathbf{G}_3 = \dot{\varepsilon}(\hat{\mathbf{d}}_1\hat{\mathbf{d}}_2 + \hat{\mathbf{d}}_2\hat{\mathbf{d}}_1) = \begin{pmatrix} 0 & \dot{\varepsilon} & 0 \\ \dot{\varepsilon} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



*reorientation  
of principal  
directions*

(Eigenvectors and eigenvalues of  $\mathbf{P} = -\boldsymbol{\sigma}$ )

$$N_1 = -2\dot{\varepsilon}\lambda_3$$

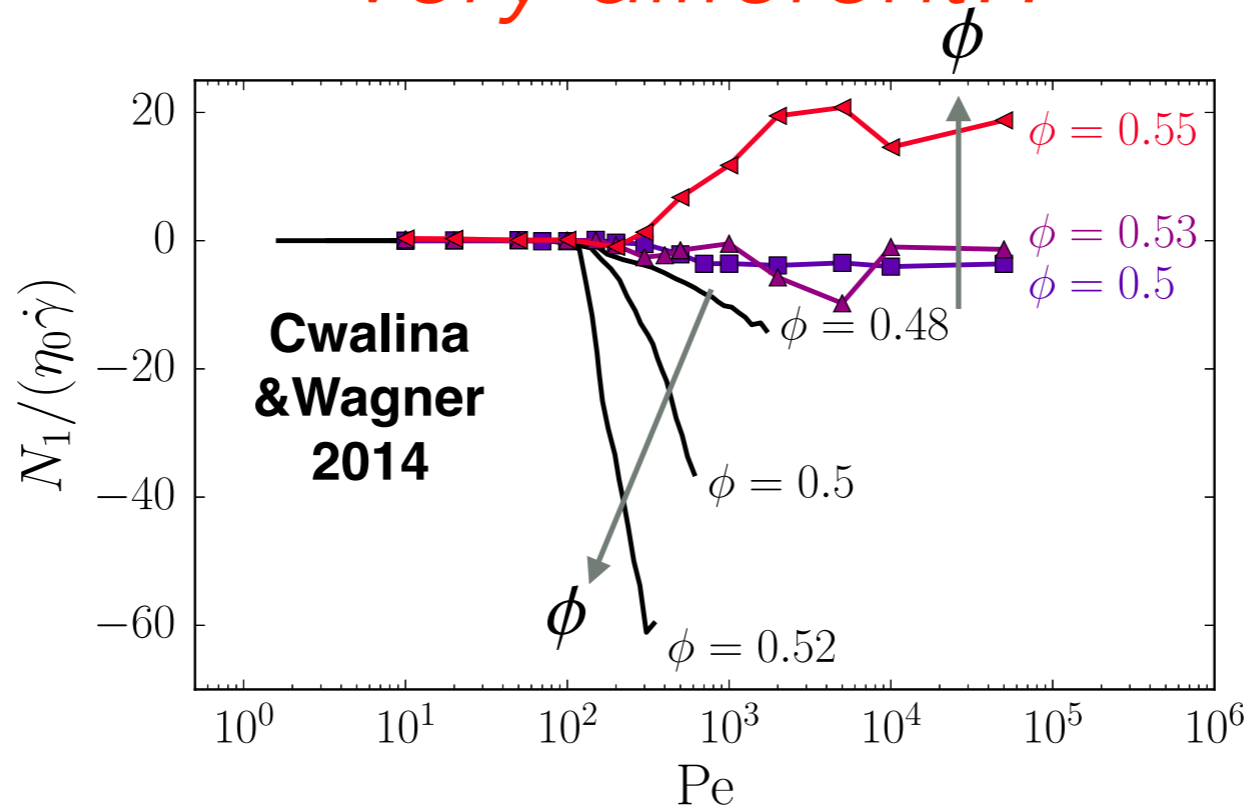
$$\theta \equiv \tan^{-1} \left( \frac{-N_1/2\sigma}{1 + \sqrt{1 + (N_1/2\sigma)^2}} \right) \approx -\frac{N_1}{4\sigma}$$

$$\sigma = \eta\dot{\gamma}$$

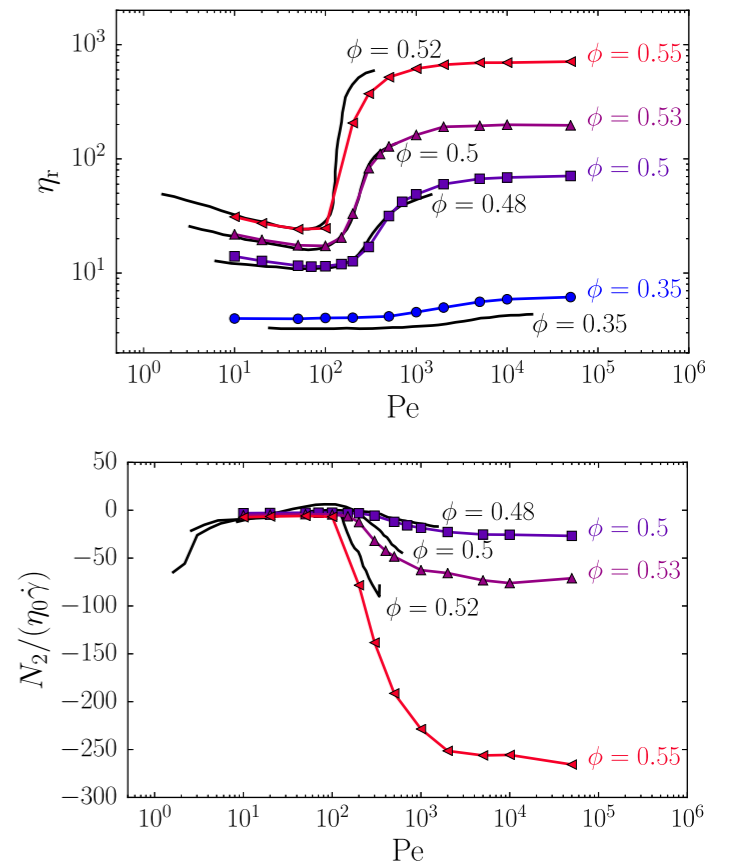
# $N_1$ issue

*very different!?*

$$\frac{N_1}{\eta_0 \dot{\gamma}}$$



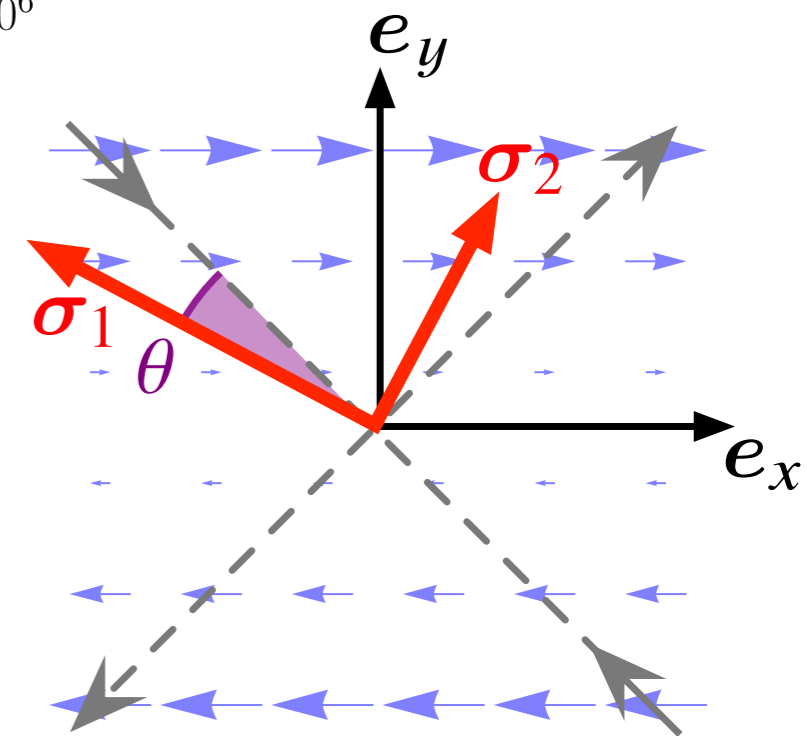
Mari et. al. 2015



reorientation angle

$$\theta \equiv \tan^{-1} \left( \frac{-N_1/2\sigma}{1 + \sqrt{1 + (N_1/2\sigma)^2}} \right) \approx -\frac{N_1}{4\sigma}$$

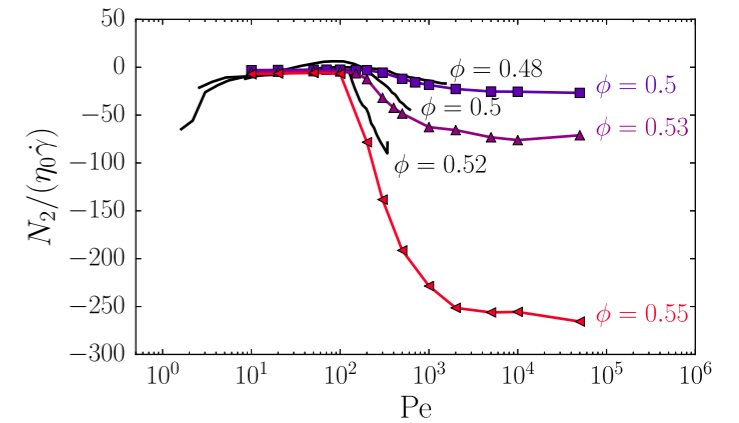
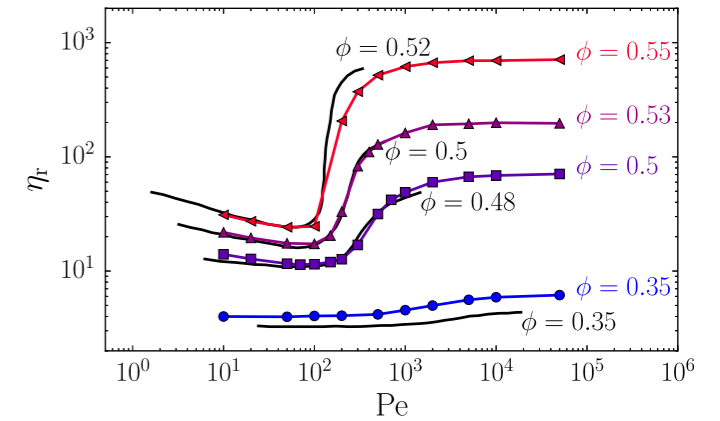
$$N_1 = -2\dot{\epsilon}\lambda_3$$



# $N_1$ issue

*very different!?*

Mari et. al. 2015



$$\frac{N_1}{\eta_0 \dot{\gamma}}$$

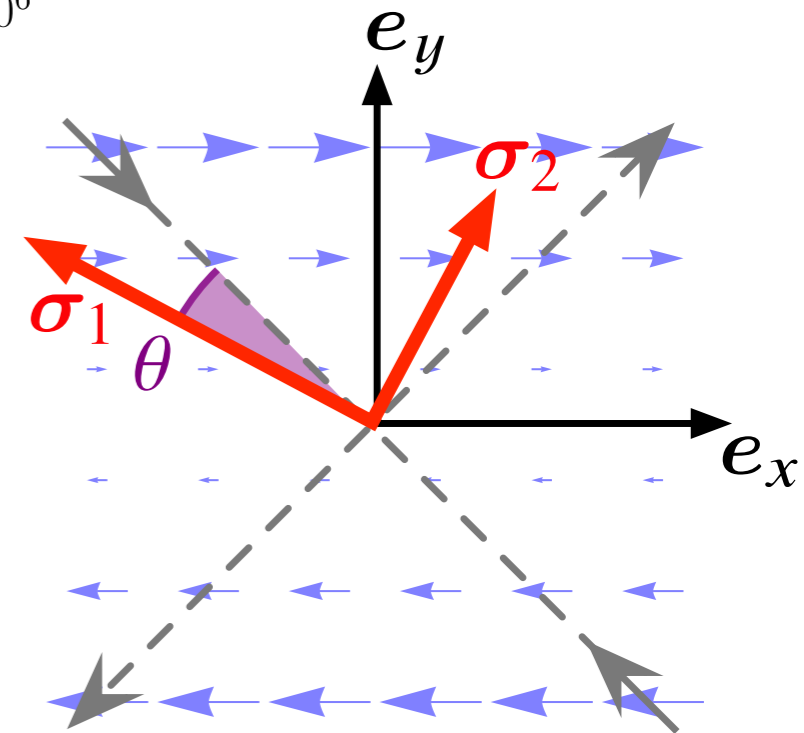
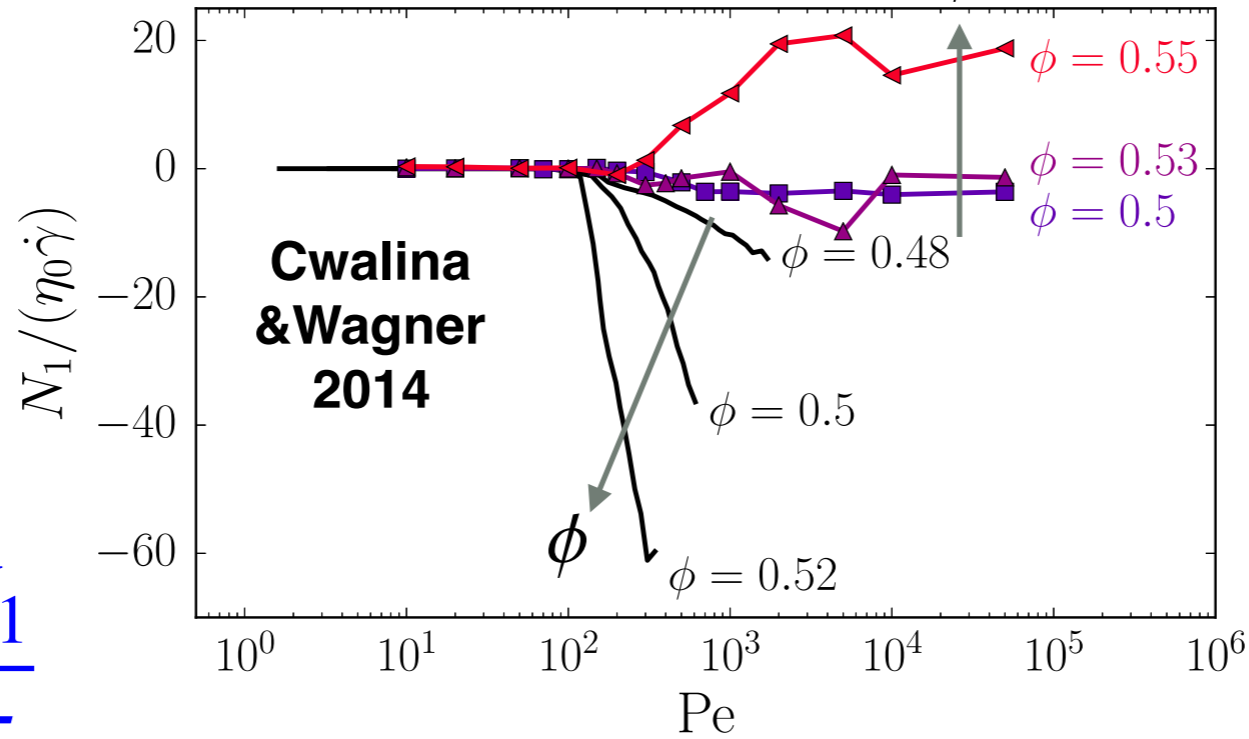


