Hydrodynamics, phase behaviour and rheology of active suspensions

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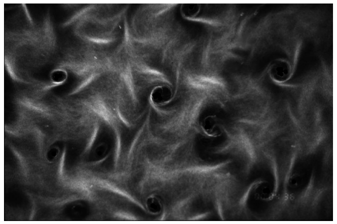
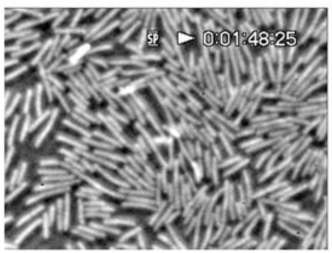
Active matter: examples

Nedelec et al.



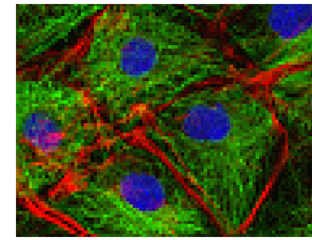
Berg et al.



Narayan et al.

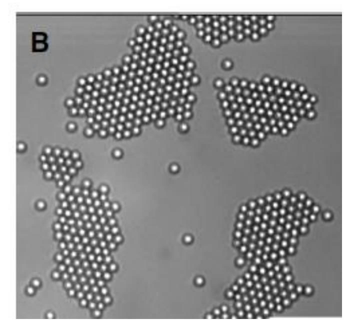
- Cytoskeleton and its extracts
- Biological tissues
- Suspensions of bacteria, protozoa
- Shoals of fish, flocks of birds
- Self-propelled synthetic colloids
- Vibrated granular monolayers

ww.bscb.org



http://angel.elte.hu

Palacci et al.



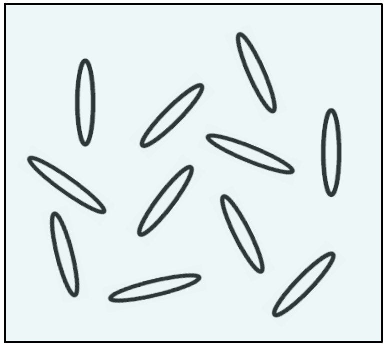
Emergent phenomena

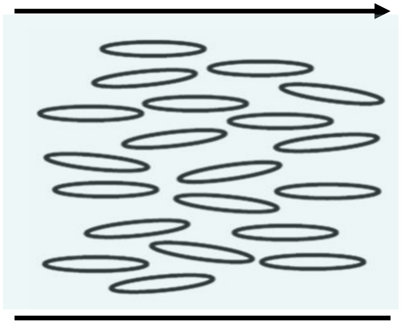
- Spontaneous flows without external driving
- Chaotic/turbulent internal flows at zero Reynolds number
- Non-equilibrium ordering transitions
- Swarming
- Giant number fluctuations
- Activity-induced phase separation

Toner, Tu, Ramaswamy Ann. Phys. (2005); Kruse et al. Phys. Rep. (2007)
Ramaswamy Ann. Rev. Cond. Matt. (2010); Marchetti et al. Rev. Mod. Phys. (2013)

Active matter as a complex fluid

Complex fluid: internal mesoscopic substructures



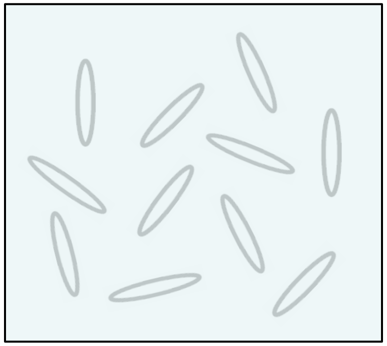


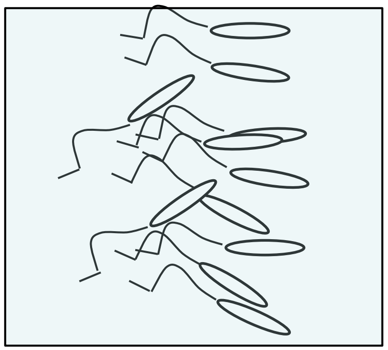
slow relaxation
processes

easily driven
out of equilibrium

Active matter as a complex fluid

Active complex fluid: self propelled substructures



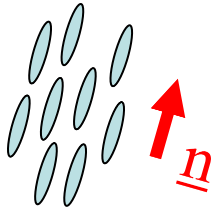


slow relaxation processes

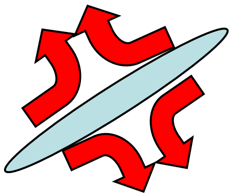
out of equilibrium “from within”

Contractile versus extensile

passive

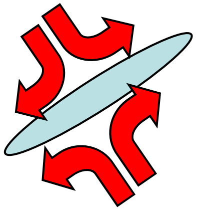


active contractile



microtubules/motors

active extensile



bacterial suspensions

Activity induces dipolar flow

Part I: Hydrodynamics, coherent structures and rheology

- Experiments
- Continuum model
- 0D active rheology: homogeneous shear flow
- 1D active rheology: shear banding
- 2D active dynamics: roll-like and chaotic flow states
- 2D active rheology
- Summary and outlook

Part II: Hydrodynamics and phase separation (or otherwise)

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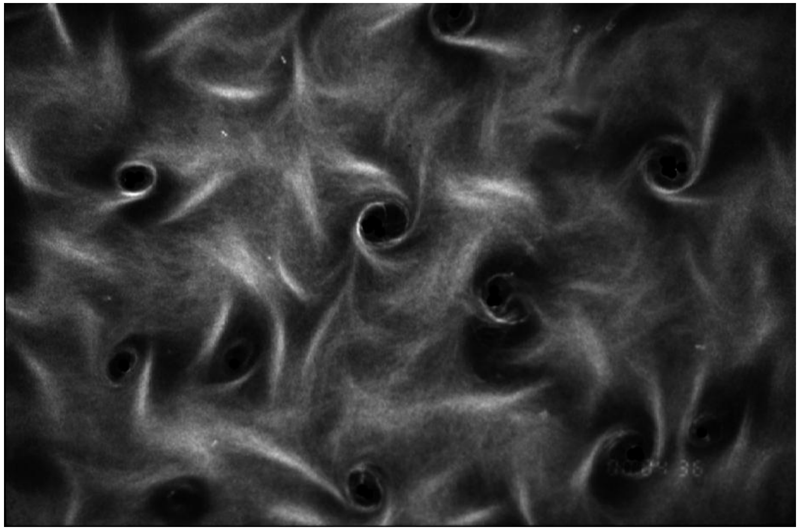
Experimental phenomenology

active contractile

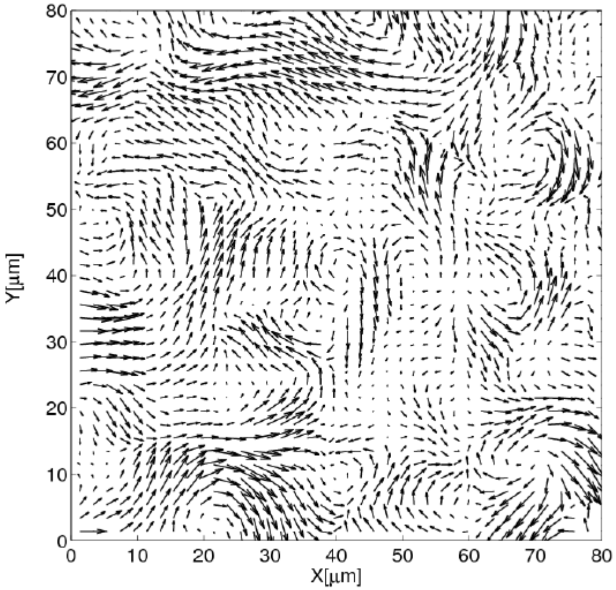


Spontaneously rotating vortices

in microtubules/motors

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

active extensile



“Bacterial turbulence”

in B subtilis suspensions

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

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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

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

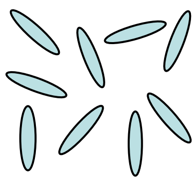
Molecular field

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

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

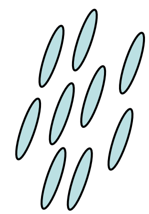
[Hatwalne et al. PRL 04; Liverpool et al. EPL 05; Kruse et al. PRL 04; Voituirez et al., EPL 05]

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

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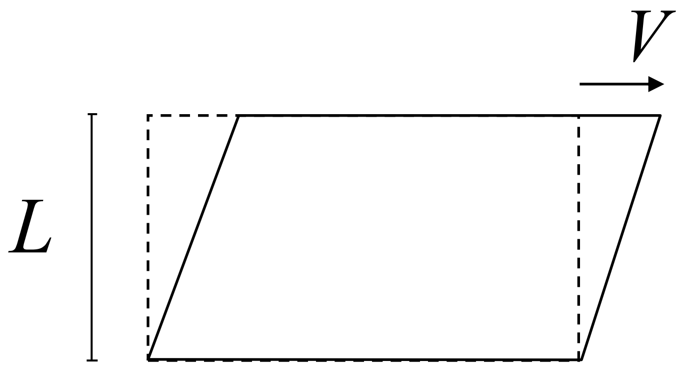
Rheology primer: Shear rheology



