Active hydrodynamics

framework & applications

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Support: J C Bose Fellowship, DST/SERB, India

Outline

- Introduction
  - motivation
  - from equilibrium Langevin to active dynamics
- Examples
- Active fluids, from bulk to confined
  - polar
  - apolar
- Summary

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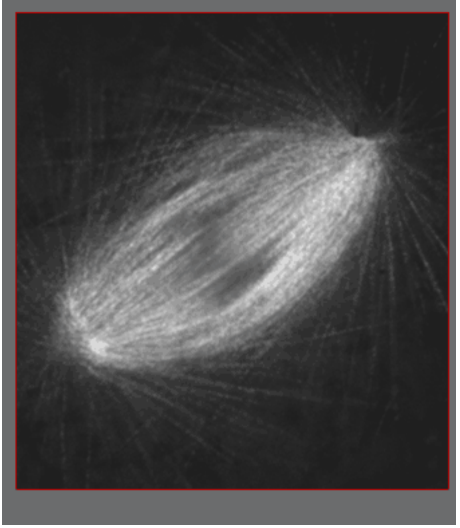
MOTIVATION

- Active particle
  - direct free-energy input to each particle
  - machinery to transduce this to movement
  - transient information: sensing and signalling
  - heritable information: self-replication
  - mutation: evolution
- Active condensed matter
  - collections of interacting active particles

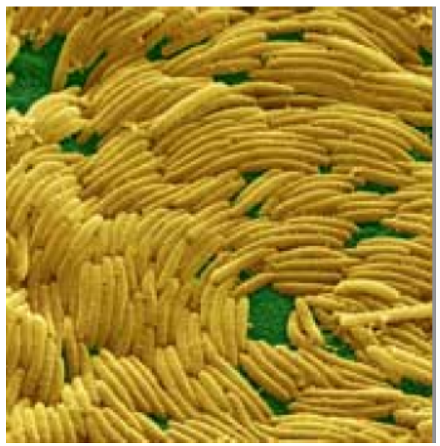
If you accept this definition then here are some active-matter systems:

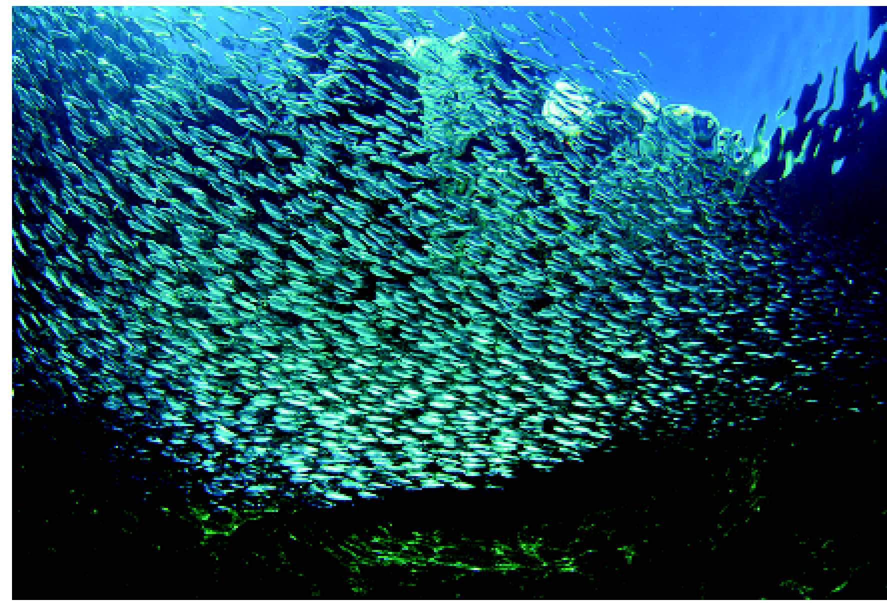
The varieties of active matter



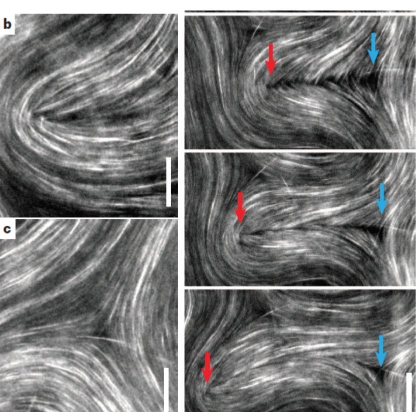
Within a cell
Dan Needleman

Many cells
G Velicer (Indiana)
J Bergen (MPI Dev Bio)

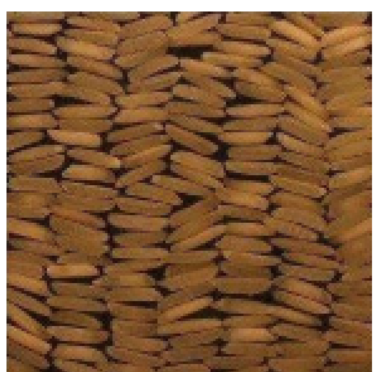




Fish schools Jon Bertsch
http://www.thalassagraphics.com/blog/?p=167

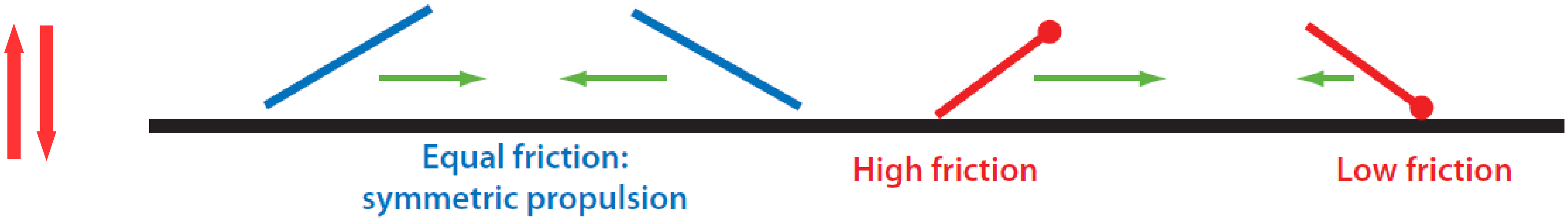


Extracts from a cell
Sanchez et al 2012



Artificial systems
V Narayan, N Menon

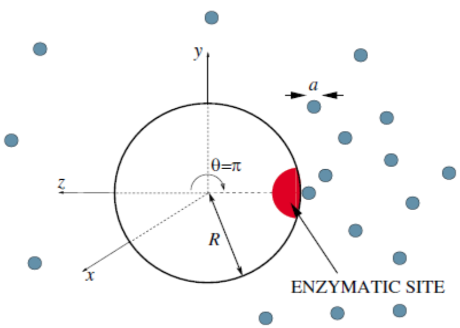
The varieties of active matter



Vertically vibrated horizontal granular monolayer

Figure 2

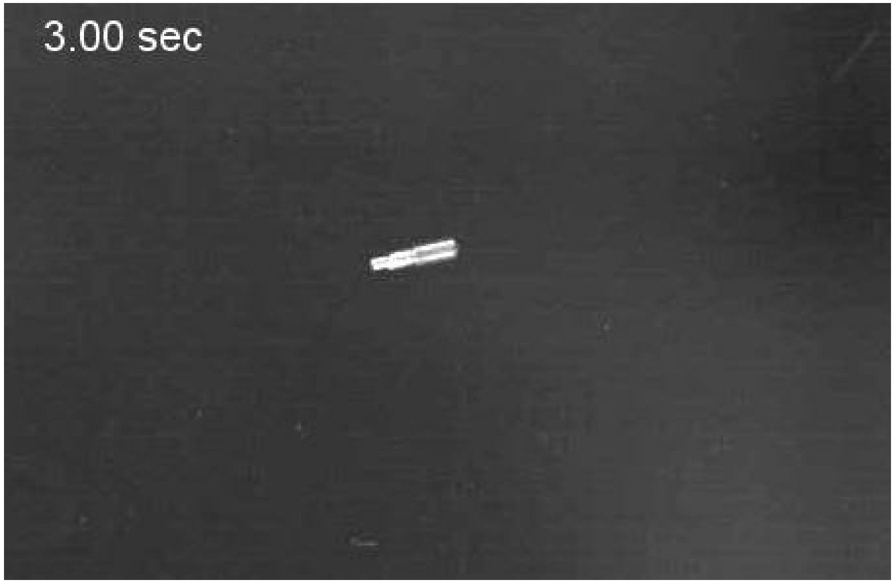
A rod landing after being tossed up will in general be impelled away from the end that makes first contact with the surface. If the two ends differ in weight, geometry, or friction, the rod will be propelled toward one end.



