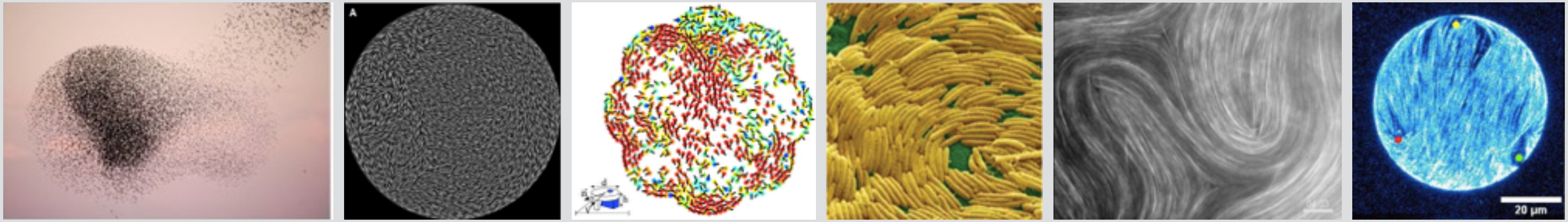
MA999: From Equilibrium to Extreme Events and Life

ACTIVE MATTER

Gareth Alexander



SUGGESTED PAPERS

General overview (theory)

Ramaswamy, The Mechanics and Statistics of Active Matter, Annu Rev Condens Matter Phys **1**, 323 (2010)

Ramaswamy, Active Matter, J Stat Mech 054002 (2017)

Active nematics

Doostmohammadi *et al*., Active nematics, Nature Comm **9**, 3246 (2018)

Sanchez *et al*., Spontaneous motion in hierarchically assembled active matter, Nature **491**, 431 (2012)

Keber *et al*., Topology and dynamics of active nematic vesicles, Science **345**, 1135 (2014)

Beng Saw *et al*., Topological defects in epithelia govern cell death and extrusion, Nature **544**, 212 (2017)

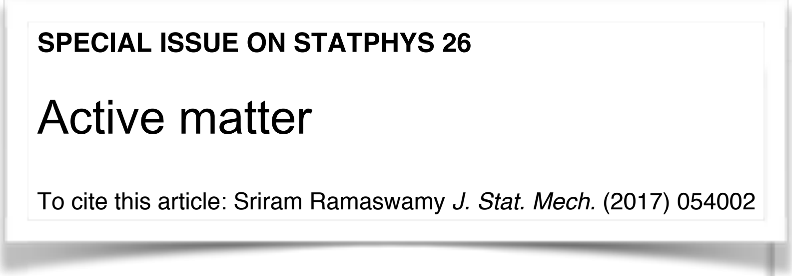
Cells, tissues

Prost, Jülicher & Joanny, Active gel physics, Nature Phys **11**, 111 (2015)

Active Brownian particles

Cates & Tailleur, Motility-Induced Phase Separation, Annu Rev Condens Matter Phys **6**, 219 (2015)

What is Active Matter?



SPECIAL ISSUE ON STATPHYS 26

Active matter

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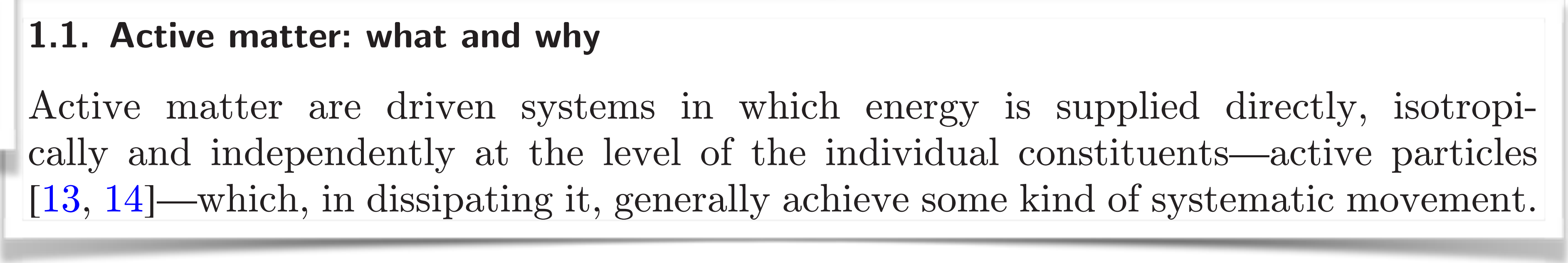


1.1. Active matter: what and why

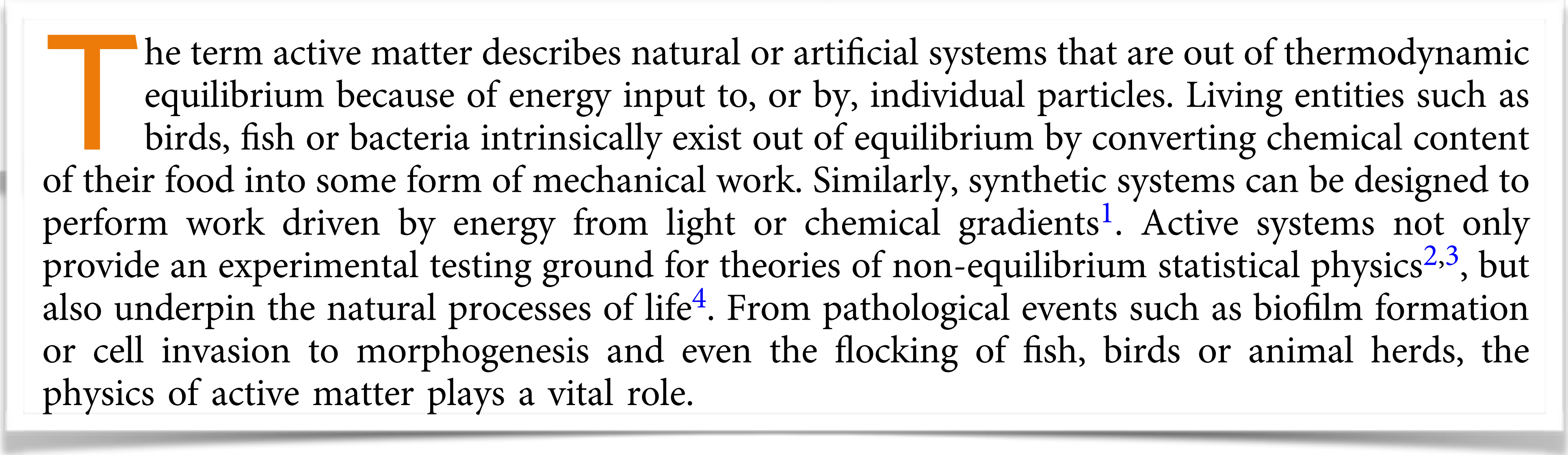
Active matter are driven systems in which energy is supplied directly, isotropically and independently at the level of the individual constituents—active particles [13, 14]—which, in dissipating it, generally achieve some kind of systematic movement.

REVIEW ARTICLE

DOI: 10.1038/s41467-018-05666-8 OPEN

Active nematics

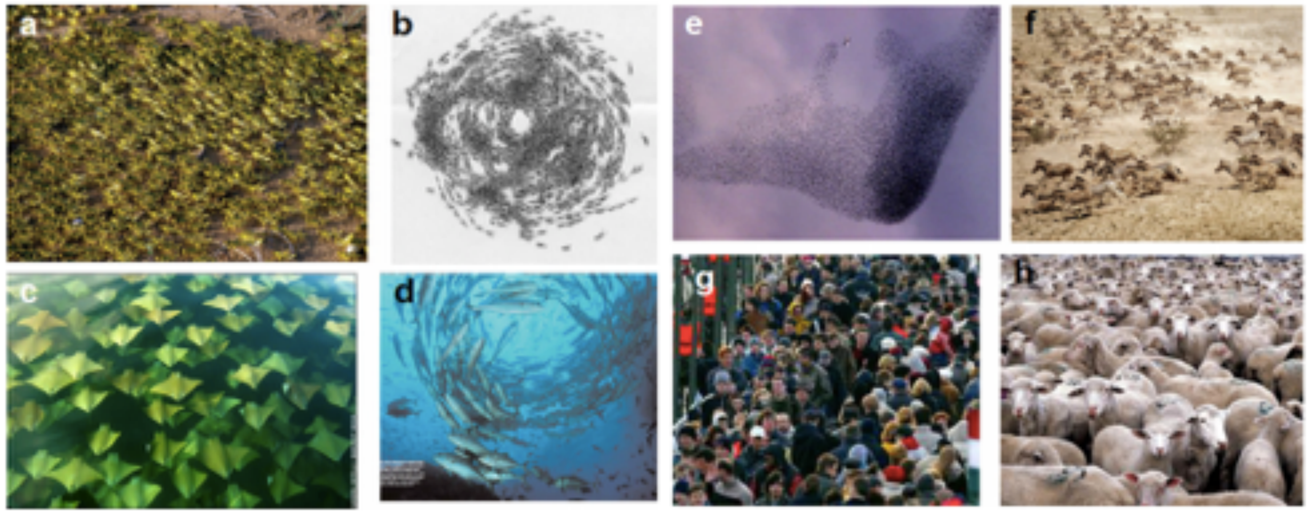
Amin Doostmohammadi[1], Jordi Ignés-Mullol[2], Julia M. Yeomans[1] & Francesc Sagués[2]



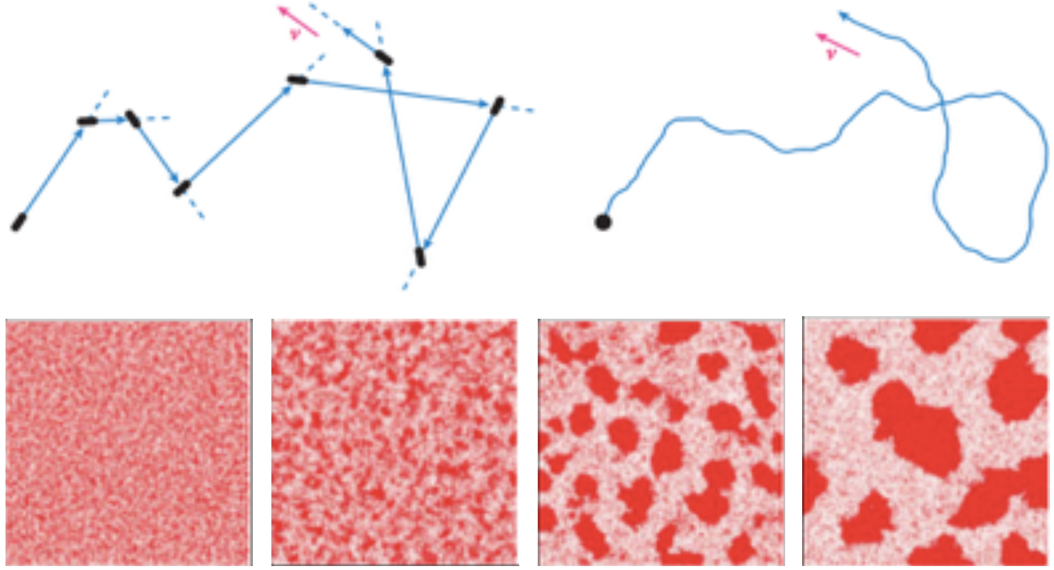
The term active matter describes natural or artificial systems that are out of thermodynamic equilibrium because of energy input to, or by, individual particles. Living entities such as birds, fish or bacteria intrinsically exist out of equilibrium by converting chemical content of their food into some form of mechanical work. Similarly, synthetic systems can be designed to perform work driven by energy from light or chemical gradients[1]. Active systems not only provide an experimental testing ground for theories of non-equilibrium statistical physics[2,3], but also underpin the natural processes of life[4]. From pathological events such as biofilm formation or cell invasion to morphogenesis and even the flocking of fish, birds or animal herds, the physics of active matter plays a vital role.

WHAT IS ACTIVE MATTER?