$$\frac{N_1}{\eta \dot{\gamma}} = \frac{N_1}{\sigma}$$

reorientation angle

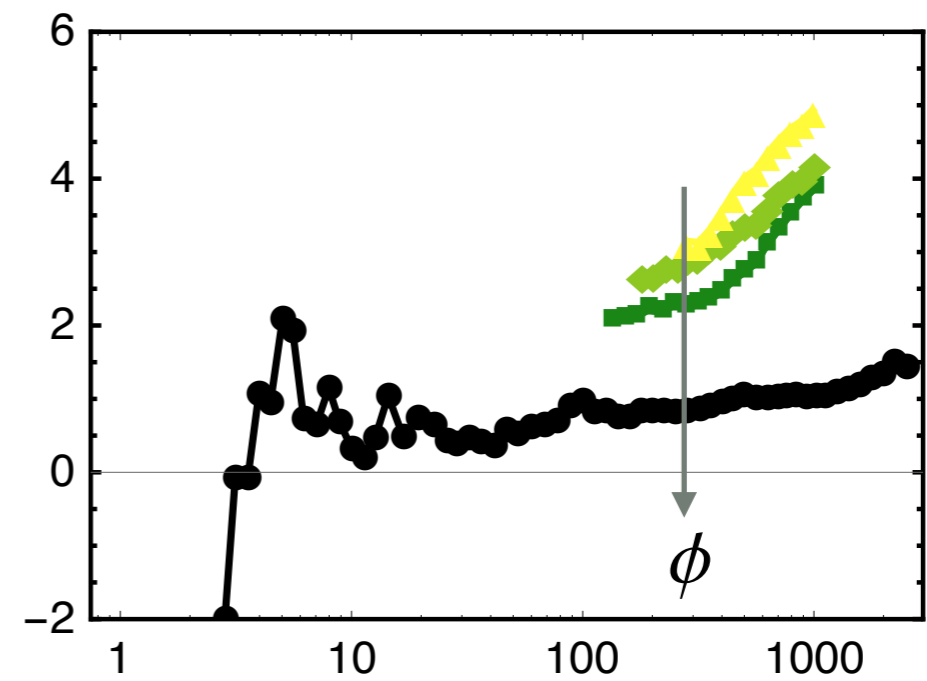
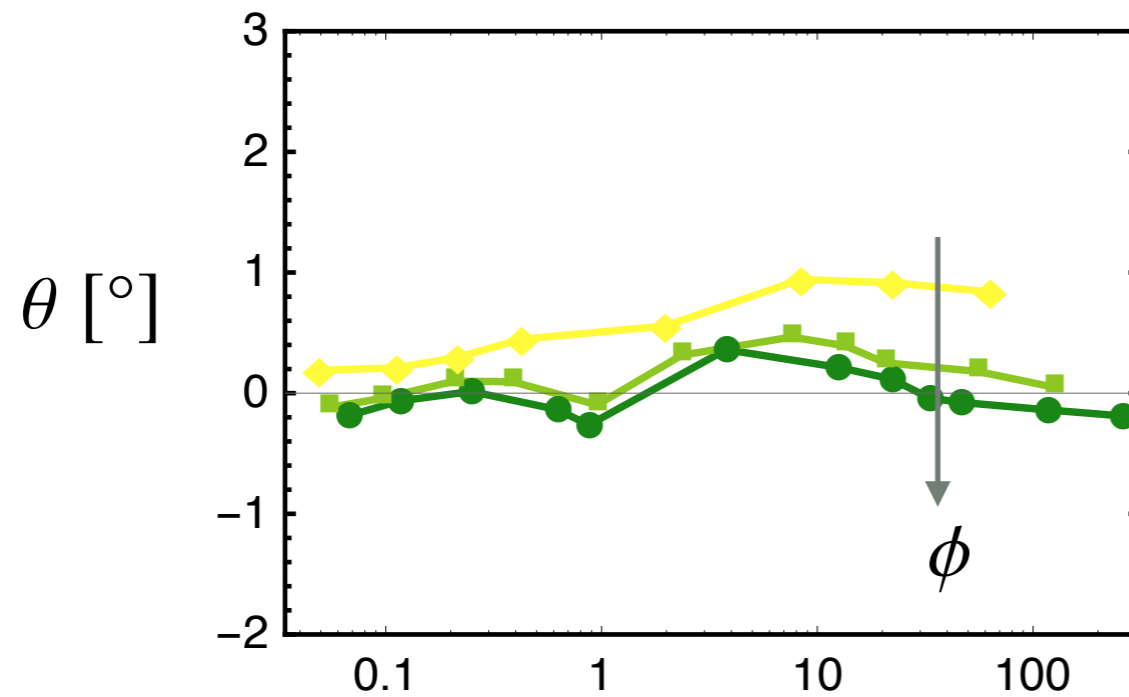
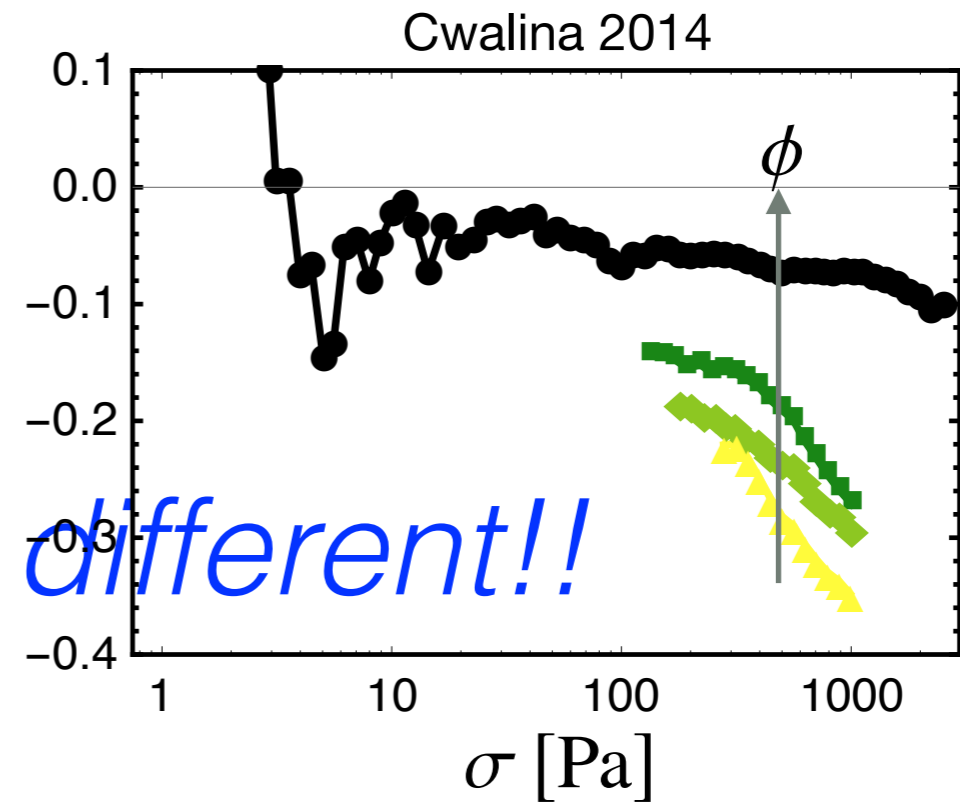
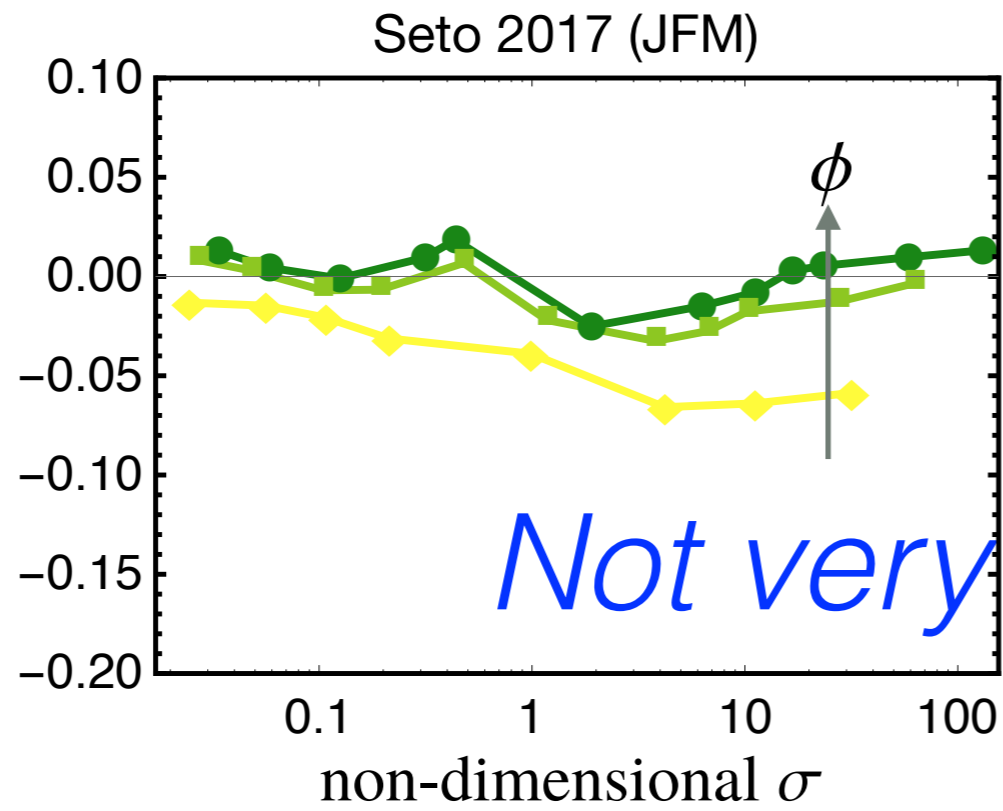
$$\theta \equiv \tan^{-1} \left( \frac{-N_1/2\sigma}{1 + \sqrt{1 + (N_1/2\sigma)^2}} \right) \approx -\frac{N_1}{4\sigma}$$

$$N_1 = -2\dot{\epsilon}\lambda_3$$

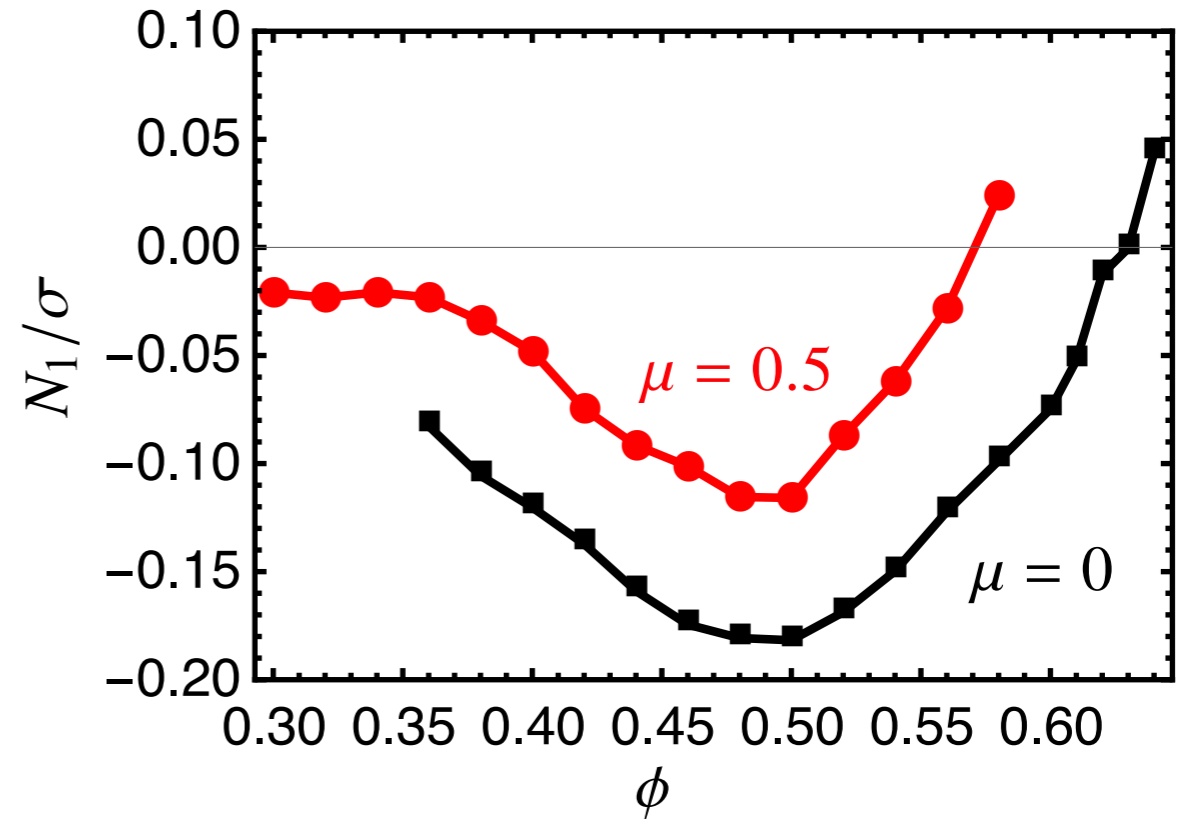
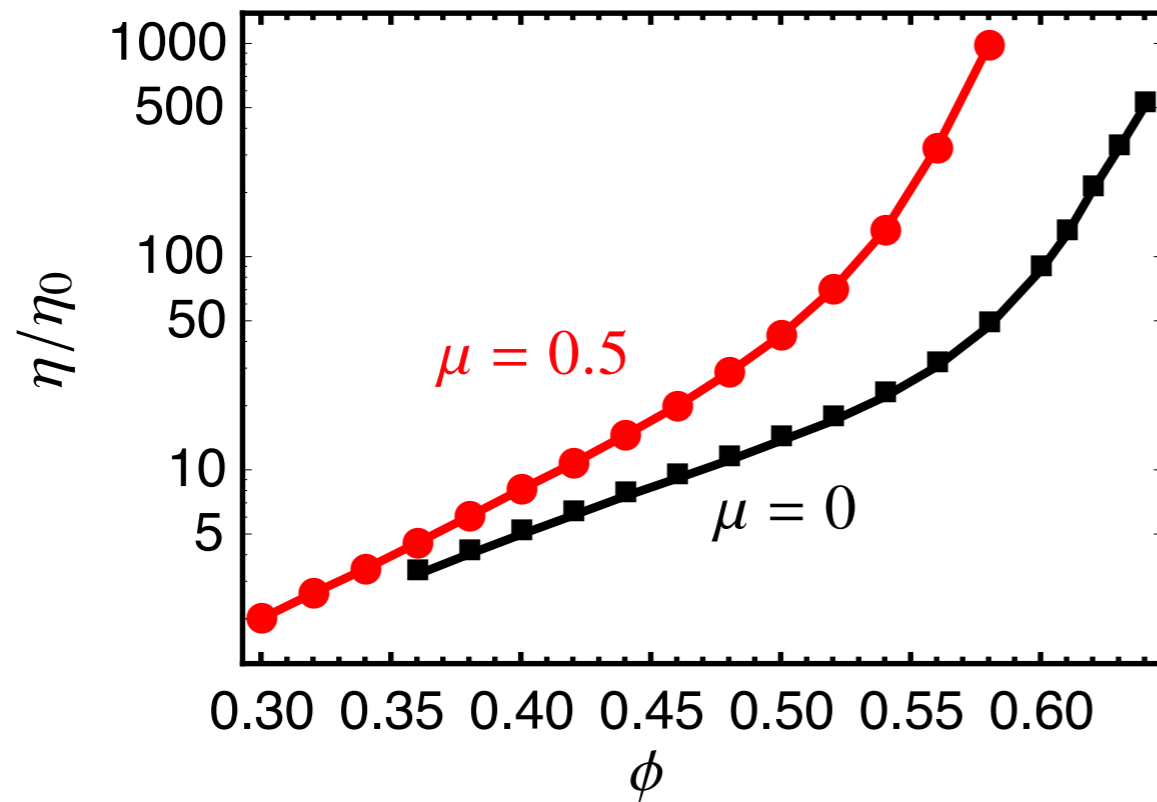


