Complex flows of complex fluids

Suzanne Fielding
Department of Physics, Durham University

Outline

A) Rheology of complex fluids

1) overview
2) continuum models
3) 0D → 1D → 2D: a study in bulk flow instabilities

B) Hydrodynamics of active fluids

1) overview
2) continuum models
3) 0D → 1D → 2D: a study in bulk flow instabilities

C) Interlude - numerical methods

D) Surface instabilities in complex fluids

1) extensional necking
2) edge fracture
3) wall slip

Outline

A) Rheology of complex fluids

1) overview

2) continuum models

3) 0D rheology – flow curves

↓ unstable

1D rheology – shear banding

↓ unstable

2D rheology – instability of interface between bands

Outline

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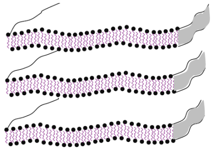
1) Rheology of complex fluids: overview

Surfactants

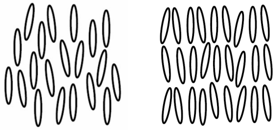
cell membranes, drug delivery



self-assembled micelles/membranes

Liquid crystals

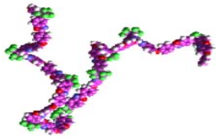
displays, viruses, cartilage



rodlike molecules

Polymers

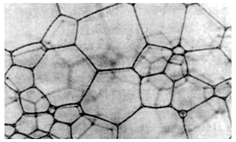
plastics, DNA, drag reduction



chainlike molecules

Foams, emulsions

fire-fighting, foods



cellular bubble packing

Colloids

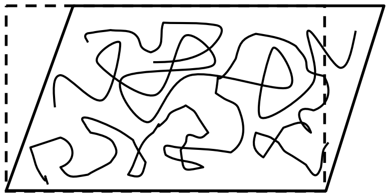
clays, inks, blood

fractal aggregates

Unifying feature: mesoscopic internal substructures – rods, chains, *etc.* – nm to μm

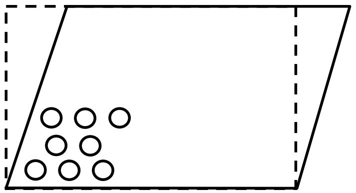
Mesostructures confer unique material properties

a) Softness under shear



soft matter

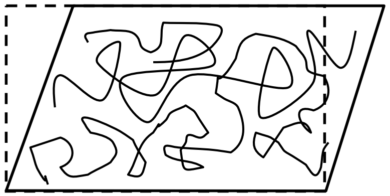
easily deformed
polymer chains



compare hard matter

Mesostructures confer unique material properties

a) Softness under shear



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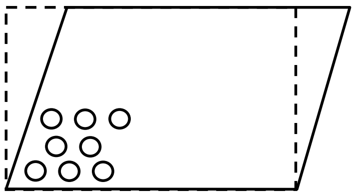


compare hard matter

b) Viscoelasticity

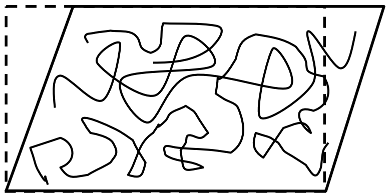
c) Easily driven into nonlinear flow states

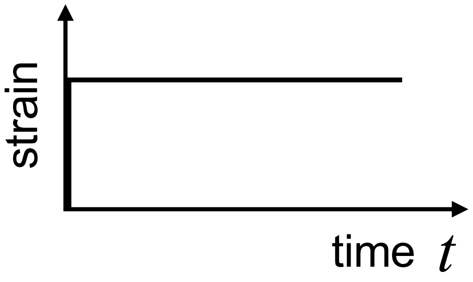
d) Show non-zero ‘normal stress differences’

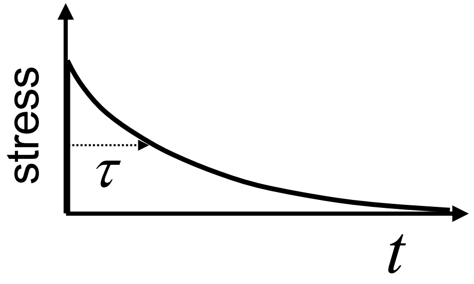
e) Display flow-induced transitions

b) Viscoelasticity

Stress relaxation after small step shear strain

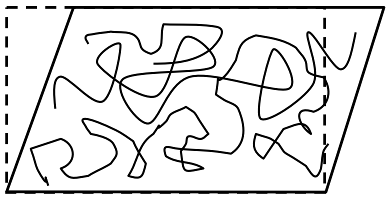


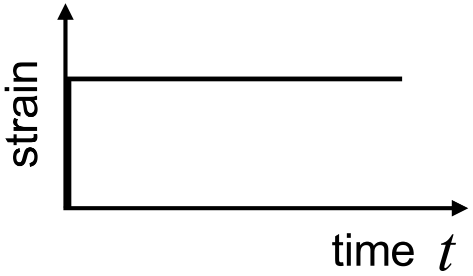


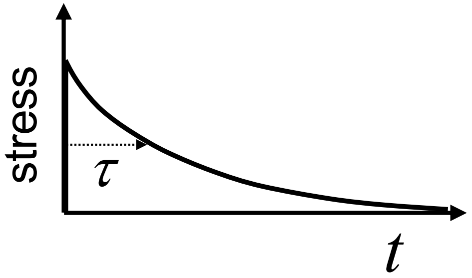


b) Viscoelasticity

Stress relaxation after small step shear strain

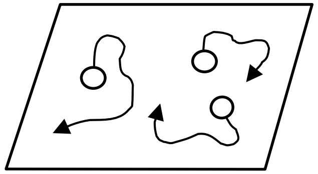




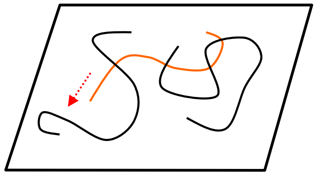


tiny — 10^{-3} to 10^{3} s — huge → relaxation time τ

simple fluids

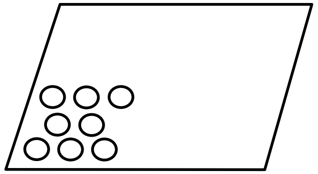


COMPLEX FLUIDS



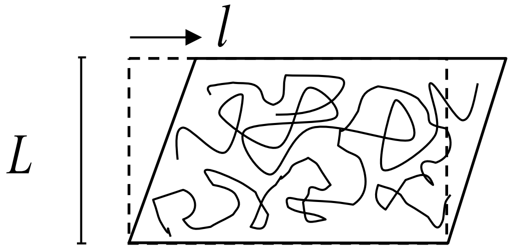
sluggish relaxation

elastic solid



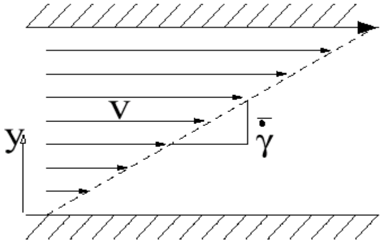
c) Easily driven into nonlinear flow regimes

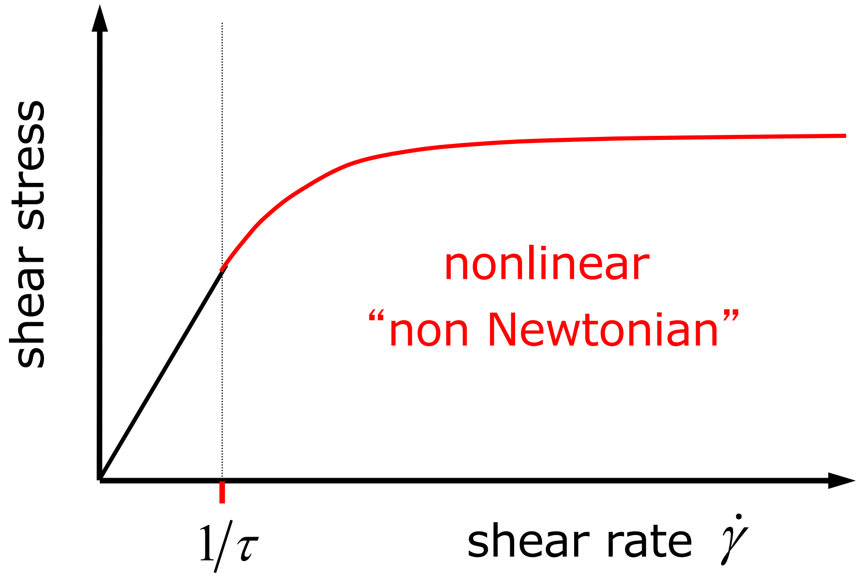
Stress response to steady applied shear flow



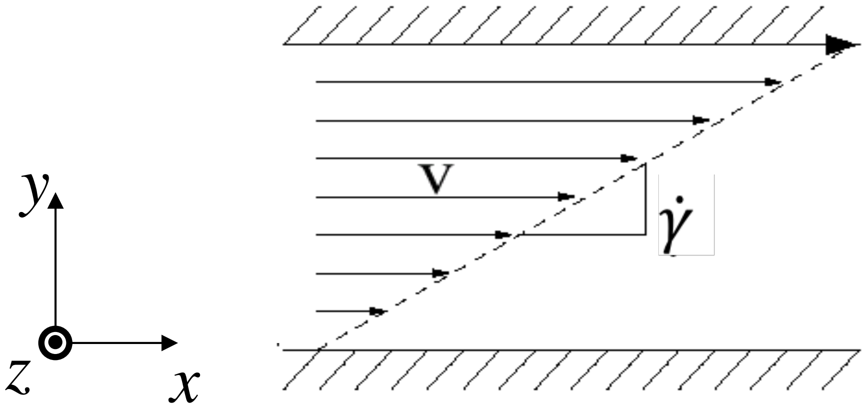
shear at constant

rate $\dot{\gamma} \equiv \frac{1}{L}\partial_t l$





d) Non-zero normal stress differences



x: flow direction

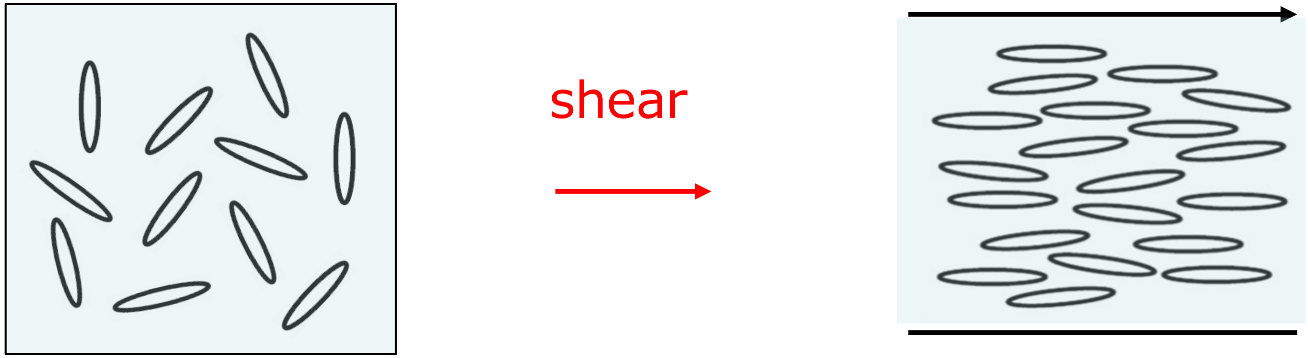
y: flow gradient direction

z: vorticity direction

shear stress	$\Sigma_{xy}(\dot{\gamma})$
first normal stress difference	$\Sigma_{xx}(\dot{\gamma}) - \Sigma_{yy}(\dot{\gamma}) = N_1(\dot{\gamma})$
second normal stress difference	$\Sigma_{yy}(\dot{\gamma}) - \Sigma_{zz}(\dot{\gamma}) = N_2(\dot{\gamma})$

e) Display non-equilibrium, flow-induced transitions and instabilities

Example: liquid crystalline phase behaviour



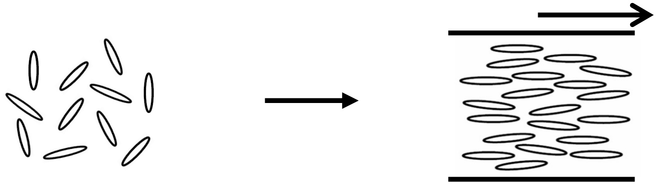
shear

isotropic

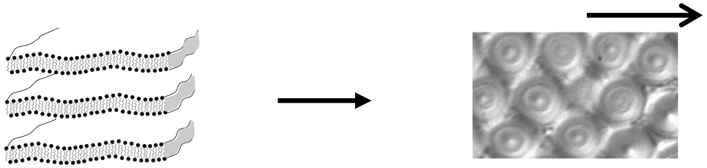
nematic

e) Display non-equilibrium, flow-induced transitions and instabilities

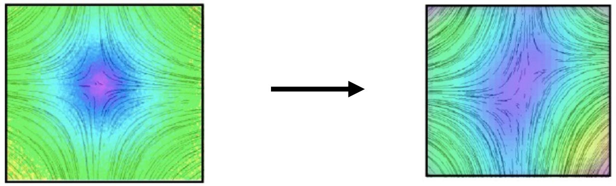
Liquid crystal



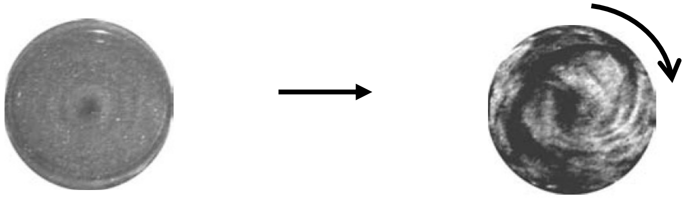
Surfactant onion phase



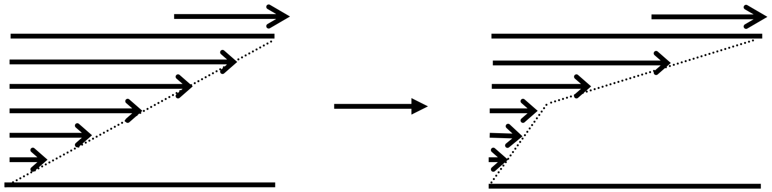
Cross slot instability



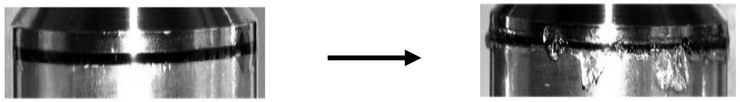
Viscoelastic turbulence



Shear banding



Edge fracture



Outline

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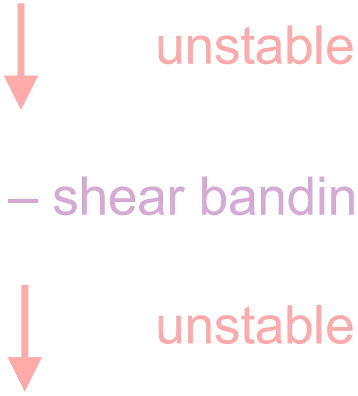
1) overview

2) continuum models

3) 0D rheology – flow curves



unstable

1D rheology – shear banding

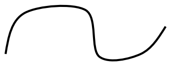
unstable

2D rheology – instability of interface between bands

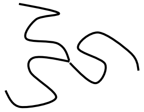
Modelling complex fluids – the basic philosophy

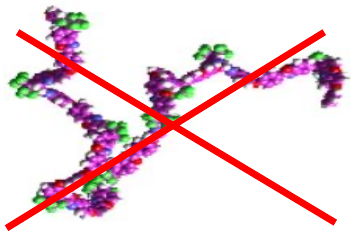
Macroscopic properties depend on dynamics at coarse-grained level of chains, rods

e.g. viscosity universally $\propto \left(\text{chain length}\right)^{3.4}$ linear polymers



$\propto \exp\left(\text{chain length}\right)$ star polymers





CHEMICAL DETAIL
NOT IMPORTANT

↑

a polymer molecule is a piece of string

So, concerned with (non-equilibrium) dynamics of chains, rods in flow

Modelling flow properties

Navier Stokes (+ incompressibility)

$$\underset{\substack{\uparrow\\ \text{inertial}}}{\rho\, D_t \mathbf{v}} = \underset{\substack{\uparrow\\ \text{viscous}}}{\eta\, \nabla^2 \mathbf{v}} - \underset{\substack{\uparrow\\ \text{pressure}}}{\nabla p}$$

viscosity η; density ρ

Modelling flow properties of complex fluids

Extended Navier Stokes (+ incompressibility)

$$\rho \underset{\substack{\uparrow\\ \text{inertial}}}{D_t}\mathbf{v} = \nabla\cdot\underset{\uparrow}{\sigma} + \eta\underset{\substack{\uparrow\\ \text{solvent}}}{\nabla^2}\mathbf{v} - \underset{\substack{\uparrow\\ \text{pressure}}}{\nabla p}$$

Viscoelastic stress σ due to internal mesoscopic substructures

Modelling flow properties of complex fluids

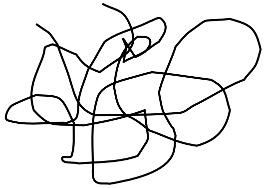
Extended Navier Stokes (+ incompressibility)

$$\underset{\substack{\uparrow\\\text{inertial}}}{\rho D_t \mathbf{v}} = \underset{\uparrow}{\nabla \cdot \sigma} + \underset{\substack{\uparrow\\\text{solvent}}}{\eta \nabla^2 \mathbf{v}} - \underset{\substack{\uparrow\\\text{pressure}}}{\nabla p}$$

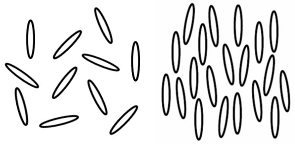
Viscoelastic stress $\sigma = \sigma(\mathbf{W})$

Generalised mesostructural variable(s), W

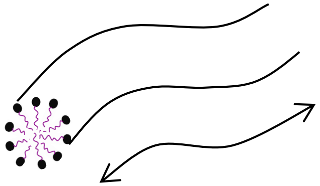
e.g. molecular strain



orientation tensor



micellar length



Modelling flow properties of complex fluids

Extended Navier Stokes (+ incompressibility)

$$\underset{\substack{\uparrow\\ \text{inertial}}}{\rho D_t \mathbf{v}} = \nabla \cdot \sigma + \underset{\substack{\uparrow\\ \text{solvent}}}{\eta \nabla^2 \mathbf{v}} - \underset{\substack{\uparrow\\ \text{pressure}}}{\nabla p}$$

Viscoelastic stress $\sigma = \sigma\left(\mathbf{W}\right)$

Equation of motion for mesostructure

$$D_t \mathbf{W} = \mathbf{N}\left(\nabla \mathbf{v}, \mathbf{W}\right)$$

Often: nonlinear PDE of
reaction-diffusion type

Modelling flow properties of complex fluids

Extended Stokes (+ incompressibility)

$$0 = \nabla \cdot \sigma + \eta \nabla^2 \mathbf{v} - \nabla p$$

inertia
free !

solvent

pressure

Viscoelastic stress

$$\sigma = \sigma\left(\mathbf{W}\right)$$

Equation of motion for mesostructure

$$D_t \mathbf{W} = \mathbf{N}\left(\nabla \mathbf{v}, \mathbf{W}\right)$$

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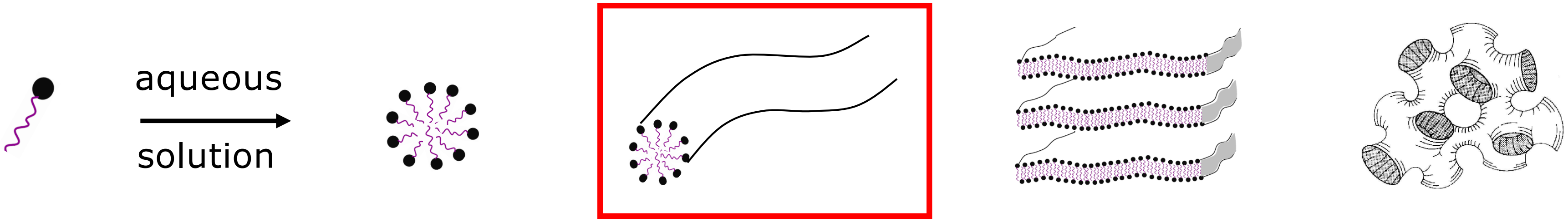
An example: wormlike micellar surfactant

Amphiphilic molecule  polar head likes water; non-polar tail hates water



aqueous

solution

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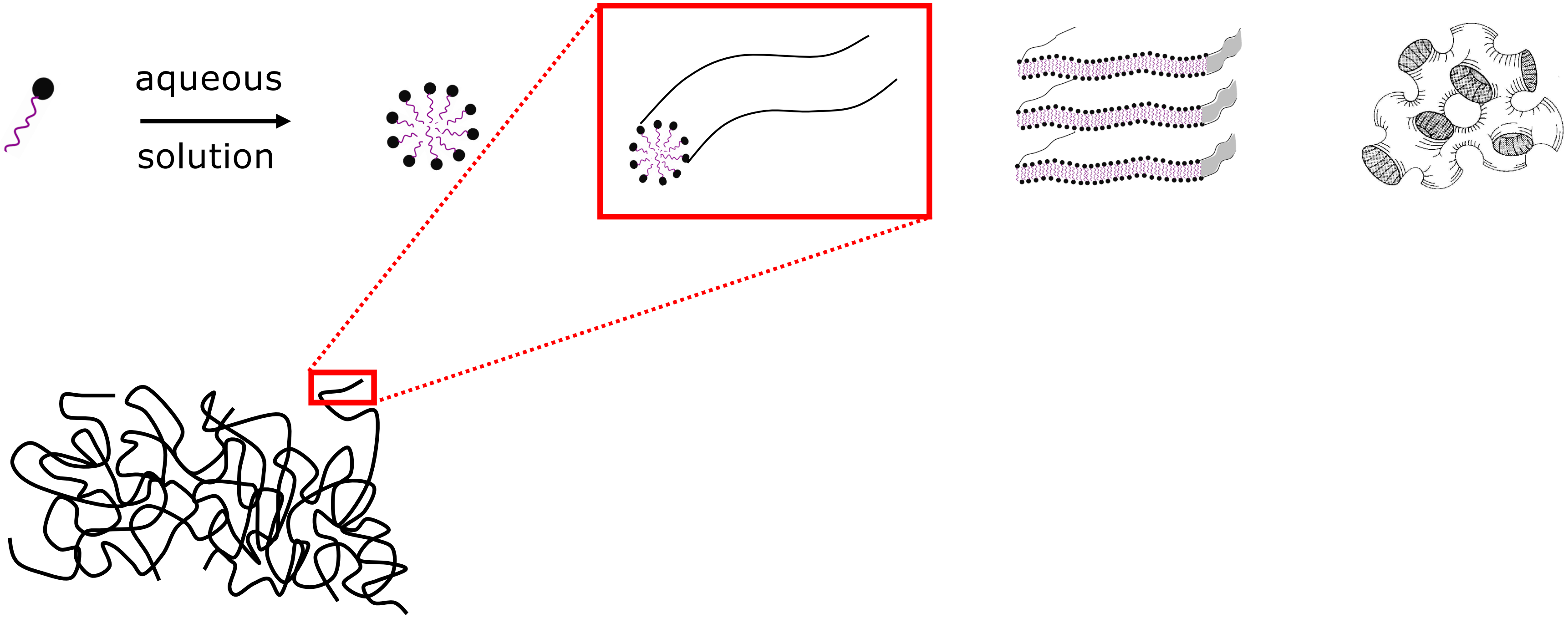

aqueous

solution

each worm constrained by
entanglements with others

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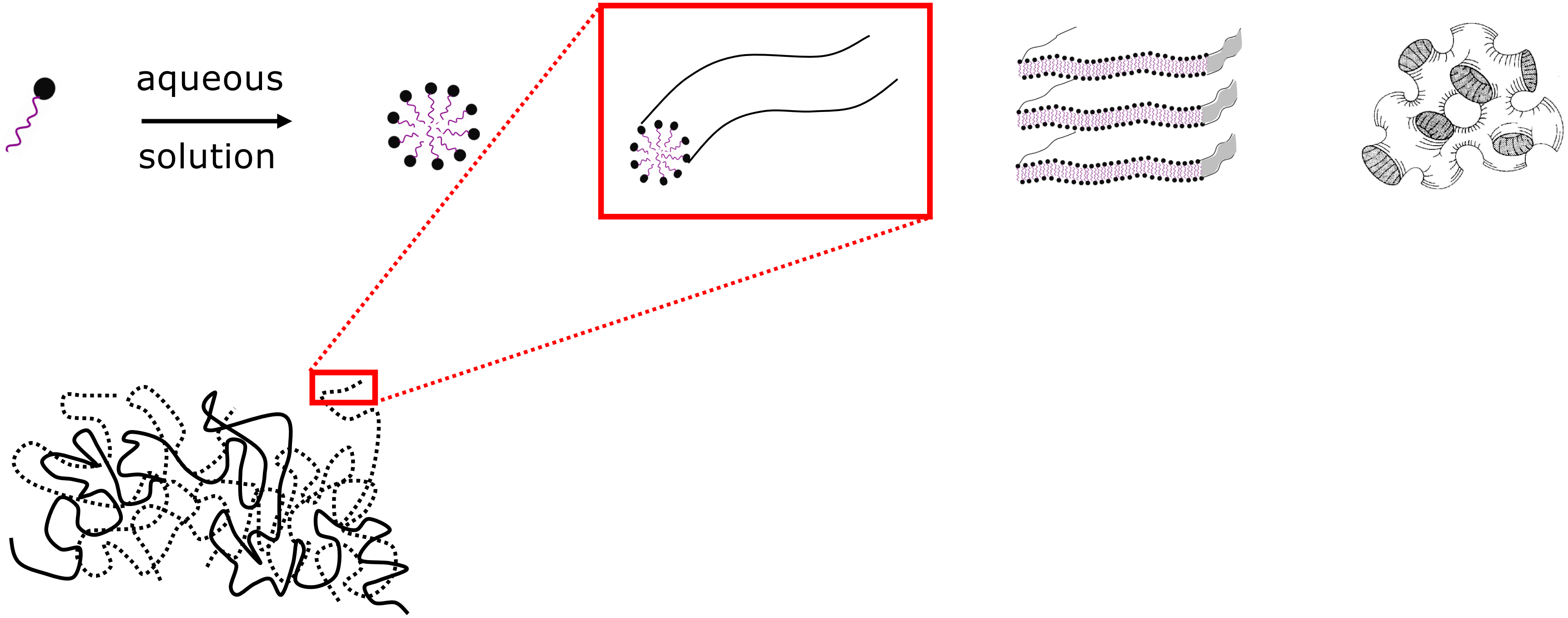

focus on single worm

An example: wormlike micellar surfactant

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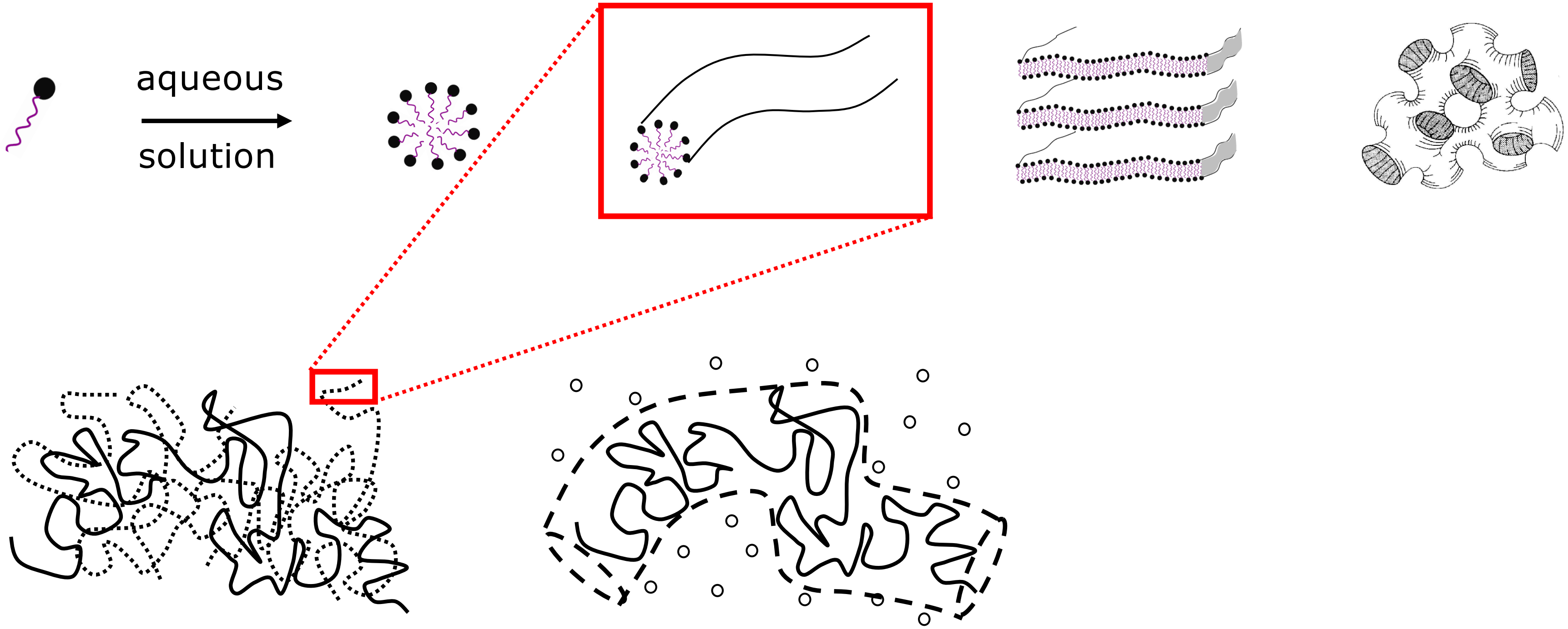

focus on single worm

“**tube**” of entanglements
constrains lateral motion

[Doi + Edwards 1986]

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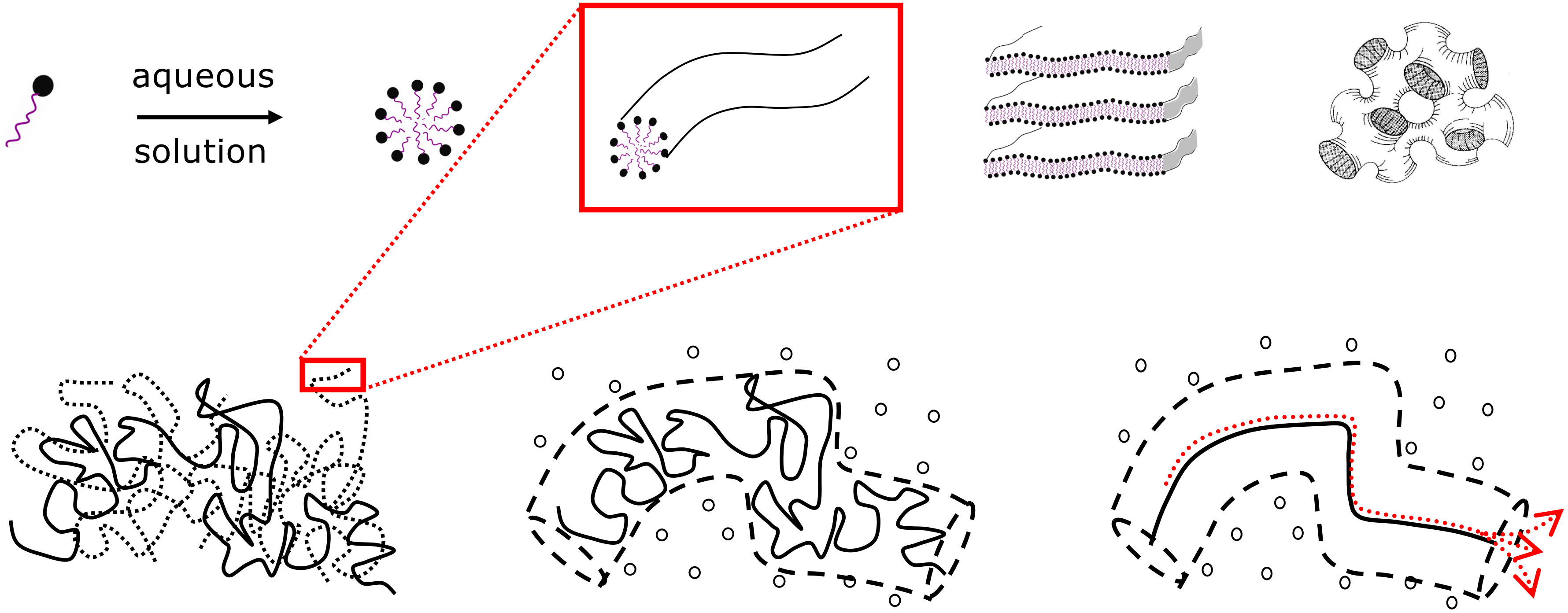

focus on single worm

“**tube**” of entanglements constrains lateral motion

escape by “**reptation**”

[Doi + Edwards 1986]

An example: wormlike micellar surfactant

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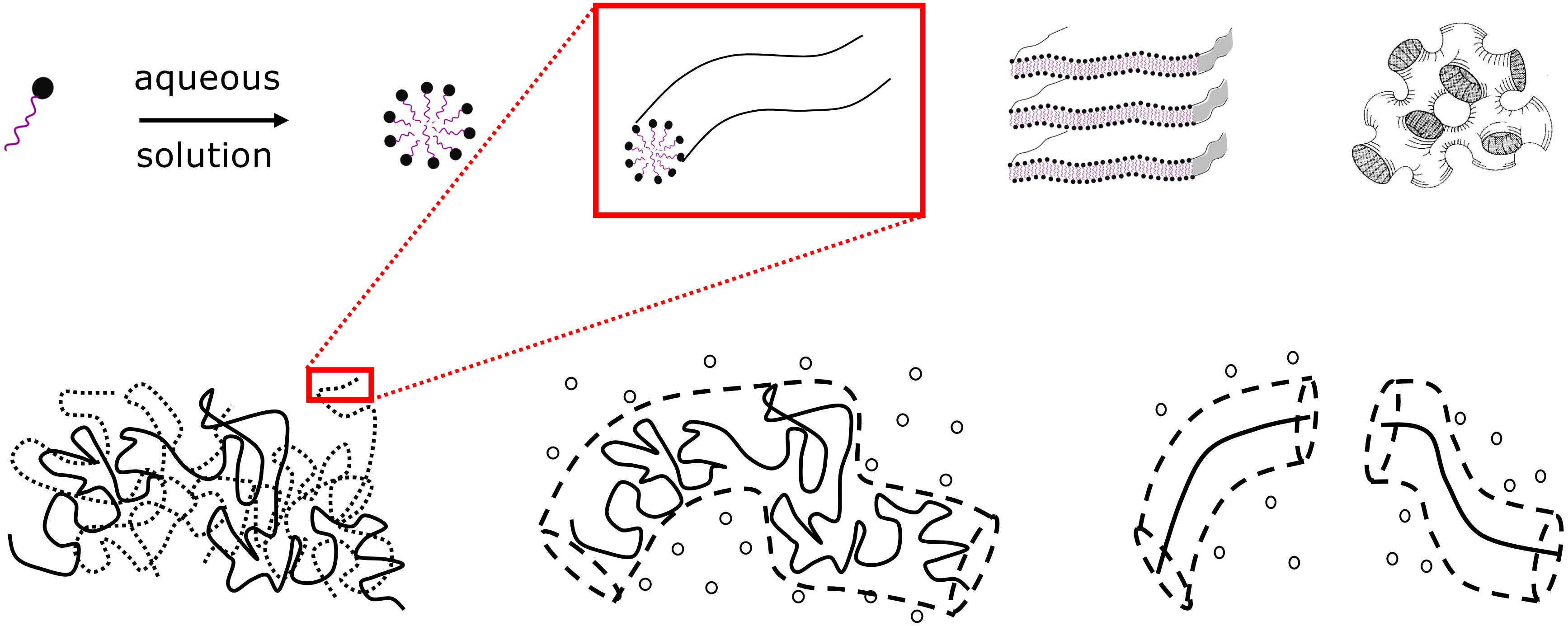

focus on single worm

“**tube**” of entanglements constrains lateral motion

and by “**reaction**”

[Cates 1987, 1990]

Modelling flow properties of wormlike micelles

Extended Stokes balance (+ incompressibility)

$$0 = \nabla \cdot \sigma + \eta \nabla^2 \mathbf{v} - \nabla p$$

solvent

pressure

Viscoelastic stress

$$\sigma = G\left(\mathbf{W} - \tfrac{1}{3}\boldsymbol{\delta}\right)$$

Reptation-reaction model for micellar deformation tensor $\mathbf{W} = \langle \mathbf{uu} \rangle_P$

$$D_t \mathbf{W} = \nabla \mathbf{v} . \mathbf{W} + \mathbf{W} . \nabla \mathbf{v} - \frac{2}{3}\left(\nabla \mathbf{v} : \mathbf{W}\right)\mathbf{W} - \frac{\mathbf{W}}{\tau} + \frac{\delta}{3\tau}$$

[Cates 1987, 1990]

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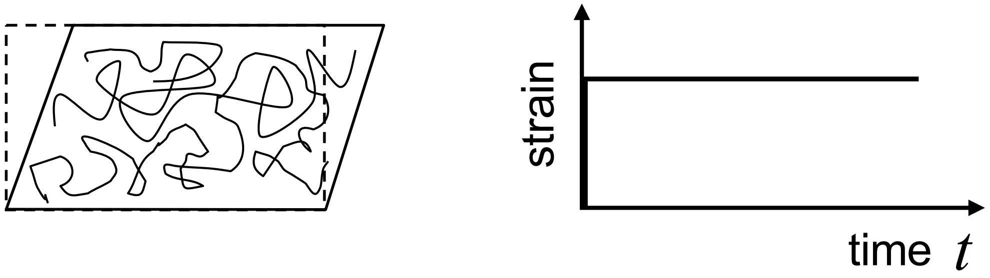
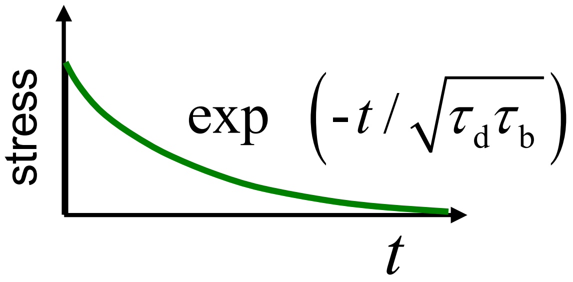
Predictions of the reptation - reaction model: 0D linear viscoelasticity

Recall: stress relaxation after small step strain



Model predicts: mono-exponential stress relaxation

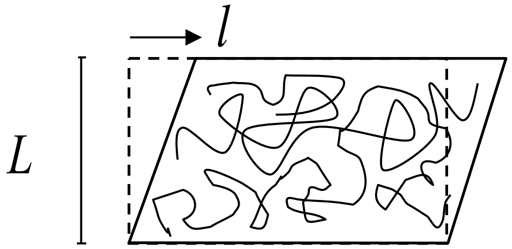


$$\exp\left(-t/\sqrt{\tau_d\tau_b}\right)$$

[Cates 1987, 1990]

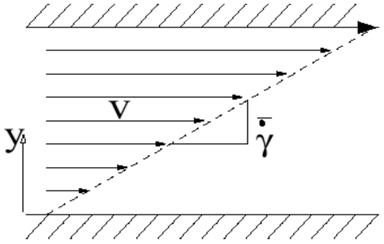
Predictions of the reptation - reaction model: 0D linear viscoelasticity

Recall: stress response to steady applied shear flow

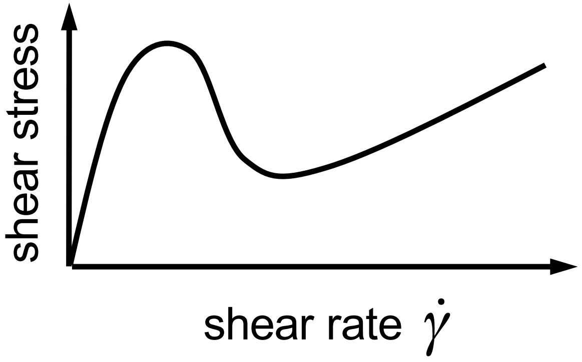


shear at constant

rate $\dot{\gamma} \equiv \frac{1}{L} \partial_t l$



Model predicts: flow curve as follows



Predictions of the reptation - reaction model: 0D linear viscoelasticity

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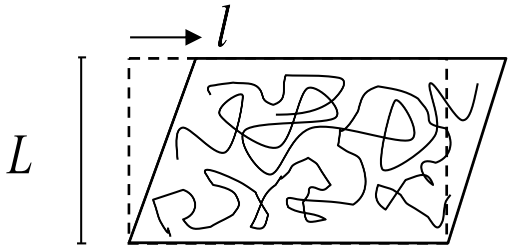

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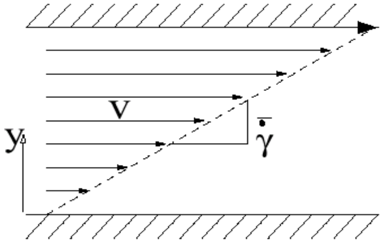

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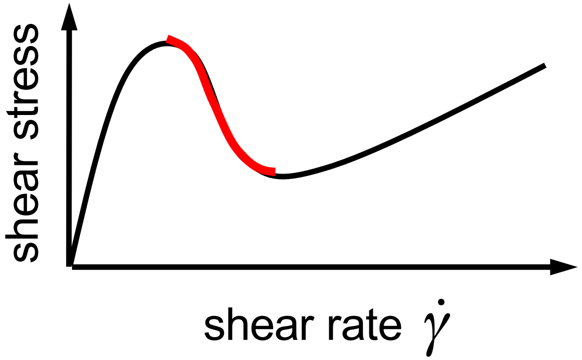

?!