apply shear flow of rate

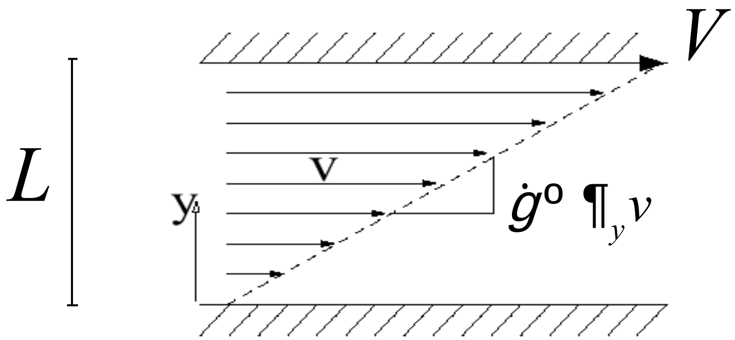
$$\dot{\gamma} \equiv V / L$$

for all times $t > 0$

Measure shear stress response $\Sigma(\dot{\gamma}, t)$

Plot “flow curve” $\Sigma(\dot{\gamma})$ in steady state $t \to \infty$

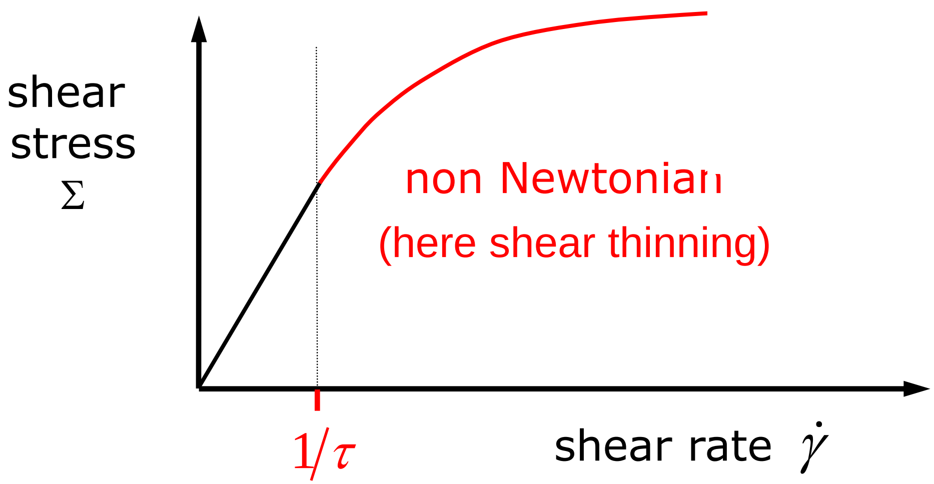
Rheology primer: steady state shear flow



$$\dot{\gamma} = \partial_y v = V / L$$

everywhere across cell

(assumed homogeneous)

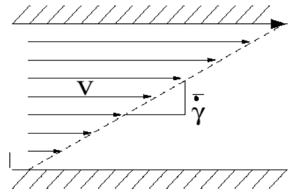


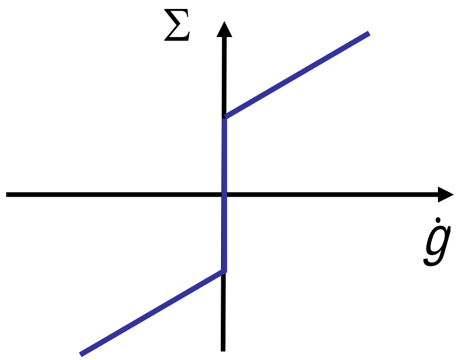
flow curve

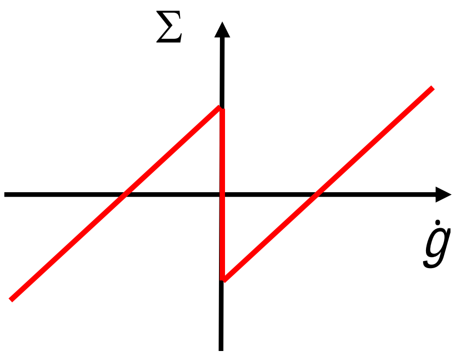
viscosity $\eta_{\mathrm{app}} = \Sigma / \dot{\gamma}$

decreases with increasing $\dot{\gamma}$

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







active contractile

active extensile

conventional yield stress

negative yield stress?!

[Cates, Fielding, Marenduzzo, Orlandini, Yeomans, PRL (08)]

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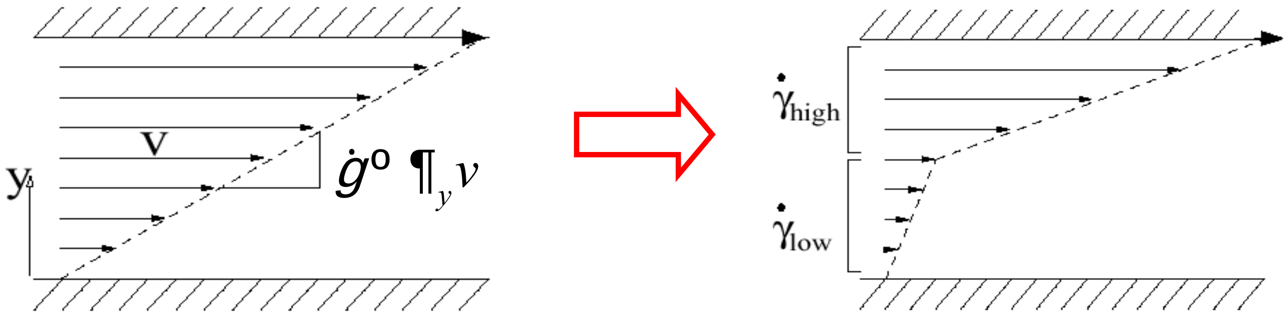
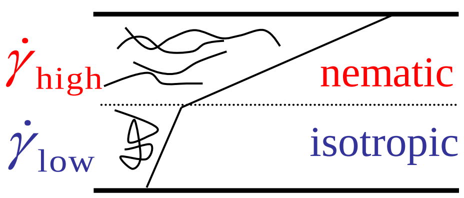
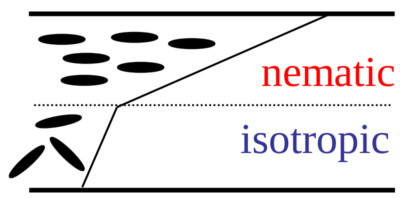
Rheology primer: shear banding - widespread in complex fluids



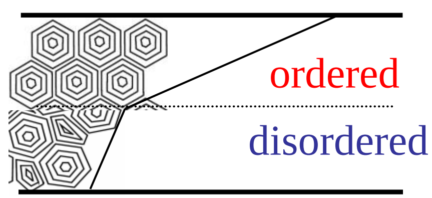
Wormlike surfactants



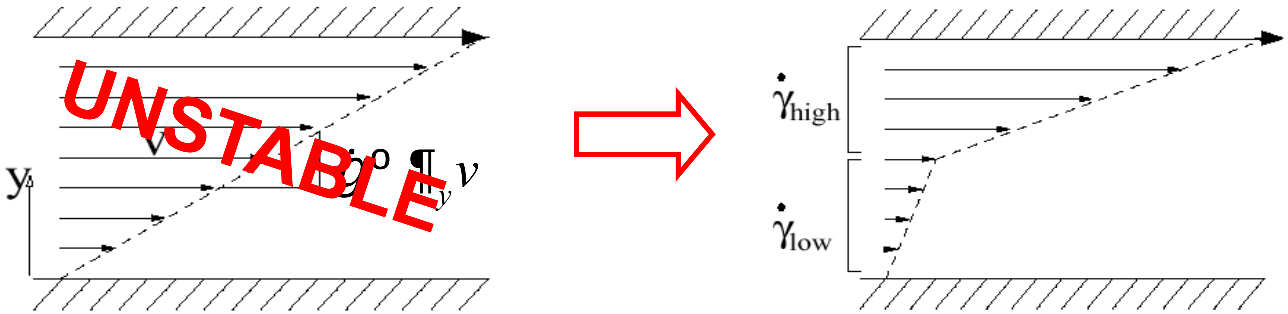
Liquid crystals

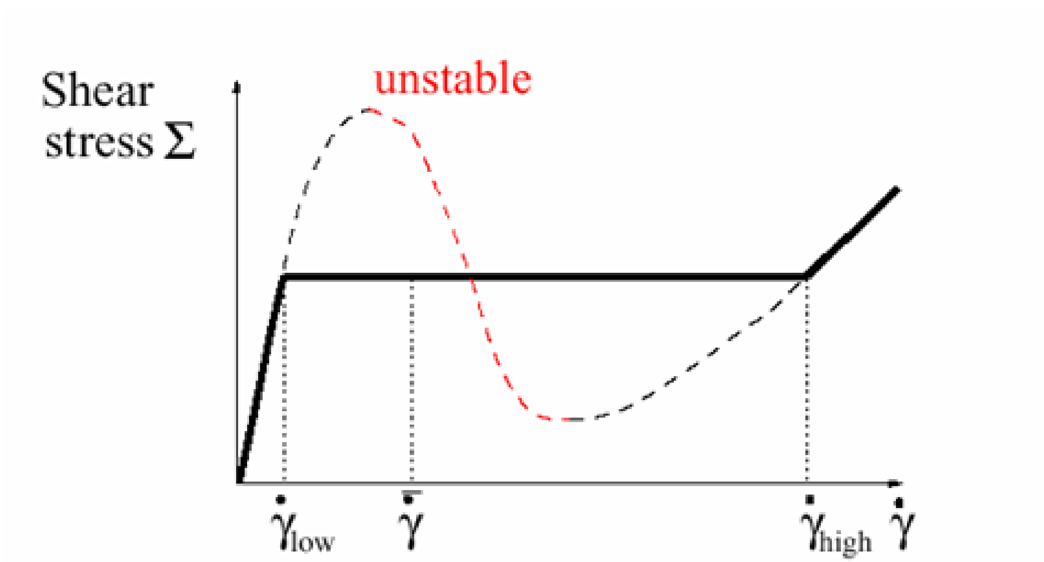


Onion surfactants



Cause: non–monotonic underlying "constitutive curve" $S(\dot{g})$





flow curve $S(\bar{\dot{g}})$

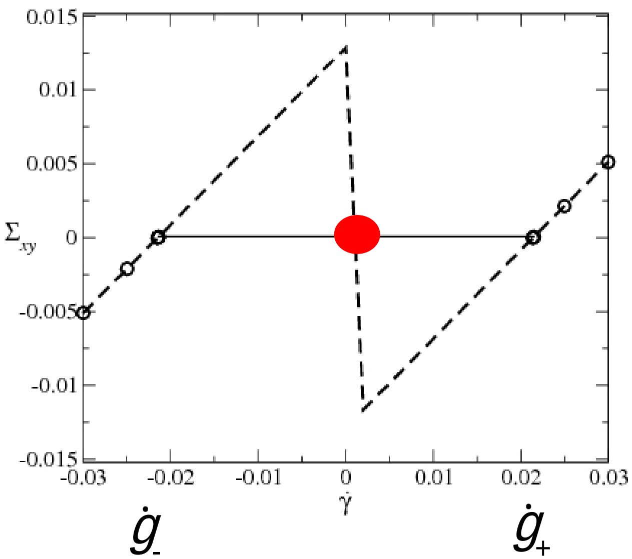
shows plateau in

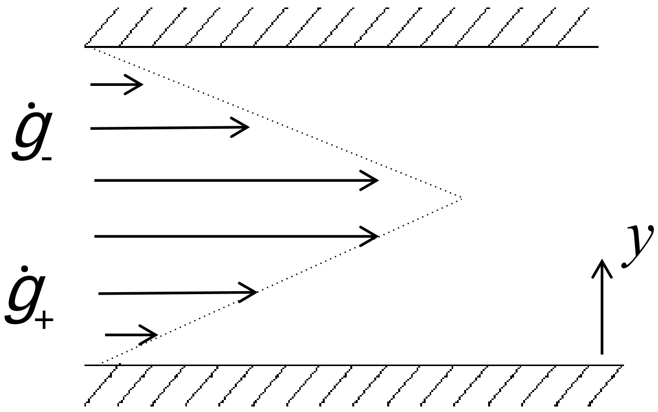
banded steady state

[Spenley, Cates, McLeish PRL 93]