Catalytic particle in a reactant bath

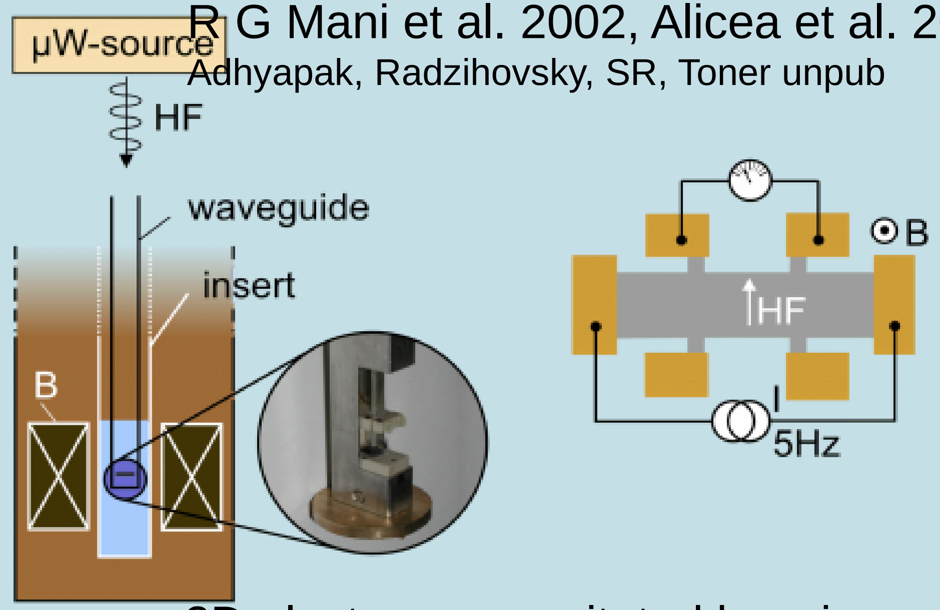
Golestanian et al., Saha et al.

Nitin Kumar
Ajay Sood



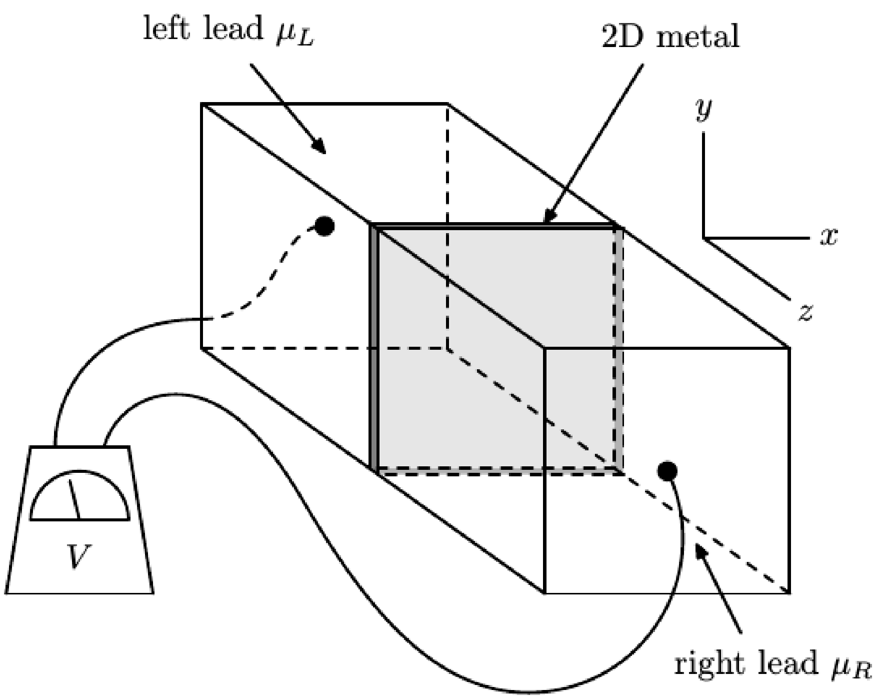
The varieties of active matter

R G Mani et al. 2002, Alicea et al. 2005
Adhyapak, Radzihovsky, SR, Toner unpub



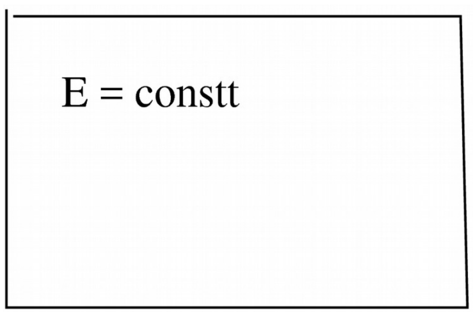
2D electron gas agitated by microwaves

Takei and Kim
Phys. Rev. B 76, 115304 (2007)

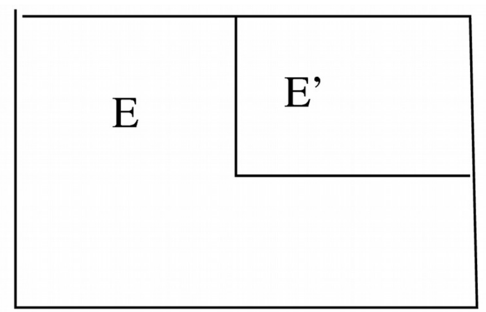


Common feature: sustained, direct driving of constituent degrees of freedom

Thermal equilibrium: “closed” systems



E = constt

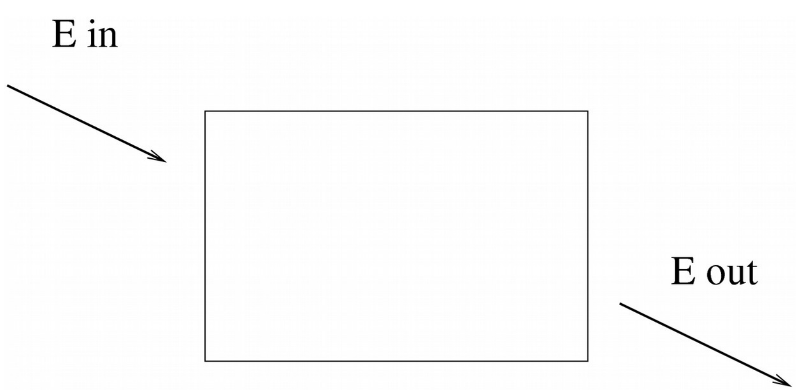


E + E’ = constt
Temperature of subsystem = constt

$t \leftrightarrow -t$

Physics students know the rules

Active matter: open systems (& questions)