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↓ unstable

1D rheology – shear banding

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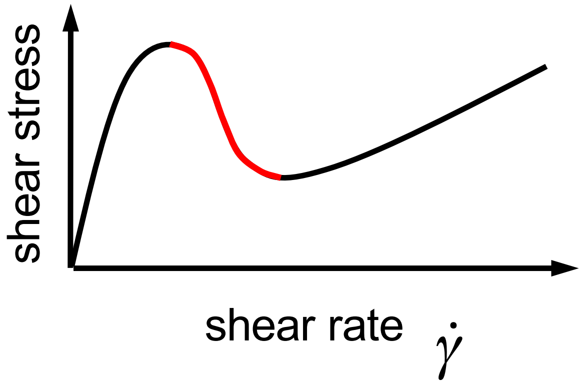
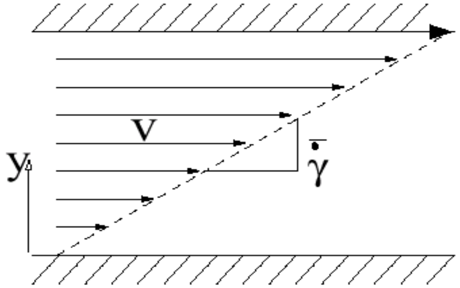
2D rheology – instability of interface between bands

[Spenley et al. PRL 93]

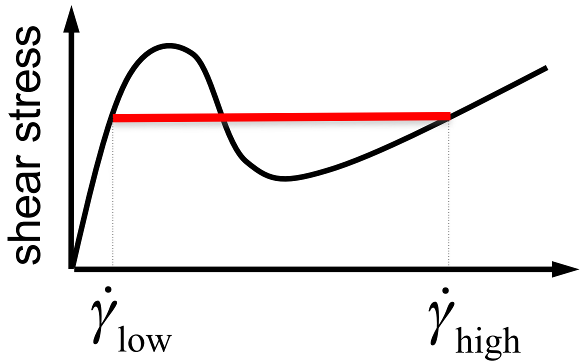
Predictions of reptation-reaction model: shear banding

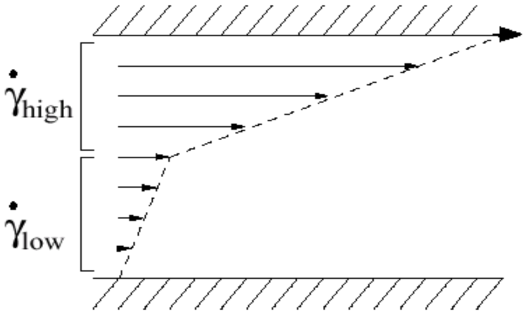
Recall: reptation-reaction model predicts non-monotonic flow curve





And so instability and transition to `shear bands’ (seen experimentally)





Tutorial: linear stability analysis for the onset of shear banding

Recall basic structure of equations:

$$\underline{0} = \nabla . \underline{\underline{\sigma}} + \eta \nabla^2 \underline{v} - \nabla p$$ ① "Stokes +"

$$\underline{\underline{\sigma}} = \underline{\underline{\sigma}} (\underline{\underline{W}})$$ ② viscoelastic stress

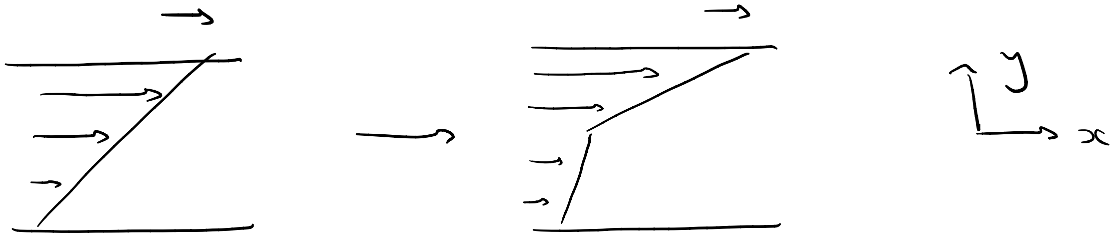
$$D_t \underline{\underline{W}} = \underline{\underline{N}} (\nabla \underline{v}, \underline{\underline{W}})$$ ③ mesostructure

Often combine ② and ③ to write simply:

$$D_t \underline{\underline{\sigma}} = \underline{\underline{\tilde{N}}} (\nabla \underline{v}, \underline{\underline{\sigma}})$$ viscoelastic constitutive equation

Tutorial: linear stability analysis for the onset of shear banding

For the essentially 1D problem of shear banding:



we specialise to consider ....

$$\underline{v} = v(y,t)\,\hat{x}$$

$$\nabla\underline{v} = \partial_y v(y,t)\,\hat{y}\hat{x} \equiv \dot{\gamma}(y,t)\,\hat{y}\hat{x}$$

} flow only in x

gradients " " y

and, for simplicity, only xy component of stress ...

$$\sigma_{xy}(y,t) \equiv \sigma(y,t)$$

ignore normal stresses, σ_{xx} etc

Tutorial: linear stability analysis for the onset of shear banding

So the Stokes + eqtn, which in general componentwise would be:

$$0_x = \cancel{\partial_x \sigma_{xx}} + \partial_y \sigma_{xy} + \eta\left(\cancel{\partial_x^2} + \partial_y^2\right) v_x - \cancel{\partial_x p}$$

$$\left[\; 0_y = \cancel{\partial_x \sigma_{xy}} + \partial_y \sigma_{yy} + \eta\left(\cancel{\partial_x^2} + \partial_y^2\right) \cancel{v_y} - \partial_y p \;\right]$$

Now, for this simpler 1D geometry, becomes:

$$0 = \partial_y \sigma + \eta\, \partial_y^2 v$$

$$0 = \partial_y \sigma + \eta\, \partial_y \dot{\gamma}$$

Integrate w.r.t. y:

$$\Sigma(t) = \sigma(y,t) + \eta\, \dot{\gamma}(y,t)$$

[Recall:

$v = v_x$

$\dot{\gamma} = \partial_y v$

$\sigma = \sigma_{xy}$]

Tutorial: linear stability analysis for the onset of shear banding

So we now have the governing equations:

- Stokes, as just discussed

$$\Sigma(t) = \sigma(y,t) + \eta\,\dot{\gamma}(y,t)$$

total shear stress, uniform   viscoelastic   Newtonian solvent

- Assume simplified scalar viscoelastic constitutive equation:

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma})$$

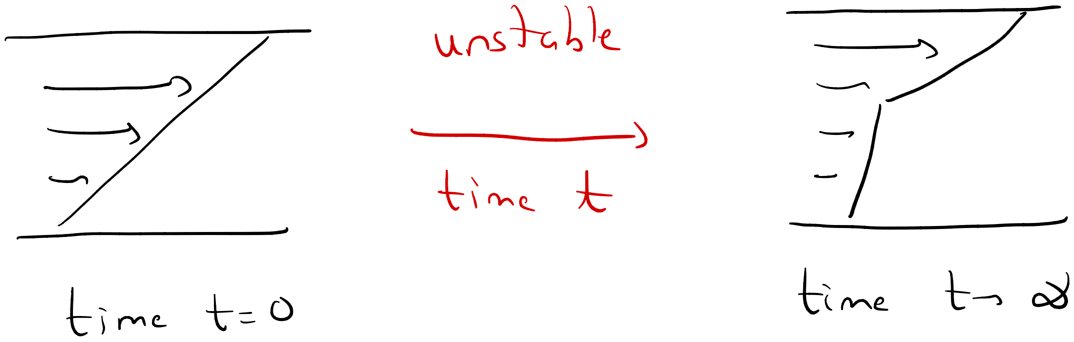
Tutorial: linear stability analysis for the onset of shear banding

Aim : use this simplified model to show that

A) when slope of $\Sigma(\dot{\gamma})$ is negative ...

$$\frac{d\Sigma}{d\dot{\gamma}} < 0$$

B) ... initially homogeneous shear is unstable to banding :



Tutorial: linear stability analysis for the onset of shear banding

A) Slope of constitutive curve : $[\cancel{y}, \cancel{t}]$

Differentiate Stokes + :

$$\Sigma = \sigma + \eta\dot{\gamma} \longrightarrow d\Sigma = d\sigma + \eta\, d\dot{\gamma}$$

Differentiate constitutive equation

$$0 = f(\sigma, \dot{\gamma}) \longrightarrow 0 = f_\sigma\, d\sigma + f_{\dot{\gamma}}\, d\dot{\gamma}$$

Combine these :

$$\frac{d\Sigma}{d\dot{\gamma}} = -\frac{f_{\dot{\gamma}}}{f_\sigma} + \eta$$

slope of constitutive curve.

Tutorial: linear stability analysis for the onset of shear banding

B) Instability to shear banding:

Recall governing equations:

$$\Sigma(t) = \sigma(y,t) + \eta\,\dot{\gamma}(y,t)$$

$$\frac{d\sigma}{dt} = f(\sigma, \dot{\gamma})$$

Assume solution = initial state, uniform shear + small perturbations, banding precursors

$$\Sigma(t) = \Sigma + 0 \quad (\text{uniform!})$$

$$\sigma(y,t) = \bar{\sigma} + \delta\sigma_k\, e^{iky}\, e^{\omega t}$$

$$\dot{\gamma}(y,t) = \bar{\dot{\gamma}} + \delta\dot{\gamma}_k\, e^{iky}\, e^{\omega t}$$

If $\omega > 0$ perturbations grow, bands form

Tutorial: linear stability analysis for the onset of shear banding

Substitute assumed solution into governing equations

Expand to 1° in size of small perturbations:

$$0 = \delta\sigma_k + \eta\,\delta\dot{\gamma}_k$$

$$\frac{d}{dt}\delta\sigma_k = f_\sigma\,\delta\sigma_k + f_{\dot{\gamma}}\,\delta\dot{\gamma}_k$$

Combine these:

$$\frac{d}{dt}\delta\sigma_k = \underbrace{\left(f_\sigma - \frac{f_{\dot{\gamma}}}{\eta}\right)}_{\omega}\delta\sigma_k \equiv \omega\,\delta\sigma_k$$

Tutorial: linear stability analysis for the onset of shear banding

A) Slope of constitutive curve:

$$\frac{d\Sigma}{d\dot{\gamma}} = -\frac{f_{\dot{\gamma}}}{f_\sigma} + \eta$$

B) Eigenvalue for growth (or decay) of perturbations:

$$\omega = f_\sigma - \frac{f_{\dot{\gamma}}}{\eta}$$

Now combine these:

$$\omega = \frac{f_\sigma}{\eta}\frac{d\Sigma}{d\dot{\gamma}} \xrightarrow{(f_\sigma < 0)} \boxed{\frac{d\Sigma}{d\dot{\gamma}} < 0 \text{ GIVES } \omega > 0}$$

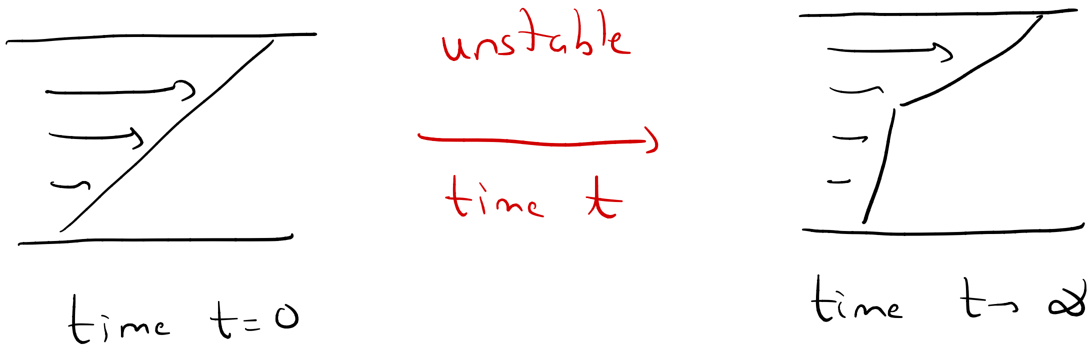
Tutorial: linear stability analysis for the onset of shear banding

So : using this simplified model, we have shown that :

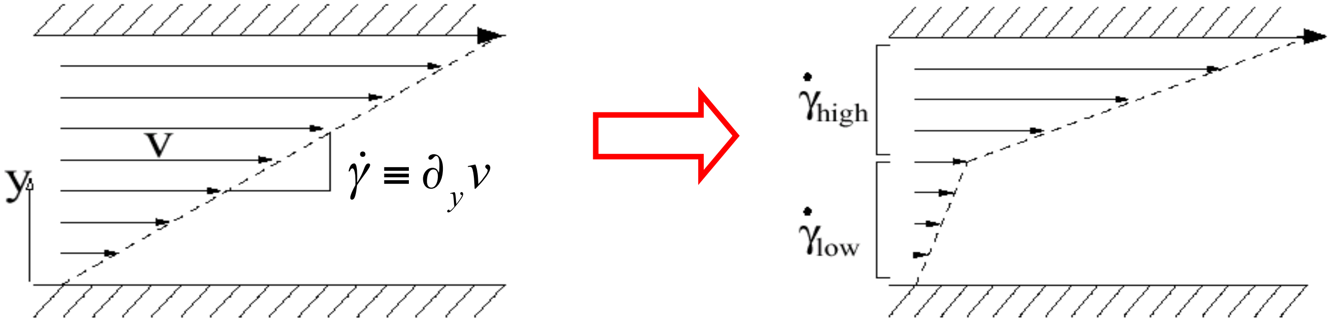
A) when slope of $\Sigma(\dot{\gamma})$ is negative . . .

$$\frac{d\Sigma}{d\dot{\gamma}} < 0$$

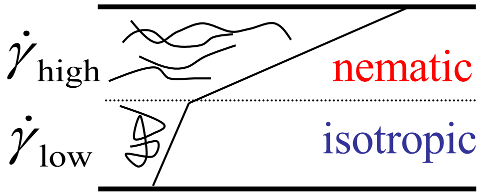
B) . . . initially homogeneous shear is unstable to banding :



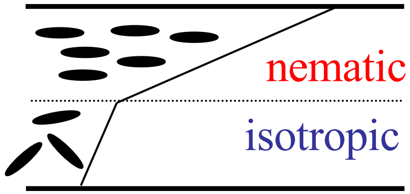
Indeed, assumption of homogeneous flow is incorrect in many complex fluids



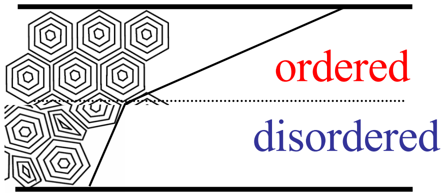
Wormlike surfactants



Liquid crystals



Onion surfactants



linear entangled polymers; star polymers; clays; colloids; etc; etc….

Reminder of yesterday's lecture

A) Rheology of complex fluids

1) overview

2) continuum models

3) 0D rheology – linear viscoelasticity and flow curves

↓ unstable

1D rheology – shear banding

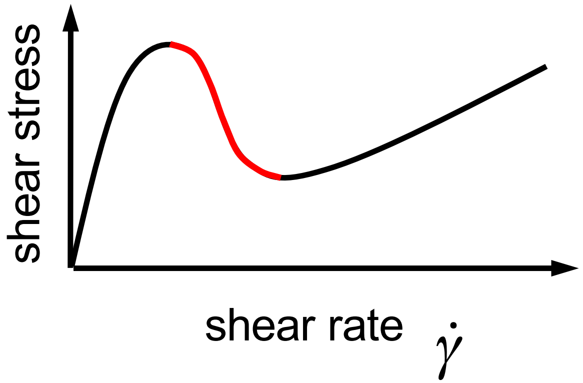
↓ unstable

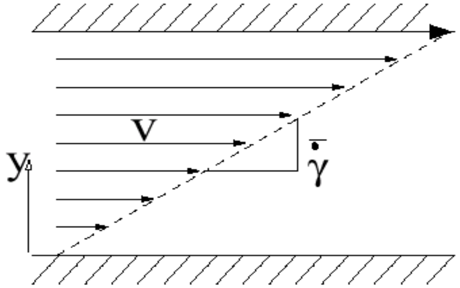
2D rheology – instability of interface between bands

[Spenley et al. PRL 93]

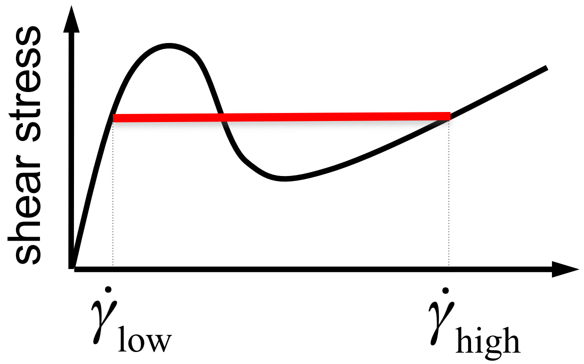
Predictions of reptation-reaction model: shear banding

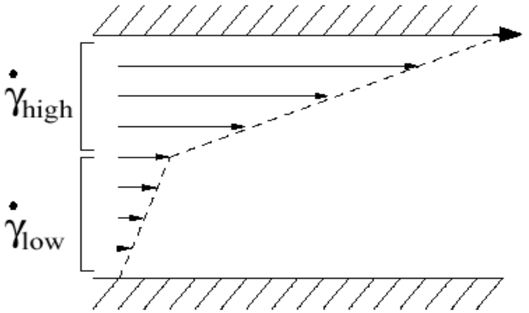
Recall: reptation-reaction model predicts non-monotonic flow curve





And so instability and transition to `shear bands’ (seen experimentally)





Outline

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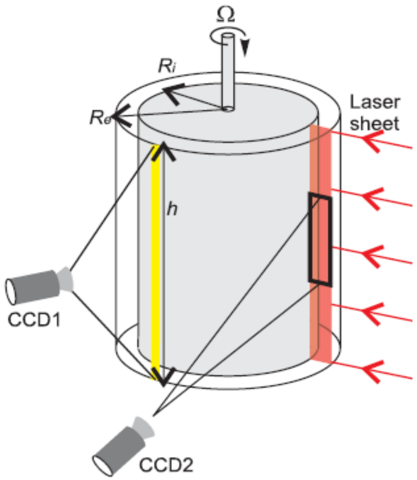
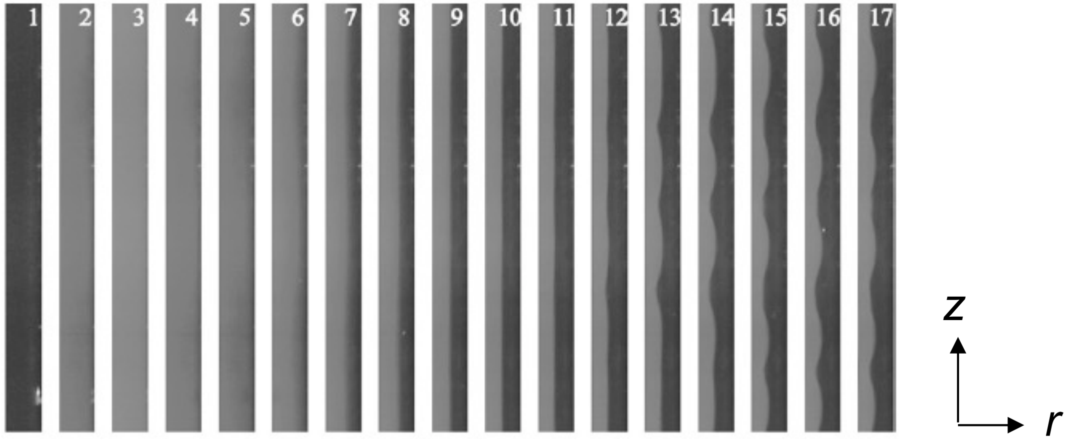
[Lerouge et al. PRL 06; PRL 09; Soft Matter 08]

2D experiments, curved Couette, Lerouge

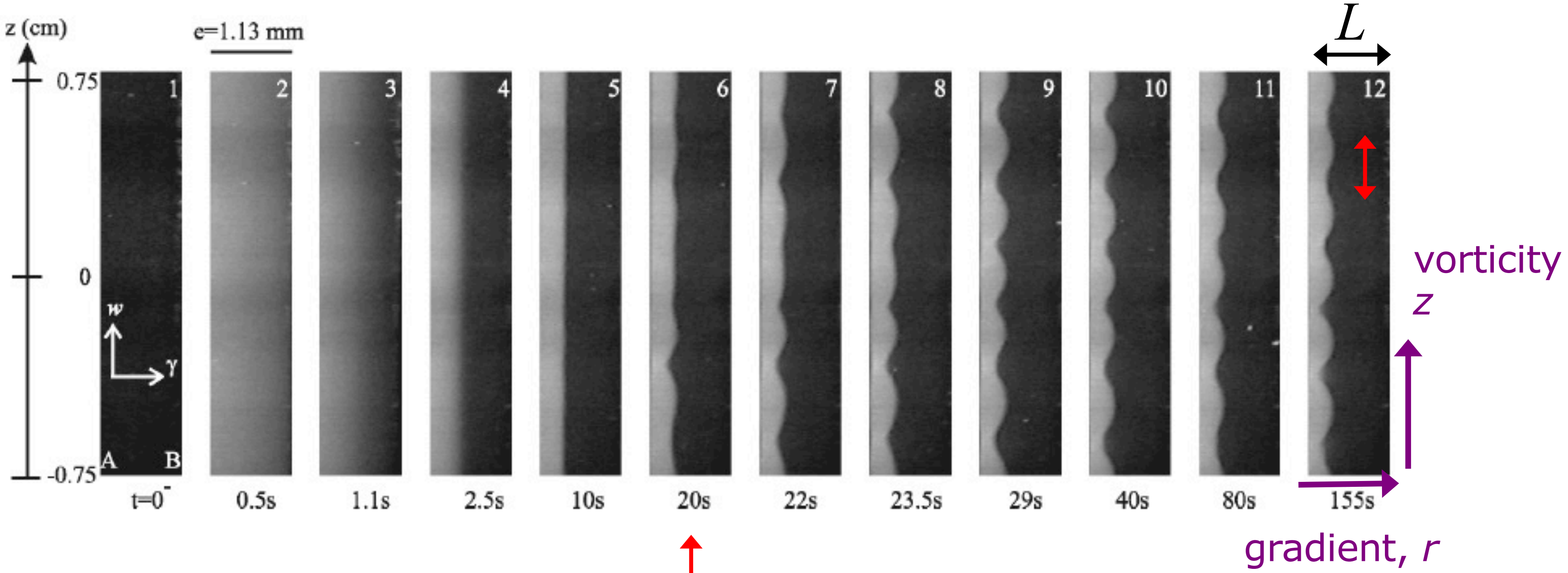


Snapshots over time in startup



[Lerouge et al. PRL 06; PRL 09; Soft Matter 08]

What quantitative information should we seek to capture?



Timescale for onset $t = O\left(100\tau_{\mathrm{R}}\right)$

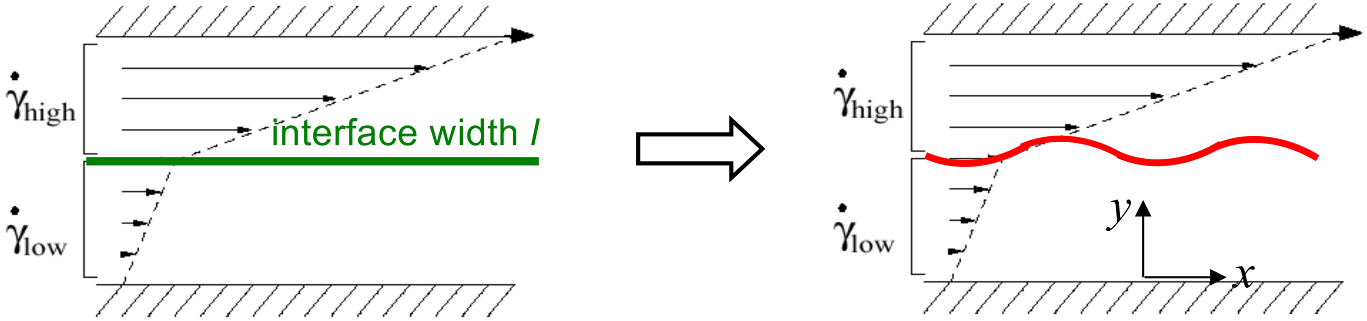
Wavelength $\lambda = O\left(L\right)$

Linear instability of the interface

$$v(x,y,t) = v_0(y) + \delta\tilde{v}(y)\exp(iq_x x + \omega t)$$

$$\mathbf{W}(x,y,t) = \mathbf{W}_0(y) + \delta\tilde{\mathbf{W}}(y)\exp(iq_x x + \omega t)$$

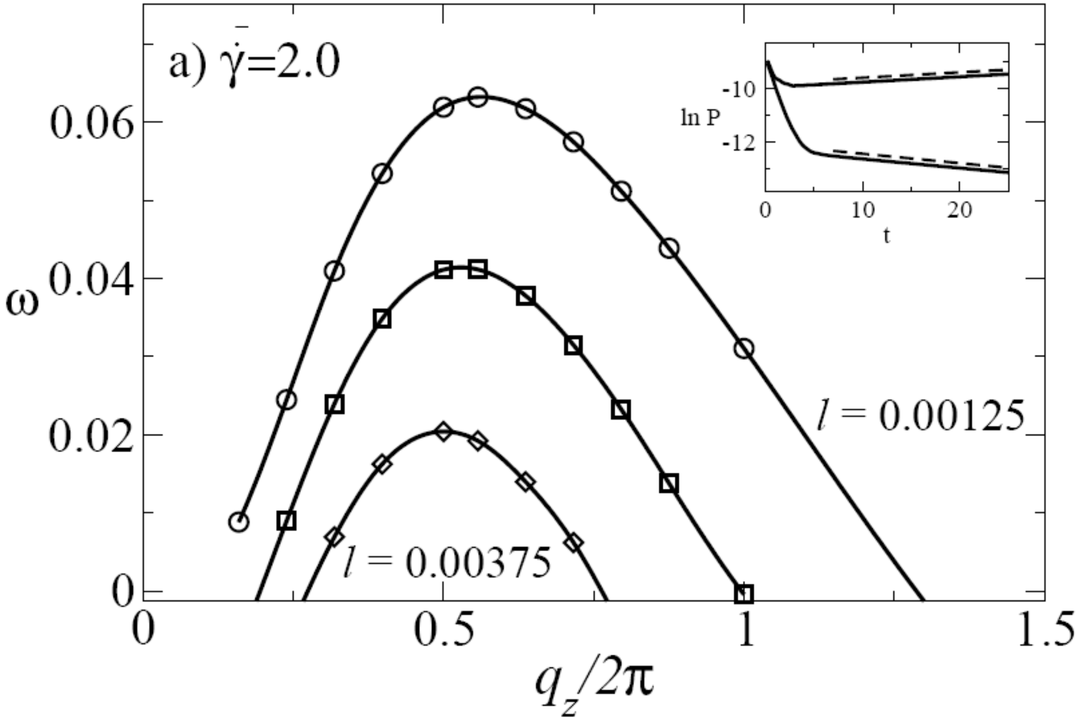
Substitute into governing equations (JS not RR) and retain only terms $O(\delta)$



1D state unstable with respect to growth of undulations along interface

for wavevectors both in flow direction *x* and in vorticity direction *z.*

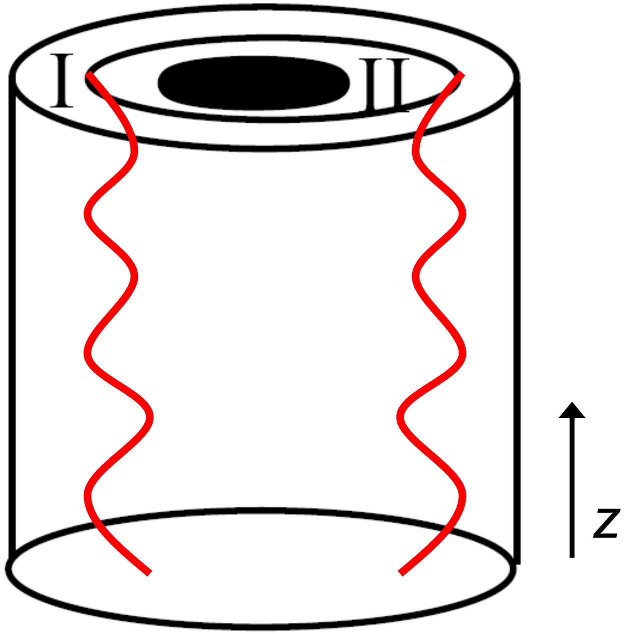
Linear instability of interface



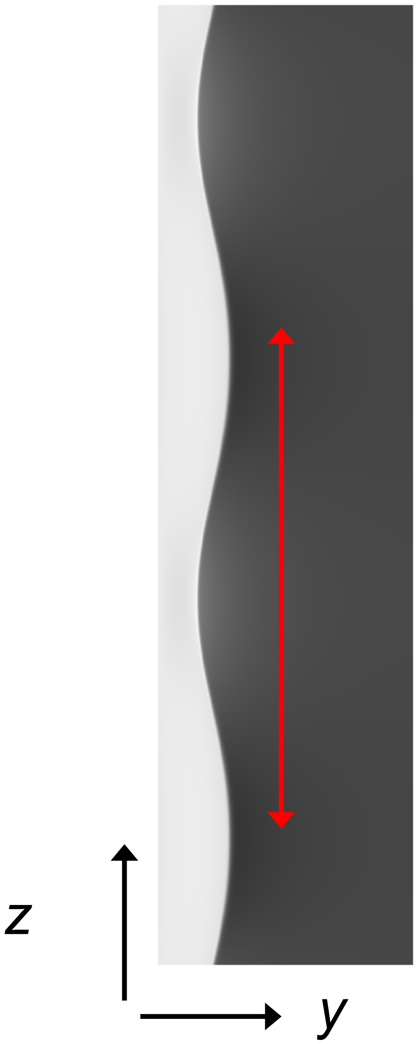
Positive growth rate → linearly unstable $\omega^{-1} = O\left(100\tau_{\mathrm{R}}\right)$

Wavelength $\lambda = O\left(L\right)$

Nonlinear steady state

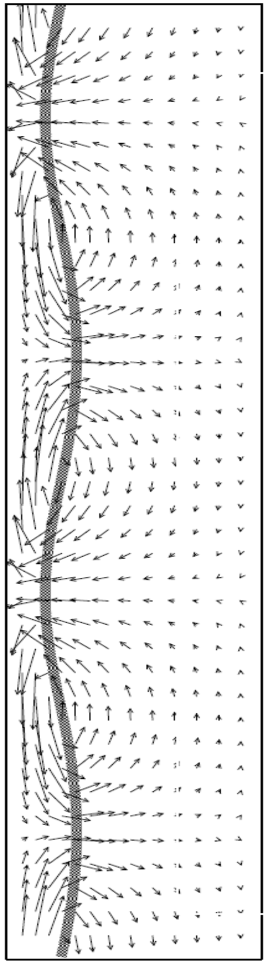


Greyscale of W_{xx}



$$\lambda = O(L)$$

Velocity rolls



Reminder so far…

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1D rheology – shear banding

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And now…

B) Hydrodynamics of active fluids

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↓ unstable

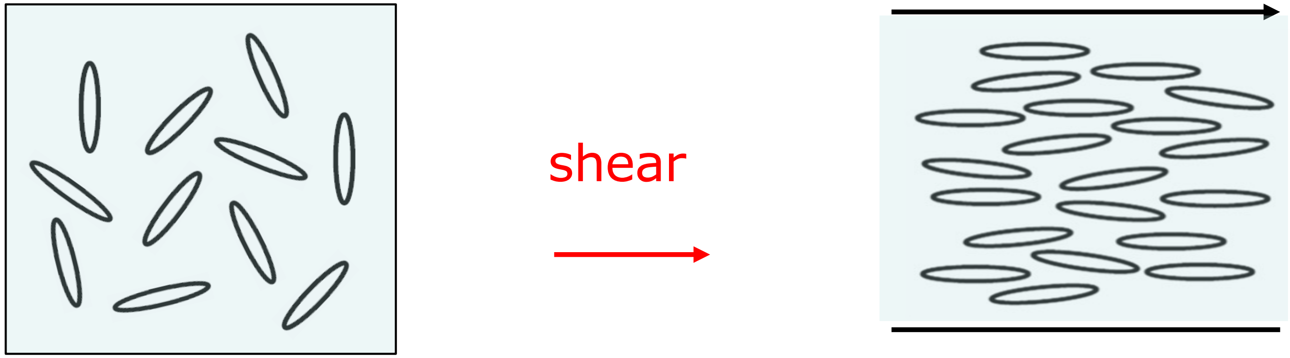
1D rheology – shear banding

↓ unstable

2D rheology – spatio-temporally complicated states

Active matter as a complex fluid

Recall complex fluid: internal mesoscopic substructures



shear

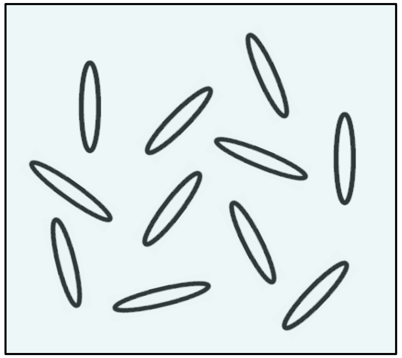
isotropic state

nematic state

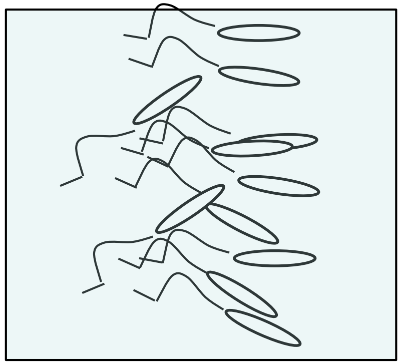
Substructures relax slowly → easily driven out of equilibrium