# $N_1$ issue

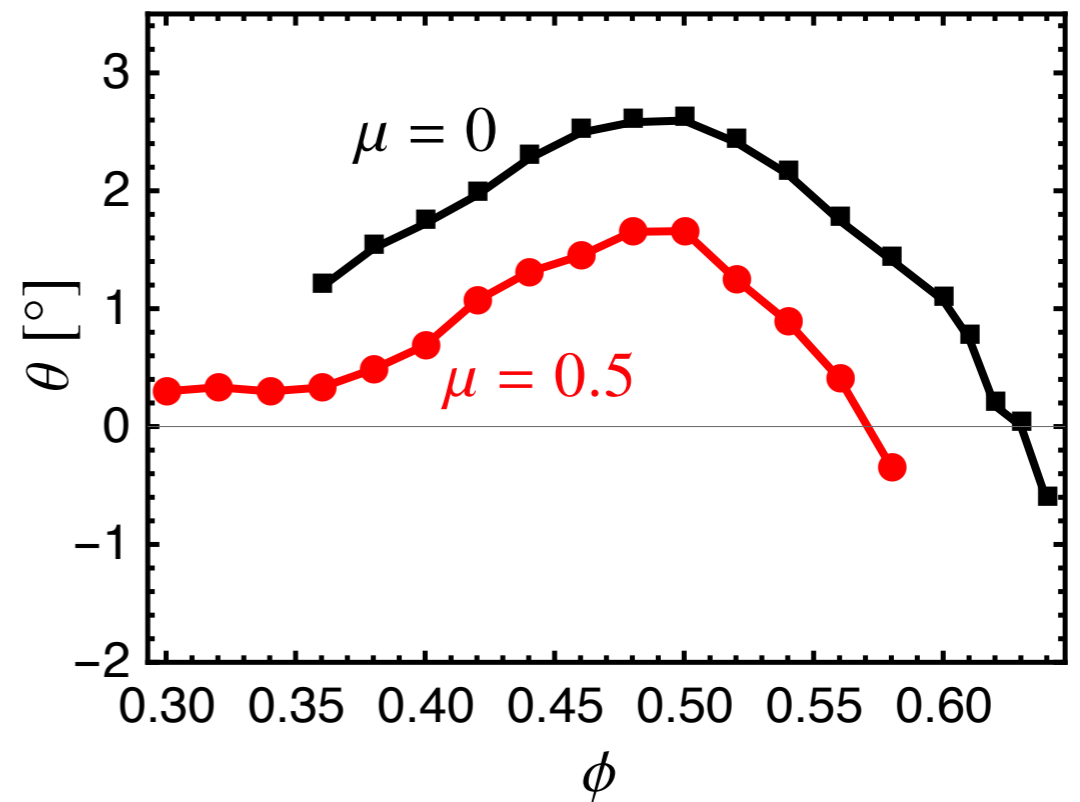
$$\frac{N_1}{\eta\dot{\gamma}} = \frac{N_1}{\sigma}$$



# The change of sign is not surprising!



$$\theta \equiv \tan^{-1} \left( \frac{-N_1/2\sigma}{1 + \sqrt{1 + (N_1/2\sigma)^2}} \right) \approx -\frac{N_1}{4\sigma}$$



# Outline

1. Periodic boundary conditions
2. Simulation model for particle dynamics
3. Material functions
4.  $N_1$  issue
5. Extensional rheology

# Planar flows

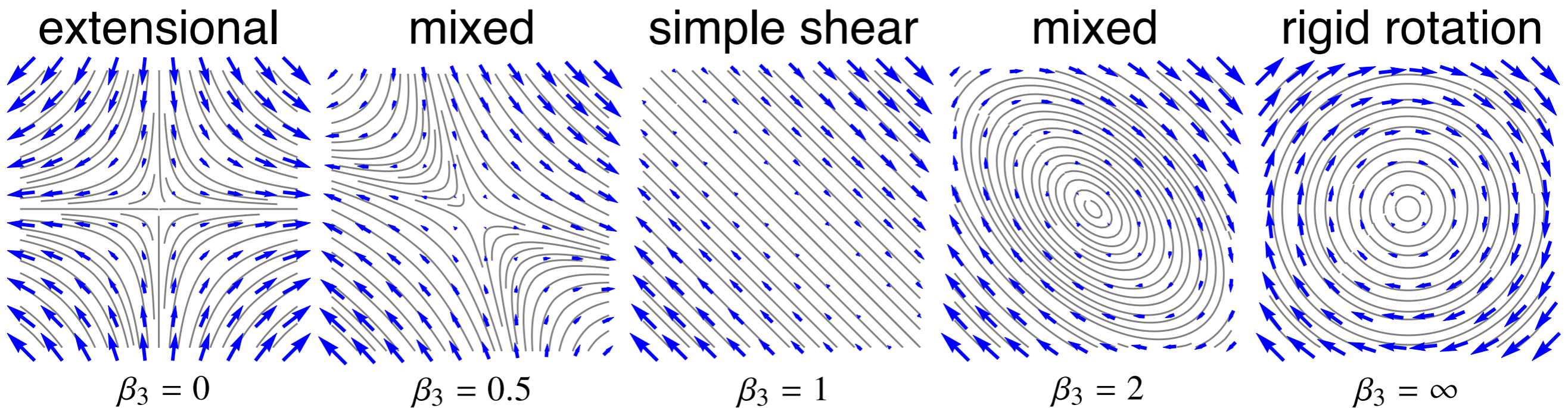
$$\boldsymbol{\sigma} = -\left[p_f + \Pi(\dot{\boldsymbol{\varepsilon}}, \beta_3)\right] \mathbf{I} + 2\eta(\dot{\boldsymbol{\varepsilon}}, \beta_3) \mathbf{D} + 2\lambda_0(\dot{\boldsymbol{\varepsilon}}, \beta_3) \mathbf{E} + 2\lambda_3(\dot{\boldsymbol{\varepsilon}}, \beta_3) \mathbf{G}_3$$

$$\nabla \mathbf{u} \begin{cases} \mathbf{D} \equiv \frac{\nabla \mathbf{u} + \nabla \mathbf{u}^\top}{2} \\ \mathbf{W} \equiv \frac{\nabla \mathbf{u} - \nabla \mathbf{u}^\top}{2} \end{cases}$$

strain rate  $\dot{\boldsymbol{\varepsilon}} \equiv \sqrt{\frac{\mathbf{D} : \mathbf{D}}{2}}$

flow type  $\beta_3 \equiv \frac{1}{2\dot{\boldsymbol{\varepsilon}}} \hat{\mathbf{d}}_3 \cdot \nabla \times \mathbf{u}$

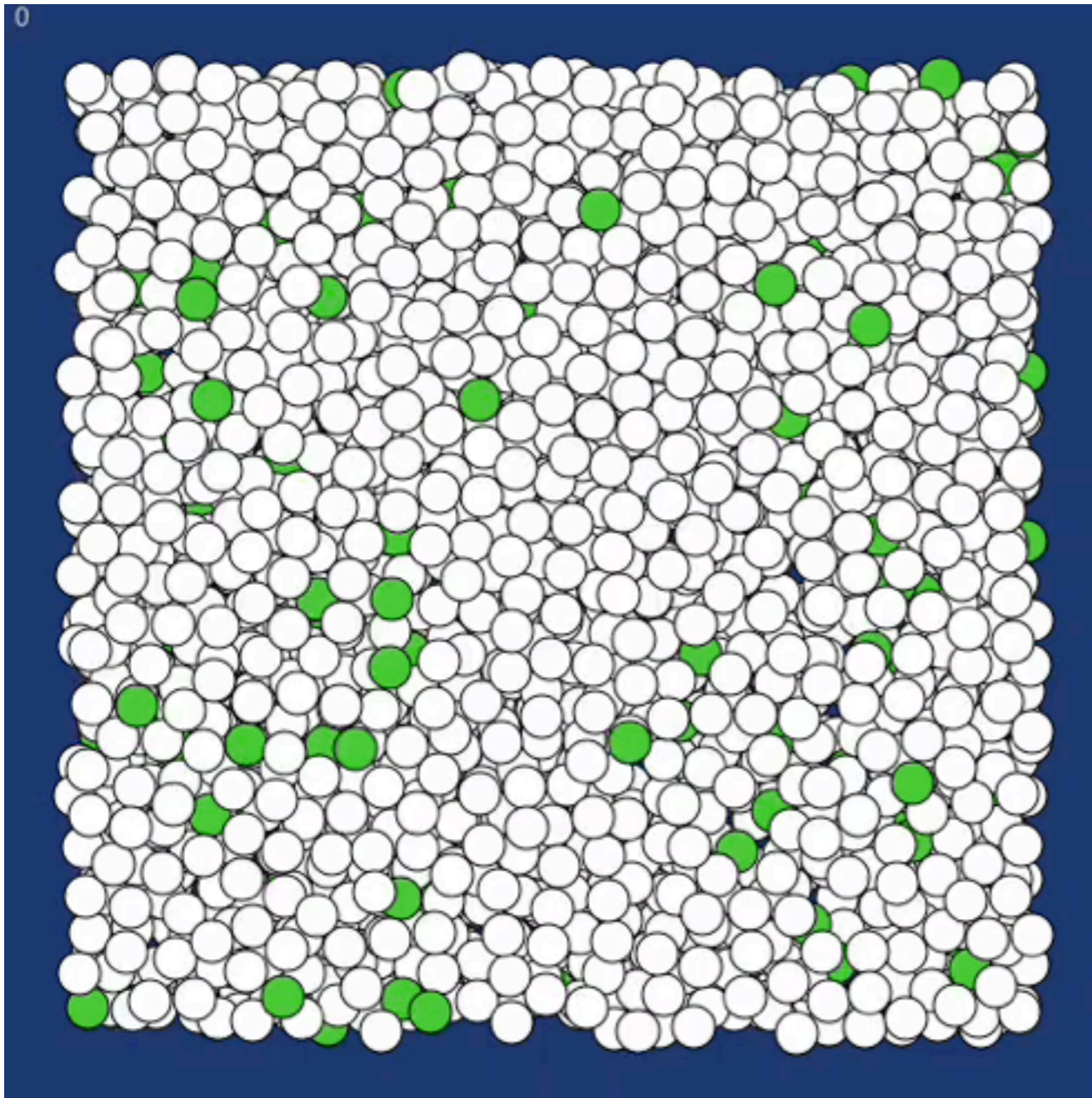
objective flow type:  $\bar{\beta}_3 = \beta_3 - \delta_3$