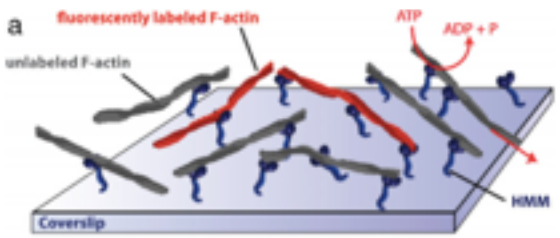
flocking, collective motion

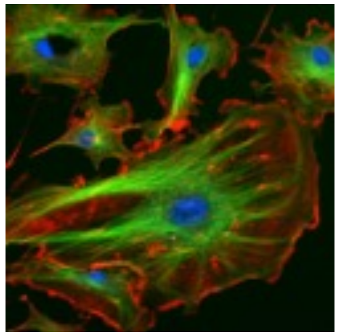


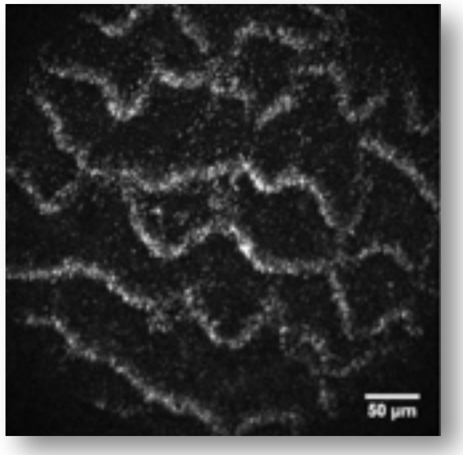
mips, active Brownian particles

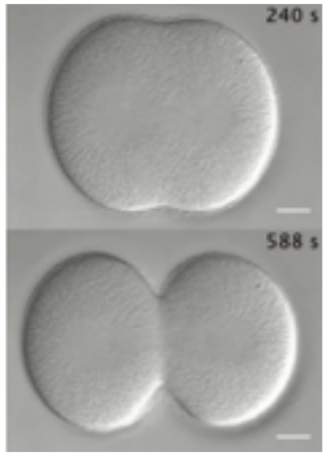


motility assays, cell cytoskeleton, tissues

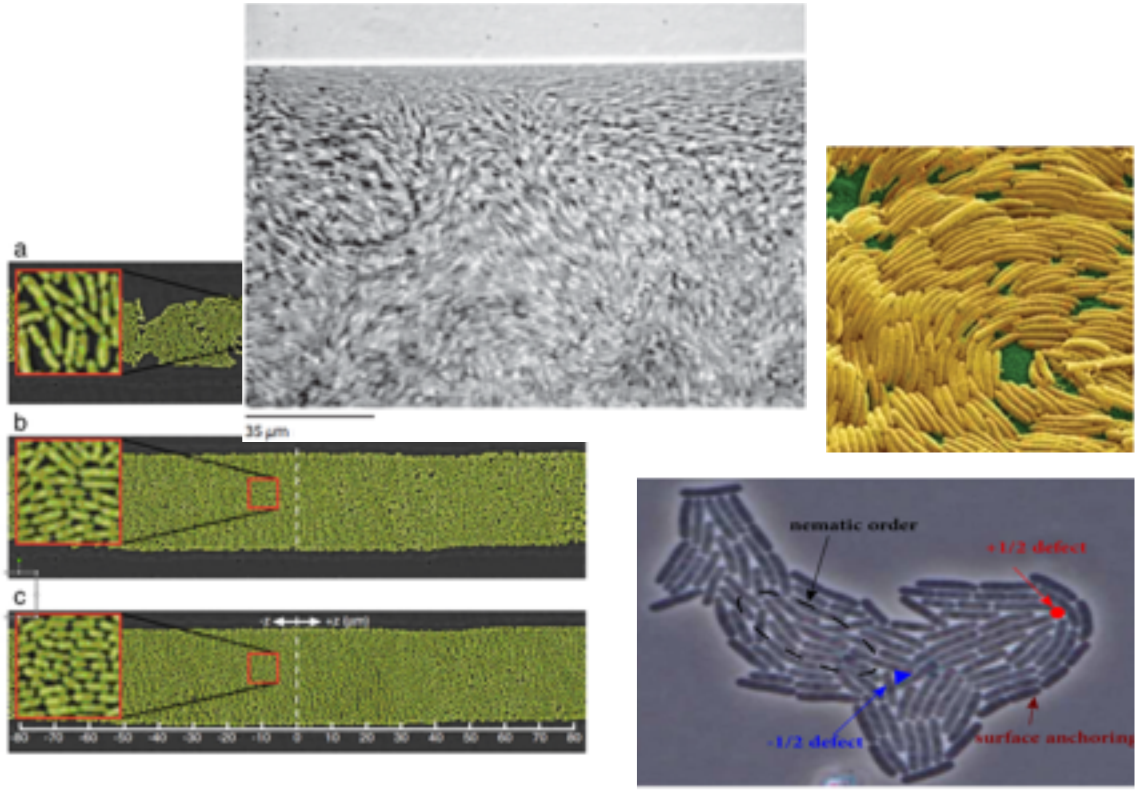




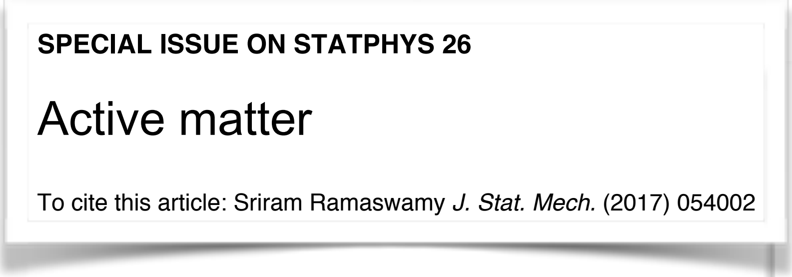




bacterial suspension, growing colonies



WHAT IS ACTIVE MATTER?



SPECIAL ISSUE ON STATPHYS 26

Active matter

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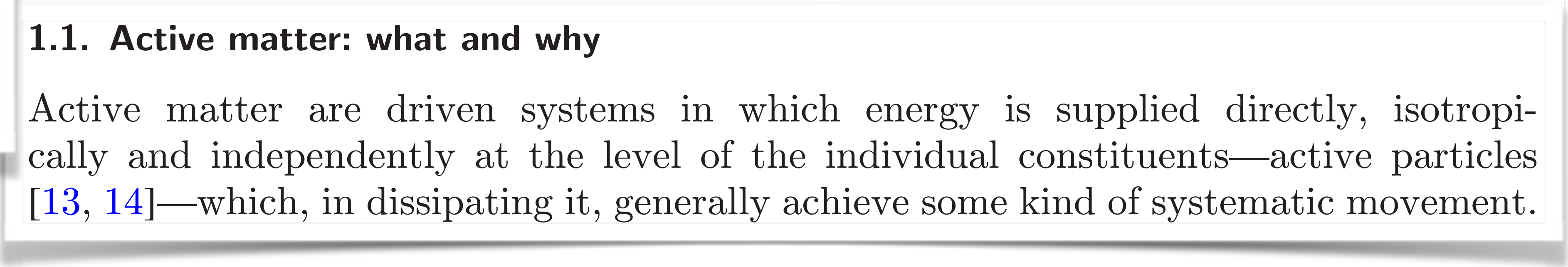

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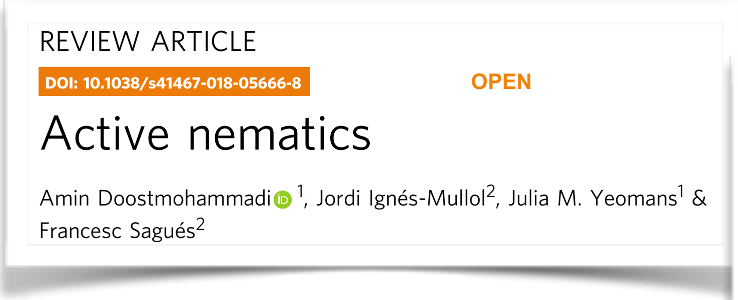


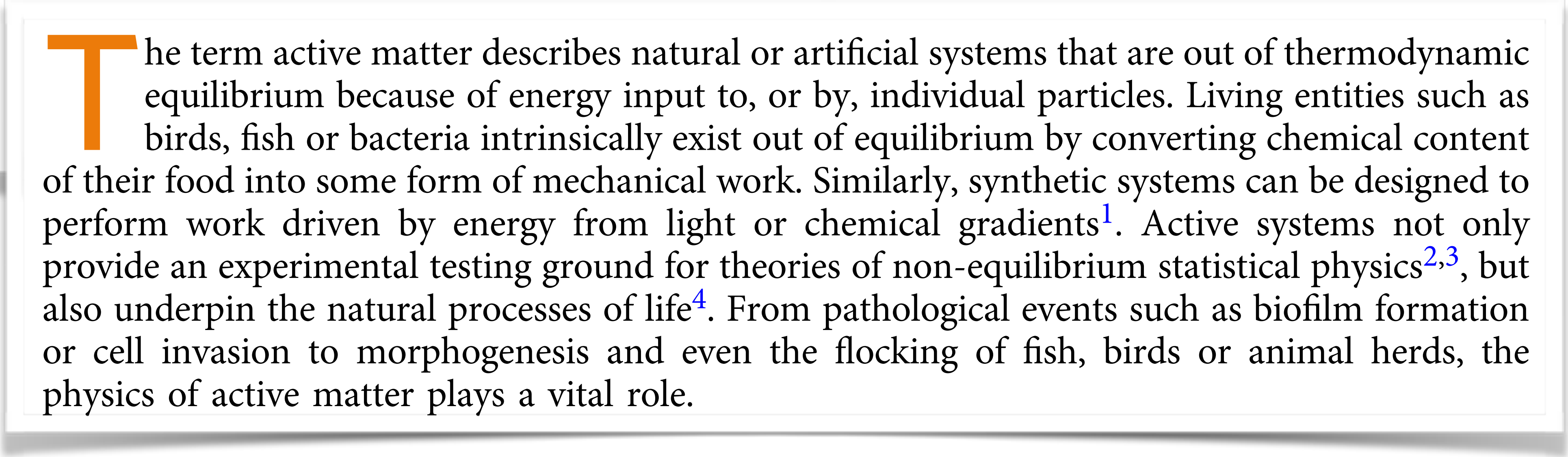
REVIEW ARTICLE

DOI: 10.1038/s41467-018-05666-8

OPEN

Active nematics

Amin Doostmohammadi[1], Jordi Ignés-Mullol[2], Julia M. Yeomans[1] & Francesc Sagués[2]



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The grand aim of the active-matter paradigm is twofold: to bring living systems into the inclusive ambit of condensed matter physics, and to discover the emergent statistical and thermodynamic laws governing matter made of intrinsically driven particles

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Active nematics

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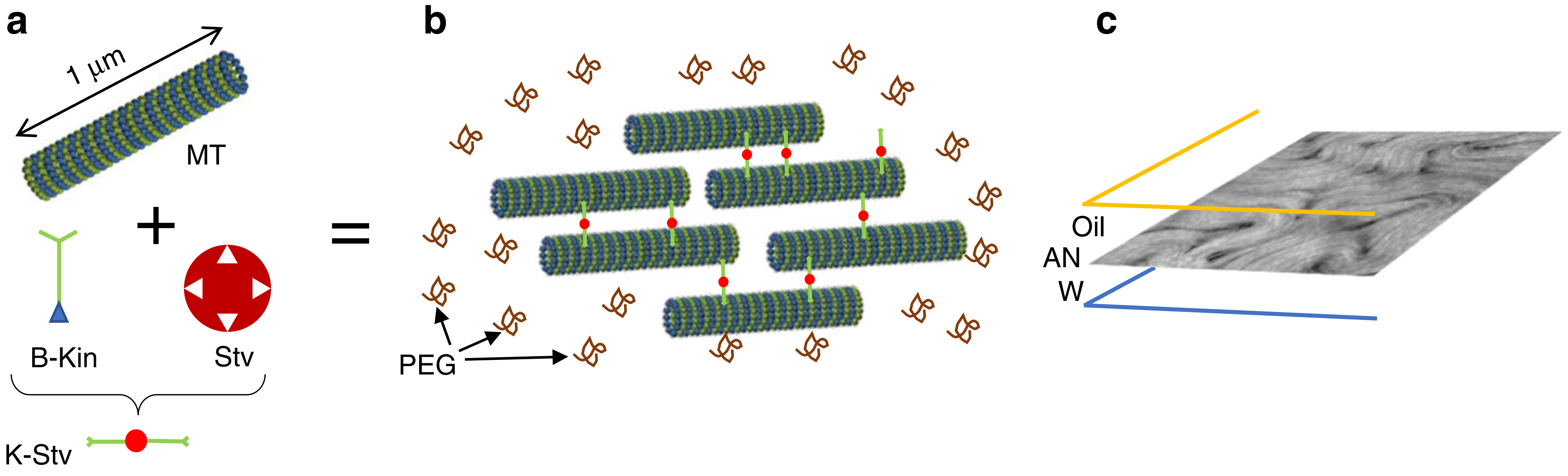
BOX 2 MT/motor protein mixtures

An experimental system that continues to be very important to developing the understanding of active nematics is a mixture of MTs and two-headed molecular motors. **a** Fluorescently tagged MTs from polymerised tubulin are brought together by the depleting action of PEG, and are cross-linked by clusters of B-Kin and Stv, resulting in active extensile MTs bundles in an aqueous suspension (**b**). As the motors walk along the MTs the bundles extend, are pushed apart, and re-form. **c** The active nematic self-assembles at the water/oil interface and gives rise to active turbulence for as long as there is sufficient ATP to fuel the motors.



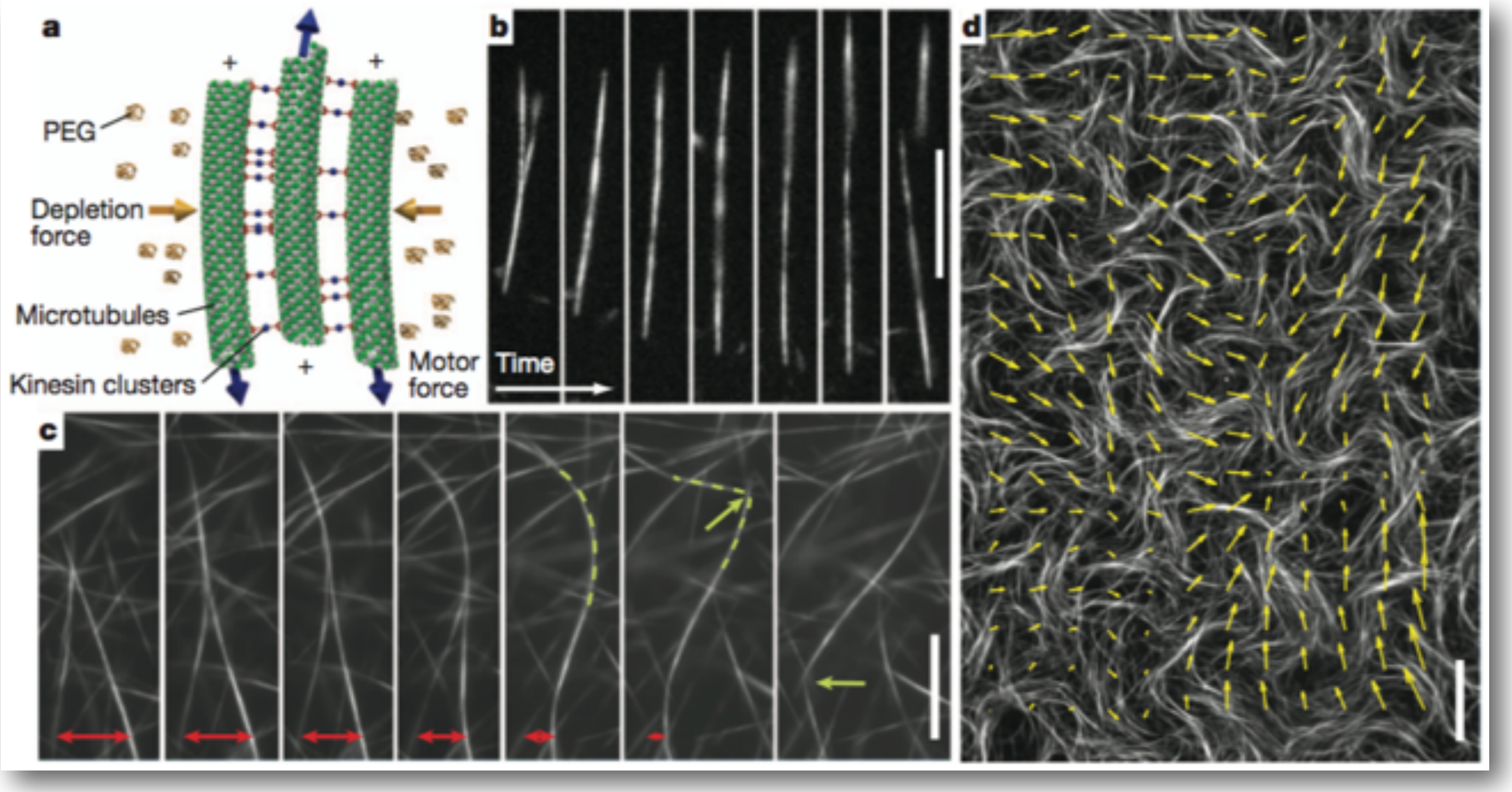
Schematic of the experimental system.