Active matter as a complex fluid

Active complex fluid: self propelled substructures



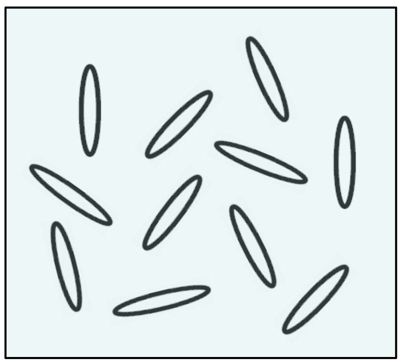
slow relaxation
processes

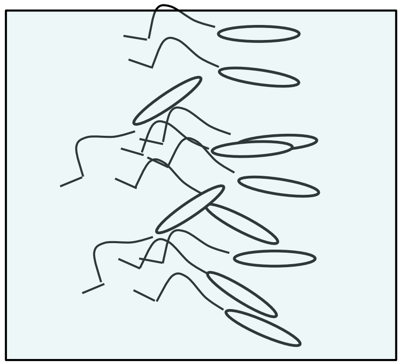


out of equilibrium
“from within”

Active matter as a complex fluid

Active complex fluid: self propelled substructures





slow relaxation processes

non-eqbm ordering transitions

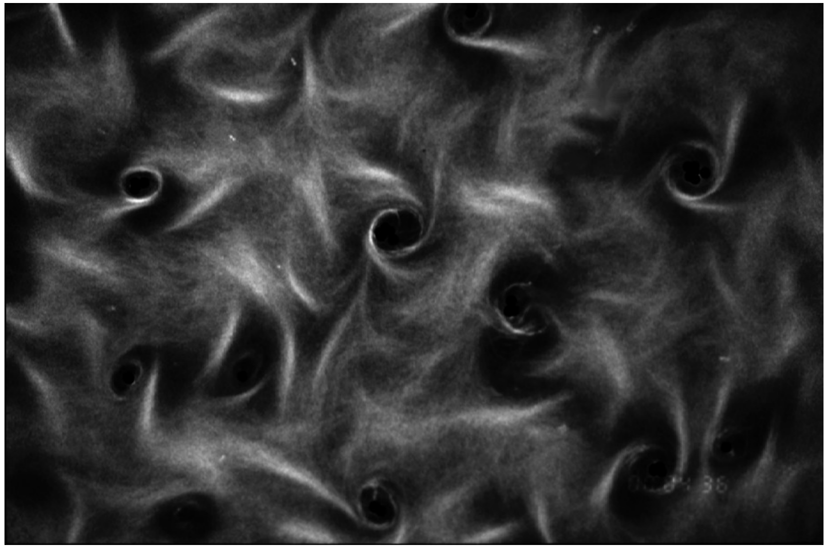
swarming

spontaneous flows / “turbulence”

activity-induced phase separation

Experimental phenomenology

active contractile

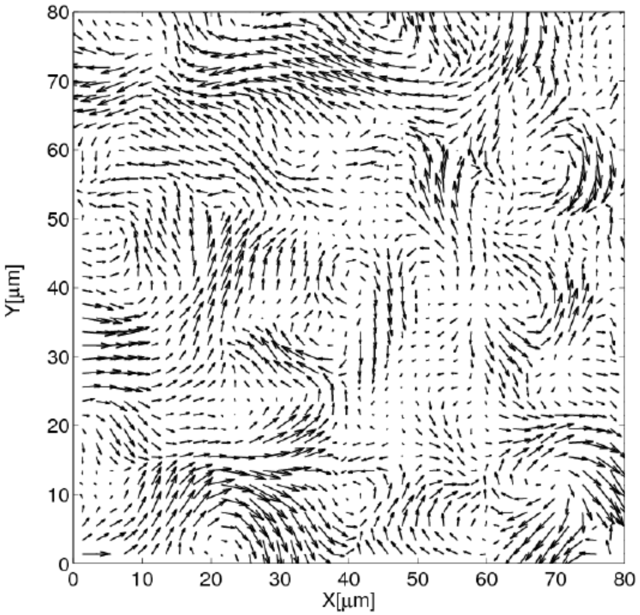


Spontaneously rotating vortices

in microtubules/motors

[F. Nedelec et al., Nature, 97]

active extensile



“Bacterial turbulence”

in B subtilis suspensions

[L. Cisneros et al., Exp. Fluids, 07]

Outline

B) Hydrodynamics of active fluids

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3) 0D rheology – flow curves

↓ unstable

1D rheology – shear banding

↓ unstable

2D rheology – spatio-temporally complicated states

Recall: Modelling flow properties of complex fluids

Navier Stokes (+ incompressibility)

$$\underset{\substack{\uparrow\\ \text{inertial}}}{\rho D_t \mathbf{v}} = \nabla \cdot \underset{\substack{\uparrow}}{\sigma} + \underset{\substack{\uparrow\\ \text{solvent}}}{\eta \nabla^2 \mathbf{v}} - \underset{\substack{\uparrow\\ \text{pressure}}}{\nabla p}$$

Viscoelastic stress $\sigma = \sigma\left(\mathbf{W}\right)$

Equation of motion for mesostructure

$$D_t \mathbf{W} = \mathbf{N}\left(\nabla \mathbf{v}, \mathbf{W}\right)$$

Often: nonlinear PDE of reaction-diffusion type

Now: Modelling flow properties of active fluids

Navier Stokes (+ incompressibility)

$$\underset{\substack{\uparrow\\ \text{inertial}}}{\rho D_t \mathbf{v}} = \nabla\cdot\sigma + \underset{\substack{\uparrow\\ \text{solvent}}}{\eta \nabla^2 \mathbf{v}} - \underset{\substack{\uparrow\\ \text{pressure}}}{\nabla p}$$

Viscoelastic stress $\sigma = \sigma(\boldsymbol{Q})$

Equation of motion for mesostructure

$$D_t \boldsymbol{Q} = \mathbf{N}(\nabla\mathbf{v}, \boldsymbol{Q})$$

Often: nonlinear PDE of
reaction-diffusion type

Continuum description: nematics hydrodynamics + activity

Navier Stokes

$$\rho(\partial_t + u_\beta \partial_\beta) u_\alpha = \partial_\beta(\Pi_{\alpha\beta}) + \eta \partial_\beta(\partial_\alpha u_\beta + \partial_\beta u_\alpha)$$

Stress tensor

$$\Pi_{\alpha\beta} = -P_0 \delta_{\alpha\beta} + 2\xi(Q_{\alpha\beta} + \frac{1}{3}\delta_{\alpha\beta}) Q_{\gamma\epsilon} H_{\gamma\epsilon} - \xi H_{\alpha\gamma}(Q_{\gamma\beta} + \frac{1}{3}\delta_{\gamma\beta})$$

$$-\xi(Q_{\alpha\gamma} + \frac{1}{3}\delta_{\alpha\gamma}) H_{\gamma\beta} - \partial_\beta Q_{\gamma\nu} \frac{\delta \mathcal{F}}{\delta \partial_\alpha Q_{\gamma\nu}} + Q_{\alpha\gamma} H_{\gamma\beta} - H_{\alpha\gamma} Q_{\gamma\beta} - \boxed{\zeta Q_{\alpha\beta}}$$

active terms

Order parameter relaxation

$$D_t Q_{\alpha\beta} = \Gamma H_{\alpha\beta}$$

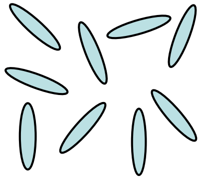
Molecular field

$$H_{\alpha\beta} = -(1 - \varphi/3 + \boxed{\lambda/\Gamma}) Q_{\alpha\beta} + \varphi(Q_{\alpha\zeta} Q_{\zeta\beta} - \delta_{\alpha\beta} Q^2_{\zeta\delta}/3)$$

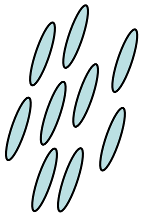
$$-\varphi Q^2_{\zeta\delta} Q_{\alpha\beta} + K \partial^2_\zeta Q_{\alpha\beta}$$

[Hatwalne et al. PRL 04; Liverpool et al. EPL 05; Kruse et al. PRL 04; Voituirez et al., EPL 05]

Isotropic – nematic transition



Isotropic (I)
for $\phi < 3$



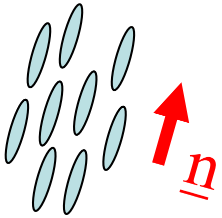
Nematic (N)
for $\phi > 3$

Here study:

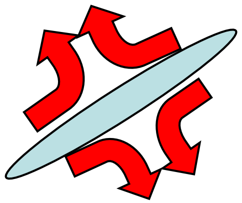
rheology of active suspension in vicinity of this I-N transition

Contractile versus extensile

passive

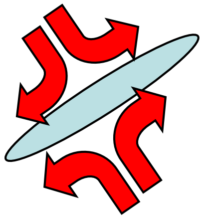


active contractile $\zeta < 0$



microtubules/motors

active extensile $\zeta > 0$



bacterial suspensions

Activity induces dipolar flow

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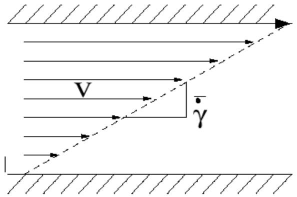
↓ unstable

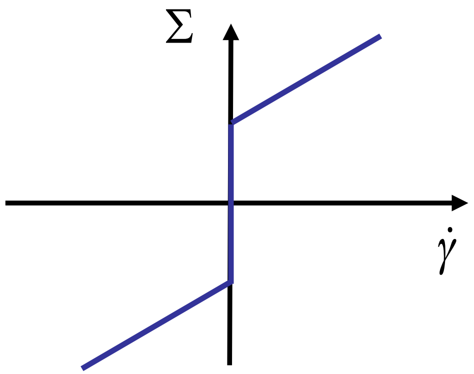
1D rheology – shear banding

↓ unstable

2D rheology – spatio-temporally complicated states

0D active rheology: homogeneous shear flow $\phi \geq 3.0$

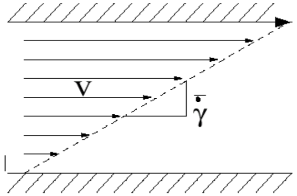


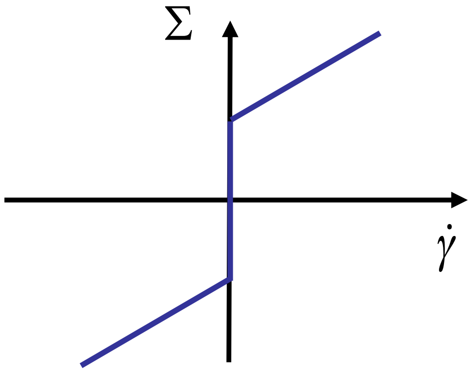


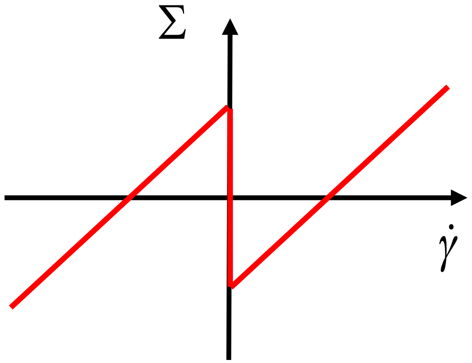
active contractile

conventional yield stress

0D active rheology: homogeneous shear flow $\phi \geq 3.0$







active contractile

conventional yield stress

active extensile

negative yield stress?!

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↓ unstable

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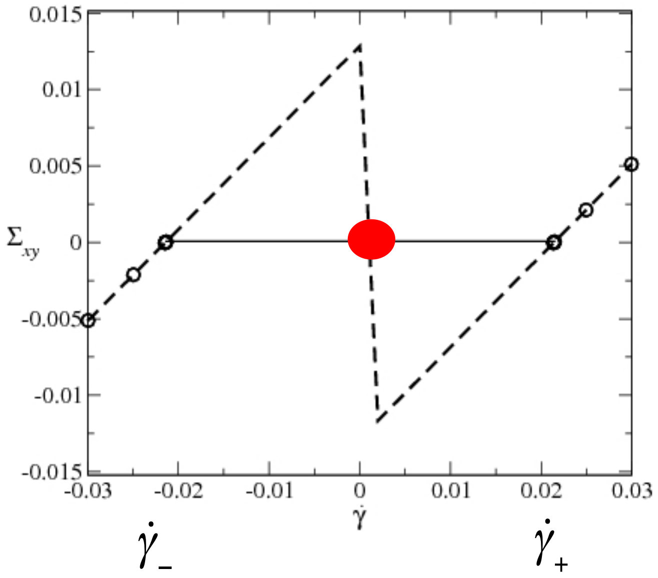
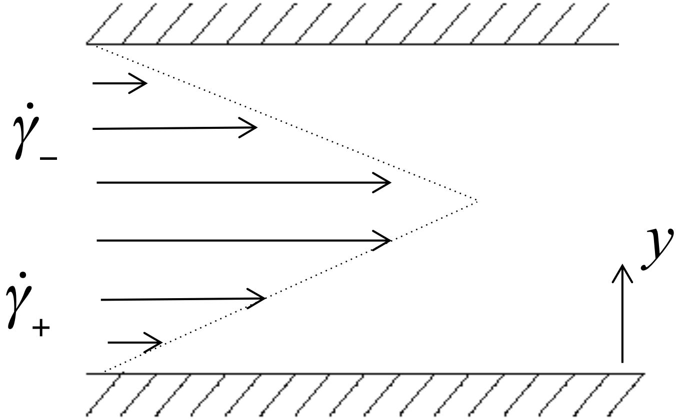
1D active rheology, extensile systems for $\phi \geq 3.0$

Negative yield stress in 0D → coexisting shear bands in 1D

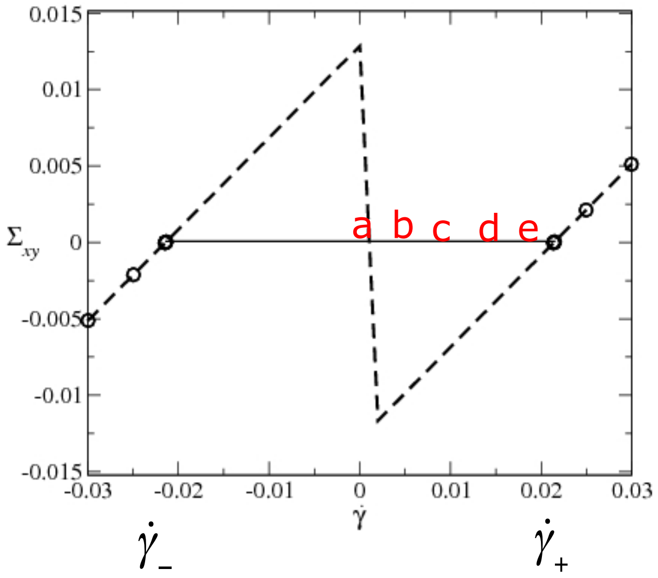


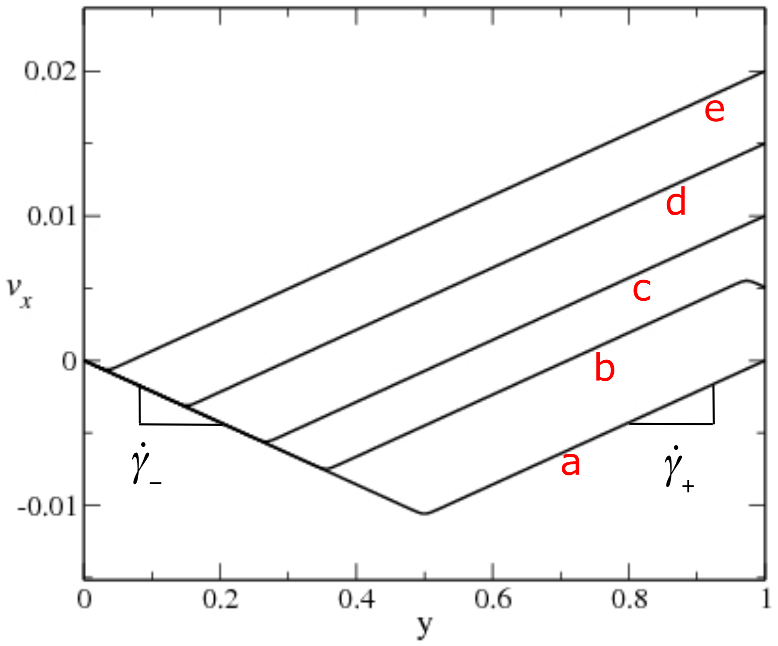


Bands of equal, opposite shear rates even in globally unsheared system!

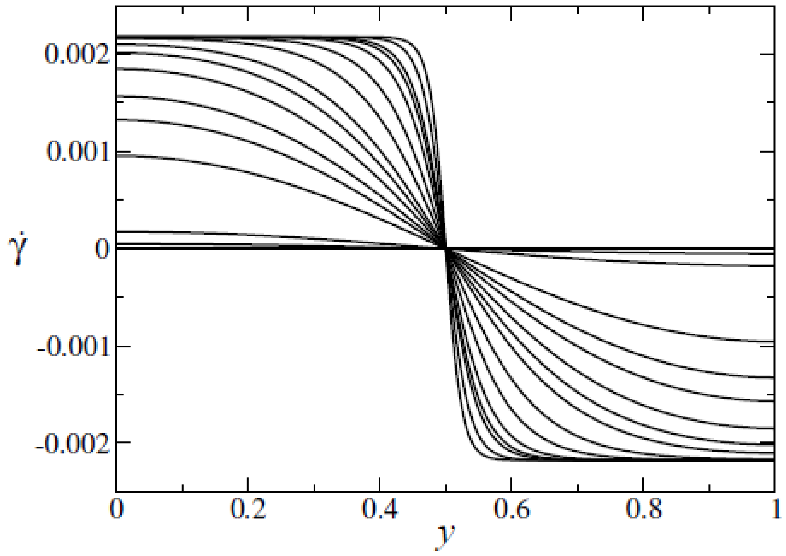
1D active rheology, extensile systems for $\phi \geq 3.0$

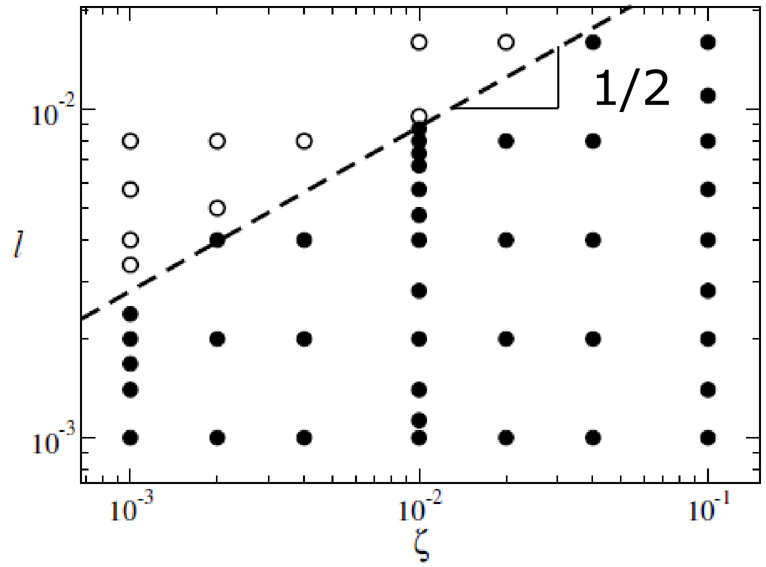
Negative yield stress in 0D → coexisting shear bands in 1D





Effect of spatial gradients $K\partial_y^2\mathbf{Q} \rightarrow l^2\partial_y^2\mathbf{Q}$





Fixed activity, ζ

No spontaneous flow for large *l*

○ No flow

● Spontaneous flow

Outline

B) Hydrodynamics of active fluids

1) overview

2) continuum models

3) 0D rheology – flow curves

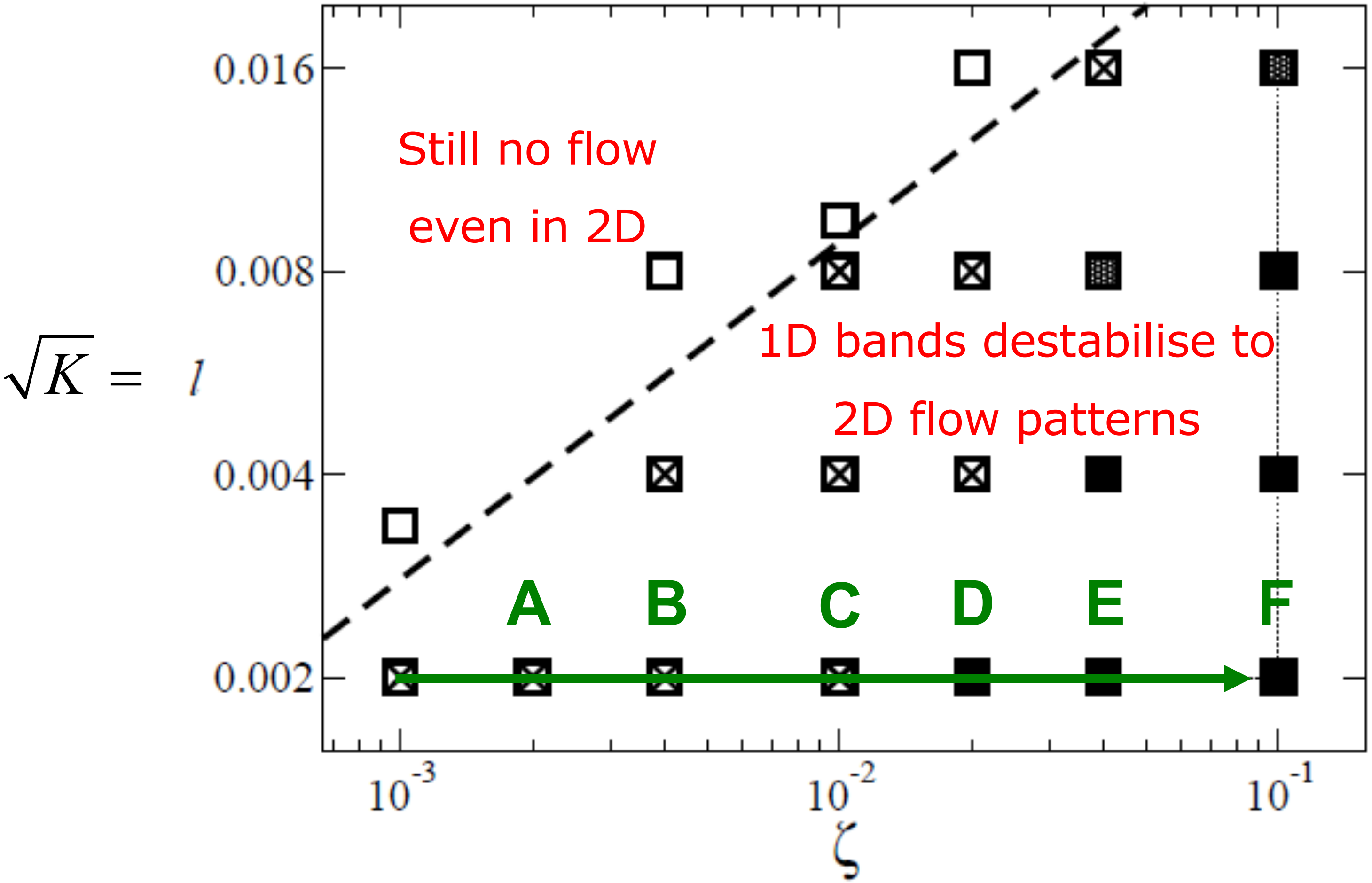
↓ unstable

1D rheology – shear banding

↓ unstable

2D rheology – spatio-temporally complicated states

2D systems: “phase diagram” for extensile at zero global shear

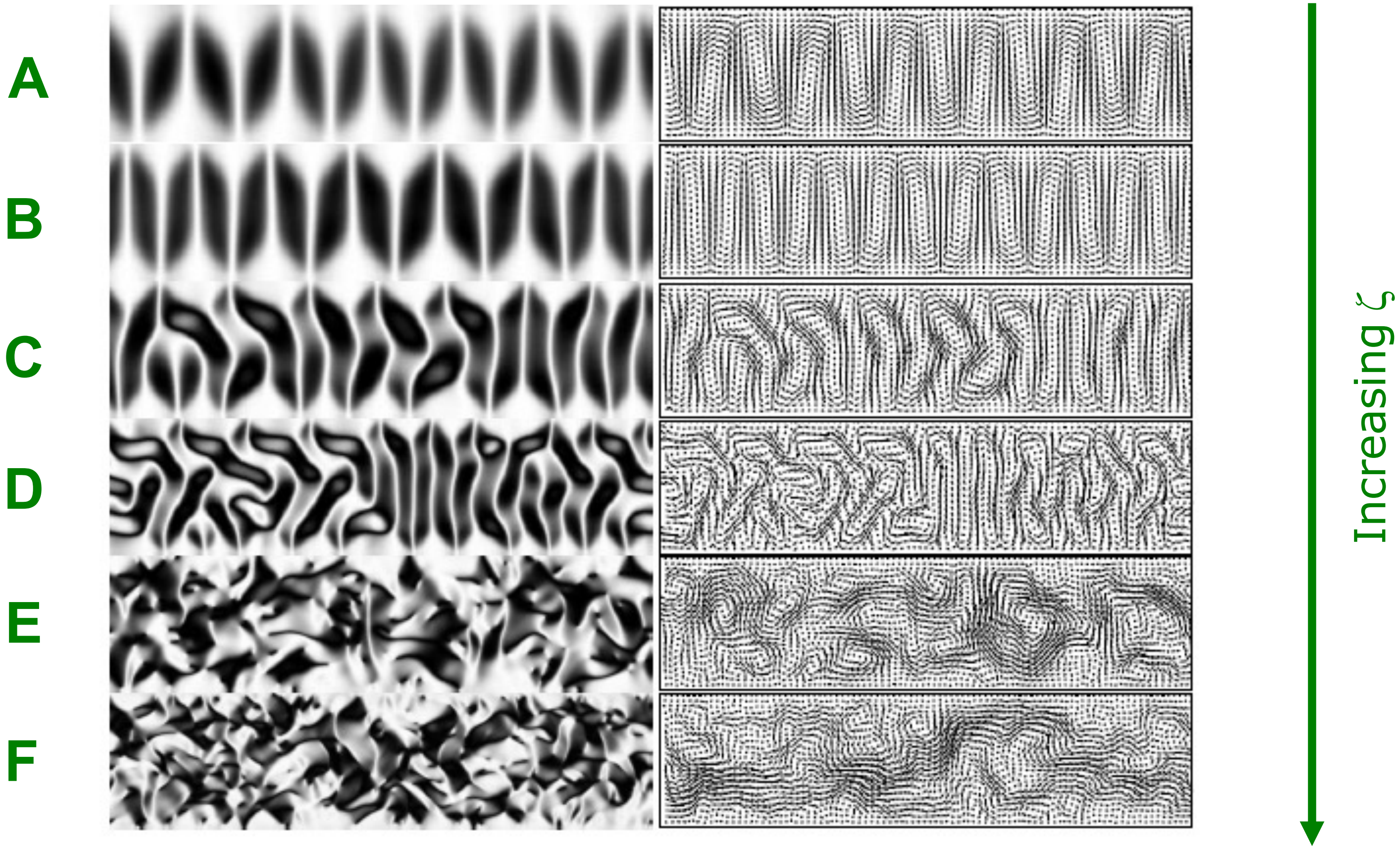


Still no flow even in 2D

1D bands destabilise to 2D flow patterns

[SMF et al. PRE 2011, Hemingway et al. PRL 2015]

2D spontaneous flow patterns

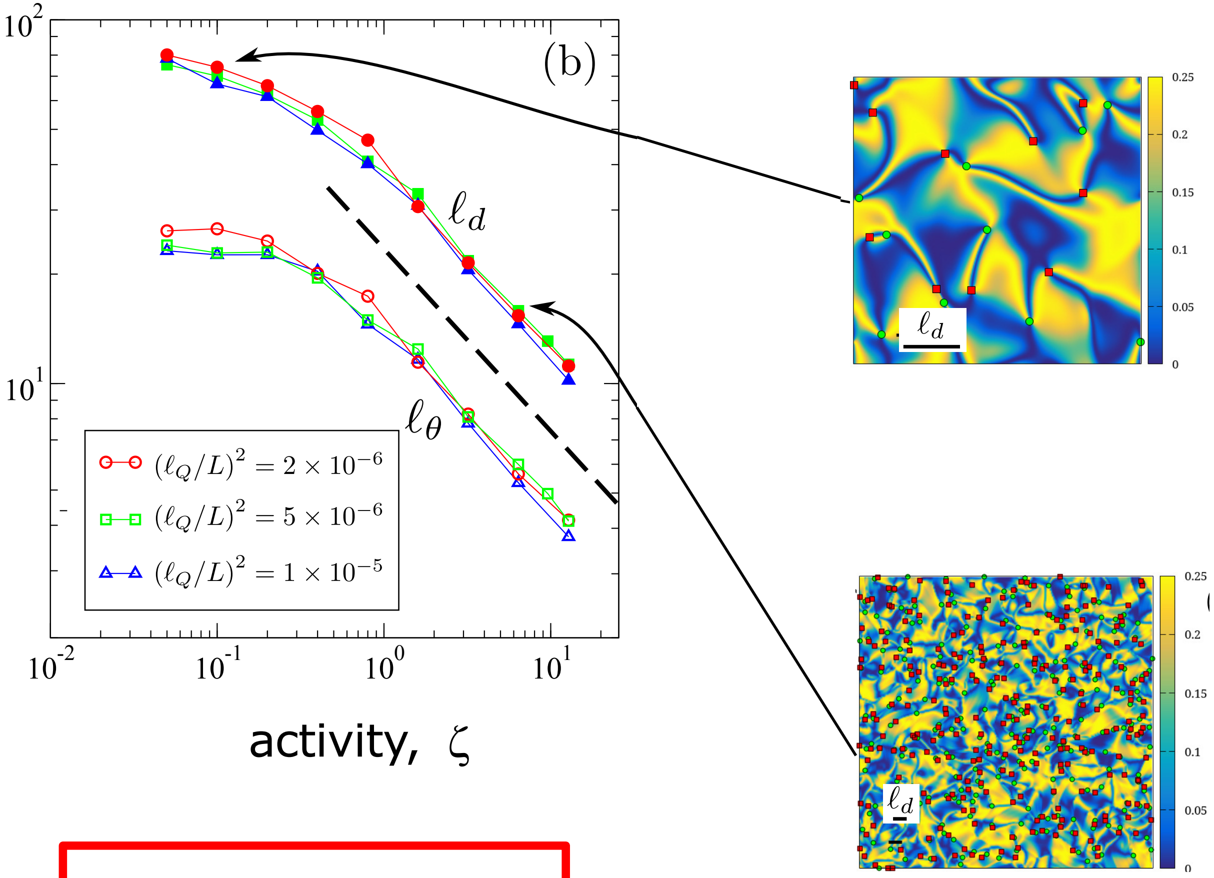


[Also: Hernandez-Ortiz et al. PRL 05; Ishikawa et al. JFM 08; Saintillan + Shelley PRL 08; Giomi + Marchetti Soft Matter 12]

2D spontaneous flow patterns: scaling of correlation lengths

defect spacing l_d

nematic correlation length l_θ



$$\boxed{\text{length } l_{d,\theta} \sim \zeta^{-1/2}}$$

[Hemingway et al., Soft Matter 2016]

Recall section A: Modelling flow properties of complex fluids

Navier Stokes (+ incompressibility)

$$\underset{\substack{\uparrow\\\text{inertial}}}{\rho D_t \mathbf{v}} = \underset{\uparrow}{\nabla \cdot \sigma} + \underset{\substack{\uparrow\\\text{solvent}}}{\eta \nabla^2 \mathbf{v}} - \underset{\substack{\uparrow\\\text{pressure}}}{\nabla p}$$

Viscoelastic stress $\sigma = \sigma(\mathbf{W})$

Equation of motion for mesostructure

$$D_t \mathbf{W} = \mathbf{N}(\nabla \mathbf{v}, \mathbf{W})$$

Often: nonlinear PDE of reaction-diffusion type

And section B so far: Modelling flow properties of active fluids

Navier Stokes (+ incompressibility)

$$\underset{\substack{\uparrow \\ \text{inertial}}}{\rho D_t \mathbf{v}} = \underset{\substack{\uparrow}}{\nabla \cdot \sigma} + \eta \underset{\substack{\uparrow \\ \text{solvent}}}{\nabla^2 \mathbf{v}} - \underset{\substack{\uparrow \\ \text{pressure}}}{\nabla p}$$

Viscoelastic stress

$$\sigma = \sigma(\boldsymbol{Q})$$

Equation of motion for mesostructure

$$D_t \boldsymbol{Q} = \mathbf{N}(\nabla \mathbf{v}, \boldsymbol{Q})$$

Often: nonlinear PDE of
reaction-diffusion type

Now include a polymeric background fluid

$\rho\left(\partial_t + v_\beta \partial_\beta\right) v_\alpha = \partial_\beta \Sigma_{\alpha\beta}$ momentum balance - as before

Stress tensor - as before plus a new polymeric stress term

$$\boldsymbol{\Sigma} = -P\mathbf{I} + 2\eta\mathbf{D} + \boxed{\boldsymbol{\Sigma}_A + \boldsymbol{\Sigma}_Q} \boxed{+ \boldsymbol{\Sigma}_C}$$

Active Q sector obeys dynamics as before

Polymeric stress obeys Johnson-Segalman constitutive dynamics

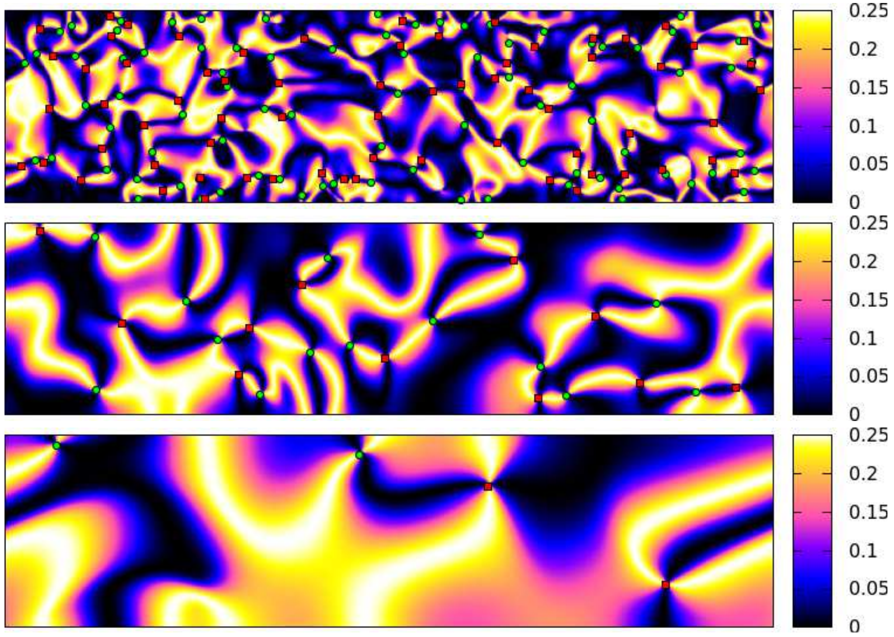
This combines rheology of passive complex fluids (section A)

With the dynamics of active nematic (section B)

[Hemingway et al., Phys. Rev. Lett. 2015, Phys. Rev. E 2016]

[Hemingway et al., Phys. Rev. Lett. 2015, Phys. Rev. E 2016]

Elastomeric limit of polymeric dynamics, $\tau_C \to \infty$



increasing time

Slow coarsening of active domains, with associated strain field

Outline

A) Rheology of complex fluids

1) overview
2) continuum models
3) 0D → 1D → 2D: a study in bulk flow instabilities

B) Hydrodynamics of active fluids

1) overview
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C) Interlude - numerical methods

