BUGS, MOTORS, COPPER RODS AND BROWNIAN INCHWORMS

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KITP May 2006

Based on

- K Vijay Kumar, SR, Madan Rao, in preparation
- S Mishra and SR, cond-mat/0603051
- V Narayan, N Menon, SR, J. Stat. Mech. (2006) P01005
- Toner, Tu, SR, Ann. Phys. **318** (2005) 170
- Hatwalne, SR, Rao, Simha, Phys Rev Lett **92** (2004) 118101
- SR, R A Simha and J Toner, Europhys Lett **62** (2003) 196-202
- R A Simha Ph D thesis, IISc 2003
- R A Simha and SR, Phys Rev Lett **89** (2002) 058101

Support

- Centre for Condensed Matter Theory: Dept of Science and Technology, India
- Students: Council for Scientific and Industrial Research, India
- Collaboration: Indo-French Centre for the Promotion of Advanced Research

DIRECTED MOTION

Herds, bird flocks

Fish schools, bacteria

Crawling cells/fragments, treadmilling actin

Cell extracts: motors $+$ filaments

Rods on a vibrating surface

MY INTEREST

Collective behaviour of *many* moving things

Approach: nonequilibrium statistical mechanics

Drawn to questions of how *one* thing moves:
noise $\rightarrow$ directed motion

For this workshop: common features of treadmilling actin, translocating motors, granular arrowheads

TALK PLAN

- Background, systems of interest
  - What are active particles?
- Self-propelled suspensions, force dipoles
  - Rheological consequences of activity
- Active granular matter
  - Apolar vs polar; giant number fluctuations
- Force dipoles, tension and propulsion from noise
  - Brownian inchworms
- Conclusion and prospect

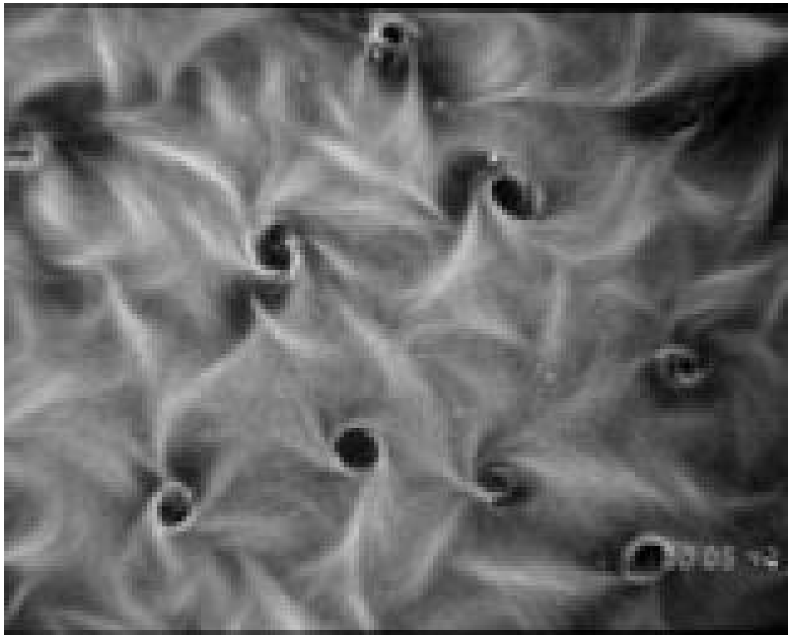
SYSTEMS OF INTEREST

Fish
liquid
crystals

http://fins.actwin.com/fish/marine-pics/anchovie.MOV

Active topological defects

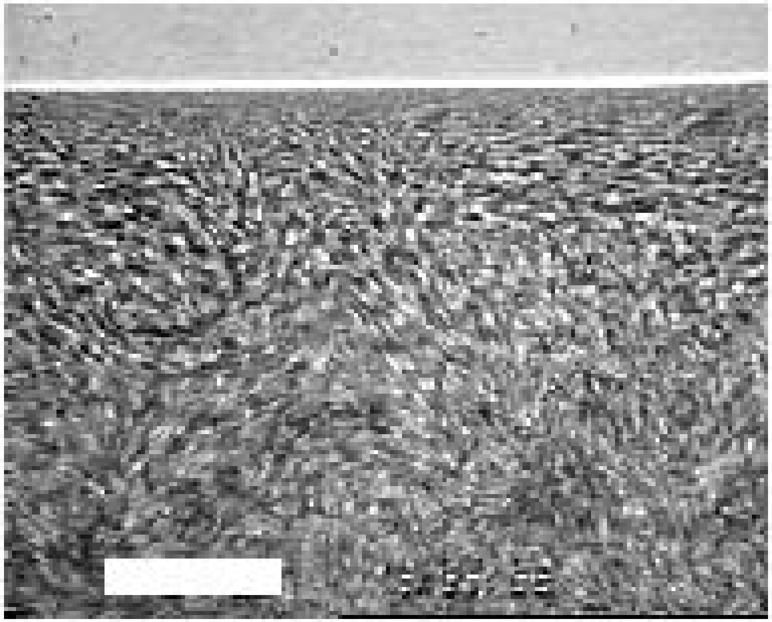
kinesin + microtubules
Nedelec et al. 1997



http://www.cytosim.org/others/princeton/

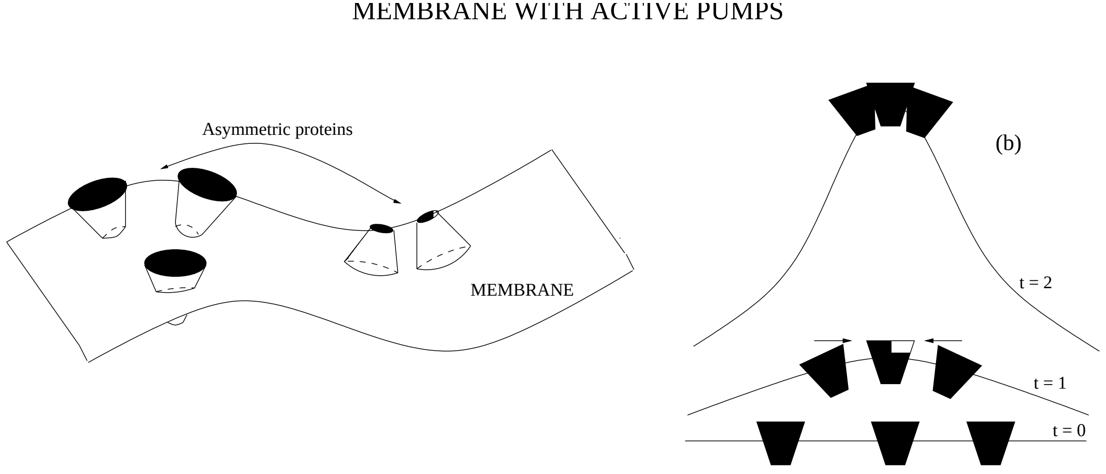
Order and instabilities in bacterial suspensions