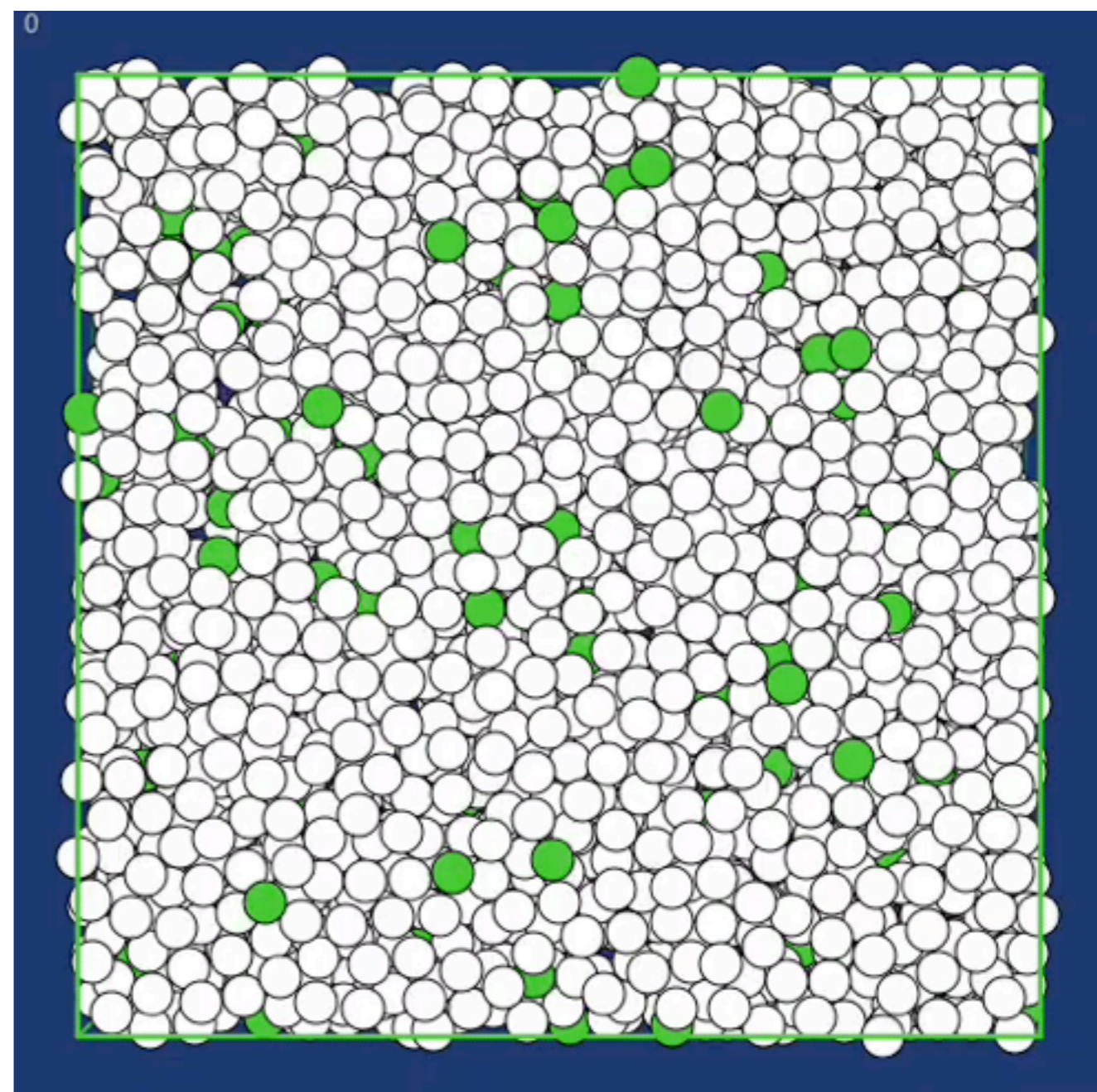
# Planar flows

flow type  $\beta_3 \equiv \frac{1}{2\dot{\epsilon}} \hat{d}_3 \cdot \nabla \times \mathbf{u}$

$\beta_3 = 1$



$\beta_3 = 0$





$$\eta(\dot{\epsilon}, \beta_3) \equiv \frac{1}{2} \frac{\sigma : \mathbf{D}}{\mathbf{D} : \mathbf{D}}$$

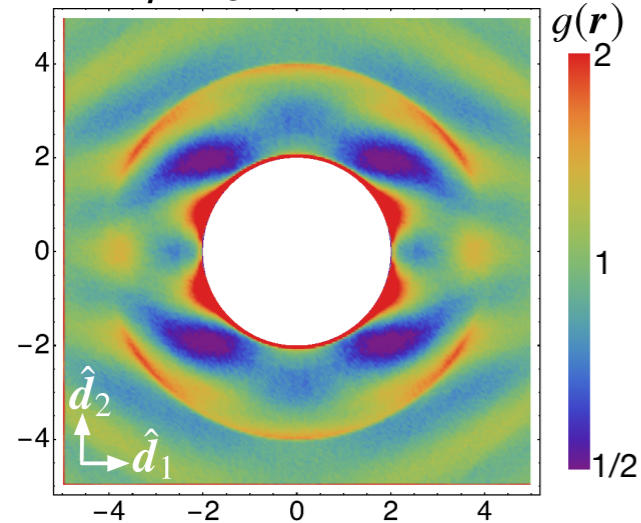
$$\text{strain rate } \dot{\epsilon} \equiv \sqrt{\frac{\mathbf{D} : \mathbf{D}}{2}}$$

— **extensional**  $\beta_3 = 0$

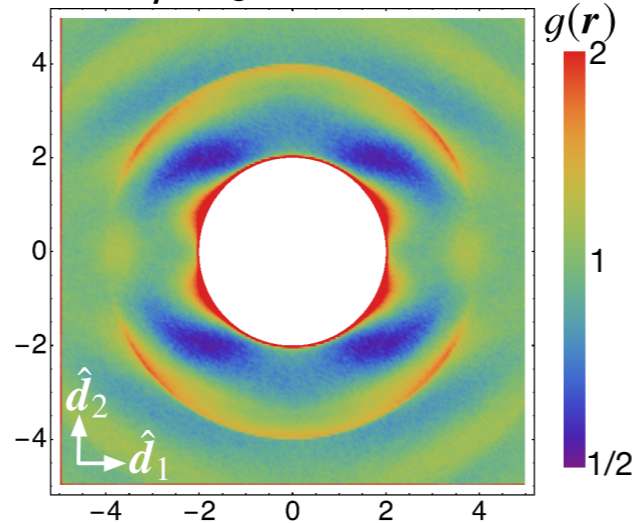
- - - **simple shear**

$\beta_3 = 1$

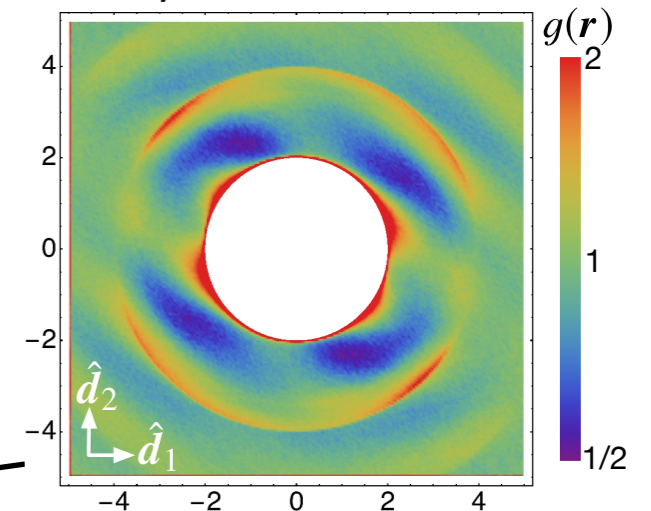
$\dot{\epsilon} / \dot{\epsilon}_0 = 0.01$



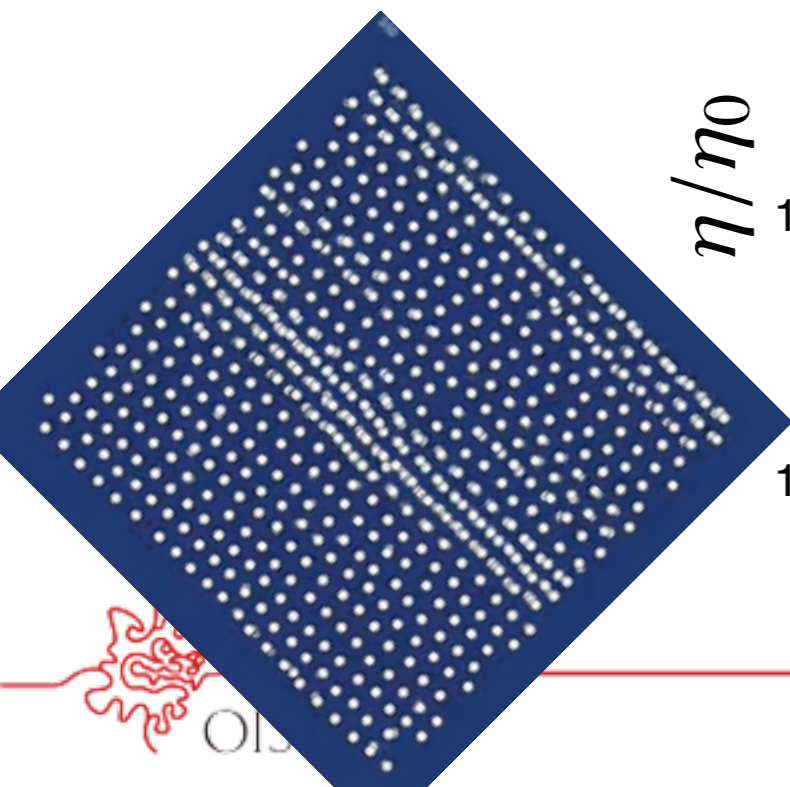
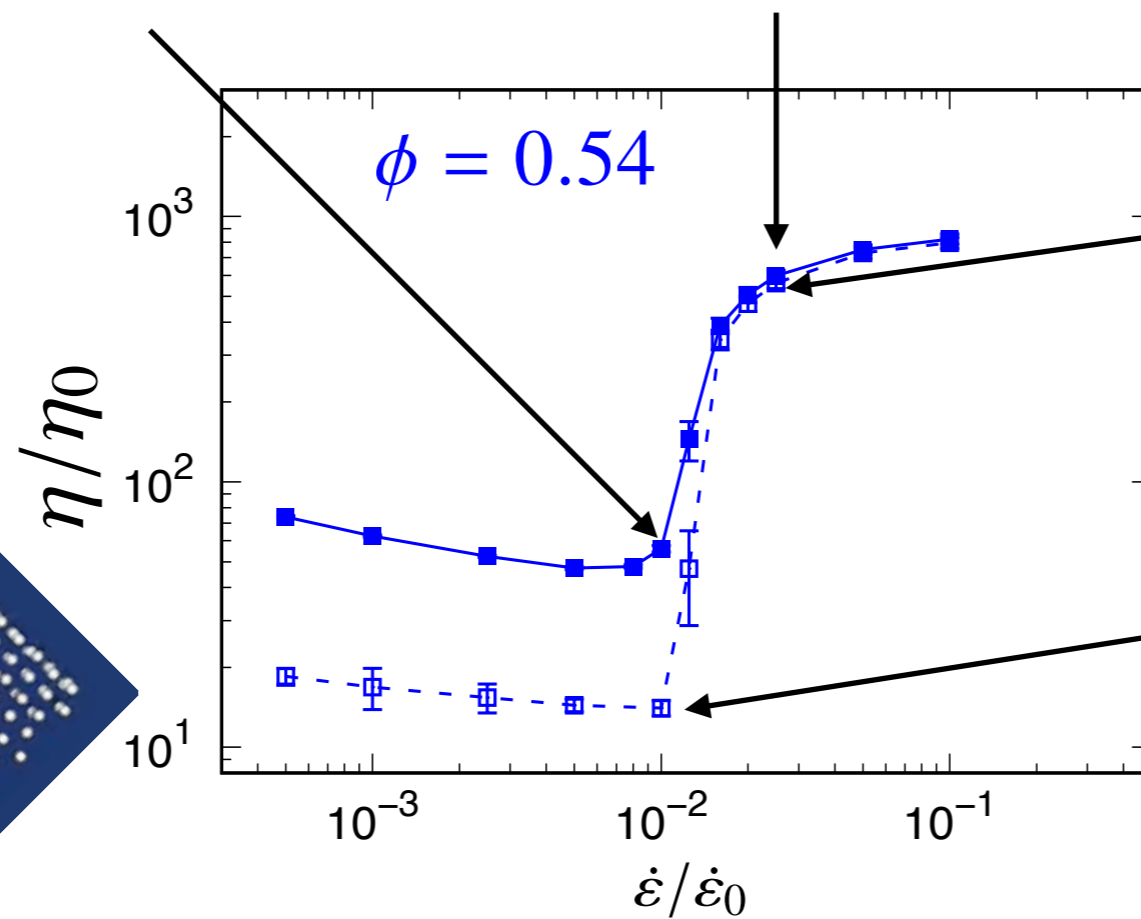
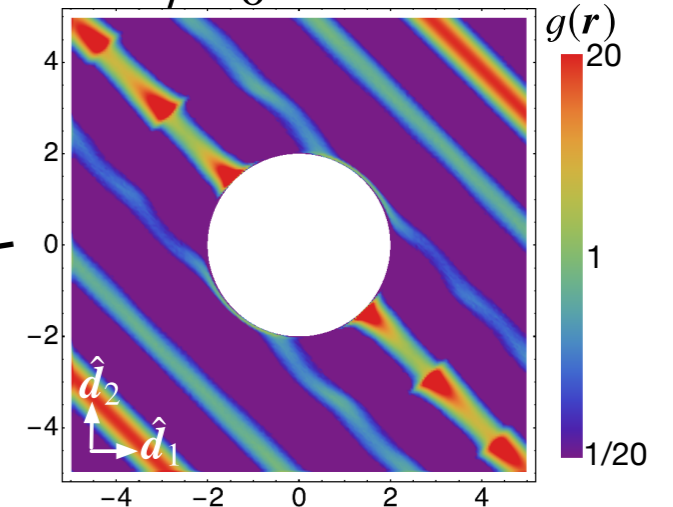
$\dot{\epsilon} / \dot{\epsilon}_0 = 0.02$