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

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



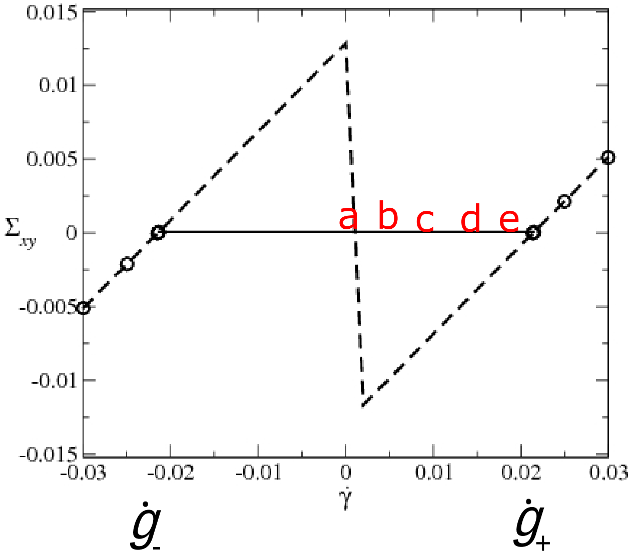


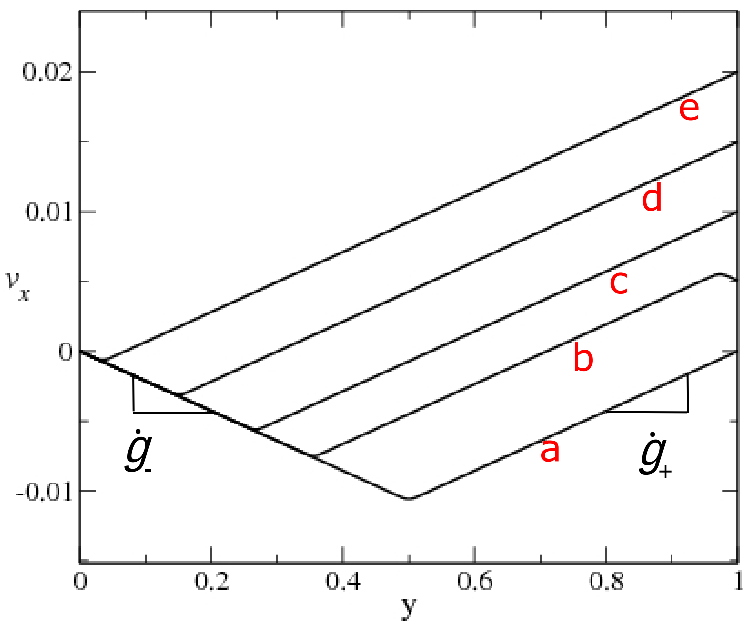
Bands of equal, opposite shear rates even in globally unsheared system!

[Cates, Fielding, Marenduzzo, Orlandini, Yeomans, PRL (08)]

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

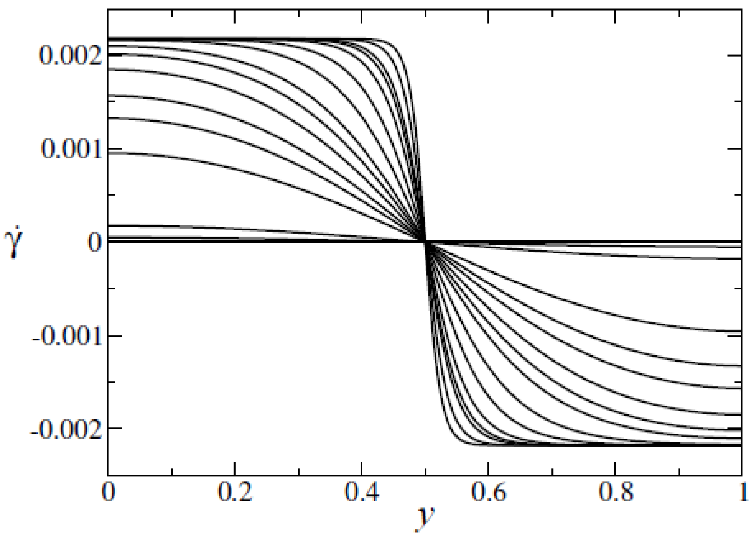
Negative yield stress in 0D → coexisting shear bands in 1D

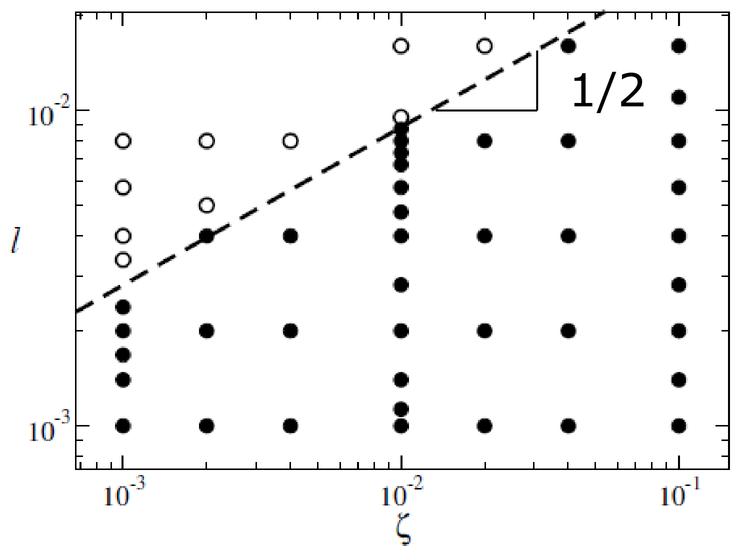




[Cates, Fielding, Marenduzzo, Orlandini, Yeomans, PRL (08)]

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*

o No flow

● Spontaneous flow

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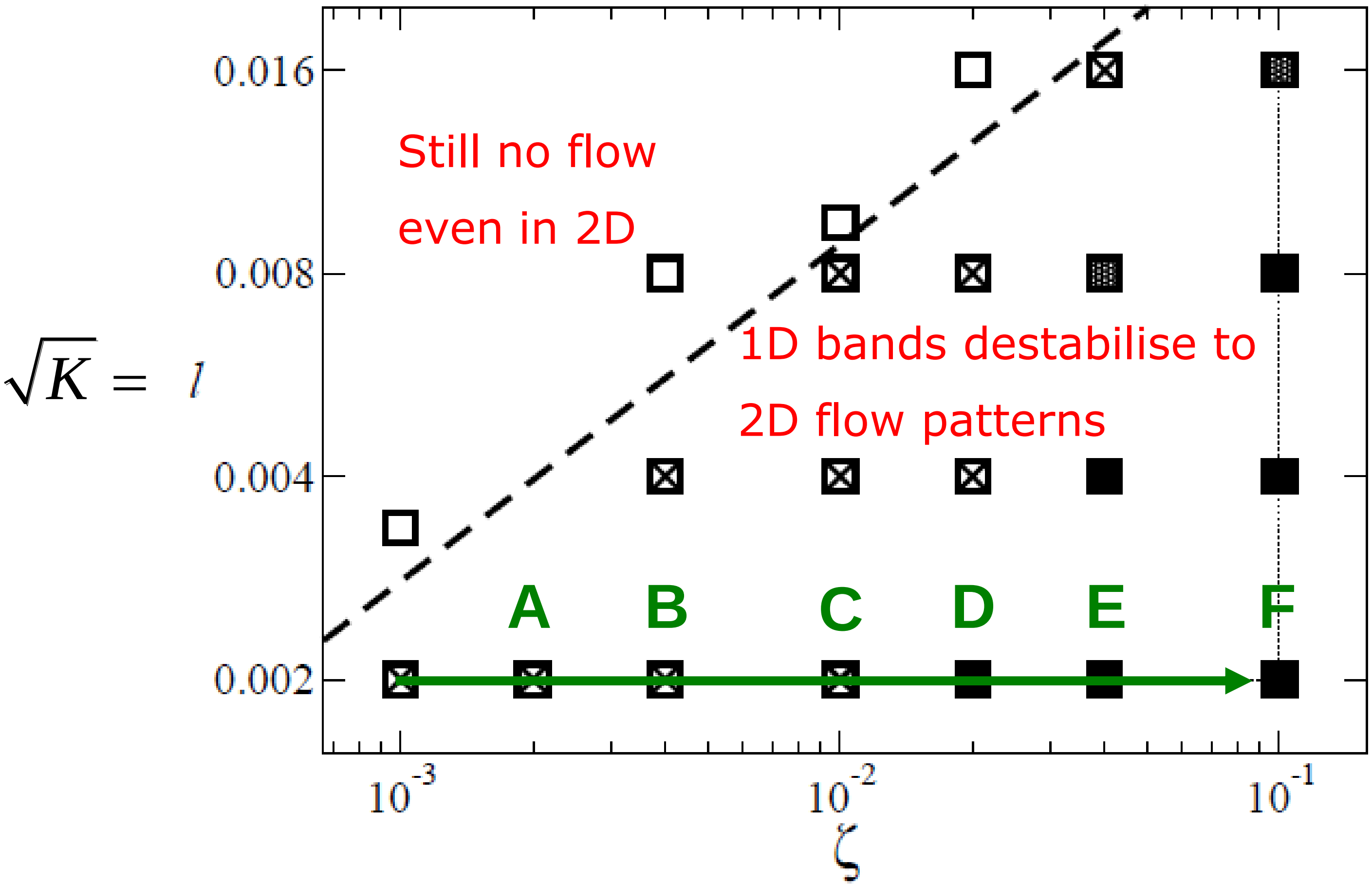
Part II: Hydrodynamics and phase separation (or otherwise)