D) Surface instabilities in complex fluids

1) extensional necking
2) edge fracture
3) wall slip

Numerical methods

Recall the equations to be solved:

a) force balance and incompressibility (`Stokes sector’):

$$\eta\nabla^2\boldsymbol{v} - \boldsymbol{\nabla}p + \boldsymbol{\nabla}\cdot\boldsymbol{\Sigma} = \boldsymbol{0}$$ Stokes force balance

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

b) viscoelastic constitutive equation

$$(\partial_t + \boldsymbol{v}\cdot\boldsymbol{\nabla})\boldsymbol{\Sigma} = 2G\mathbf{D} + f(\boldsymbol{\Sigma}, \boldsymbol{\nabla}\boldsymbol{v}) - \frac{1}{\tau}g(\boldsymbol{\Sigma}) + \ell^2\nabla^2\boldsymbol{\Sigma}$$

At any timestep in code, have two substeps:

First, solve Stokes sector at fixed $\boldsymbol{\Sigma}$ to calculate $\boldsymbol{v}$ (and p)

Second, update constitutive equation at fixed $\boldsymbol{v}$ to calculate $\boldsymbol{\Sigma}$

Will describe methods for periodic domain, give refs later for channels, etc

First substep: solve the Stokes sector

$$\begin{aligned} \eta\nabla^2\boldsymbol{v} - \boldsymbol{\nabla}p + \boldsymbol{f} &= \boldsymbol{0} \\ \boldsymbol{\nabla}\cdot\boldsymbol{v} &= 0 \end{aligned}$$

Stokes force balance

Incompressibility

These are linear and non-local, so best handled in Fourier space (FFTW)

$$\begin{aligned} \eta(ik)^2\widehat{\boldsymbol{v}}_{\boldsymbol{k}} - \mathrm{i}k\hat{p}_{\boldsymbol{k}} + \widehat{\boldsymbol{f}}_{\boldsymbol{k}} &= \boldsymbol{0} \\ \mathrm{i}\mathbf{k}\cdot\widehat{\boldsymbol{v}}_{\boldsymbol{k}} &= 0 \end{aligned}$$

Stokes force balance

Incompressibility

Take divergence $(i\boldsymbol{k}\,\cdot)$ of force balance eqn. to find pressure

$$\hat{p}_{\boldsymbol{k}} = -i\,\frac{\boldsymbol{k}\cdot\widehat{\boldsymbol{f}}_{\boldsymbol{k}}}{k^2}$$

Substituting this back into force balance equation gives

$$\widehat{\boldsymbol{v}}_{\boldsymbol{k}} = \underbrace{\frac{1}{\eta k^2}\left(\boldsymbol{\delta} - \frac{\boldsymbol{k}\boldsymbol{k}}{k^2}\right)}\cdot\widehat{\boldsymbol{f}}_{\boldsymbol{k}}$$

This is called the Oseen tensor (and is calculated just once, at each $\boldsymbol{k}$)

Second substep: updating dynamical equations (at fixed v)

Recall the equation to be solved:

$$(\partial_t + \boxed{\boldsymbol{v}\cdot\boldsymbol{\nabla})\boldsymbol{\Sigma}} = \boxed{2G\mathbf{D} + f(\boldsymbol{\Sigma},\boldsymbol{\nabla}\boldsymbol{v}) - \frac{1}{\tau}g(\boldsymbol{\Sigma})} + \boxed{\ell^2\nabla^2\boldsymbol{\Sigma}}$$

The essence of this is captured in: $\partial_t c + v\cdot\nabla c = \mathrm{f}(c) + \nabla^2 c$

So we have three ‘types’ of term (written now for our generalised variable c):

$\partial_t c = -v\cdot\nabla c$ Spatially non-local, quasi-linear advective terms

$\partial_t c = \nabla^2 c$ Spatially non-local, linear diffusive terms

$\partial_t c = \mathrm{f}(c)$ Spatially local, non-linear terms

Split the operator and solve these successively in turn

I will illustrate in one spatial dimension, but easily generalises…

Spatially local, non-linear term

Recall the general form of the equation:

$$\partial_t c + v \cdot \nabla \mathrm{c} = \mathrm{f}(c) + \nabla^2 c$$

Spatially local, non-linear term f(c) time-stepped in real space, eg via:

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = f(c_i^n)$$

This is `explicit Euler' update and works OK for small enough Δt

More sophisticated methods e.g. Runge Kutta - can use larger Δt

Spatially non-local, linear diffusion term

Recall the general form of the equation:

$$\partial_t c + v \cdot \nabla \mathrm{c} = \mathrm{f}(c) + \nabla^2 c$$

Spatially non-local, linear diffusion term is time-stepped in Fourier space:

$\partial_t c = \nabla^2 c$ Form in real space

$\partial_t \hat{c}_k = (ik)^2 \hat{c}_k$ After taking Fourier transform

Use semi-implicit time-stepping algorithm:

$$\frac{\hat{c}_k^{n+1} - \hat{c}_k^n}{\Delta t} = (ik)^2 \left(\frac{\hat{c}_k^{n+1} + \hat{c}_k^n}{2} \right)$$

Other time-stepping algorithms are possible, e.g., implicit Euler

Spatially non-local, quasi-linear advection term

Recall the general form of the equation:

$$\partial_t c + v \cdot \nabla \mathrm{c} = \mathrm{f}(c) + \nabla^2 c$$

Spatially non-local, quasi-linear advection term:

$$\partial_t c = -v \cdot \nabla \mathrm{c}$$

Handle in real space using `third order upwinding', and Euler time-stepping

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + \left(a^+ c_{x,i}^- + a^- c_{x,i}^+\right) = 0 \qquad a^+ = \max(v_i, 0)\,, a^- = \min(v_i, 0)$$

$$c_{x,i}^- = \frac{+2c_{i+1} + 3c_i - 6c_{i-1} + c_{i-2}}{6\Delta x} \qquad c_{x,i}^+ = \frac{-c_{i+2} + 6c_{i+1} - 3c_i - 2c_{i+1}}{6\Delta x}$$

Summary of numerical methods

Time-stepping algorithm

Spatially local, non-linear terms handled in real space

Spatially non-local diffusive terms terms handled in Fourier space

Advective term handled in real space using third order upwinding

Stokes sector handled using Oseen tensor (for biperiodic flow)

For methods in channel, and details of algorithms used, see:

C. Canuto et al. *Spectral Methods in Fluid Dynamics*, 1988.

C. Canuto et al. *Spectral Methods: Evolution to Complex Geometries and Applications to Fluid Dynamics*., 2007.

R. Peyret. *Spectral Methods for Incompressible Viscous Flow*, 2002.

C. Pozrikidis, *Introduction to Theoretical and Computational Fluid Dynamics*, 2011.

Reminder so far

A) Rheology of complex fluids

1) overview
2) continuum models
3) 0D → 1D → 2D: a study in bulk flow instabilities

B) Hydrodynamics of active fluids

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C) Interlude - numerical methods

D) Surface instabilities in complex fluids

1) extensional necking
2) edge fracture
3) wall slip

Today's lecture

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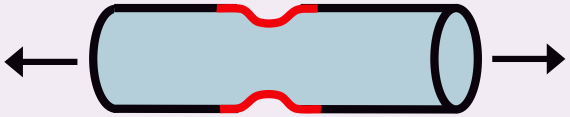
Surface instabilities: three major challenges in experimental rheometry

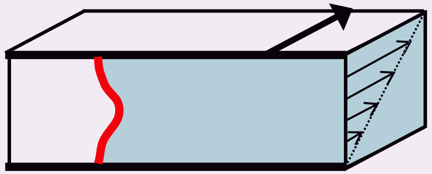
Extension:



“necking”

of filament

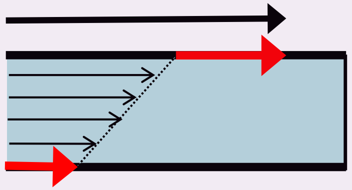
Shear:



“edge fracture”

of fluid-air interface

Shear:



“wall slip”

of fluid w.r.t. plates

Theoretical goals:

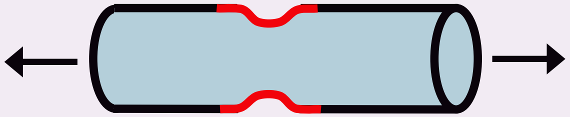
derive fluid-universal criterion for the onset of instability

understand the physical mechanism of instability

suggest practical strategies to mitigate instability

The three major challenges in experimental rheometry…?

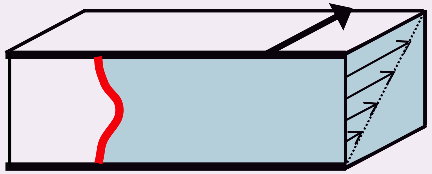
Extension:



“necking”

of filament

Shear:



“edge fracture”

of fluid-air interface

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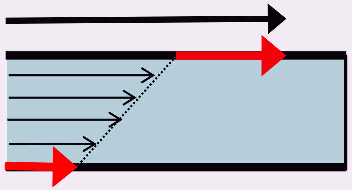


“wall slip”

of fluid w.r.t. plates

Theoretical goals:

derive fluid-universal criterion for the onset of instability

understand the physical mechanism of instability

suggest practical strategies to mitigate instability

[Review: McKinley + Sridhar, Ann. Rev. Fluid Mech. 2002]

Necking in extensional filament stretching rheometry

Experimental aim:

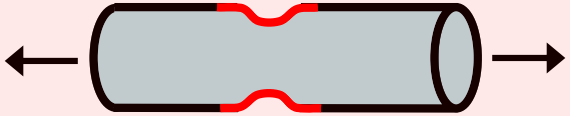
achieve homogeneous filament stretching.

Measure extensional e.g. constitutive curve: $\sigma_E(\dot{\varepsilon})$

σ_E = tensile stress (force/area)

$\dot{\varepsilon}$ = Hencky strain rate

Experimental practice:

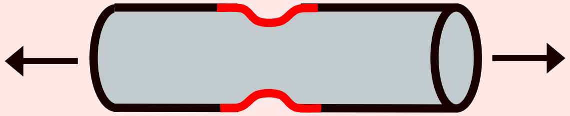


“necking” of filament hampers measurement.

(Partially controlled by feedback strategies e.g. Hoyle et al. JoR 2013.)

Necking in extensional filament stretching

Extension:



"necking"

of filament

Introduction: experimental observations

Pre-existing criterion in an elastic solid: Considère criterion

Here: criterion for necking in viscoelastic fluids

Calculation 0): "back of a postage stamp"

Calculation 1): constant imposed tensile stress

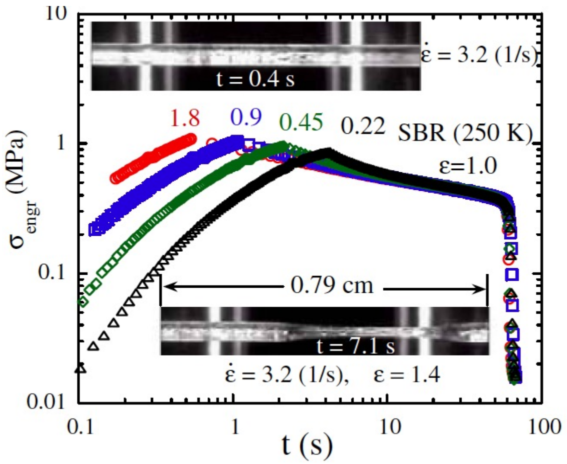
Calculation 2): constant imposed Hencky strain rate

Necking - conclusions

Introduction to necking: widely seen in complex fluids

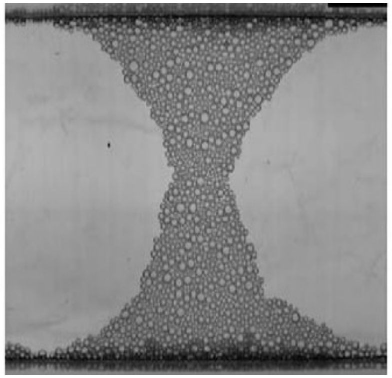
Step strain, entangled melts

[Wang et al. PRL 2007]



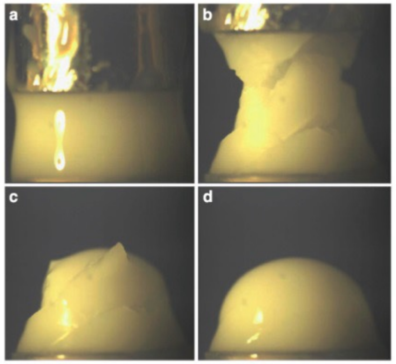
Bubble raft

[Kuo + Dennin JoR 2012]



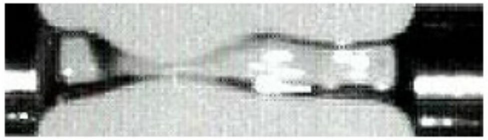
Dense colloids

[Smith et al Nat. Comm. 2010]



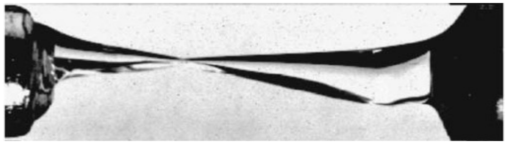
Associative polymers

[Tripathi et al. Macromol. 2006]



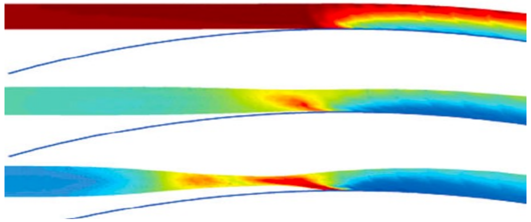
Wormlike micelles

[Bhardwaj et al. J. Rheol. 2007]

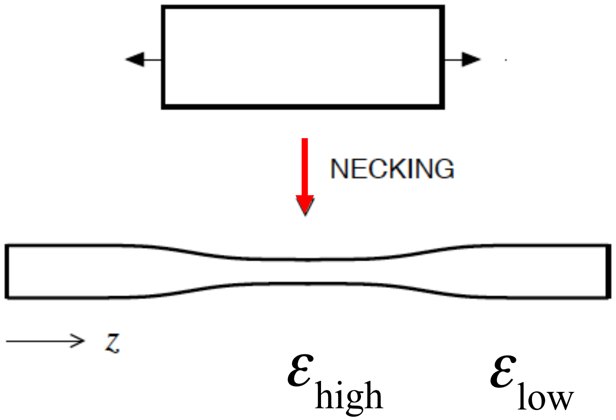


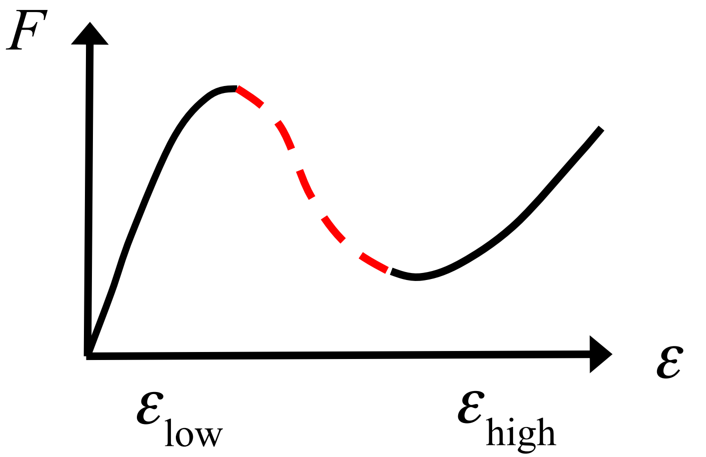
Doi Edwards + chain stretch

[Lyhne et al PRL 2009]



Pre-existing criterion: necking in a nonlinear elastic solid





Considère criterion:

Necking arises if tensile force is non-monotonic in extensional strain

[Considère Ann. Ponts Chausees 1885]

Criterion for onset of necking instability in complex fluids?

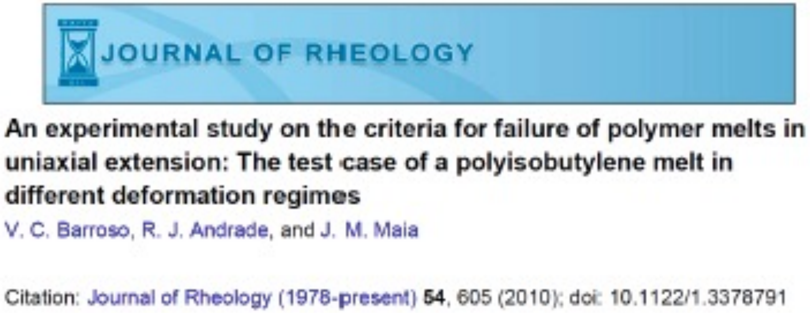
Considère criterion widely discussed...

JOURNAL OF RHEOLOGY

Uniaxial extensional rheology of well-characterized comb polymers

H. Lentzakis, D. Vlassopoulos, D. J. Read, H. Lee, T. Chang, P. Driva, and N. Hadjichristidis

Citation: Journal of Rheology **57**, 605 (2013); doi: 10.1122/1.4789443

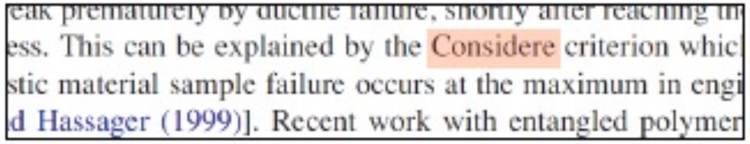


JOURNAL OF RHEOLOGY

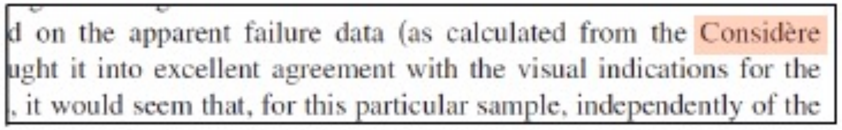
An experimental study on the criteria for failure of polymer melts in uniaxial extension: The test case of a polyisobutylene melt in different deformation regimes

V. C. Barroso, R. J. Andrade, and J. M. Maia

Citation: Journal of Rheology (1978-present) **54**, 605 (2010); doi: 10.1122/1.3378791



eak prematurely by ductile failure, shortly after reaching th
ess. This can be explained by the Considere criterion whic
stic material sample failure occurs at the maximum in engi
d Hassager (1999)]. Recent work with entangled polymer



d on the apparent failure data (as calculated from the Considère
ught it into excellent agreement with the visual indications for the
, it would seem that, for this particular sample, independently of the

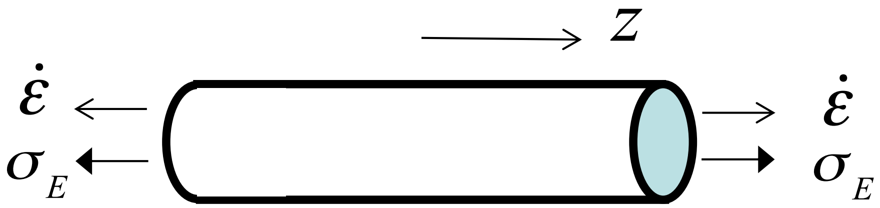
… but has obvious shortcomings:

- Takes force = force (strain) only. For fluids, strain rate is important too
- Static criterion: can’t predict dynamical rate of necking onset

[Ide + White JNNFM 1977; Olagunju JNNFM 1999 & Int J. Nonlin Mech. 2011]

Criterion for onset of necking instability in complex fluid

Initially uniform cylinder

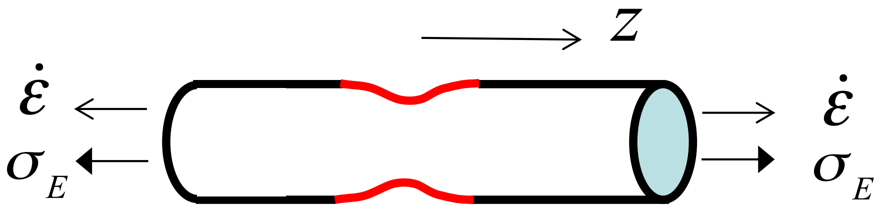


$A(t)$	cross sectional area
$\dot{\varepsilon}(t)$	Hencky strain rate
$\sigma_E(t)$	tensile stress
$F(t)$	tensile force $= A(t)\sigma_E(t)$

[Ide + White JNNFM 1977; Olagunju JNNFM 1999 & Int J. Nonlin Mech. 2011]

Criterion for onset of necking instability in complex fluid

How/why does it just start to neck



$A(z,t)$	cross sectional area
$\dot{\varepsilon}(z,t)$	Hencky strain rate
$\sigma_E(z,t)$	tensile stress
$F(t)$	tensile force

Consider small perturbations, i.e.,

perform linear stability analysis.

Consider long wavelengths, i.e.,

use slender filament approach.

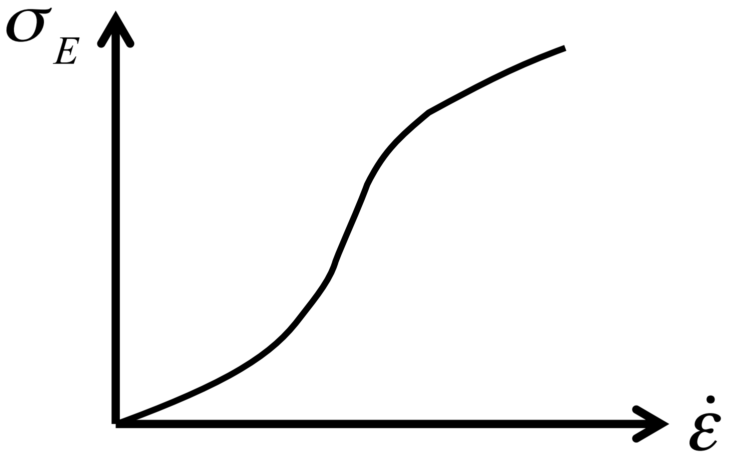
Neglect surface tension, i.e.,

study highly viscoelastic filaments.

Criterion for onset of necking instability in complex fluid

How/why does it just start to neck

Extensional constitutive curve



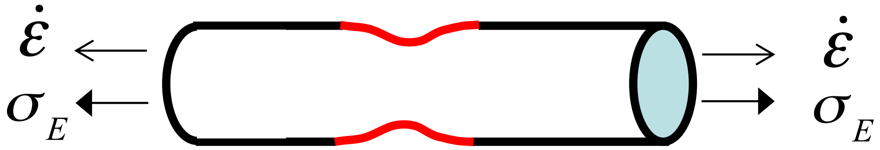
If attainable, defines steady

state stress *vs.* strain rate in

in uniformly thinning filament

Criterion for onset of necking instability in complex fluid

How/why does it just start to neck



Calculation 0)

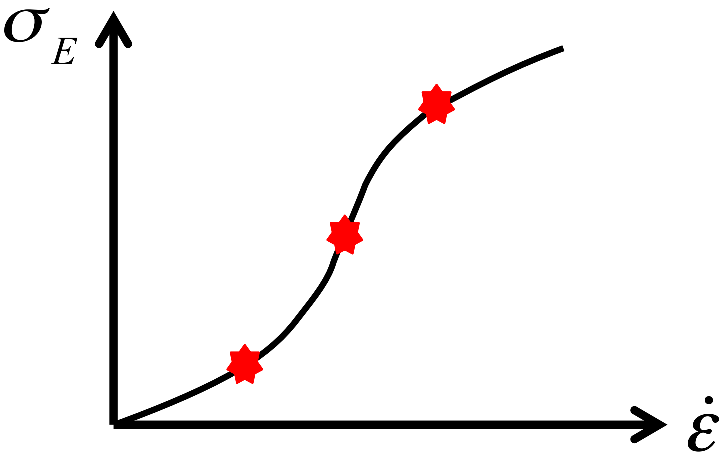
Initially uniform thinning cylinder

with steady state $\dot{\varepsilon}$ and $\sigma_E\left(\dot{\varepsilon}\right)$

on constitutive curve.

(Idealised. Unrealistic…?)

Extensional constitutive curve



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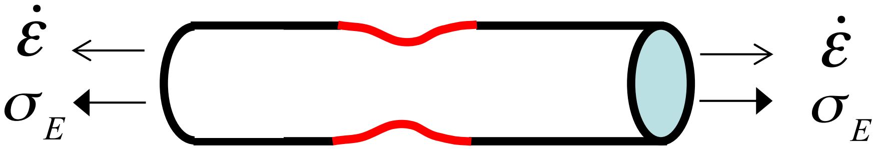
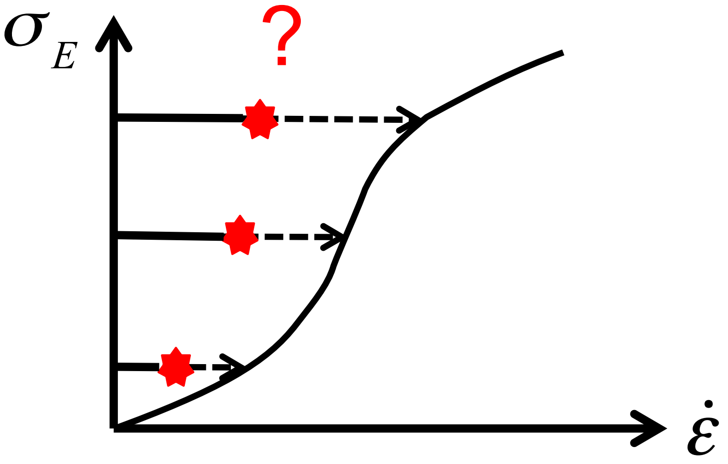
Criterion for onset of necking instability in complex fluid

How/why does it just start to neck



Extensional constitutive curve



Calculation 1)

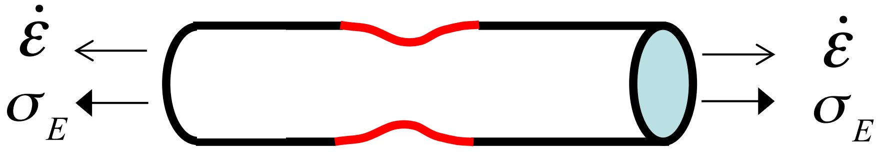
Initially unloaded cylinder

then subject to switch on

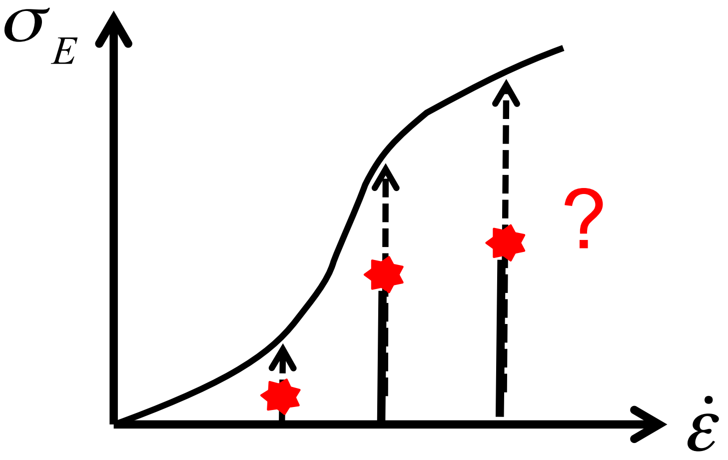
of a constant stress σ_E

Criterion for onset of necking instability in complex fluid

How/why does it just start to neck



Extensional constitutive curve



Calculation 2)

Initially undeformed cylinder

then subject to switch on

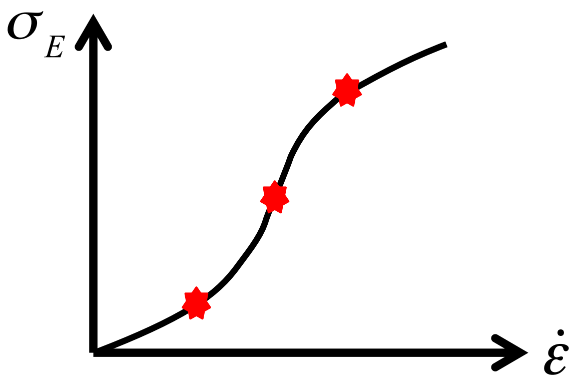
of a constant strain rate $\dot{\varepsilon}$

Calculation 0) initial uniform cylinder that already attained constitutive curve

Back of postage stamp calculation

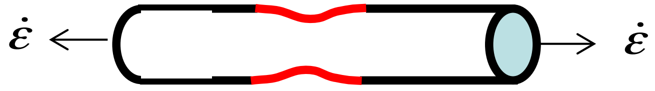
$\dot{A} = -\dot{\varepsilon} A$ mass conservation

$F = A\sigma_E\left(\dot{\varepsilon}\right)$ uniform force



Initially perfectly uniform cylinder with thinning area $A = A_0 \exp\left(-\dot{\varepsilon} t\right)$

plus spatially varying perturbations of small amplitude $\delta\dot{\varepsilon}\left(z,t\right), \delta a\left(z,t\right)$

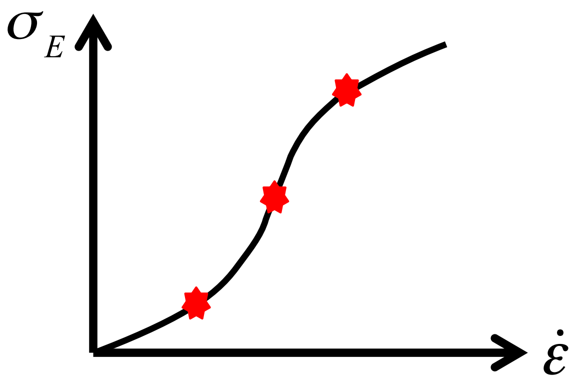


Calculation 0) initial uniform cylinder that already attained constitutive curve

Back of postage stamp calculation

$\dot{A} = -\dot{\varepsilon} A$ mass conservation

$F = A\sigma_E\left(\dot{\varepsilon}\right)$ uniform force

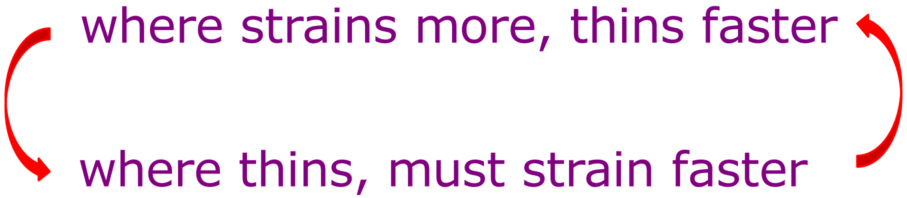


Initially perfectly uniform cylinder with thinning area $A = A_0 \exp\left(-\dot{\varepsilon} t\right)$

plus spatially varying perturbations of small amplitude $\delta\dot{\varepsilon}\left(z,t\right), \delta a\left(z,t\right)$

$$\delta\dot{a} = -\delta\dot{\varepsilon}$$

$$\delta F = 0 = \sigma_E \delta a + \left(d\sigma_E / d\dot{\varepsilon}\right)\delta\dot{\varepsilon}$$



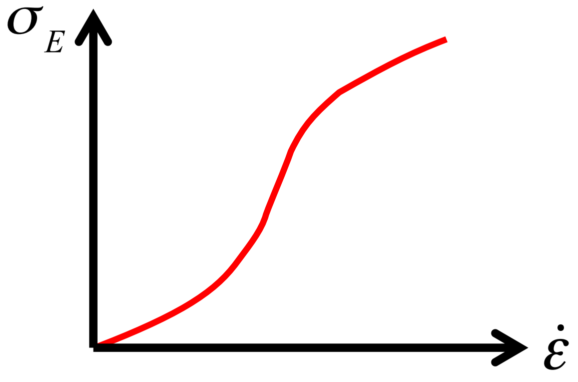
where strains more, thins faster

where thins, must strain faster

- ➢ Simple mechanistic understanding of the physics of necking instability

Calculation 0) initial uniform cylinder that already attained constitutive curve

Back of postage stamp calculation



$\dot{A} = -\dot{\varepsilon} A$ mass conservation

$F = A\sigma_E\left(\dot{\varepsilon}\right)$ uniform force

Initially perfectly uniform cylinder with thinning area $A = A_0 \exp\left(-\dot{\varepsilon} t\right)$

plus spatially varying perturbations of small amplitude $\delta\dot{\varepsilon}\left(z,t\right), \delta a\left(z,t\right)$

$$\delta\dot{a} = \frac{\sigma_E}{\sigma_E{}'}\delta a$$

Any constitutive curve with positive slope $\sigma_E{}' > 0$

gives instability to necking

[prime denotes derivative w.r.t. strain rate $\dot{\varepsilon}$]

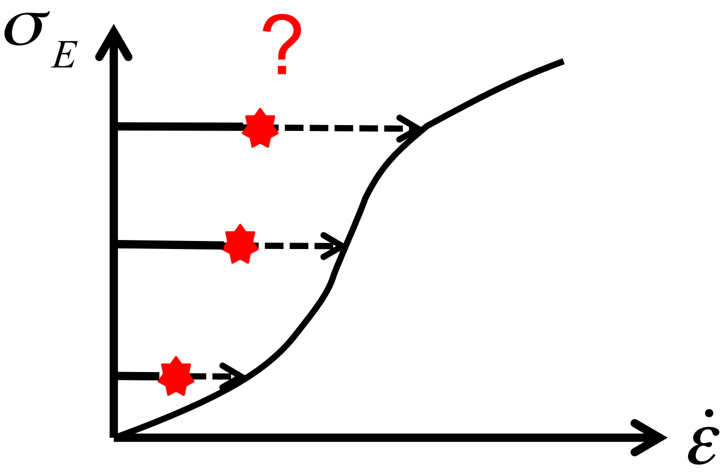
Calculation 1) Necking following imposition of a step stress

$\dot{A} = -\dot{\varepsilon} A$ mass conservation

$F = A\sigma_E$ uniform force

$\sigma_E = GW + 3\eta\dot{\varepsilon}$ viscoelastic + solvent

$\dot{W} = \ldots$ viscoelastic constitutive eqn.