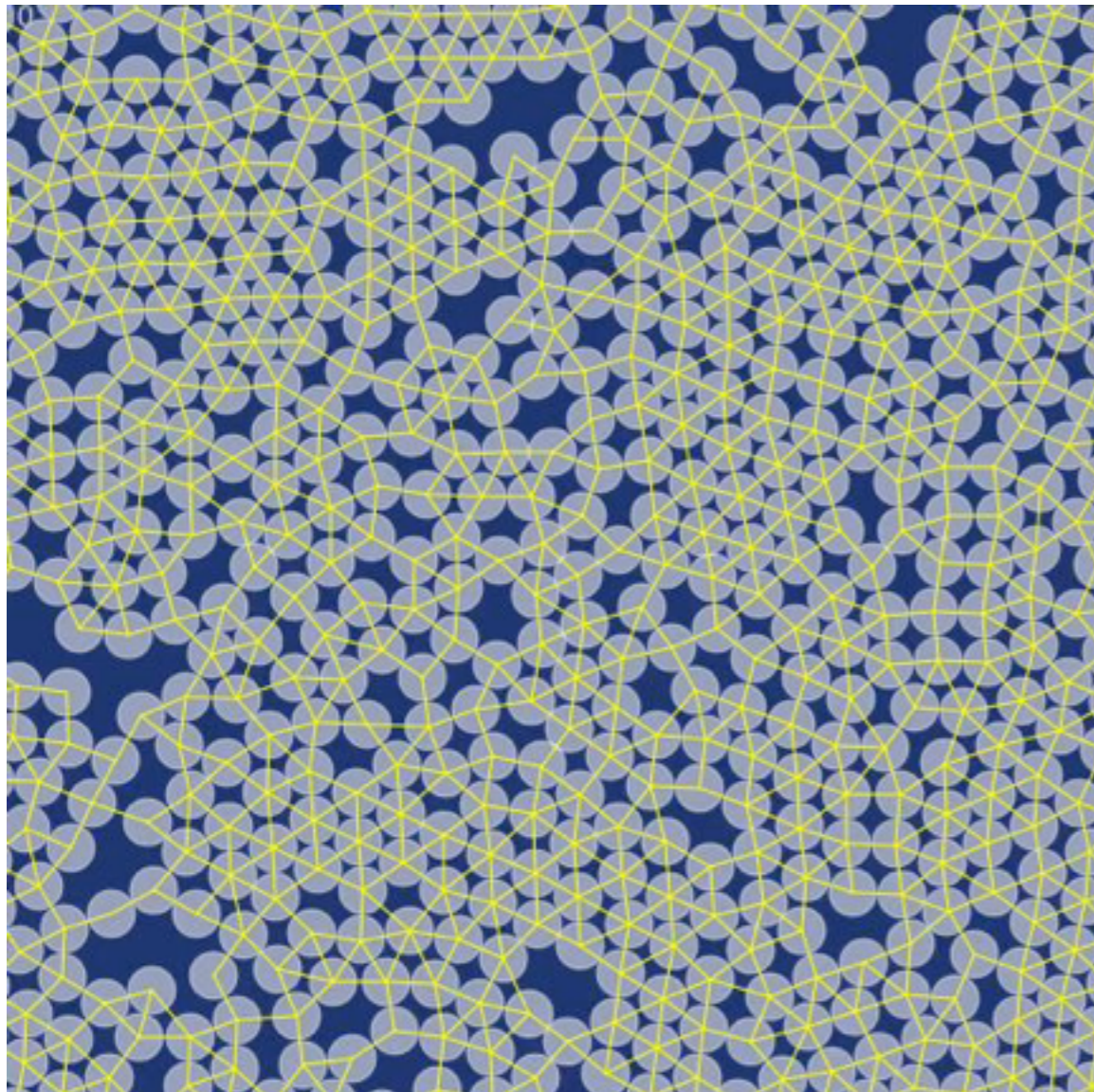
$\dot{\epsilon} / \dot{\epsilon}_0 = 0.02$



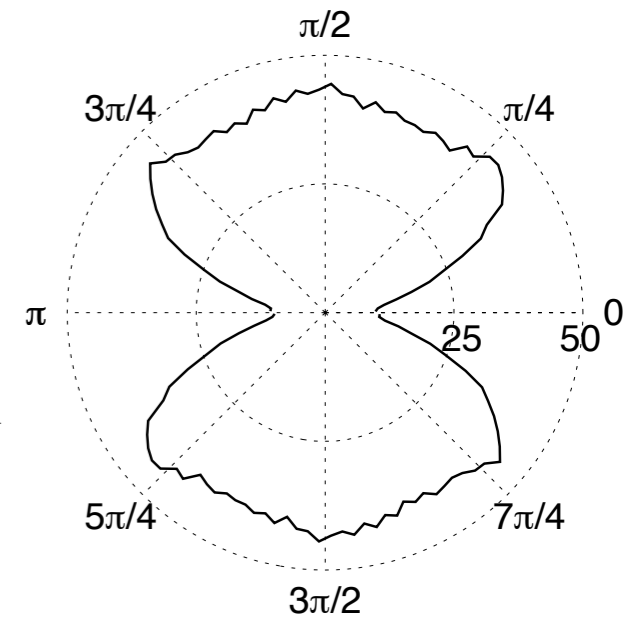
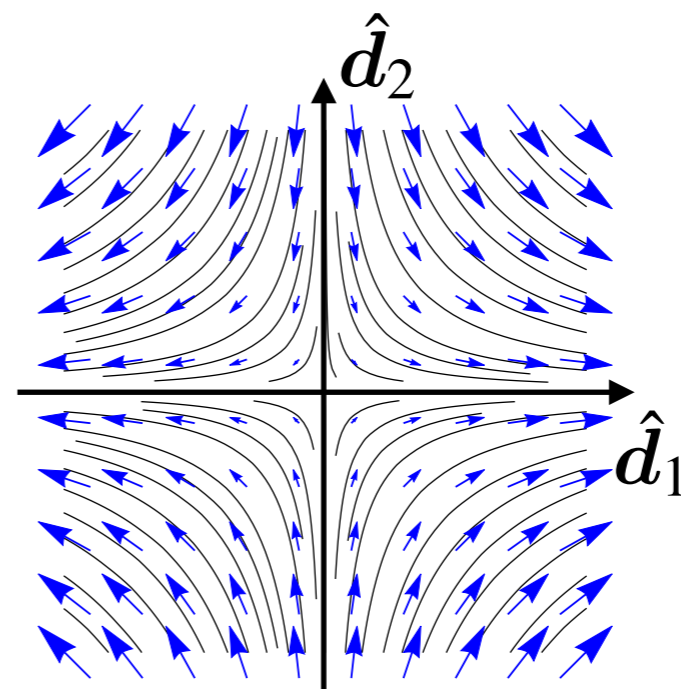
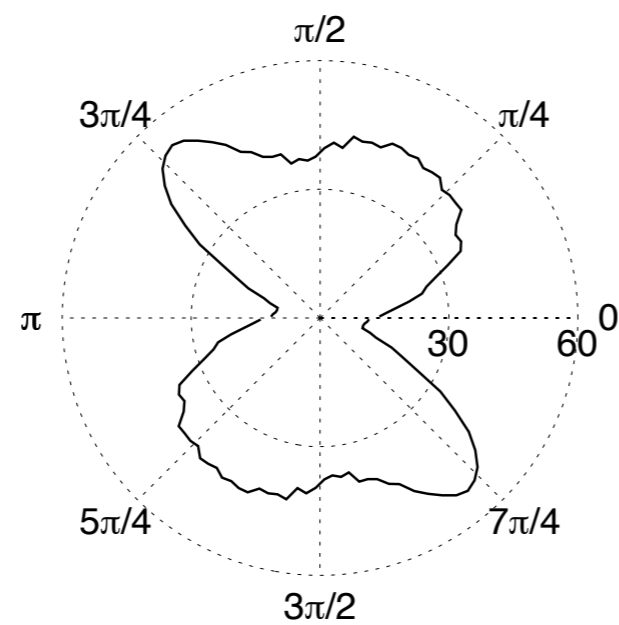
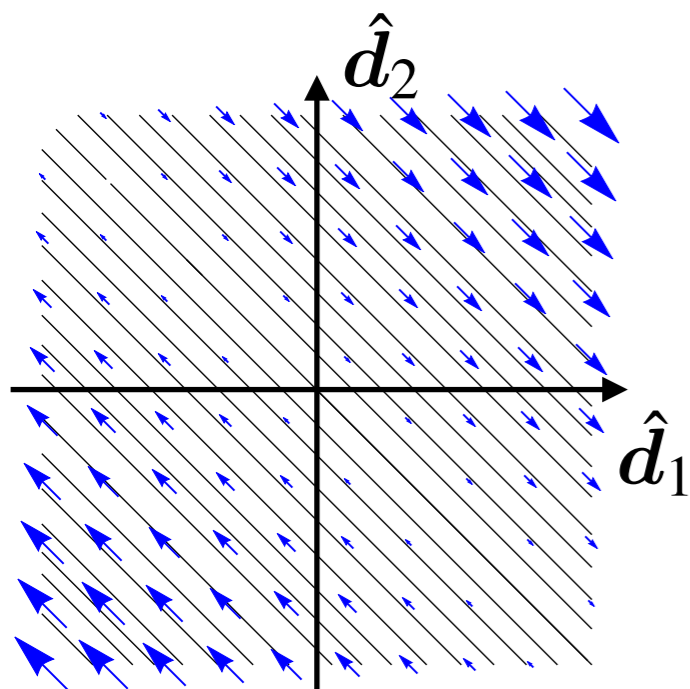
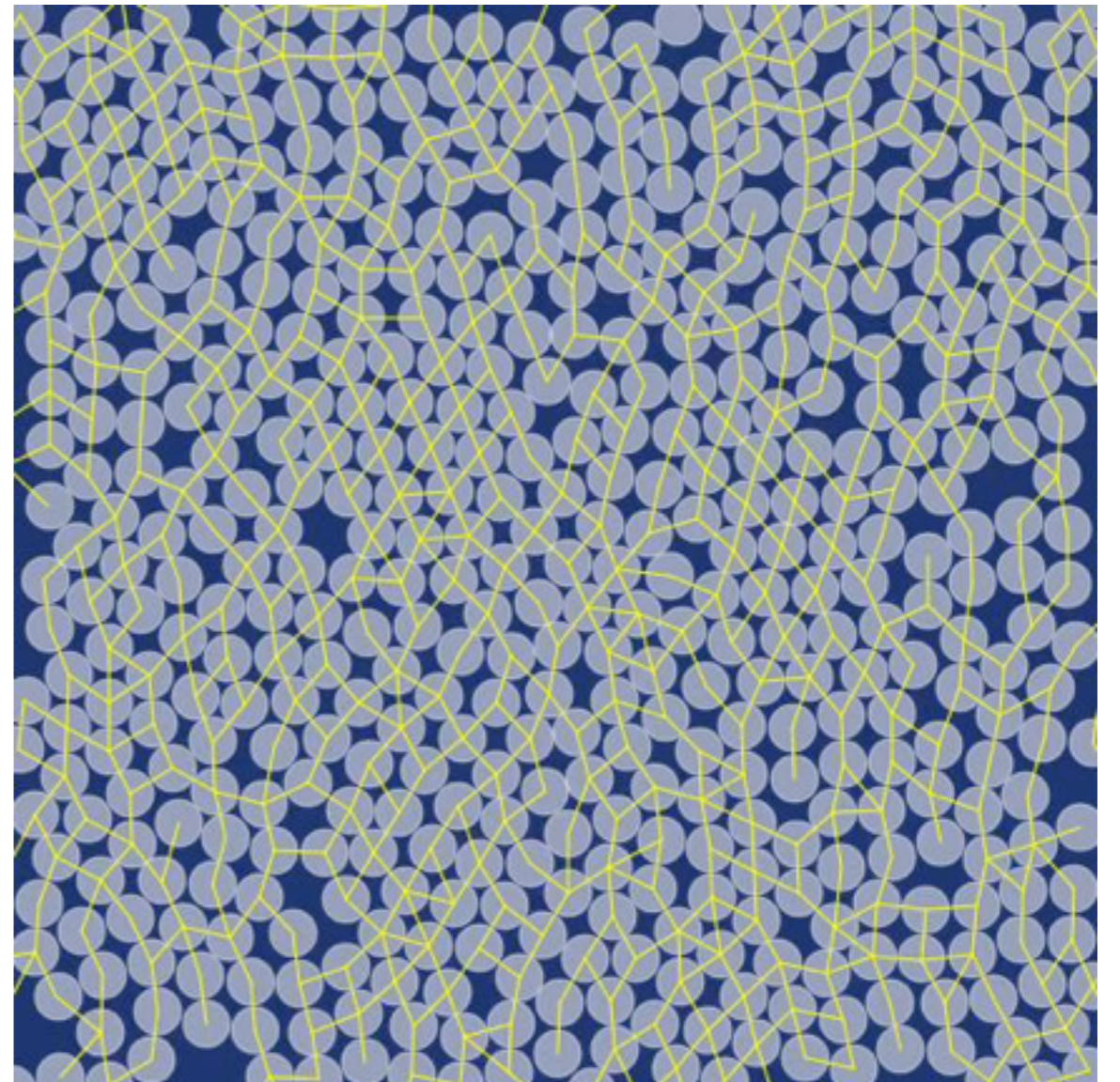
$\dot{\epsilon} / \dot{\epsilon}_0 = 0.01$