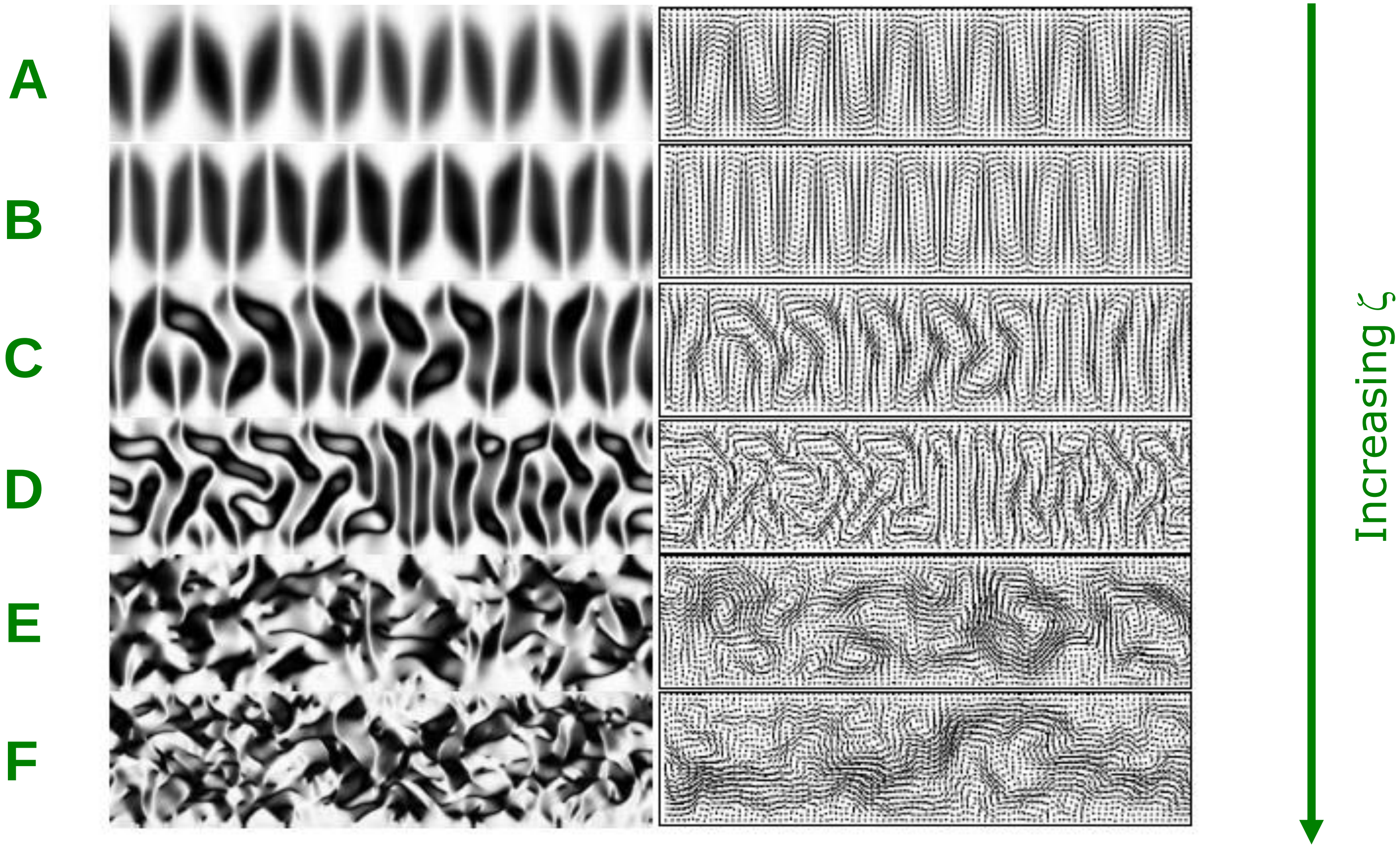
2D systems: "phase diagram" for extensile at zero global shear



[SMF et al. PRE 2011]

[SMF et al. PRE 2011]

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]

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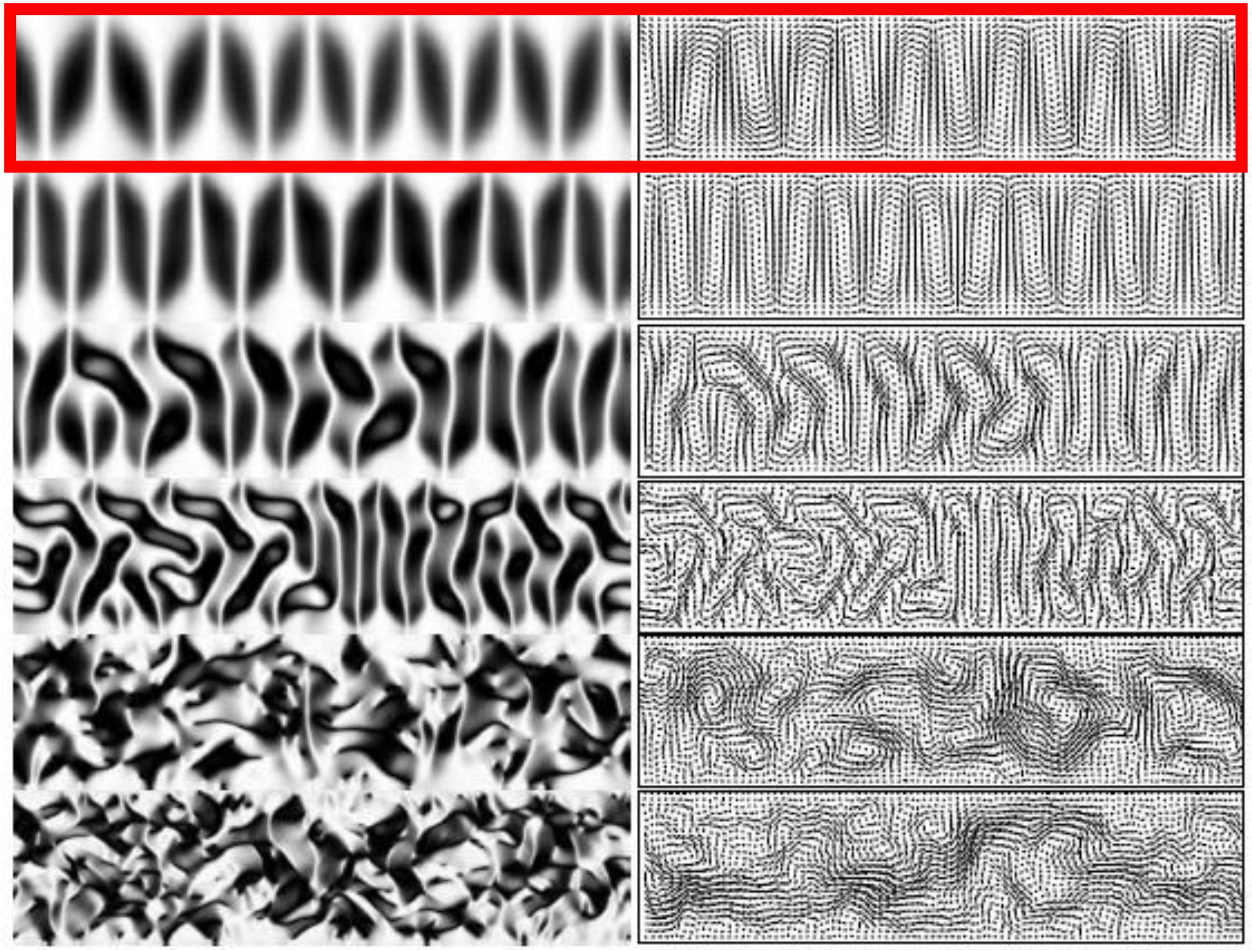
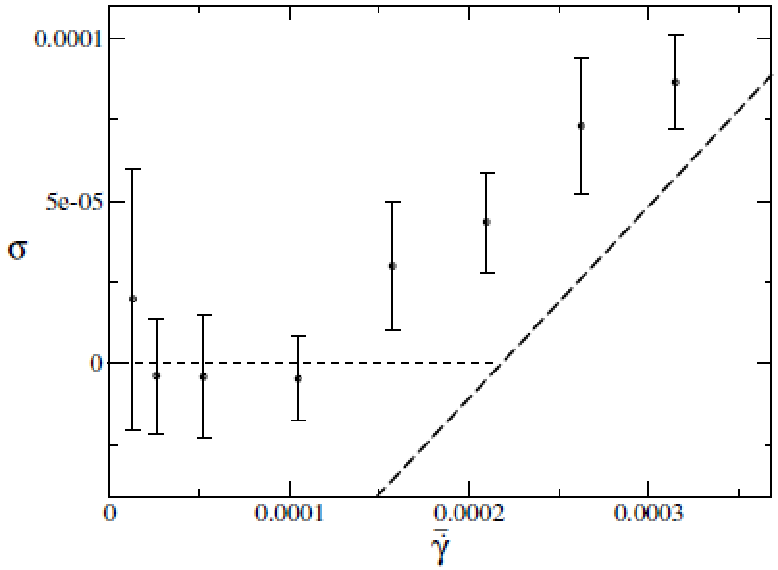
Shear roll-like state (next slide)

