Modelling Dense Suspension Flows

- Dense suspensions: Quasi-Newtonian expectation

- Shear thickening: Frictional mechanism

- Mechanistic insight from particle-based simulation

- Contact engineering

- Flow protocol engineering

- Flow reversal as a challenge to constitutive models

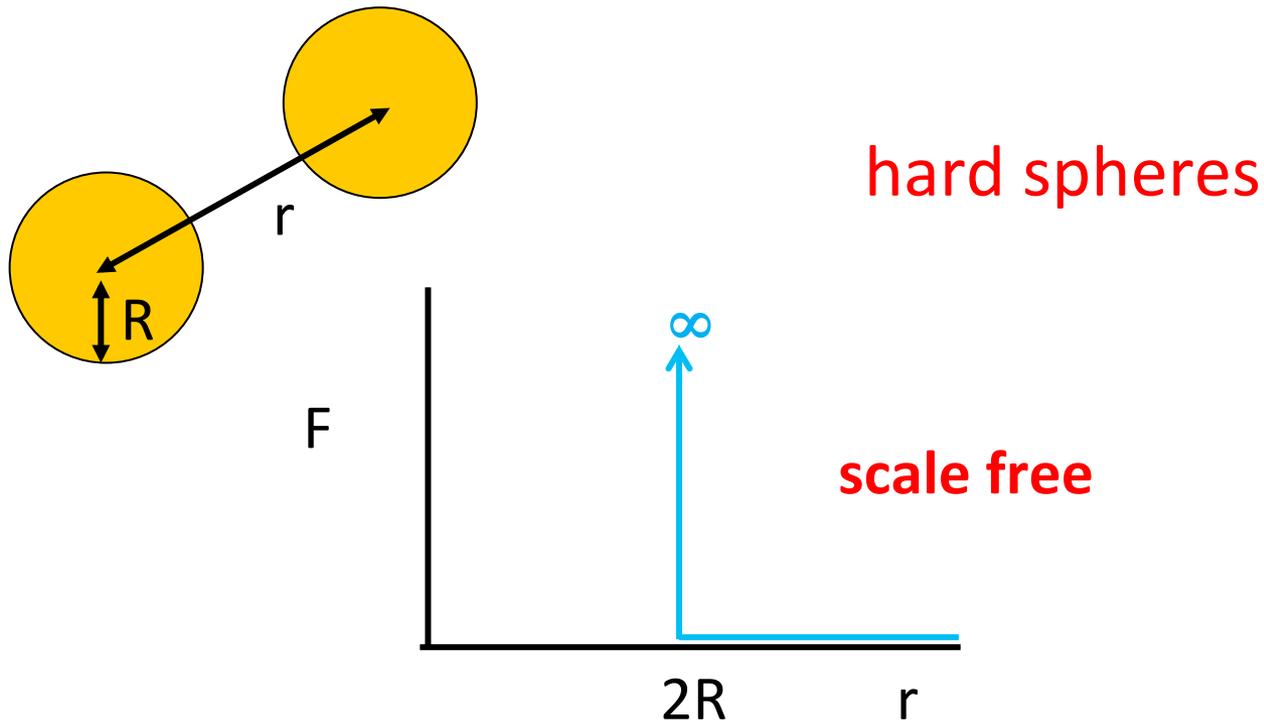Collaborators: M. Wyart (EPFL); R. Mari (Grenoble)

S. Fielding + R. Chacko (Durham); C. Ness (Cambridge)

Experiments: Poon Group (Edinburgh)

Standard Model: Hard Particle Suspensions

- hard particles in a viscous solvent ($\eta = \eta_s$)

- negligible: Brownian motion, inertia

- steady shear flow

hard spheres

scale free

Standard Model: Hard Particle Suspensions

- hard particles in a viscous solvent ($\eta = \eta_s$)

- negligible: Brownian motion, inertia

- steady shear flow

Theorem: (Stokes, Batchelor)
Any H.P.S. is either <u>quasi</u>-Newtonian, or solid

normal stresses:
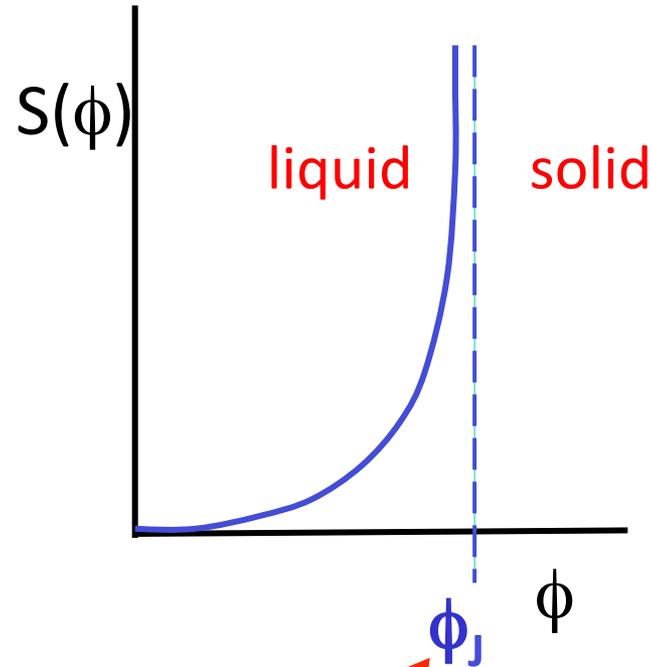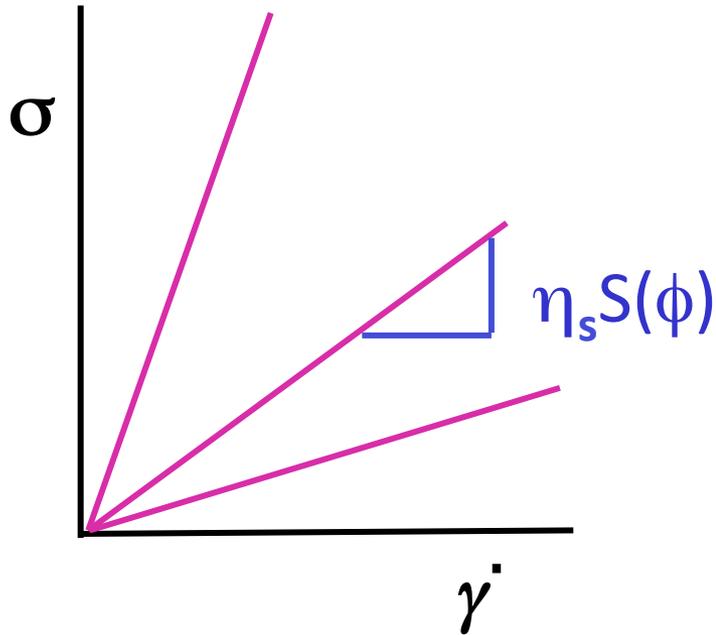also linear in $\dot{\gamma}$

Proof:

No force scale: $\sigma(\dot{\gamma}) = \eta_s \, \dot{\gamma} \; S(\phi, \dot{\gamma}\tau)$

No time scale τ: $S = S(\phi)$ only

$S < \infty$: fluid $\qquad S = \infty$: solid

Standard Model: Hard Particle Suspensions

- hard particles in a viscous solvent ($\eta = \eta_s$)

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- steady shear flow

$\eta_s S(\phi)$

σ

$\dot{\gamma}$

$S(\phi)$

liquid   solid

ϕ_J

ϕ

key parameter!!

What Governs ϕ_J ?

"friction" at interparticle "contacts"

Boyer et al 2011, Fernandez et al 2013, Seto et al 2013

Particle Contacts vs Hydroclusters

Shear thickening in colloidal dispersions

Norman J. Wagner and John F. Brady

Shampoos, paints, cements, and soft body armor that stiffens under impact are just a few of the materials whose rheology is due to the change in viscosity that occurs when colloidal fluids experience shear stress.
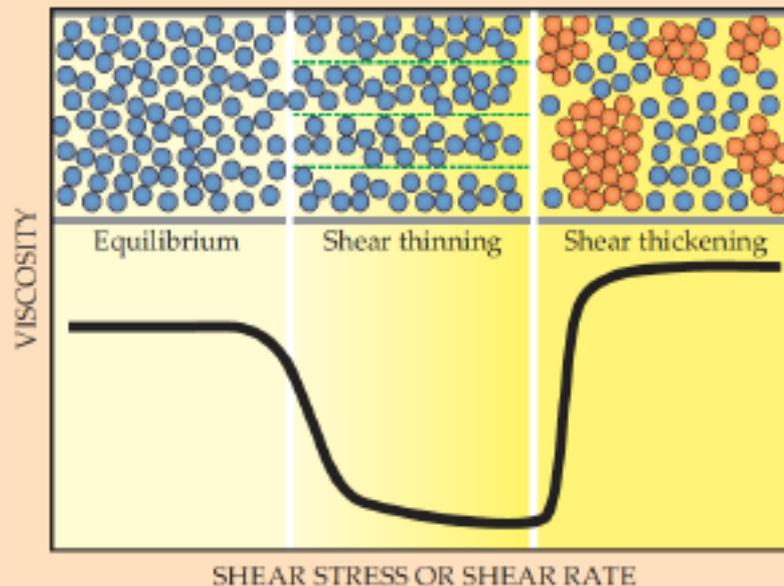
ganized, low-dissipation flow may be helpful. Unlike the seemingly random microstructure observed close to equilibrium, however, this microstructure is highly organized and

Figure 2. The change in microstructure of a colloidal dispersion explains the transitions to shear thinning and shear thickening. In equilibrium, random collisions among particles make them naturally resistant to flow. But as the shear stress (or, equivalently, the shear rate) increases, particles become organized in the flow, which lowers their viscosity. At yet higher shear rates, hydrodynamic interactions between particles dominate over stochastic ones, a change that spawns hydroclusters (red)—transient fluctuations in particle concentration. The difficulty of particles flowing around each other in a strong flow leads to a higher rate of energy dissipation and an abrupt increase in viscosity.

Particle Contacts vs Hydroclusters

Hydrodynamic forces

Cannot support static stress

Flow reversal

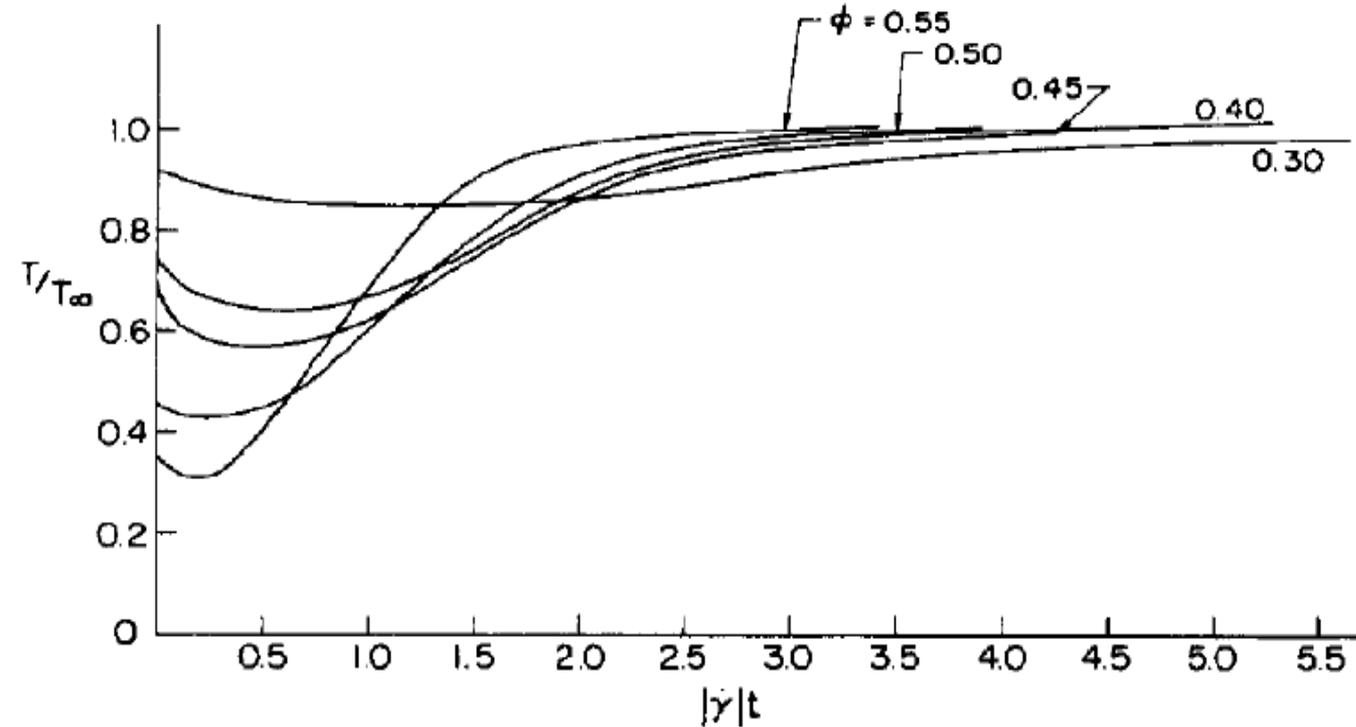σ instantly reverses (Stokes)

Contact forces

Support static stress

Flow reversal

σ instantly falls to zero

Particle Contacts vs Hydroclusters

evidence from flow reversal (quasi-Newtonian)

Hydro- and contact forces **both** matter
Stress is contact-dominated for $\phi > 0.5$
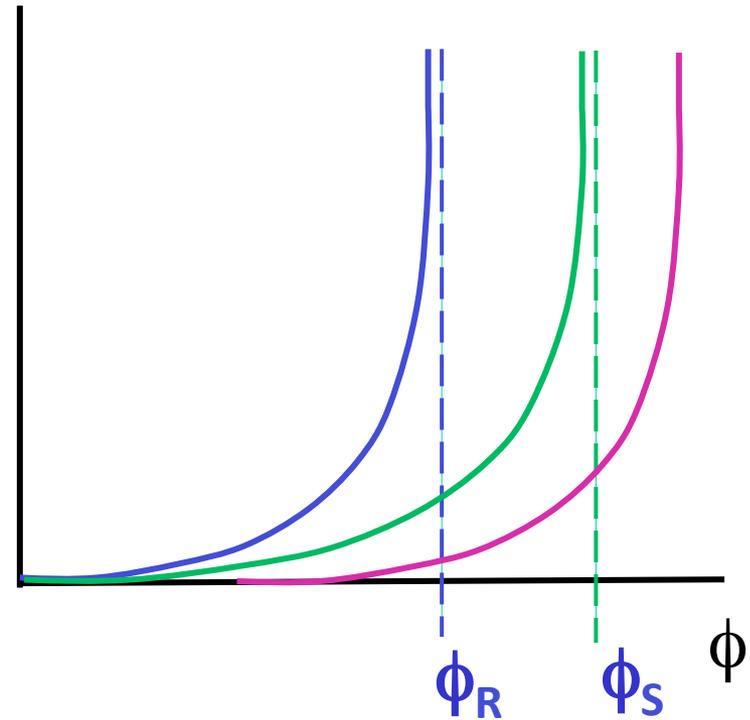Acrivos + Galada-Maria 1980

Why Friction Matters

max friction (all rolling $S(\phi)$

$\phi_J = \phi_R = 0.58$

typical friction ($\mu \approx 1$):

$\phi_J = 0.60$

zero friction (all sliding):