$$\beta_3 = 1$$



$$\beta_3 = 0$$



# If ordering is suppressed, flow type dependence is subtle

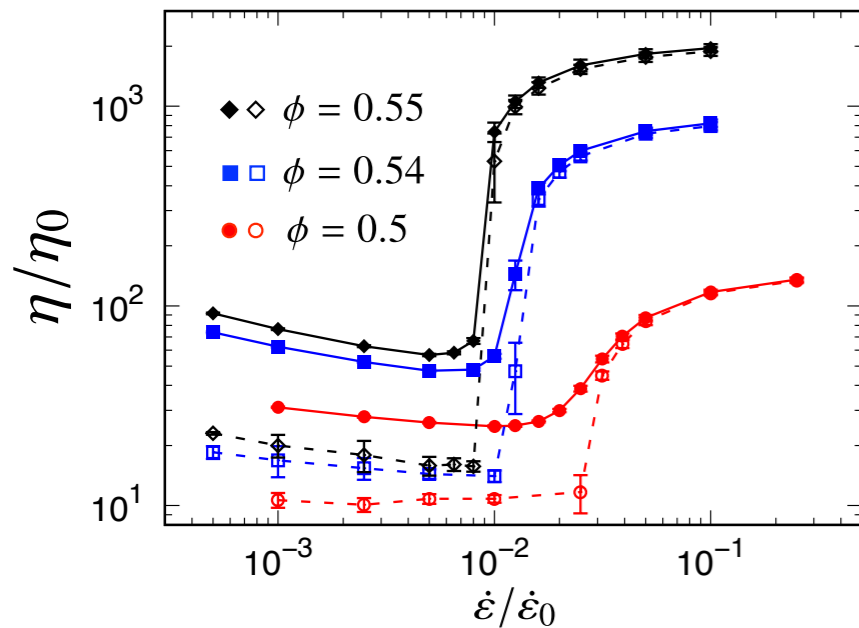
— extensional

$\beta_3 = 0$

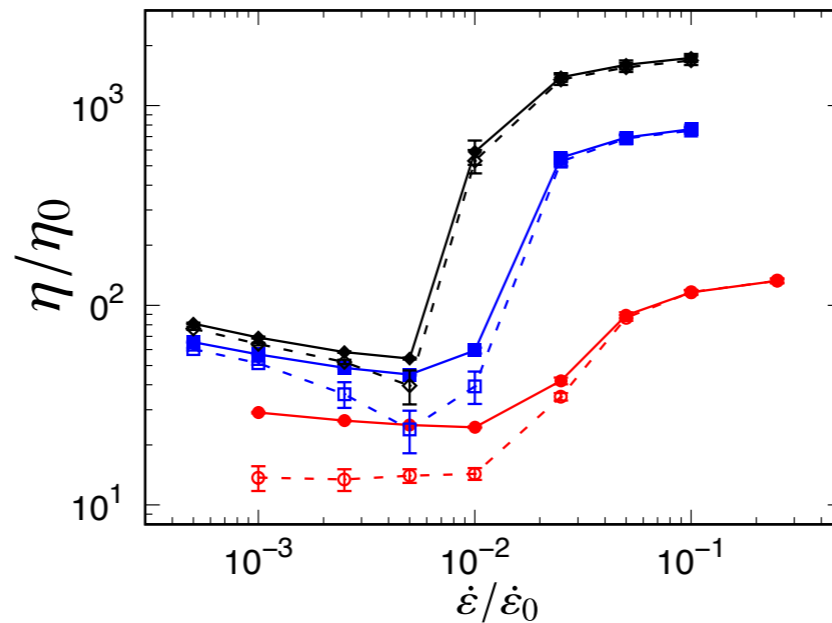
- - - simple shear

$\beta_3 = 1$

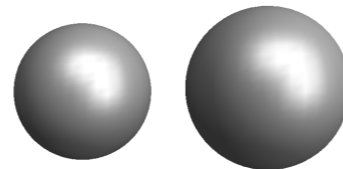
monodisperse



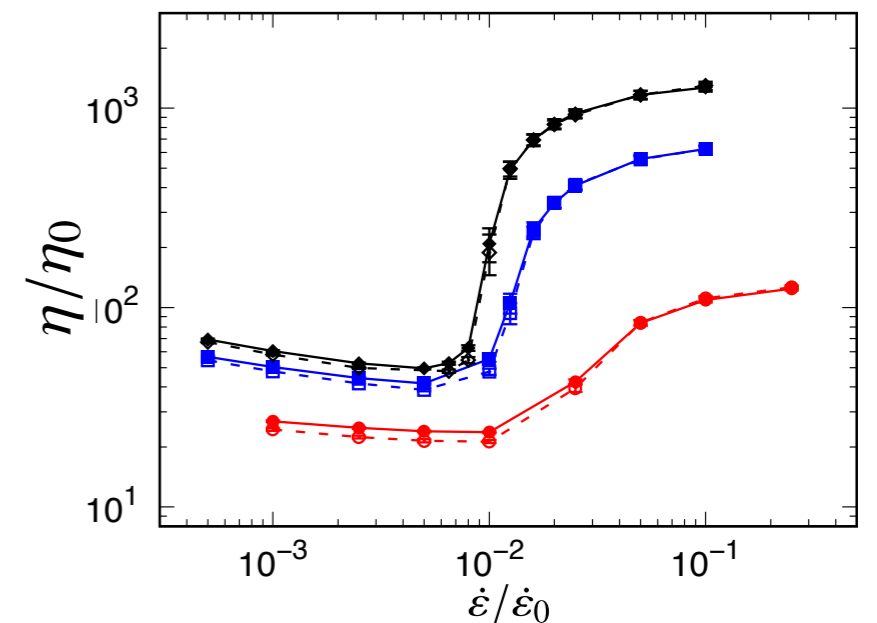
bidisperse



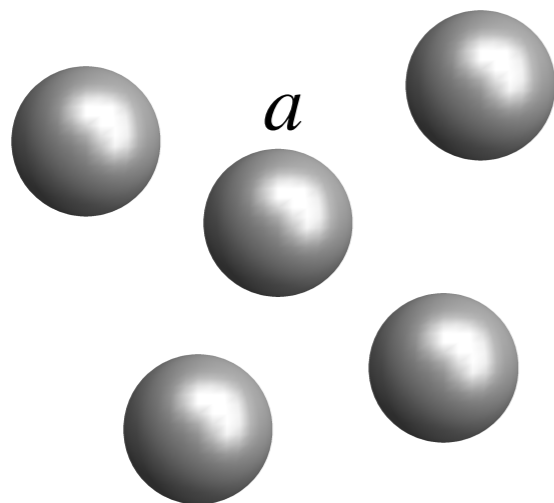
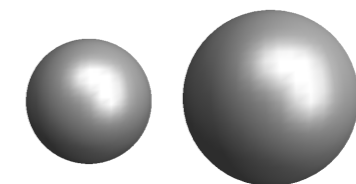
$$\frac{a_2}{a_1} = 1.2$$



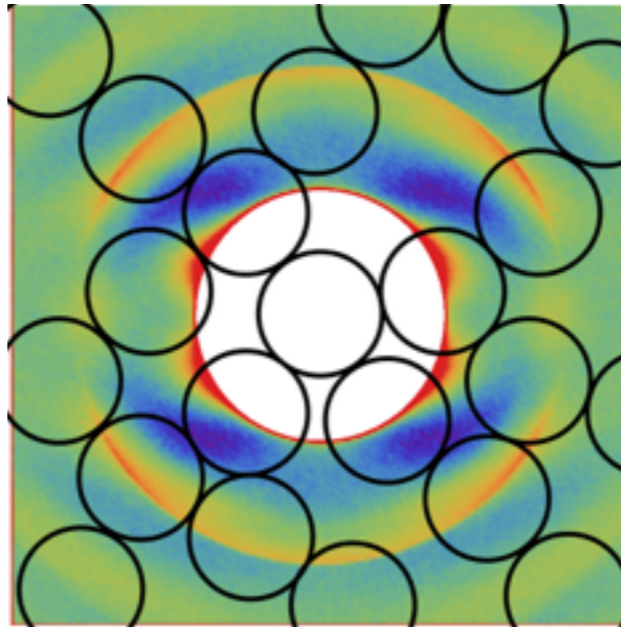
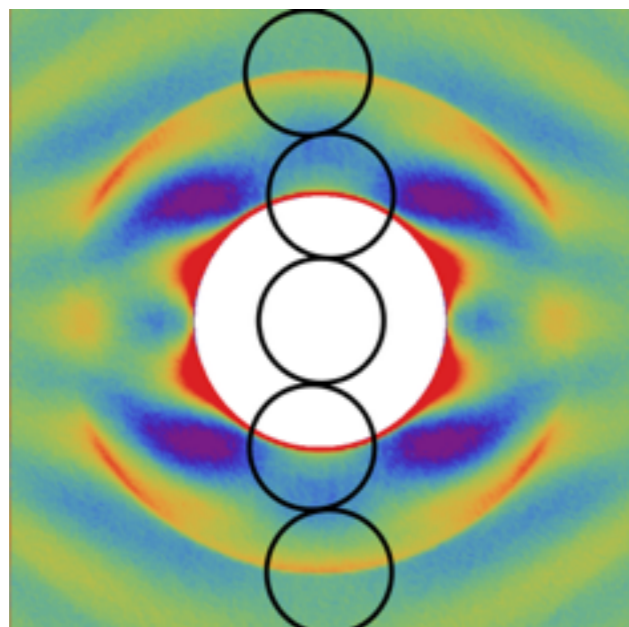
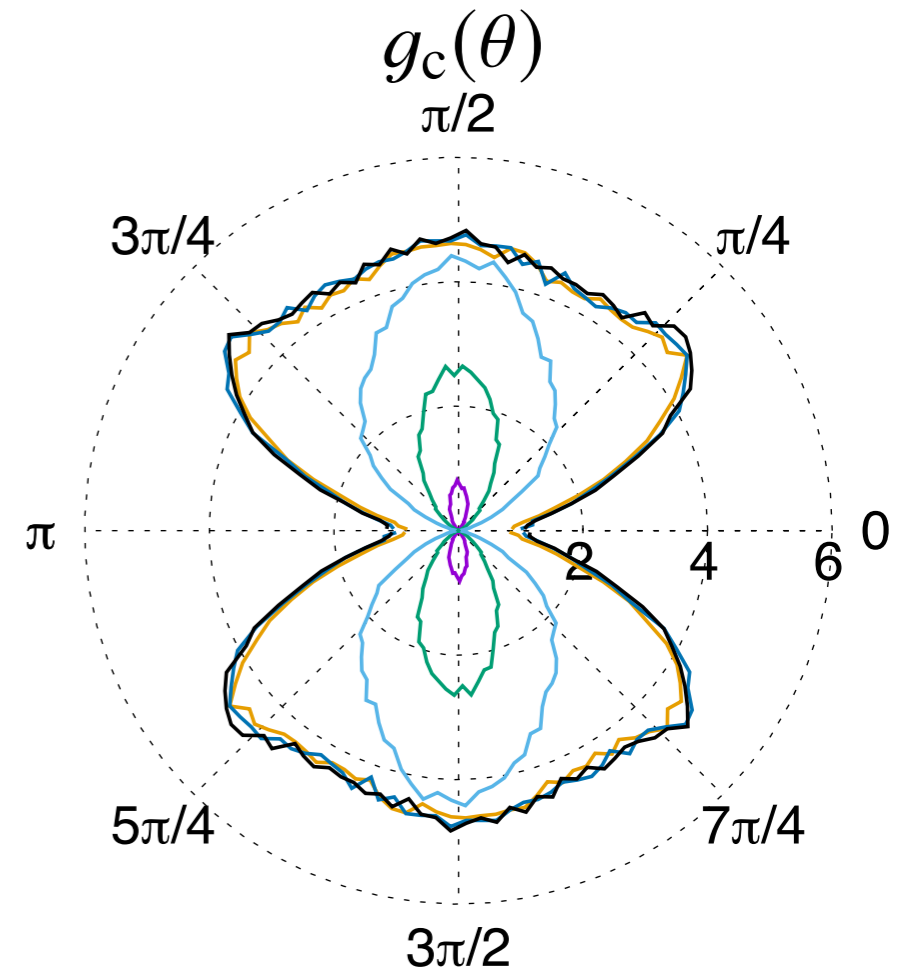
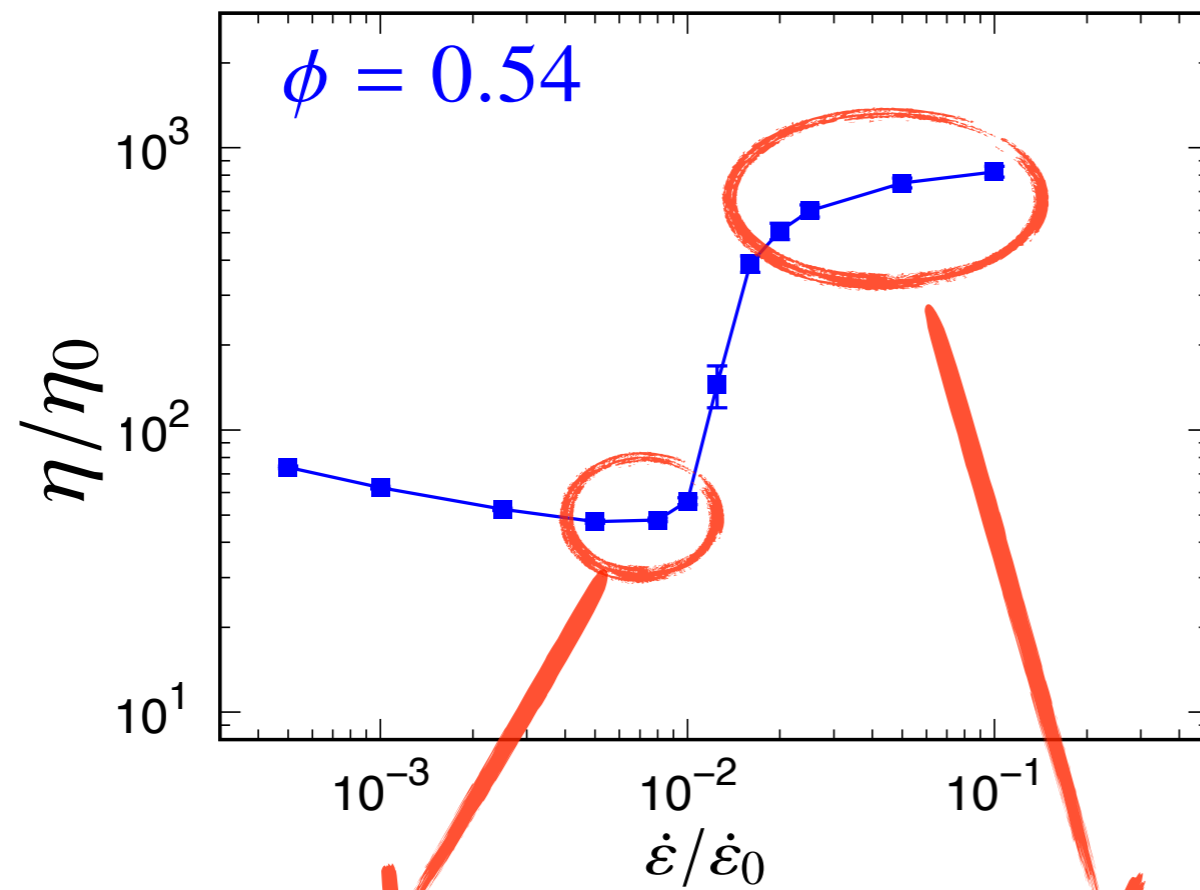
bidisperse