Impose stress σ_E in initially undeformed, unloaded sample

Calculation 1) Necking following imposition of a step stress

$\dot{A} = -\dot{\varepsilon} A$ mass conservation

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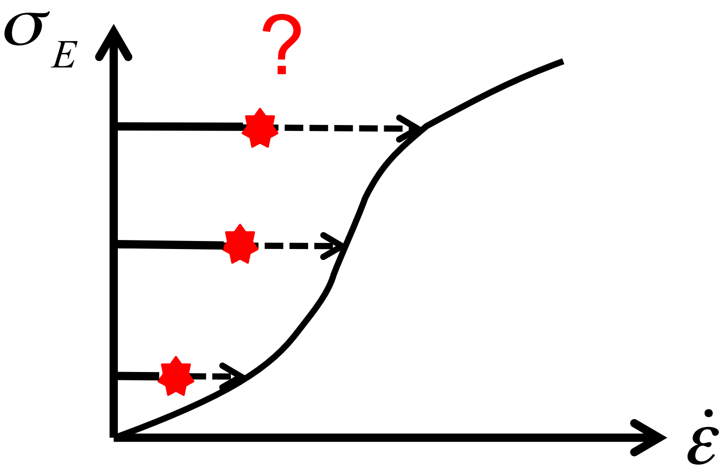

Impose stress σ_E in initially undeformed, unloaded sample

Strain rate quickly attains constitutive curve

No significant necking during that fast evolution to constitutive curve

Calculation 1) Necking following imposition of a step stress

$\dot{A} = -\dot{\varepsilon} A$ mass conservation

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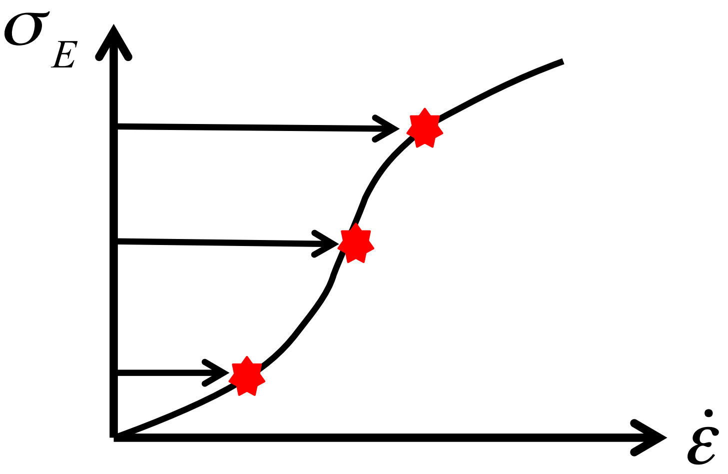


Impose stress σ_E in initially undeformed, unloaded sample

Strain rate quickly attains constitutive curve

No significant necking during that fast evolution to constitutive curve

Once attains constitutive curve, necks as per calculation 0) $\delta\dot{a} = \frac{\sigma_E}{\sigma_E'}\delta a$

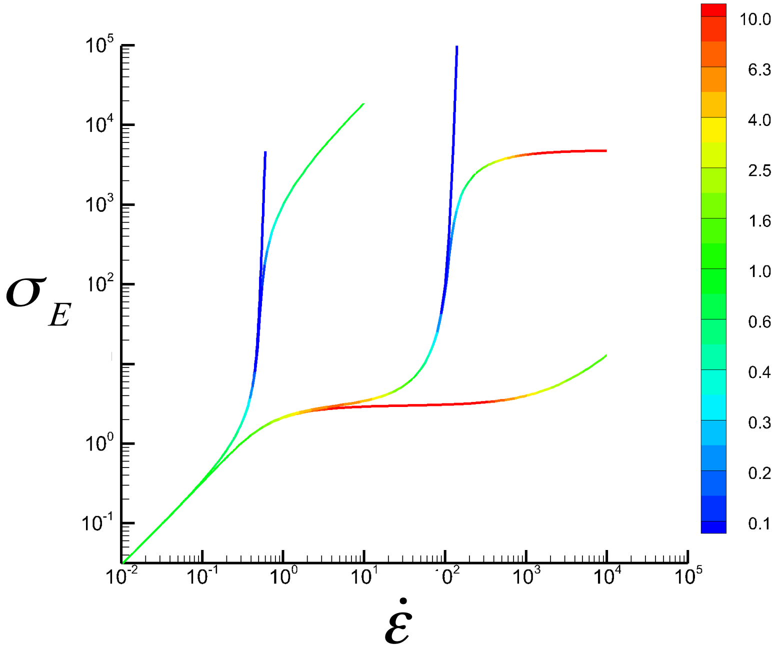
Calculation 1) Necking following imposition of a step stress

Colourscale: normalised necking rate

$$\widehat{\omega} = \omega \big/ \dot{\varepsilon} = \sigma_E \big/ \dot{\varepsilon}\sigma_E{}'$$

for (curves clockwise)

- Oldroyd B
- Giesekus , fene P (indistinguishable)
- Rolie-poly + chain stretch
- Rolie-poly + finite chain stretch
- Rolie-poly without chain stretch



Flatter constitutive slope → more spectacular necking

[Likhtman and Graham JNNFM 2003]

Calculation 1) Necking following imposition of a step stress

Colourscale: normalised necking rate

$$\widehat{\omega} = \omega / \dot{\varepsilon} = \sigma_E / \dot{\varepsilon}\sigma_E'$$

For Rolie-poly + finite chain stretch

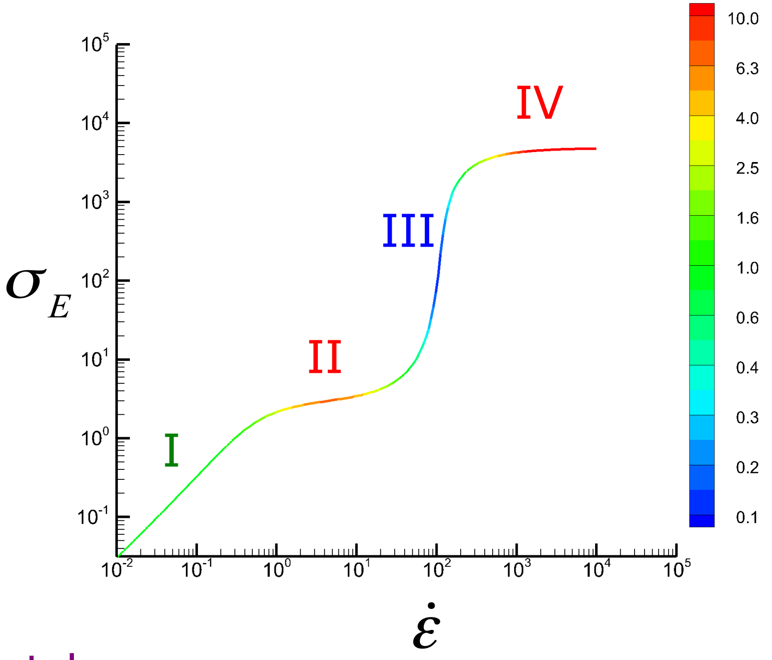
Four regimes:

I: Unstable even in slow flow limit

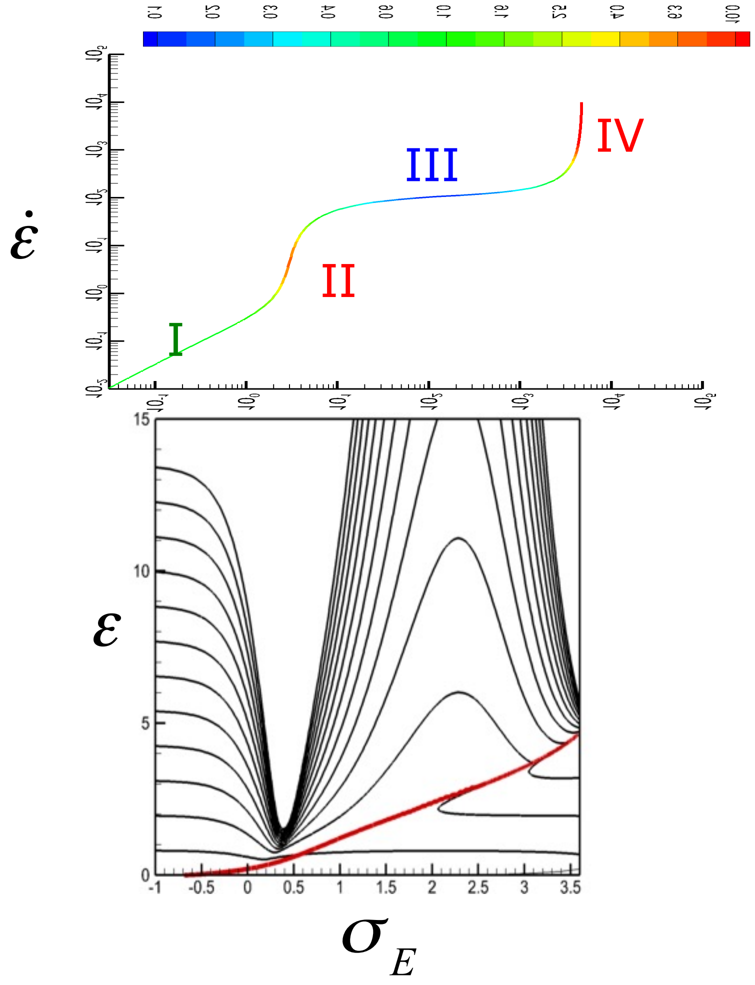
II: saturated orientation → highly unstable

III: strongly stabilised by increasing chain stretch

IV: saturated chain stretch → highly unstable



Calculation 1) Necking following imposition of a step stress

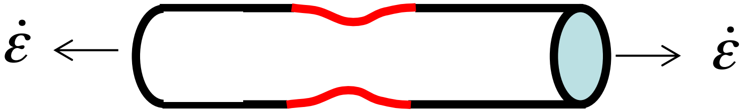


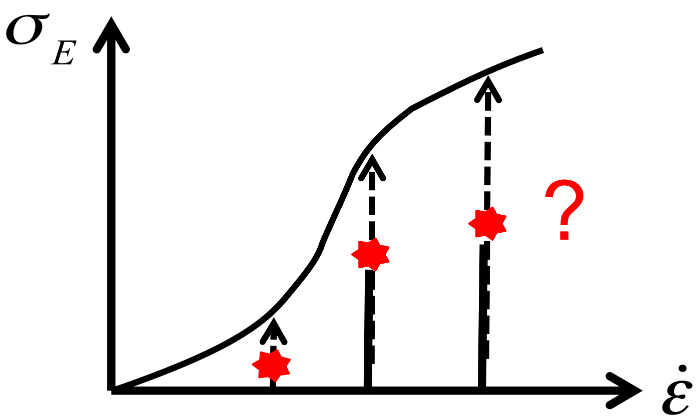
inverted constitutive curve $\dot{\varepsilon}\left(\sigma_E\right)$

🟥 attains constitutive curve

⬛ contours of constant δa

Calculation 2) Necking in filament stretching at constant Hencky strain rate





In any filament stretching experiment:

At what time (or strain) does necking start?

Does this correspond to experimentally identifiable rheological signature…

… such as an overshoot in the force as a function of strain $dF/d\varepsilon < 0$?

…or some characteristic feature in the time evolving stress signal $\sigma_E(t)$?

[note we can equivalently report evolution with time t or strain $\varepsilon = \dot{\varepsilon}t$]

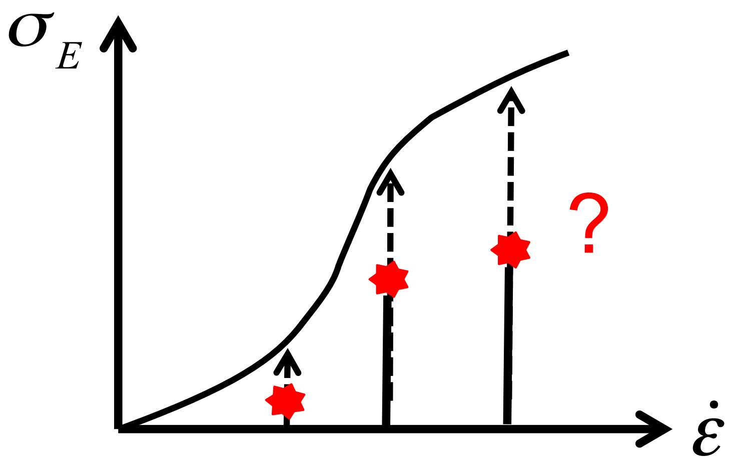
Calculation 2) Necking in filament stretching at constant Hencky strain rate

$\dot{A} = -\dot{\varepsilon} A$ mass conservation

$F = A\sigma_E$ uniform force

$\sigma_E = GW + 3\eta\dot{\varepsilon}$ viscoelastic + solvent

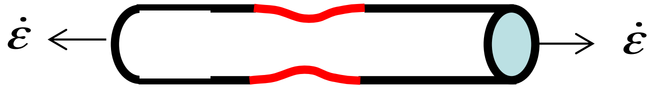
$\dot{W} = \ldots$ viscoelastic constitutive eqn.



Initial uniform cylinder (“base state”) has time-evolving area and stress

$A = A_0 \exp\left(-\dot{\varepsilon}t\right)$ and $\sigma_E = \sigma_E\left(t\right)$

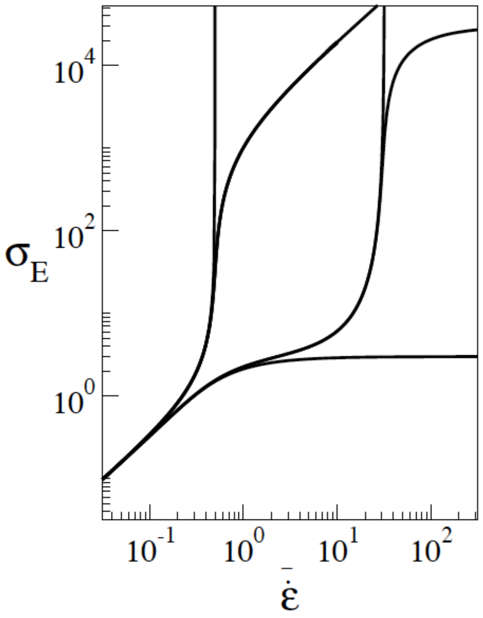
Small amplitude spatially varying fluctuations to onset of necking



$\delta\dot{\varepsilon}\left(z,t\right), \delta W\left(z,t\right), \delta a\left(z,t\right)$

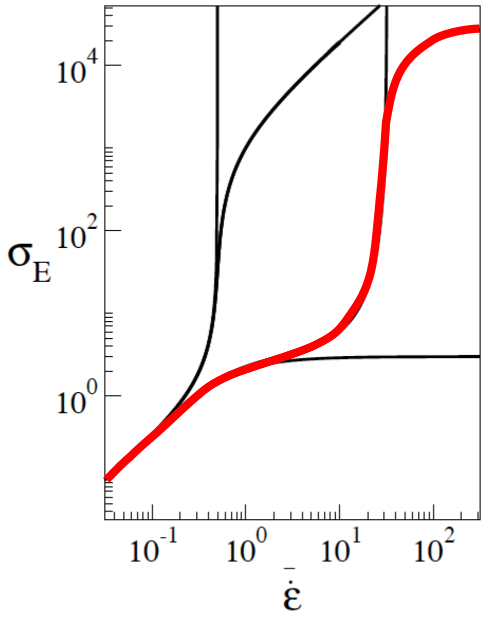
Onset of necking and its rheological signature

constitutive curve



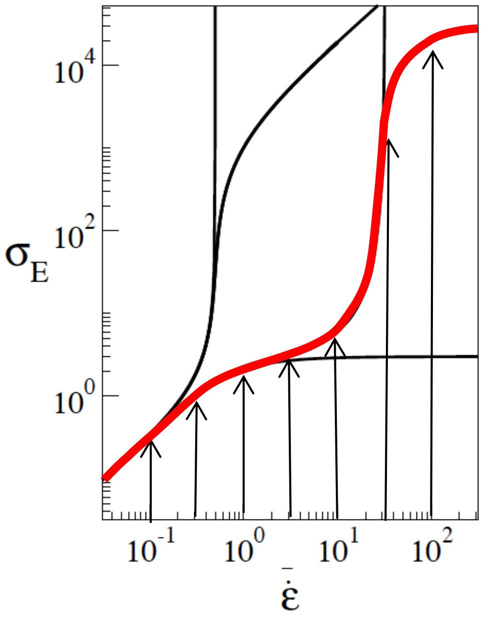
Onset of necking and its rheological signature

constitutive curve

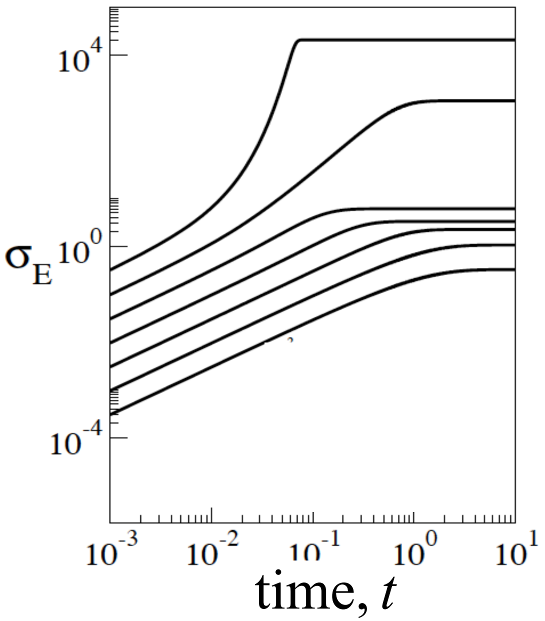


Onset of necking and its rheological signature

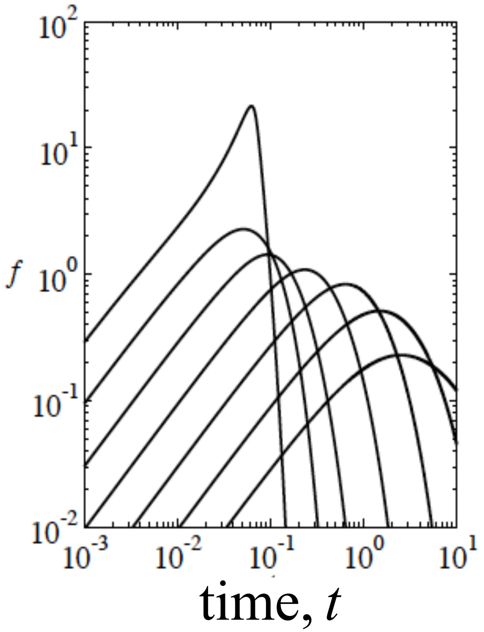
constitutive curve



stress transient



force evolution

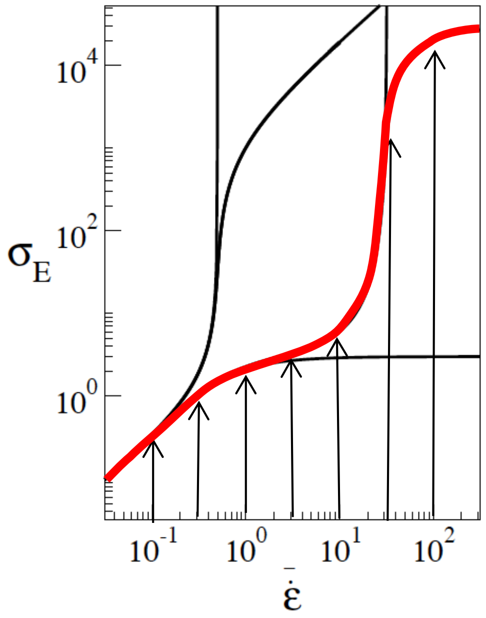


Onset of necking and its rheological signature

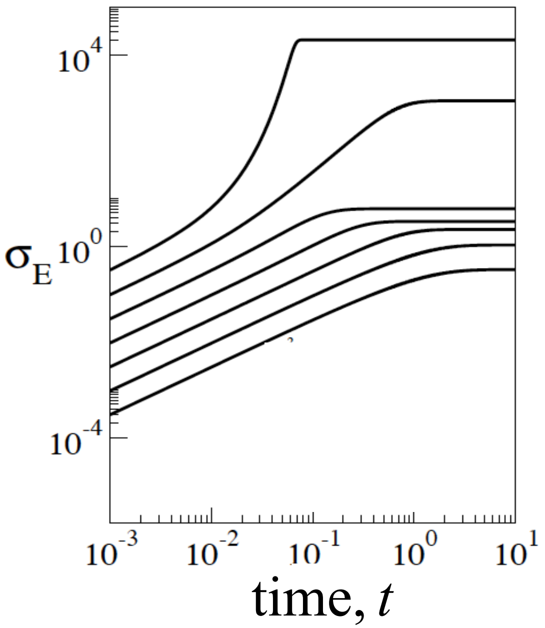
Recall: the Considere criterion predicts necking when $F' < 0$

[prime now denotes derivative w.r.t. strain and so equivalently w.r.t. time]

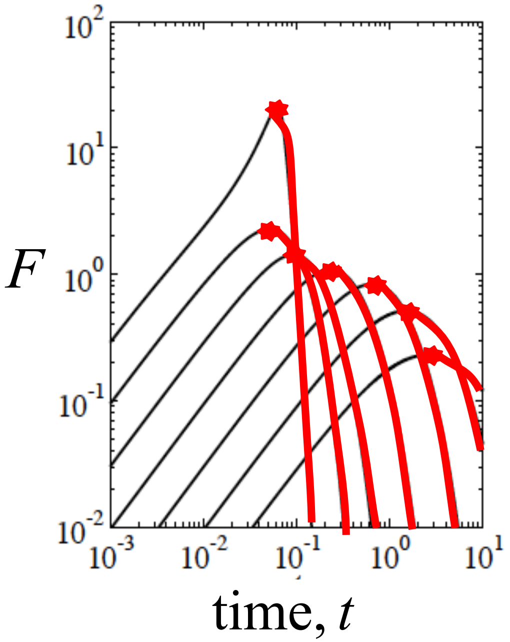
constitutive curve



stress transient



force evolution

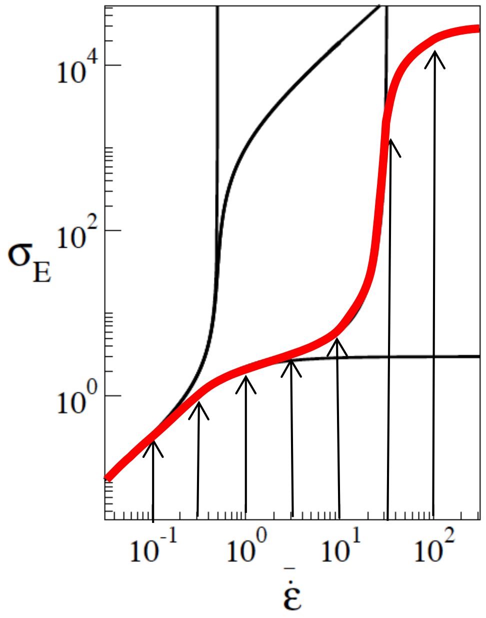


Onset of necking and its rheological signature

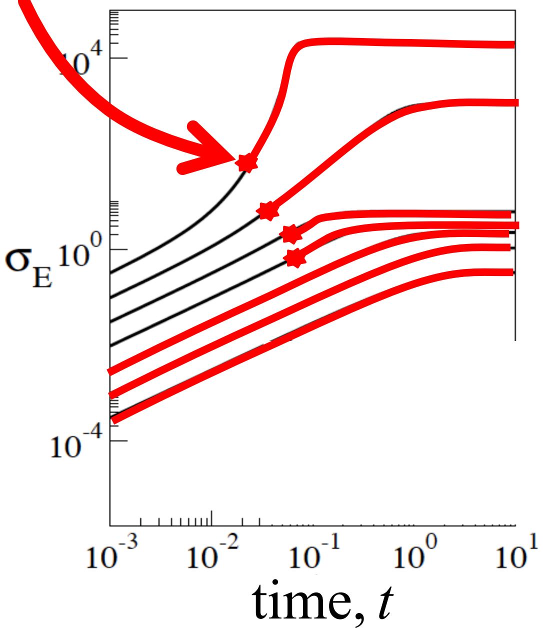
We find: stress curvature

$$\omega = -O\left(\dot{\varepsilon}\right)\boxed{\sigma_E{}''}\big/\sigma_E{}'$$

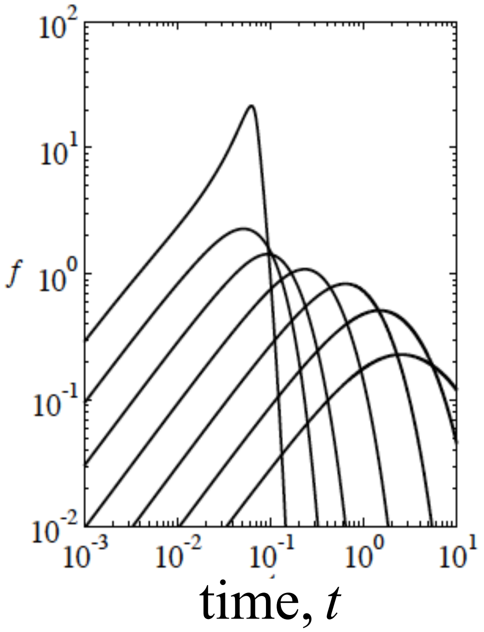
constitutive curve



stress transient



force evolution

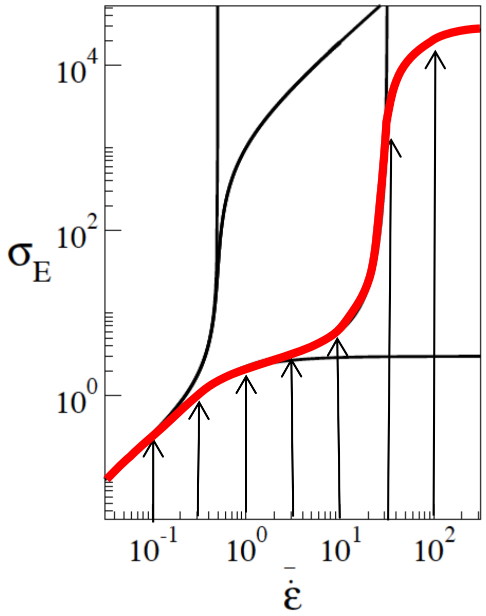


Onset of necking and its rheological signature

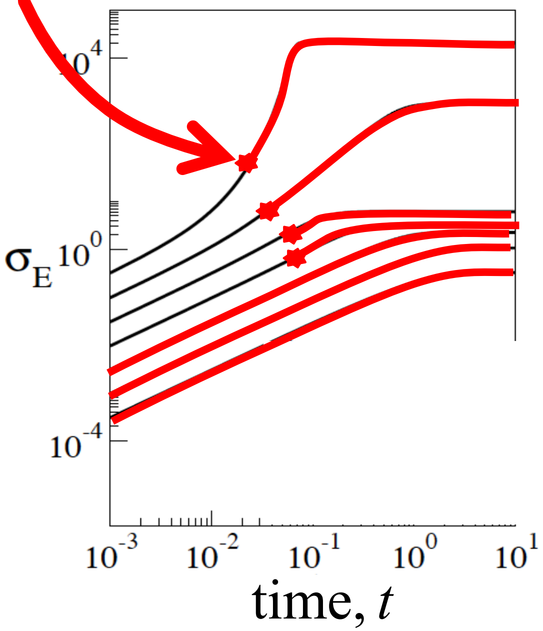
We find: stress curvature and modified Considere

$\omega = -O\left(\dot{\varepsilon}\right)\boxed{\sigma_E''}/\sigma_E'$ and $\omega = -O\left(\frac{1}{\eta}\right)\boxed{F'_{\text{elastic}}}$

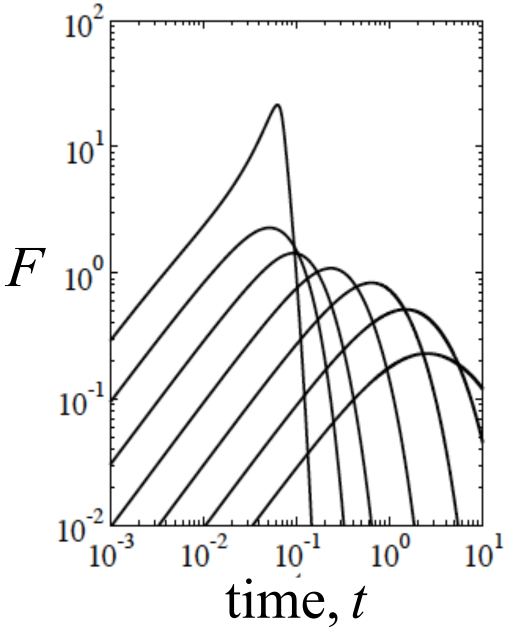
constitutive curve



stress transient



force evolution



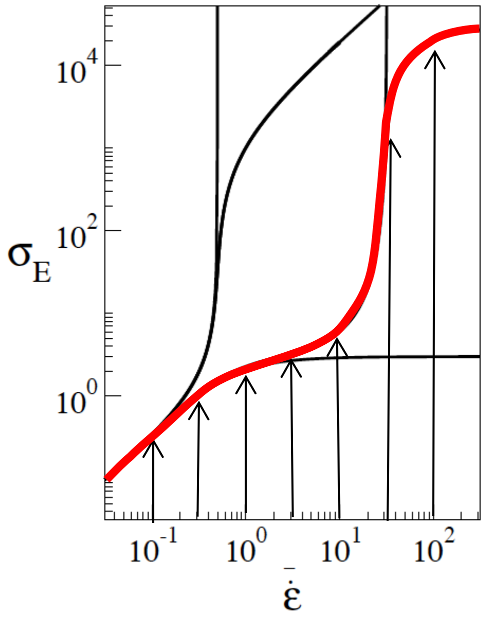
Onset of necking and its rheological signature

We find: stress curvature and modified Considere

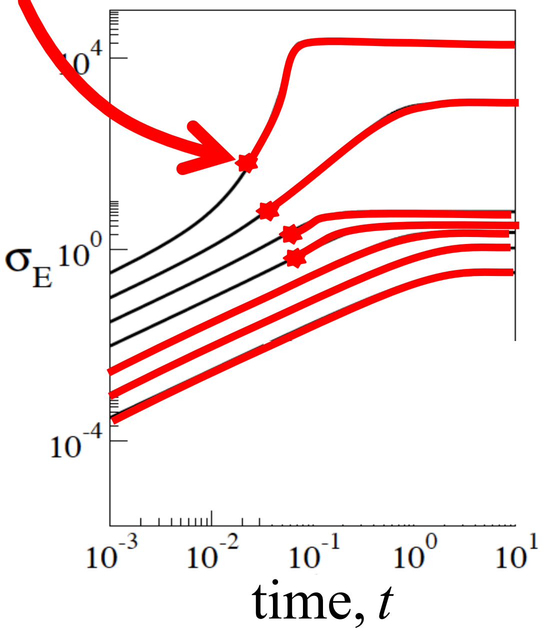
$$\omega = -O\left(\dot{\varepsilon}\right)\boxed{\sigma_E''}/\sigma_E' \quad \text{and} \quad \omega = -O\left(\tfrac{1}{\eta}\right)\boxed{F'_{\text{elastic}}}$$

NOT

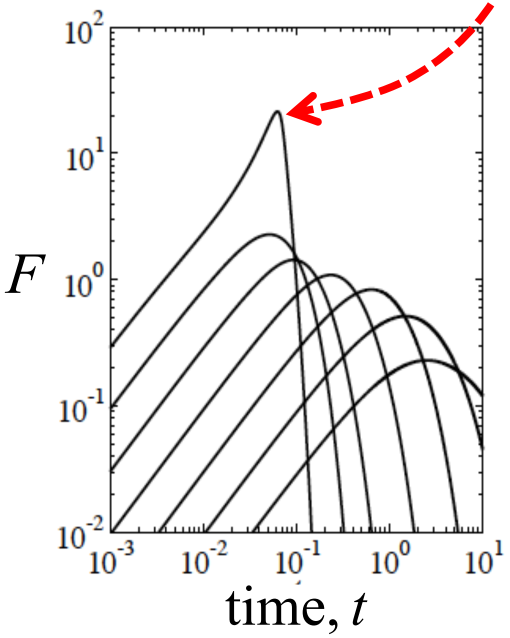
constitutive curve



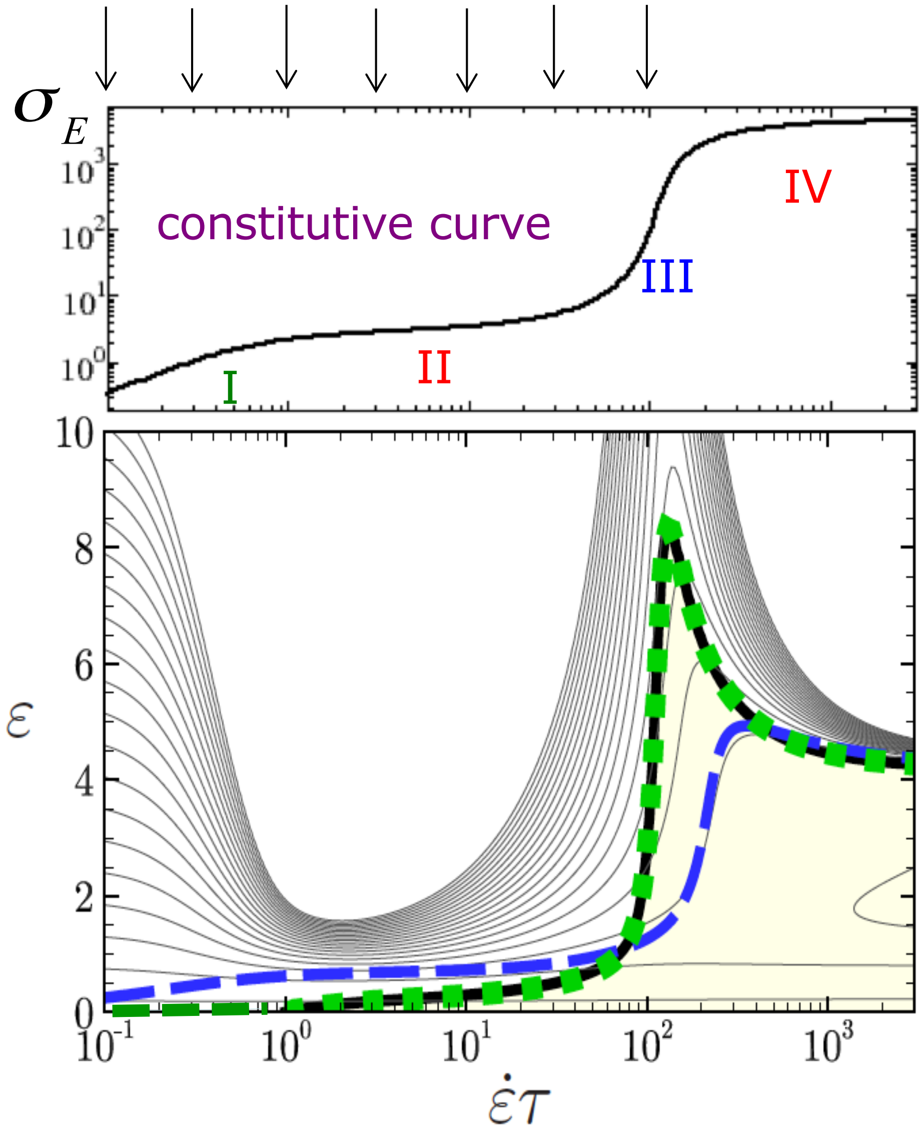
stress transient



force evolution



Numerical results: Rolie-poly model with finite chain stretch



I: slow flow regime

II: saturated orientation

III: increasing chain stretch

IV: saturated chain stretch

—— contours of constant δa

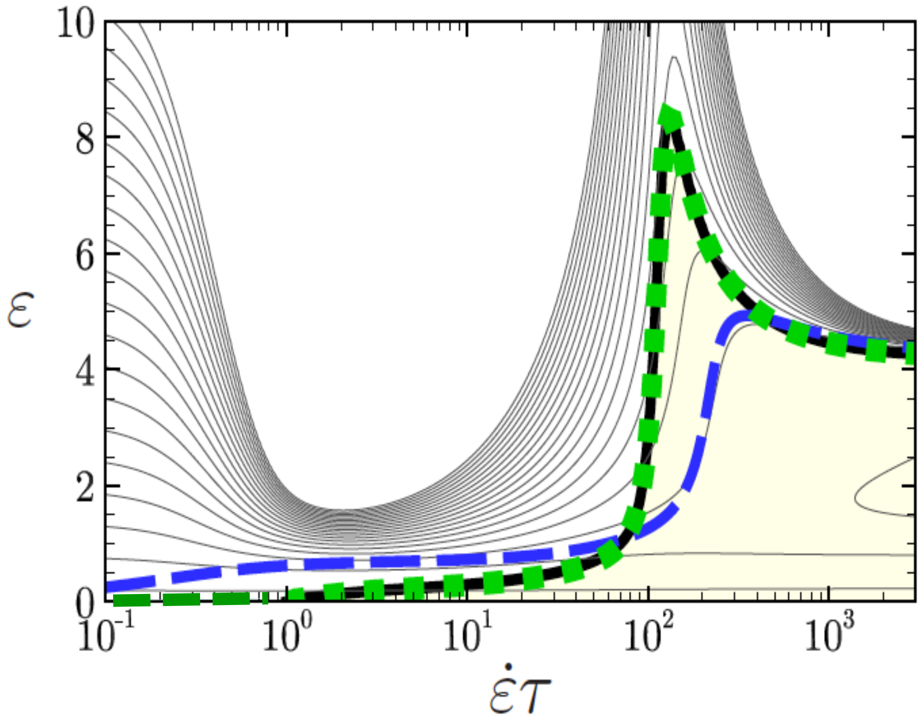
▬ ▬ ▬ stress curvature criterion $\sigma_E'' = 0$
describes necking onset well

▬ ▬ ▬ Considere criterion $F' = 0$
force overshoot exists but describes
necking onset much less well

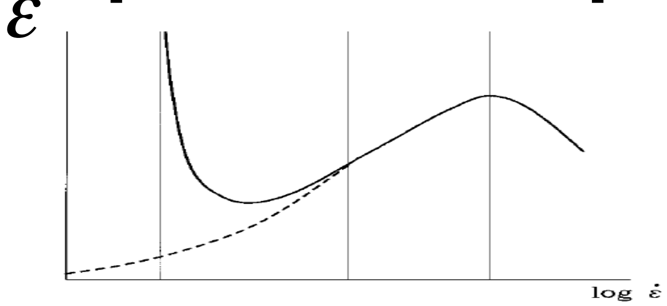
▬ ▬ ▬ modified Considere mode $F'_{\text{elastic}} = 0$
only unstable without chain stretch
(so not here!)

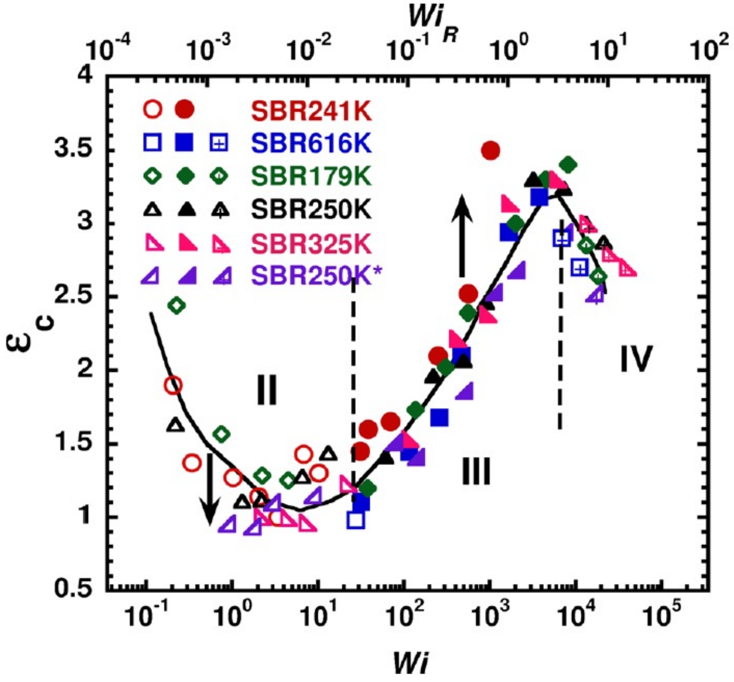
Rolie-poly model with finite chain stretch: compare with experiment

Strain at failure vs strain rate



[Malkin + Petrie 1997]





[Zhu and Wang 2013]

Necking of a filament in extensional stretching: conclusions

- Predicted necking will inevitably arise in (most) complex fluids
- Moved beyond Considère criterion of elastic solids $dF / d\varepsilon < 0$
- Constant stress: necking rate goes as inverse slope of constitutive curve
- Constant strain rate: identified curvature criterion $d^2\sigma_{\mathrm{E}} / d\varepsilon^2 < 0$….