Ott, Kessler, Goldstein
U. of Arizona
B. subtilis

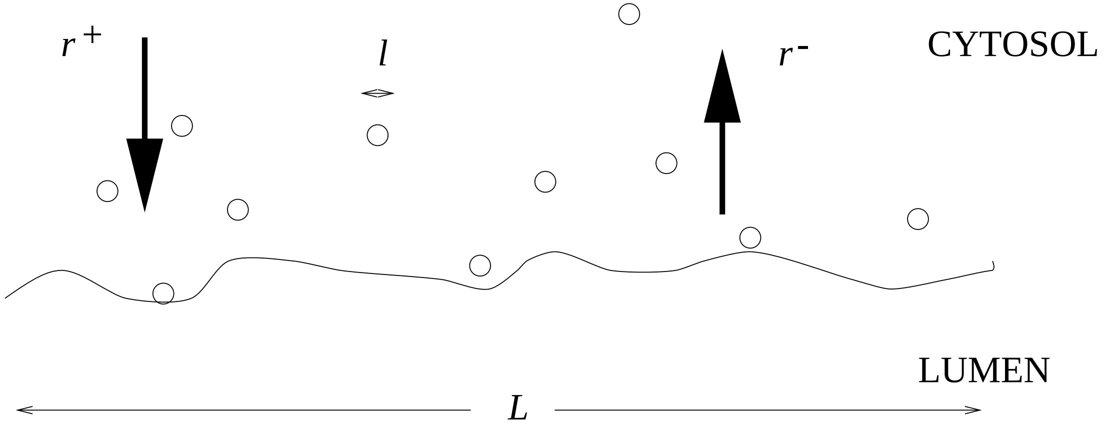


http://math.arizona.edu/ lega/UG/Colonies/Colonies.htm

Active membranes



Membranes
+ pumps
SR/Toner/Prost 2000
Bassereau *et al.* 2001

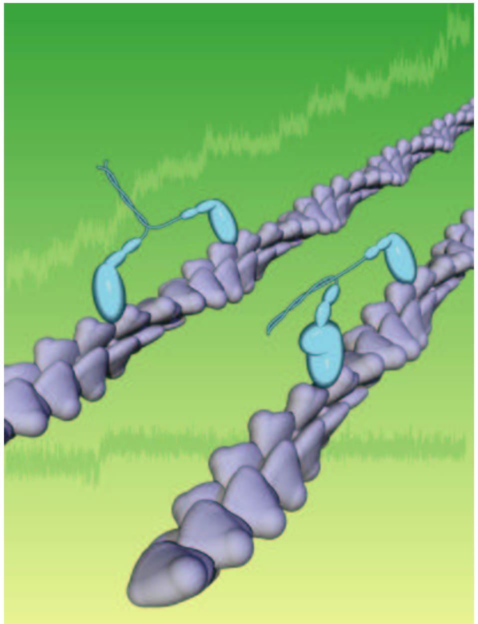


Active
fission-fusion
Sarasij/Rao 2001

C.R. Acad. Sci. Paris **2** (2001), Série IV, 817

Active filaments

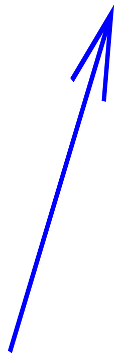
Actin-myosin (Spudich), treadmilling actin (Theriot), helicase (Schulten, Ha)



http://www.dictybase.org/tutorial/myosinassays.htm

http://cmgm.stanford.edu/theriot/movies.htm

Polar and apolar particles

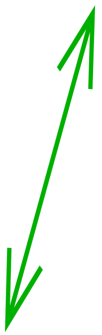


POLAR

FISH, BACTERIA

MOTOR−FILAMENT

fore-aft asymmetric



APOLAR

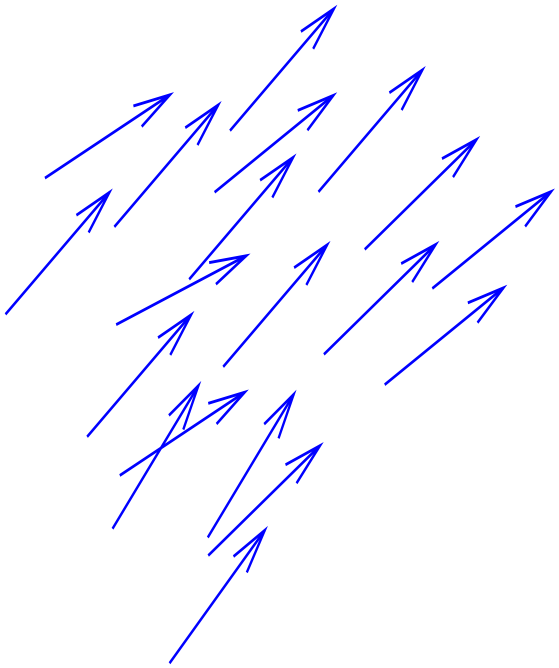
MELANOCYTES,

SYMMETRIC RODS,

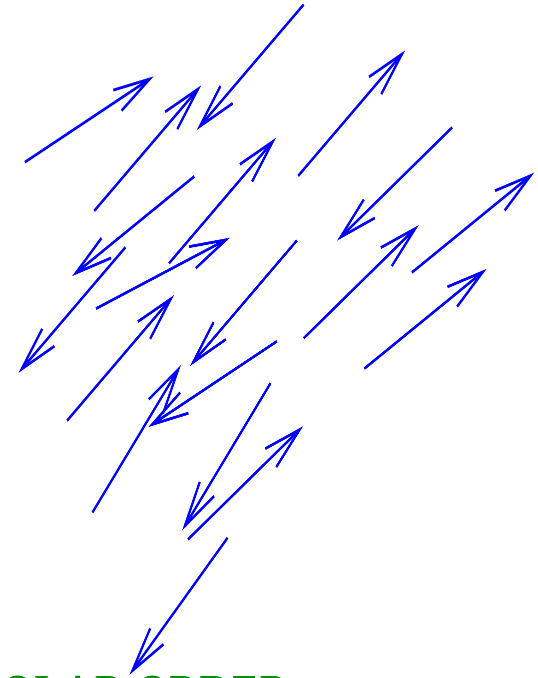
BUNDLES

symmetric

Polar and apolar order



POLAR ORDER



APOLAR ORDER

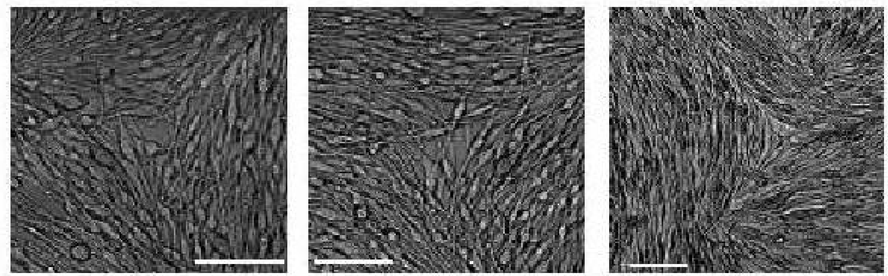
fore-aft asym particles

can order symmetrically

APOLAR active systems

Melanocyte aggregates Kemkemer *et al.* 2000

R. Kemkemer *et al.*: Elastic properties of nematoid arrangements formed by amoeboid cells 223



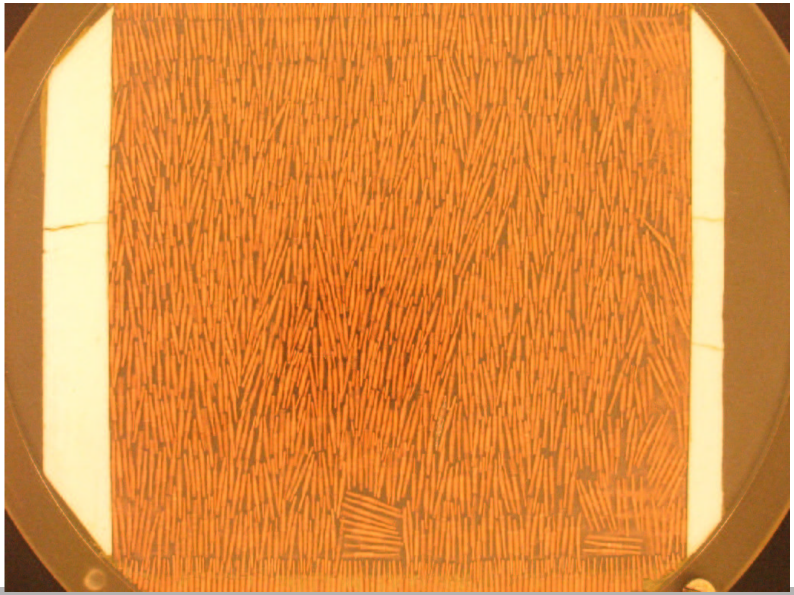
(a) (b) (c)

Fig. 8. A $m = -1/2$ disclination is shown for melanocytes. The bar is 100 μm. Different possibilities are shown: (a) the core of the disclination is an area free of cells. (b) The core of the disclination is an area with isotropically distributed cell. (c) The core of the disclination is occupied by a star-shaped cell. The cells which form the nematoid fluid are in an elongated bipolar state.