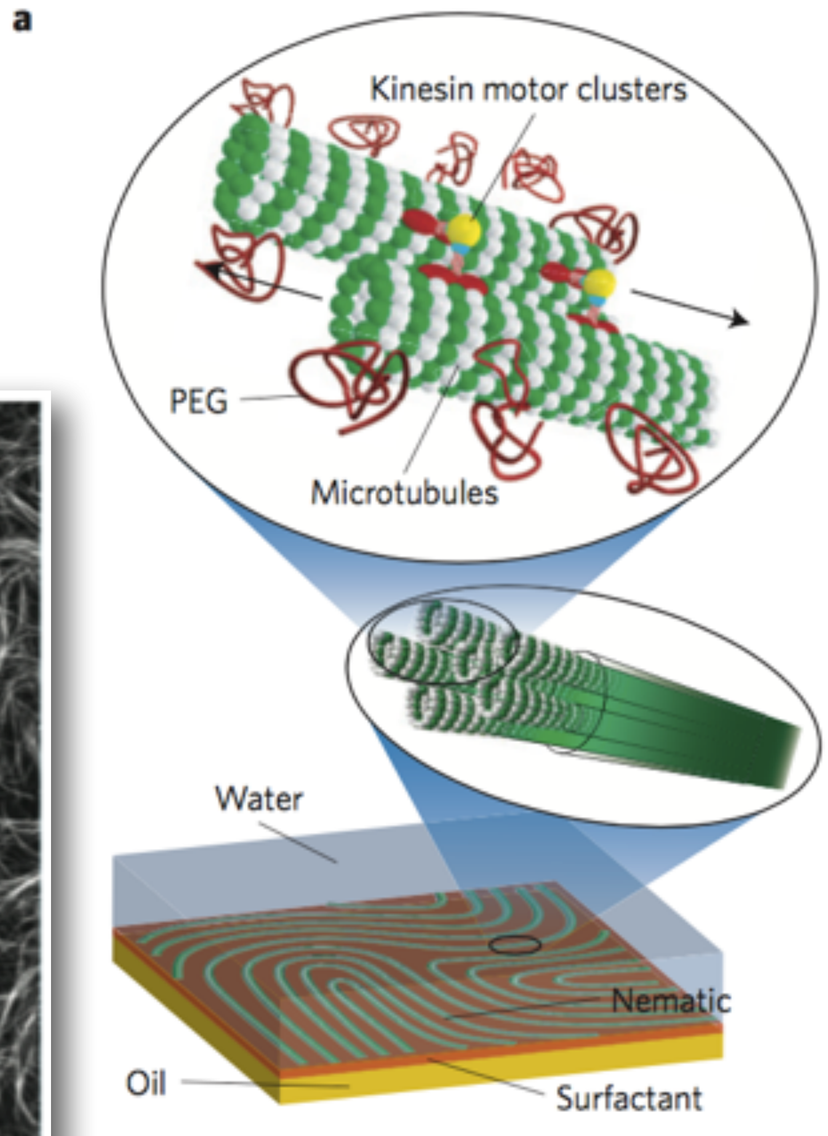
LETTER

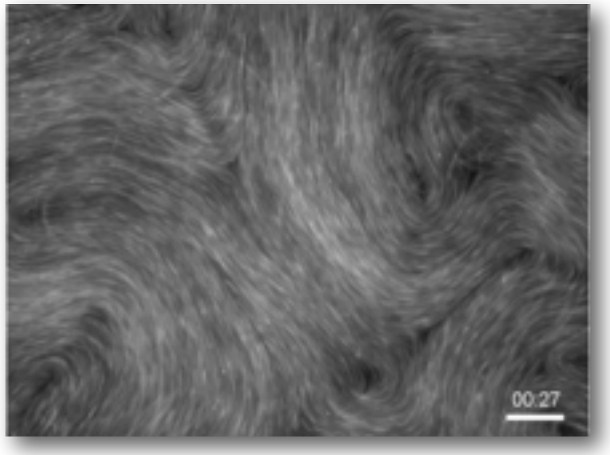
doi:10.1038/nature11591

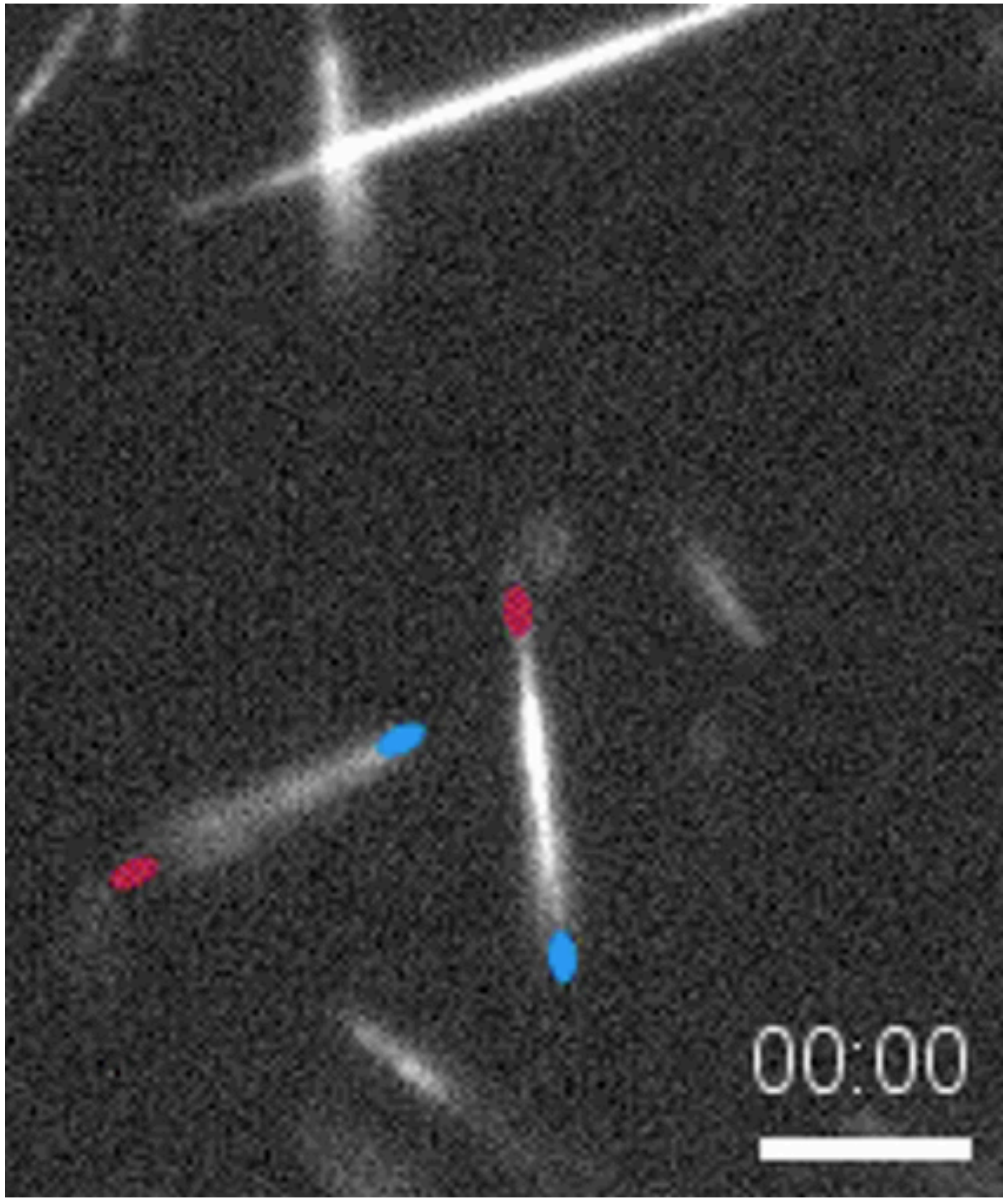
Spontaneous motion in hierarchically assembled active matter

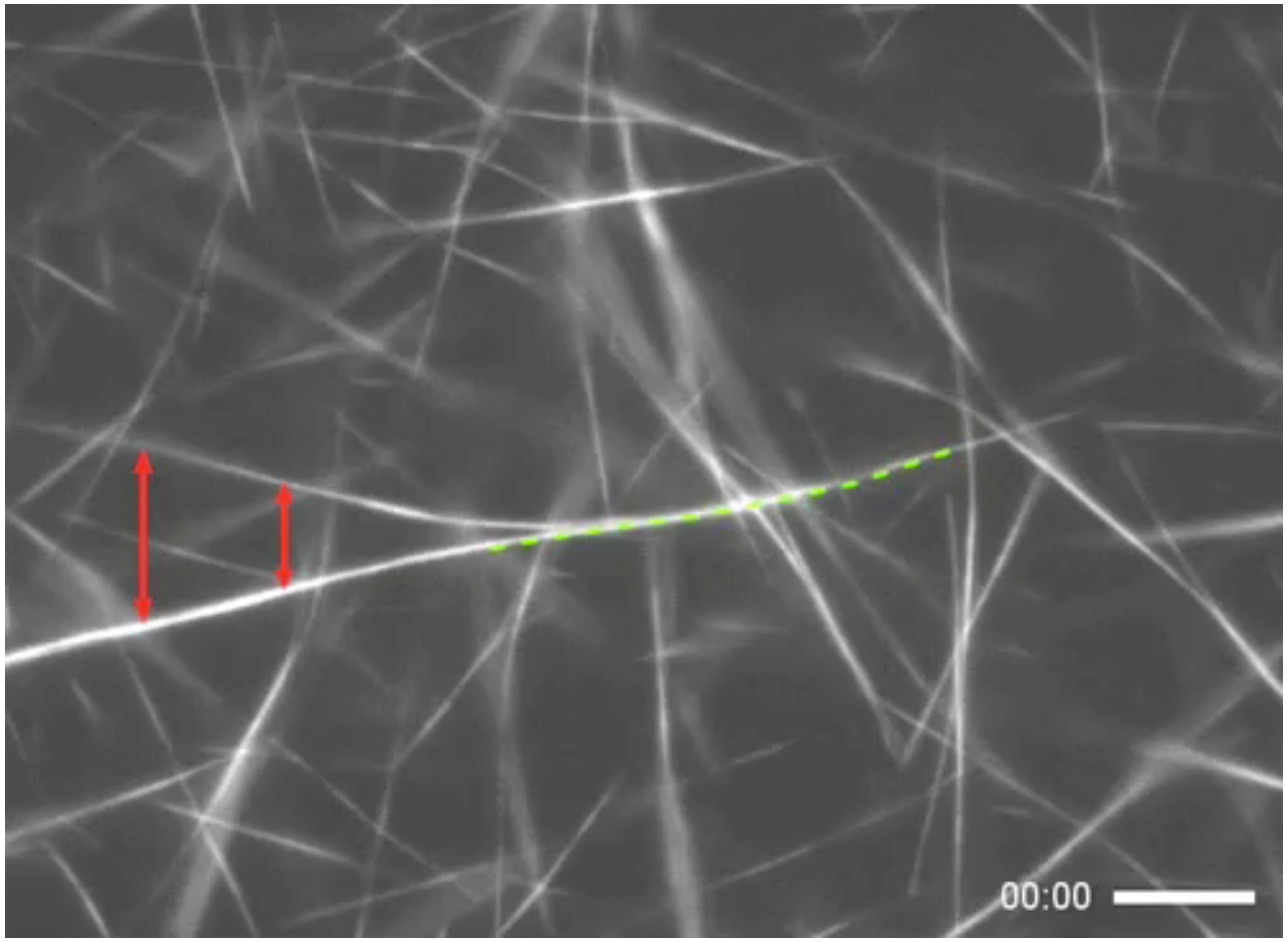
Tim Sanchez[1]*, Daniel T. N. Chen[1]*, Stephen J. DeCamp[1]*, Michael Heymann[1,2] & Zvonimir Dogic[1]











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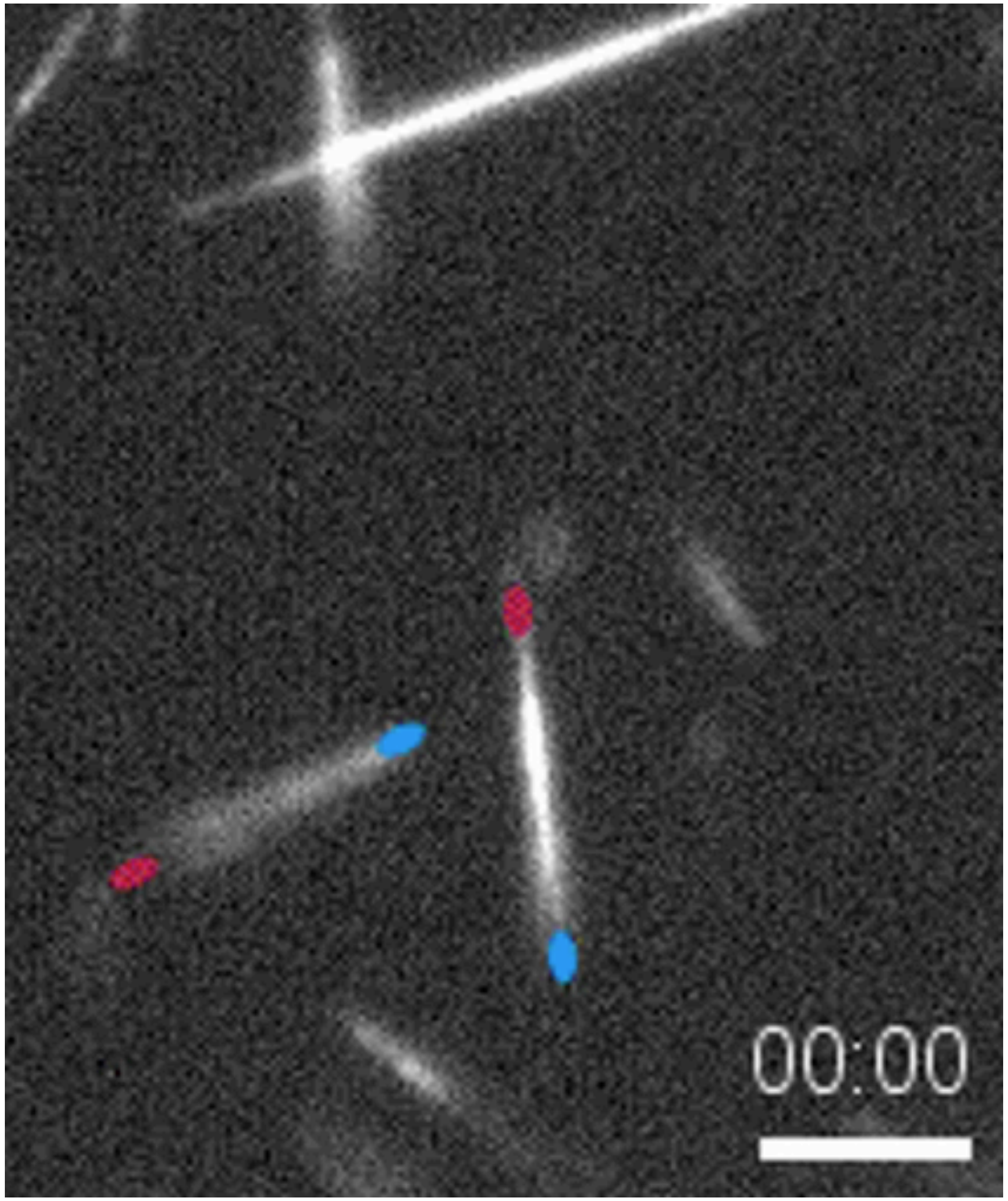