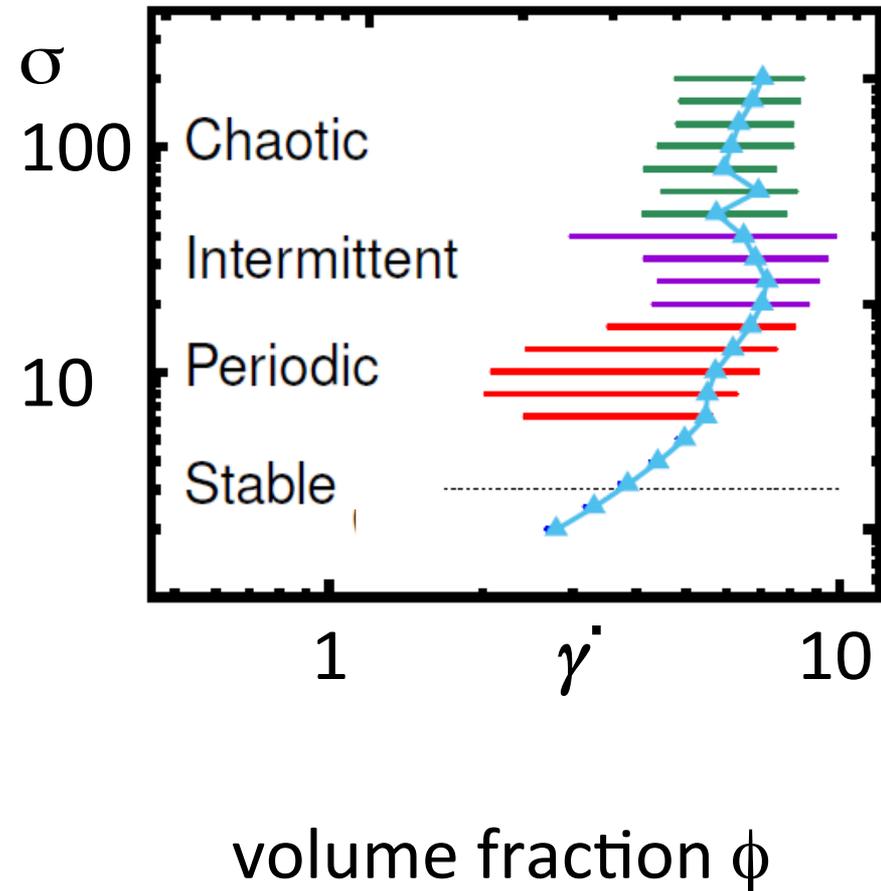$\phi_J = \phi_S = 0.64$

Hard Particle Suspensions: Summary
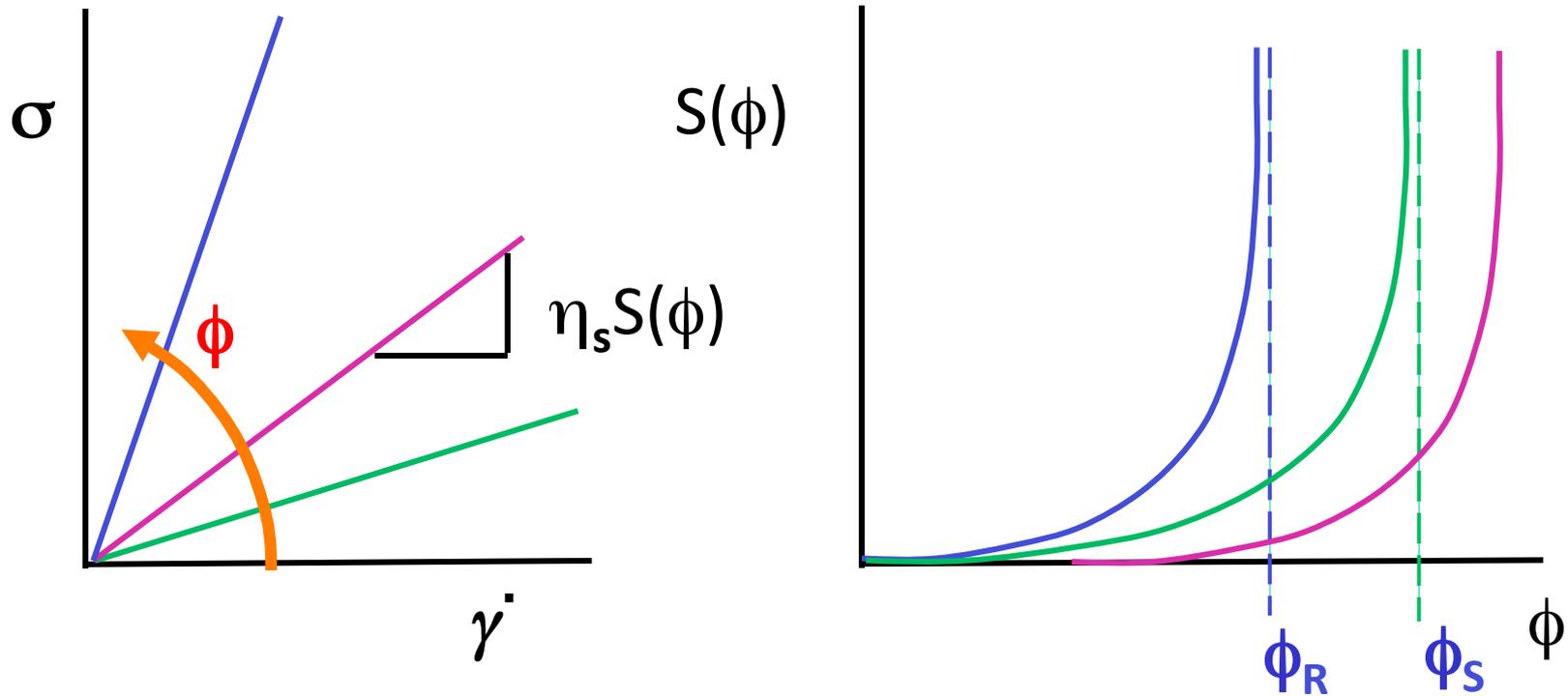
- Quasi-Newtonian

- viscosity diverges at a <u>friction-dependent</u> density

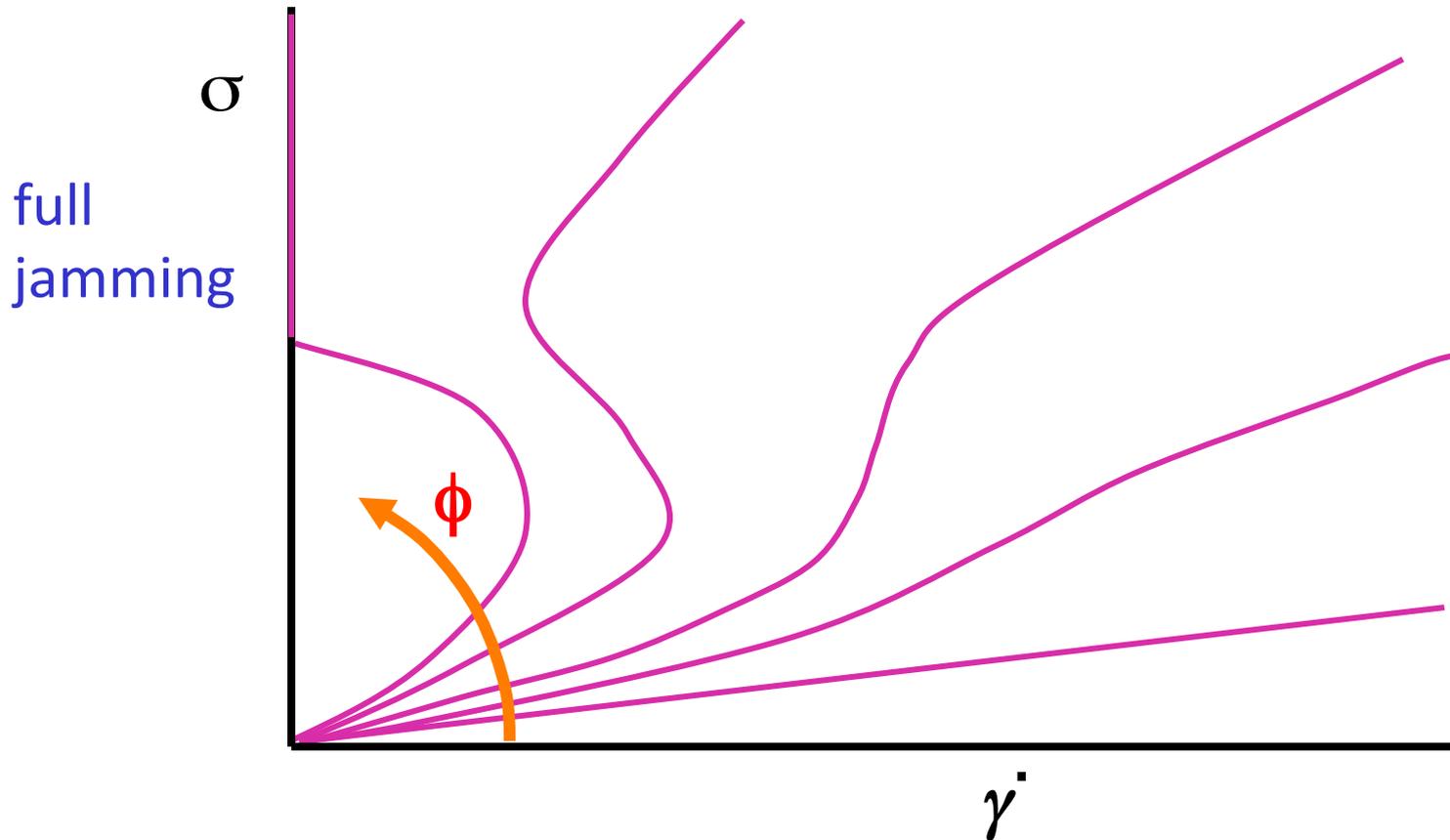# Shear-Thickening Suspensions
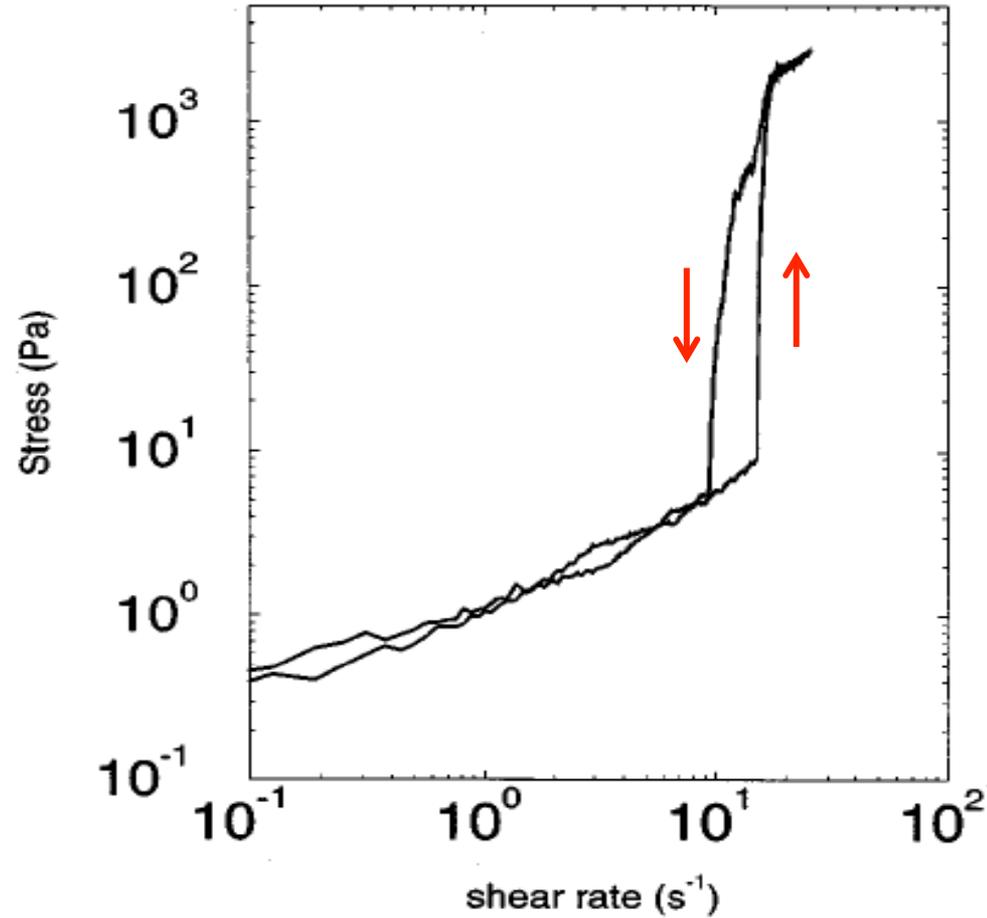
Bender + Wagner 1996

Shear-Thickening Suspensions
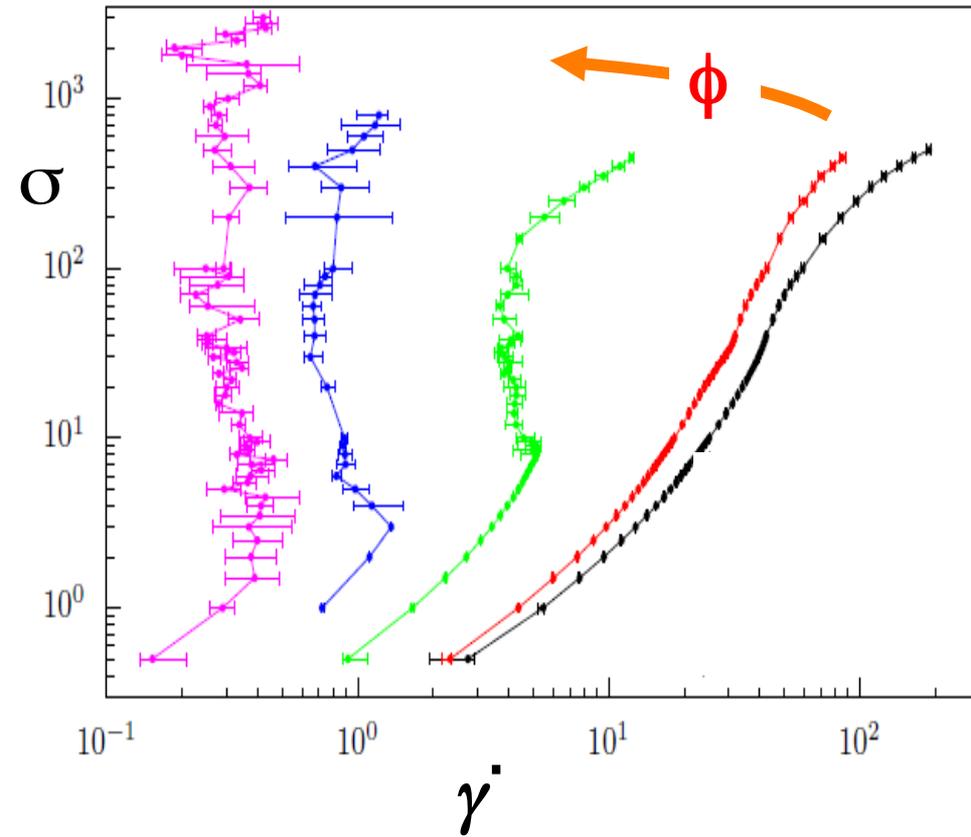
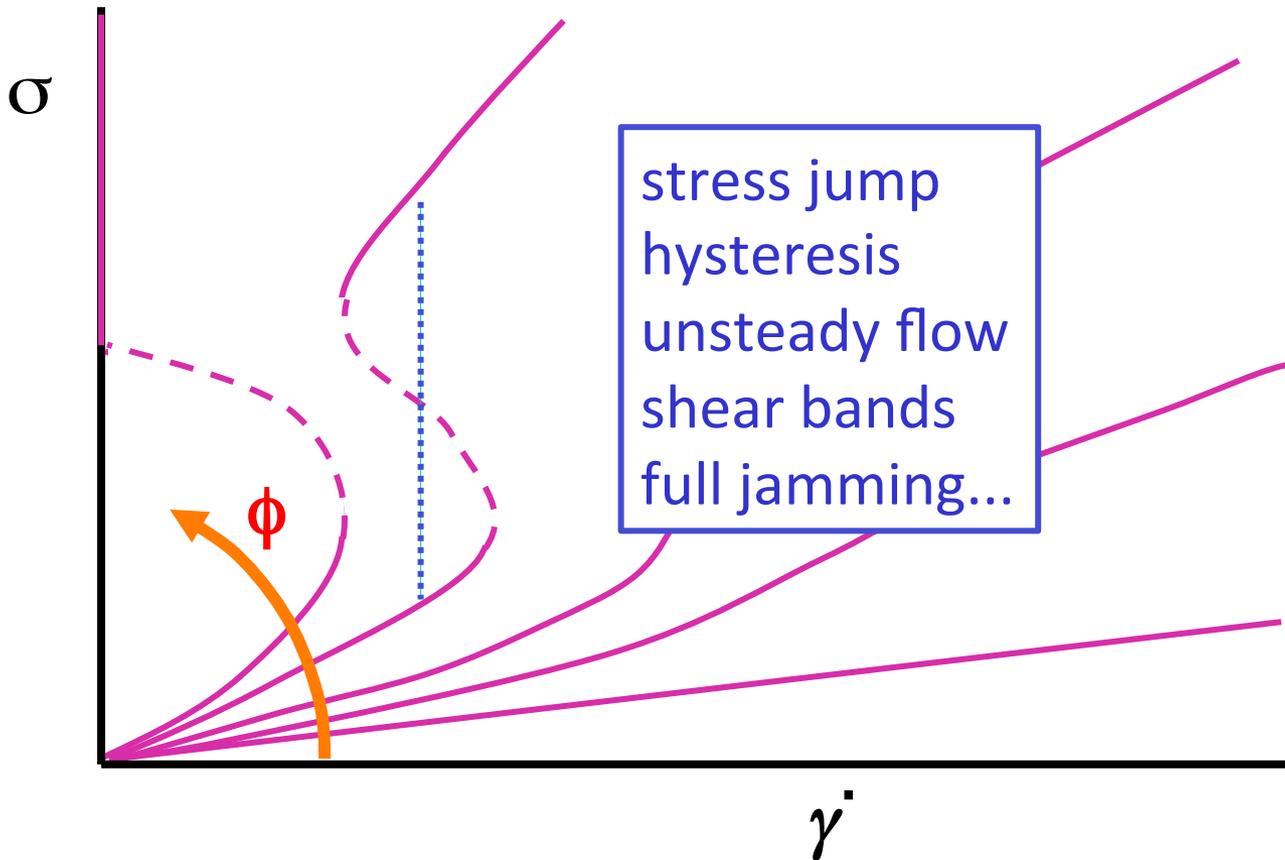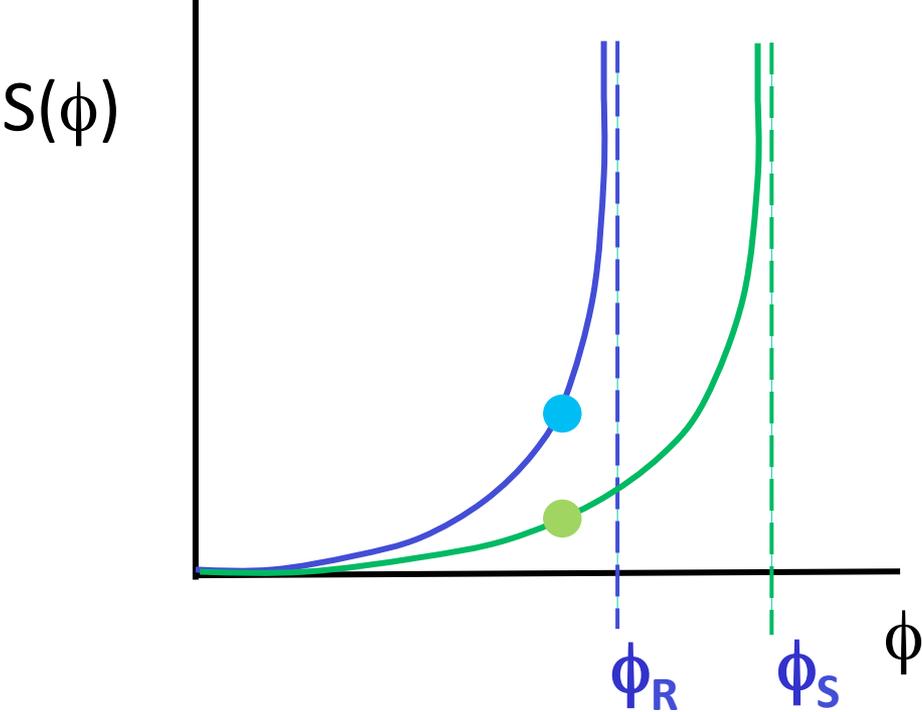Hermes et al J Rheol 2016