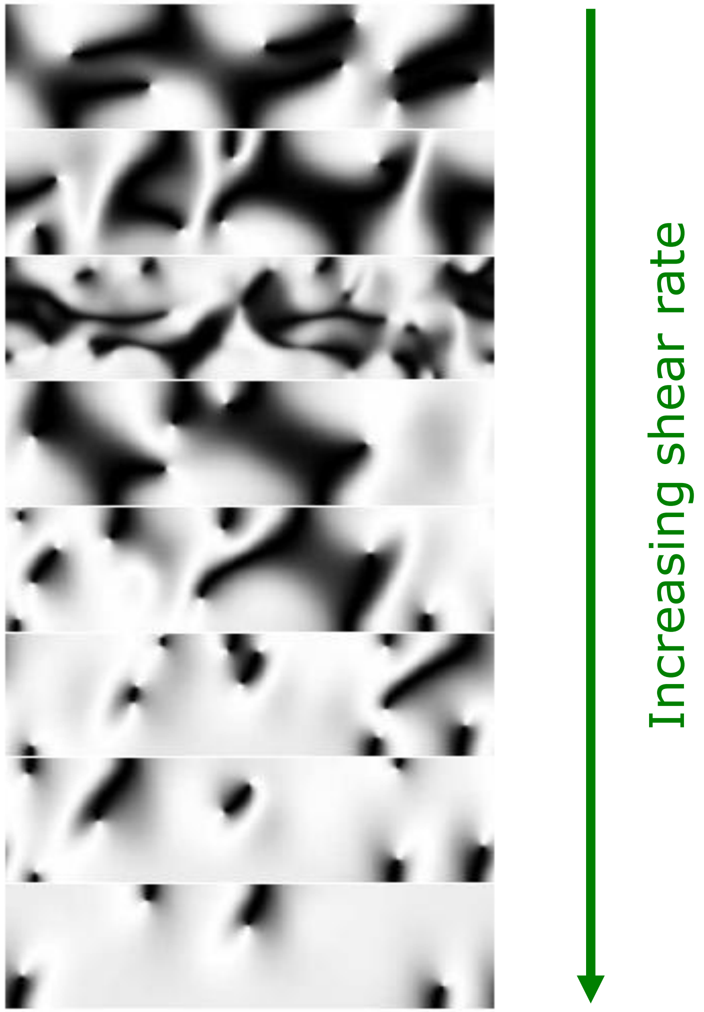


[SMF et al. PRE 2011]

Shearing roll-like state

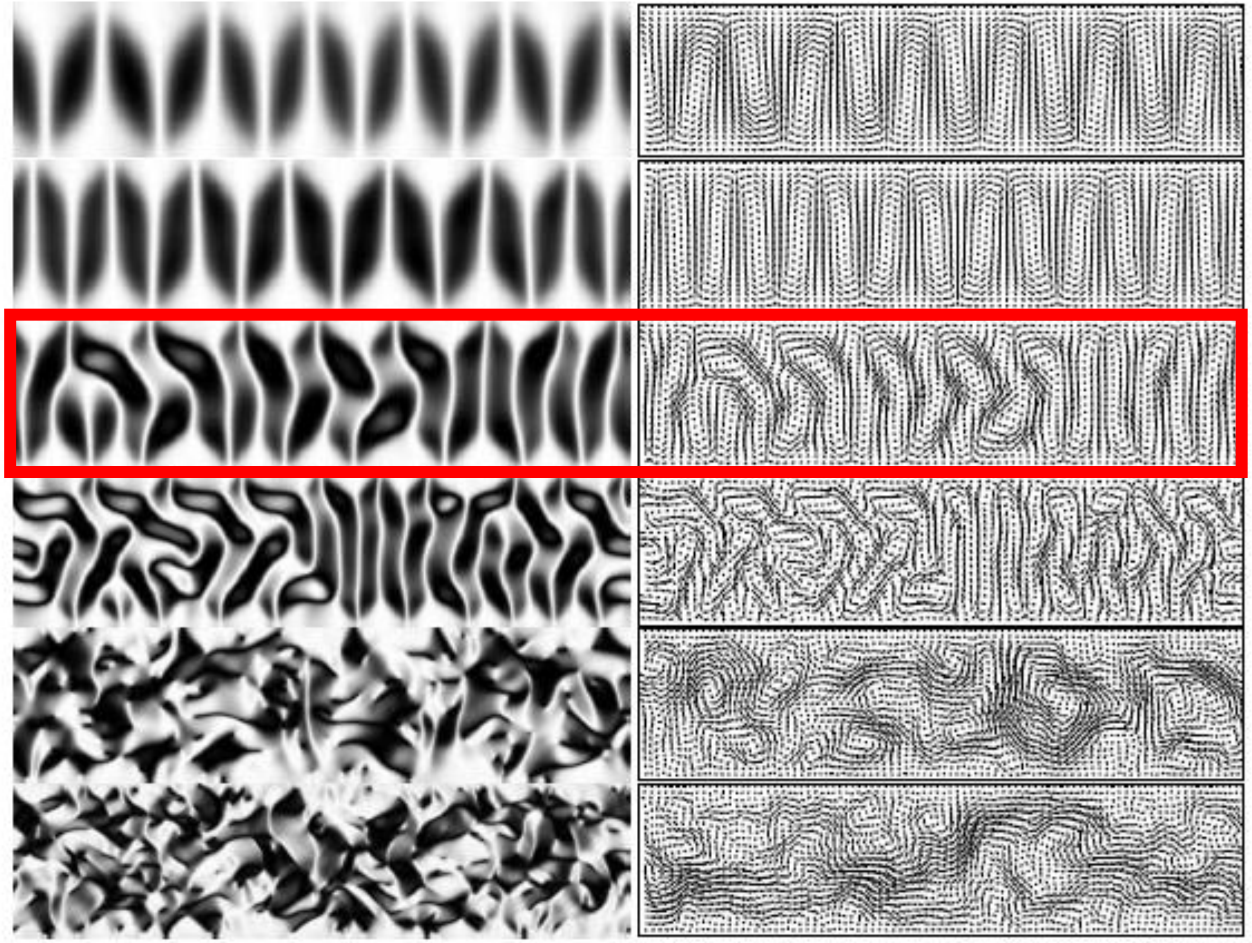
Flow curve





[SMF et al. PRE 2011]

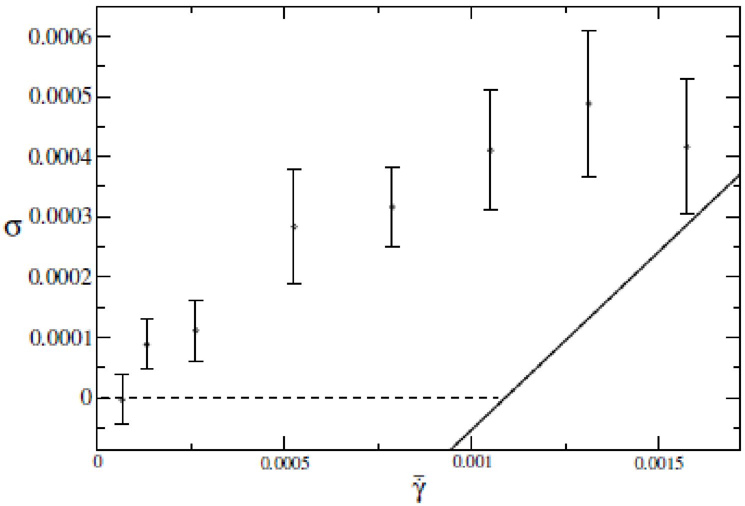
Shear wavy rolls (next slide)

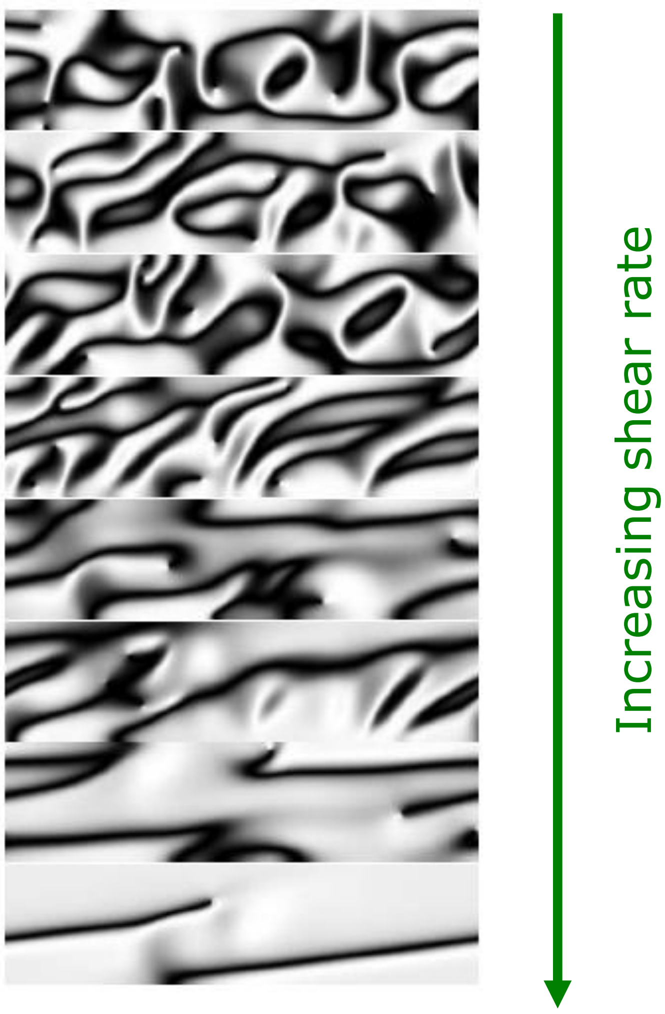


[SMF et al. PRE 2011]