- running engine + fuel
- living organism + food

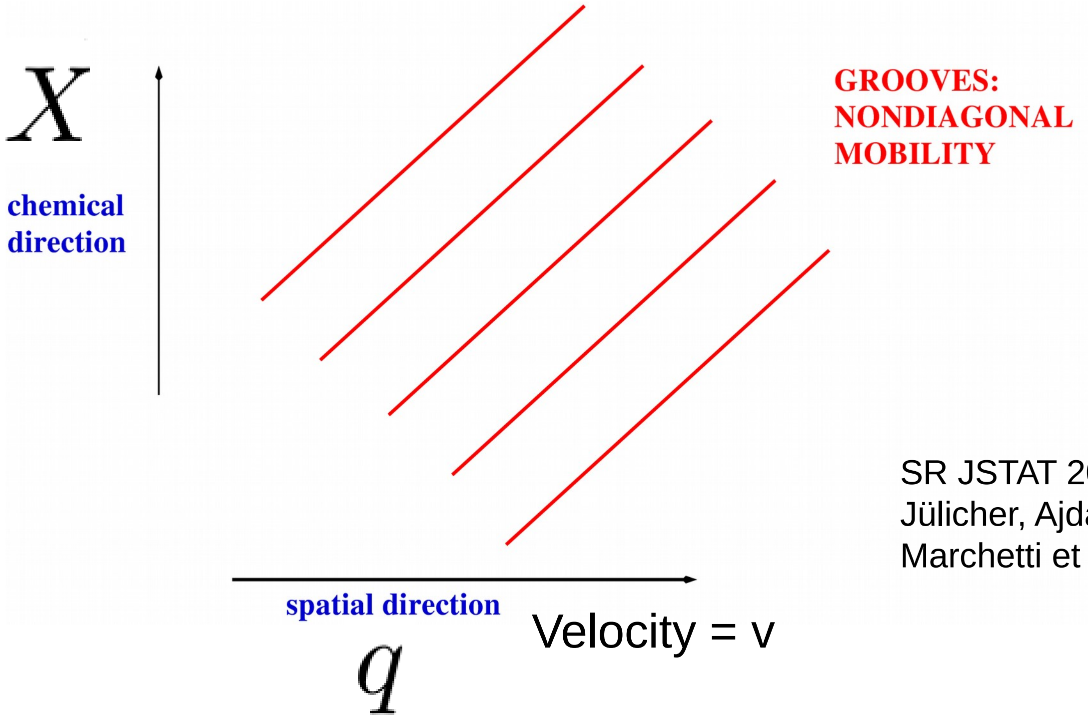
~~$t \leftrightarrow -t$~~

Actually no CPT

FROM EQUILIBRIUM LANGEVIN TO ACTIVE DYNAMICS

Active: “New” terms, ruled out in equilibrium dynamics?

Velocity = r



Velocity = v

SR JSTAT 2017
Jülicher, Ajdari, Prost RMP Colloq 1993
Marchetti et al. RMP 2013

Motor: catalyst for fuel breakdown; 2d configuration space

Driving force $\Delta\mu = \mu_{\text{reactant}} - \mu_{\text{product}}$ in *chemical* direction

Mobility nondiagonal

Velocity = Mobility * Force has component in *spatial* direction

FROM EQUILIBRIUM LANGEVIN TO ACTIVE DYNAMICS

Temperature T; Effective free energy $H(q,p,X) \sim \log P_{equil}$

q (time-rev even), p (odd), X (extra degree of freedom)

$$\begin{aligned} \dot{q} + \gamma \partial_q H &= \partial_p H + \theta \\ \dot{p} + \Gamma_{11} \partial_p H + \Gamma_{12}(q) \partial_\Pi H &= -\partial_q H + \eta \\ \dot{\Pi} + \Gamma_{21}(q) \partial_p H + \Gamma_{22} \partial_\Pi H &= -\partial_X H + \xi \\ \dot{X} &= \partial_\Pi H \end{aligned}$$

noises (θ, η, ξ) $\qquad$ $\langle \eta(0) \xi(t) \rangle = 2 k_B T \Gamma_{12}(q) \delta(t)$

FROM EQUILIBRIUM LANGEVIN TO ACTIVE DYNAMICS

Temperature T; Effective free energy $H(q,p,X) \sim \log P_{equil}$

q (time-rev even), p (odd), X (extra degree of freedom)

Off-diagonal q-dependent Onsager coefficients

$$\begin{aligned}
\dot{q} + \gamma \partial_q H &= \partial_p H + \theta \\
\dot{p} + \Gamma_{11} \partial_p H + \underline{\Gamma_{12}(q)} \partial_\Pi H &= -\partial_q H + \eta \\
\dot{\Pi} + \underline{\Gamma_{21}(q)} \partial_p H + \Gamma_{22} \partial_\Pi H &= -\partial_X H + \xi \\
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\end{aligned}$$

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noises (θ, η, ξ)

$$\langle \eta(0)\xi(t)\rangle = 2k_B T\Gamma_{12}(q)\delta(t)$$

FROM EQUILIBRIUM LANGEVIN TO ACTIVE DYNAMICS

Temperature T; Effective free energy $H(q,p,X) \sim \log P_{equil}$

q (time-rev even), p (odd), X (no. of fuel mols consumed)

$$\begin{aligned} \dot{q} + \gamma \partial_q H &= \partial_p H + \theta \\ \dot{p} + \Gamma_{11} \partial_p H + \Gamma_{12}(q) \dot{X} &= -\partial_q H + \eta \\ \Gamma_{21}(q) \partial_p H + \Gamma_{22} \dot{X} &= -\partial_X H + \xi \end{aligned}$$

noises (θ, η, ξ) $\langle \eta(0) \xi(t) \rangle = 2 k_B T \Gamma_{12}(q) \delta(t)$

From equilibrium Langevin equations to active matter

$$\begin{aligned} \dot{q} + \gamma \partial_q H &= \partial_p H + \theta \\ \dot{p} + \Gamma_{11} \partial_p H + \Gamma_{12}(q) \dot{X} &= -\partial_q H + \eta \\ \Gamma_{21}(q) \partial_p H + \Gamma_{22} \dot{X} &= -\partial_X H + \xi \end{aligned}$$

eliminate $\dot{X}$ from the p equation

in favour of corresponding force $-\partial_X H$

From equilibrium Langevin equations to active matter

$$\dot{q} + \gamma\partial_q H = \partial_p H + \theta$$

$$\dot{p} + \Gamma\partial_p H - \frac{\Gamma_{12}(q)}{\Gamma_{22}}\partial_X H = -\partial_q H + f$$

$$\dot{X} + \frac{\Gamma_{12}(q)}{\Gamma_{22}}\partial_p H = -\frac{1}{\Gamma_{22}}\partial_X H + \frac{\xi}{\Gamma_{22}}$$

equilibrium dynamics of q, p and X

$$f \equiv \eta - (\Gamma_{12}/\Gamma_{22})\xi \longleftrightarrow \Gamma \equiv \Gamma_{11} - \Gamma_{12}^2(q)/\Gamma_{22}$$

$$[X, p] = \Gamma_{12}(q)/\Gamma_{22}$$

From equilibrium Langevin equations to active matter

$$\dot{q} + \gamma \partial_q H = \partial_p H + \theta$$

$$\dot{p} + \Gamma \partial_p H - \frac{\Gamma_{12}(q)}{\Gamma_{22}} \partial_X H = -\partial_q H + f$$

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$$-\partial_X H \equiv -\Delta\mu$$

From equilibrium Langevin equations to active matter

$$\begin{aligned}
\dot{q} + \gamma \partial_q H &= \partial_p H + \theta \\
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\dot{X} + \frac{\Gamma_{12}(q)}{\Gamma_{22}} \partial_p H &= -\frac{1}{\Gamma_{22}} \partial_X H + \frac{\xi}{\Gamma_{22}}
\end{aligned}$$

Active? Hold chemical force

$$-\partial_X H \equiv -\Delta\mu$$

= constant

From equilibrium Langevin equations to active matter

Including chemical fluctuations

$$\dot{q} + \gamma \partial_q H \;=\; \partial_p H + \theta$$

$$\dot{p} + \Gamma \partial_p H \;=\; \frac{\Delta\mu}{\Gamma_{22}} \Gamma_{12}(q) - \partial_q H + f$$

$$\dot{X} + \frac{\Gamma_{12}(q)}{\Gamma_{22}} \partial_p H \;=\; -\frac{1}{\Gamma_{22}} \Delta\mu + \frac{\xi}{\Gamma_{22}}$$

From equilibrium Langevin equations to active matter

$$\dot{q} + \gamma \partial_q H = \partial_p H + \theta$$

$$\dot{p} + \Gamma \partial_p H = \boxed{\frac{\Delta\mu}{\Gamma_{22}} \Gamma_{12}(q)} - \partial_q H + f$$

"New" terms, ruled out in equilibrium dynamics

No inertia: q-only equation of motion

$$\dot{q} + (\gamma + \Gamma^{-1}) \partial_q H = \boxed{\frac{\Delta\mu}{\Gamma_{22}\Gamma} \Gamma_{12}(q)} + \theta + \Gamma^{-1} f$$

Examples: active interface

$$q \to h(\mathbf{x}, t) = \text{height field of interface}$$

$$\text{Invariance: } h \to h + \text{constant } \textbf{but not } h \to -h$$

$$\dot{h} + \frac{1}{\zeta}\frac{\delta H}{\delta h} = \frac{\Delta\mu}{\Gamma_{22}\Gamma}\underline{\Gamma_{12}}(h, \nabla h, ...) + \sqrt{\frac{2k_B T}{\zeta}}f$$

$$\text{Symmetries} \to \underline{\Gamma_{12}} = \text{constt} + (\nabla h)^2$$

KPZ equation

Examples: dry polar active system

$$q \to \mathbf{w}(\mathbf{x}, t) = \text{vector orientation field of SPPs}$$

$$\dot{\mathbf{w}} + \frac{1}{\zeta}\frac{\delta H}{\delta \mathbf{w}} = \frac{\Delta\mu}{\Gamma_{22}\Gamma}\Gamma_{12}(\mathbf{w}, \nabla\mathbf{w}, ...) + \sqrt{\frac{2k_B T}{\zeta}}\mathbf{f}$$

$$\Gamma_{12} \text{ must be a vector}$$

$$\Gamma_{12} = \text{all possible contractions of } \mathbf{w}\nabla\mathbf{w}$$