Shear-Thickening Suspensions

Data is explicable if:

σ

full
jamming

φ

γ̇

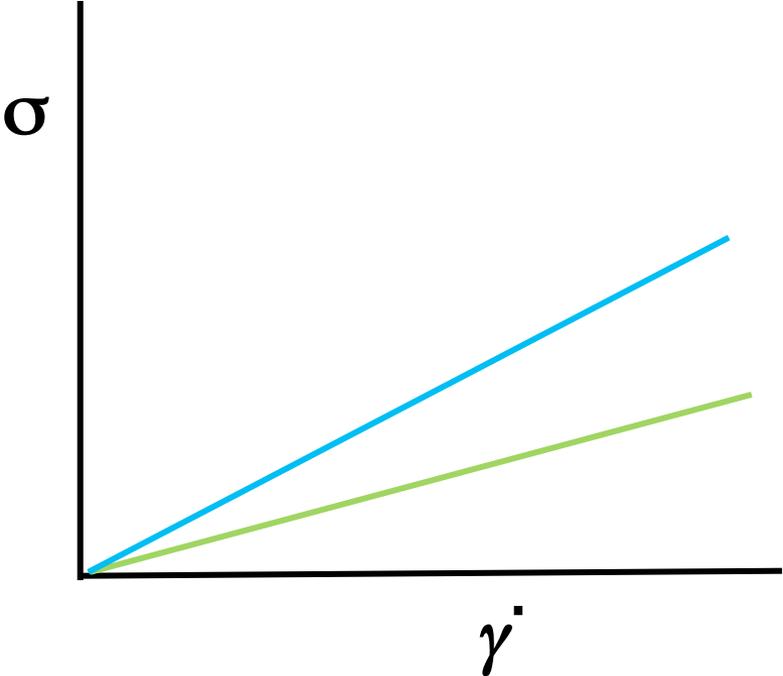Bashkirtseva et al 2009, Wyart + MEC 2014, Holmes et al 2004

Shear-Thickening Suspensions

Data is explicable if:

σ

ϕ

$\dot{\gamma}$

stress jump
hysteresis
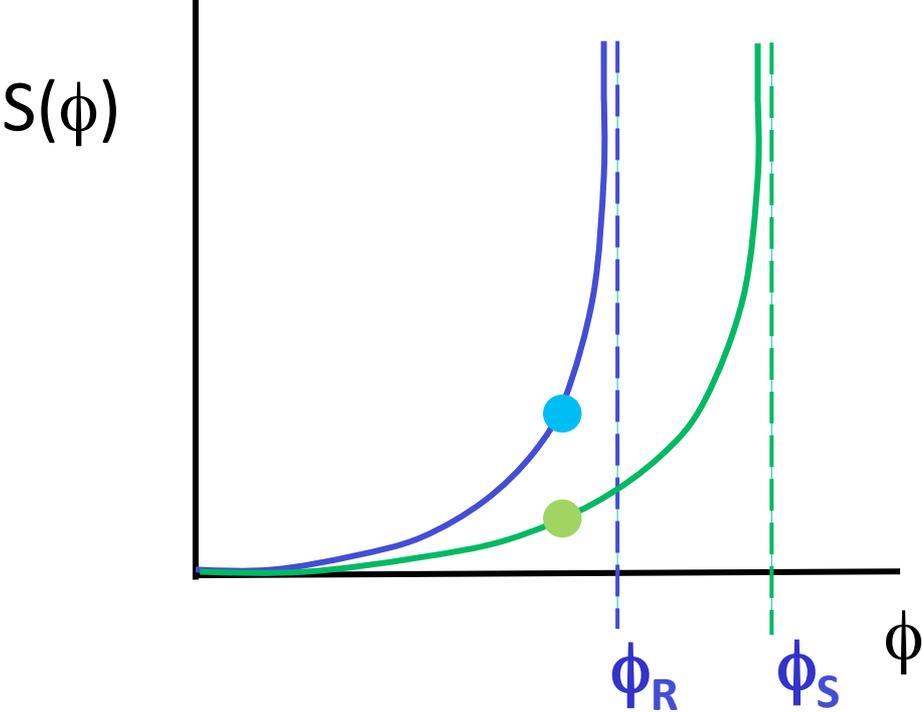unsteady flow
shear bands
full jamming...

Bashkirtseva et al 2009, Wyart + MEC 2014, Holmes et al 2004

Stress-Dependent Friction
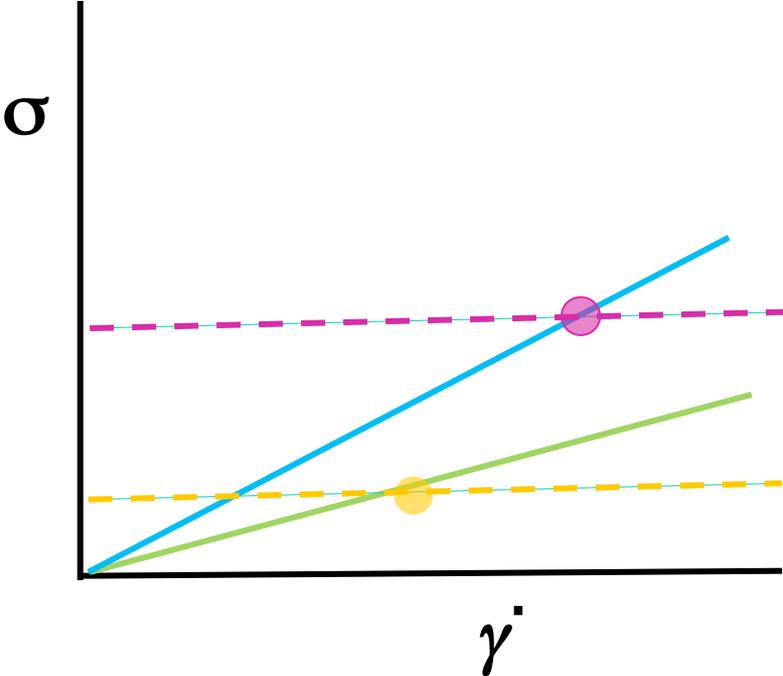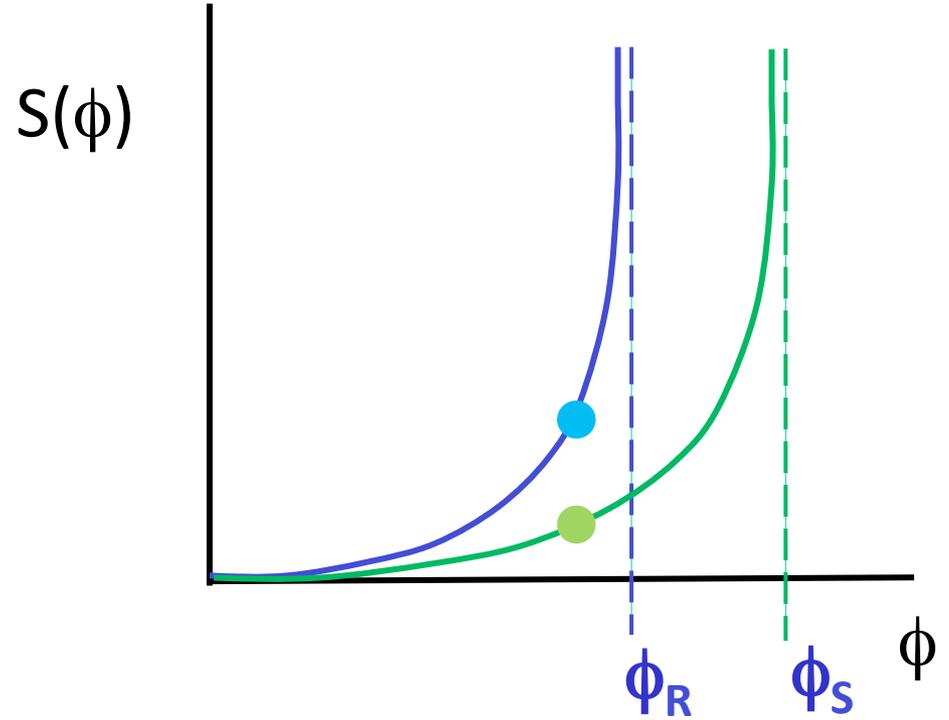