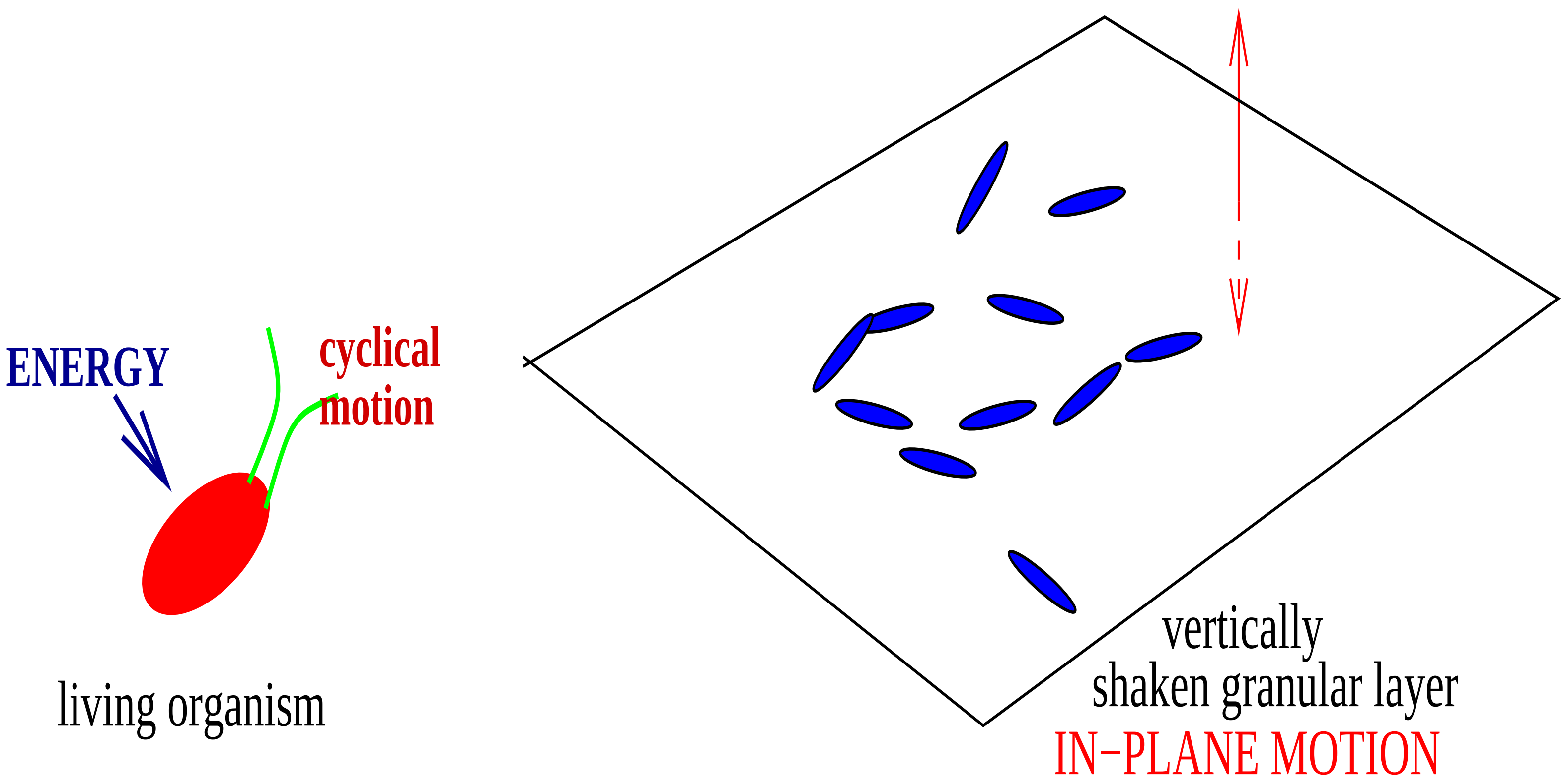
rotation

ordering

V Narayan, N Menon, SR



Active particle: working definition



Absorb and dissipate energy: nonequilibrium steady state

Motion self-directed

D. Chowdhury 2005, S. Sinha 2003, Ebeling *et al.* 2002

Common features of our systems

Self-driven, interacting, correlated, noisy

Orientable particles: ordering?

Fixed energy *throughput*, not budget

All particles forced independently, not from boundary

not like shear flow or $3d$ granular

SELF-PROPELLED SUSPENSIONS

Why do they form?
Mechanism of motion?

HARD

ASSUME in or near ordered state

EASIER

Response to disturbance?

Fluctuation statistics?

Hydrodynamic approach

Construct equations of motion for slow variables

Related: Lau, Lubensky PRL 2003, Kruse *et al.* PRL 2004

Our interest

Symmetry, conservation laws $\rightarrow$ coarse-grained eqns of motion

Nonequilibrium steady state; infer statistics from eqns of motion: no Gibbs distribution, no Onsager symmetry.

Focus: qualitative difference from dead Brownian particles

Earlier work

Reynolds 1987: computer graphics for movies

Vicsek et al 1995: simulations

Toner and Tu 1998: field theory – moving XY model

Only polar order: can't describe nematics

No fluid flow: misses physics of suspensions

Fluid dynamics literature (Lighthill, Pedley-Kessler): doesn't consider ordering

Results

Generic hydrodynamic eqns for active-particle systems

Ordered phases

- Travelling waves
- Giant number fluctuations, tails
- Ordered low-Re swimmers always break up into finite domains (expts)

Isotropic phase: novel rheology; nonequilibrium noise

- Increase correlations $\rightarrow$ stiffen or soften
- activity $\rightarrow$ giant noise-temperature, tails

HOW?

Hydrodynamic approach; slow variables

Active-particle concentration $c(\mathbf{x}, t)$

Momentum density of particles $+$ fluid $\mathbf{g}(\mathbf{x}, t) = \rho\mathbf{u}$

$\mathbf{u} =$ hydrodynamic velocity field

Incompressible: $\rho =$ constant; $\nabla \cdot \mathbf{u} = 0$

Polar order parameter: active-particle velocity relative to solvent: $\mathbf{v}(\mathbf{x}, t)$

Simha and SR PRL 2002

See also Kruse *et al.* “active gels” PRL 2004

Building equations of motion

Number conservation: $\partial_t c = -\nabla \cdot \mathbf{J}$

Newton II: $\partial_t \mathbf{g} = -\nabla \cdot \boldsymbol{\sigma} + \mathbf{F}_{ext}$

Order-parameter: $\partial_t \mathbf{v} =$ Forces and Torques

Express $\boldsymbol{\sigma}$, $\mathbf{J}$, forces and torques in terms of slow variables.

Easiest: concentration equation

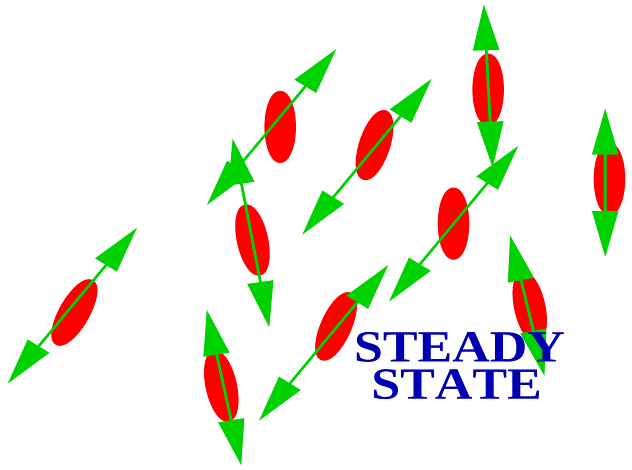
$$\partial_t c = -\nabla \cdot \mathbf{J}$$

$$\mathbf{J} = c(\mathbf{v} + \mathbf{u})$$

$\mathbf{v}$ is velocity *relative* to medium

Galilean invariance of particles $+$ fluid

Momentum equation



Activity: internal forces: Total momentum (particles + solvent) conserved

$$\partial_t \mathbf{g} \equiv \partial_t(\rho \mathbf{u}) = -\nabla \cdot \boldsymbol{\sigma}$$

$$\underline{\underline{\sigma}} = -\eta \nabla \mathbf{u} + p\mathbf{I} + \boldsymbol{\sigma}^a$$

viscosity pressure activity

Modelling active stresses

Guess (symmetry permits)

$$\boldsymbol{\sigma}^{a}_{ij}(\mathbf{x}, t) \propto c v_i v_j$$

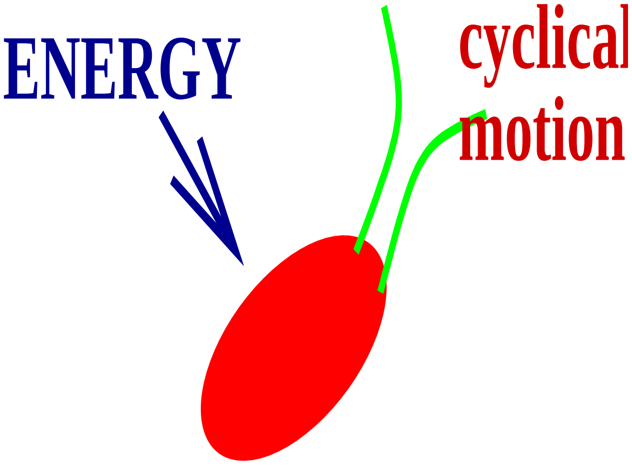
because of noneq activity

CONTRAST: for *thermal equilibrium* uniaxial phase

structure anisotropic, mean stress isotropic

More microscopically:

One active particle



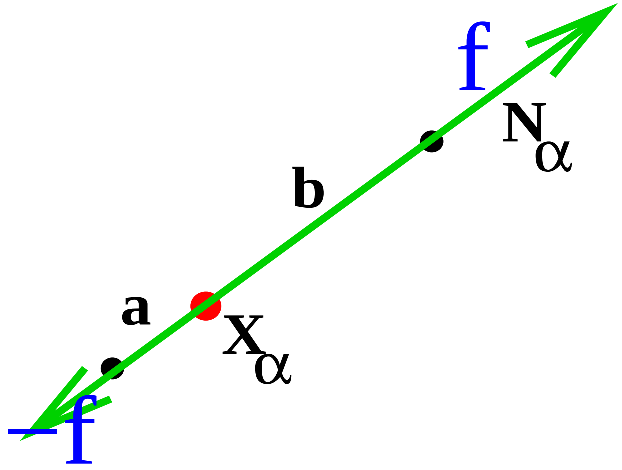
$$F_{ptcl-med} = -F_{med-ptcl}$$

Force-density has zero monopole moment

Active particle = permanent force dipole

Brennen and Winet 1977

Force dipole model: movers and shakers



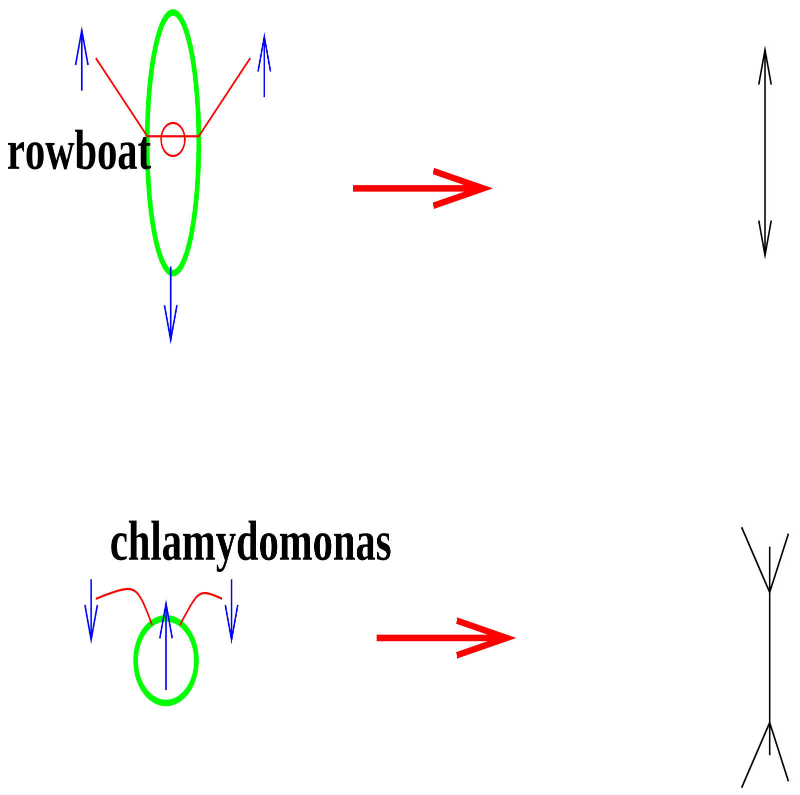
Point forces, equal magnitude, opposite direction

$a \neq b$: mover (polar, vectorial); velocity $\mathbf{v}_\alpha = v_0 \mathbf{N}_\alpha$

$a = b$: shaker (apolar, nematic); velocity $= 0$

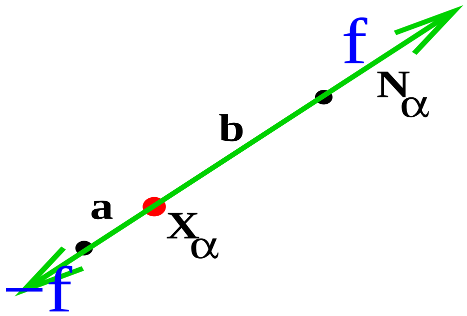
Coarse-grain: $\mathbf{v}_\alpha \to \mathbf{v}(\mathbf{x}, t)$; $\mathbf{v}_\alpha \mathbf{v}_\alpha - \frac{1}{3} v_\alpha^2 \to \mathbf{Q}(\mathbf{x}, t)$

Examples



steady-state activity $\leftrightarrow$ permanent force dipoles

$$\sigma^a = K\mathbf{Q};\ \text{sgn}(K)?$$



Force density $= \rightarrow (a+b) f \nabla \cdot c\mathbf{Q} + (a-b) f \mathrm{O}(\nabla\nabla)$

in continuum limit

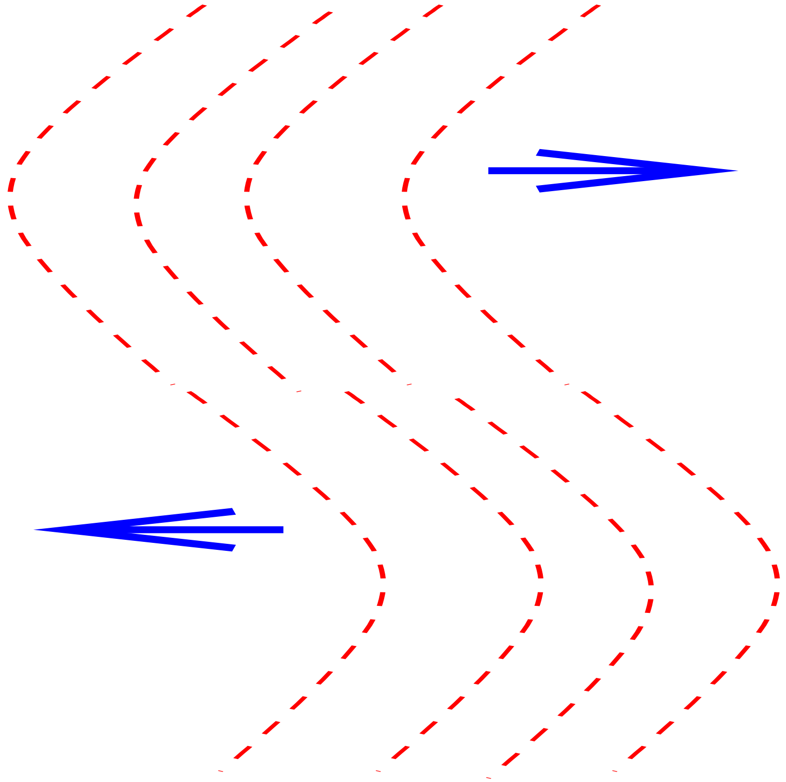
c = local concentration

$\mathbf{Q} \sim \mathbf{vv}$ = local alignment tensor

Simha and SR PRL 2002

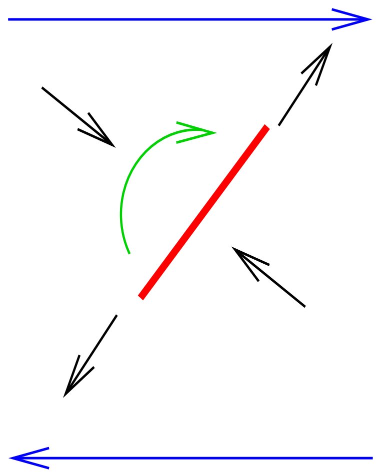
Motor-filament calculation: Liverpool and Marchetti 2006

Consequences



Driven state: curvature (asymmetry) $\rightarrow$ flow (Curie)

Polar order-parameter dynamics



$$\dot{\mathbf{v}} \sim +(\nabla \mathbf{u}\,\mathbf{v}) + \alpha \mathbf{v} - \beta |\mathbf{v}|^2 \mathbf{v} - \nabla(c\mathbf{Q}) + O(\nabla\nabla\mathbf{v}) + \cdot^{\cdot^{\cdot}}$$

advection speed limit stress elasticity

Toner-Tu $+$ fluid flow

Flow rotates orientation

Bacteria: stokesian limit

Include viscosity, ignore inertia

Viscous forces balance active forces

$$-\eta\nabla^2\mathbf{u}_\perp \sim \partial_z\delta\mathbf{n}_\perp - \nabla c + \ldots$$

$$\partial_t c \sim -\partial_z c - \nabla\cdot\delta\mathbf{n}_\perp + \ldots$$

$$\partial_t\delta\mathbf{n}_\perp \sim \partial_z\mathbf{u}_\perp + \nabla_\perp c + \ldots$$

$\Rightarrow$ Effective eqn of motion

$$(\partial_t + v_0\partial_z)\delta\mathbf{n}_\perp \sim \tau^{-1}\cos 2\theta\delta\mathbf{n}_\perp$$

Instability near 45°!

Numbers?

$\tau \sim \eta / a c_0 f \sim$ .1 sec

$a =$ particle size, $c_0 =$ mean conc., f = active force

Convective instability for Re $\ll qa \ll 1$

$q =$ wavenumber

Relevant regime for bacteria

Only *finite-scale* ordered domains!