Orientation advects itself

Toner-Tu nonlinearities emerge naturally

Examples: dry polar active system

$$q \to \rho(\mathbf{x}, t) = \text{density field of SPPs}$$

$$\dot{\rho} - M\nabla^2 \frac{\delta H}{\delta \rho} = \frac{\Delta\mu}{\Gamma_{22}\Gamma}\underline{\Gamma_{12}} + \sqrt{2k_B T M}\nabla \cdot \mathbf{f}$$

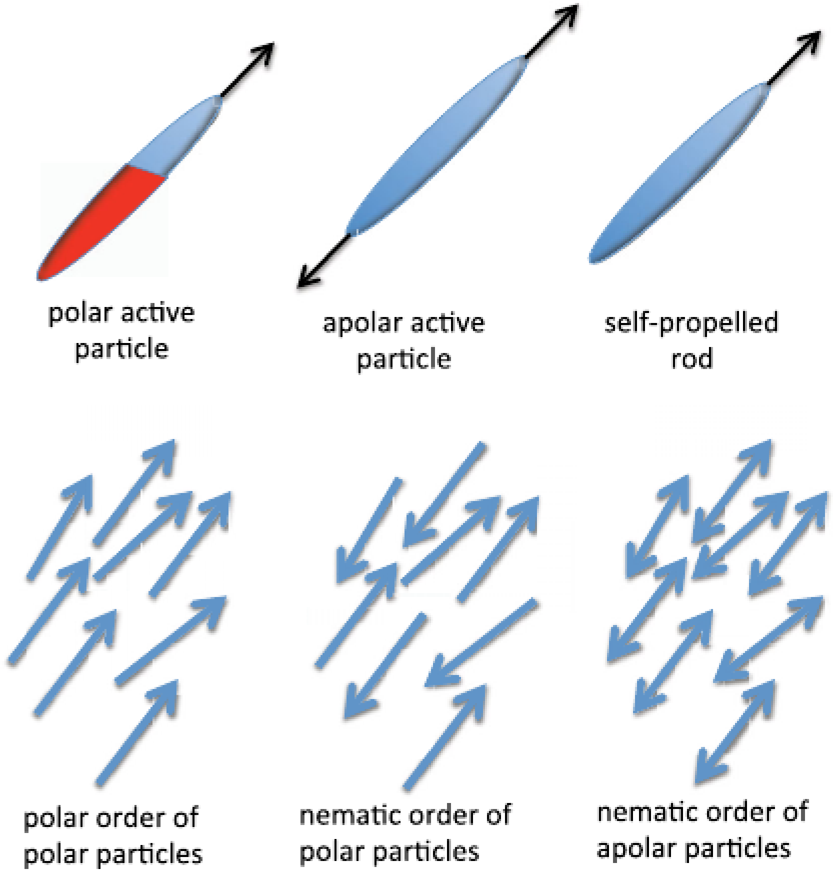
$$\Gamma_{12} \text{ must conserve } \int d^d x \rho$$

$$\underline{\Gamma_{12}} = \nabla \cdot \mathbf{w} + \ldots.$$

Orientation “becomes” a current

ORIENTATIONAL ORDER NEED NOT BE AN ARROW

$\mathbf{n}_\alpha$



Polar order parameter

$\boldsymbol{p}(\boldsymbol{r}) = \langle \mathbf{n}_\alpha \rangle$

Apolar order parameter

$\boldsymbol{Q}(\boldsymbol{r}) = \langle \mathbf{n}_\alpha\, \mathbf{n}_\alpha - \boldsymbol{I}/3 \rangle$

Examples: dry apolar active system

$$q \to \rho(\mathbf{x}, t) = \text{density field of SPPs}$$

$$\dot{\rho} - M\nabla^2 \frac{\delta H}{\delta \rho} = \frac{\Delta\mu}{\Gamma_{22}\Gamma}\underline{\Gamma_{12}} + \sqrt{2k_B T M}\nabla \cdot \mathbf{f}$$

$$\Gamma_{12} \text{ must conserve } \int d^d x \rho$$

$$\underline{\Gamma_{12}} = \nabla\nabla : \mathbf{Q} + \ldots.$$

Curvature-induced current in *apolar* systems

Examples: orientable active *fluid*

$$q \to \mathbf{Q}(\mathbf{x}, t) = \text{nematic order parameter}$$

$$\text{or vector order parameter } \mathbf{w}$$

$$p \to \mathbf{g}(\mathbf{x}, t) = \text{momentum density field}$$

$$\partial_t \mathbf{g} = [\mathbf{g}, \mathbf{Q}] \frac{\delta H}{\delta \mathbf{Q}} - \hat{\eta} \frac{\delta H}{\delta \mathbf{g}} + \frac{\Delta\mu}{\Gamma_{22}\Gamma} \underline{\Gamma_{12}} + \sqrt{2k_B T \hat{\eta}}\mathbf{f}$$

Momentum conservation
vectorial symmetry

$$\underline{\Gamma_{12}} = \nabla \cdot \mathbf{Q} + \nabla\nabla\mathbf{w} \ldots.$$

Active stresses

Liquid-crystal hydrodynamics with a difference

F = free energy relative to isotropic fluid
Tensors **Q** = orientation, $\mathbf{\Omega}$ = vorticity, **A** = deformation rate

Extensional flow: Orienting torque

Thermodynamic relaxation

Comoving co-rotating derivative

$$(\partial_t + \mathbf{u}\cdot\nabla)\mathbf{Q} - (\mathbf{\Omega}\cdot\mathbf{Q} - \mathbf{Q}\cdot\mathbf{\Omega}) = \left[\lambda_0 \mathbf{A} + \lambda_1 \mathbf{A}\cdot\mathbf{Q} - \Gamma \frac{\delta F}{\delta \mathbf{Q}}\right]_{\mathrm{ST}}$$

Symmetrised, traceless

$$-\eta\nabla^2\mathbf{u} = \nabla\cdot\left[\left(\lambda_0\frac{\delta F}{\delta\mathbf{Q}} - \lambda_1\mathbf{Q}\cdot\frac{\delta F}{\delta\mathbf{Q}}\right)_{\mathrm{ST}} - W_2 c\mathbf{Q}\right] - \nabla p$$

Viscosity

pressure

Ericksen stresses

ACTIVE STRESS

Simha and SR 2002; Hatwalne *et al.* 2004
Kruse, Juelicher, Joanny, Prost, Voituriez, Sekimoto 2004

CONSEQUENCES →

Ignore inertia and acceleration
Go to zero wavevector – unbounded system
Direction matters: along or transverse to axis
A single timescale: viscosity/active stress

$$\partial_t Q_{xz} = -\frac{\alpha c_0 W_2}{\eta} Q_{xz}$$

Transverse to axis:
Splay instability
if contractile ($W_2<0$)