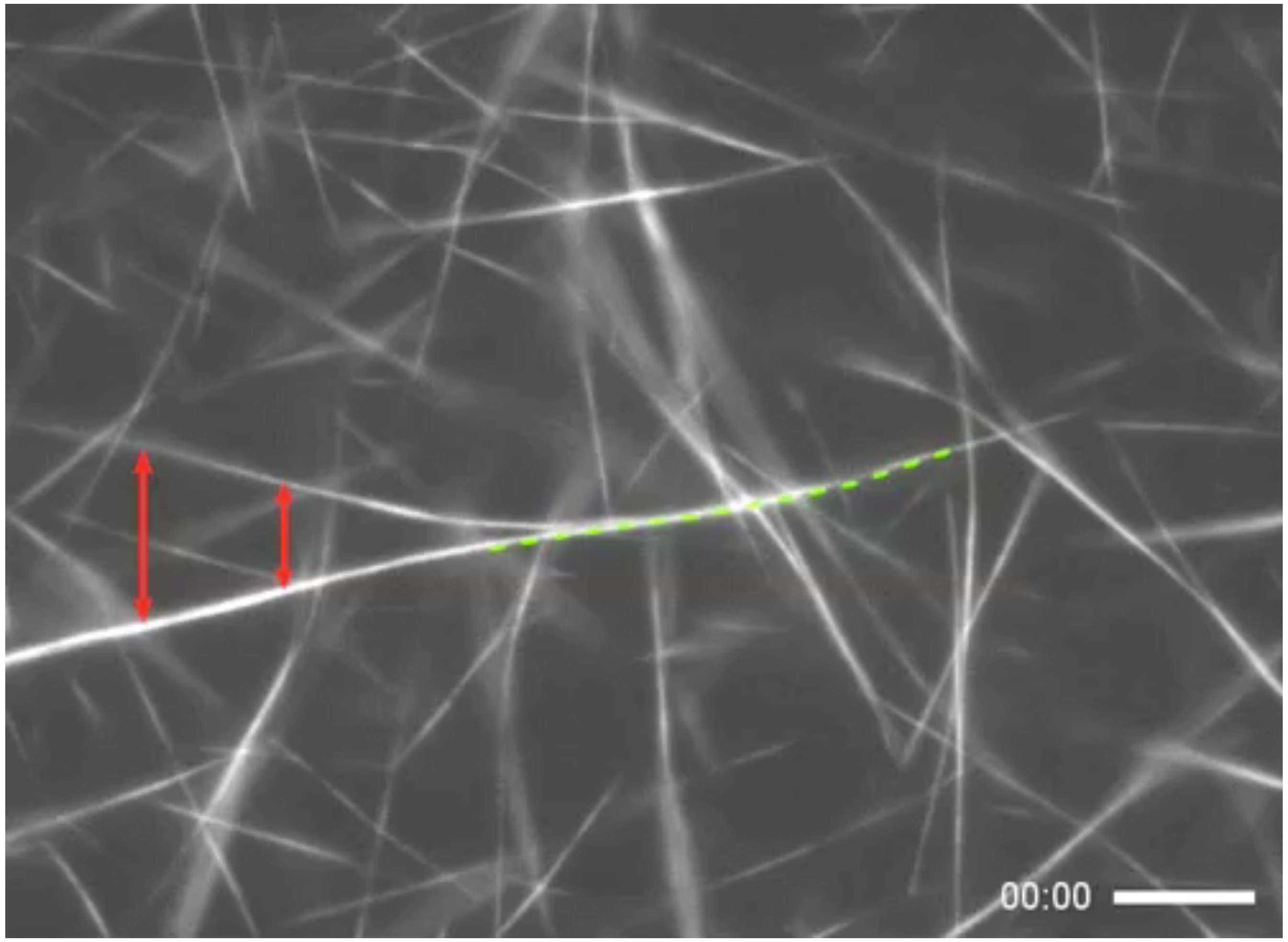

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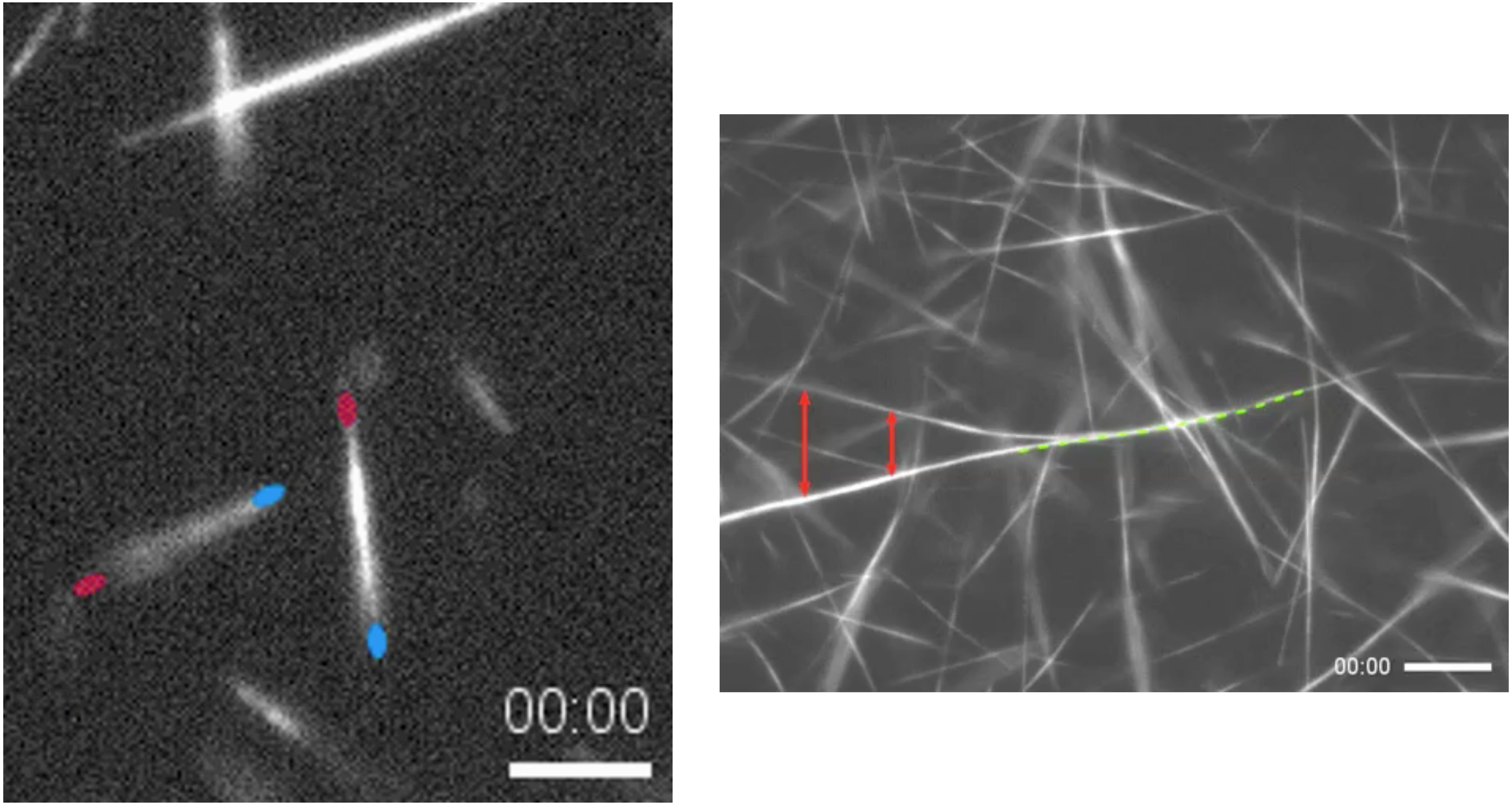

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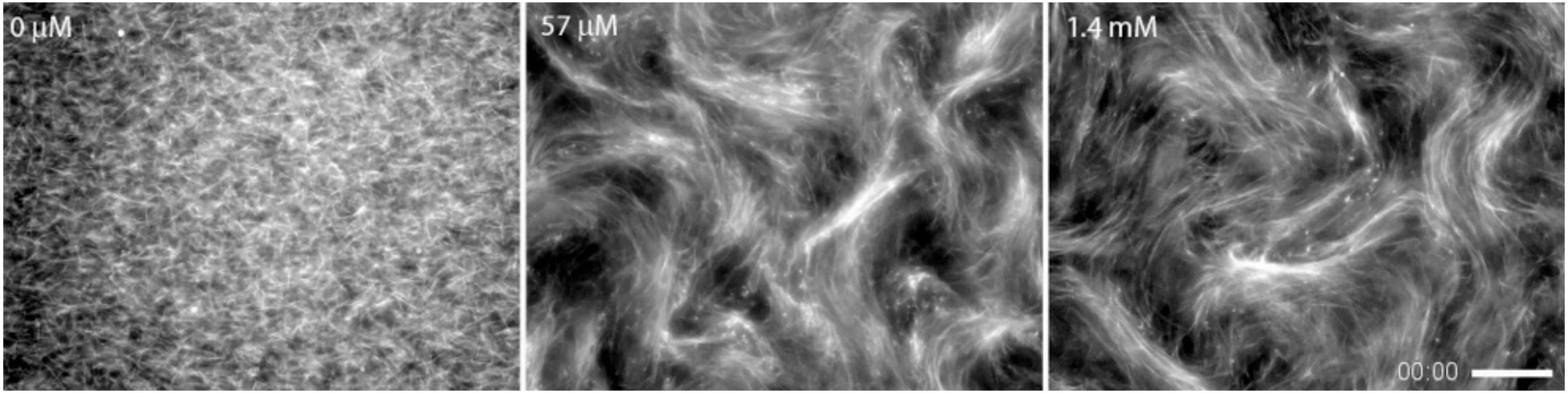

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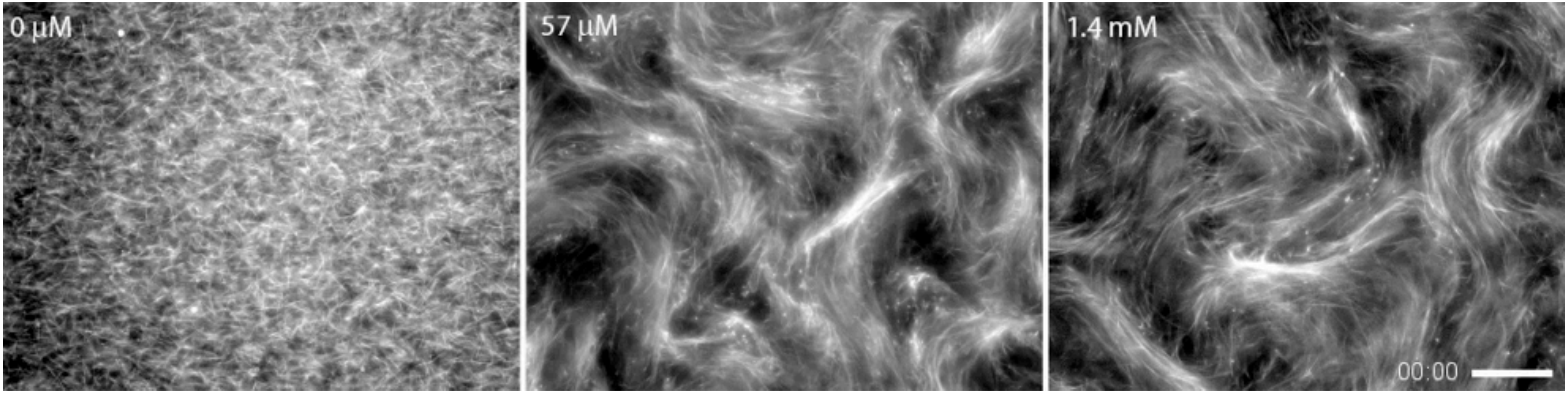

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Active 2D nematic
Low curvature interface
60X mag
15μm bar