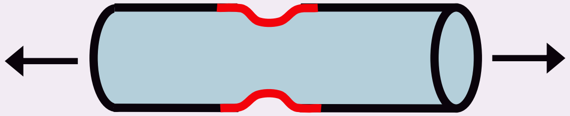
…. and modified-Considere criterion, carefully interpreted for liquids !

- Criteria hold in six popular constitutive models…
- …and capture four different regimes seen experimentally in entangled polymers

D. M. Hoyle and S. M. Fielding,	J. Nonnewton. Fluid Mech. **247** (2017) 32
D. M. Hoyle and S. M. Fielding,	J. Rheol. **60** (2016) 1347(a), 1377 (b)
D. M. Hoyle and S. M. Fielding,	Phys. Rev. Lett. **114** (2015) 158301
S. M. Fielding,	Phys. Rev. Lett. **107** (2011) 258301

Three key challenges in experimental rheometry

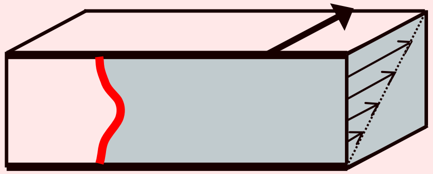
Extension:



“necking”

of filament

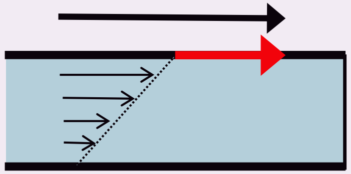
Shear:



“edge fracture”

of fluid-air interface

Shear:

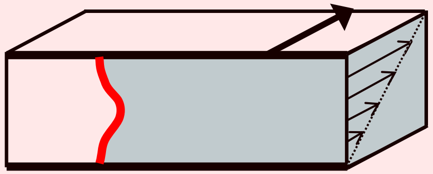


“wall slip”

of fluid w.r.t. plate

Outline: edge fracture in sheared complex fluids

Shear:



“edge fracture”

of fluid-air interface

Introduction to edge fracture: experimental observations

Early scaling criterion for the onset of edge fracture

Here: new criterion

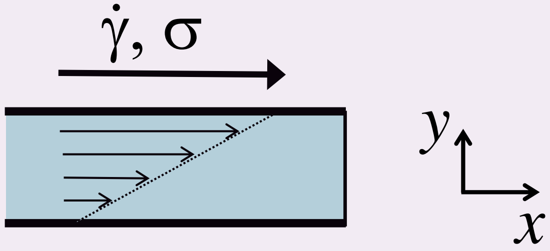
- Nonlinear simulation study of edge fracture
- Linear stability analysis for onset of edge fracture
- Mechanism and possible mitigation of edge fracture

Edge fracture - conclusions

[Mall-Gleissle et al. Rheol. Acta 2002; Schweizer JoR 2003; Costanzo Rheol. Acta 2018]

Edge fracture in shear rheometry

Experimental aim:



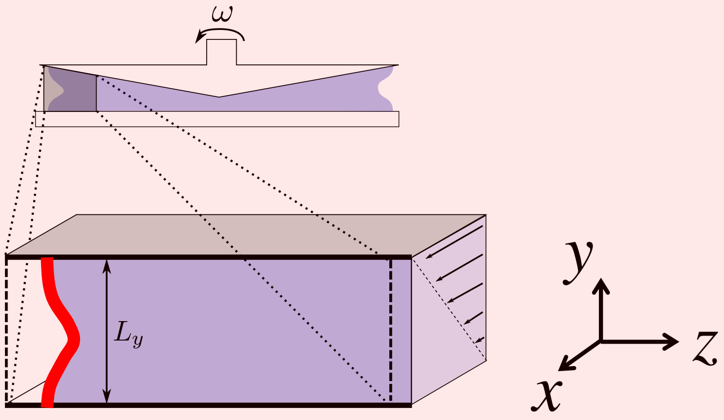
measure shear e.g.

flow curve $\sigma\,(\dot{\gamma})$

σ = shear stress

$\dot{\gamma}$ = shear rate

Experimental practice:



“edge fracture” of fluid-air interface hampers rheometry.

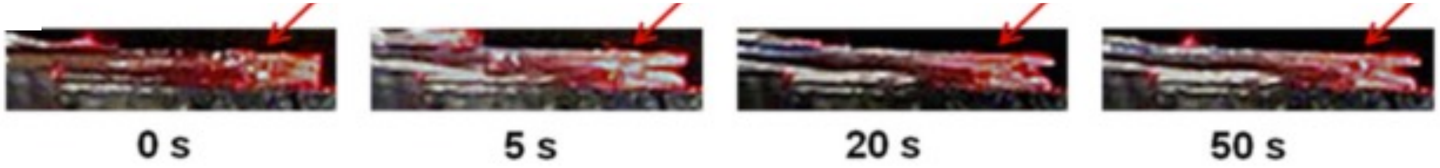
Mitigation strategies:

guard rings; cone-partitioned plates

x = flow, y = flow-gradient, z = vorticity

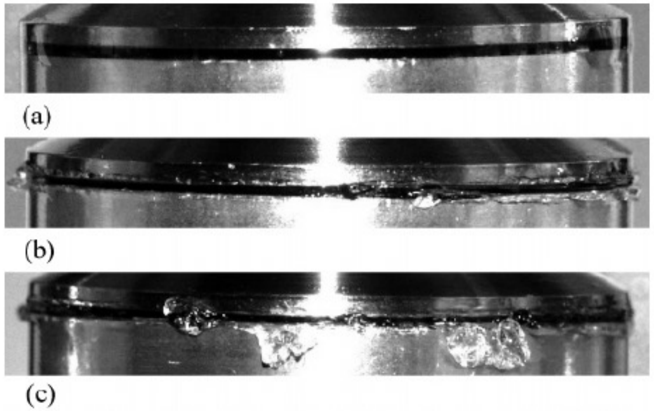
Experimental observations of edge fracture

Entangled polybutadiene solution: Li et al. J. Rheol. 2013

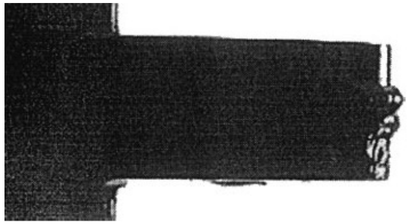


Entangled polybutadiene solution:

Inn, Wissbrun + Denn Macromol 2005.



Keentok & Xue, Rheol. Acta (1999)



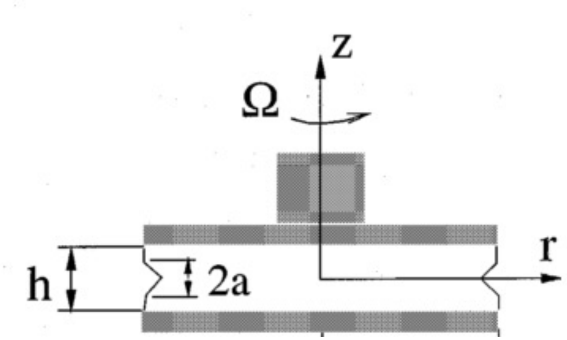
Shell Barbatia grease

“Edge fracture is the limiting factor in rotational rheometry”

Jensen & Christiansen, JNNFM (2008)

[Tanner and Keentok, J. Rheol (1983); Lee, Tripp, Magda, Rheol. Acta (1992)]

Early scaling criterion for edge fracture



Assume initial semi-circular `crack' of radius a

Assume flow only in main flow (theta) direction

Assume flow field has form as for Newtonian fluid

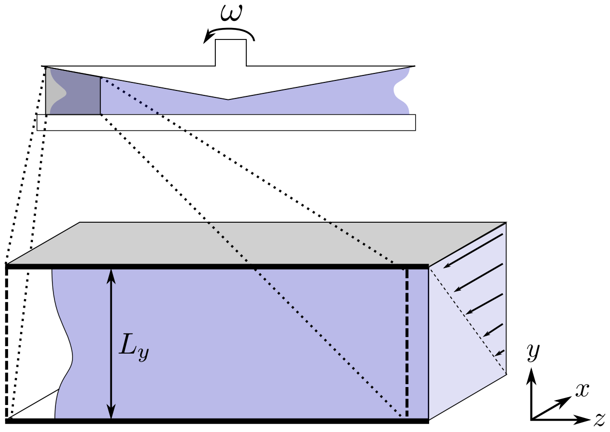
Viscoelastic constitutive equation: second order fluid

Second normal stress N_2 destabilising, surface tension Γ stabilising

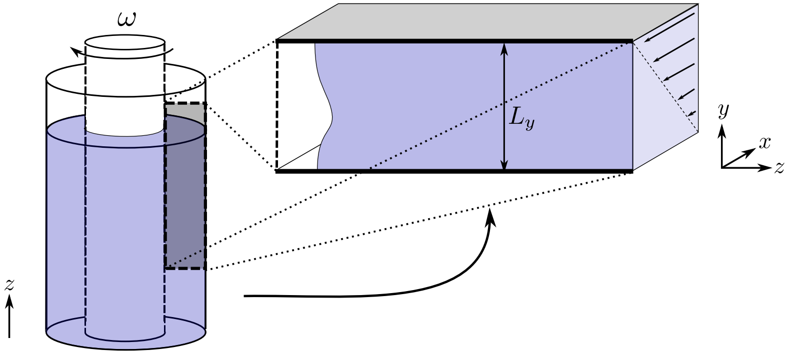
Expect fracture for $\boxed{|N_{2c}| > 2\Gamma/3a.}$

Simulation study of edge fracture

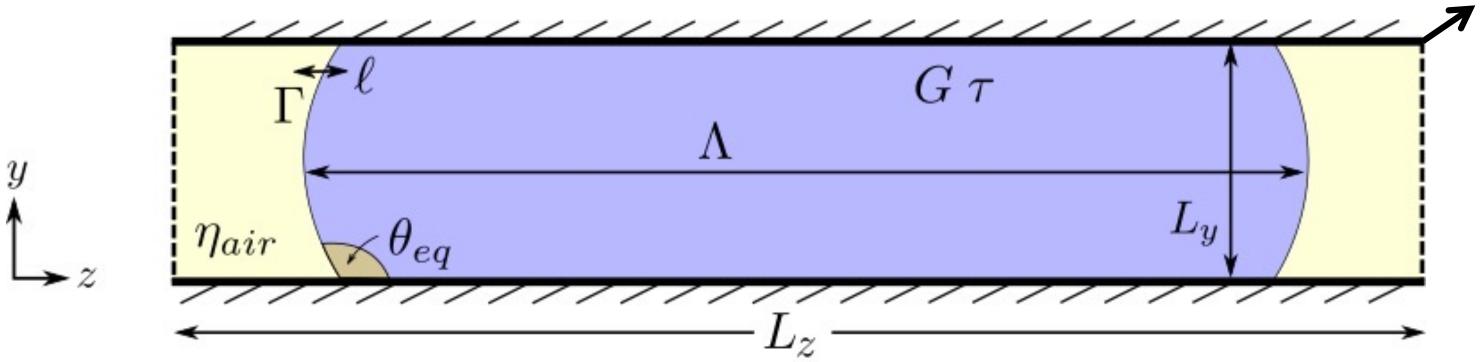
Cone and plate cartoon



Curved Couette cartoon

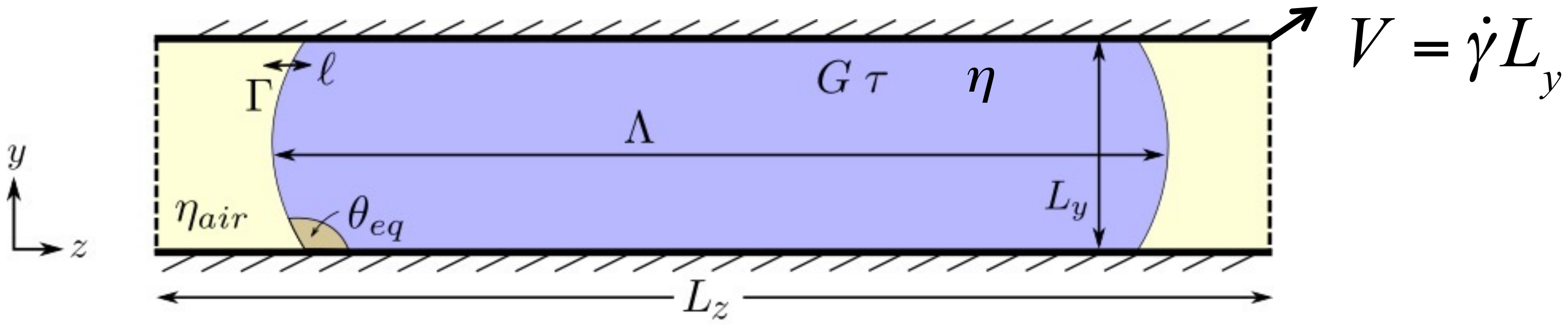


Our simulation: plane of flow gradient y, vorticity z



$$V = \dot{\gamma} L_y$$

Simulation study of edge fracture



Sketched structure of equations (with no slip/permeation at walls)

$$0 = \nabla . v$$ incompressible

$$0 = \eta \nabla^2 v + \nabla . \Sigma - \phi \nabla \mu - \nabla p$$ generalised Stokes balance

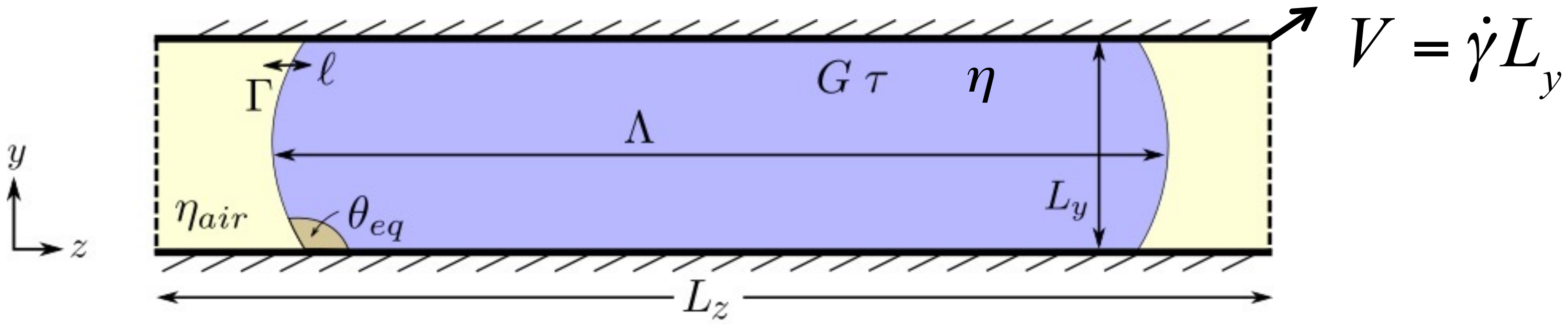
$$D_t \Sigma = \ldots$$ viscoelastic constitutive model

$$D_t \phi = M \nabla^2 \mu$$ phase field = 1 inside fluid and = -1 in air

Chemical potential μ → diffuse interface (width *l*) → contact line motion

Interfacial surface tension Γ. Boundary condition → contact angle

Simulation study of edge fracture



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$0 = \eta \nabla^2 v + \nabla . \Sigma - \phi \nabla \mu - \nabla p$ generalised Stokes balance

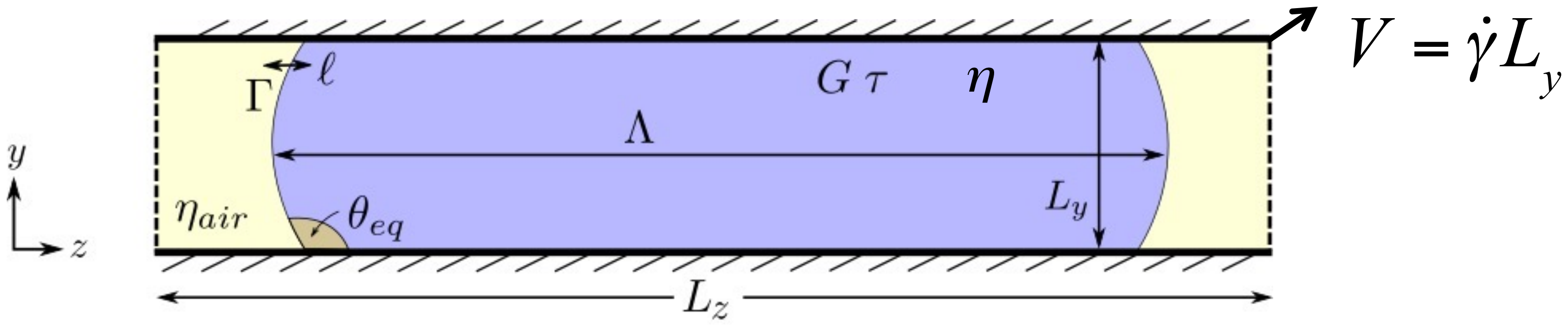
$D_t \Sigma = \ldots$ Johnson Segalman or Giesekus model

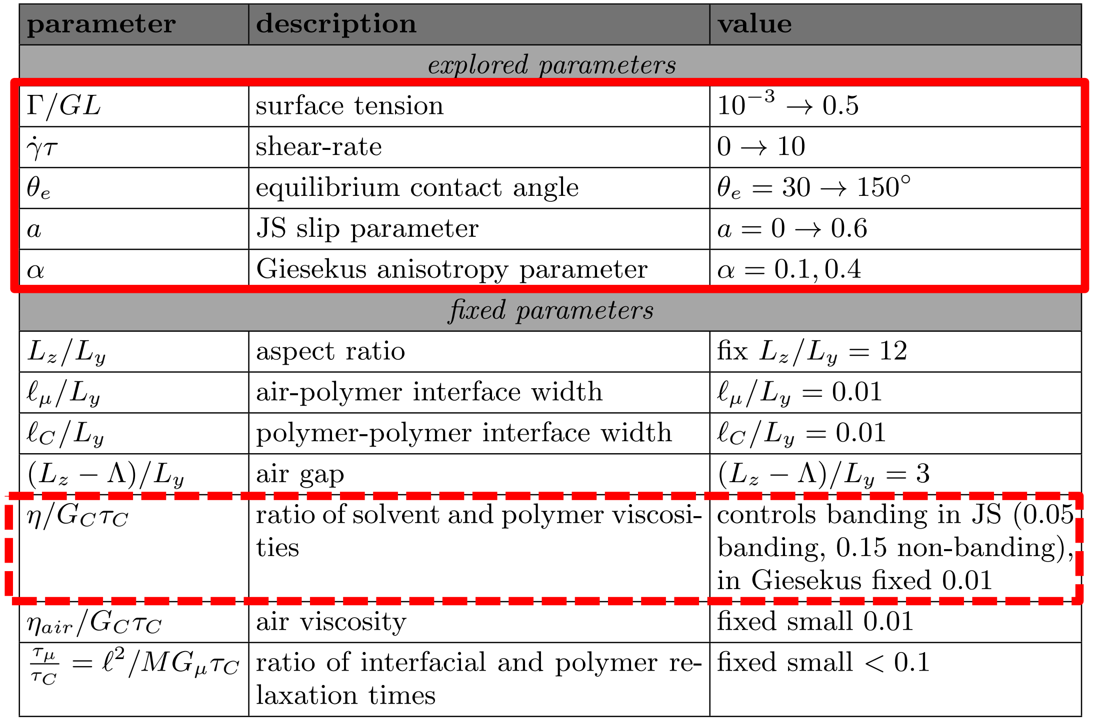
$D_t \phi = M \nabla^2 \mu$ phase field = 1 inside fluid and = -1 in air

Chemical potential μ → diffuse interface (width *l*) → contact line motion

Interfacial surface tension Γ. Boundary condition → contact angle

Simulation study of edge fracture



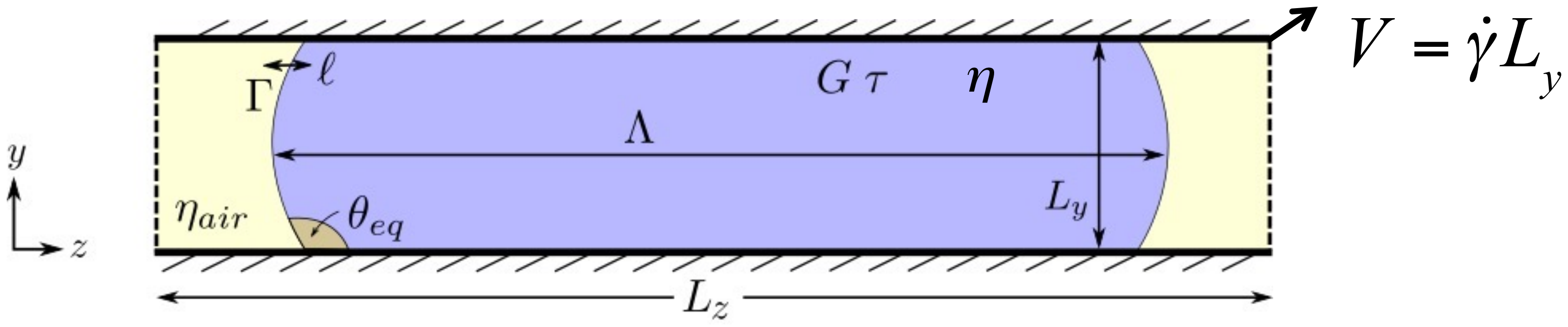


parameter	description	value
explored parameters		
Γ/GL	surface tension	$10^{-3} \rightarrow 0.5$
$\dot{\gamma}\tau$	shear-rate	$0 \rightarrow 10$
θ_e	equilibrium contact angle	$\theta_e = 30 \rightarrow 150^\circ$
a	JS slip parameter	$a = 0 \rightarrow 0.6$
α	Giesekus anisotropy parameter	$\alpha = 0.1, 0.4$
fixed parameters		
L_z/L_y	aspect ratio	fix $L_z/L_y = 12$
ℓ_μ/L_y	air-polymer interface width	$\ell_\mu/L_y = 0.01$
ℓ_C/L_y	polymer-polymer interface width	$\ell_C/L_y = 0.01$
$(L_z - \Lambda)/L_y$	air gap	$(L_z - \Lambda)/L_y = 3$
$\eta/G_C\tau_C$	ratio of solvent and polymer viscosities	controls banding in JS (0.05 banding, 0.15 non-banding), in Giesekus fixed 0.01
$\eta_{air}/G_C\tau_C$	air viscosity	fixed small 0.01
$\frac{\tau_\mu}{\tau_C} = \ell^2/MG_\mu\tau_C$	ratio of interfacial and polymer relaxation times	fixed small < 0.1

Key parameters to explore

converge to small or large

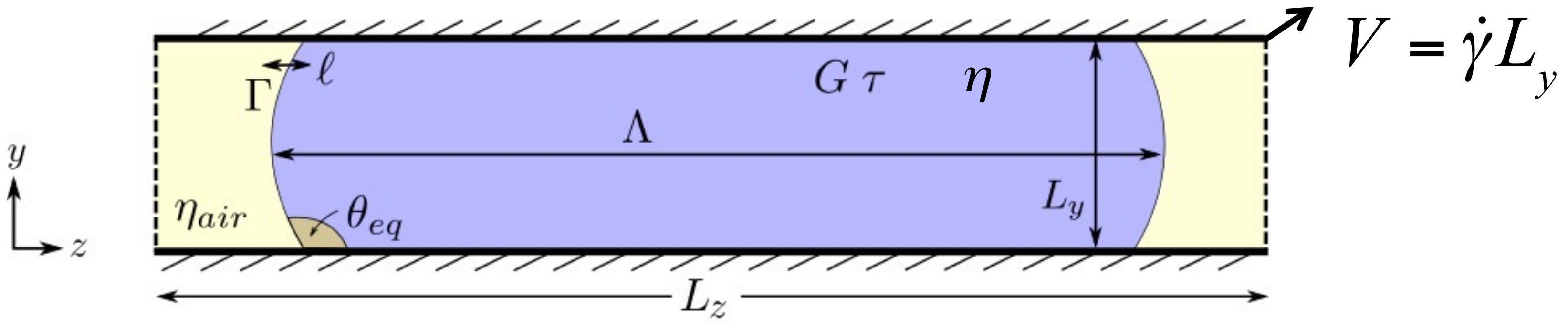
Simulation study of edge fracture



Surface tension	$\Gamma / G L_y$
Equilibrium contact angle	θ_{eq}
Imposed shear rate	$\dot{\gamma}\tau$
Johnson Segalman slip parameter	a
Solvent viscosity	$\eta / G\tau$

Key parameters to explore

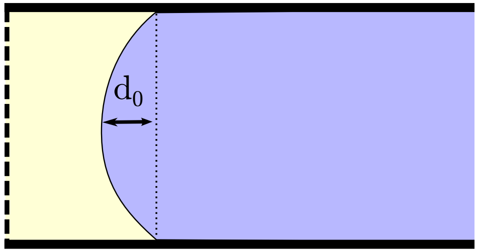
Simulation study of edge fracture



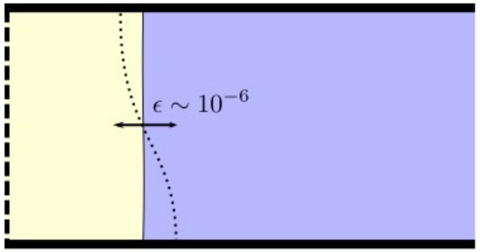
Surface tension	$\Gamma / G L_y$
Equilibrium contact angle	θ_{eq}
Imposed shear rate	$\dot{\gamma}\tau$
Giesekus anisotropy parameter	α
Solvent viscosity	$\eta / G\tau$

Key parameters to explore

Initial condition to shear simulations



Equilibrate liquid/air phase field without shear



Then slightly perturb the interface

(only need to do this for contact angle $\theta_{eq} = 90^o$)

$$h(y) \rightarrow h(y) + \varepsilon \cos(\pi y)$$

JS, a = 0.3, $\eta=0.15$, θ_{eq} = 90°

Simulation results

stable flat interface

stationary bowed interface

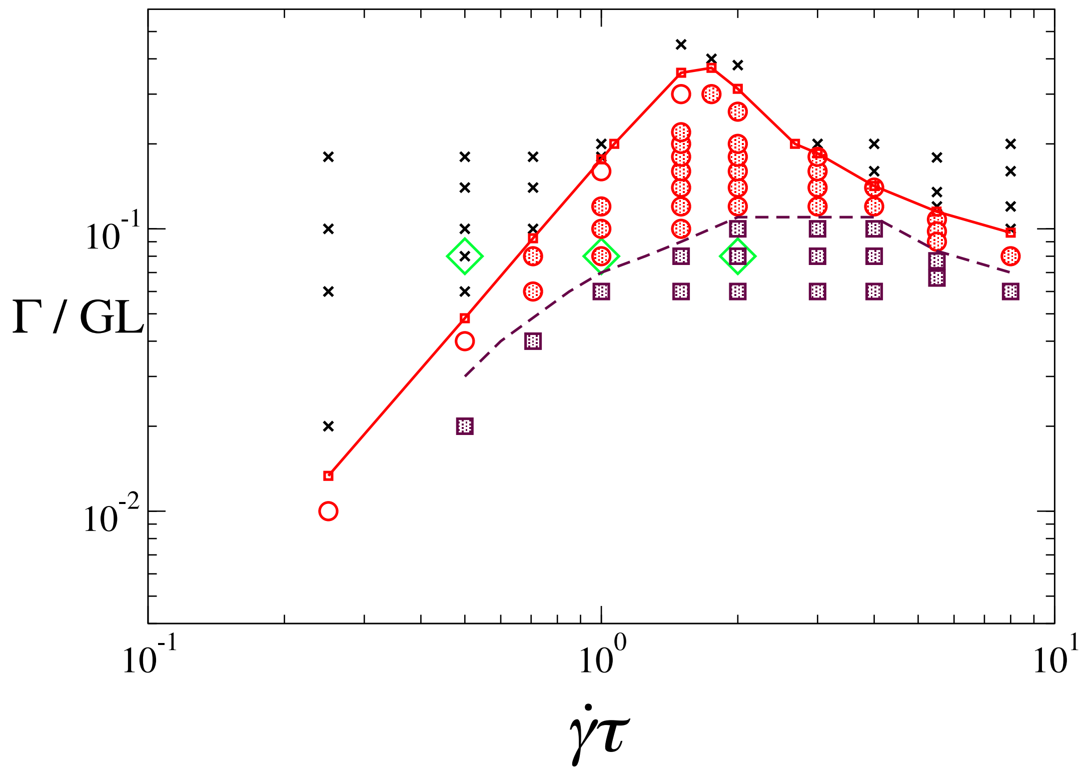
propagating fracture at wall

increasing shear rate $\dot{\gamma}\tau$

at fixed surface tension Γ/GL_y

JS, a = 0.3, $\eta=0.15$, θ_{eq} = 90°

Simulation results

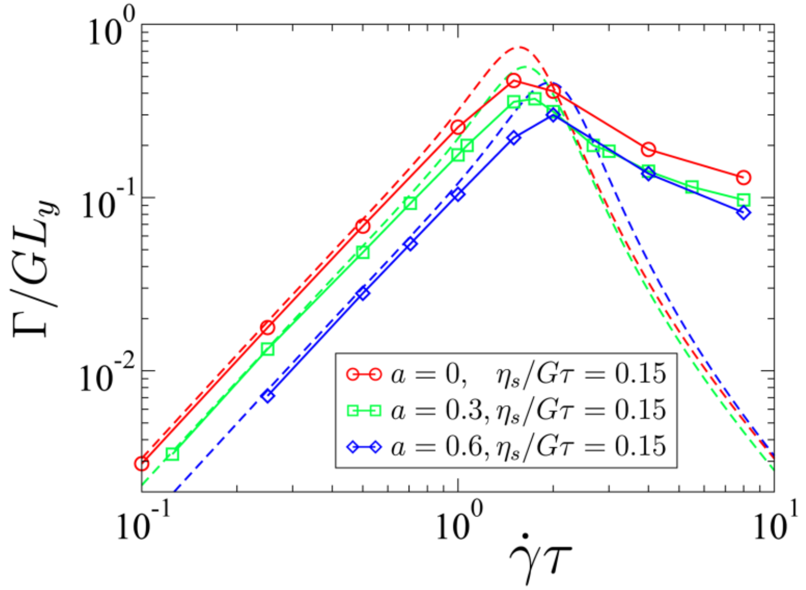


X stable flat interface

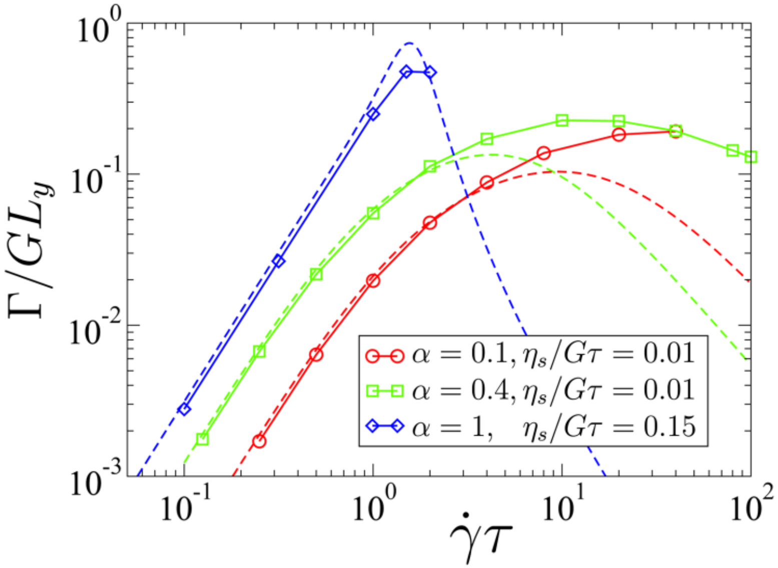
● stationary bowed interface

▨ propagating fracture at wall

Results: robustness against choice of constitutive model



Johnson-Segalman model



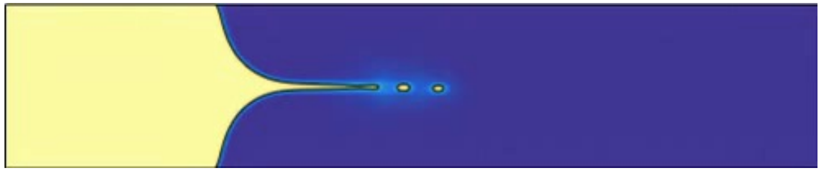
Giesekus model

Broadly the same behaviour in both constitutive models

Stability against edge fracture recovered for a = 1 (JS) or α = 0 (Gk)

where each model reduces to Oldroyd B model, with no N_2

Some movies (and effect of wetting angle…)



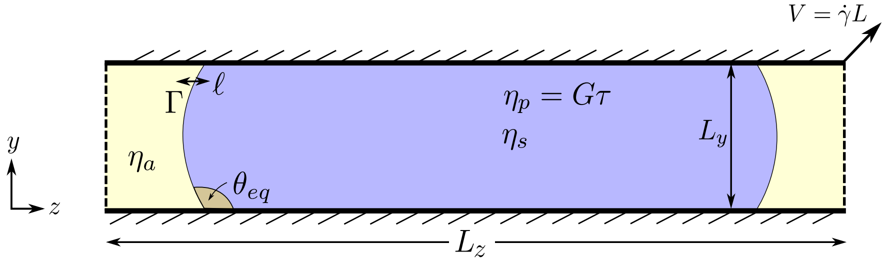
more wetting θ_{eq} = 60º

neutrally wetting θ_{eq} = 90º

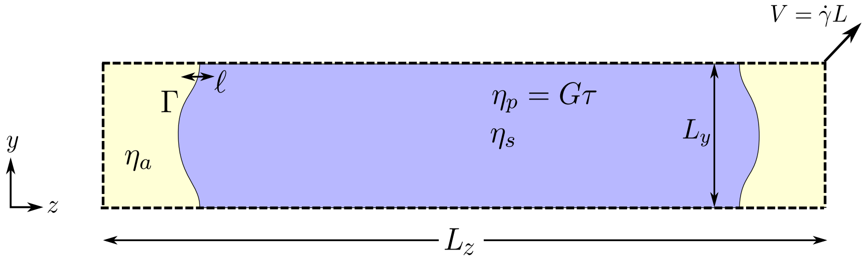
less wetting θ_{eq} = 120º

Linear stability analysis of edge fracture

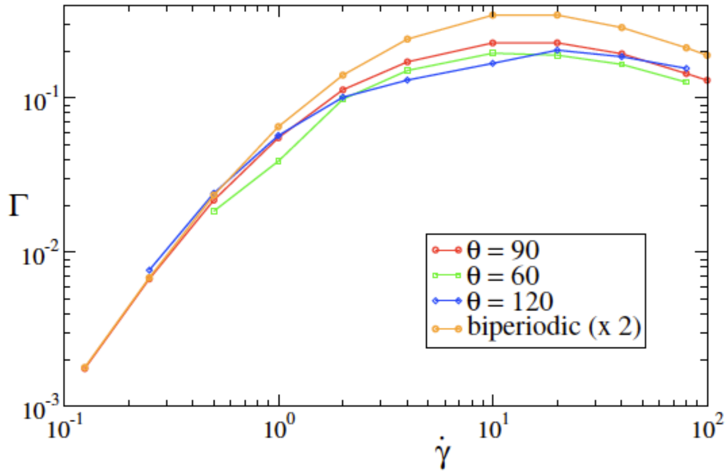
Simulations (just discussed) with walls



Also simulated sheared periodic BCs



Essentially same phase diagram in both



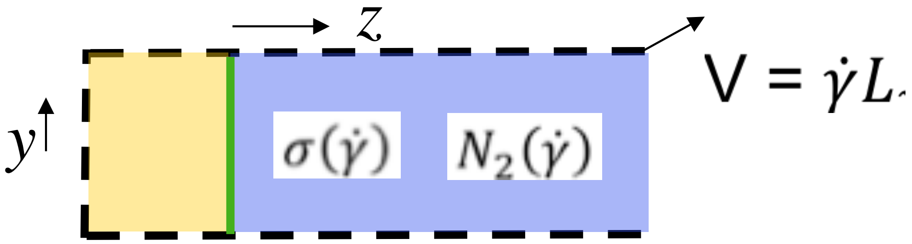
<u>Simplifications in linear analysis:</u>

Periodic BCs

Sharp interface $l = 0$
(still with surface tension)

Air viscosity $\eta_a = 0$

Linear stability analysis of edge fracture

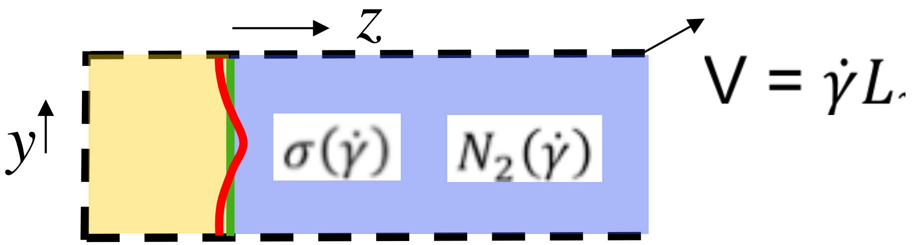


- Work in limit of slow imposed shear flow, $\dot{\gamma}\tau \to 0$

- Initial base state with stationary flat interface

Shear stress $\sigma(\dot{\gamma})$ and second normal stress $N_2(\dot{\gamma})$ in fluid