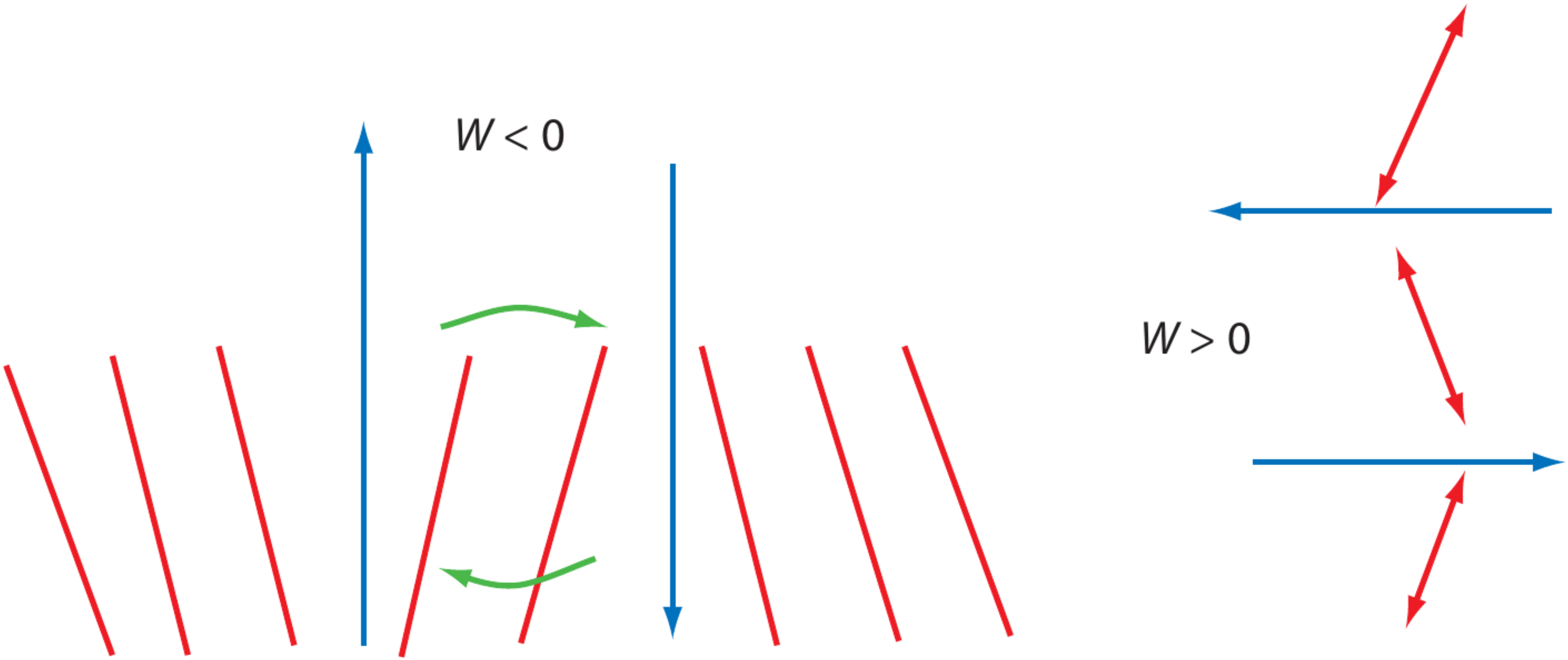
Growth rate nonzero
for wavenumber → 0

$$\partial_t Q_{xz} = +\frac{\alpha c_0 W_2}{\eta} Q_{xz}$$

Along axis:
Bend instability
if extensile ($W_2>0$)

$\alpha > 0$ = flow-director coupling
c_0=concentration, η = viscosity

Splay or bend instability: spontaneous flow

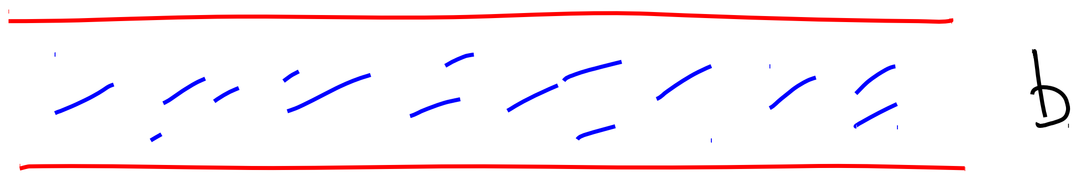


R A Simha & SR PRL 2002, '04
Joanny, Julicher, Kruse, Prost, Voituriez 2004,5,6
SR + Rao NJP 2007

Expts: Dombrowski *et* al. 2005;
Simulations: Saintillan and Shelley 2007
Wolgemuth bacterial turbulence 2008

Confinement

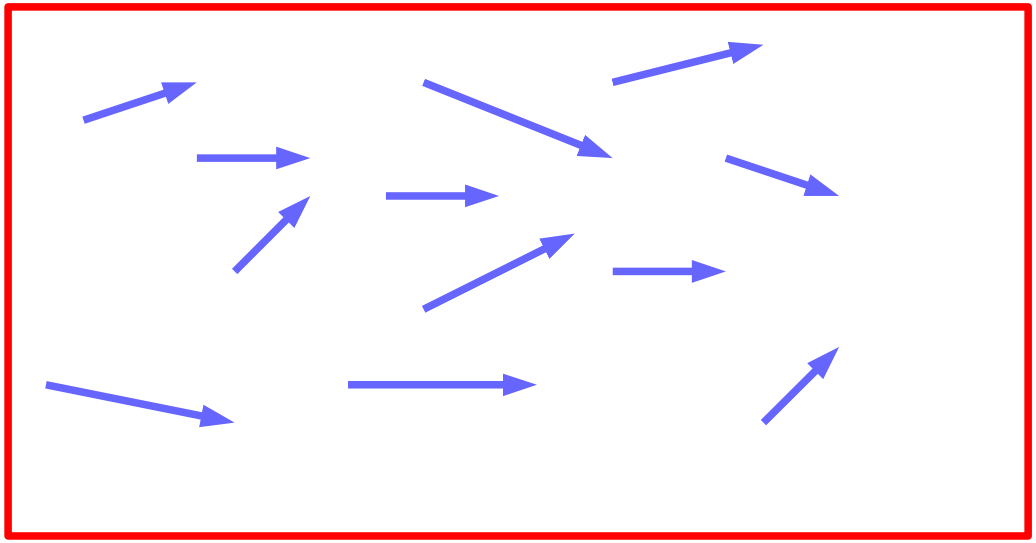
SR and M. Rao, New J Phys 2007
Muhuri et al 2007 -- shear



$$\partial_t Q_{xz} = -\left[\frac{\alpha c_0 W_2}{q_x^2 + (\pi/b)^2} + K\right]\frac{q_x^2}{\eta} Q_{xz}$$

K = Frank elastic constant of underlying liq crystal
Length scale $\xi = (K/c_0 W_2)^{1/2}$; stable if $b < \xi$
Fix b, increase activity W_2: diffusive instability
Is that all?

Confined active fluids

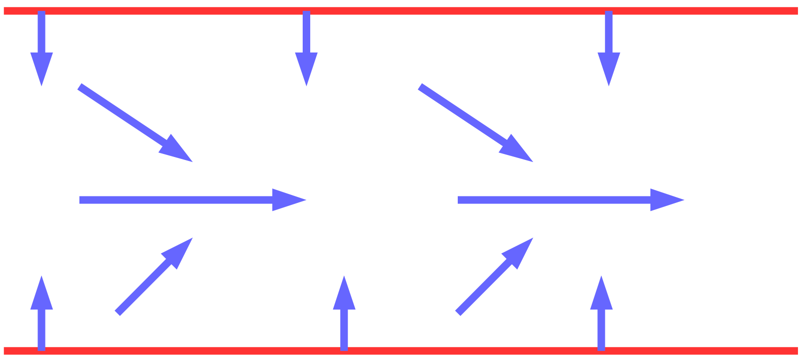


Top view

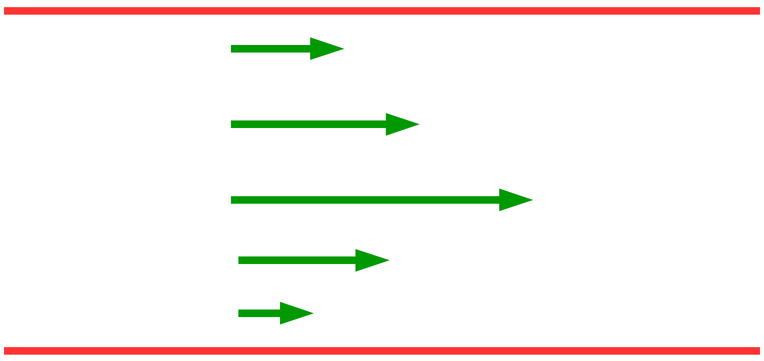
Extended in XY plane, confined in z

- bounding walls are a preferred frame
- forget momentum conservation?
- 2d confined = dry flocking model?