σ

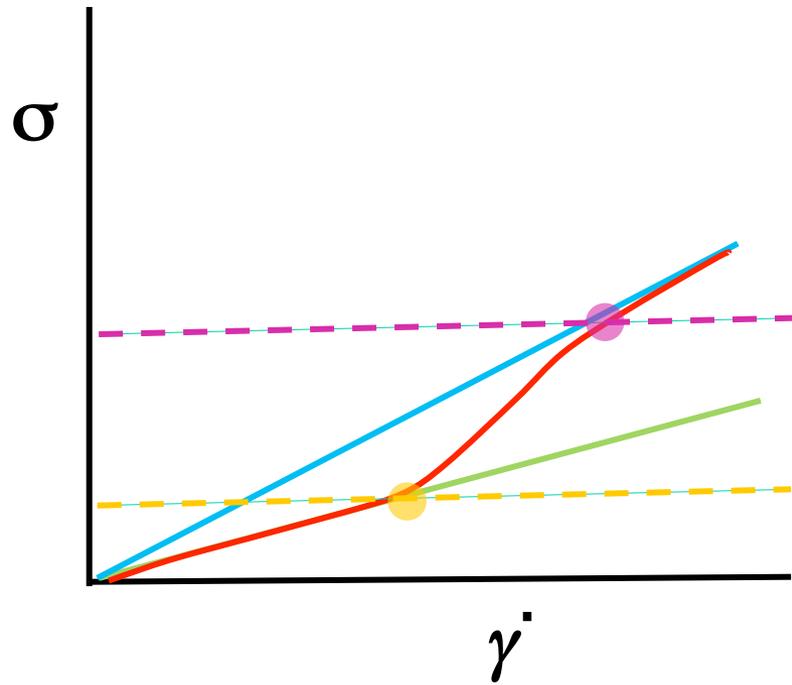$\dot{\gamma}$

$S(\phi)$

ϕ_R ϕ_S

ϕ

Wyart + MEC 2014

Stress-Dependent Friction

Wyart + MEC 2014

Stress-Dependent Friction

σ

$\dot{\gamma}$
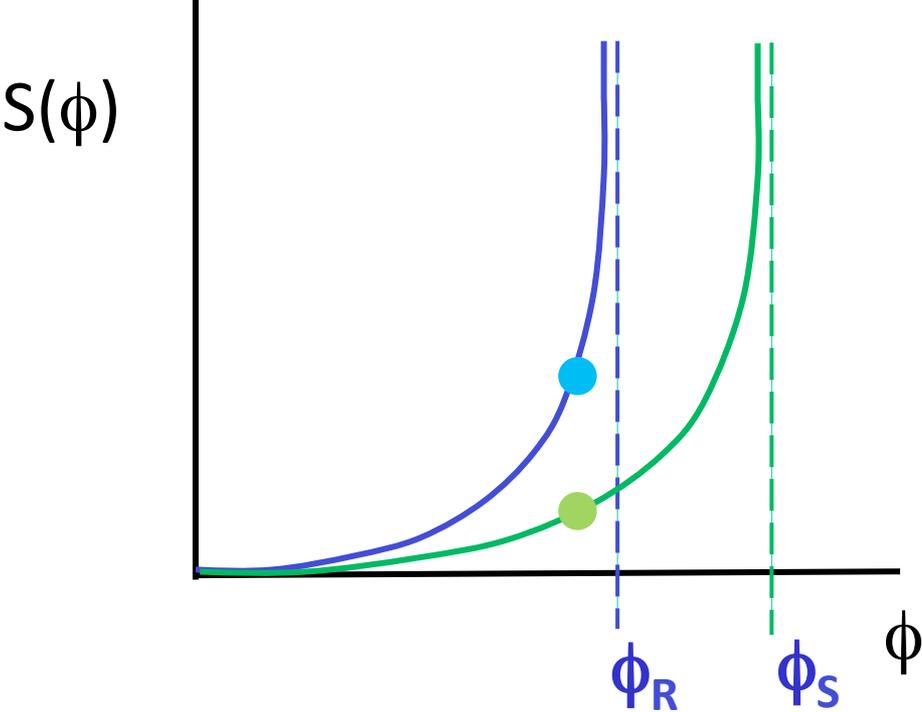
$S(\phi)$

ϕ_R ϕ_S ϕ
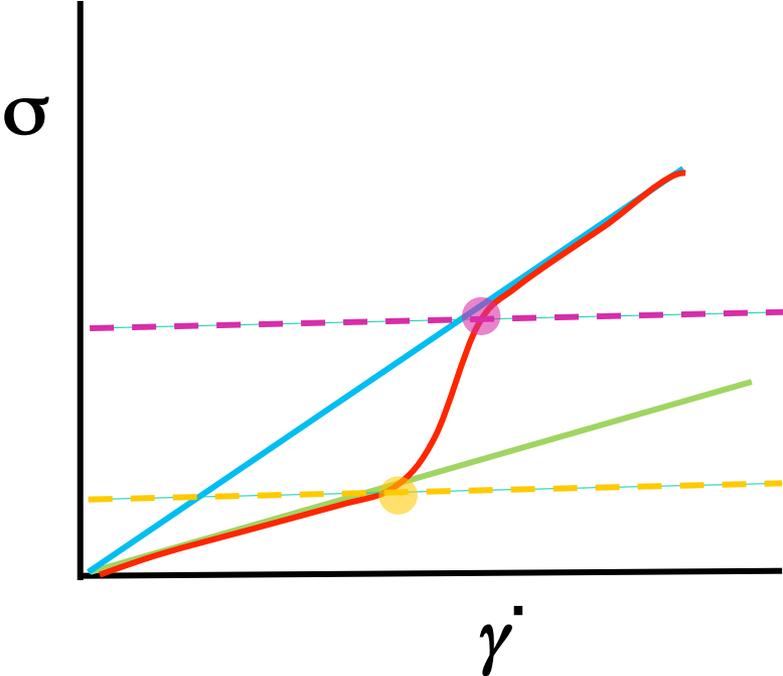
Wyart + MEC 2014

Stress-Dependent Friction

Wyart + MEC 2014

Stress-Dependent Friction

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Wyart + MEC 2014

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Stress-Dependent Friction
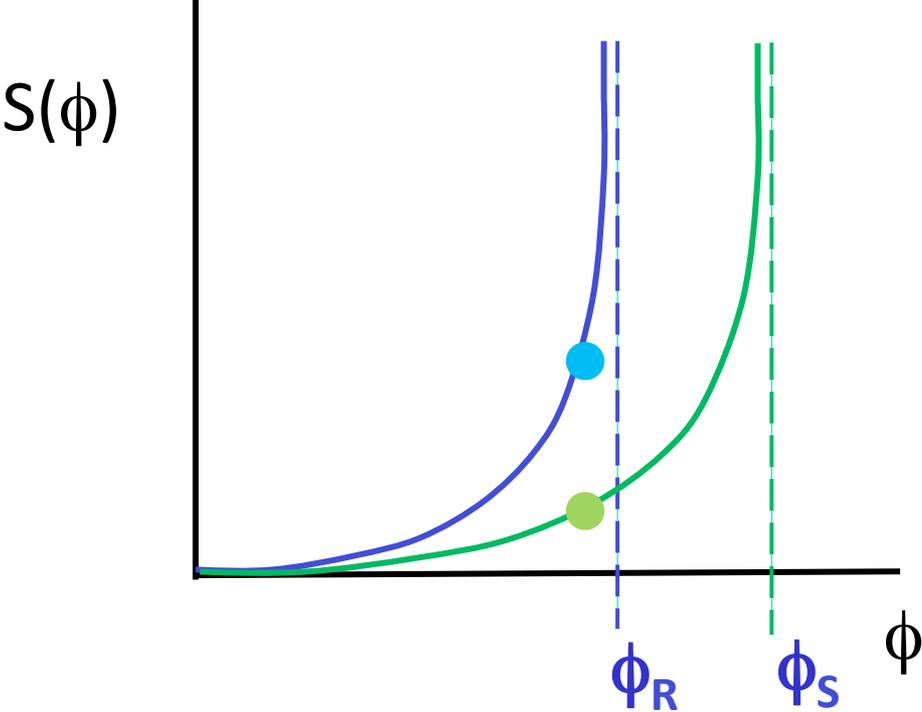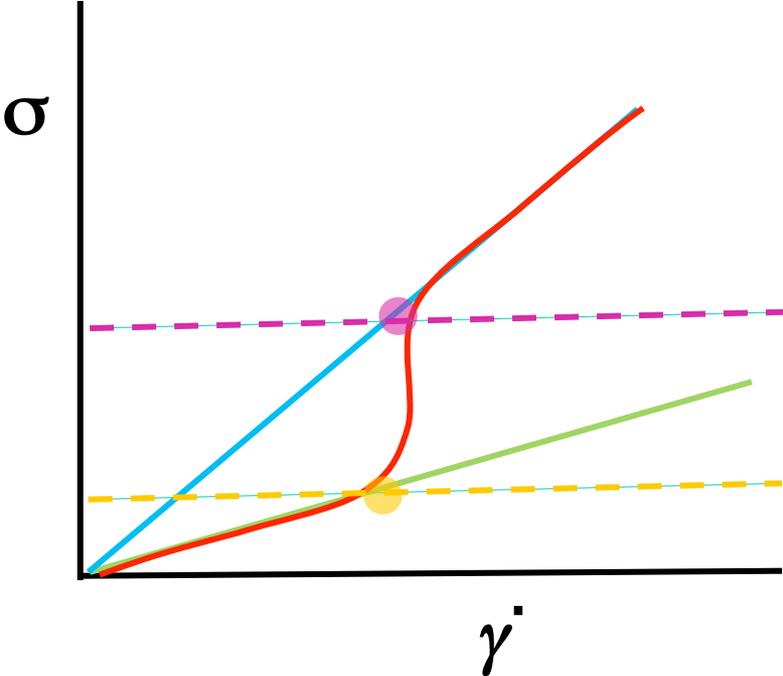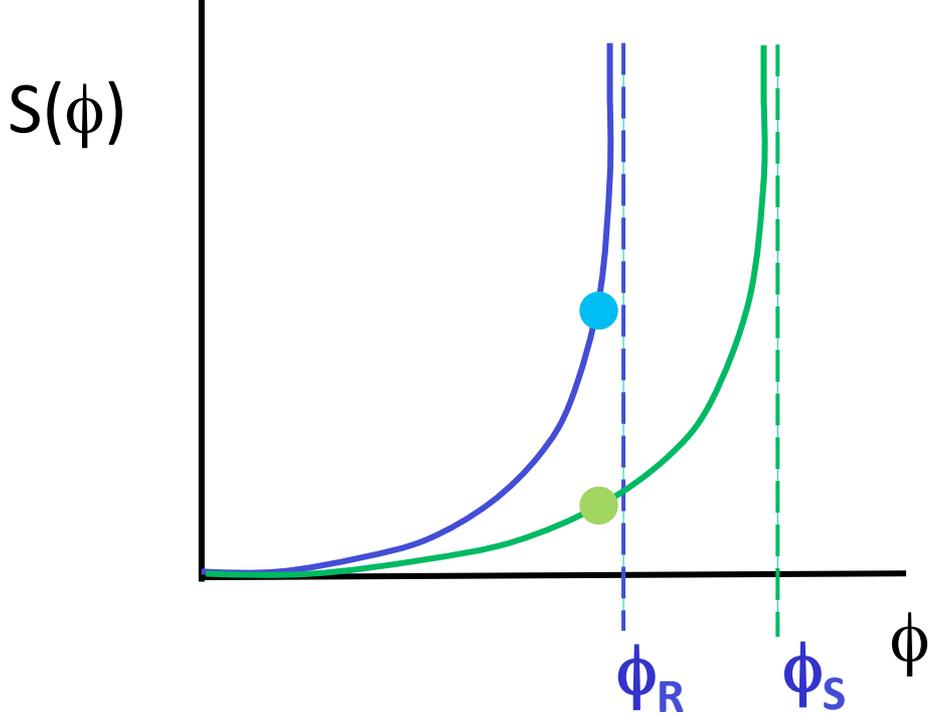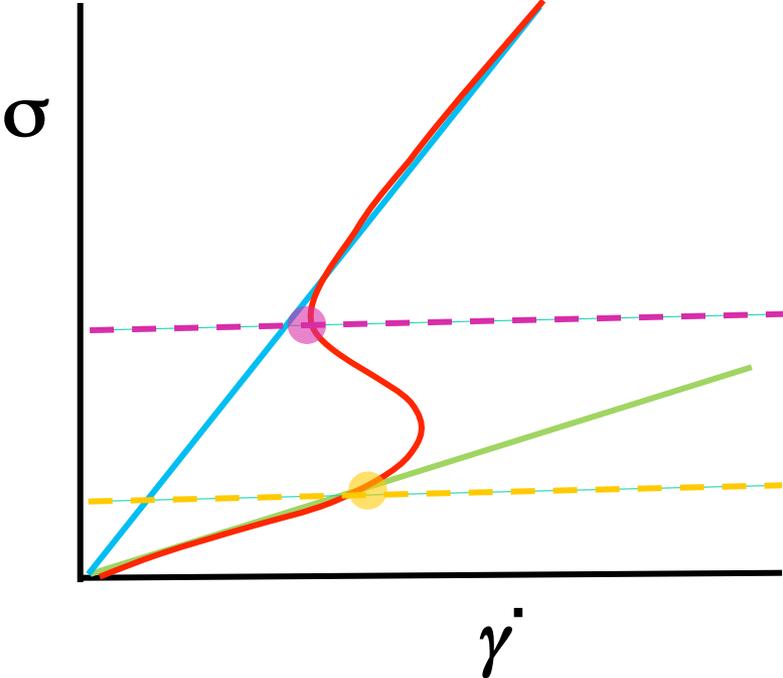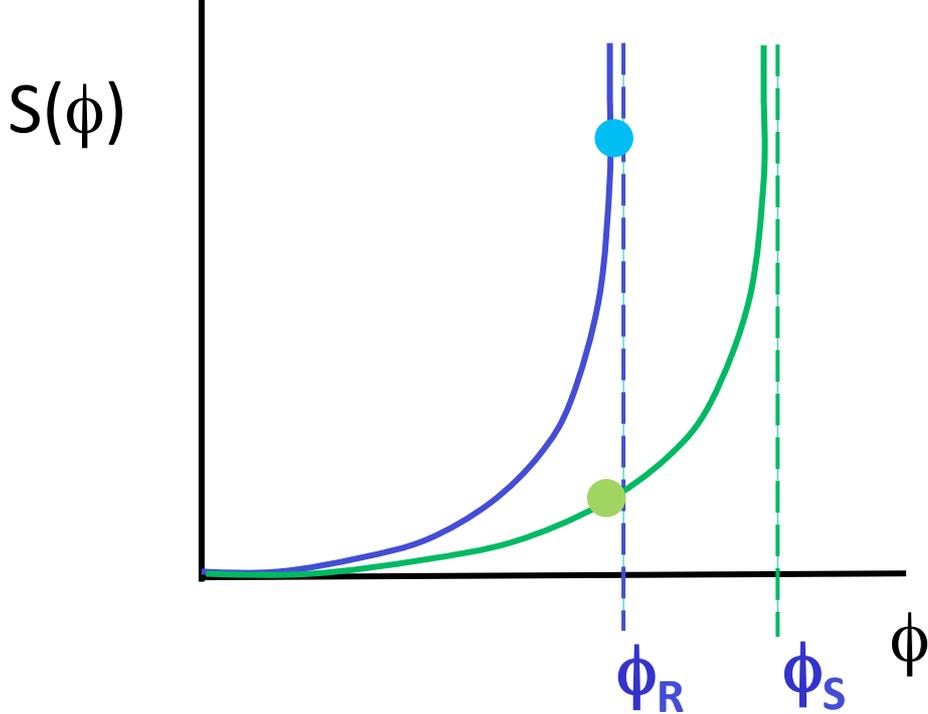

σ

$\dot{\gamma}$

$S(\phi)$

ϕ_R ϕ_S ϕ
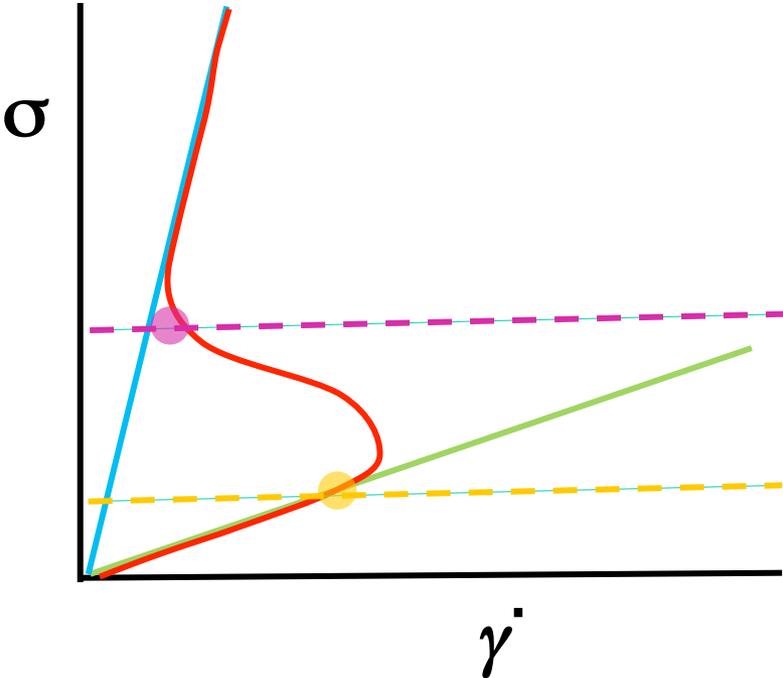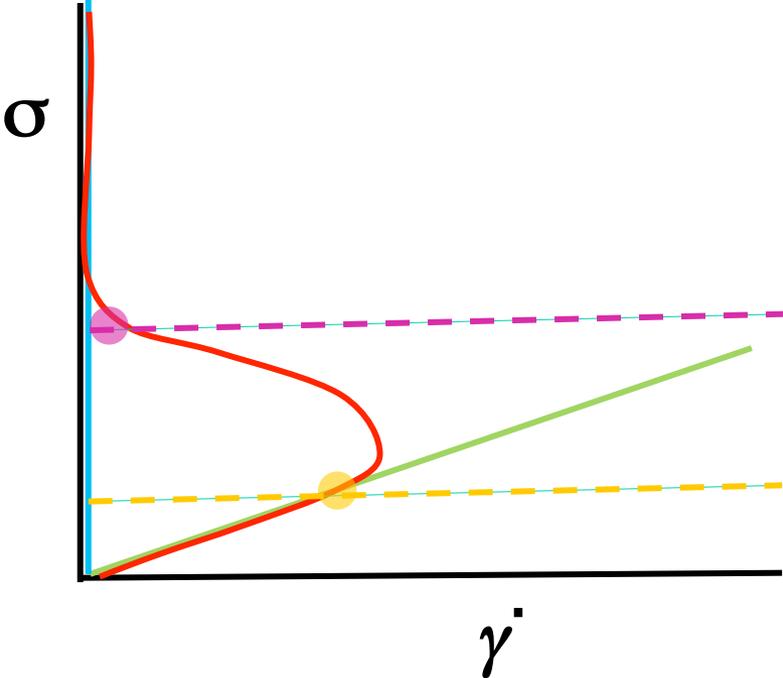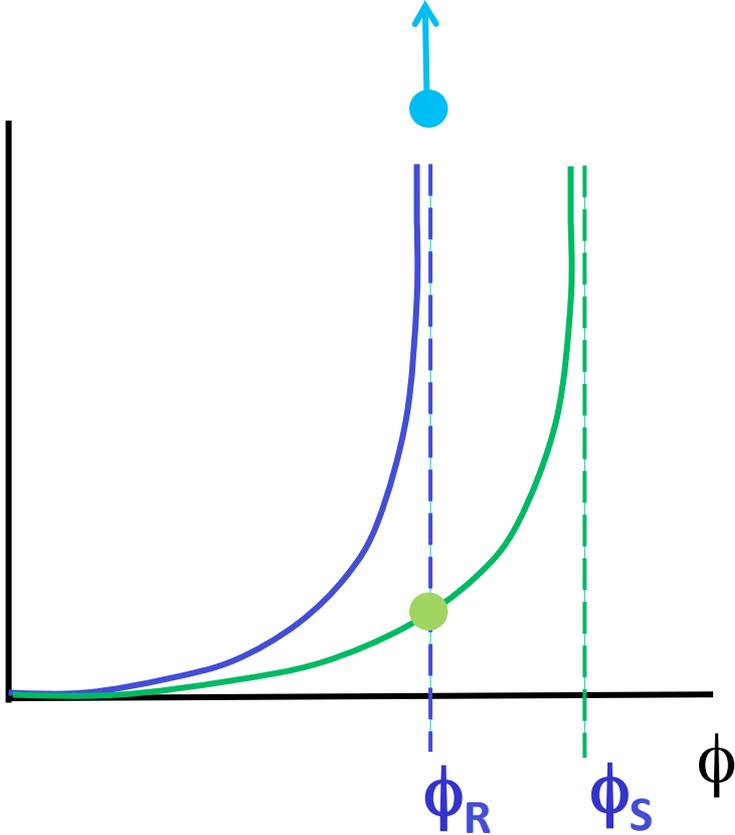
Wyart + MEC 2014