Linear stability analysis of edge fracture

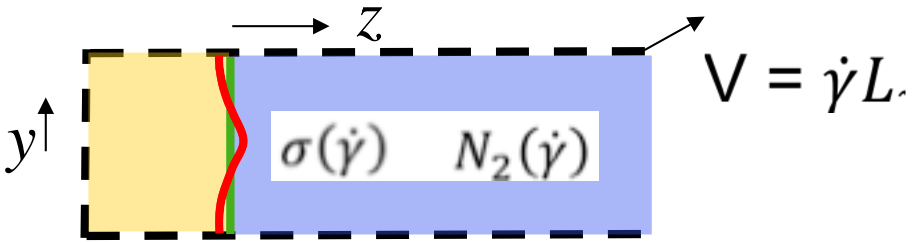


- Work in limit of slow imposed shear flow, $\dot{\gamma}\tau \rightarrow 0$
- Initial base state with stationary flat interface

Shear stress $\sigma(\dot{\gamma})$ and second normal stress $N_2(\dot{\gamma})$ in fluid

- Add small amplitude perturbations in interfacial profile, flow fields, stresses
- Substitute base state + perturbations into governing equations
- Expand in powers of perturbation amplitude, keep only first order terms

Linear stability analysis of edge fracture



- Work in limit of slow imposed shear flow, $\dot{\gamma}\tau \to 0$

- Initial base state with stationary flat interface

  Shear stress $\sigma(\dot{\gamma})$ and second normal stress $N_2(\dot{\gamma})$ in fluid

- Add small amplitude perturbations in interfacial profile, flow fields, stresses

in-plane streamfunction: $\tilde{\psi}(y,z,t) = \left(Ae^{-qz} + Be^{-kz}\right)e^{wt}e^{iqy},$

out-of-plane velocity: $\tilde{v}(y,z,t) = Ce^{-qz}e^{wt}e^{iqy},$

interfacial profile: $\tilde{h}(y,t) = iqDe^{wt}e^{iqy}$

Linear stability analysis of edge fracture

- Resulting eigenvalue is positive (giving instability) when:

surface tension
(stabilising)

$$\frac{1}{2q}\sigma\frac{\partial|N_2|}{\partial\dot{\gamma}}\Big/\frac{\partial\sigma}{\partial\dot{\gamma}} > \Gamma$$

wavevector of
perturbation

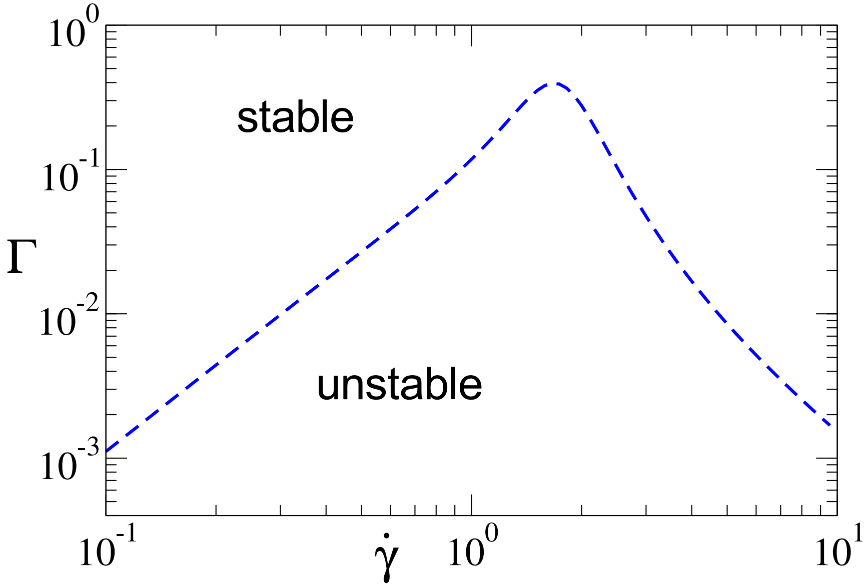
polymer stresses
(destabilising)

Compare linear stability prediction against simulations

- Predicted threshold for instability

$$\frac{1}{2q}\sigma\frac{\partial|N_2|}{\partial\dot{\gamma}}\Big/\frac{\partial\sigma}{\partial\dot{\gamma}} > \Gamma$$

- Longest wavelength mode, i.e., the one with $q=2\pi/L_y$, is first to go unstable



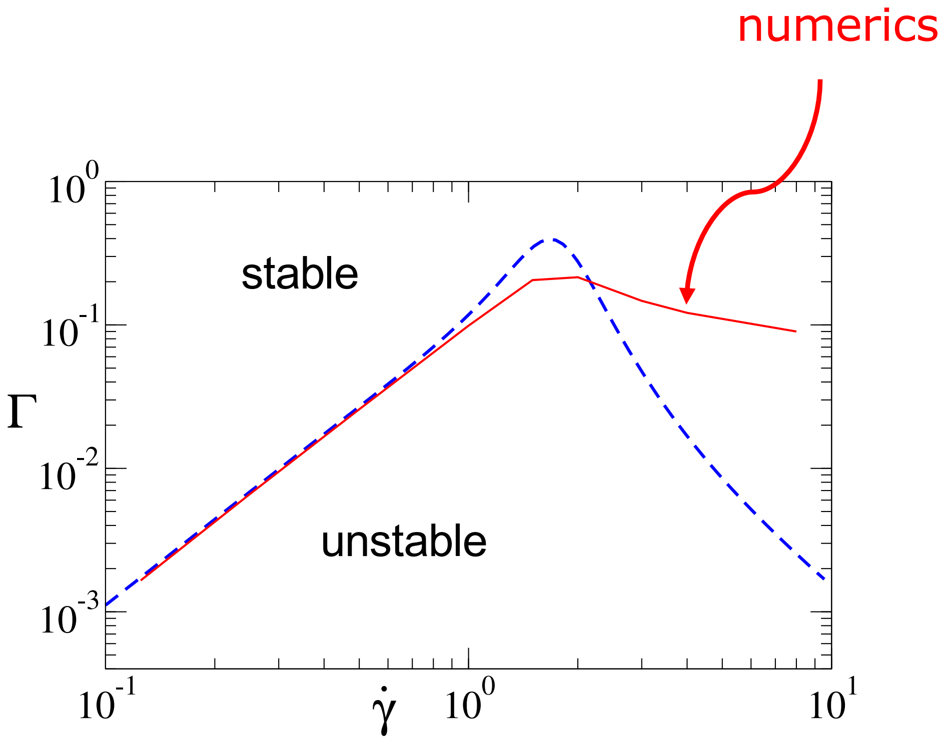
- So threshold for this mode gives threshold for edge first to destabilise

- Re-entrance due to saturating $N_2(\dot{\gamma})$

Compare linear stability prediction against simulations

- Predicted threshold for instability

$$\frac{1}{2q}\sigma\frac{\partial|N_2|}{\partial\dot{\gamma}}\Big/\frac{\partial\sigma}{\partial\dot{\gamma}} > \Gamma$$



- Longest wavelength mode, i.e., the one with $q=2\pi/L_y$, is first to go unstable

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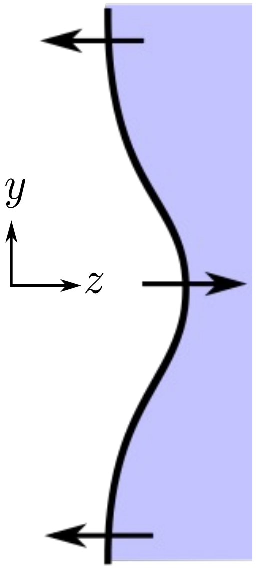
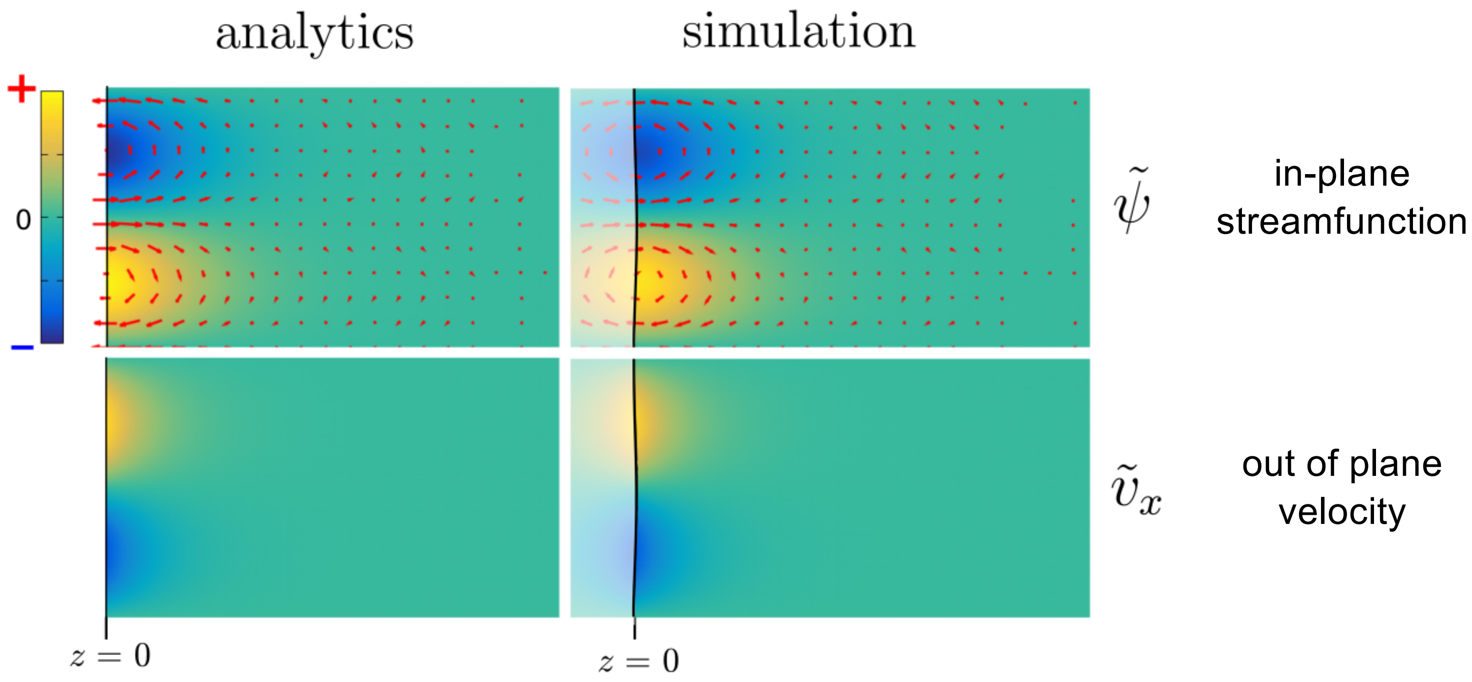
Compare linear stability prediction against simulations

- Eigenfunction of stability analysis (left) compared with simulation (right)





[Tanner and Keentok, *J. Rheol* (1983),   Keentok and Xue, *Rheol. Acta* (1999)]

Comparison with Tanner's original prediction

- Our linear analysis gives

$$\frac{1}{2q}\sigma\frac{\partial|N_2|}{\partial\dot{\gamma}}\Big/\frac{\partial\sigma}{\partial\dot{\gamma}} > \Gamma$$

- Tanner's scaling predicted

$$a\,|N_2| > 2\Gamma/3$$

- Our calculation: identifies role of shear stresses as well as N_2

  identifies differential nature of criterion

  considers all wavelengths, without pre-assuming a crack size

  reveals mechanism of instability and possible mitigation

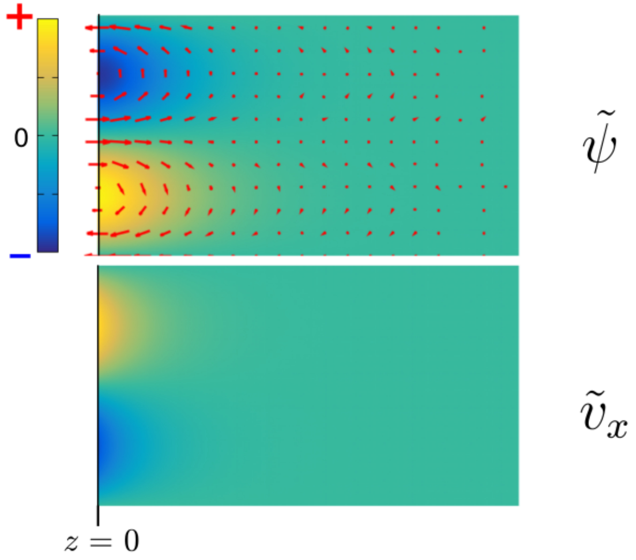
- Setting $q^{-1} = a$ and noting that for weak shear $\sigma{\sim}\dot{\gamma}$ and $|N_2|{\sim}\dot{\gamma}^2$

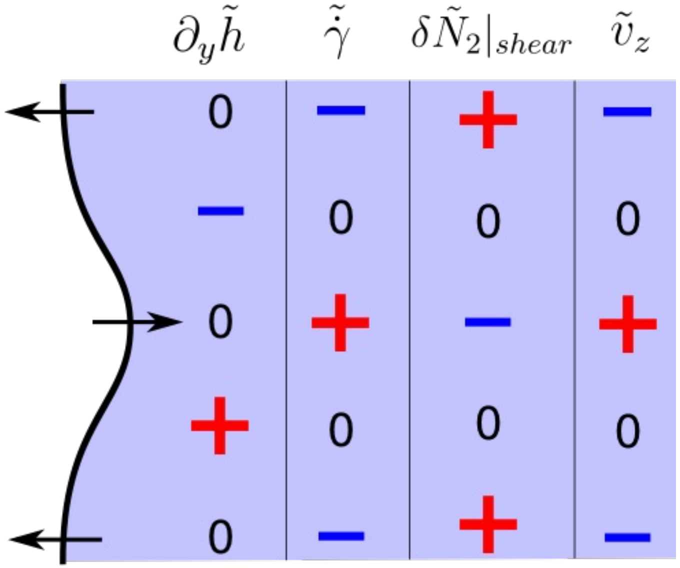
  we find our predictions and Tanner's happen to give same low $\dot{\gamma}$ scaling

- In strong shear, the two criteria depart markedly from each other

Hemingway et al. PRL (2017) cf. Hinch, Harris, Rallison, *JNNFM* (1992) , Wilson & Rallison, *JNNFM* (1997)

Mechanism of the edge fracture instability (zero surface tension here)





$\partial_y \tilde{h}$	$\tilde{\dot{\gamma}}$	$\delta \tilde{N}_2\|_{shear}$	$\tilde{v}_z$
0	−	+	−
−	0	0	0
0	+	−	+
+	0	0	0
0	−	+	−

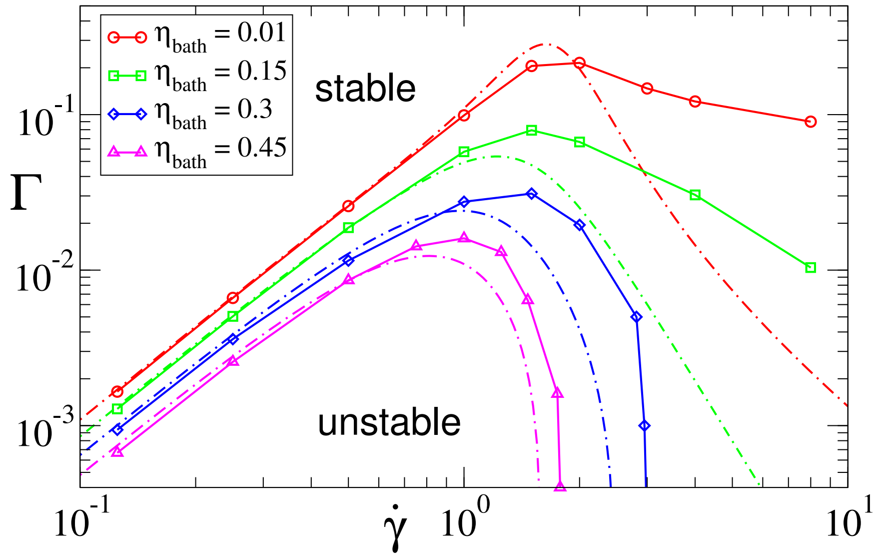
1. Tilt $\partial_y \tilde{h}$ in interface exposes jump in shear-stress $\Delta\sigma$

2. To maintain force balance, need shear-rate perturbation $\tilde{\dot{\gamma}}$

3. N_2 then suffers a shear perturbation, $\tilde{N}_2 = dN_2/d\dot{\gamma} \times \tilde{\dot{\gamma}}$

4. This must be balanced by opposite extensional perturbation, which is achieved by a flow field $\tilde{v}_z$ that enhances original tilt $\partial_y \tilde{h}$

How might we seek to mitigate edge fracture ?



$$\frac{1}{2q}\sigma\frac{\partial|N_2|}{\partial\dot{\gamma}}\Big/\frac{\partial\sigma}{\partial\dot{\gamma}} > \Gamma$$

"air" (i.e., bathing fluid)

viscosity increases

in curves downwards

- Now re-do linear analysis with non-negligible viscosity for outside "air"
- *i.e.*, in experimental practice, bathe flow cell in an immiscible Newtonian fluid
- Destabilising jump $\Delta\sigma$ in shear stress between fluid & "air" reduced

Edge fracture: conclusions, outlook….

Edge fracture near ubiquitous and limits rheological measurements

Linear stability analysis and nonlinear simulations of edge fracture

New criterion for, mechanism and possible mitigation of edge fracture

E. J. Hemingway, H. Kusumaatmaja + S. M. F. Phys. Rev. Lett., **119**, 029006 (2017)

E. J. Hemingway and S. M. Fielding, J. Rheol, **63**, 138002 (2019)

Modest precursors of edge fracture can cause (apparent) bulk shear banding

E. J. Hemingway and S. M. Fielding, Phys. Rev. Lett., **120**, 138002 (2018)

Bulk shear banding can cause edge fracture

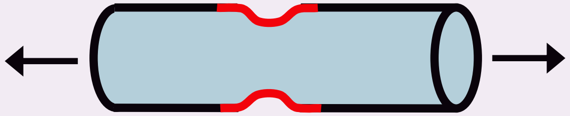
S. Skorski and P. D. Olmsted, J. Rheol., **55**, 1219 (2011)

There is a complicated interplay between shear banding and edge fracture

E. J. Hemingway and S. M. Fielding, J. Rheol., **64**, 1147 (2020)

Three key challenges in experimental rheometry

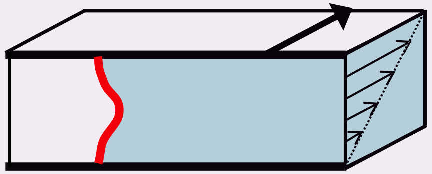
Extension:



“necking”

of filament

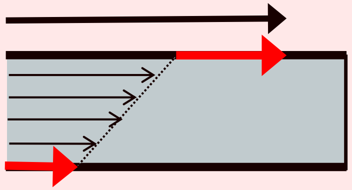
Shear:



“edge fracture”

of fluid-air interface

Shear:



“wall slip”

of fluid w.r.t. plates

Wall slip in shear rheometry

Introduction to wall slip in soft jammed suspensions

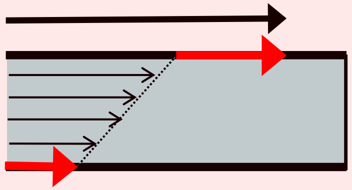
Experimental observations

Immersed boundary simulation method

Results

Slip - conclusions

Shear:

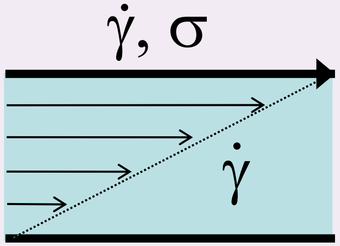


“wall slip”

of fluid w.r.t. plates

Wall slip in shear rheometry

Experimental aim:



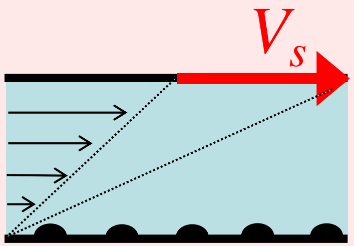
measure shear e.g.

flow curve $\sigma(\dot{\gamma})$

σ = shear stress

$\dot{\gamma}$ = shear rate

Experimental practice:



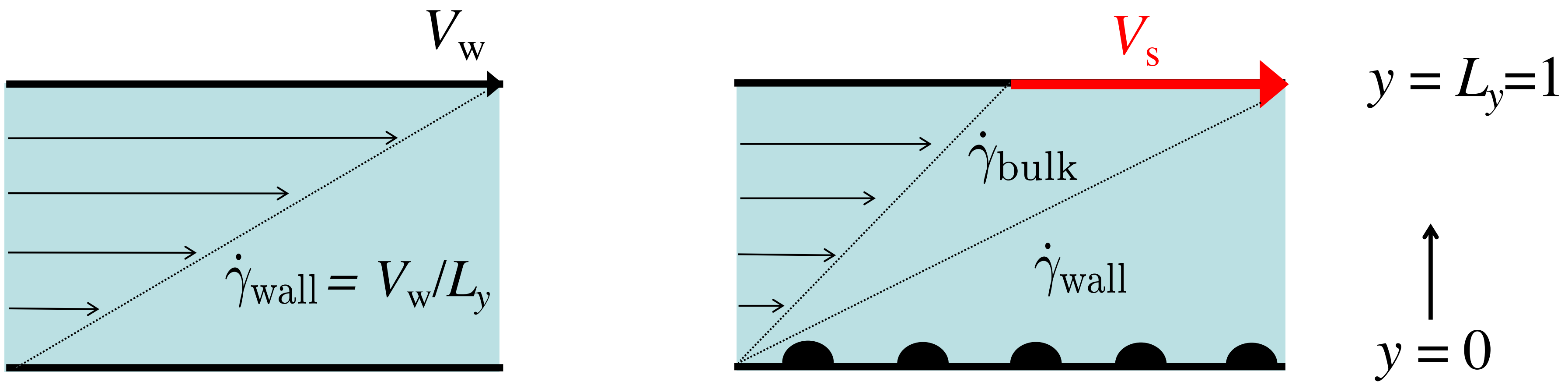
"wall-slip" where fluid meets plate(s) hampers rheometry.

Common mitigation strategies:

chemically coat or

physically roughen wall

Introduction to wall slip: key measurements



$v = v\,(y)$ velocity profile across gap coordinate, y

$V_\mathrm{s} = V_\mathrm{s}\,(\sigma)$ slip velocity, often as function of shear stress, σ

$\sigma = \sigma\,(\dot\gamma)$ flow curve, using either…

shear rate from plate velocities, including slip $\dot\gamma_\mathrm{wall}$

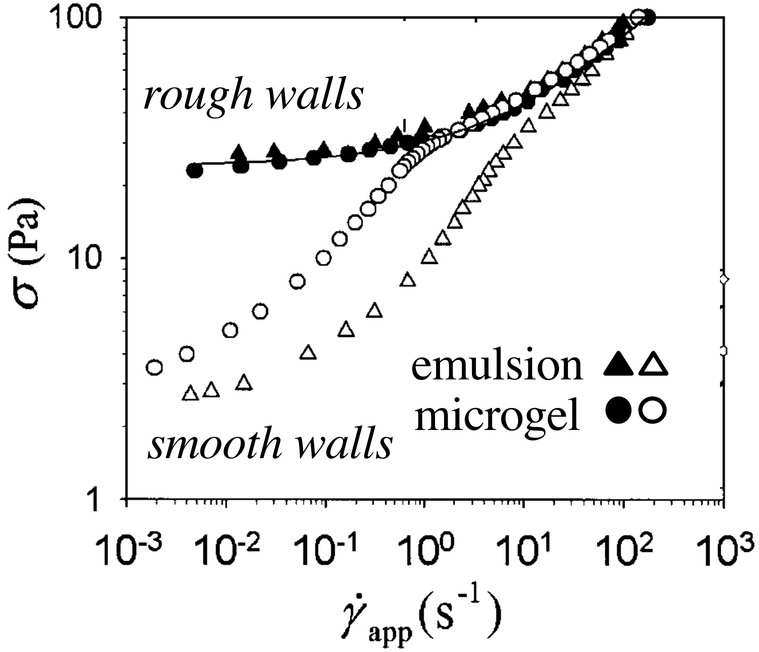
shear rate within fluid bulk, removing slip $\dot\gamma_\mathrm{bulk}$

[Zhang et al. PRL 2017; Review: Cloitre, Bonnecaze, Rheol. Acta 2017 + refs therein]

Slip in jammed suspensions of soft particles (emulsions, microgels…)

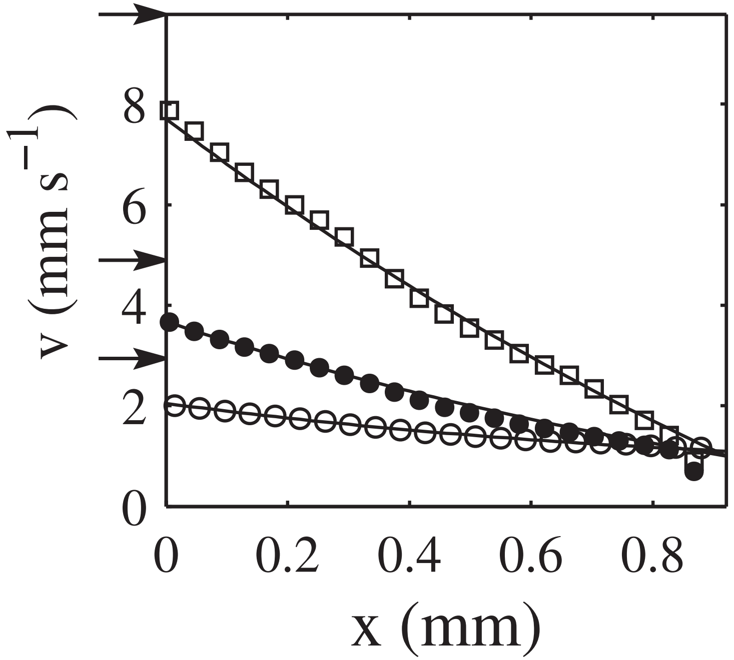
flow curve, including slip

[Cloitre et al. PRL 2004]



velocity profiles across gap

[Becu et al. PRL 2006]

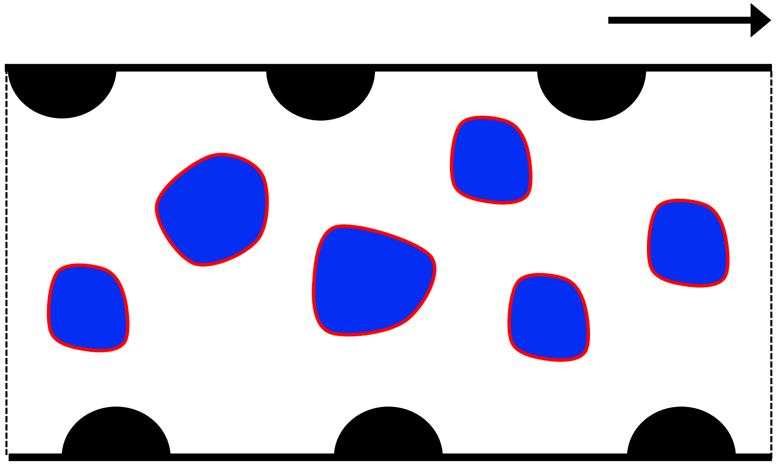


Slip velocity versus stress: usually fit to $V_s \sim \sigma^{p}$

but exponent controversial (p = 1 → 2) , and different above/below yield

[See also: Pelusi et al. Europhys. Lett. 2019]

Simulate densely packed soft particles sheared between hard bumpy walls



hard walls with hard bumps

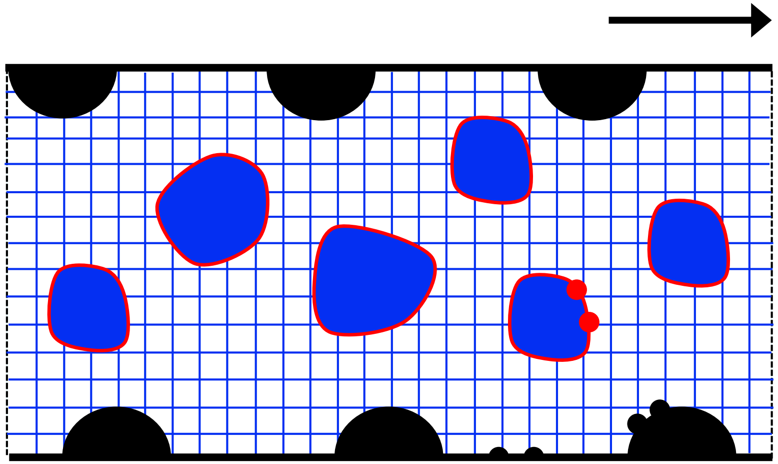
Stokes fluid inside particles

elastic soft particle perimeters

Stokes fluid between particles

[Review of immersed boundary methods: Peskin Acta Numerica 2002]

Simulate densely packed soft particles sheared between hard bumpy walls



hard walls with hard bumps

(*Lagrangian `immersed boundary'* ●)

elastic soft particle perimeters

(*Lagrangian `immersed boundary'* ●)

Stokes fluid inside particles

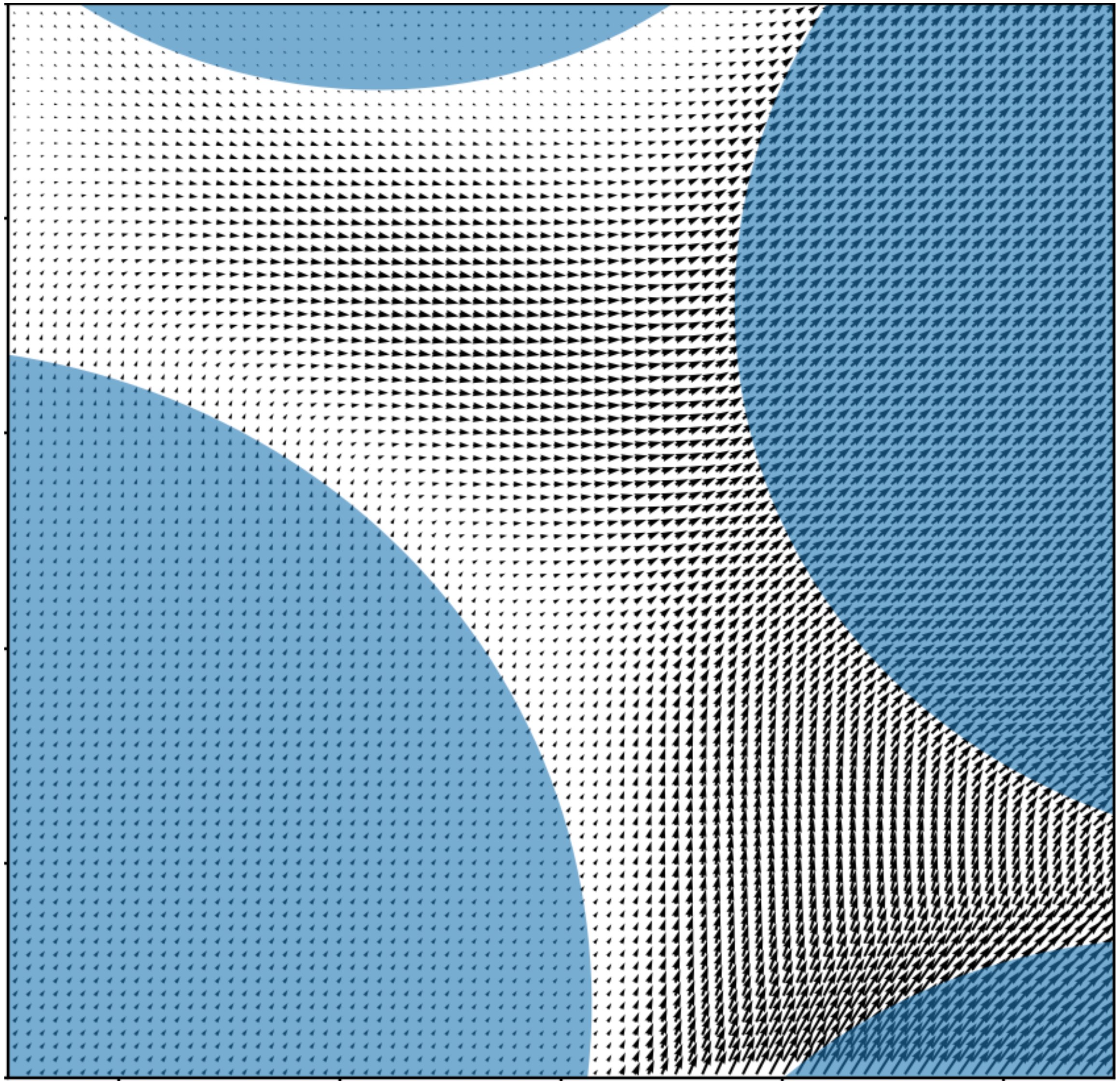
(*solve Stokes eqn on Eulerian grid* +)

Stokes fluid between particles

(*solve Stokes eqn on Eulerian grid* +)

Peskin delta functions

Typical resolution of Stokes flow between particles



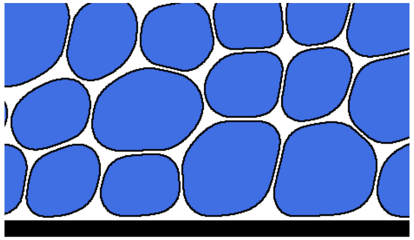
Capture fluid mechanics in particle-particle and particle-wall gaps

(rather than assuming simple relative drag)

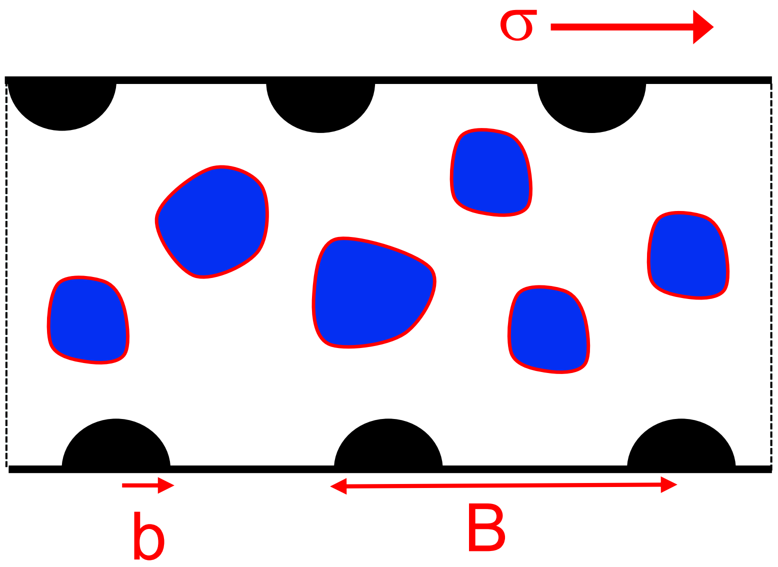
Capture solid mechanics of particle shape changes

(rather than assuming simple spherical potential)