$$\frac{a_2}{a_1} = 1.4$$



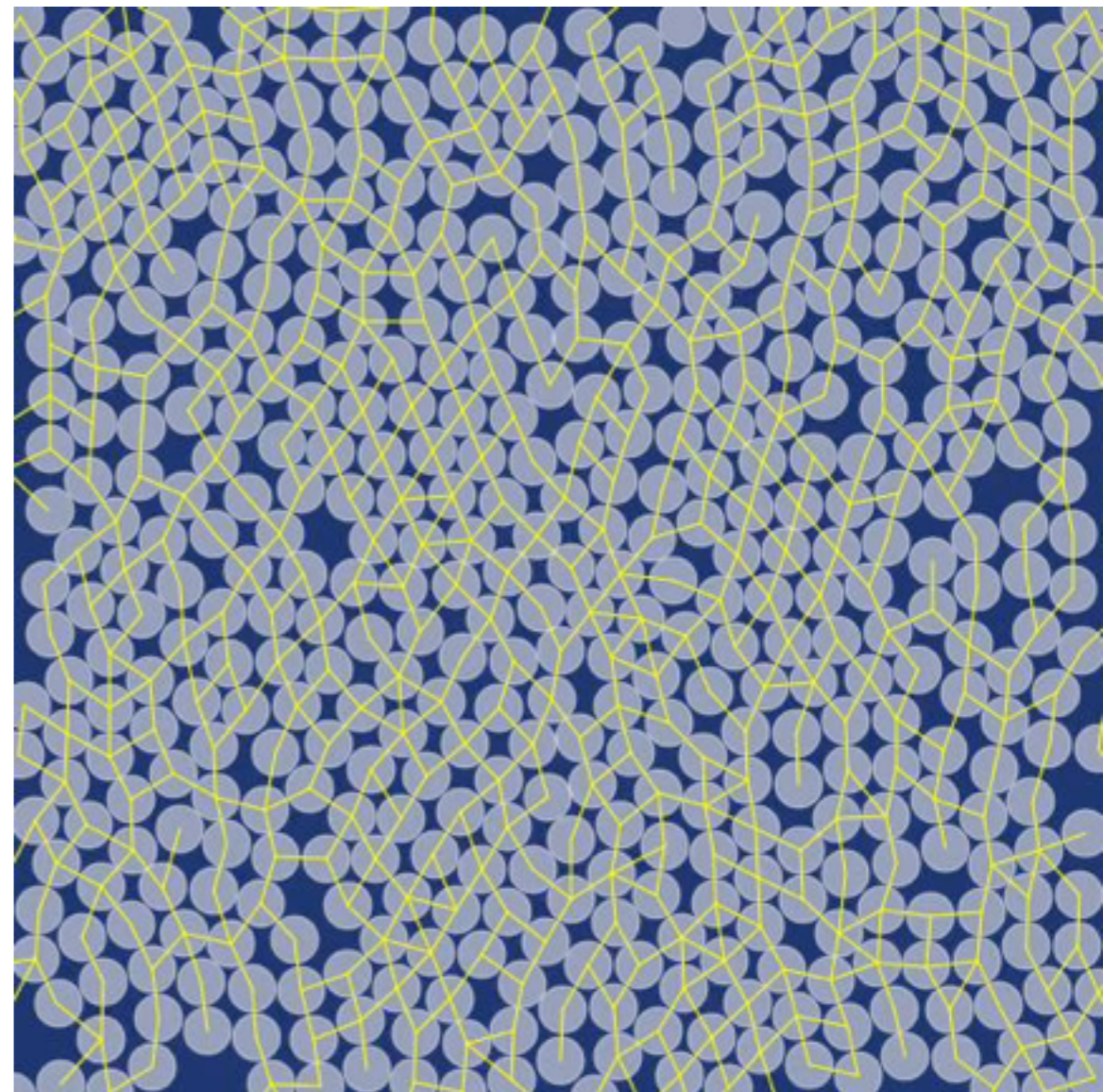
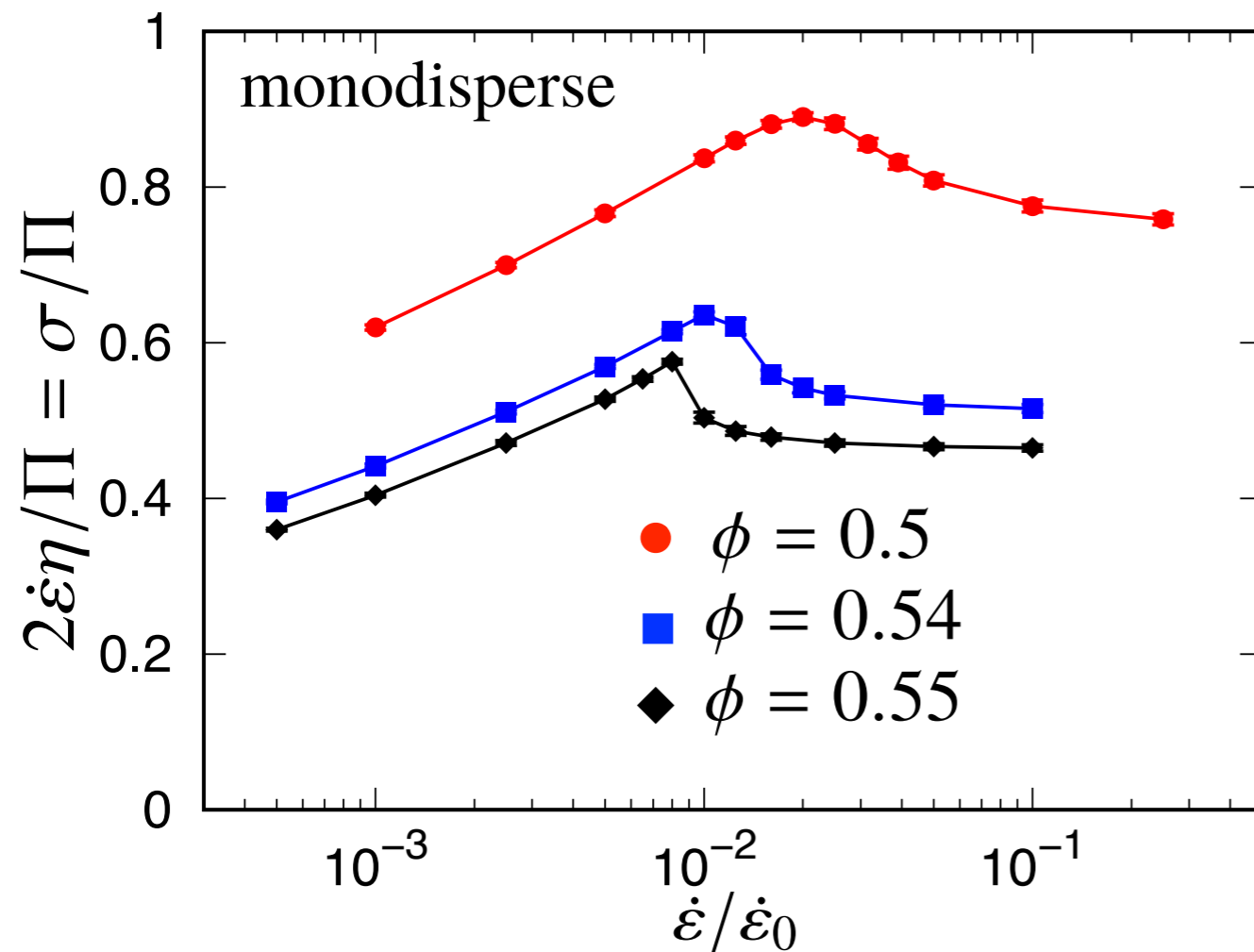
# Angular distributions for frictional contacts



# Particle pressure

$$\boldsymbol{\sigma} = -\Pi(\dot{\boldsymbol{\varepsilon}}, \beta_3)\mathbf{I} + 2\eta(\dot{\boldsymbol{\varepsilon}}, \beta_3)\mathbf{D} + 2\lambda_0(\dot{\boldsymbol{\varepsilon}}, \beta_3)\mathbf{E} + 2\lambda_3(\dot{\boldsymbol{\varepsilon}}, \beta_3)\mathbf{G}_3$$

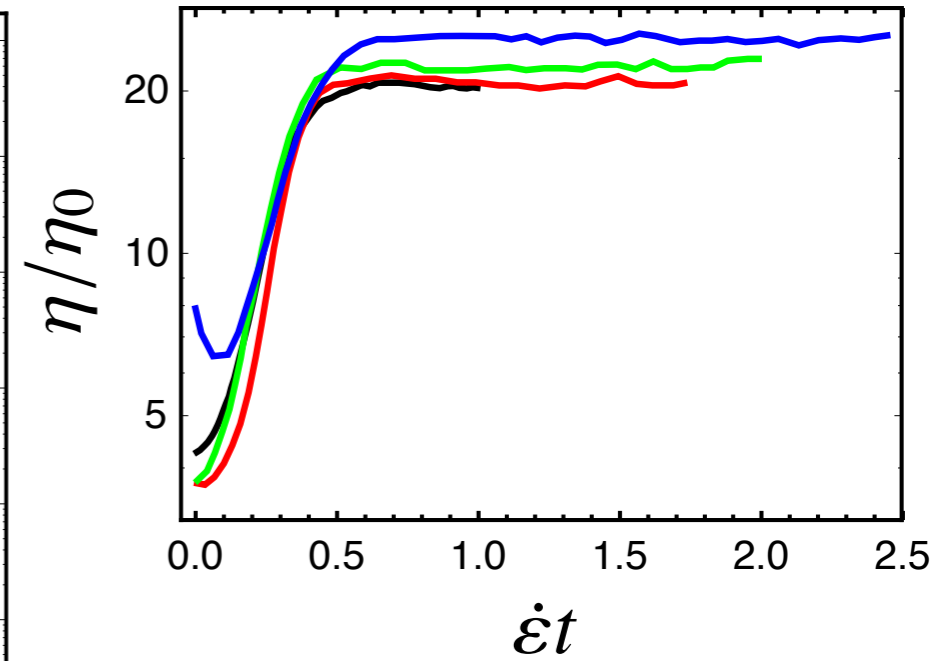
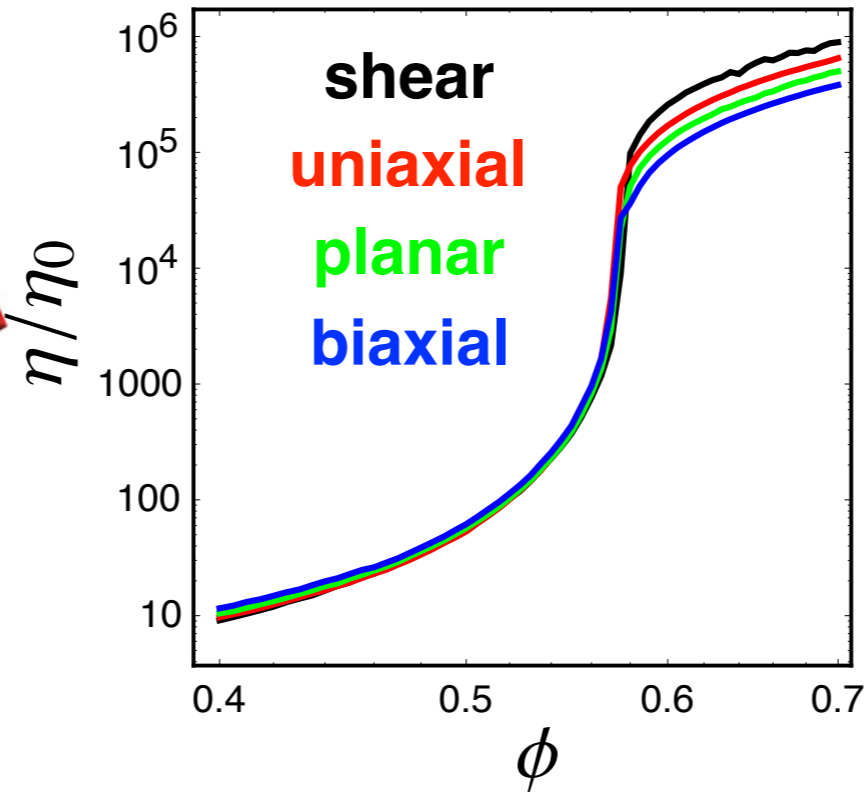
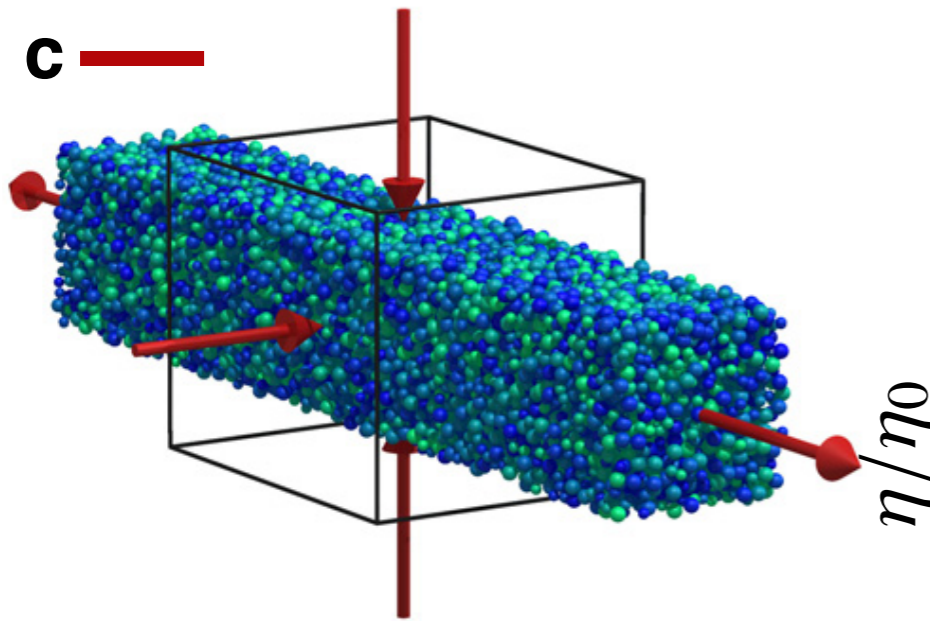
$$\Pi = -\frac{\boldsymbol{\sigma} : \mathbf{I}}{\mathbf{I} : \mathbf{I}} = -\frac{\text{Tr } \boldsymbol{\sigma}}{3}$$



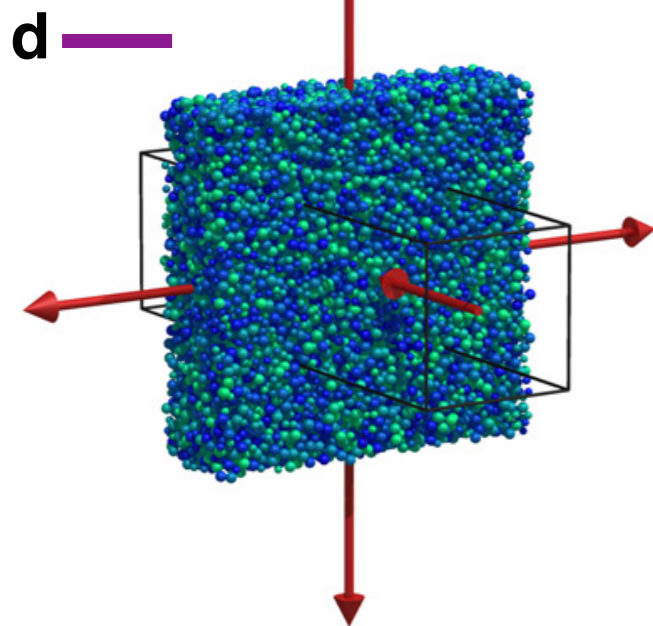
# Uniaxial, planar, and biaxial extensional flows