Stress-Dependent Friction

⇒ **what we wanted**
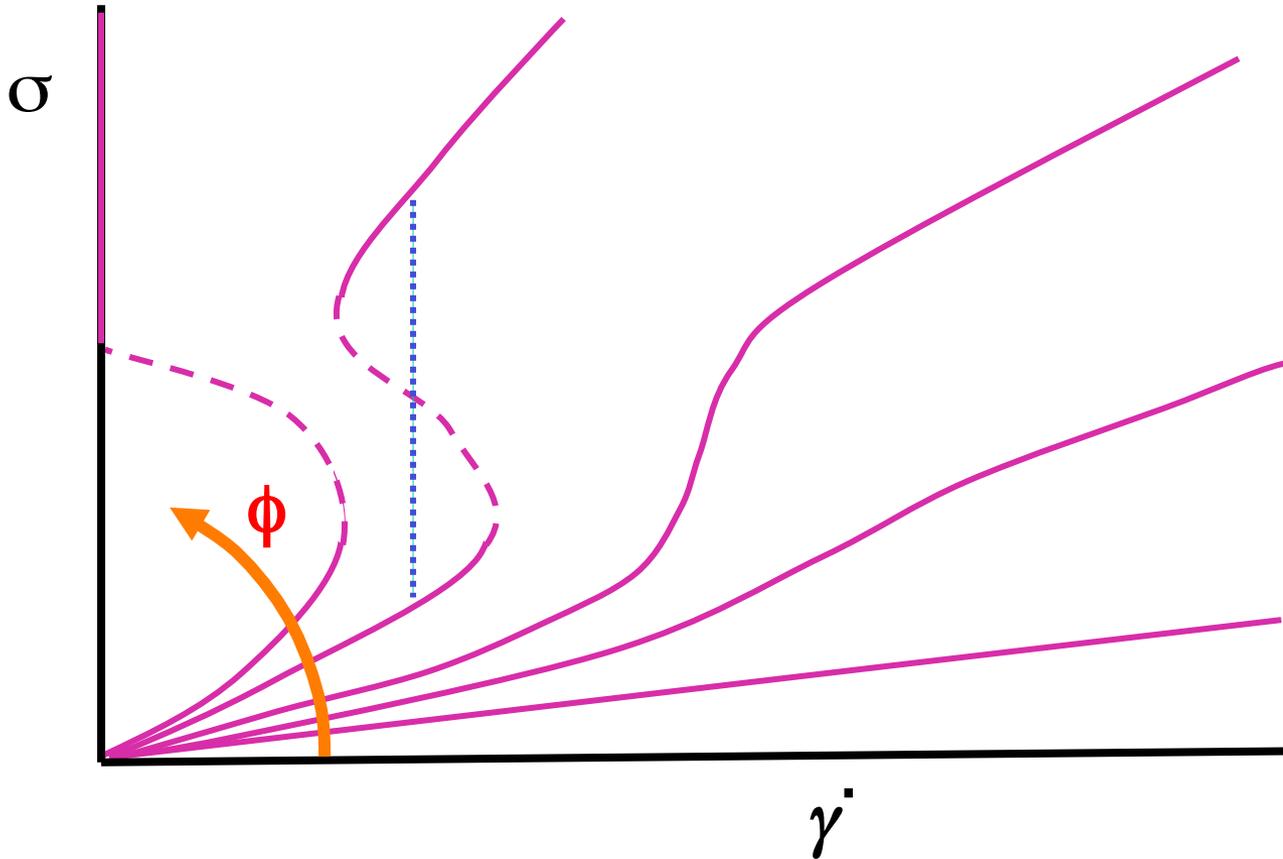
Mechanistic Insight from Particle-Based Simulations

Simulation approach for non-Brownian suspensions

A. Quasi-Newtonian

- Almost hard particles

- Contact forces + hydrodynamic lubrication forces

  Long-range hydro generally omitted

B. Shear thickening

- Additional contact friction below critical separation

- CLM: friction switches on at critical normal load

Mari et al 2014/18… Melrose+Ball 1997… Brady+Bossis 1985 … Cundell+Strack 1979

Mechanistic Insight from Particle-Based Simulations

time-averaged flow curves
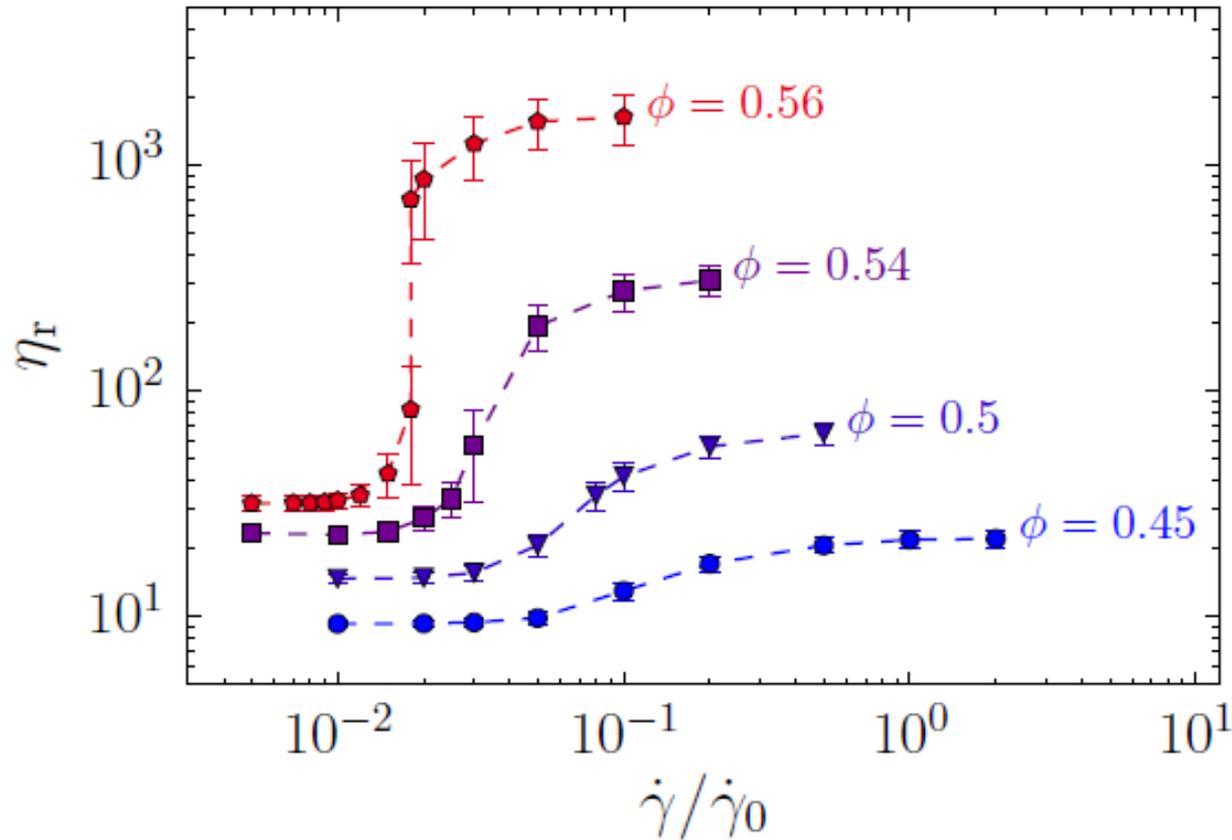
Simulations: Critical load model, Mari et al 2014

Mechanistic Insight from Particle-Based Simulations

macroscopic singularities despite smooth f(σ)

f(σ) = fraction of frictional contacts
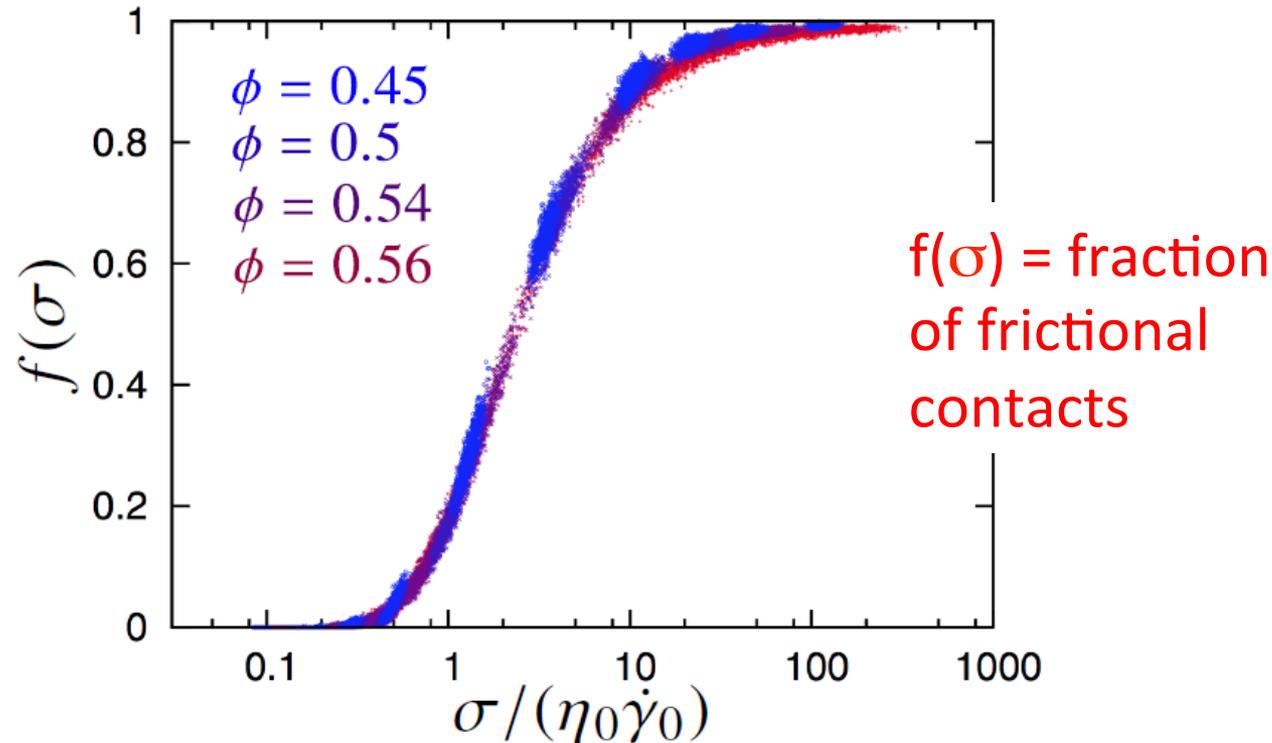
Simulations: Critical load model, Mari et al 2014

Dense Suspensions: Contact Engineering
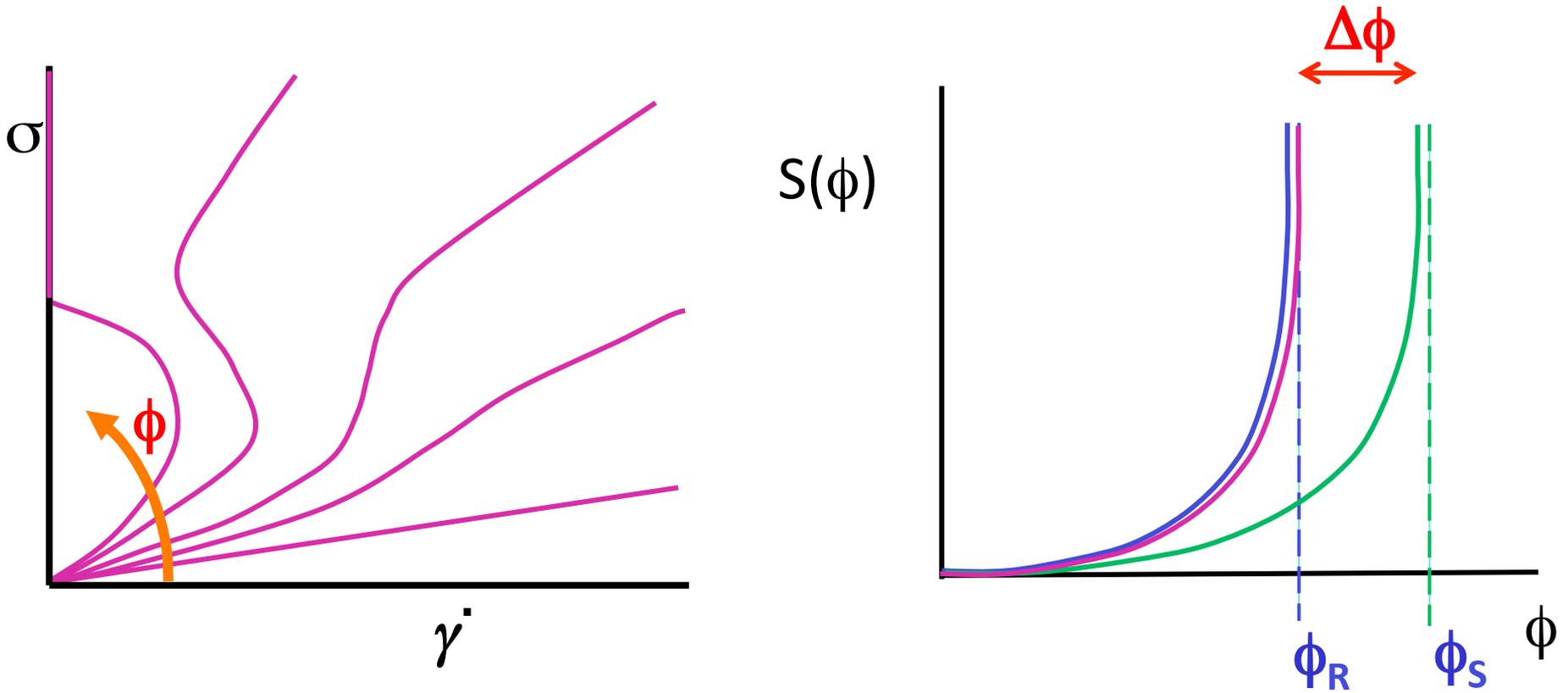
friction modifiers change everything!

Dense Suspensions: Contact Engineering

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Dense Suspensions: Contact Engineering

friction modifiers change everything!