Simha and SR PRL 2002

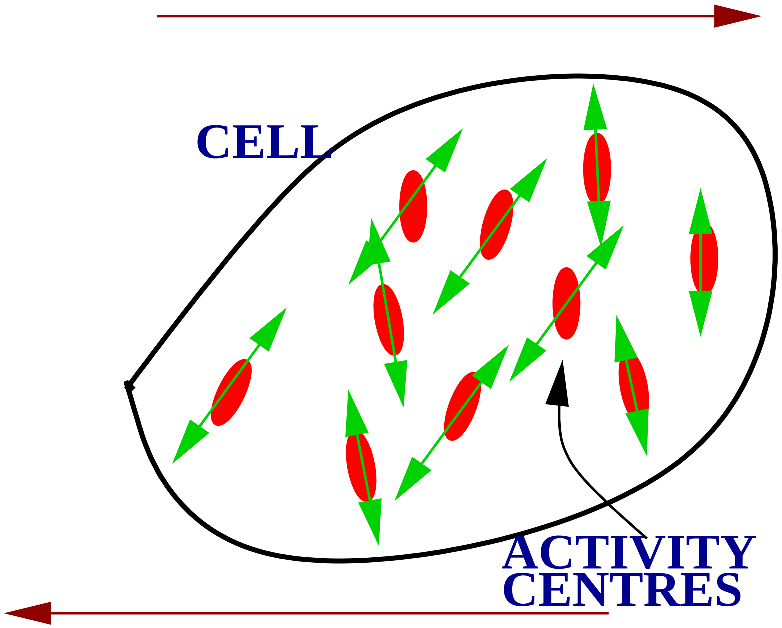
Experiments? Dombrowski *et al.* PRL 2004

Effect of shear (S Muhuri, Raman Instt)

Instabilities in film flow: SR in preparation

Isotropic phase: active rheology

Y Hatwalne, S.R., M Rao, R A Simha PRL **98** (2004) 118101

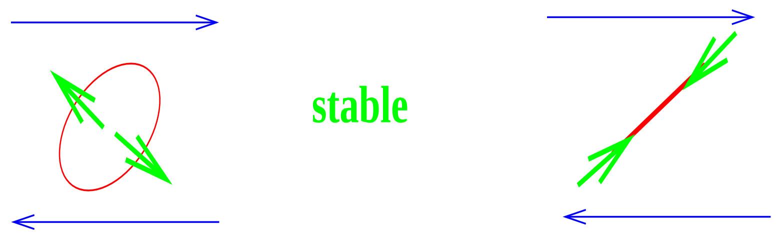


$$\frac{\text{stress}}{\text{strain}} \equiv \frac{\sigma(\omega)}{\epsilon(\omega)} = G^{*}(\epsilon,\omega) = G^{*}_{struc} + G^{*}_{activ}$$

Liverpool et al 2001 (polymers) Liverpool-Marchetti, Fabry *et al.*, Lau, Lubensky

Shape and activity

Assume flow-aligning



SHEAR -- ORIENTED ACTIVITY

ACTIVITY -- REDUCES FLOW

SHEAR -- ORIENTED ACTIVITY

ACTIVITY ENHANCES FLOW

Active viscoelasticity

In general $\rightarrow \partial_t \mathbf{Q} + \tau^{-1}\mathbf{Q} \sim \nabla \mathbf{u}$

relaxation, coupling to flow

Active:

$\partial_t \sigma^a + \tau^{-1}\sigma^a \sim K\dot{\epsilon}$ (shear-rate)

$$G'_{activ} \sim K \frac{(\omega\tau)^2}{1+(\omega\tau)^2}$$

Strong viscoelasticity if $K > 0$; strong softening if $K < 0$. This plus instability: fragile jammed matter à la Cates (SR + M Rao 2006)?

Not like equilibrium

Contrast: equilibrium systems near orientational ordering transitions:

$\sigma \sim \frac{\delta F}{\delta \mathbf{Q}}$ (field conjugate to **Q**; $\rightarrow 0$ at transition) $\sim T - T_*$

$G'_{passive} \sim \frac{\omega^2 \tau}{1+(\omega\tau)^2}$

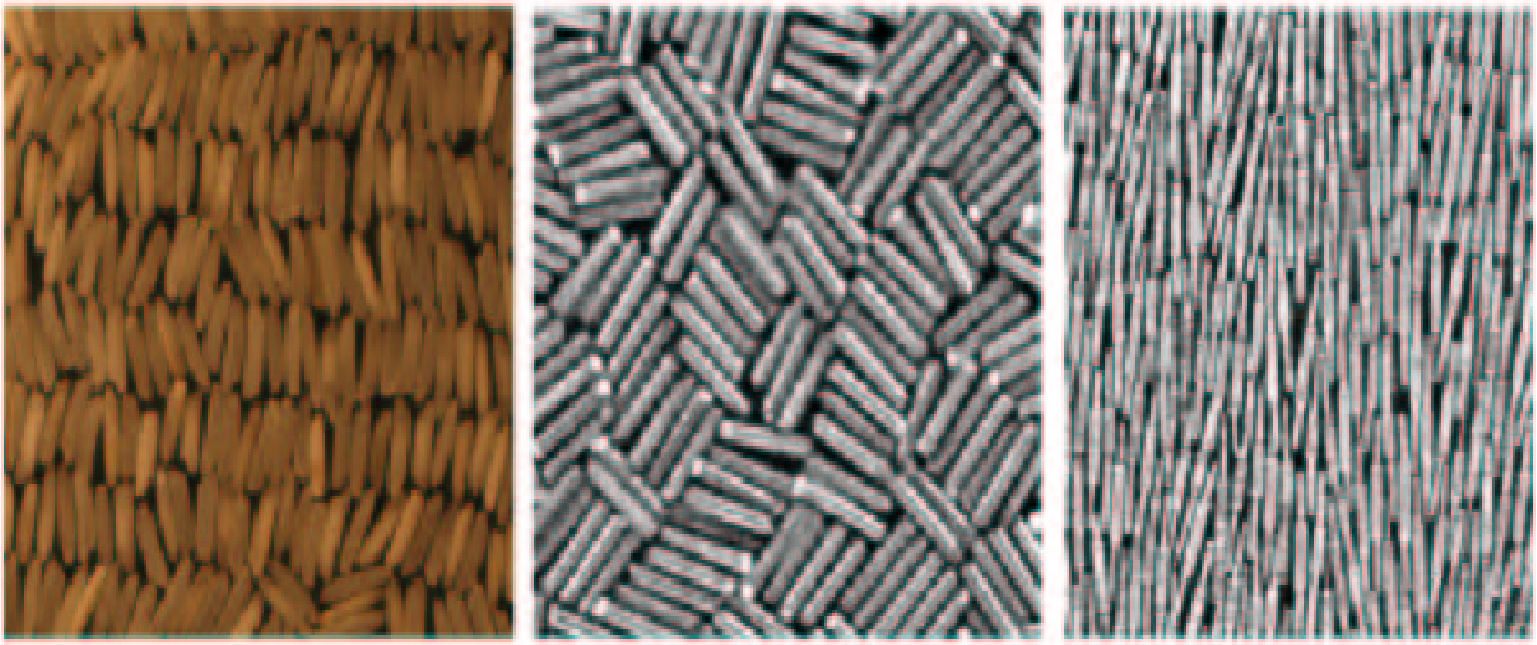
All effects discussed on previous slide $\rightarrow 0$ as system approaches ordering transition

Isotropic phase

Wu-Libchaber, Soni *et al.* – bacterial swimming

- Active stresses: noise source for dynamics of fluid velocity
- Estimate T_{eff} from variance of $\boldsymbol{\sigma}^a$
- Find $10^5 - 10^6$ Kelvin, similar to Wu-Libchaber bacterial water-polo