Shearing wavy rolls

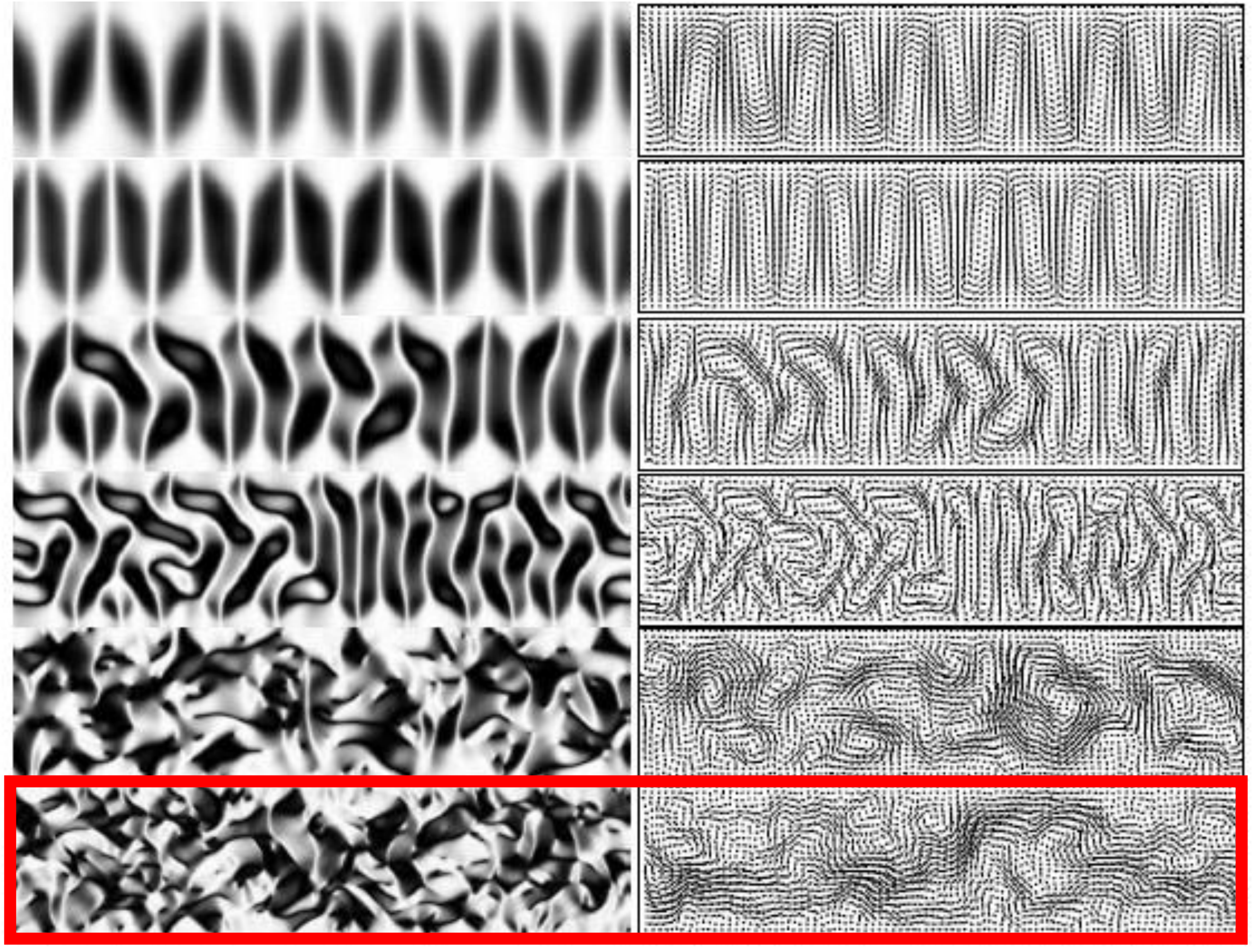
Flow curve





[SMF et al. PRE 2011]

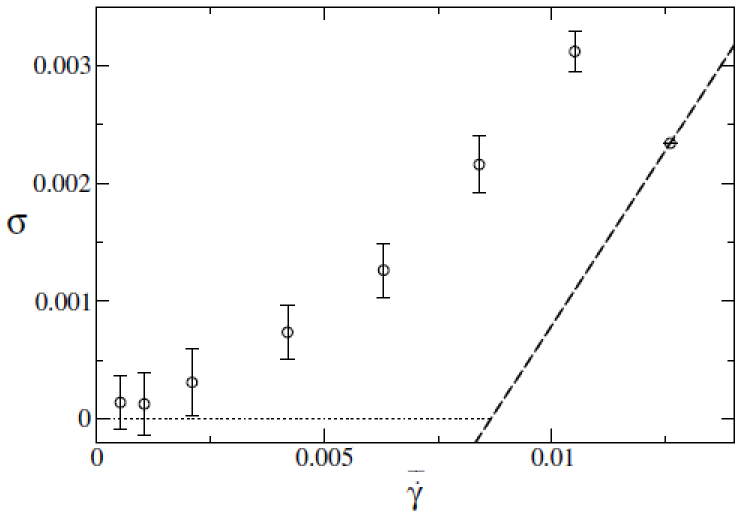
Shear “turbulent” state (next slide)

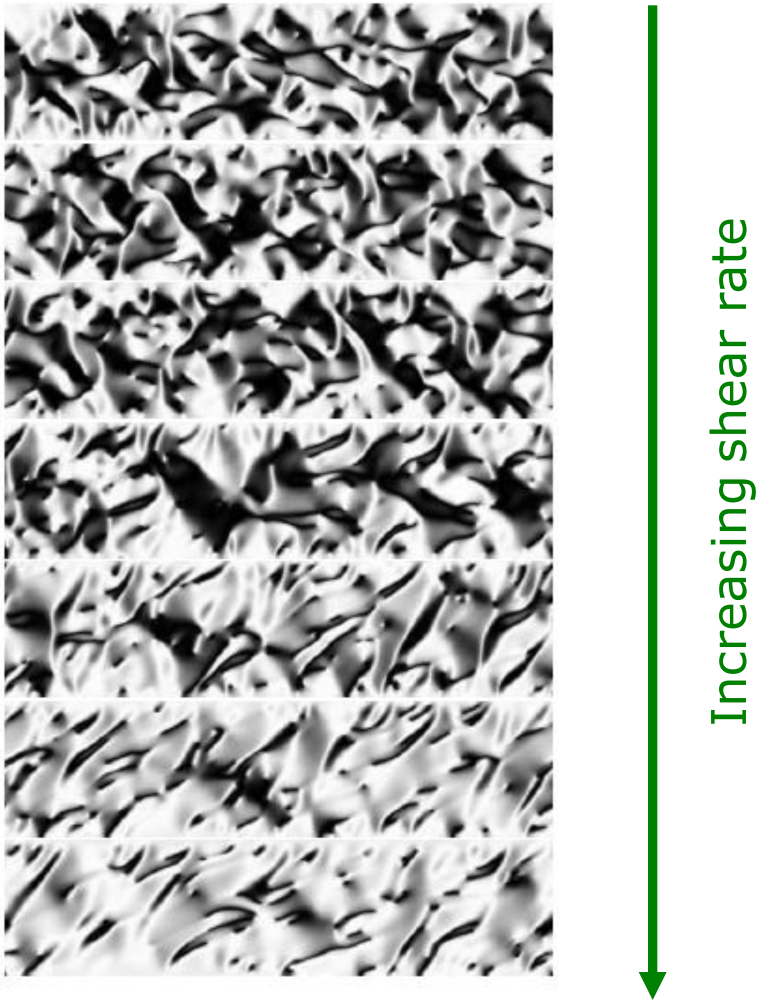


[SMF et al. PRE 2011]

Shearing "turbulent" state

Flow curve





[SMF et al. PRE 2011]

Summary of part I

Explored hydrodynamics and rheology of active gels

- Used Lattice Boltzmann & finite difference simulations
- Both methods well placed to explore strongly nonlinear regimes
- Need much more insight into parameter values
- Viscosity divergence (contractile)
- Superfluidity (extensile)
- Mechanistic link to bulk flow curve
- Shear banding in 1D
- Modulated by boundary terms (not shown here)
- Spontaneous rolls and turbulent states in 2D (extensile)

Part II: Hydrodynamics & activity induced phase separation (or not)

- Mechanisms for motility induced phase separation (MIPS)
- Presence of MIPS in suspensions of active Brownian discs
- Absence of MIPS in suspensions of active squirming discs (cylinders!)
- Possibility mechanism of suppression of MIPS by hydrodynamics
- Conclusions

Emergent phenomena: activity induced phase separation

- Mechanism I: [Narayan et al. Science (2007); Chate et al. PRL (2006)]

number density fluctuations

steric tendancy to align,
in elongated particles

coupled by activity

- Mechanism II: [Tailleur + Cates PRL (2008)]

"Motility-induced phase separation" (MIPS)

Predicted even without particle elongation

Emergent phenomena: activity induced phase separation

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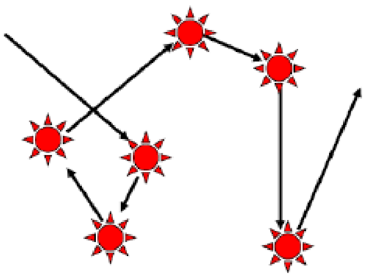
"Motility-induced phase separation" (MIPS)

Predicted even without particle elongation

Here: simulation study of when this does/doesn't arise (for disks)

Motility-induced phase separation (MIPS): prediction

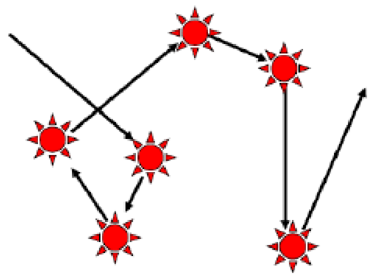


volume fraction of particles f

run → speed v

tumble  event rate $1/t_o$

Motility-induced phase separation (MIPS): prediction



volume fraction of particles f

run → speed $v = v(f)$

tumble  event rate $1/t_o$

Positive feedback mechanism

particles accumulate $f\uparrow$ where slow down $v\downarrow$

particles slow down $v\downarrow$ where crowded $f\uparrow$

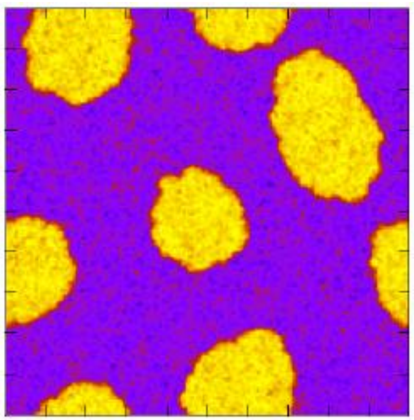
Spinodal onset of phase separation

$$\frac{d\ln v}{d\ln f} < -1$$

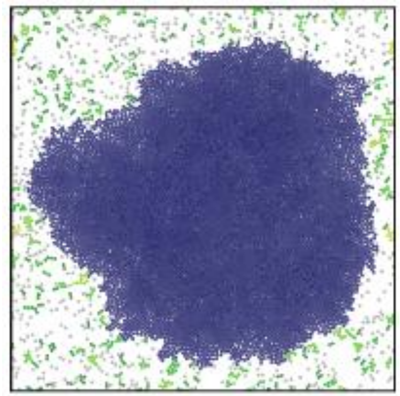
[Tailleur + Cates PRL (2008)]