Dense Suspensions: Contact Engineering

σ

ϕ

$\dot{\gamma}$

$S(\phi)$

$\Delta\phi$

ϕ_R ϕ_S ϕ
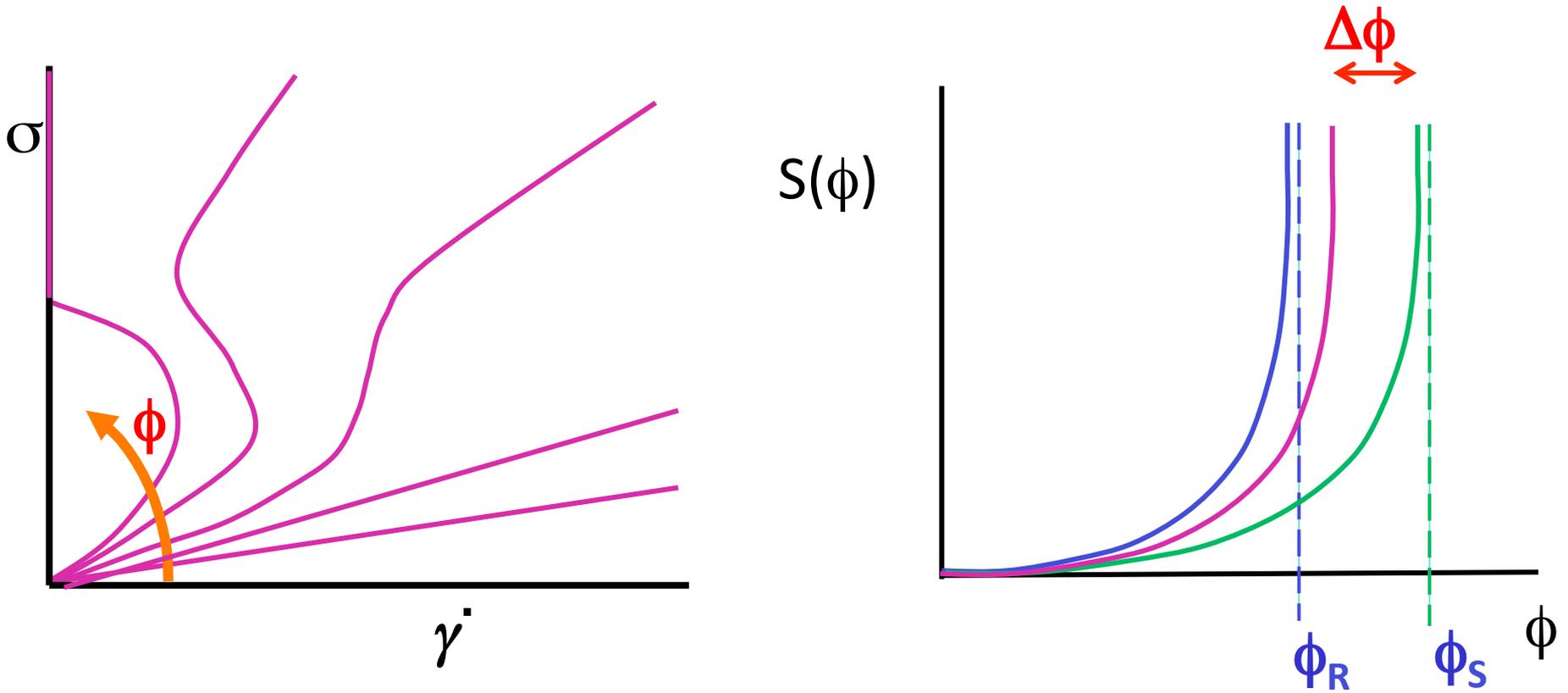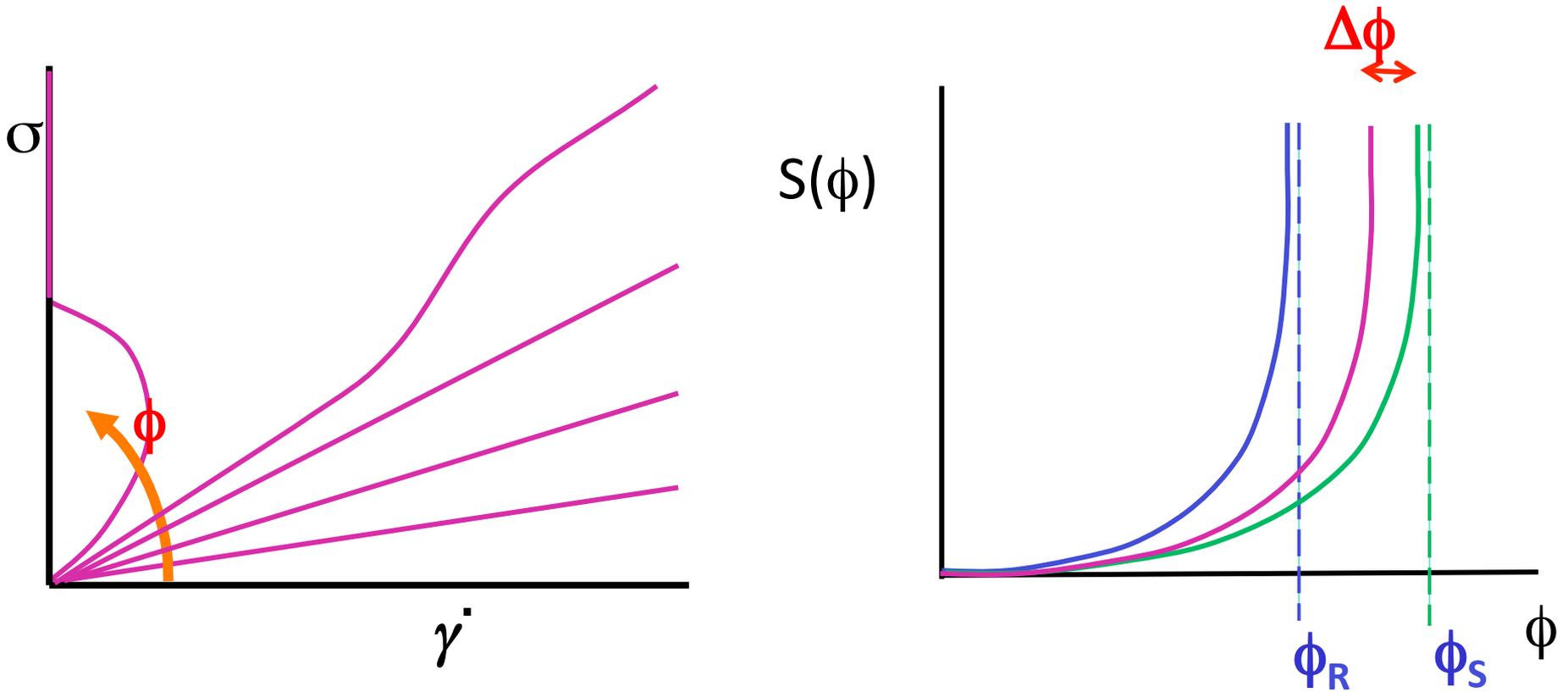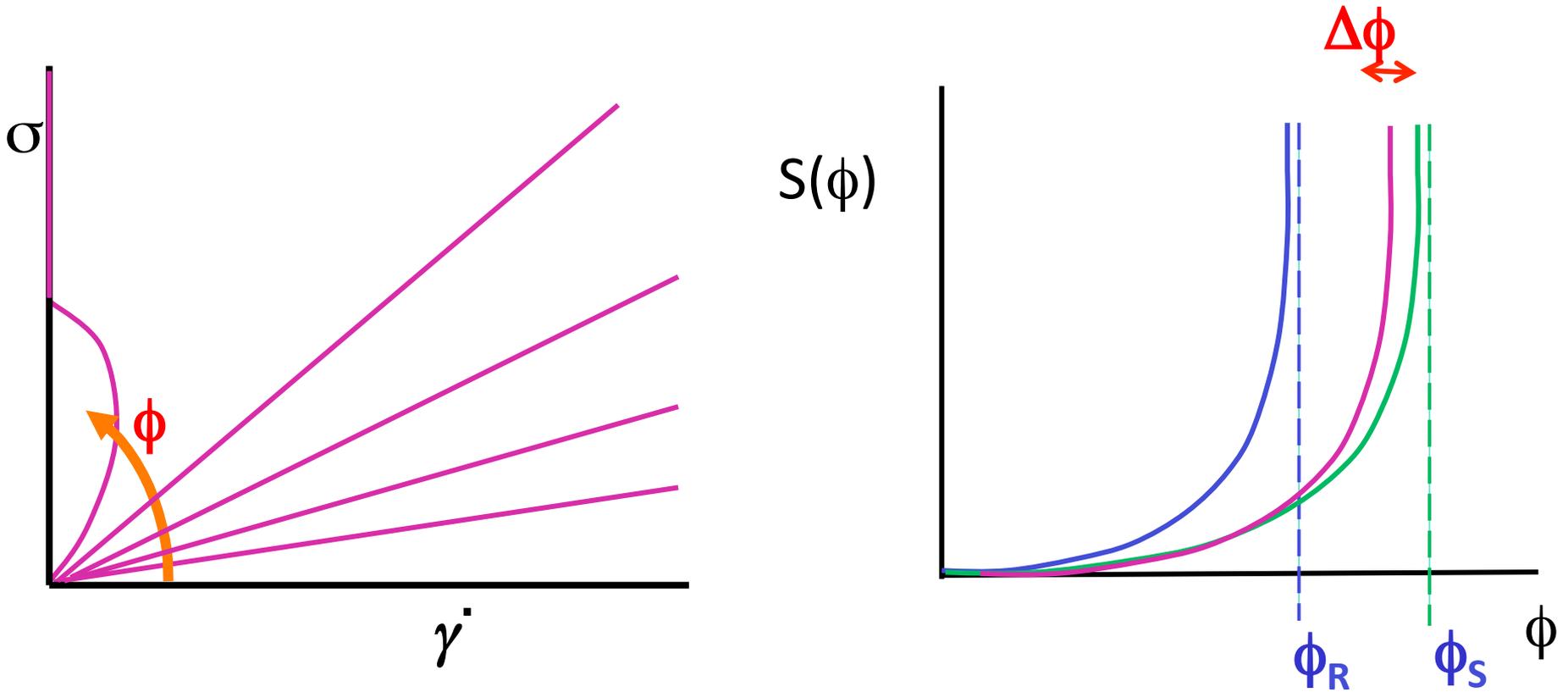
friction modifiers change everything!

Dense Suspensions: Contact Engineering
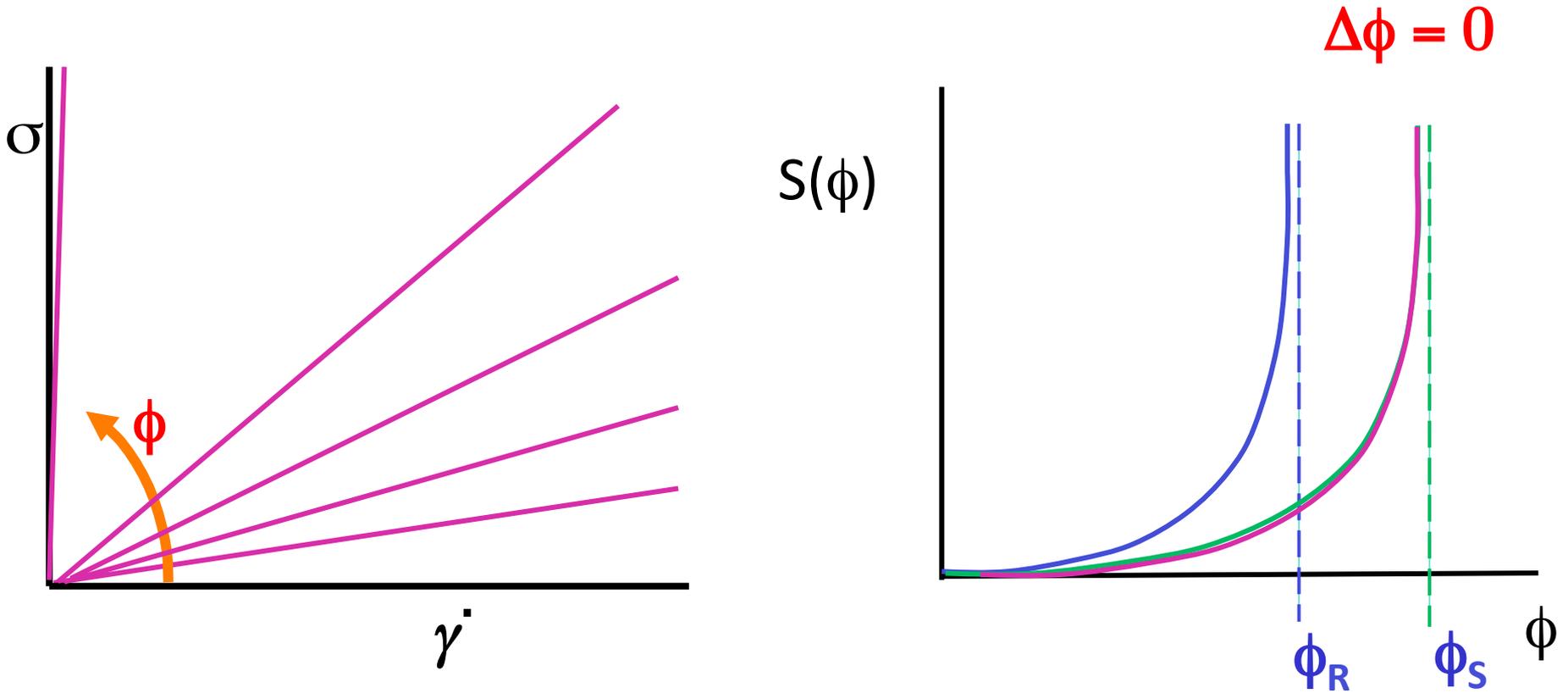
friction modifiers change everything!

Flow Protocol Engineering: OSP

Can we overcome jamming by massaging the flow?
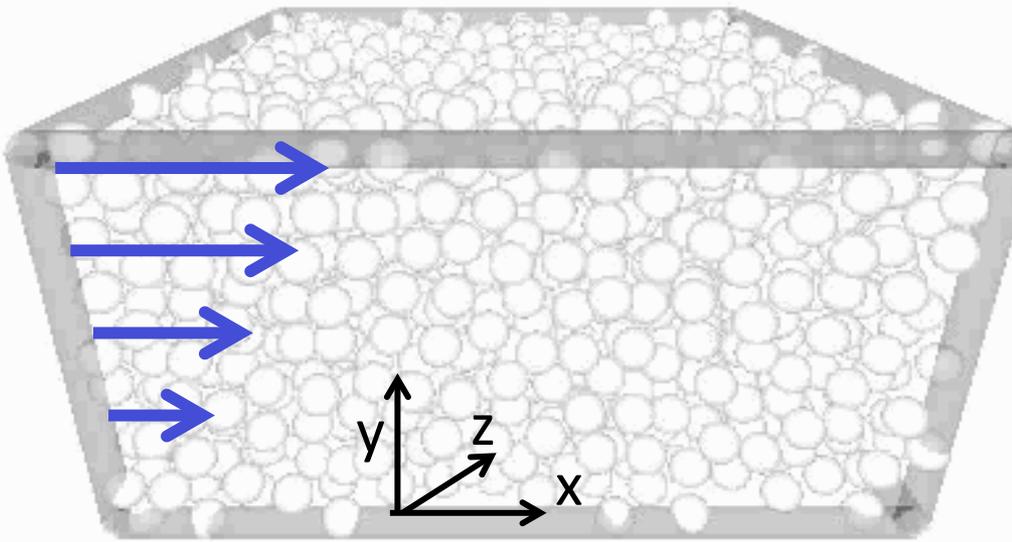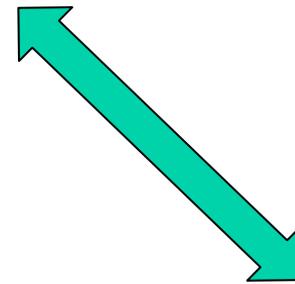
$$v_x = \dot{\gamma}\, y \qquad\qquad v_z = A \cos(\omega t)$$