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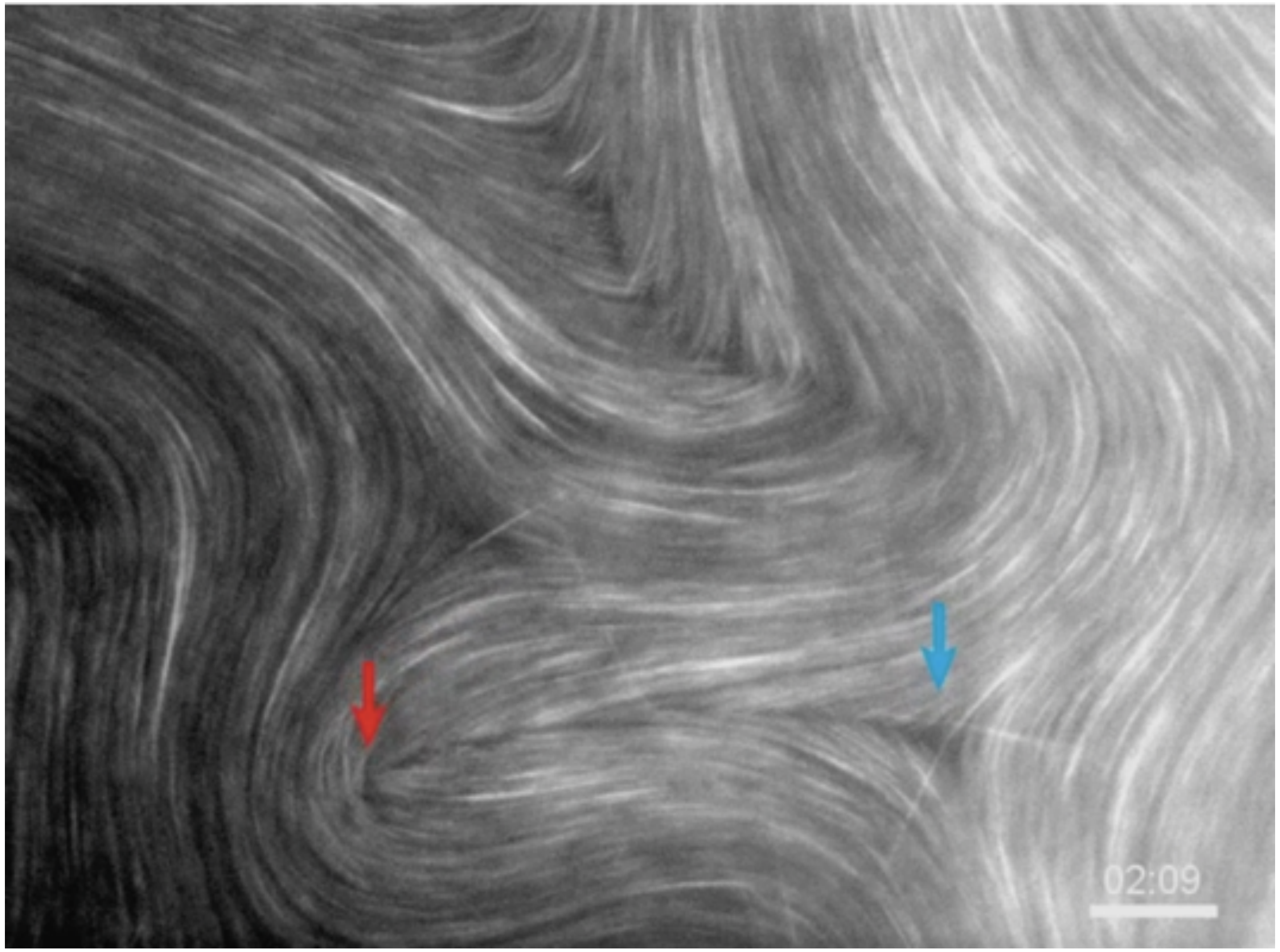
Active Nematics

macroscopic properties: local alignment; nematic order; fluid flows

model as a continuum liquid crystal



the effect of activity is to induce ***local stresses*** and create local flows with the character of ***force dipoles***

EQUATIONS

dynamics is (minimal) Stokesian liquid crystal hydrodynamics augmented by activity

conservation of mass,
momentum

$$\partial_i v_i = 0, \quad \partial_j \sigma_{ij} = 0$$

continuity *Stokes*

stress tensor

$$\sigma_{ij} = -P\delta_{ij} + 2\eta u_{ij} + \frac{\nu}{2}\big(n_i h_j + h_i n_j\big) + \frac{1}{2}\big(n_i h_j - h_i n_j\big)$$
$$- \frac{\delta F}{\delta(\partial_i n_k)}\big(\delta_{jk} - n_j n_k\big)\partial_j n_k - \zeta n_i n_j$$

active stress

director relaxation

$$\partial_t n_i + v_j \partial_j n_i + \omega_{ij} n_j = -\nu u_{ij} n_j + \frac{1}{\gamma} h_i$$

elastic relaxation

LIQUID CRYSTALS

Liquid crystals are beautiful and mysterious; I am fond of them for both reasons. My hope is that some readers of this book will feel the same attraction, help to solve the mysteries, and raise new questions.

Pierre-Gilles de Gennes, The Physics of Liquid Crystals, 1972

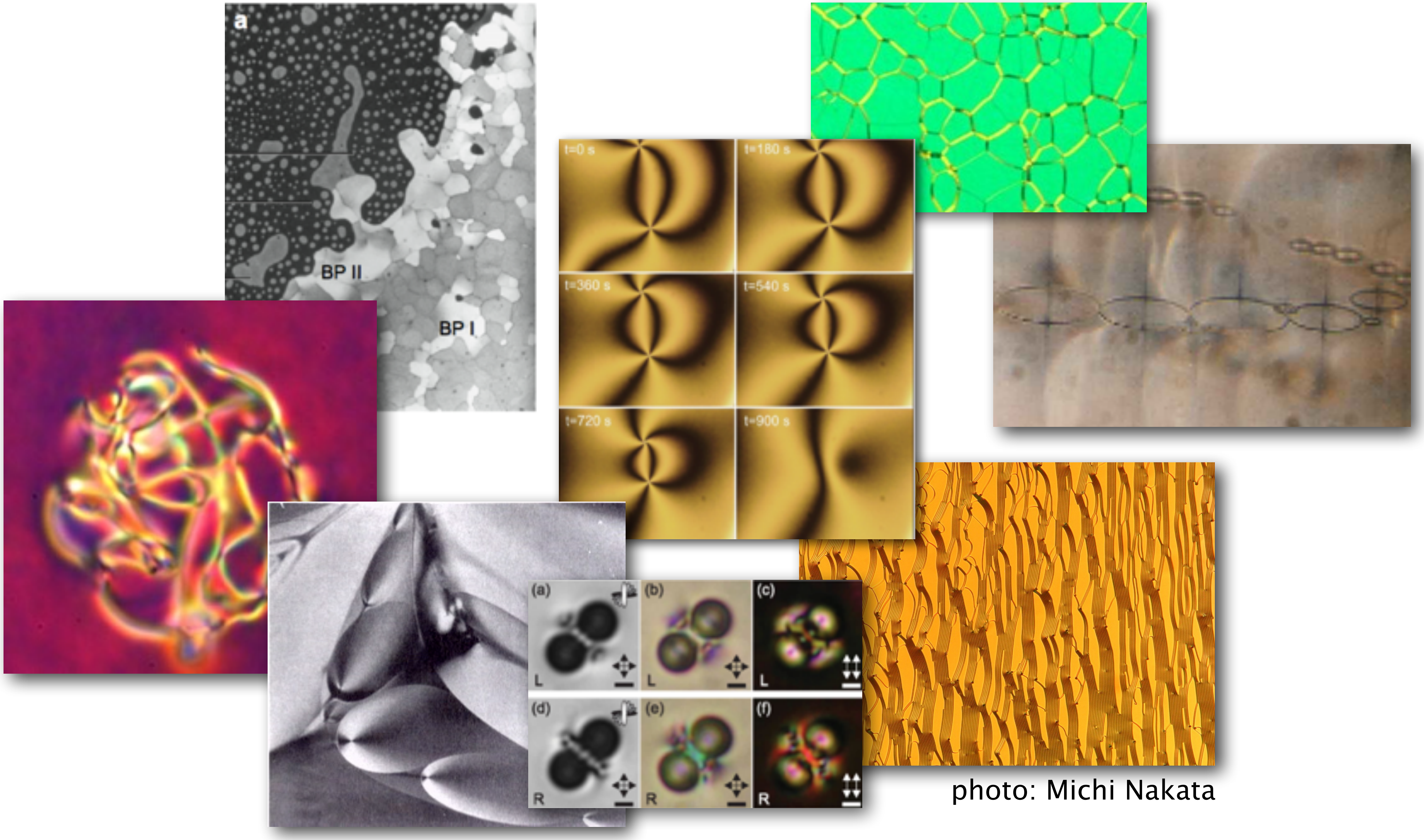
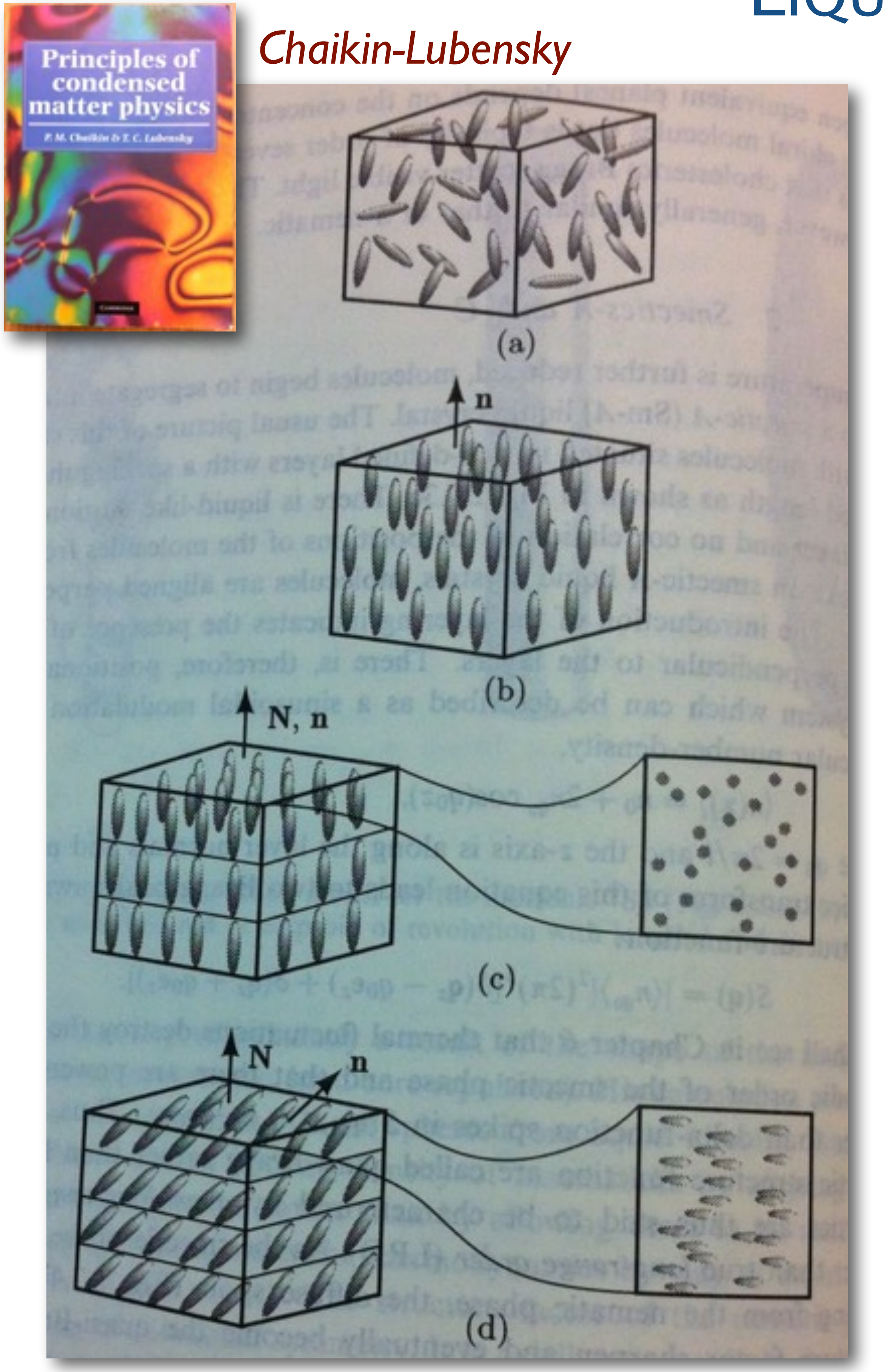


photo: Michi Nakata

LIQUID CRYSTALS



Chaikin-Lubensky

- broken symmetry ordered mesophases
- composed of long, thin, rod-like molecules

nematic
- *broken rotational symmetry*
- *molecules align along a common axis (director)*

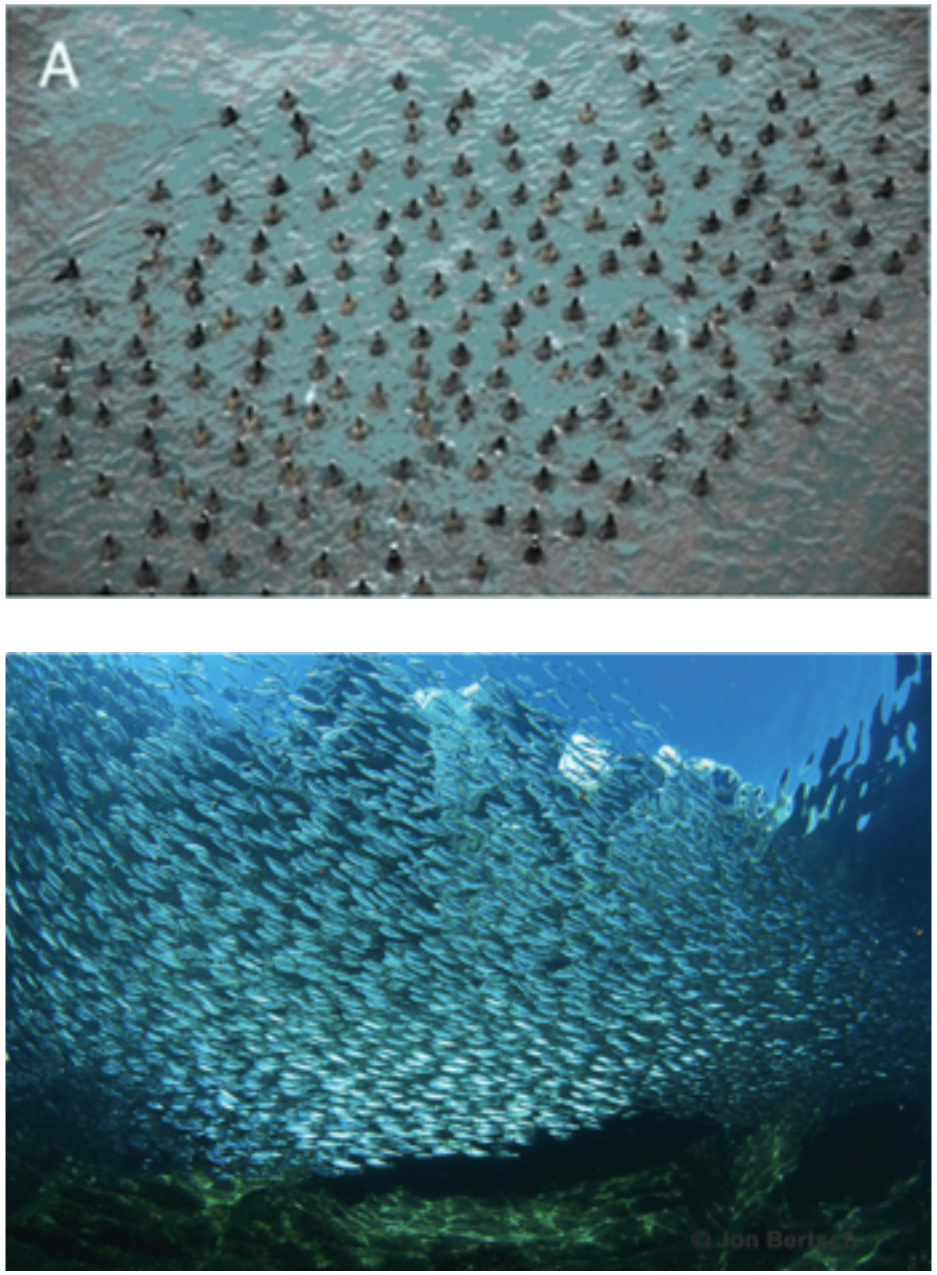
smectic A
- *1d broken translational symmetry*
- *molecules form (fluid) layers*