Confined active fluids



Side view



- Polar vs apolar: how different?
- Confined geometry
  - bounding walls: momentum sink
  - velocity field relaxes "fast"
- But: incompressibility
  - can't forget velocity field
  - "dry" flocking models not enough

Maitra, Srivastava, Marchetti, Lintuvuori, Lenz, SR preprint 2017

Confined active fluids

- So far: bounding surfaces --> no slip and parallel alignment
- OK for apolar systems
- Polar more interesting: wall anchoring --> profile
- Will assume perpendicular anchoring, parallel also works

Maitra, Srivastava,
Marchetti, Lintuvuori,
Lenz, SR preprint 2017

Building equations of motion: polar

- Start: 3d dynamics
- Polar order param $\boldsymbol{p}$, velocity field $\boldsymbol{u}$
- Project onto 2d by averaging over z
- Crucial: $\boldsymbol{p}$, $\boldsymbol{u}$ have profiles
- $\boldsymbol{u}$ in $\boldsymbol{p}$ equation: grad^2 $\boldsymbol{u}$ --> $\boldsymbol{u}$
- Active force density div $\boldsymbol{pp}$ --> $\boldsymbol{p}$

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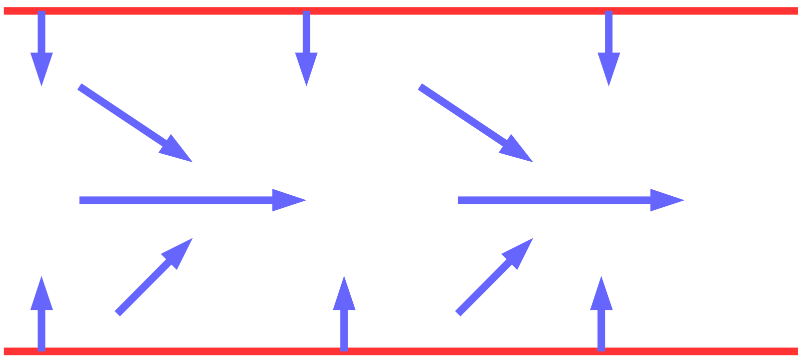
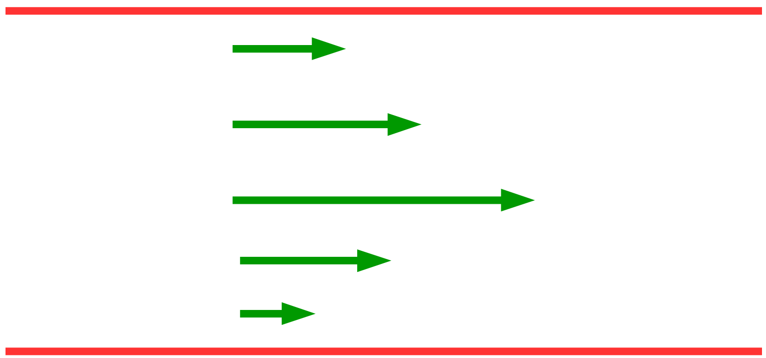
Marchetti, Lintuvuori,
Lenz, SR preprint 2017

Projected 2d dynamics



Orientation **p**



Velocity **v**

Flow-orientation coupling

relaxation

$$\partial_t \mathbf{p} = \Lambda \mathbf{v} + U \mathbf{p}$$

Forcing by polar active stresses

$$\mathbf{v} = \frac{w}{\Gamma}\mathbf{p} - \frac{1}{\Gamma}\nabla_\perp \Pi$$

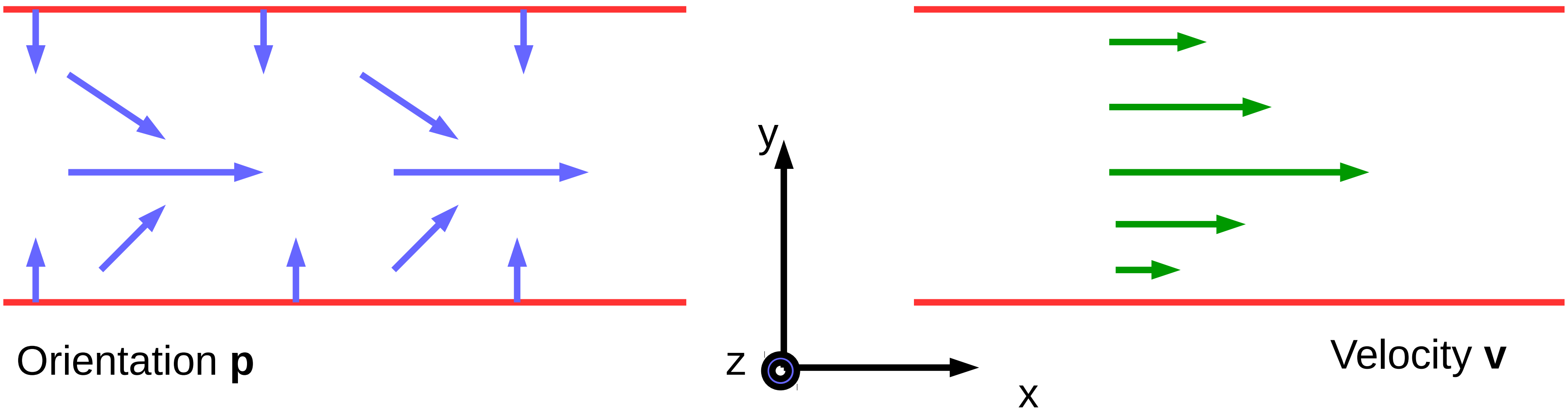
Projected pressure

$$\nabla_\perp \cdot \mathbf{v} = 0$$

Solve for v and 2d pressure Π, get effective dynamics of p

Maitra, Srivastava, Marchetti, Lintuvuori, Lenz, SR preprint 2017

Projected 2d dynamics



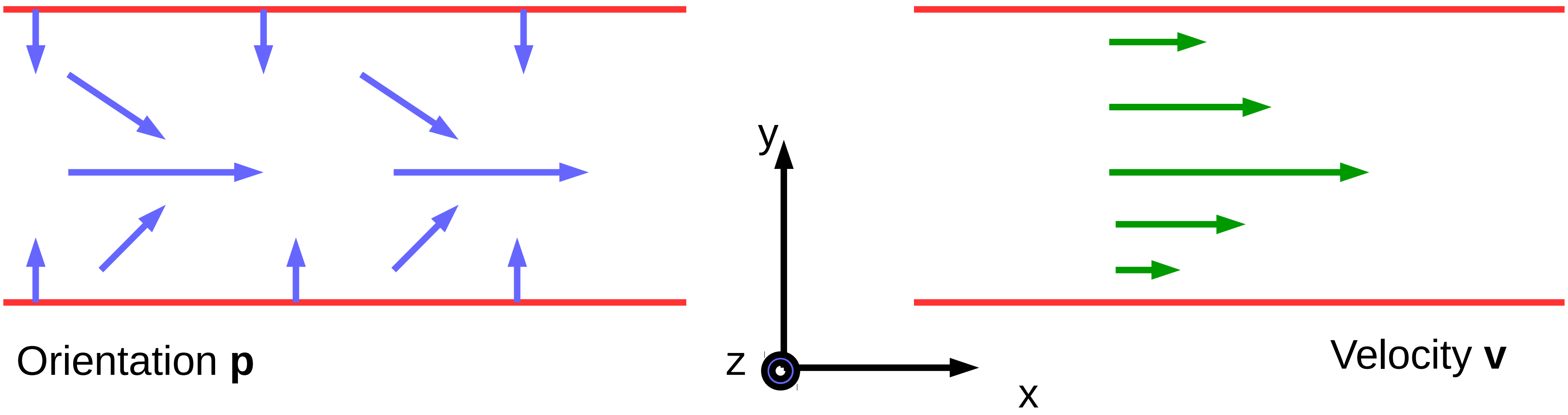
Ordered state, $\mathbf{p} = |\mathbf{p}|(\cos\Theta, \sin\Theta)$, $|\mathbf{p}|$ fixed

Fourier components Θ^q (q = wavenumber)

$$\partial_t \Theta^q = -\frac{\Lambda v}{\Gamma}(q_y^2/q^2)\Theta^q$$

Maitra, Srivastava, Marchetti, Lintuvuori, Lenz, SR preprint 2017

Projected 2d dynamics



$$\partial_t \Theta^q = -\frac{\Lambda v}{\Gamma}(q_y^2/q^2)\Theta^q$$

Orientational fluctuations relax/grow at nonzero rate for q --> 0

True for ***all*** directions except strictly along alignment direction.