Steady shear base flow   +   Orthogonal Superimposed Perturbation

N. Lin et al, PNAS 113, 10774 (2016)
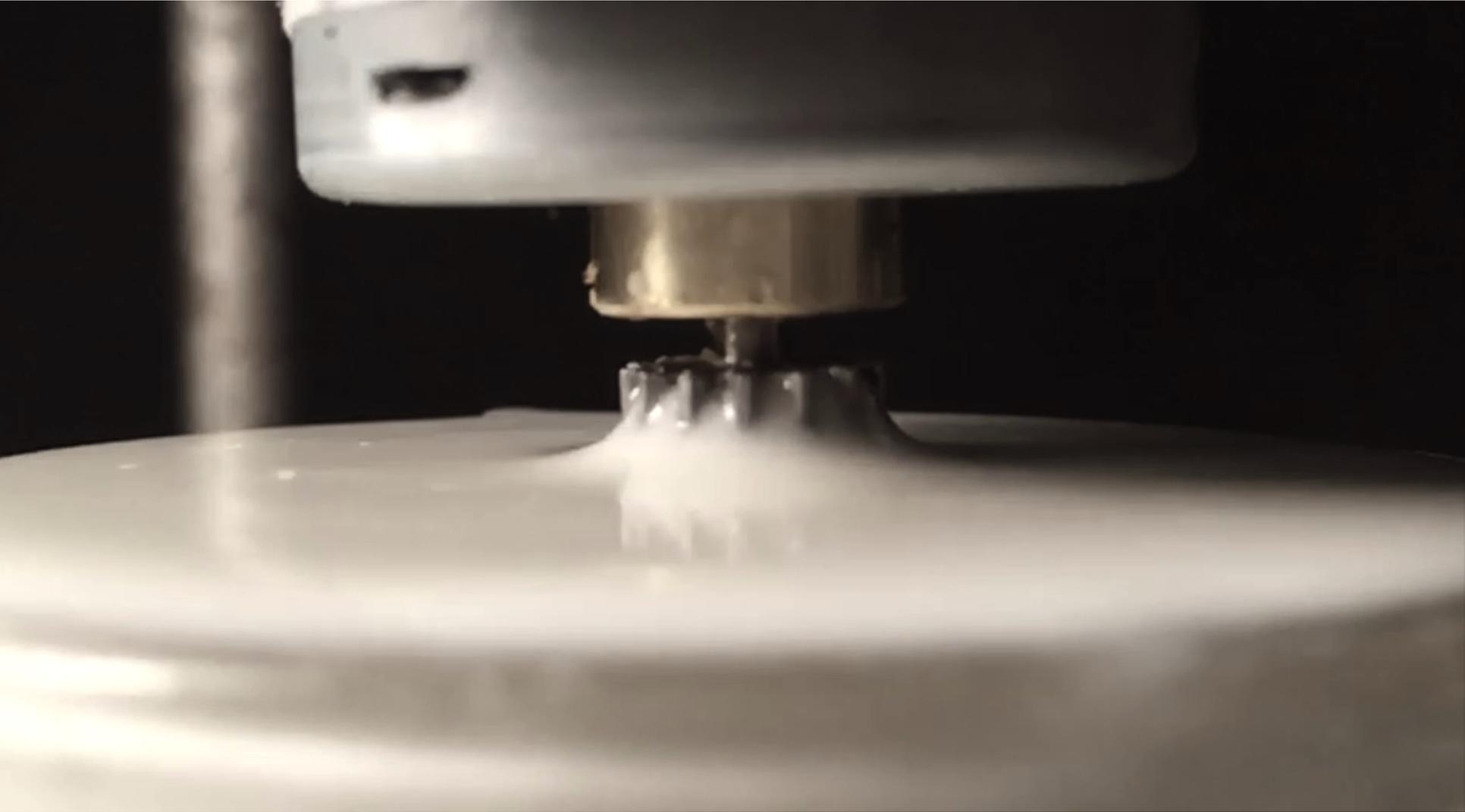
Flow Protocol Engineering: OSP

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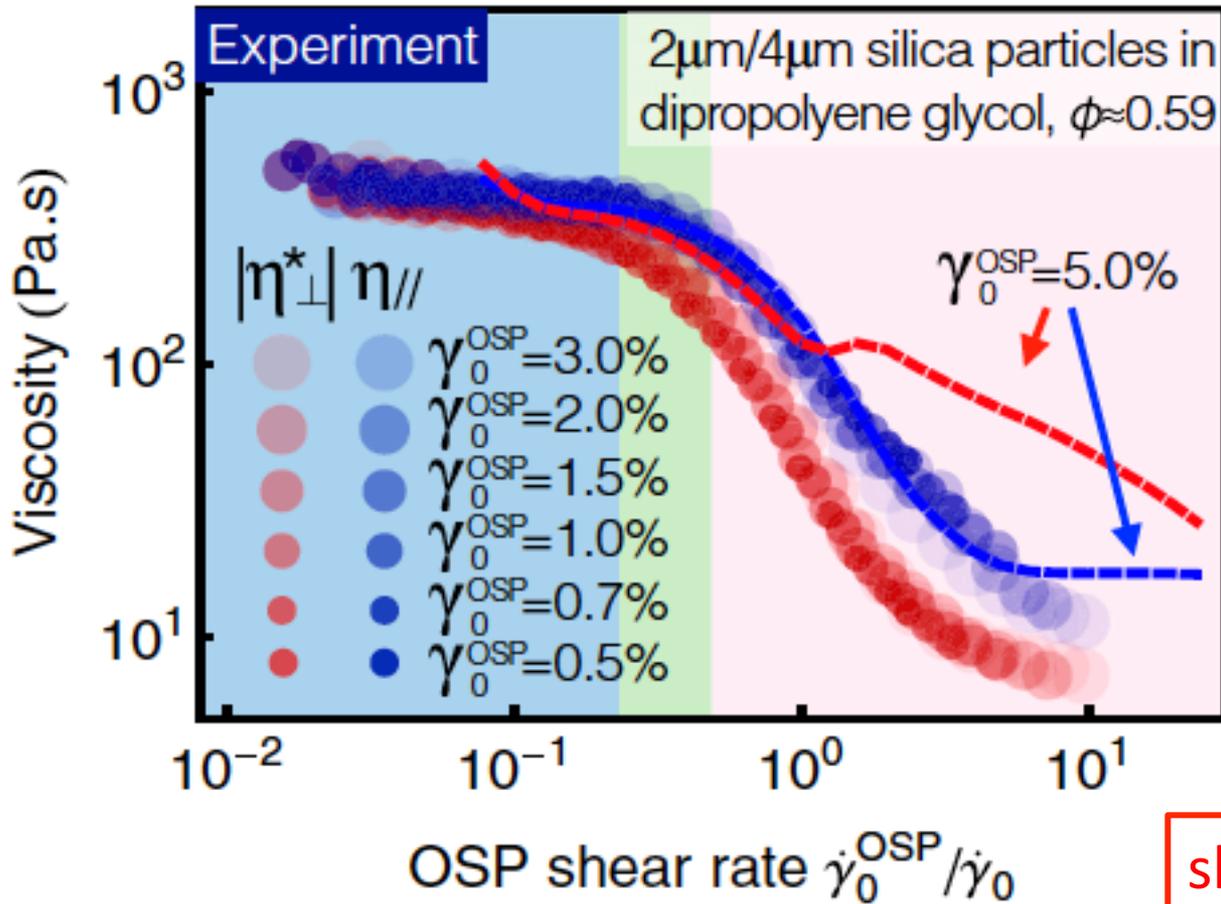
Flow Protocol Engineering: OSP

OSP amplitude:
$A = \gamma_0^{OSP}$

shear thickening material

N. Lin et al, PNAS 113, 10774 (2016)

Flow Protocol Engineering: OSP

OSP amplitude:
$A = \gamma_0^{OSP}$

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Viscosity Reduction of Frictional Suspensions

quasi-Newtonian material

R. Mari, C. Ness and MEC, Sci Advances 2018

Viscosity Reduction of Frictional Suspensions

R. Mari, C. Ness and MEC, Sci Advances 2018

Viscosity Reduction of Frictional Suspensions

R. Mari, C. Ness and MEC, Sci Advances 2018
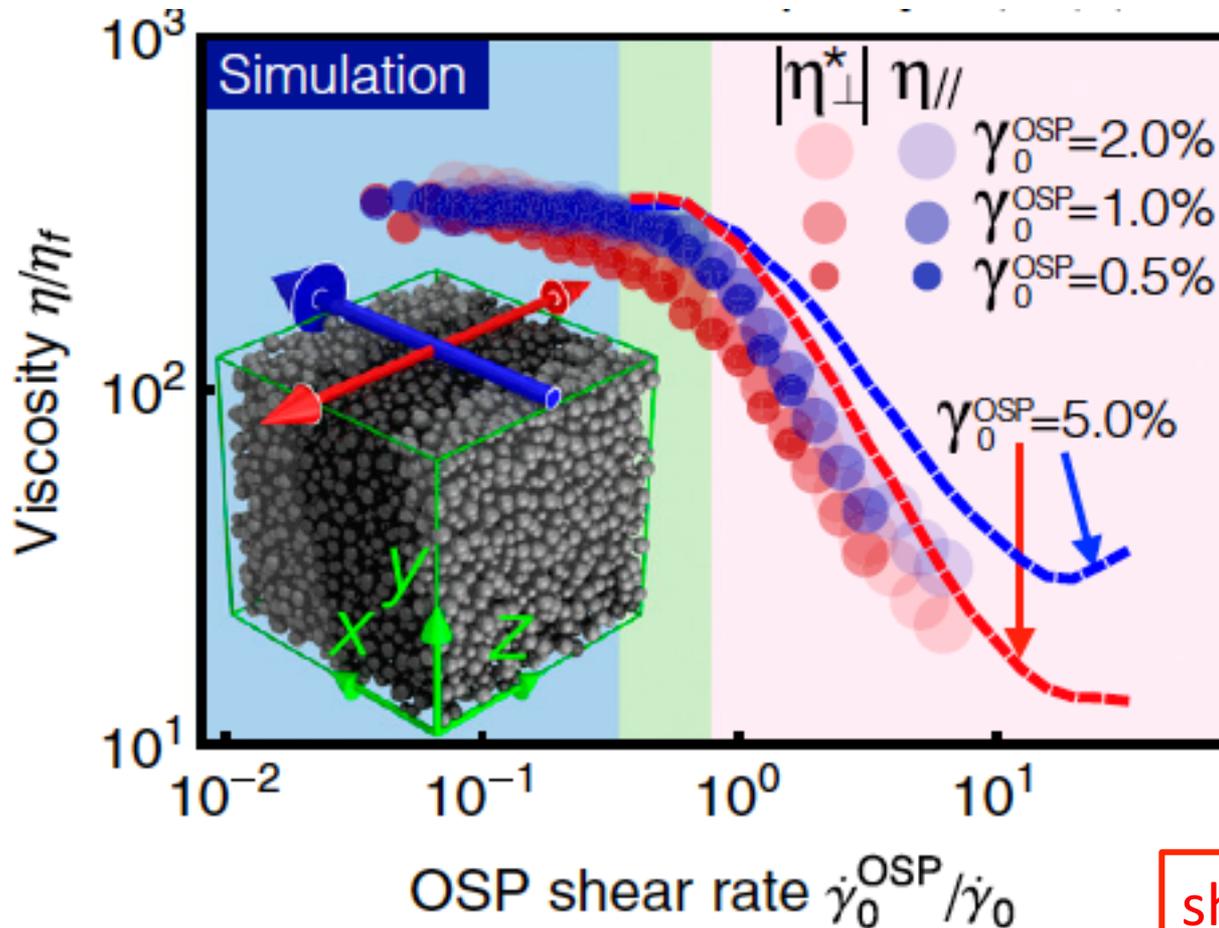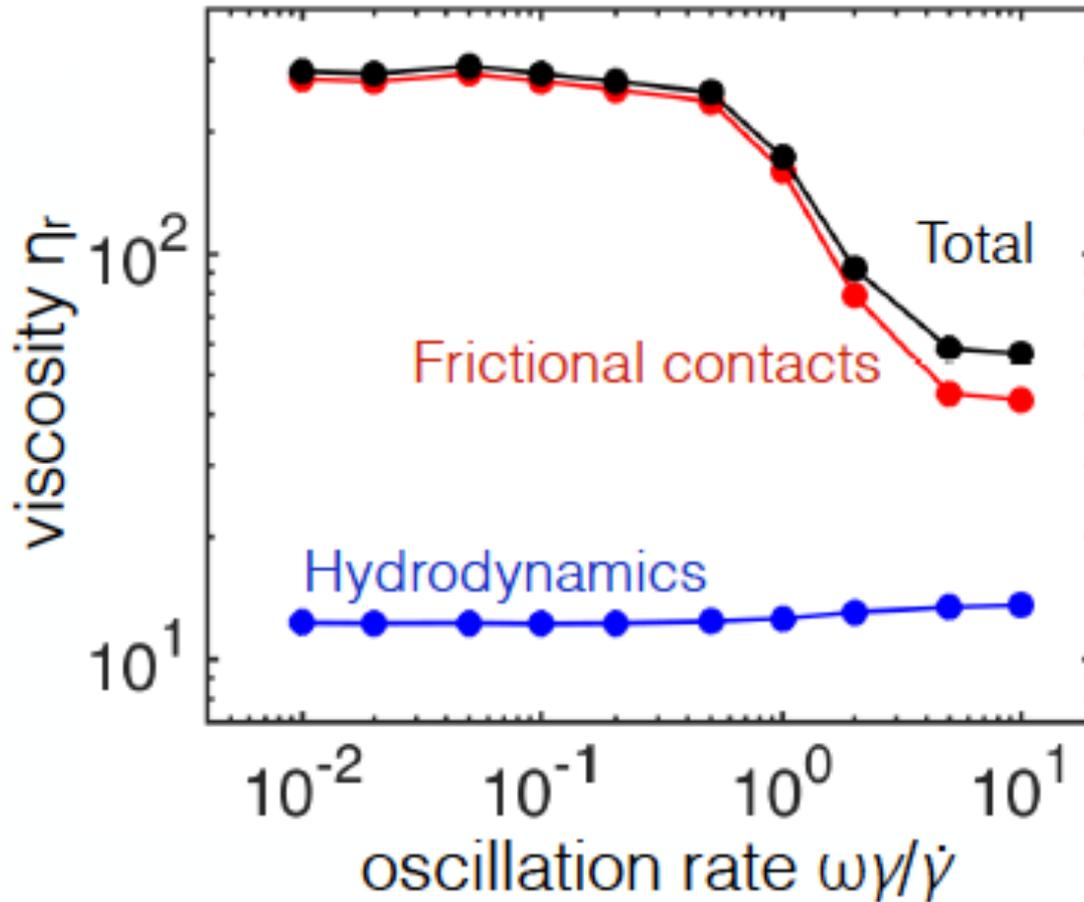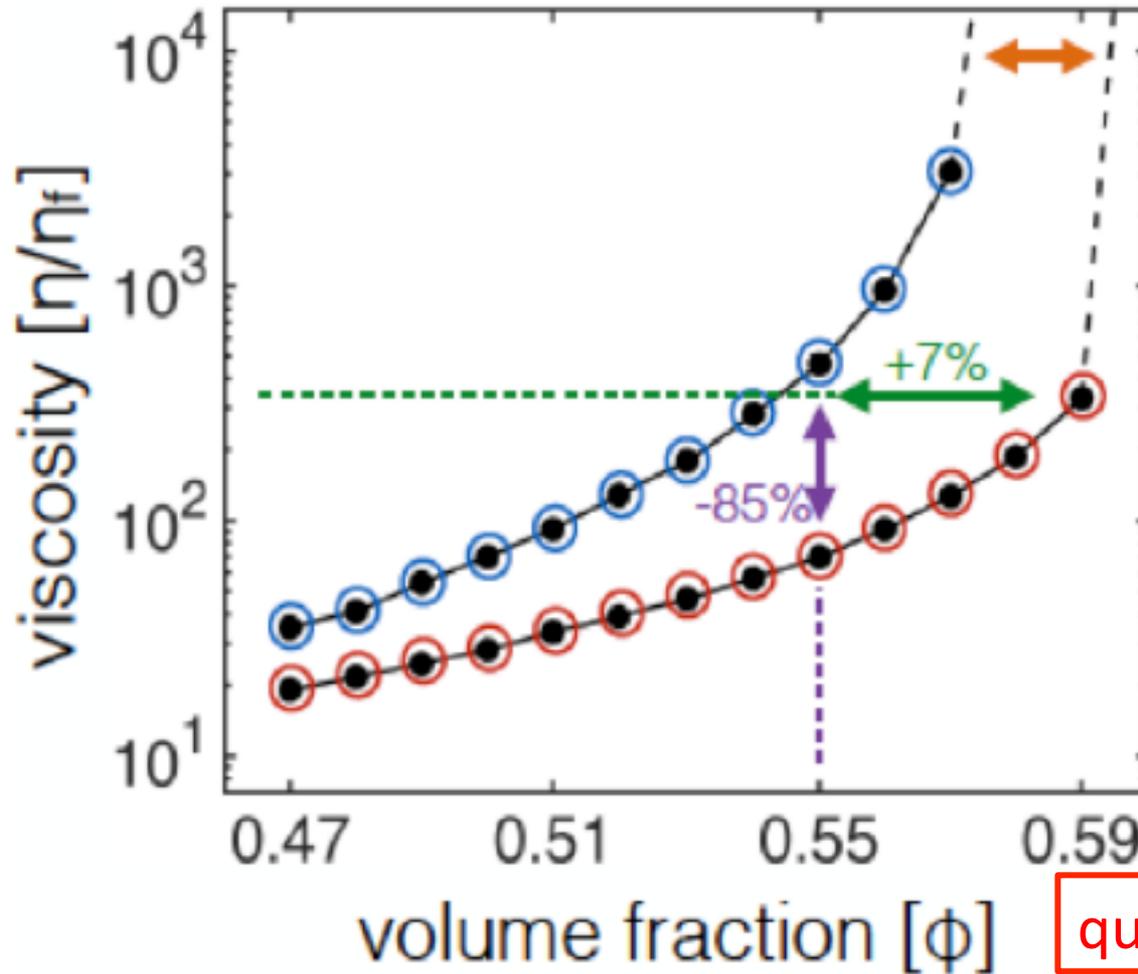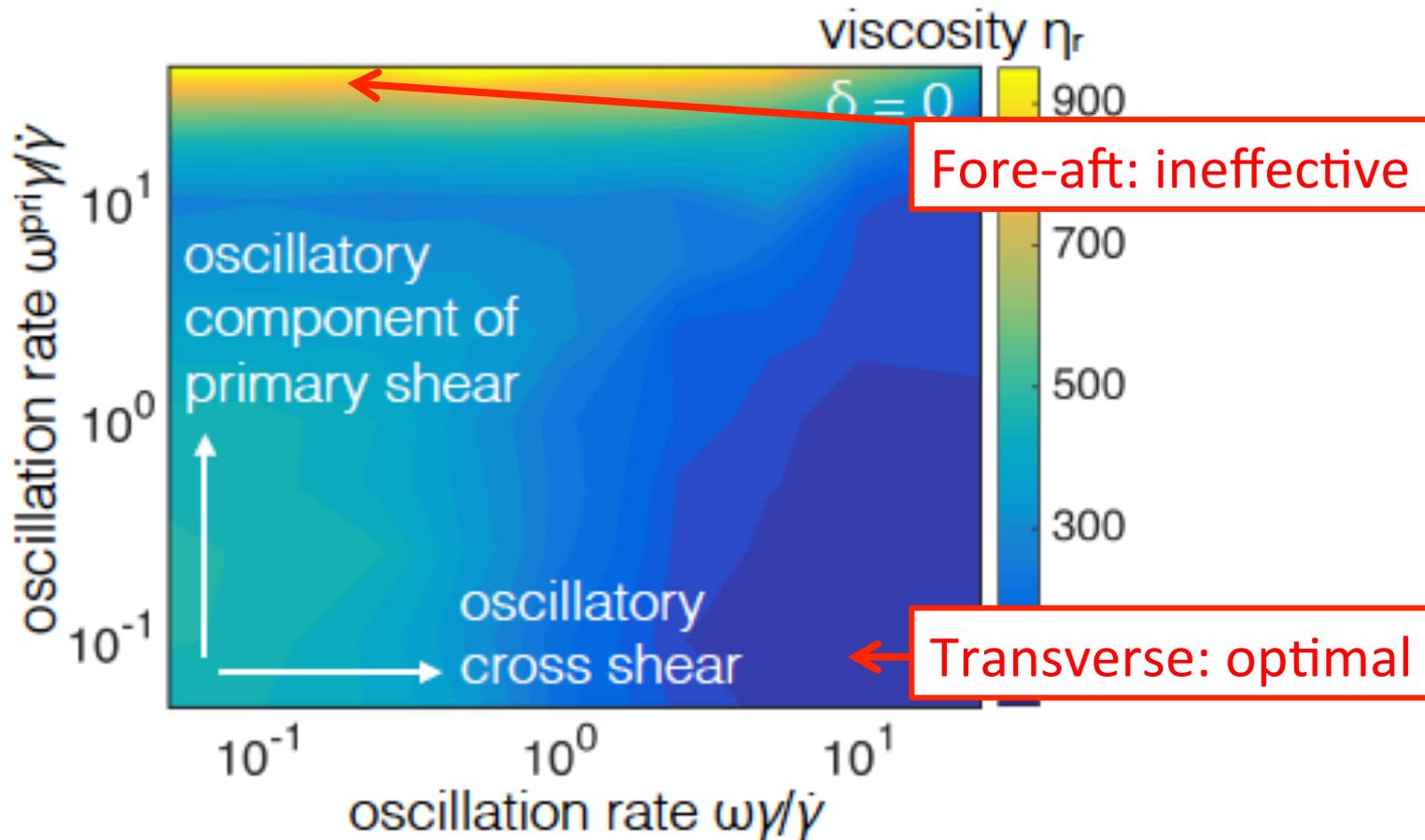
Optimize Dissipation at Fixed Mean Flow Rate