→ capture dynamics at wall



Units and key parameters



fix B/b = 5.0

Key parameters:

particle area fraction ϕ

wall roughness $\beta = b / R$

imposed stress σ

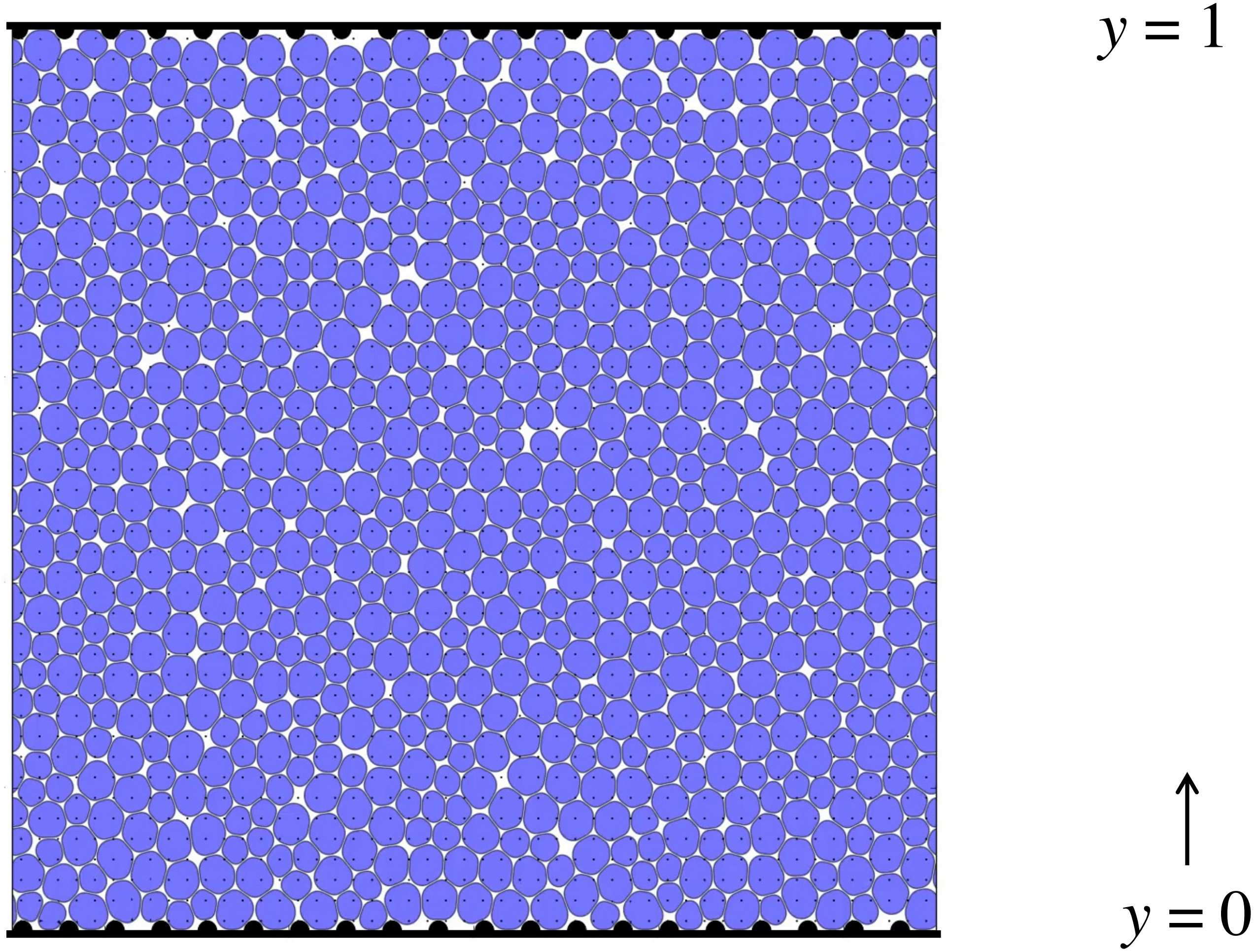
Units:

average particle radius, R

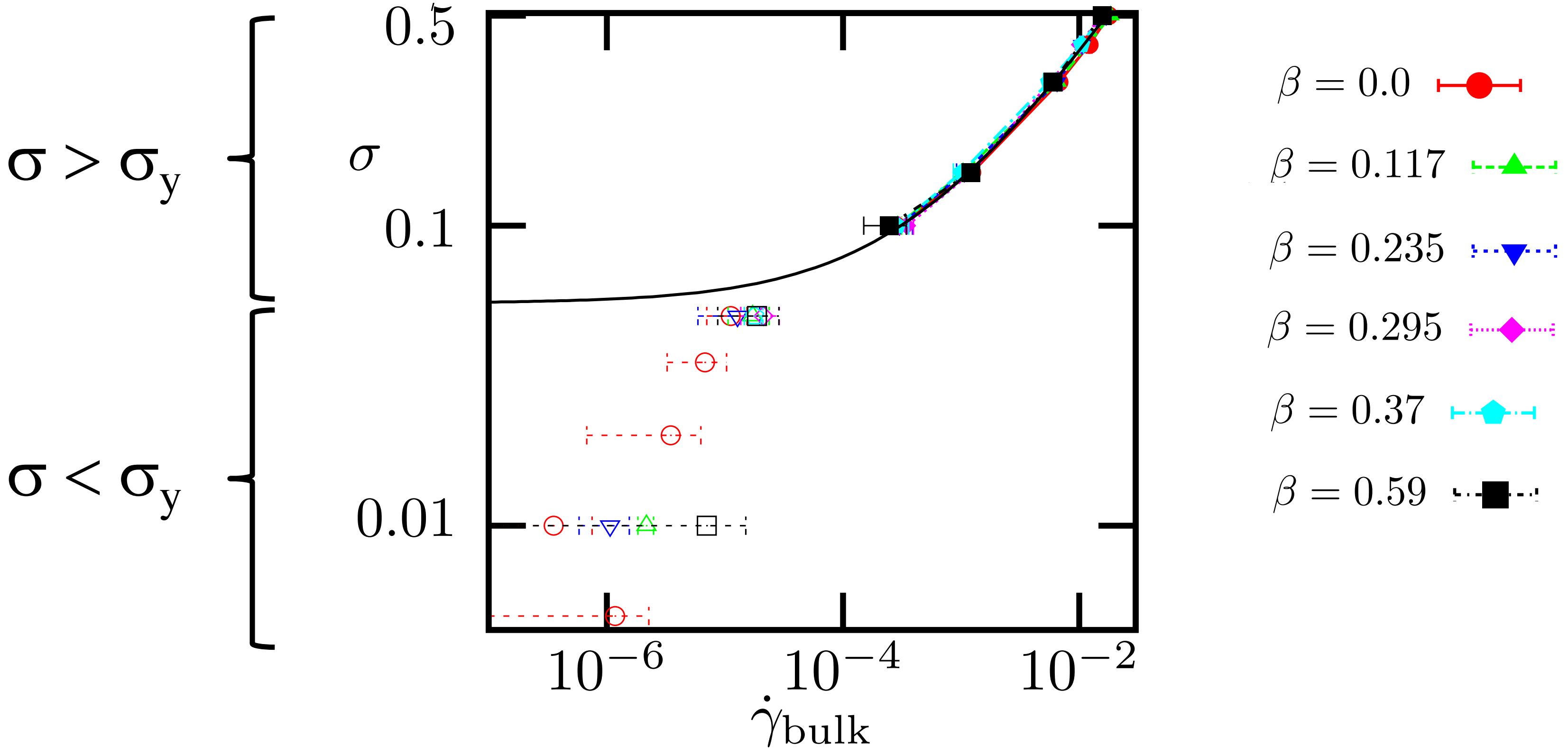
particle surface elastic constant

viscosity of Stokes fluids

A movie

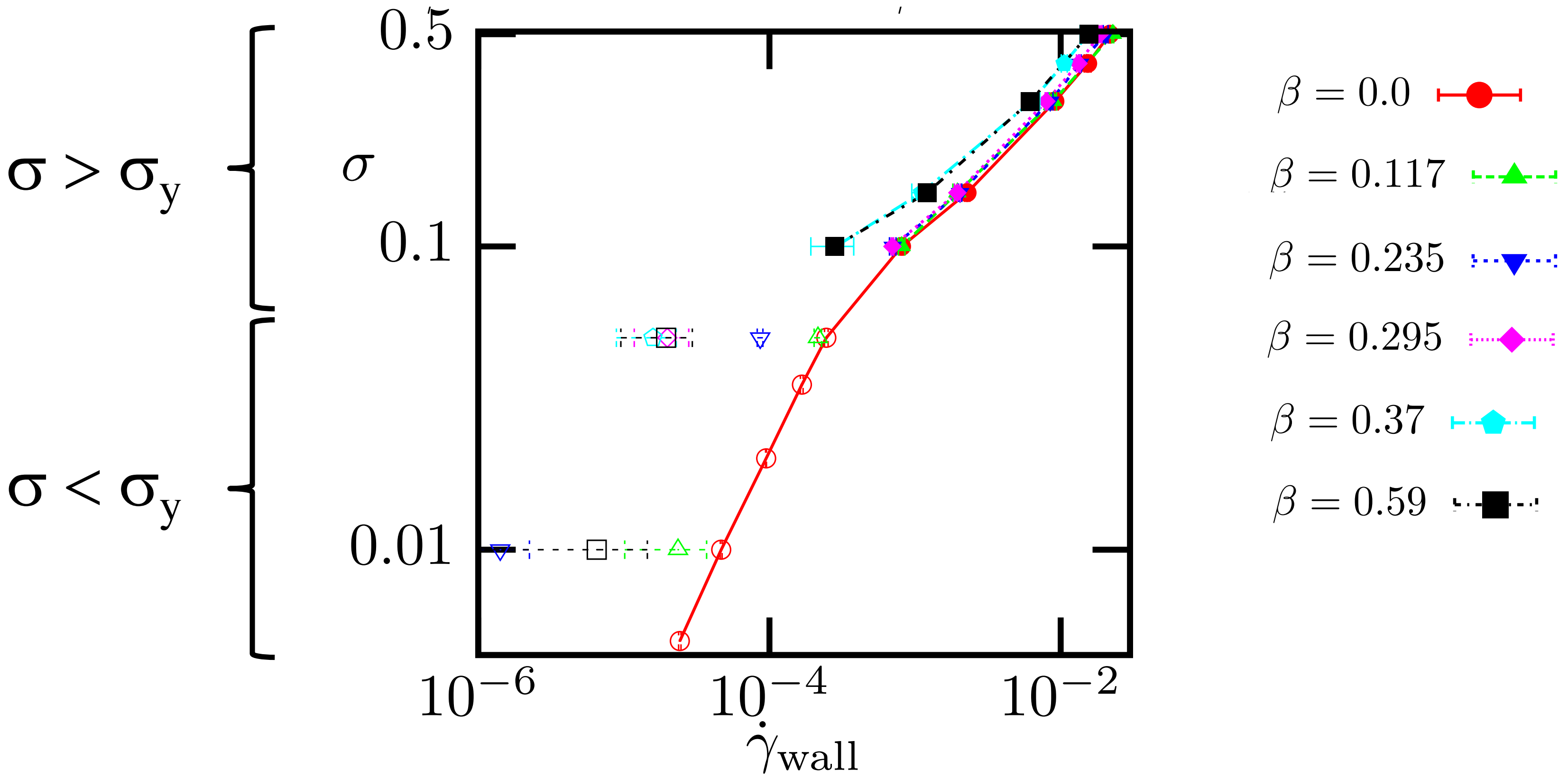


Steady state flow curve (removing slip)



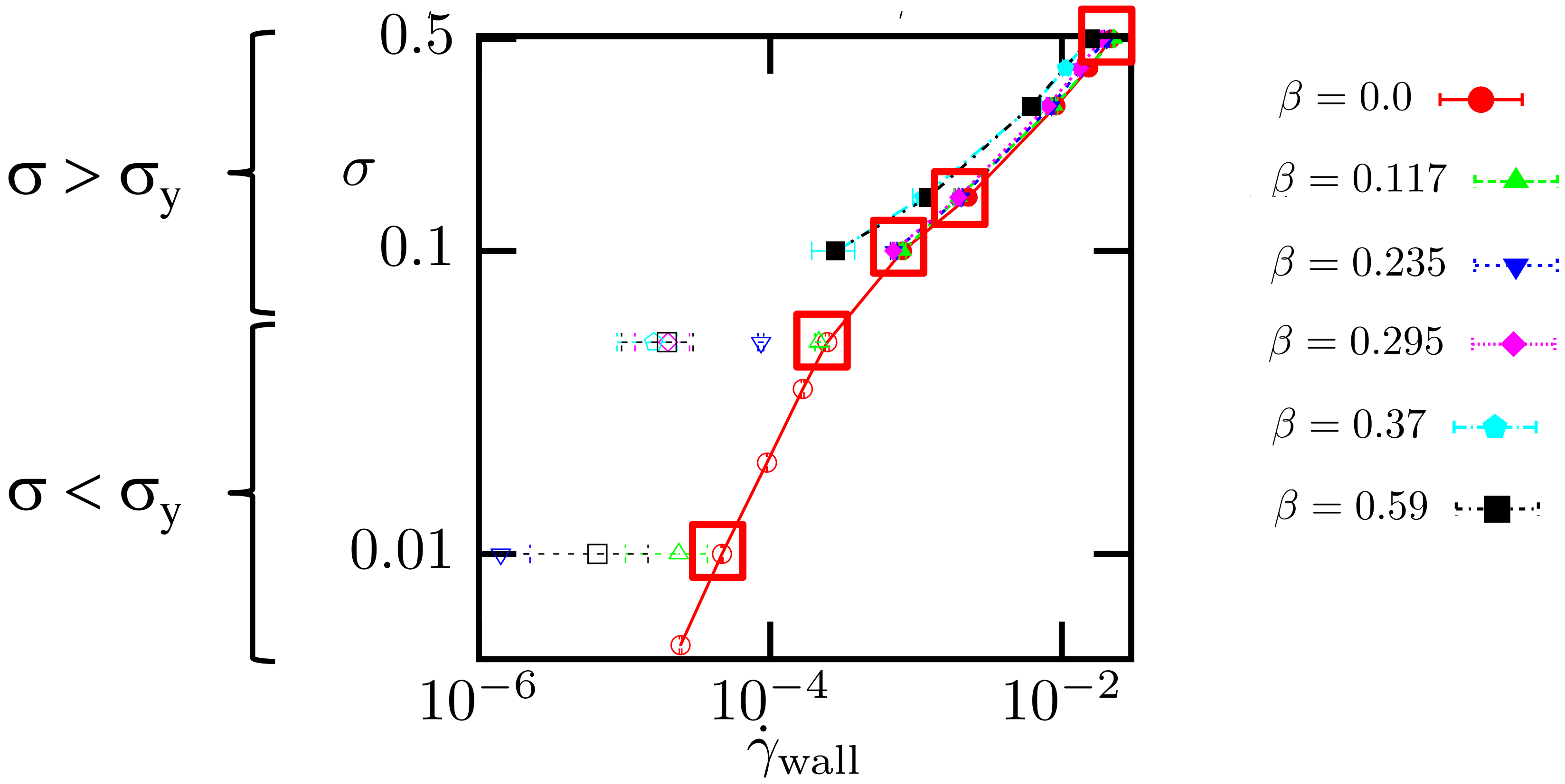
- Steady shear above yield stress, with Herschel-Bulkley fit
- Indefinitely slowing creep below yield stress, with no steady state

Steady state flow curve (including slip)



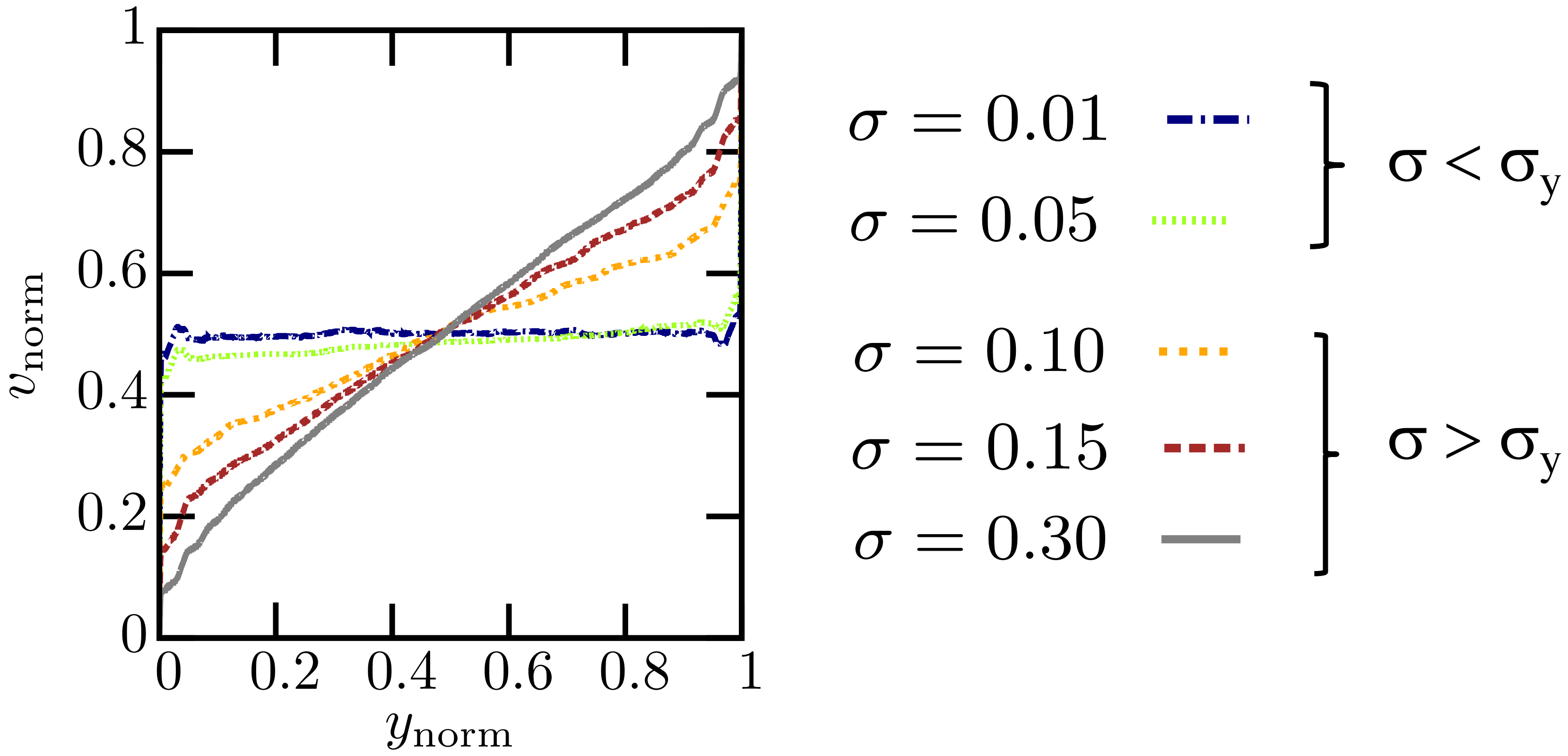
- Steady shear above yield stress, with Herschel-Bulkley fit
- Apparent steady shear below yield stress, for smooth walls, due to slip

Steady state flow curve (including slip)



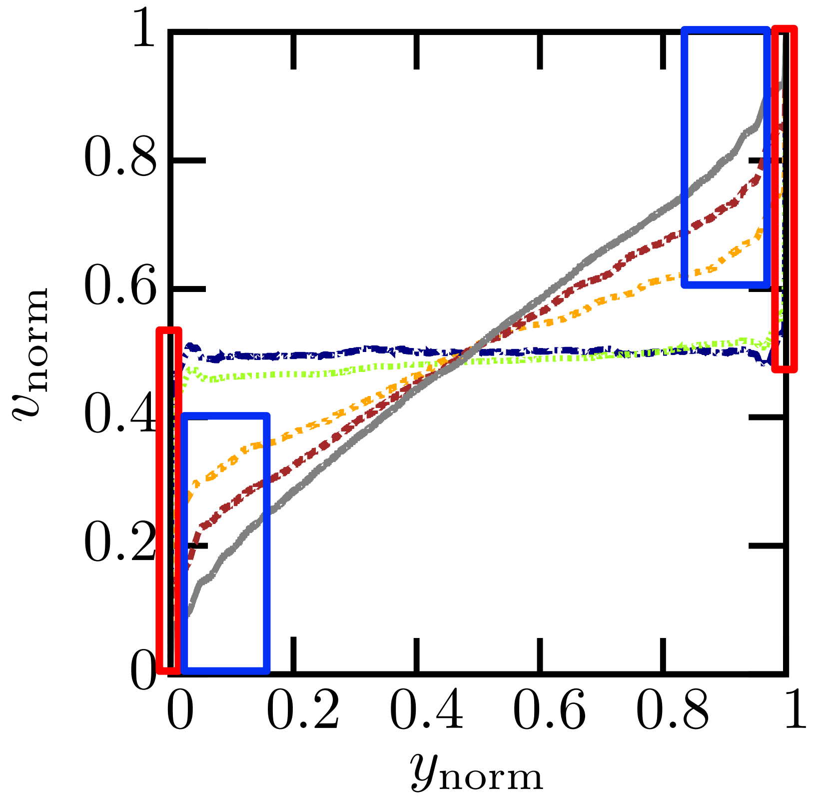
- Steady shear above yield stress, with Herschel-Bulkley fit
- Apparent steady shear below yield stress, for smooth walls, due to slip

Normalized profiles of velocity across gap with smooth walls



- Almost total slip below yield stress. Partial slip above yield stress.

Normalized profiles of velocity across gap with smooth walls



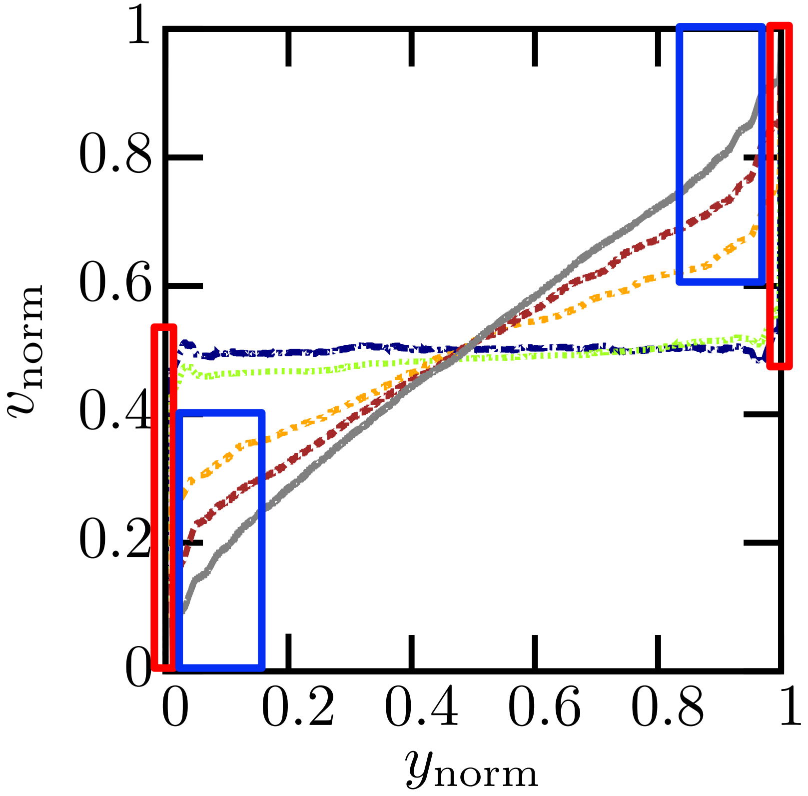
1. Thin Newtonian solvent layer,
   depleted of particles,
   immediately adjacent to wall
   (above and below yield stress)

2. Enhanced fluidisation
   of first few particles layers
   into the bulk
   (only above yield stress)

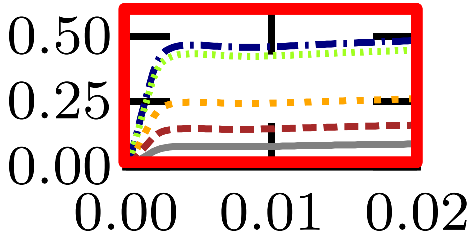
- There are two separate contributions to the slip, with different physics

  (Only one involves depletion of final layer of particles away from wall.)

Normalized profiles of velocity across gap with smooth walls



1. Thin Newtonian solvent layer



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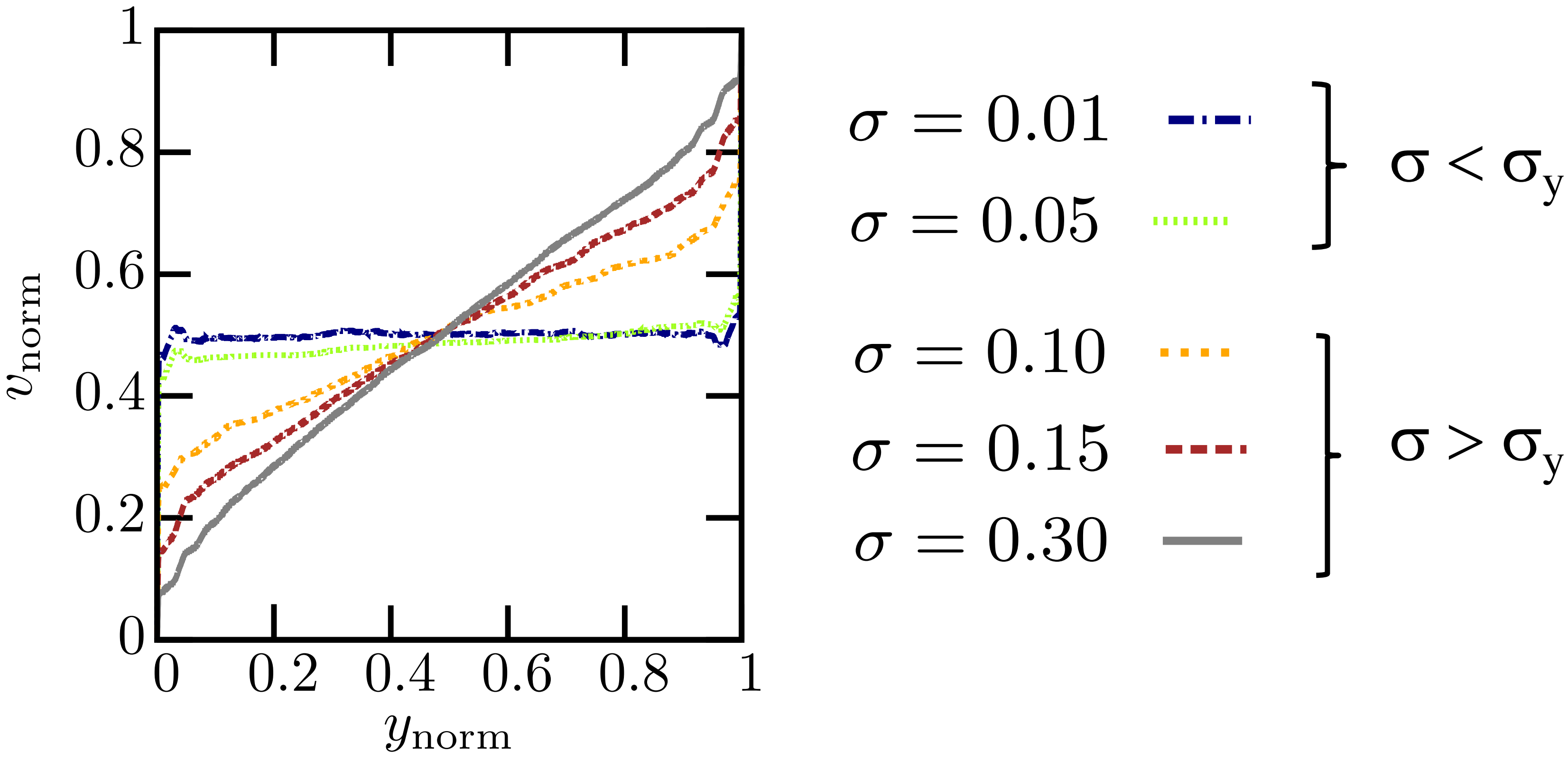
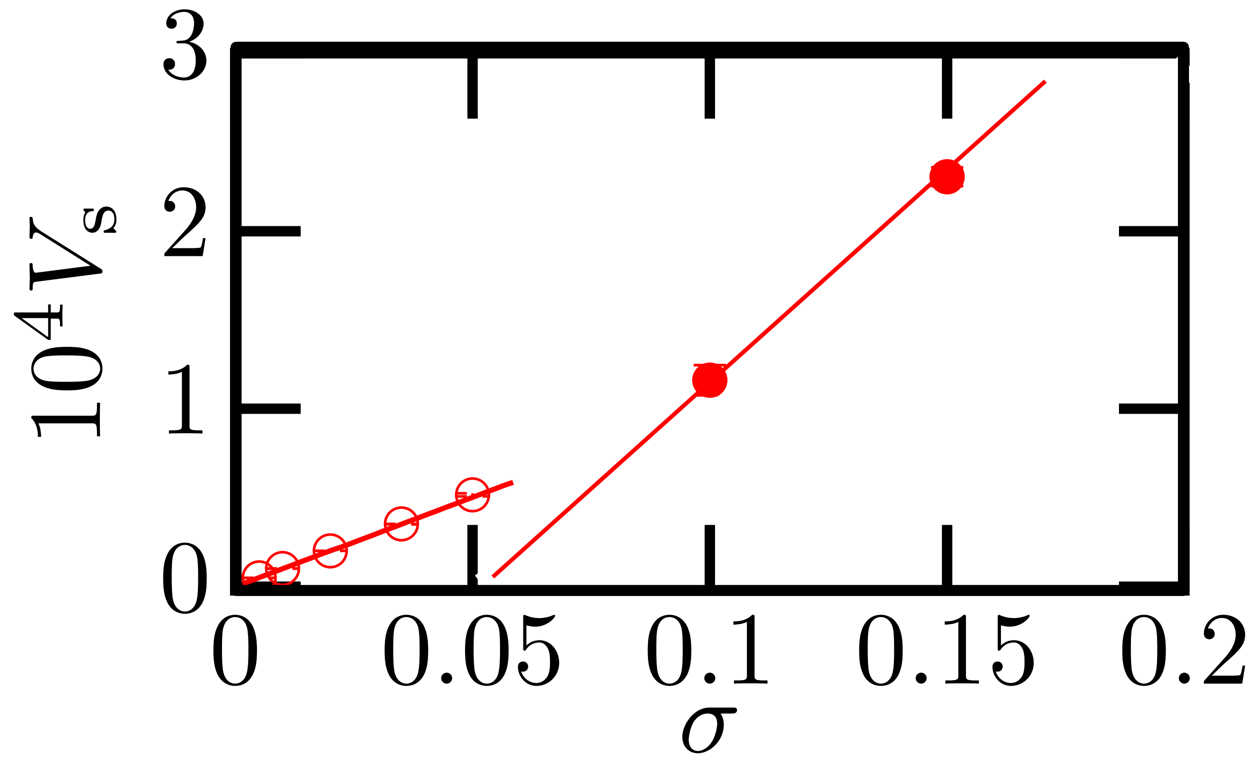
Normalized profiles of velocity across gap with smooth walls



- Almost total slip below yield stress. Partial slip above yield stress.

Slip velocity vs. shear stress for smooth walls

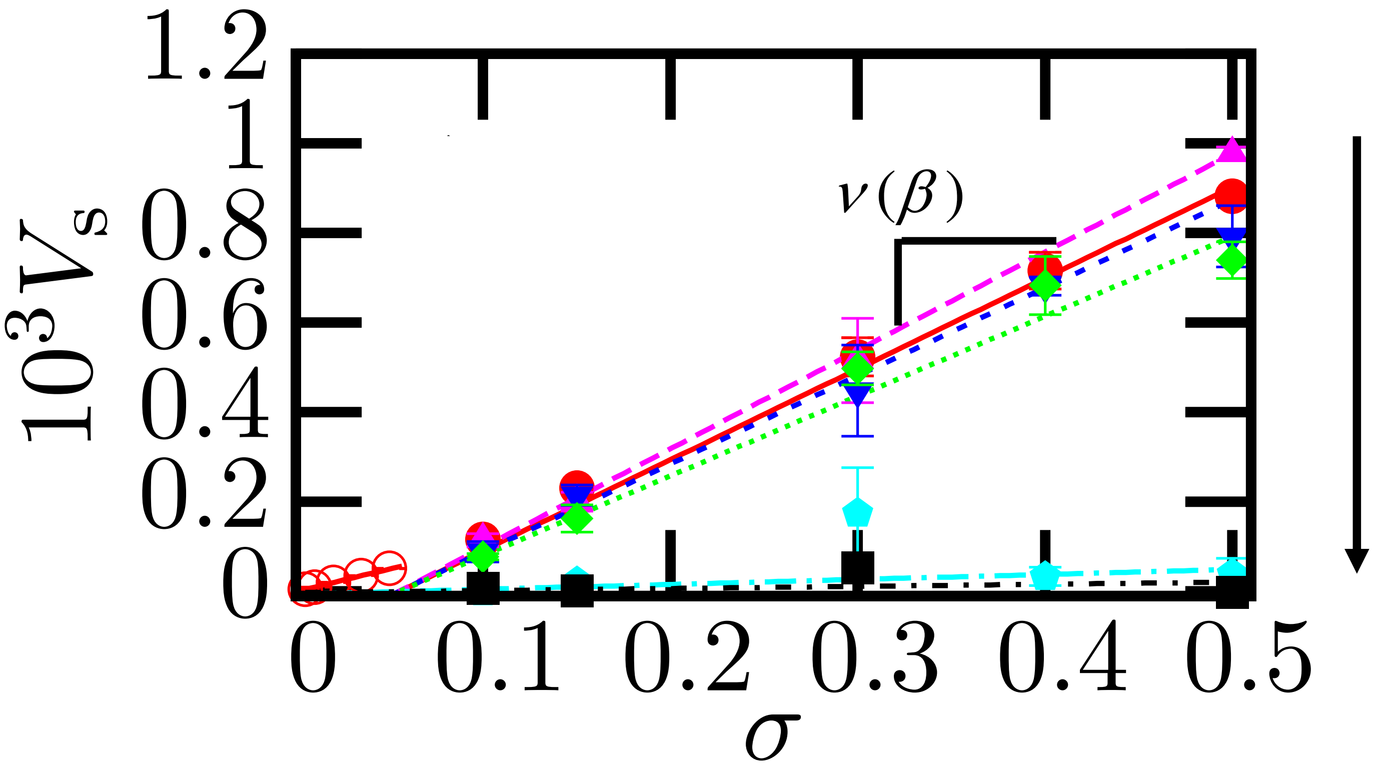


Fit to two separate linear scalings:

$$V_{\mathrm{s}}(\sigma < \sigma_{\mathrm{y}}) = \nu_{\mathrm{N}}(\beta)\sigma$$

$$V_{\mathrm{s}}(\sigma > \sigma_{\mathrm{y}}) = \nu(\beta)(\sigma - \sigma_{\mathrm{y}})$$

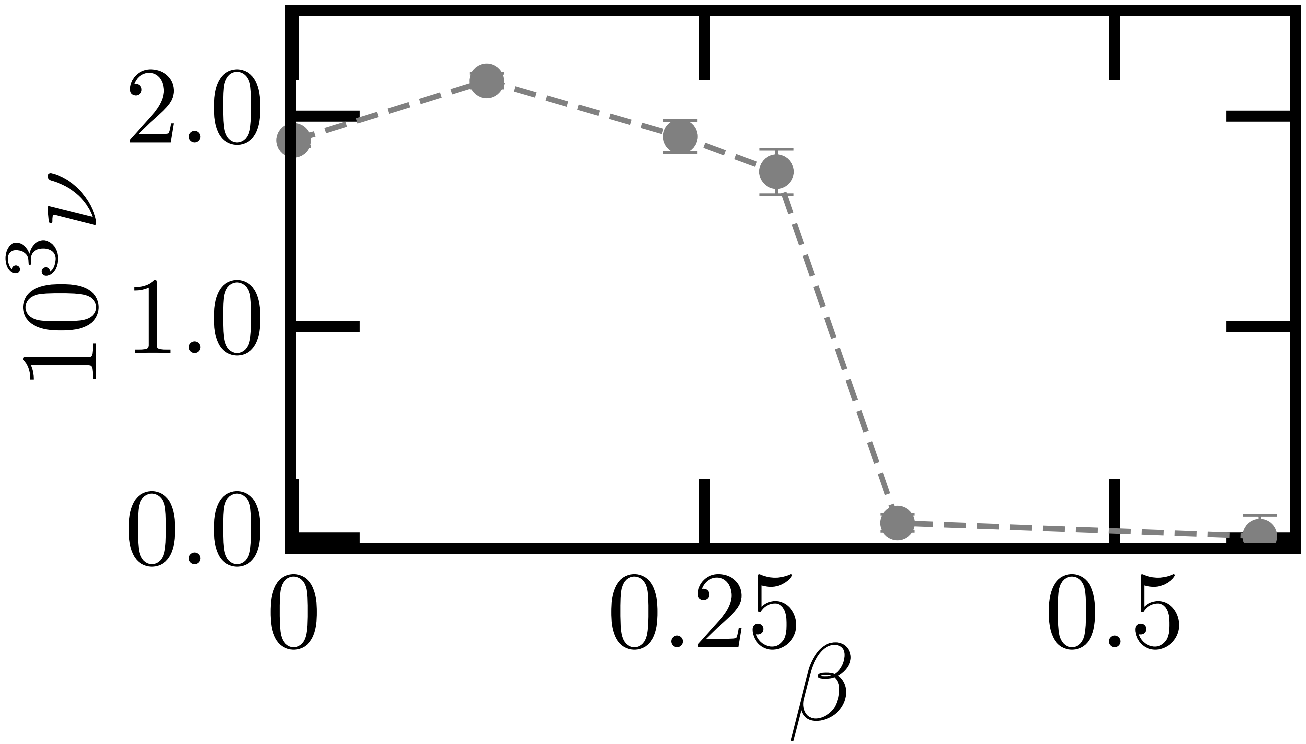
Slip velocity vs. shear stress for increasing wall roughness



roughness of wall, β, increases

- For walls rough enough compared with particle radius, slip is suppressed

Slope of slip velocity with shear stress vs. wall roughness, β



- For walls rough enough compared with particle radius, slip is suppressed

Wall slip: conclusions, outlook…

Wall slip occurs widely in sheared complex fluids

In jammed soft particle suspensions, it dominates flow curve at low shear

Immersed boundary simulation method capable of properly capturing slip

Find flow curve indeed strongly modified at low shear

Two contributions to slip: Newtonian layer at wall; fluidised particle layers

Separate linear scalings of slip velocity with stress above and below yield

Strong suppression of slip above a critical wall roughness

[G. Jung and S. M. Fielding, submitted for publication]

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