smectic C
- *+ tilt relative to the layer normal*

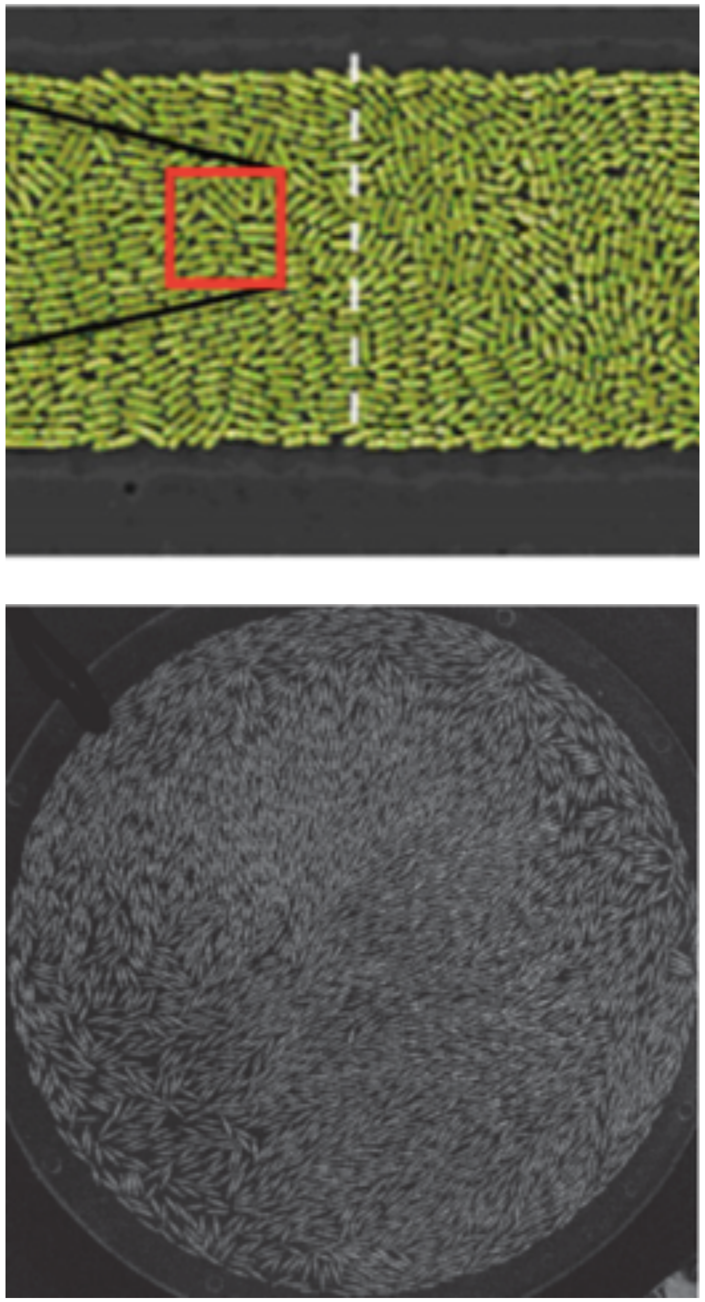
The Type of Order in Active Matter

Flocks are **polar** — they have a *macroscopic* direction

Many other systems are **apolar**, or **nematic** — there is alignment but it is *not* a vector



polar



nematic

Polar or Nematic

Equilibrium concepts of symmetry apply also to active systems to characterise the nature of their order

first moment

$$p_i(\mathbf{r}) = \langle \nu_i \rangle = \int \nu_i P(\mathbf{r}, \boldsymbol{\nu}) \, d\Omega$$

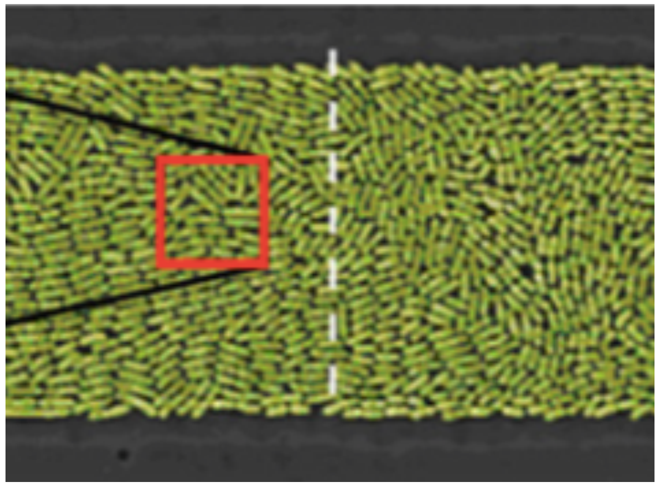
individual orientation

orientational probability distribution

second moment

$$Q_{ij}(\mathbf{r}) = \langle \nu_i \nu_j \rangle - \frac{1}{d}\delta_{ij} = \int \nu_i \nu_j \, P(\mathbf{r}, \boldsymbol{\nu}) \, d\Omega - \frac{1}{d}\delta_{ij}$$

result for isotropic distribution



Nematics: vanishing first moment; anisotropic second moment

SEEING NEMATIC ORDER

The order in nematics is ***not*** a vector; it is a ***line field***

Vectors have defects with **integer** winding; line fields can have **half integers**

$$S^1 \to \{\text{orientations}\} = \mathbb{RP}^1$$

loop in sample

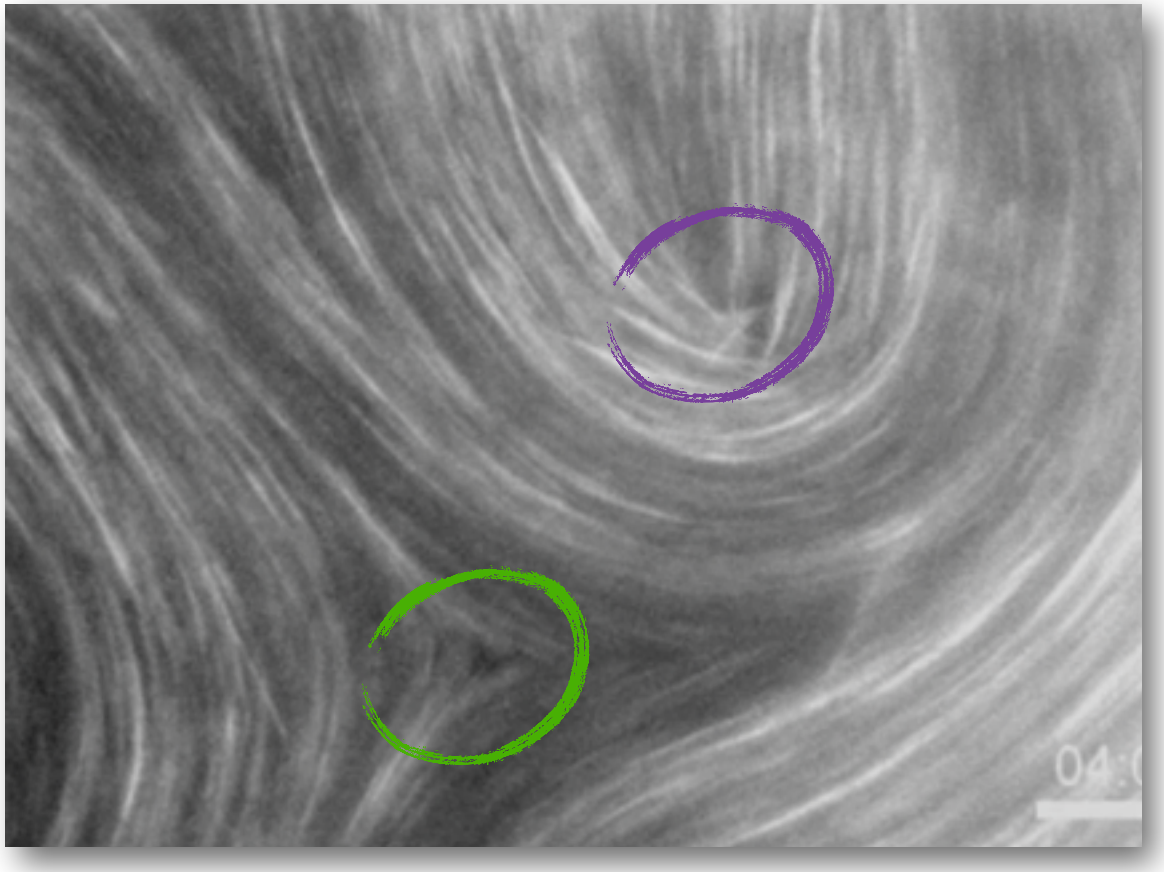
classify up to continuous changes

homotopy theory

$$\pi_1(\mathbb{RP}^1) \cong \frac{1}{2}\mathbb{Z}$$

classification is by winding number

defects combine, and behave, much like charges



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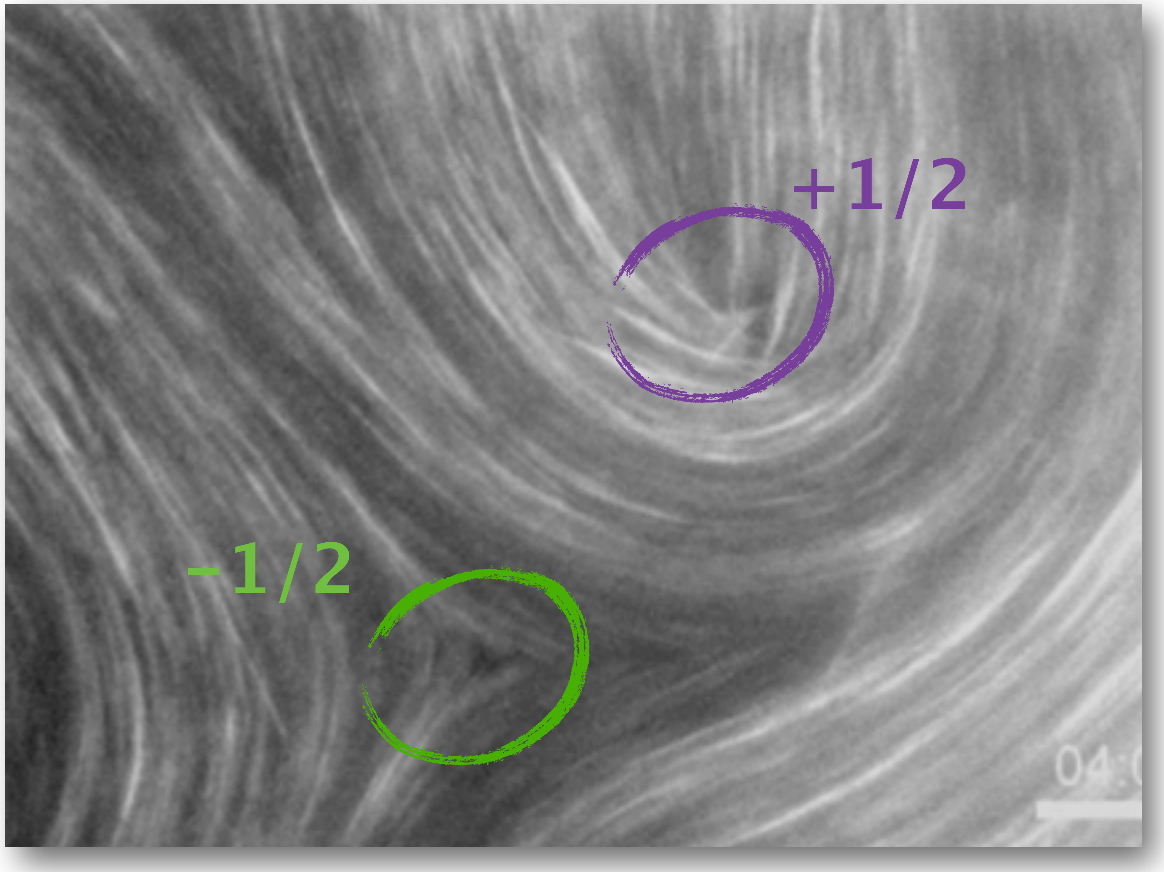


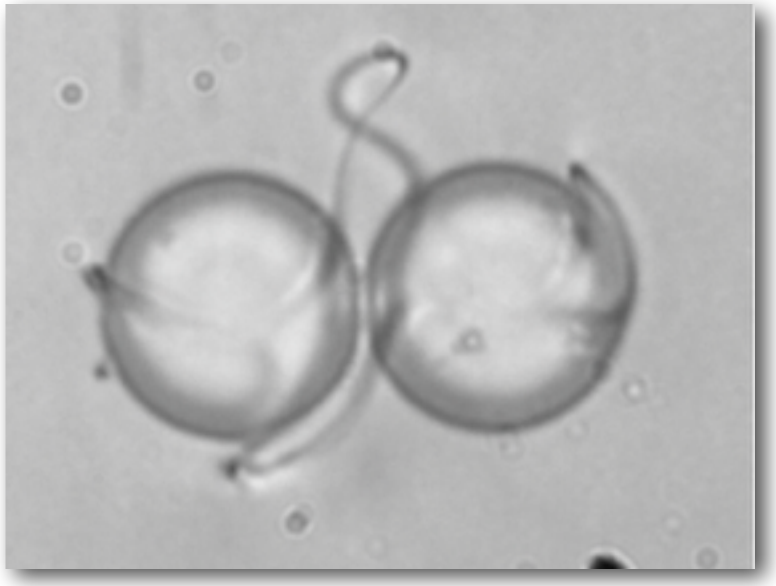
3d

$$S^1 \to \{\text{orientations}\} = \mathbb{RP}^2$$

$$\pi_1(\mathbb{RP}^2) \cong \mathbb{Z}/2$$

*defects are **lines** rather than points*

*there is only **one** type of defect*



Seeing Nematic Order

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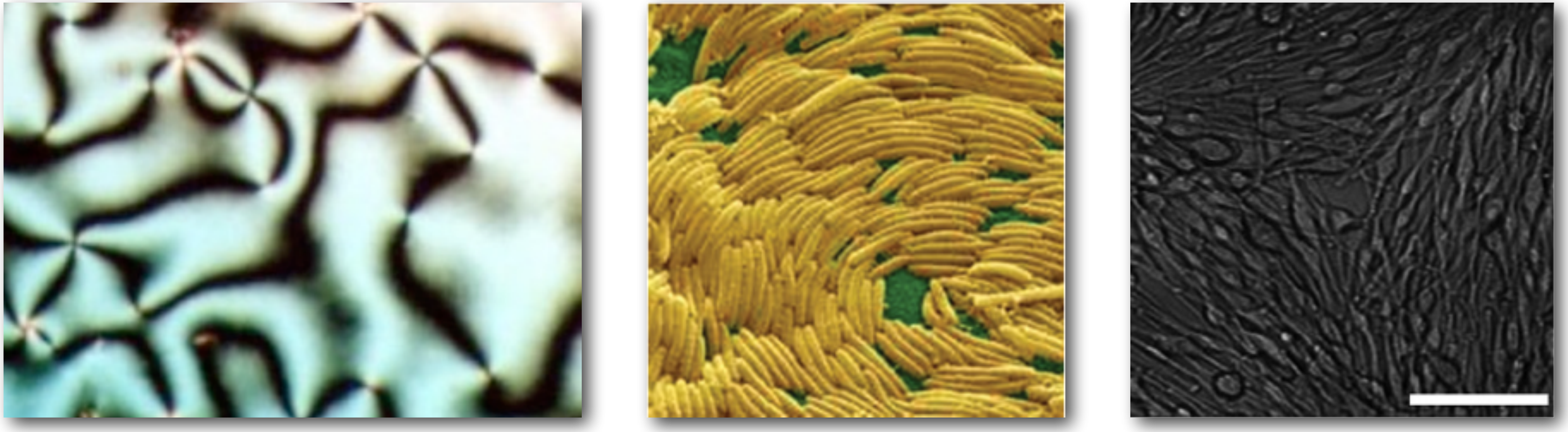


when you know what to look for, it is easy to tell what you are seeing

DIRECTOR FIELD

It is common to describe the order using a direction, rather than the full Q-tensor