MIPS in simulations of dense packings of disks

Thompson et al.
J. Stat. Mech. (2011)



run + tumble
lattice model



Fily + Marchetti PRL (‘12);

See also:
Redner et al. PRL (‘13)

$$\dot{\mathbf{r}}_i = v_0 \hat{\mathbf{v}}_i + \mu \sum_{j \neq i} \mathbf{F}_{ij}$$

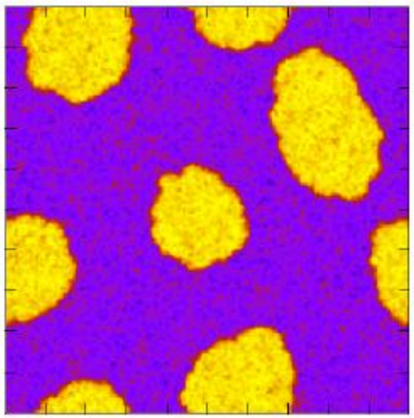
run + excluded volume

$$\dot{\theta}_i = \eta_i(t), \quad \langle \eta_i(t) \eta_j(t') \rangle = 2\nu_r \delta_{ij} \delta(t - t')$$

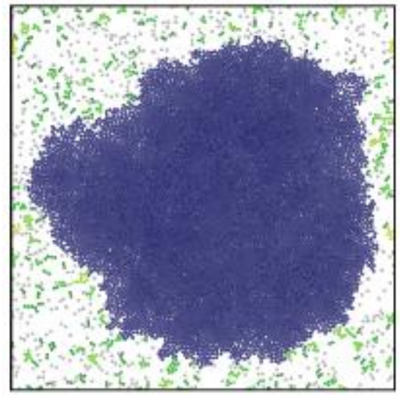
Brownian angular dynamics

MIPS in simulations of dense packings of disks

Thompson et al.
J. Stat. Mech. (2011)



run + tumble
lattice model



Fily + Marchetti PRL (‘12);

See also:
Redner et al. PRL (‘13)

$$\dot{\mathbf{r}}_i = v_0 \mathbf{v}_i + \mu \sum_{j \neq i} \mathbf{F}_{ij}$$

run + excluded volume

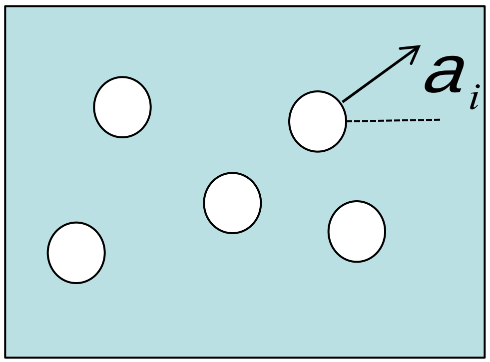
$$\dot{\theta}_i = \eta_i(t), \quad \langle \eta_i(t)\eta_j(t') \rangle = 2\nu_r \delta_{ij} \delta(t - t')$$

Brownian angular dynamics

But hydrodynamics unaccounted for. What effect will this have?

Ishikawa, Pedley, et al. PRL 2008, JFM 2008; Blake JFM 1971

Simulation: active squirming disks with full hydrodynamics



tangential velocity round i[th] disc edge

$$v_{\text{slip},\ i} = B_1 \sin(q_i - a_i) + B_2 \sin 2(q_i - a_i)$$

free swim speed $B_1/2$; direction a_i

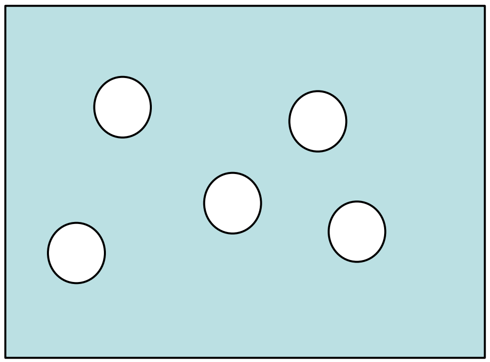
Fully solve Stokes equation for so fully capture:

- far-field power-law propagators
- near-field lubrication effects

Computer effort $O(N^3)$ so far smaller N than for Brownian

Hydrodynamics *vs.* Brownian

Squirm + excl. vol. + hydrodyn.



$N = 256$ disks

$R = 1$ disk radius

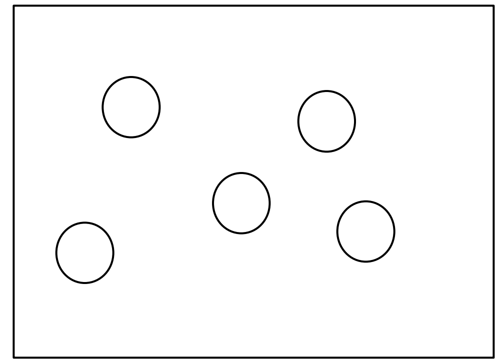
L box size

$h = 1$ fluid viscosity

$\frac{1}{2} B_1 = v_0 = 1$ free swim speed

B_2 push vs pull

Run + excl. vol. + Brownian



$N = 256$ disks

$R = 1$ disk radius

L box size

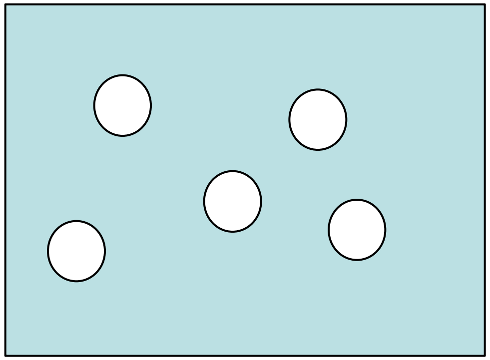
$m^{-1} = 1$ drag

$v_0 = 1$ free swim speed

$n_r = t_0^{-1}$ reorient rate

Hydrodynamics *vs.* **Brownian**

Squirm + excl. vol. + hydrodyn.