Cheal & Ness (JOR 2018)

In our representation for the data from C. Ness



$$\dot{\epsilon} \equiv \sqrt{\mathbf{D} : \mathbf{D} / 2}$$



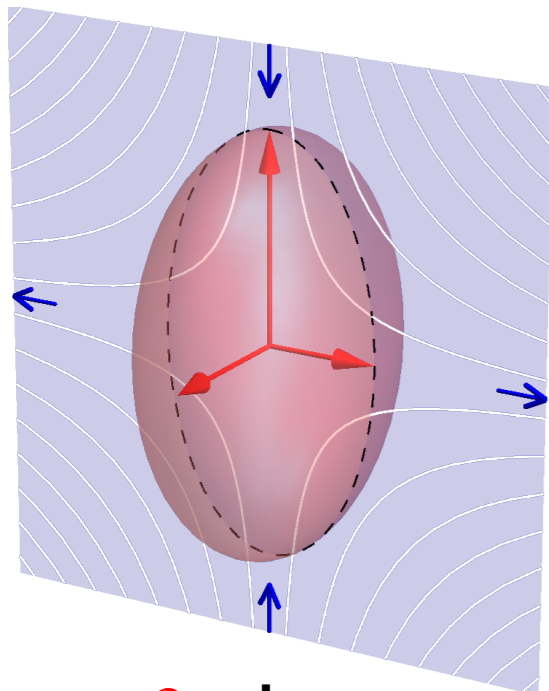
$$\mathbf{D} = \frac{2\dot{\epsilon}}{\sqrt{3 + 4\alpha^2}} \left[ \hat{d}_1 \hat{d}_1 - (1/2 + \alpha) \hat{d}_2 \hat{d}_2 - (1/2 - \alpha) \hat{d}_3 \hat{d}_3 \right]$$

$$\eta(\dot{\epsilon}, \alpha) \equiv \frac{1}{2} \frac{\boldsymbol{\sigma} : \mathbf{D}}{\mathbf{D} : \mathbf{D}}$$

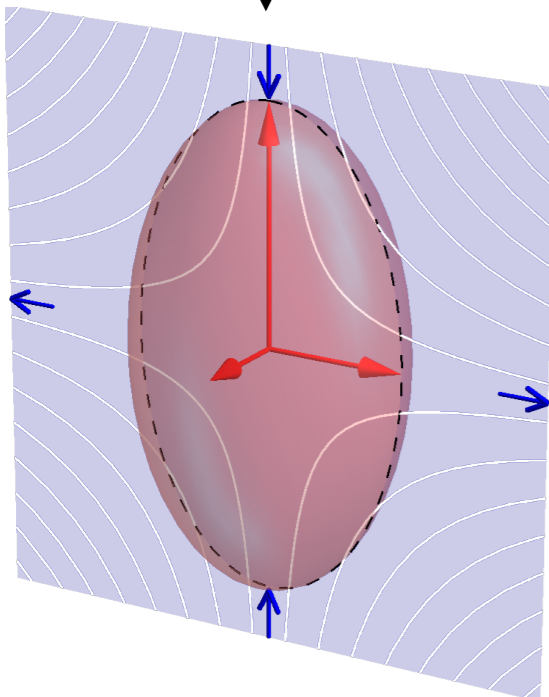
- $\alpha = 0$  &  $\dot{\epsilon} > 0 \rightarrow$  uniaxial
- $\alpha = 0$  &  $\dot{\epsilon} < 0 \rightarrow$  biaxial
- $\alpha = 1/2 \rightarrow$  planar

# The material function $\lambda_0$

$$\lambda_0(\dot{\epsilon}, \beta_3) = \frac{\sigma : \mathbf{E}}{2\mathbf{E} : \mathbf{E}} \longrightarrow \text{ellipsoidal factor} \quad \frac{2\dot{\epsilon}\lambda_0}{p}$$

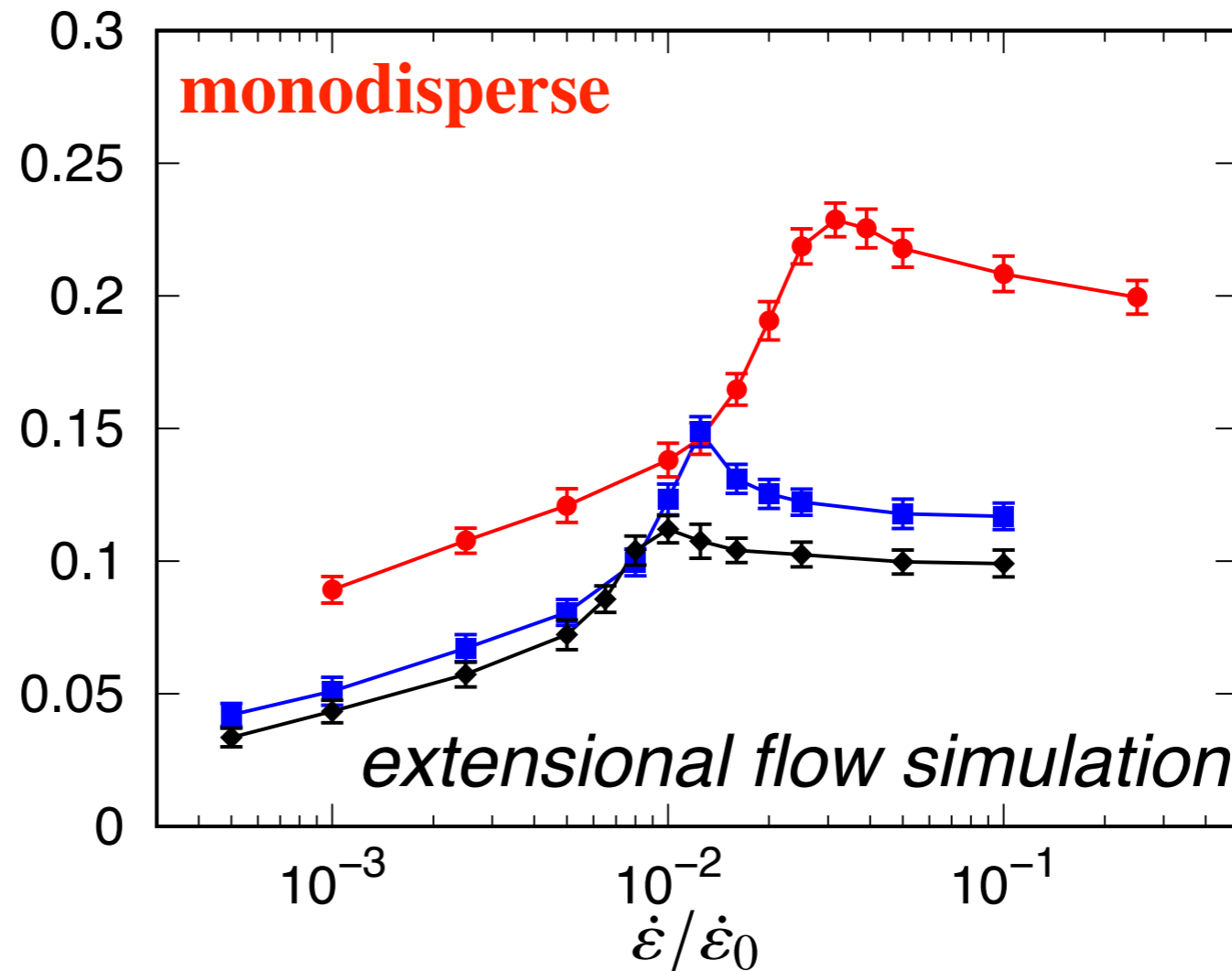


$\lambda_0$



$$\frac{2\dot{\epsilon}\lambda_0}{p}$$

$$\begin{cases} p_{\text{in}} \equiv p + \frac{1}{2}\dot{\epsilon}\lambda_0 \\ p_{\text{out}} \equiv p - \dot{\epsilon}\lambda_0 \end{cases}$$



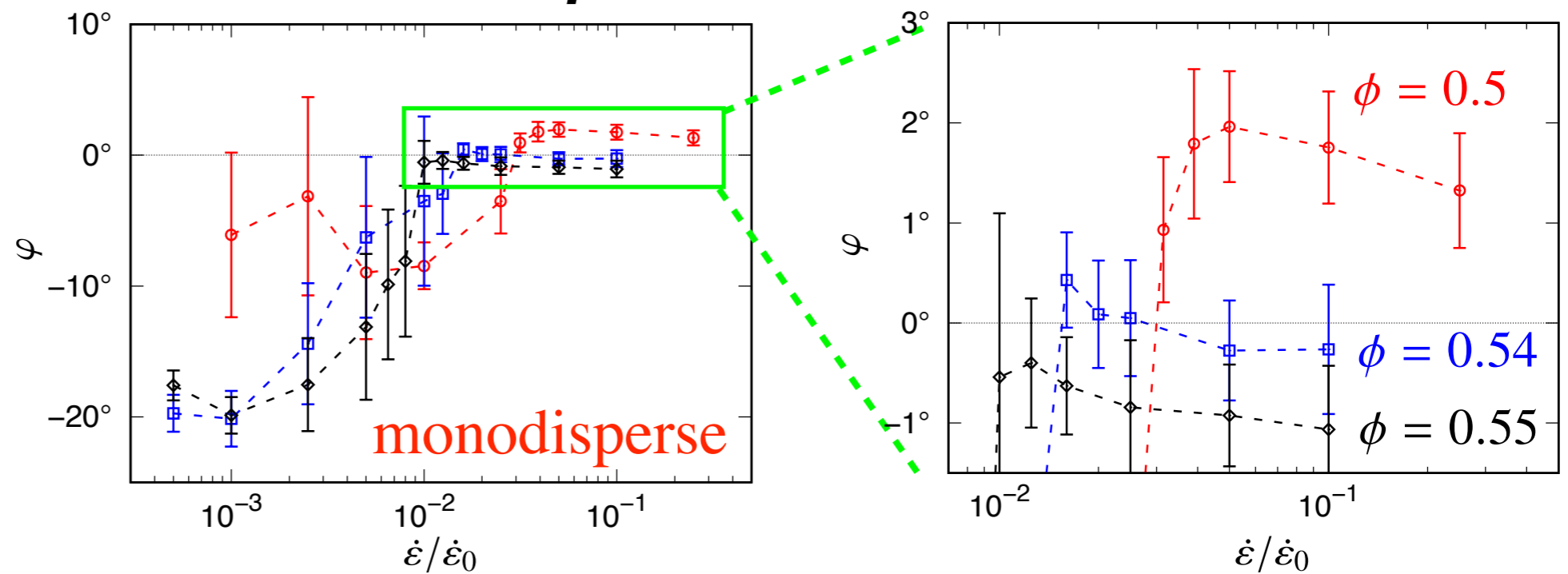
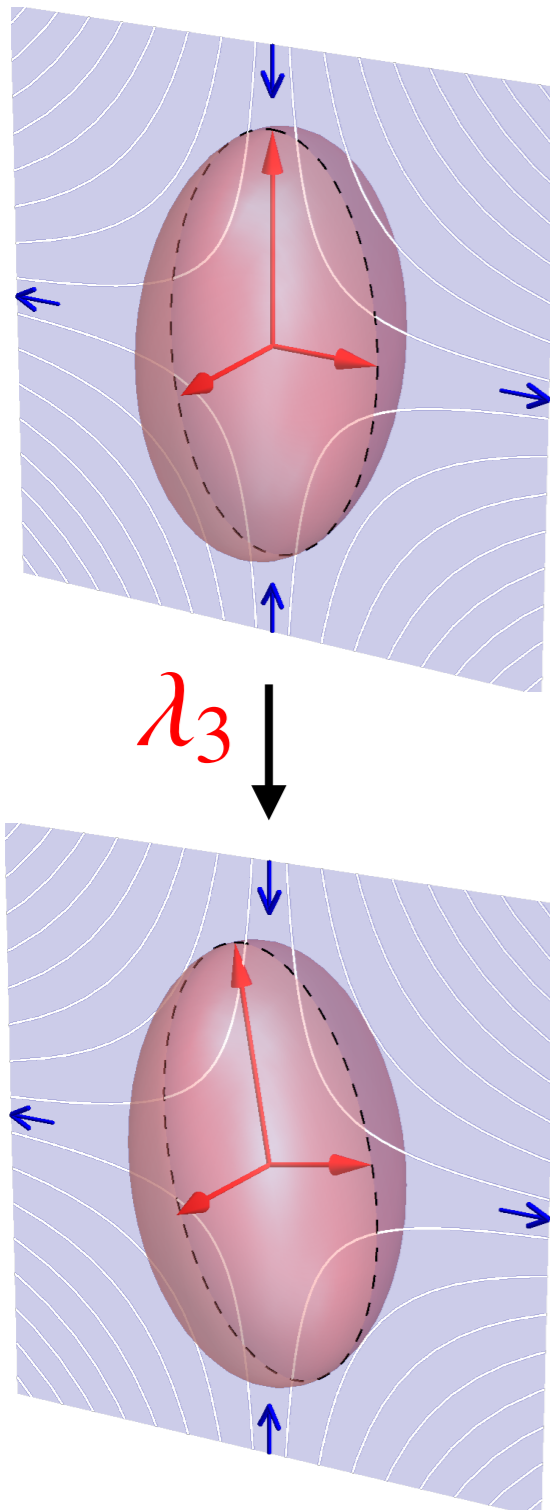
- $\phi = 0.5$
- $\phi = 0.54$
- ◆  $\phi = 0.55$

# The material function $\lambda_3$

$$\lambda_3(\dot{\epsilon}, \beta_3) = \frac{\sigma : \mathbf{G}_3}{2\mathbf{G}_3 : \mathbf{G}_3} \rightarrow \text{reorientation factor} \quad \frac{\lambda_3}{2\eta}$$

$$\tan \theta \equiv \frac{\lambda_3}{\eta + \sqrt{\eta^2 + \lambda_3^2}} \approx \frac{\lambda_3}{2\eta}$$

**simple-shear simulation**



$$N_1 = -2\dot{\epsilon}\lambda_3$$

$$\tan \theta = \frac{-N_1/2\sigma}{1 + \sqrt{1 + (N_1/2\sigma)^2}} \approx -\frac{N_1}{4\sigma} \quad \sigma: \text{shear stress}$$



# Outline

1. Periodic boundary conditions
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3. Material functions
4.  $N_1$  issue
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*We are ready  
to tackle macroscopic flow problems  
of dense suspensions!*