This is the nematic ***director*** — it is a **line field**, not a vector field

It is the eigenvector of **Q** associated to its largest eigenvalue

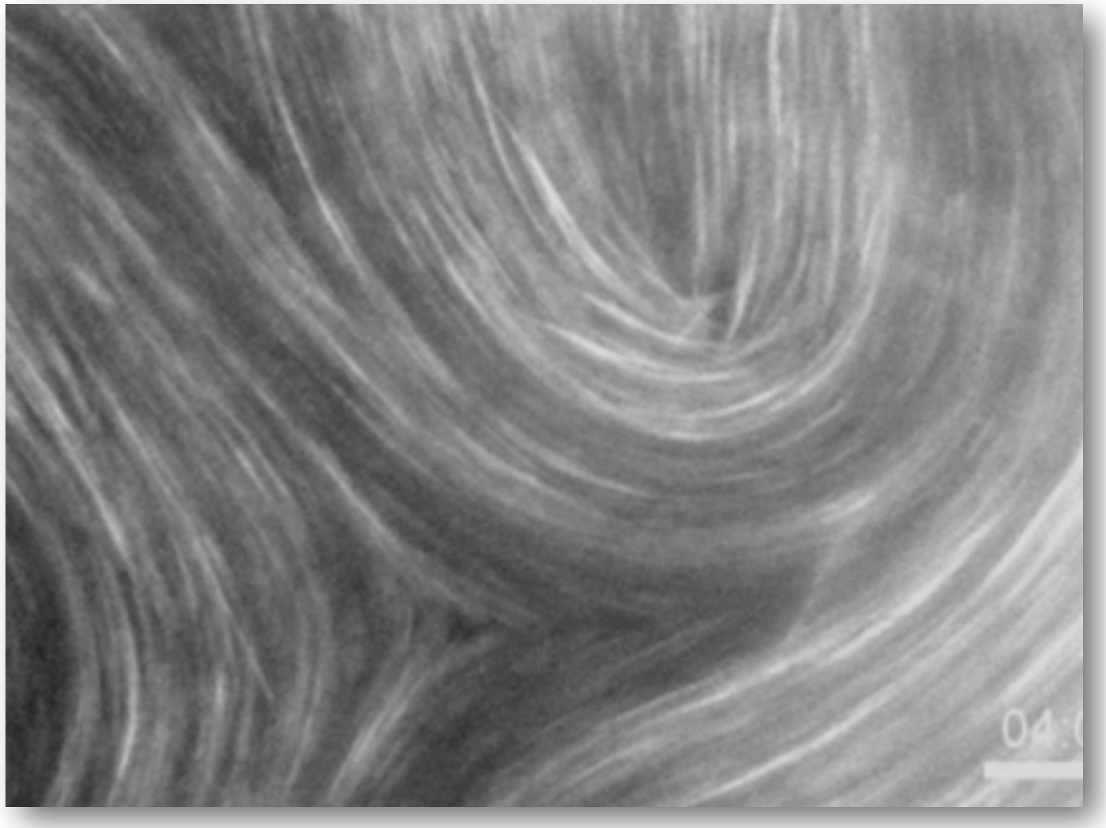
uniaxial form

$$Q_{ij} = s\left(n_i n_j - \frac{1}{d}\delta_{ij}\right)$$

magnitude of order

director

$$n_i \sim -n_i$$



THEORY OF LIQUID CRYSTALS

The order parameter is a traceless, symmetric, rank 2 tensor $\mathbf{Q}$ or Q_{ij}

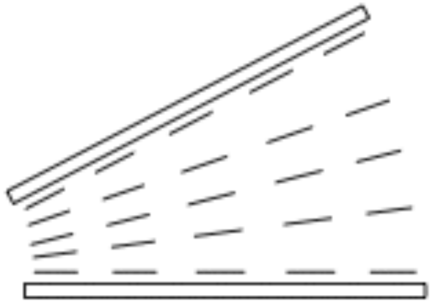
Landau theory

$$F = \int d^d r \left[\frac{A}{2} Q_{ij} Q_{ij} - \frac{B}{3} Q_{ij} Q_{jk} Q_{ki} + \frac{C}{4} \left(Q_{ij} Q_{ij} \right)^2 + \frac{K}{2} \left(\partial_k Q_{ij} \right) \left(\partial_k Q_{ij} \right) \right]$$

bulk terms

elasticity

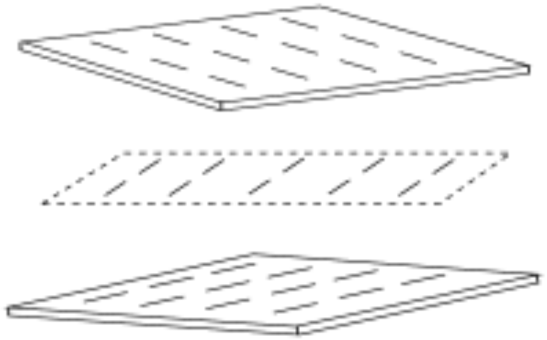
phase transition Q=0 to Q≠0



$\mathbf{n}(\nabla \cdot \mathbf{n})$

splay

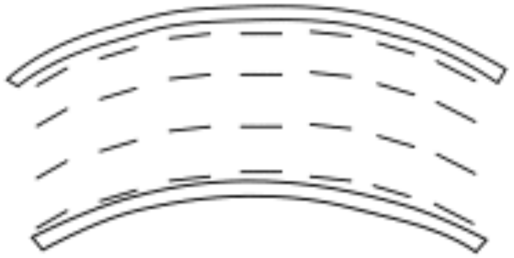
mean curvature



$\mathbf{n} \cdot \nabla \times \mathbf{n}$

twist

mean torsion



$(\mathbf{n} \cdot \nabla)\mathbf{n}$

bend

geodesic curvature of integral curves

THEORY OF LIQUID CRYSTALS

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bulk terms

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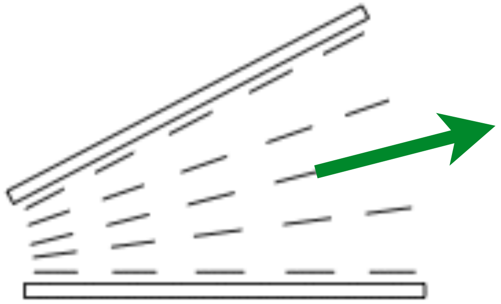
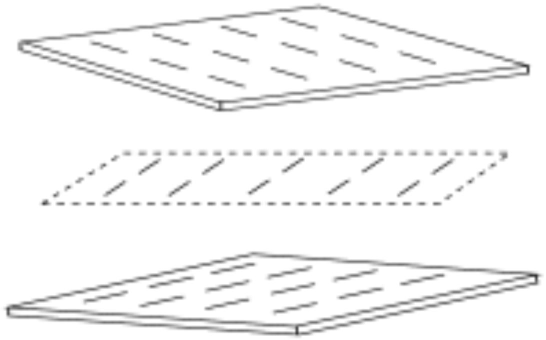


$\mathbf{n}(\nabla \cdot \mathbf{n})$

splay

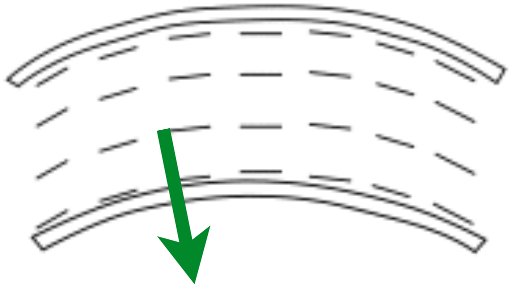
vector



$\mathbf{n} \cdot \nabla \times \mathbf{n}$

twist

pseudoscalar



$(\mathbf{n} \cdot \nabla)\mathbf{n}$

bend

vector

THEORY OF LIQUID CRYSTALS

Frank free energy

$$F = \int \left[\frac{K_1}{2} (\nabla \cdot \mathbf{n})^2 + \frac{K_2}{2} (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{K_3}{2} ((\mathbf{n} \cdot \nabla)\mathbf{n})^2 \right] d^d x = \int \frac{K}{2} (\nabla \mathbf{n})^2 \, d^d x$$

one-constant approximation

dynamics

$$\partial_t n_i + v_j \partial_j n_i + \omega_{ij} n_j = -\nu u_{ij} n_j + \frac{1}{\gamma} h_i$$

elastic relaxation

$$h_i = -\frac{\delta F}{\delta n_i}$$

symmetric and anti-symmetric velocity gradients

$$u_{ij} = \tfrac{1}{2}(\partial_i v_j + \partial_j v_i)$$
$$\omega_{ij} = \tfrac{1}{2}(\partial_i v_j - \partial_j v_i)$$

fluid flow

conservation of mass,
momentum

$$\partial_i v_i = 0, \qquad \partial_j \sigma_{ij} = 0$$

continuity *Stokes*

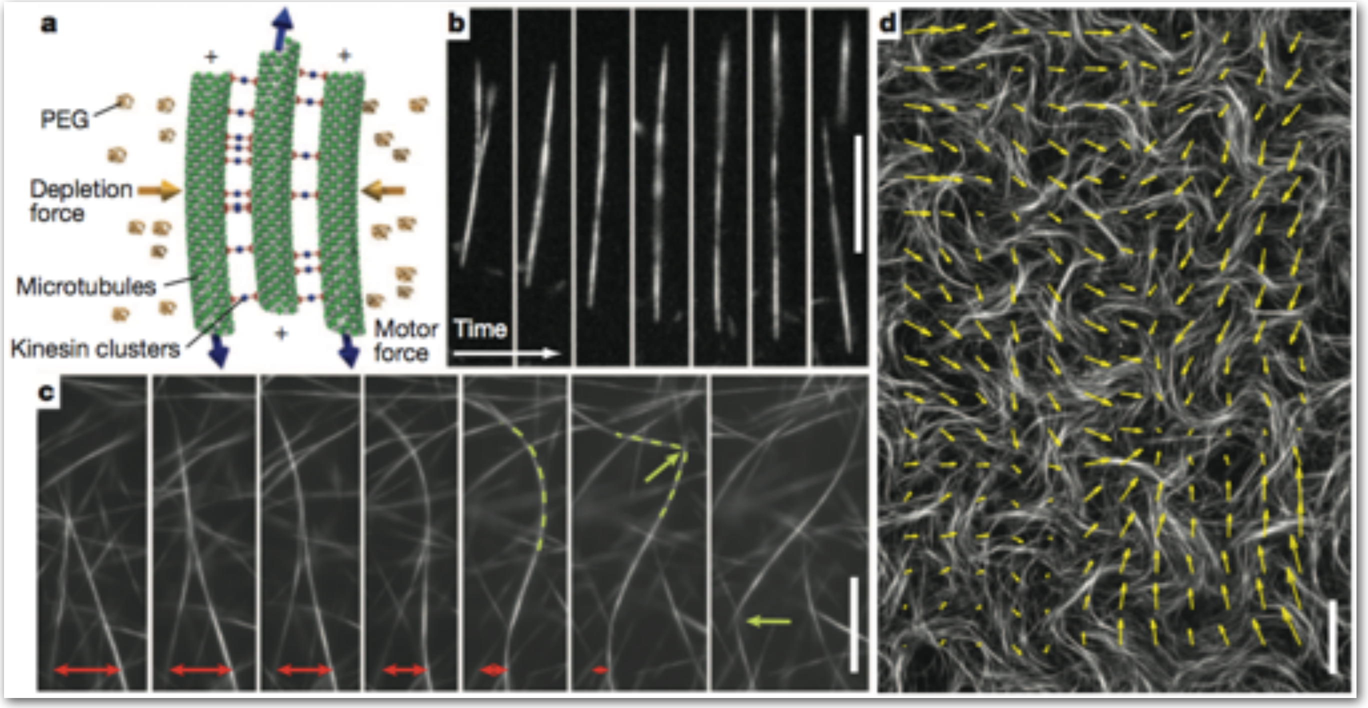
stress tensor

$$\sigma_{ij} = -P\delta_{ij} + 2\eta u_{ij} + \frac{\nu}{2}(n_i h_j + h_i n_j) + \frac{1}{2}(n_i h_j - h_i n_j)$$
$$- \frac{\delta F}{\delta(\partial_i n_k)} (\delta_{jk} - n_j n_k) \partial_j n_k - \zeta n_i n_j$$