contrary to Brotto et al. 2013

Stable/unstable: depends on sign of flow coupling Λ

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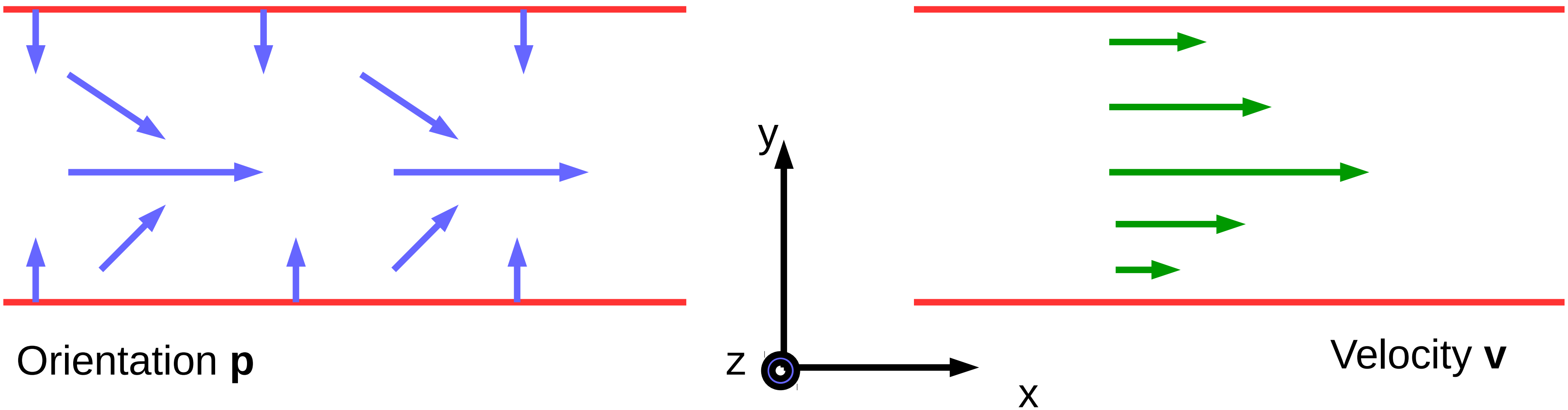
Projected 2d dynamics

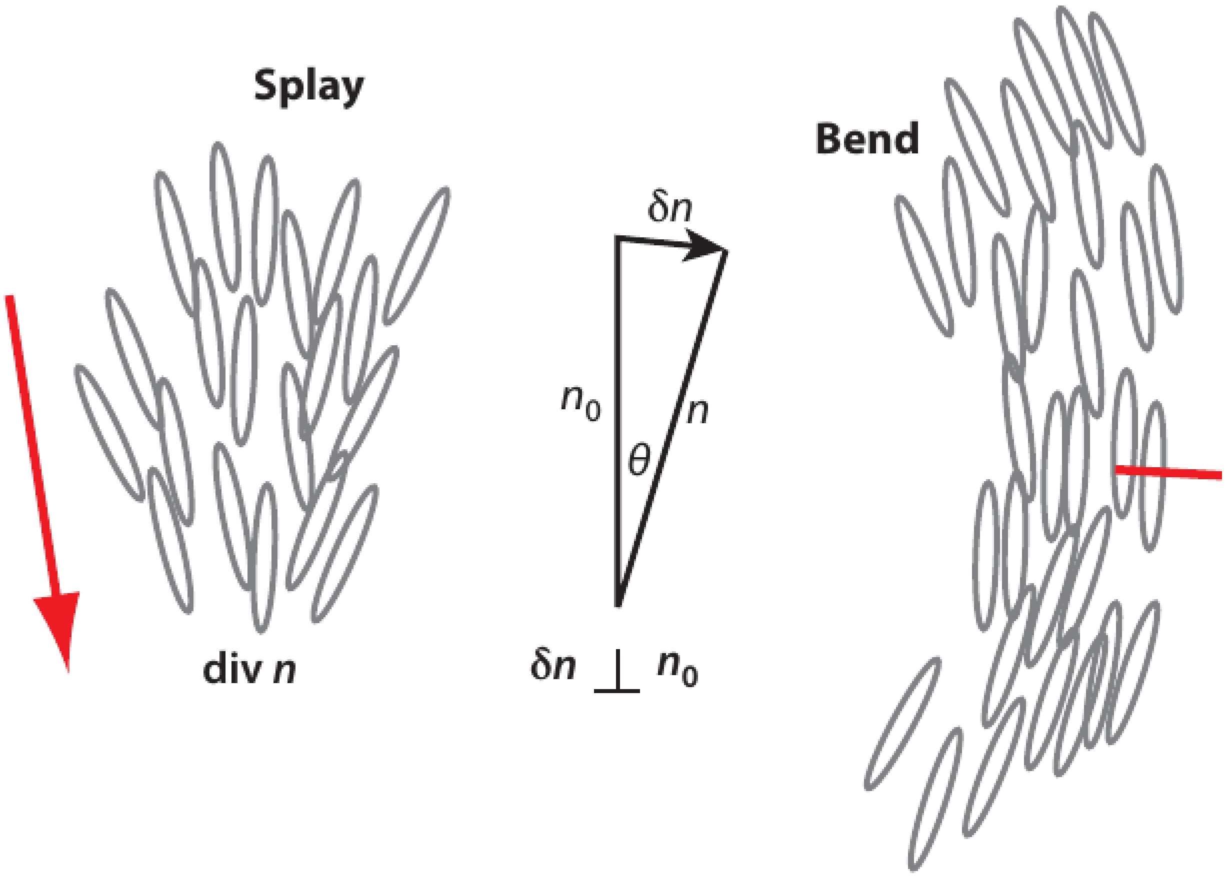


$$\partial_t \Theta^q = -\frac{\Lambda v}{\Gamma}(q_y^2/q^2)\Theta^q$$

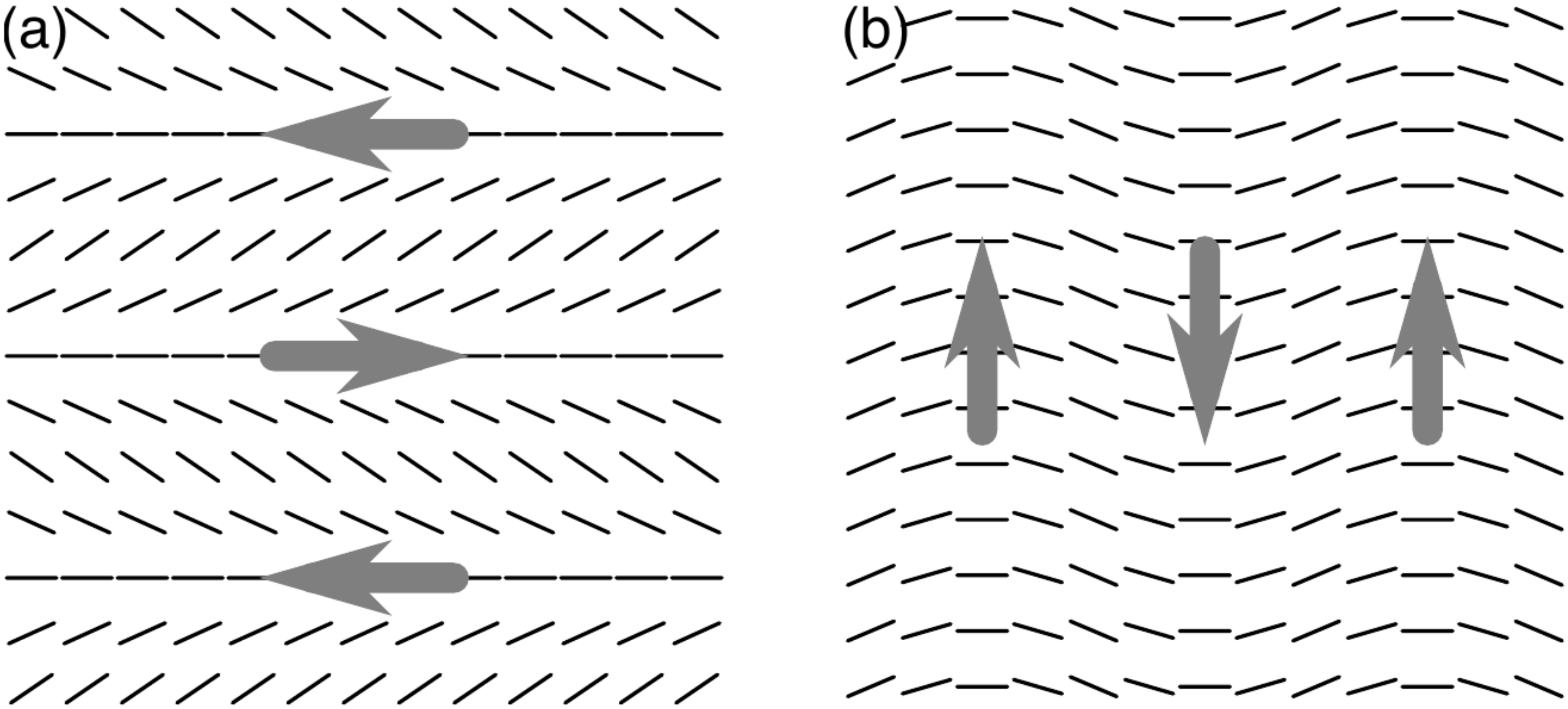
Assume Λ>0.
Add noise: angle fluctuations finite, long-range order.
Polar order crucial.
Nothing analogous for *apolar* case.