Pause forward flow to unjam with OSP:
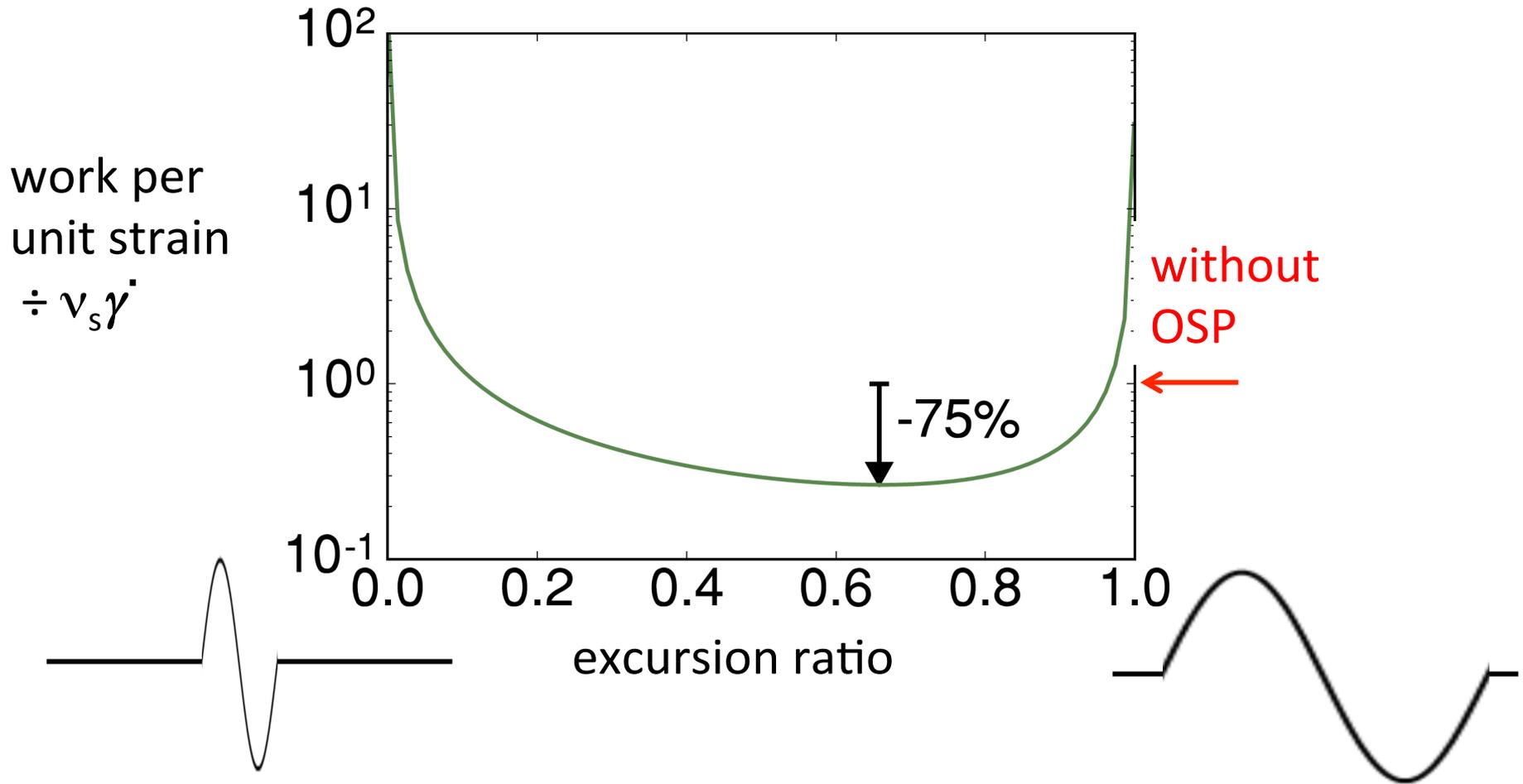
work per
unit strain
$\div \, \nu_s \dot{\gamma}$

without
OSP

-75%

excursion ratio

R. Mari, C. Ness and MEC, Sci Advances 2018

Constitutive Modelling: The Flow Reversal Challenge

So far:

       theory of steady-state flow curves only

       via graphical math ± microscopic models for $f(\sigma)$

Constitutive models:

       stress tensor as functional of flow history

       polymeric systems: successes since 1980s
       (Doi/Edwards, Larson, Marucci, McLeish, Likhtman....)

       very dense suspensions: mechanistic insights
       (Hinch, Brady, Wagner, Morris, Denn...)

       but nothing workable as constitutive model!

Constitutive Modelling: The Flow Reversal Challenge

So far:

      theory of steady-state flow curves only
      via graphical math ± microscopic models for f(σ)

Constitutiv

      str

> The challenge is already severe for quasi-Newtonian materials

      polymeric systems: successes since 1980s
      (Doi/Edwards, Larson, Marucci, McLeish, Likhtman....)

      very dense suspensions: mechanistic insights
      (Hinch, Brady, Wagner, Morris, Denn...)

      but nothing workable as constitutive model!

Constitutive Modelling

Hoped for form: $\quad$ **Q** = <**pp**> - **I**/3, **p** ≈ contact

$$\Sigma = \Sigma(Q, K)$$

stress = function of current structure and strain rate

Q = coarse-grained 'fabric': 2nd rank tensor

$$\dot{Q} = \dot{Q}(Q, K)$$

Q dynamics is <u>approximately</u> closed

compare polymers:
UCM, J-S, Rolie-Poly etc (**Q** = conformation)

Constitutive Modelling

Hoped for form:

$$\Sigma = \Sigma(\mathbf{Q}, \mathbf{K})$$ singular on reversal

stress = function of current structure and strain rate

$\mathbf{Q}$ = coarse-grained 'fabric': 2nd rank tensor

$$\dot{\mathbf{Q}} = \dot{\mathbf{Q}}(\mathbf{Q}, \mathbf{K})$$ smooth evolution

$\mathbf{Q}$ dynamics is <u>approximately</u> closed

compare polymers:
UCM, J-S, Rolie-Poly etc (Q = conformation)

Constitutive Modelling

Frame indifference (Hand 1962):

$$\frac{\mathrm{d}\boldsymbol{Q}}{\mathrm{d}t} = \boldsymbol{WQ} - \boldsymbol{QW} + \alpha_0\boldsymbol{I} + \alpha_1\boldsymbol{Q} + \alpha_2\boldsymbol{E} + \alpha_3\boldsymbol{Q}^2 + \alpha_4\boldsymbol{E}^2 + \alpha_5\left(\boldsymbol{EQ} + \boldsymbol{QE}\right)$$
$$+ \alpha_6\left(\boldsymbol{EQ}^2 + \boldsymbol{Q}^2\boldsymbol{E}\right) + \alpha_7\left(\boldsymbol{E}^2\boldsymbol{Q} + \boldsymbol{QE}^2\right) + \alpha_8\left(\boldsymbol{E}^2\boldsymbol{Q}^2 + \boldsymbol{Q}^2\boldsymbol{E}^2\right),$$

with $\alpha_{1\text{-}8}$ analytic functions of 8 scalar invariants of $(\boldsymbol{Q},\boldsymbol{E})$
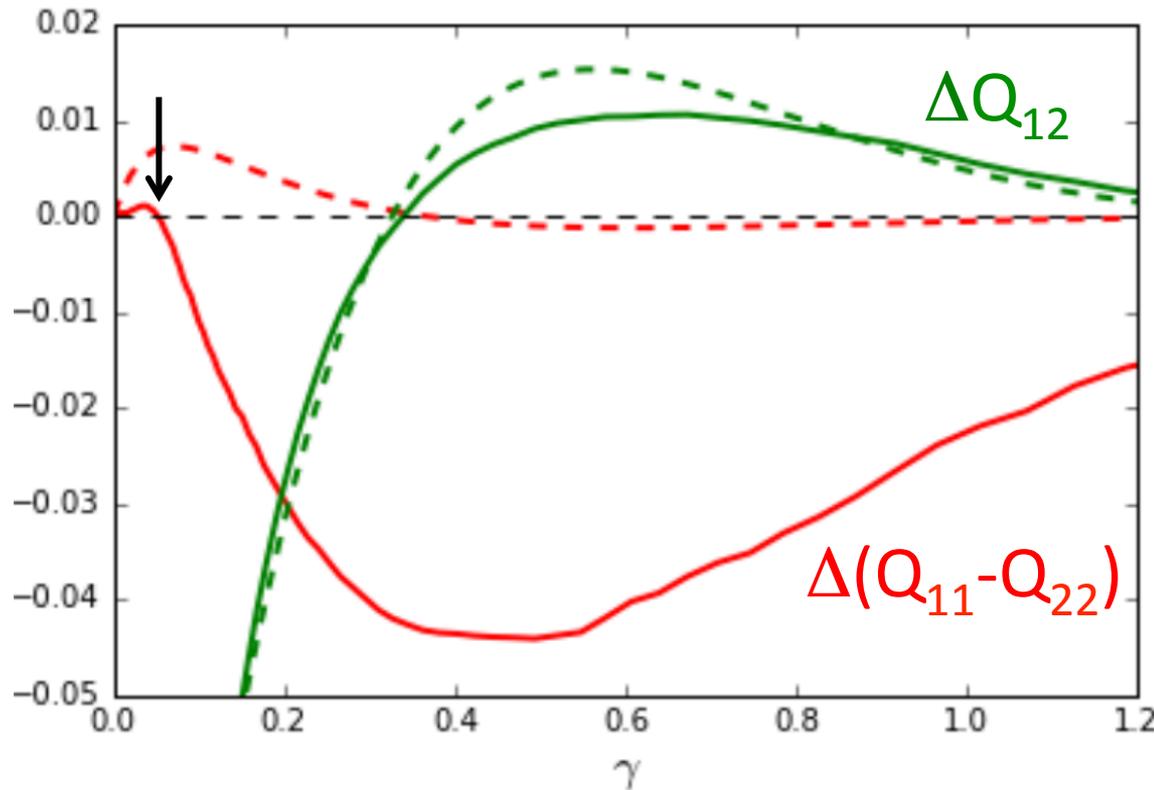$2\boldsymbol{W} = \boldsymbol{K}\text{-}\boldsymbol{K}^\mathsf{T}$, $2\boldsymbol{E} = \boldsymbol{K}\text{+}\boldsymbol{K}^\mathsf{T}$

Confront with particle-based simulations:

- **microscopic** information on contact forces

- **macroscopic** information on $\boldsymbol{Q}$, Σ

- more stringent test than current experiments

Constitutive Modelling

Linear models ruled out by reversal data:

ΔQ_{12} must change sign before $\Delta(Q_{11}-Q_{22})$

$\Delta Q := Q(\gamma) - Q_{steady}$

ΔQ_{12}

$\Delta(Q_{11}-Q_{22})$

solid: data

dashed: fit

R Chacko, R Mari, S Fielding and MEC, JFM 2018

Constitutive Modelling

Linear models ruled out by reversal data

Quadratic models OK in 3D but poor in 2D

The real physics in reversal is **not second rank**

$\gamma = 0.2$ post-reversal: contact statistics P(**p**)

$4\pi P(\mathbf{p}) = 1 + 15\mathbf{Q:pp}/2$

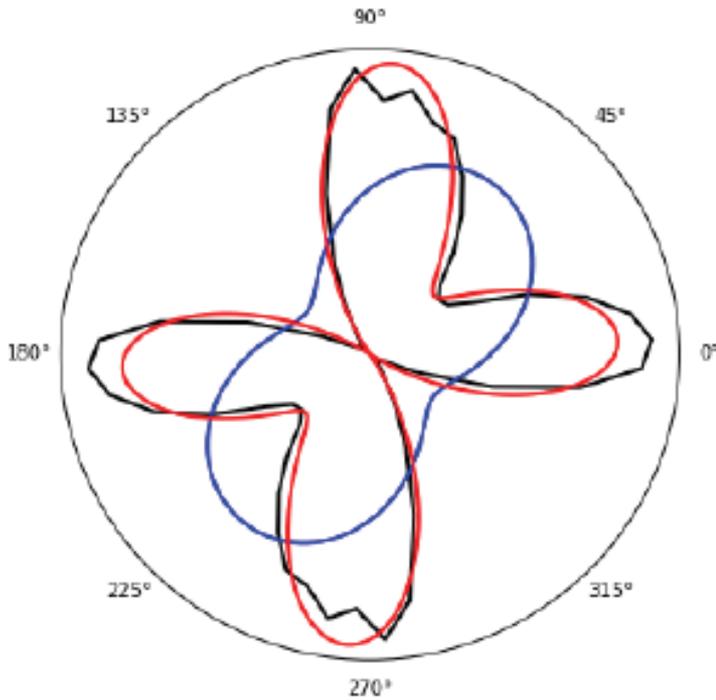$4\pi P(\mathbf{p}) = 1 + 15\mathbf{Q:pp}/2 + 315\mathbf{C::pppp}/8$

R Chacko, R Mari, S Fielding and MEC, JFM 2018

Constitutive Modelling

Linear models ruled out by reversal data

Quadratic models OK in 3D but poor in 2D

The real physics in reversal is **not second rank**

$$\Sigma = \Sigma(\mathbf{Q}, \mathbf{K})$$ singular on reversal

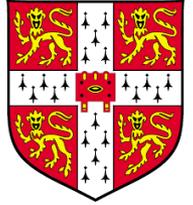$$\dot{\mathbf{Q}} = \dot{\mathbf{Q}}(\mathbf{Q}, \mathbf{C}, \mathbf{K})$$ smooth

$$\dot{\mathbf{C}} = \dot{\mathbf{C}}(\mathbf{Q}, \mathbf{C}, \mathbf{K})$$ smooth

Possibly – but still many parameters…

open question; once answered…
return to shear-thickening!

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