Narayan et al. J Stat Mech 2005

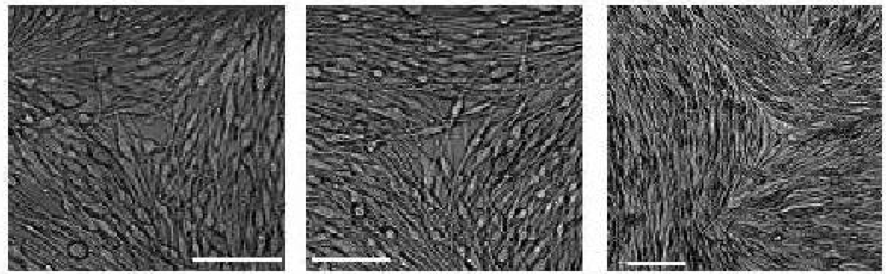


Basmati: smectic?
flat tip: tetratic?
tapered: nematic

Other apolar active systems

Melanocyte aggregates Kemkemer *et al.* 2000

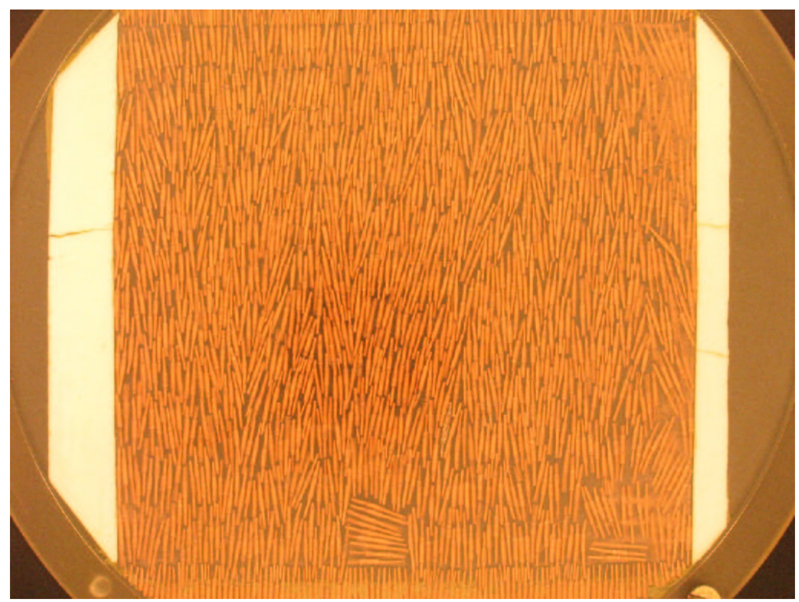
R. Kemkemer *et al.*: Elastic properties of nematoid arrangements formed by amoeboid cells 223



(a) (b) (c)

Fig. 8. A $m = -1/2$ disclination is shown for melanocytes. The bar is 100 μm. Different possibilities are shown: (a) the core of the disclination is an area free of cells. (b) The core of the disclination is an area with isotropically distributed cell. (c) The core of the disclination is occupied by a star-shaped cell. The cells which form the nematoid fluid are in an elongated bipolar state.

rod monolayer
V Narayan, N Menon, SR



Shaken monolayers of rods

Blair, Neicu and Kudrolli 2003, Galanis *et al.* 2005, Fraden 2005

V Narayan, N Menon, SR 2006

rod swirls

polar rods move

Driven steady state

Not thermal equilibrium

Don't have Boltzmann-Gibbs

Must construct equations of motion by "pure thought"

Infer statistics from dynamics

Active nematics: different

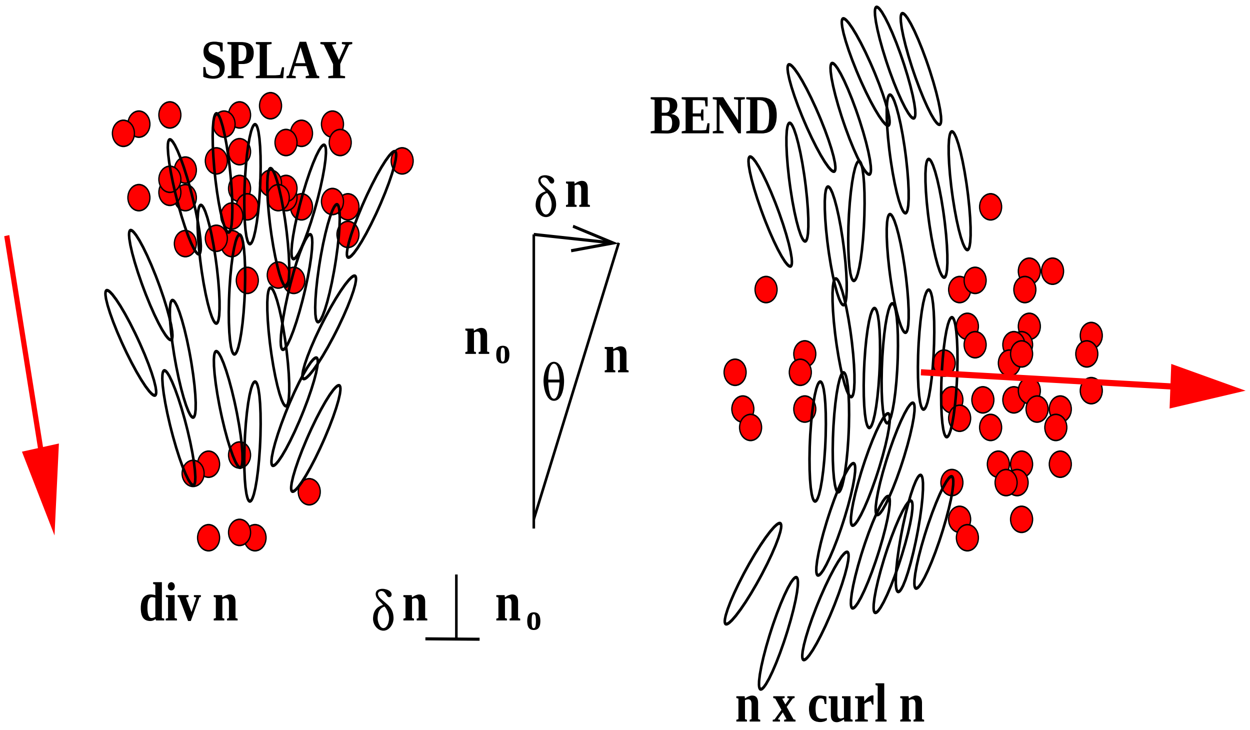
True nematic order: fore-aft symmetric, mean velocity zero
Just like equilibrium nematic? Effective temperature?

Variables:

Concentration c, 1 order parameter fluctuation $\delta \mathbf{n}_\perp$

Ignore velocities
Substrate: momentum sink

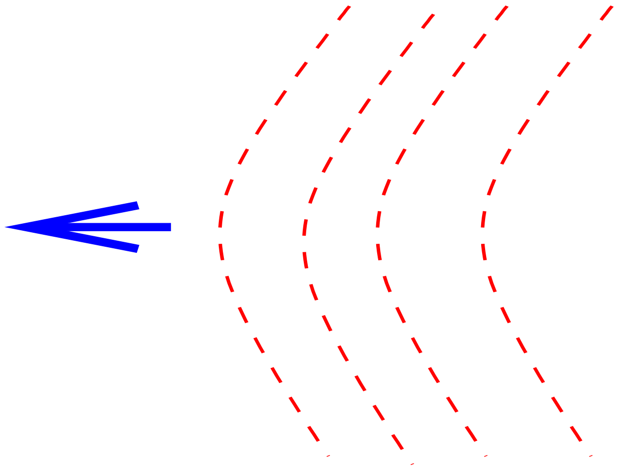
Splay or bend → current



ASYMMETRY LEADS TO CURRENT

$$J_x \propto \partial_z \theta \qquad J_z \propto \partial_x \theta$$

Curvature $\rightarrow$ current



$$\mathbf{J}^{(a)} \propto \nabla \cdot \mathbf{Q}$$

Curvature $\Rightarrow$ left-right asymmetry $\Rightarrow$ current

Giant number fluctuations

Recall

$$\langle (\delta\theta)^2 \rangle \sim \frac{T}{K} \ln \frac{L}{a}$$

and

Flux $\propto \delta\theta$

Thus concentration fluctuation (almost) indep of L.
Hence $\delta N_{rms} \propto N$.

Cf. particles sliding down fluctuating surface
Das-Barma-Majumdar, Drossel-Kardar

Not an effective temperature

Note:

$$\langle |c(\mathbf{q})|^2 \rangle \sim q^{-2}$$

system size $L \Rightarrow \langle (\delta N)^2 \rangle / N \propto L^2 \propto N^{2/d}$

$d = 2$: standard deviation $\propto$ mean!

$$\langle \delta c(x,0) \delta c(x,t) \rangle \sim \ln(1/t)$$

None of this can be described by effective temperature

Phase separation?