Maitra, Srivastava,
Marchetti, Lintuvuori,
Lenz, SR preprint 2017

Apolar active fluids



Angle field θ



Curvature actively produces flow

High activity --> always unstable?

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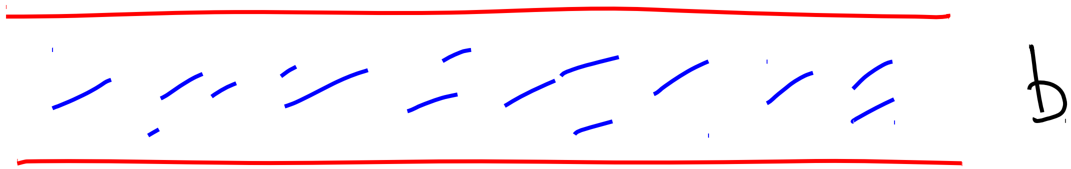
Confinement

SR and M. Rao, New J Phys 2007
Muhuri et al 2007 -- shear



$$\partial_t Q_{xz} = -\left[\frac{\alpha c_0 W_2}{q_x^2 + (\pi/b)^2} + K\right]\frac{q_x^2}{\eta} Q_{xz}$$

K = Frank elastic constant of underlying liq crystal

Length scale $\xi = (K/c_0 W_2)^{1/2}$; stable if $b < \xi$

Fix b, increase activity W_2: diffusive instability

Is that all?

$$\dot{\theta} = \frac{1-\lambda}{2}\partial_x v_y - \frac{1+\lambda}{2}\partial_y v_x - \Gamma_\theta \frac{\delta \mathcal{H}}{\delta \theta};$$

Passive and active forcing

$$\Gamma \mathbf{v} = -\nabla \Pi + \mathbf{f}^p + \mathbf{f}^a$$

$$\mathbf{f}^p = -\frac{1+\lambda}{2}\partial_y \left(\frac{\delta \mathcal{H}}{\delta \theta}\right)\hat{\mathbf{x}} + \frac{1-\lambda}{2}\partial_x \left(\frac{\delta \mathcal{H}}{\delta \theta}\right)\hat{\mathbf{y}}$$

$$f_x^a = -(\zeta_1 \Delta\mu + \underline{\zeta_2 \Delta\mu})\partial_y \theta$$

$$f_y^a = -(\zeta_1 \Delta\mu - \underline{\zeta_2 \Delta\mu})\partial_x \theta$$

NEW
Two-activity
constant
nematic

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Deriving from 3D active hydro

The second activity constant follows from bulk apolar active hydro
Apparently at higher order in gradients

$$\sigma_{ij} = \zeta_2 \Delta\mu [\nabla_j (Q_{km} \nabla_m Q_{ki}) + \nabla_i (Q_{km} \nabla_m Q_{kj})]$$

$$\eta \nabla^2 v_i = \zeta_2 \Delta\mu \nabla^2 (Q_{km} \nabla_m Q_{ki}) + \nabla_i \Pi$$

z-averaging

$$v_i = \frac{\zeta_2 \Delta\mu}{\eta} P_{ij} Q_{km} \nabla_m Q_{kj}$$

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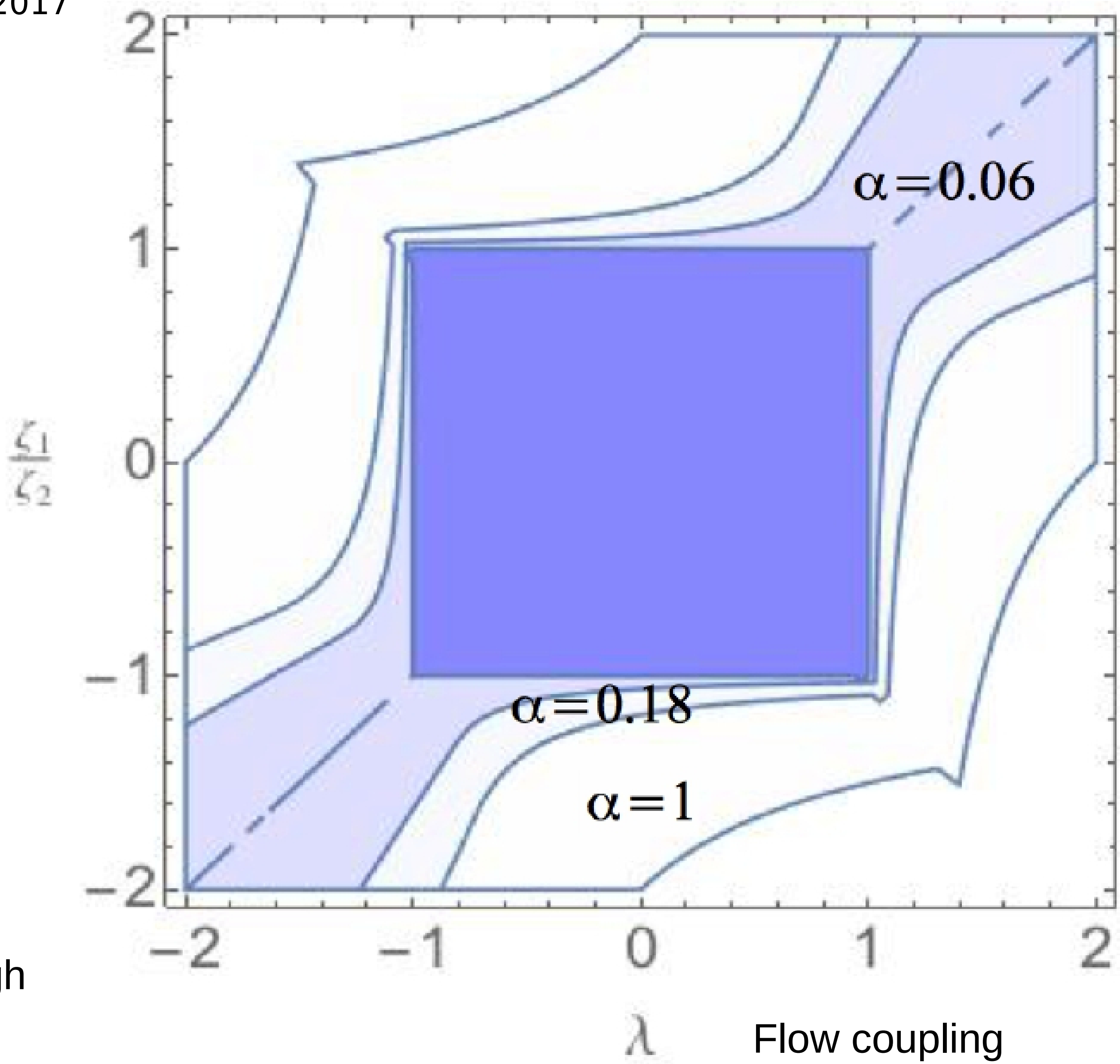

activity

Dark square stable for arbitrarily high activity

Flow coupling

Summary

- Active dynamics: forced equilibrium Langevin
  - apply to understand heat and work?

- Unifies all standard active dynamic models

- Confined active fluids
  - polar: super-stable or super-unstable
  - apolar: can be invulnerable to instability

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