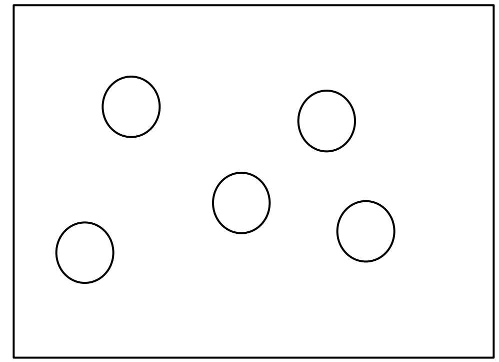


→ explore

area fraction $$f = Np\frac{R^2}{L^2}$$

push vs pull $$b = \frac{B_2}{B_1}$$

Run + excl. vol. + Brownian



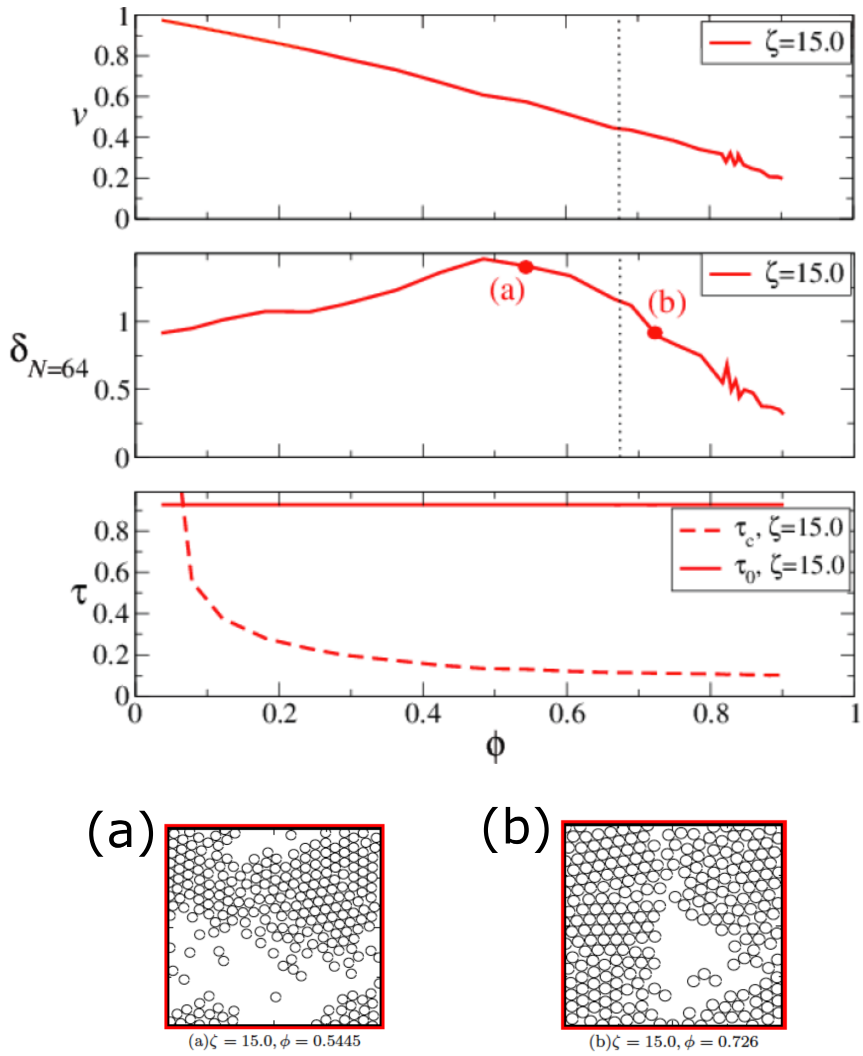
→ explore

area fraction $$f = Np\frac{R^2}{L^2}$$

reorient time/

scatter time $$z = \sqrt{\frac{p}{f}\,\frac{t_o}{t_c}}$$

Results: Brownian dynamics → phase separation



By imposing large z

reorientation slower

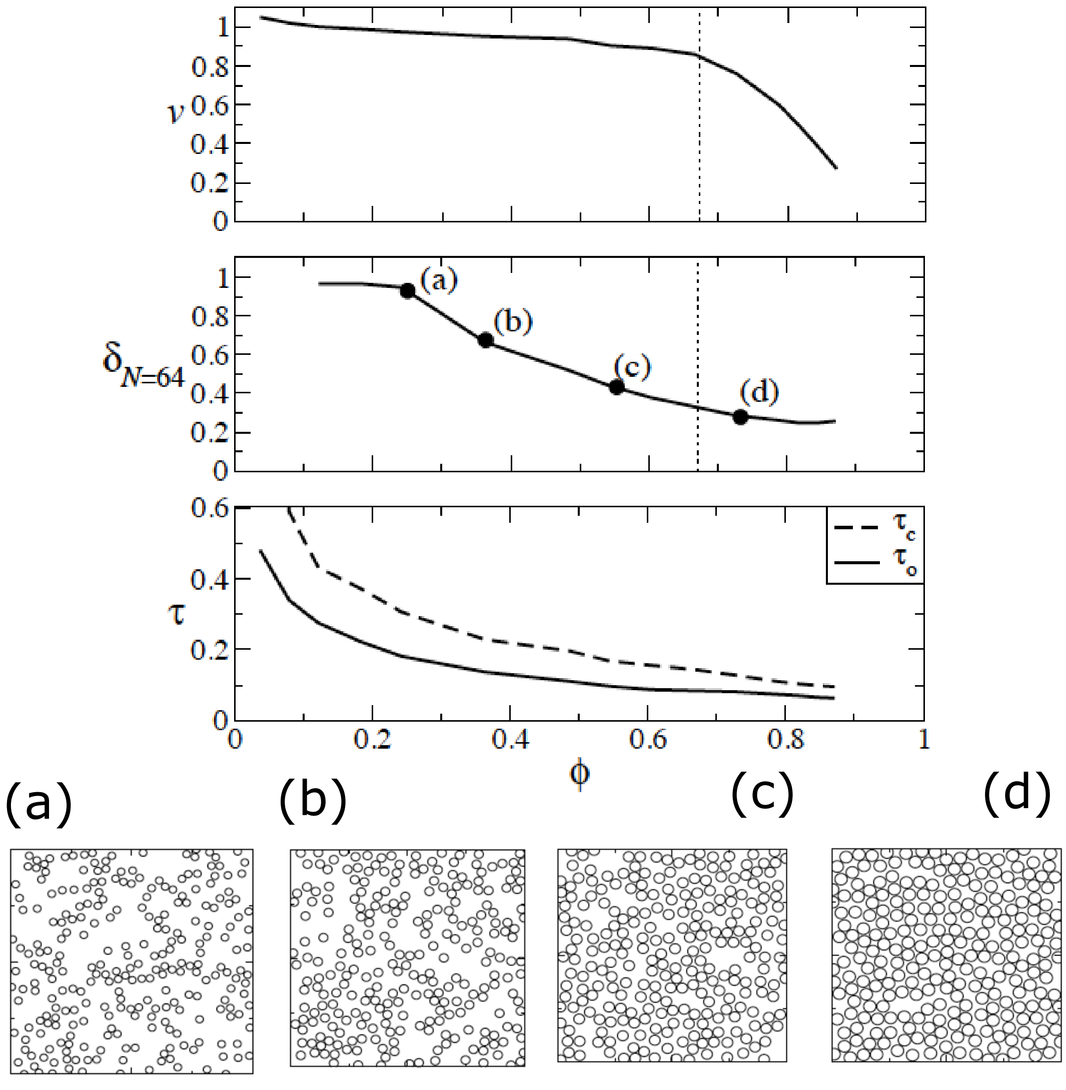
than collision time,

as in earlier work

Recall $$z = \sqrt{\frac{p}{f}\frac{t_o}{t_c}}$$

Fily + Marchetti PRL '12

Results: hydrodynamics → no phase separation



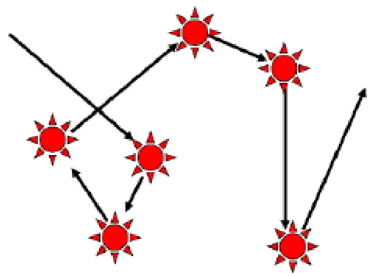
No way of imposing $\frac{t_o}{t_c}$

Reorientation emerges naturally due to hydrodynamic interactions as particles collide

So $t_o » t_c$

Checked $b = \pm¥, \pm 5, \pm 1, 0$

Why no phase separation with hydrodynamics? Revisit…



volume fraction of particles f

run → speed $v = v(f)$

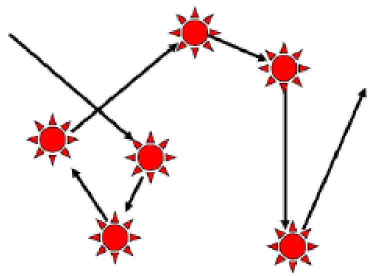
tumble ✱ event rate $1/t_o$

Positive feedback mechanism

particles accumulate $f \uparrow$ where slow down $v \downarrow$

particles slow down $v \downarrow$ where crowded $f \uparrow$

Why no phase separation with hydrodynamics? Revisit…



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Positive feedback mechanism

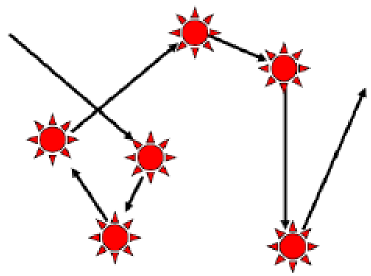
particles accumulate $f\uparrow$ where slow down $v\downarrow$

particles slow down $v\downarrow$ where crowded $f\uparrow$

To experience a decreasing $v = v(f)$ during runs, must collide

many times during a run, between tumbles, *i.e.* $t_o >> t_c$

Why no phase separation with hydrodynamics? Revisit…



volume fraction of particles f

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tumble ✸ event rate $1/t_{o}$

Positive feedback mechanism

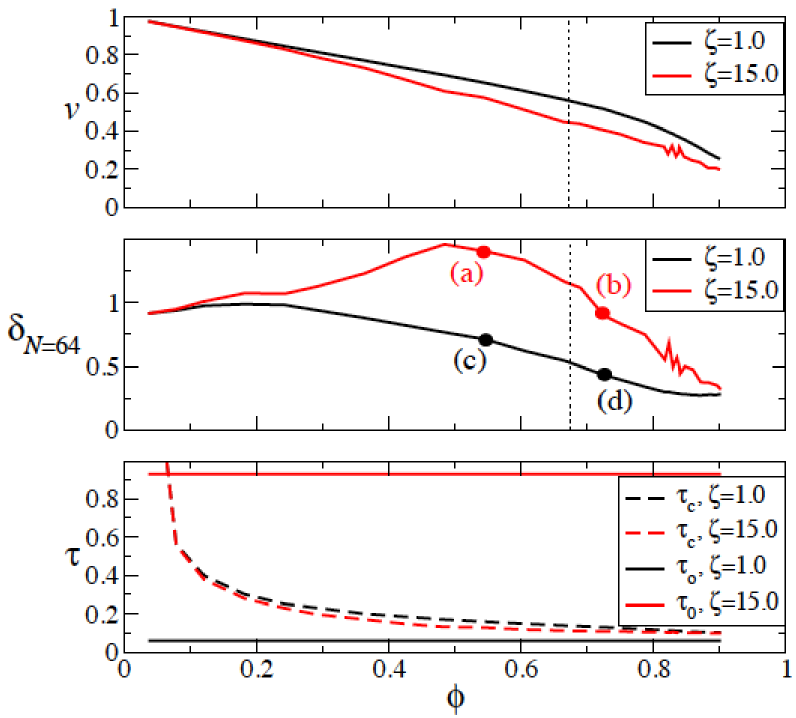
particles accumulate $f \uparrow$ where slow down $v \downarrow$

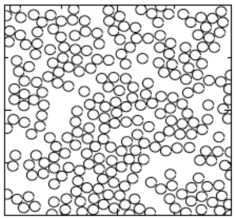
particles slow down $v \downarrow$ where crowded $f \uparrow$

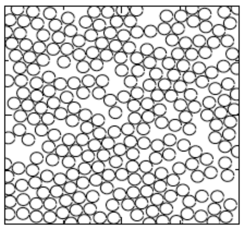
Hydrodynamic system has $t_{o} \gg t_{c}$

Feedback mechanism breaks down → no phase separation

Test this idea: re do Brownian dynamics



(c) 

(d) 

Now impose $z = O(1)$

Reorientation same order as

collision time,

Recall $z = \sqrt{\frac{p}{f}\frac{t_o}{t_c}}$

Phase separation suppressed

as in hydrodynamic case

Preprint arxiv.org/abs/1210.5464, submitted.

See also arxiv.org/abs/1309.4352 Zottl + Stark PRL 2013

Conclusions, perspectives…

- MIPS predicted to arise generically in active matter
- May be suppressed in systems where hydrodynamics important
- Suggest mechanism concerns $t_o \gg t_c$

- Effects of particle elongation and link with "mechanism 1"?
- Effects of dimensionality (hydrodynamics + packings) ?

Ishikawa et al. JFM 2008 3D + 3D -> no phase separation

Ishikawa + Pedley PRL 2008 3D + 2D -> phase separation

Durham University

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