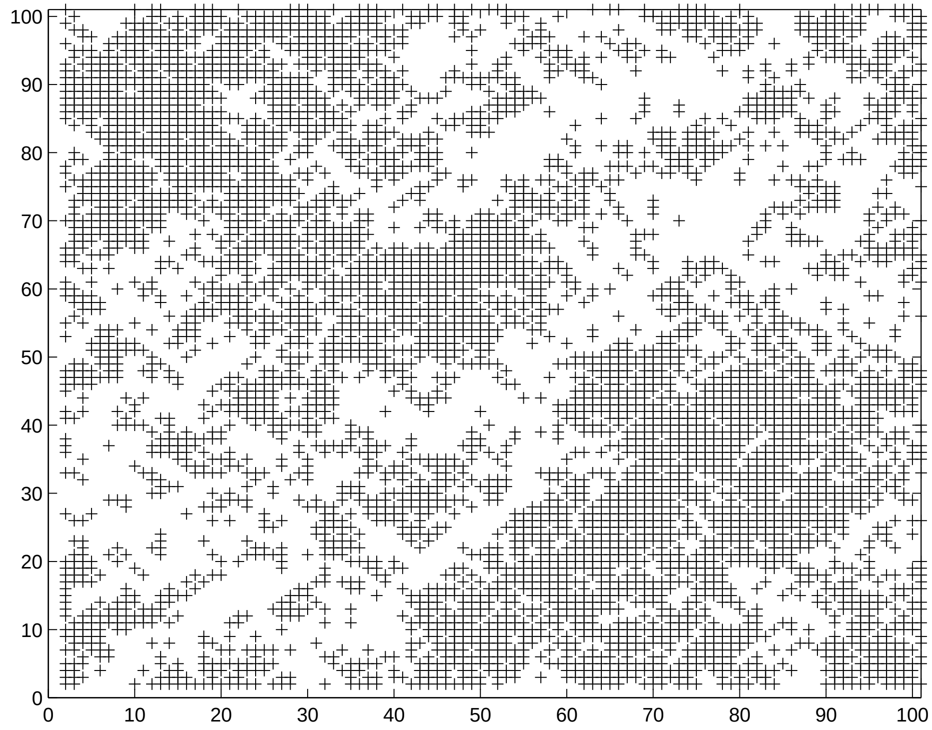
Simulation: Mishra and SR cond-mat/0603051 — particles actively advected by nematic fluctuations
Uniform distribution $\rightarrow$ coarsening:

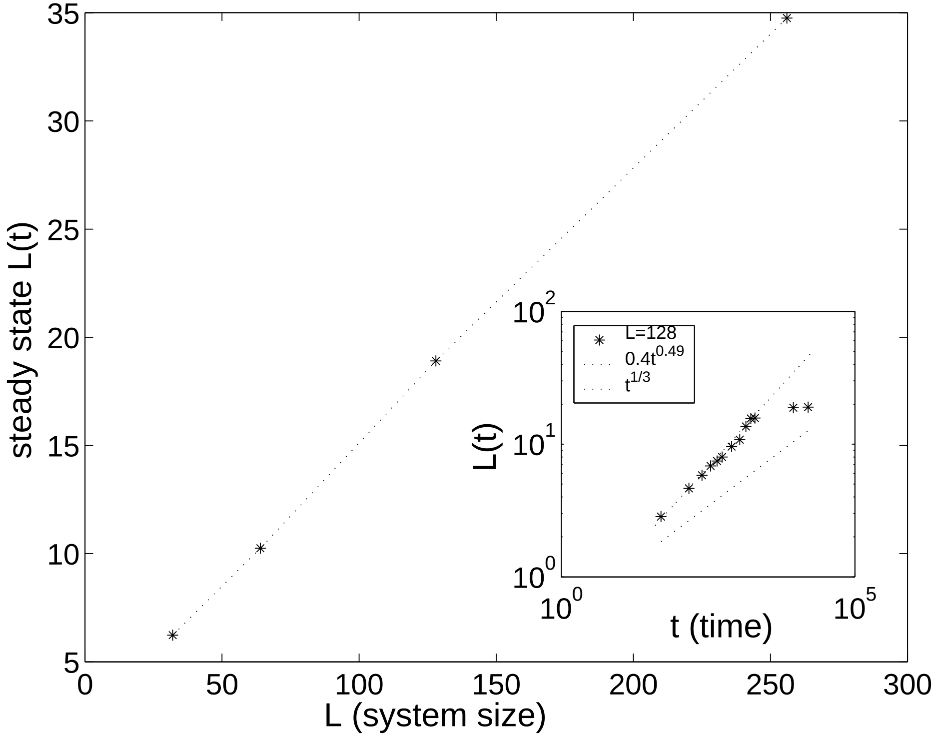
fluctuation dominated phase separation
Das, Barma, Majumdar 2000

Chaté *et al.* PRL 2006: independent confirmation in computer experiment

Experiments on biological systems?

Shradha's results



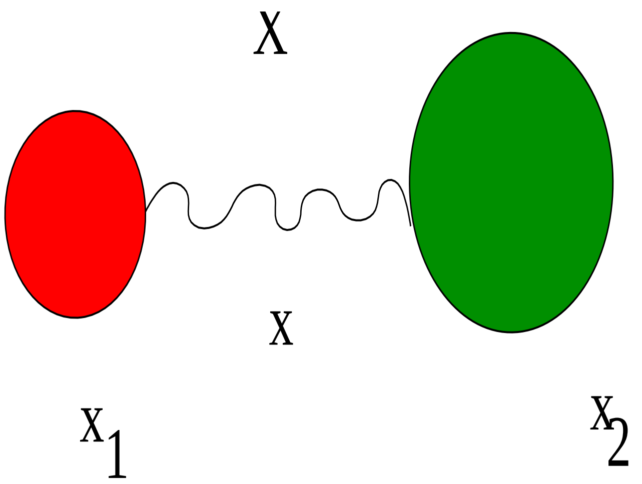


A BROWNIAN INCHWORM

Turn noise into directed motion?

No substrate sawtooth potential?

Build a moving dimer: K Vijay Kumar and M Rao



Equations of motion

$$m_i\ddot{x}_i + \zeta_i\dot{x}_i = -\partial_i U(x) + f_i$$

x, X = relative and C of M coordinates

$$\langle f_i(0) f_j(t)\rangle = A_i\delta_{ij}\delta(t)$$

Only ζ_1 depends on x, ζ_2, A_1, A_2 don't.

U symmetric, ζ_1 asymmetric, or vice versa $\rightarrow$ drift of X.

The Brownian inchworm

one moving dimer

Features

Clear analogy to Ha-Schulten 2006

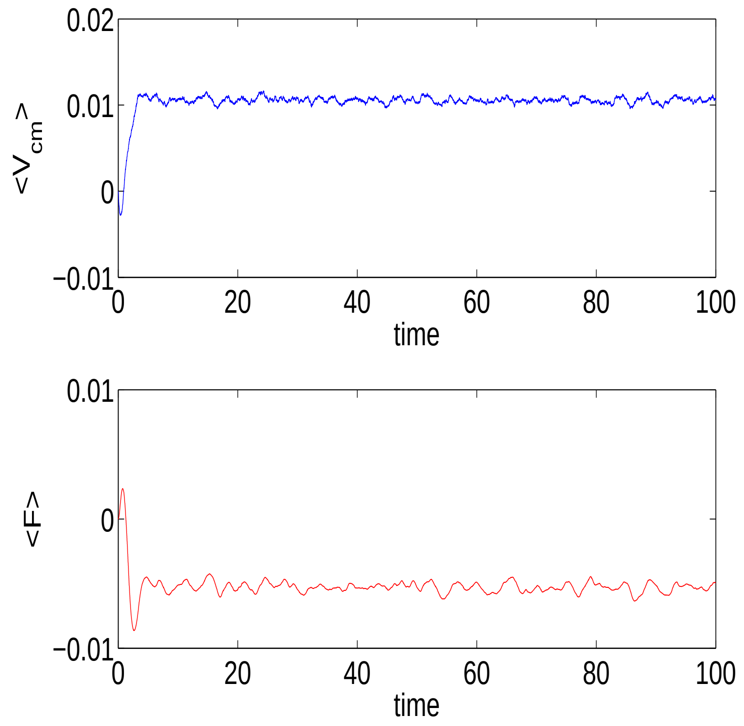
Relate their parameters to these?

Restoring equilibrium: $A_1 \propto \sqrt{\zeta_1}$ kills drift

In noneq steady state, $\langle \partial_1 U \rangle \neq 0$

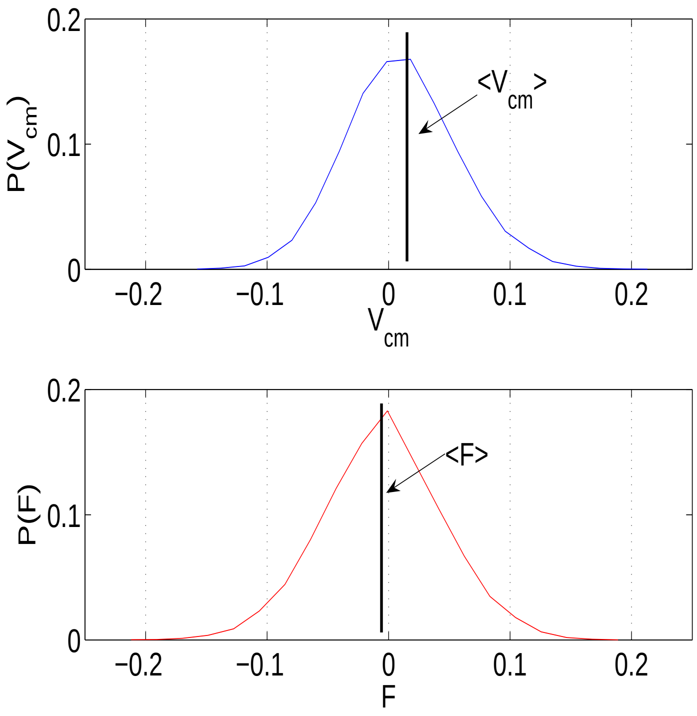
Velocity and force time-series

Asymmetric damping, harmonic $U(x)$, no FDT



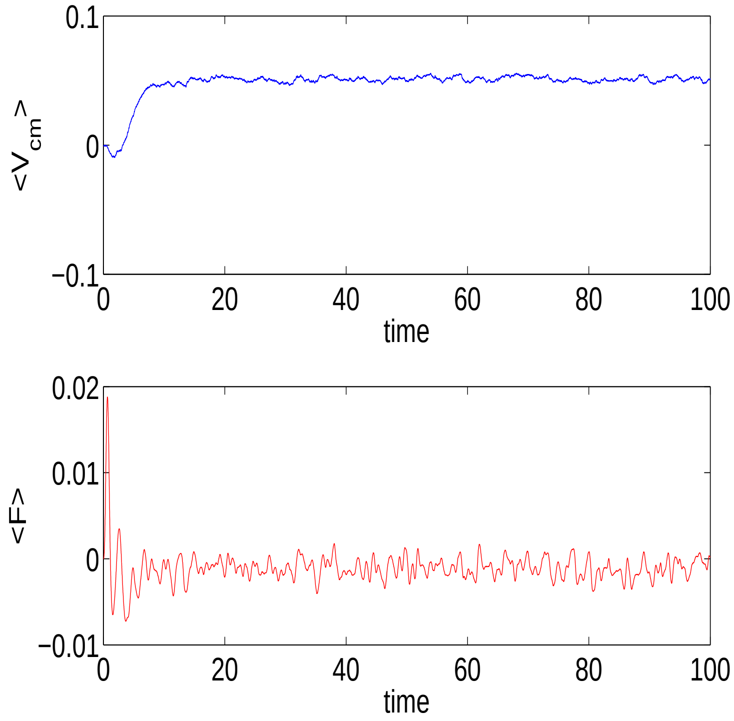
Probability distributions

Asymmetric damping, harmonic $U(x)$, no FDT



Velocity and force time-series

Symmetric damping, noncentrosym $U(x)$, no FDT



Probability distributions

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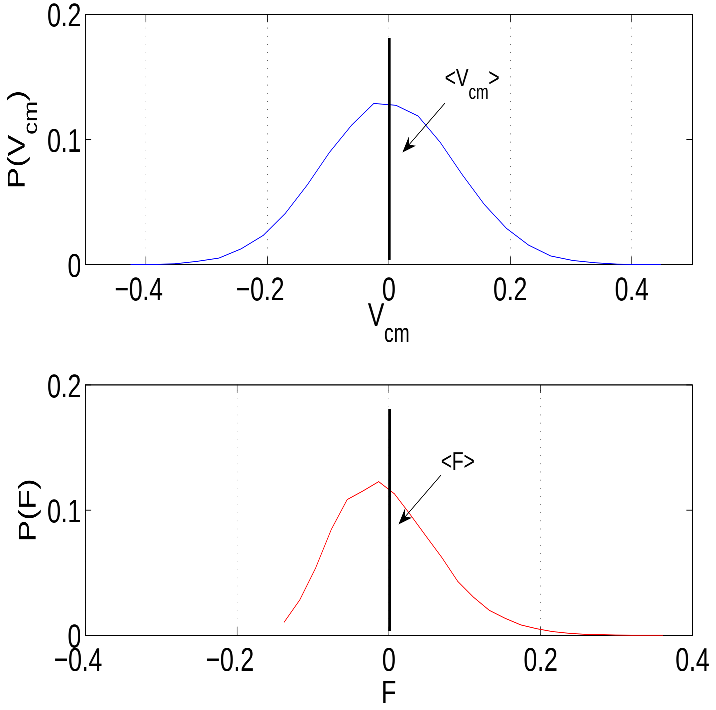
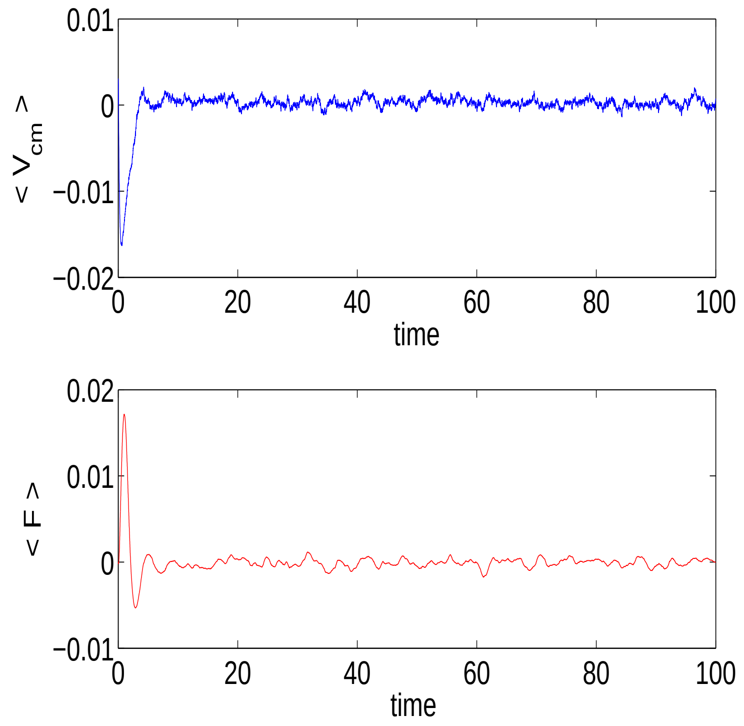


Velocity and force time-series

Asymmetric damping, harmonic $U(x)$, with FDT



Probability distributions

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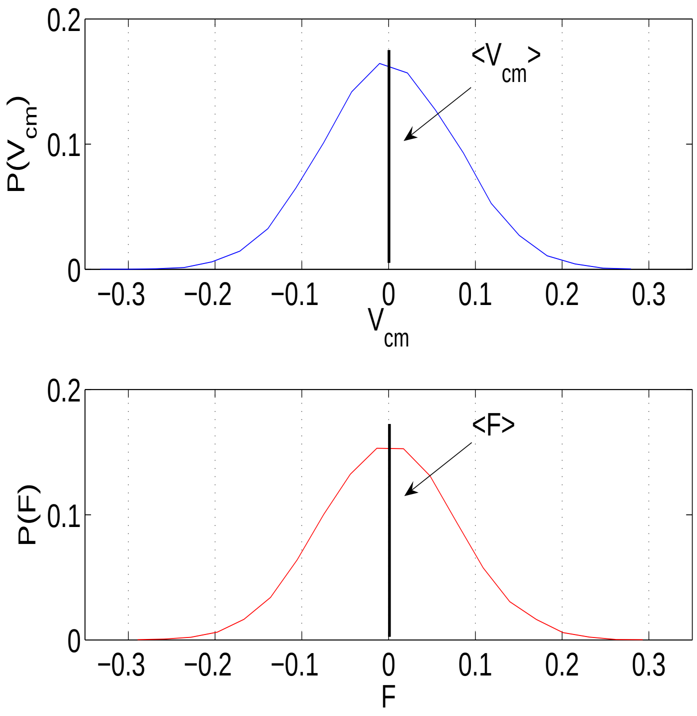

Dynamics of the distribution

distributions from an ensemble: equil vs noneq

Features

Thus: steady state tension, spontaneous motion, force dipole

Can interpret x as length of actin treadmill, tilt of polar granular rod

Many obvious generalisations: collections of inchworms, longitudinal or transverse chain, immerse in fluid etc.

CONCLUSION AND THE FUTURE

- Framework for mechanics of living soft matter
- Ordered phases
  - Orientational order $\rightarrow$ shear rigidity, waves
  - Giant number fluctuations, long-time tails
  - Long-ranged order unstable for low Reynolds no.
- Isotropic phase
  - Active shear-thickening of contractile filaments
  - Giant noise-temperature as in bacteria experiments
- Rod monolayers: promising analogue
- Simple Brownian inchworm model for individual active particles