↑

active stress

ACTIVE STRESSES



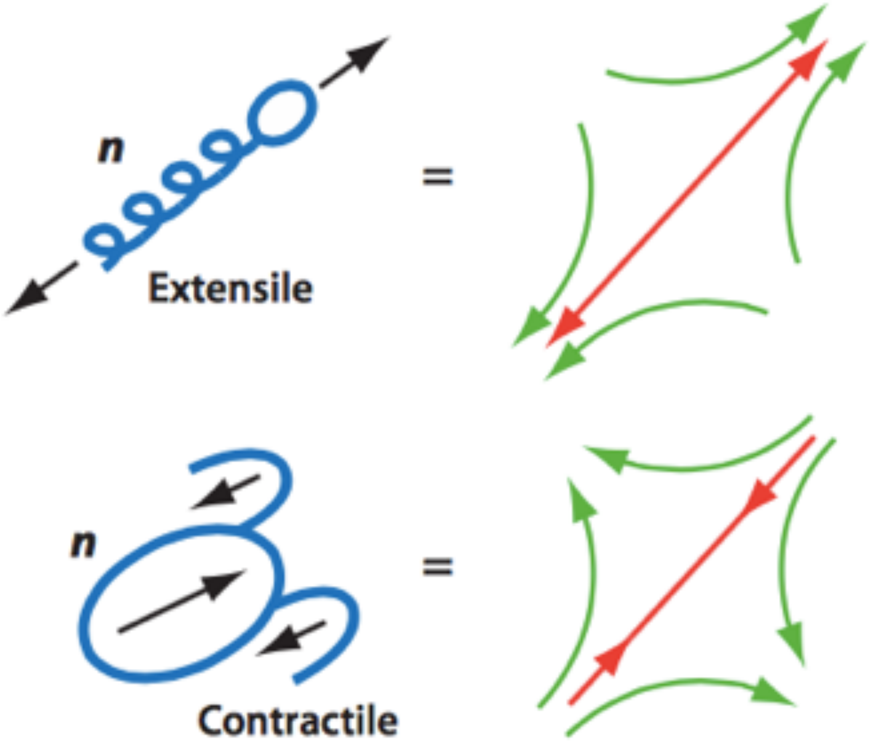
[Sanchez et al., Nature 2012]

at a microscopic scale the motility arises from kinesin walking along microtubules by hydrolysis of ATP

microtubules slide relative to each other

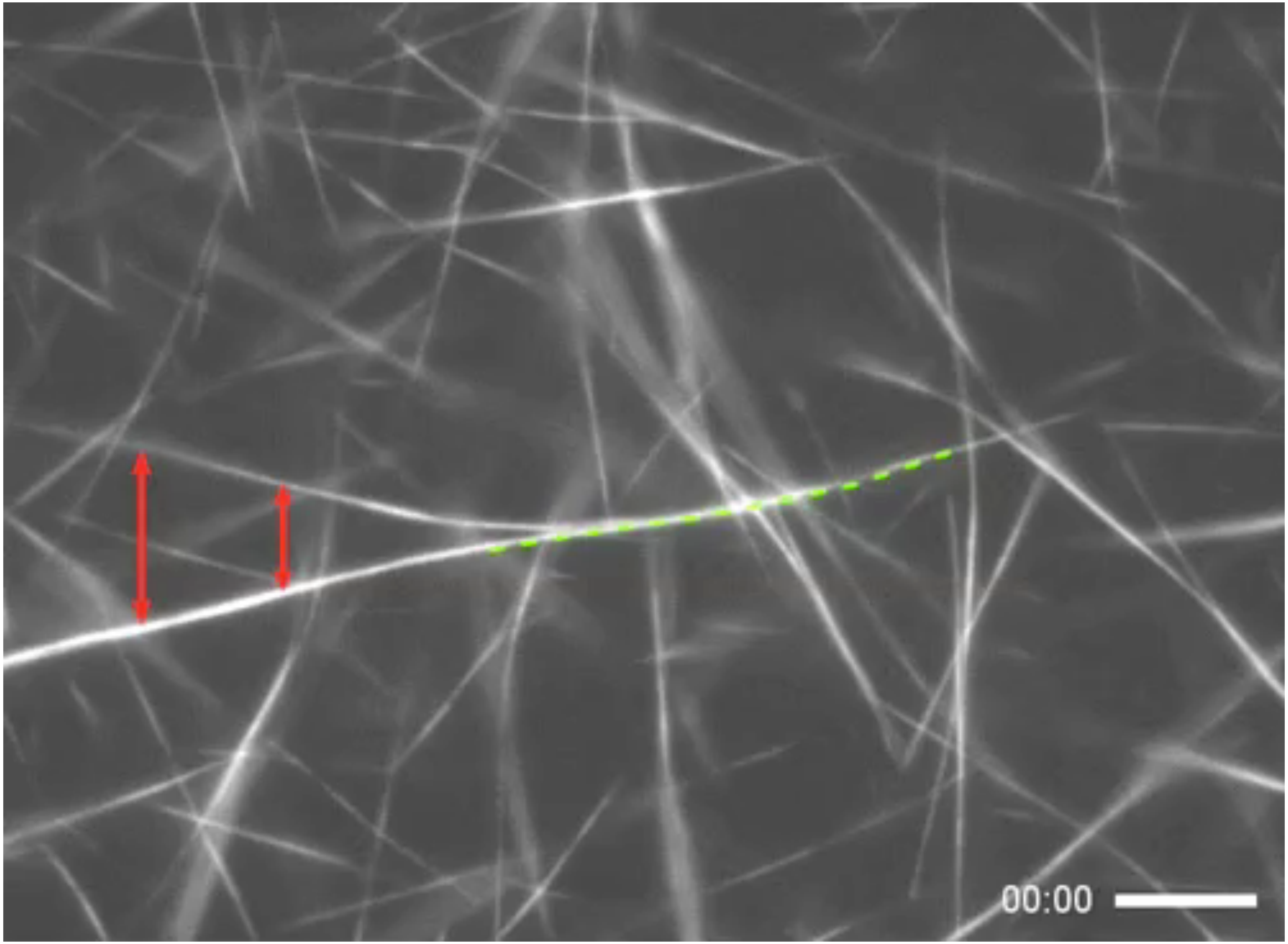
this exerts stresses that are force dipoles aligned along the microtubules

fundamental dichotomy between extensile and contractile systems



Spontaneous motion in hierarchically assembled active matter

Tim Sanchez[1]*, Daniel T. N. Chen[1]*, Stephen J. DeCamp[1]*, Michael Heymann[1,2] & Zvonimir Dogic[1]



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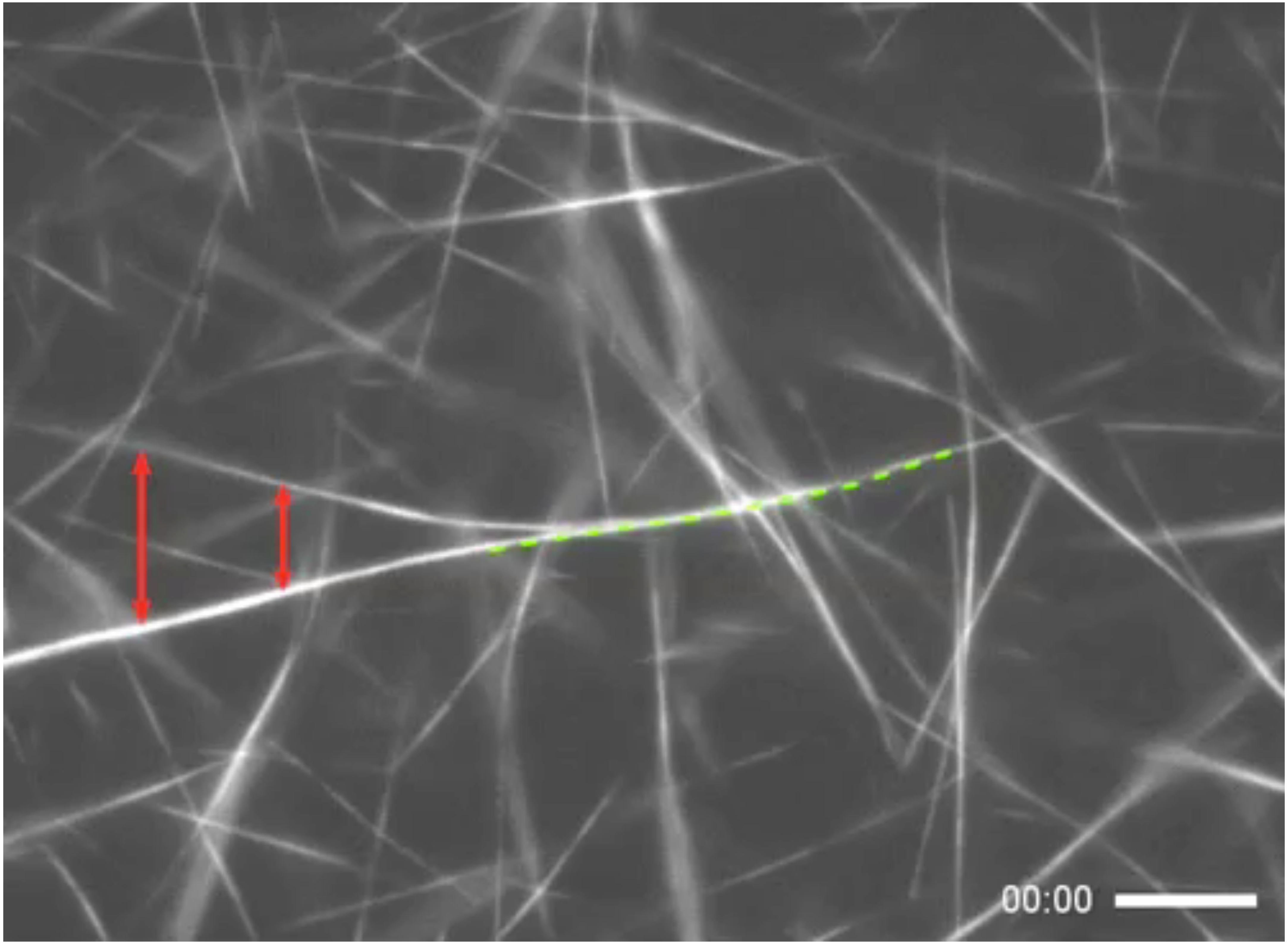
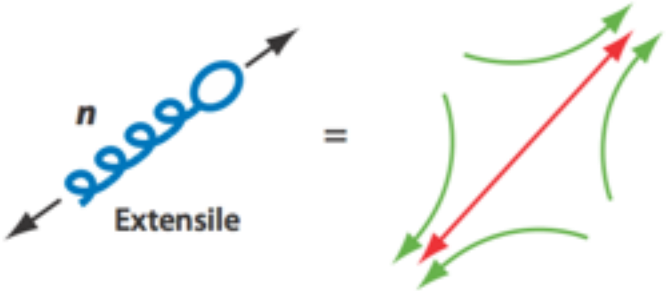


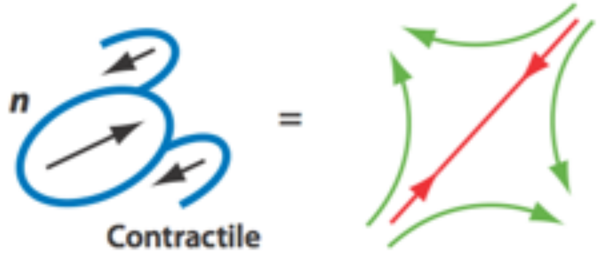
ACTIVE STRESSES AND ACTIVE FORCE

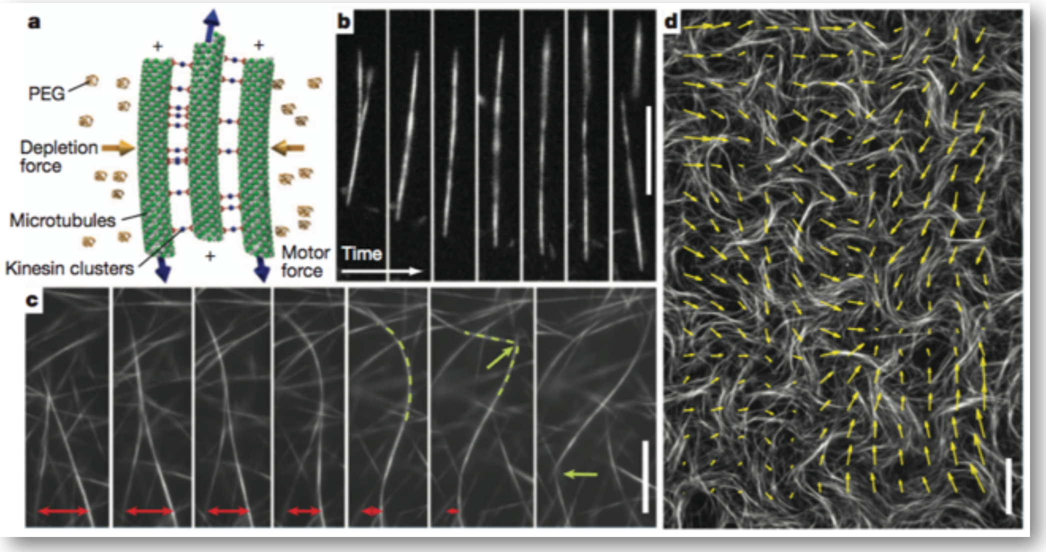
active stress $\sigma_{ij}^{\text{active}} = -\zeta n_i n_j$ *force dipole*

$\zeta > 0$



$\zeta < 0$





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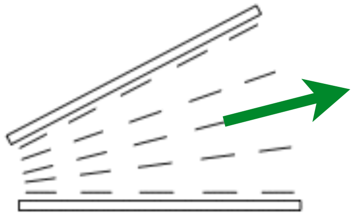
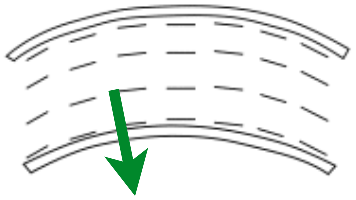
active force $f_i^{\text{active}} = \partial_j \sigma_{ij}^{\text{active}} = -\zeta \left[n_i (\partial_j n_j) + (n_j \partial_j) n_i \right]$



splay

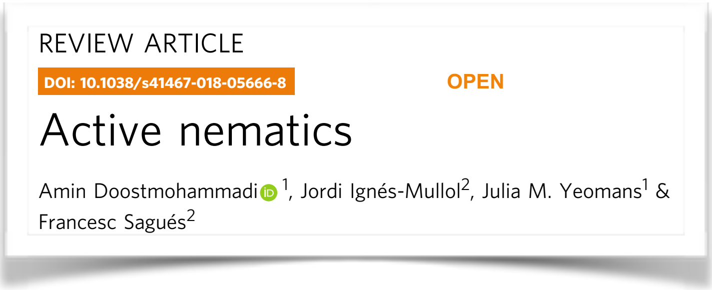


bend

Aditi Simha, Ramaswamy, Phys. Rev. Lett. **89**, 058101 (2002)

PROPERTIES OF ACTIVE NEMATICS

- simple uniformly aligned phases are ***unstable***
- ***defects*** are spontaneously created and control material properties
- flows develop ***vortices*** ("active turbulence") which are stable under confinement

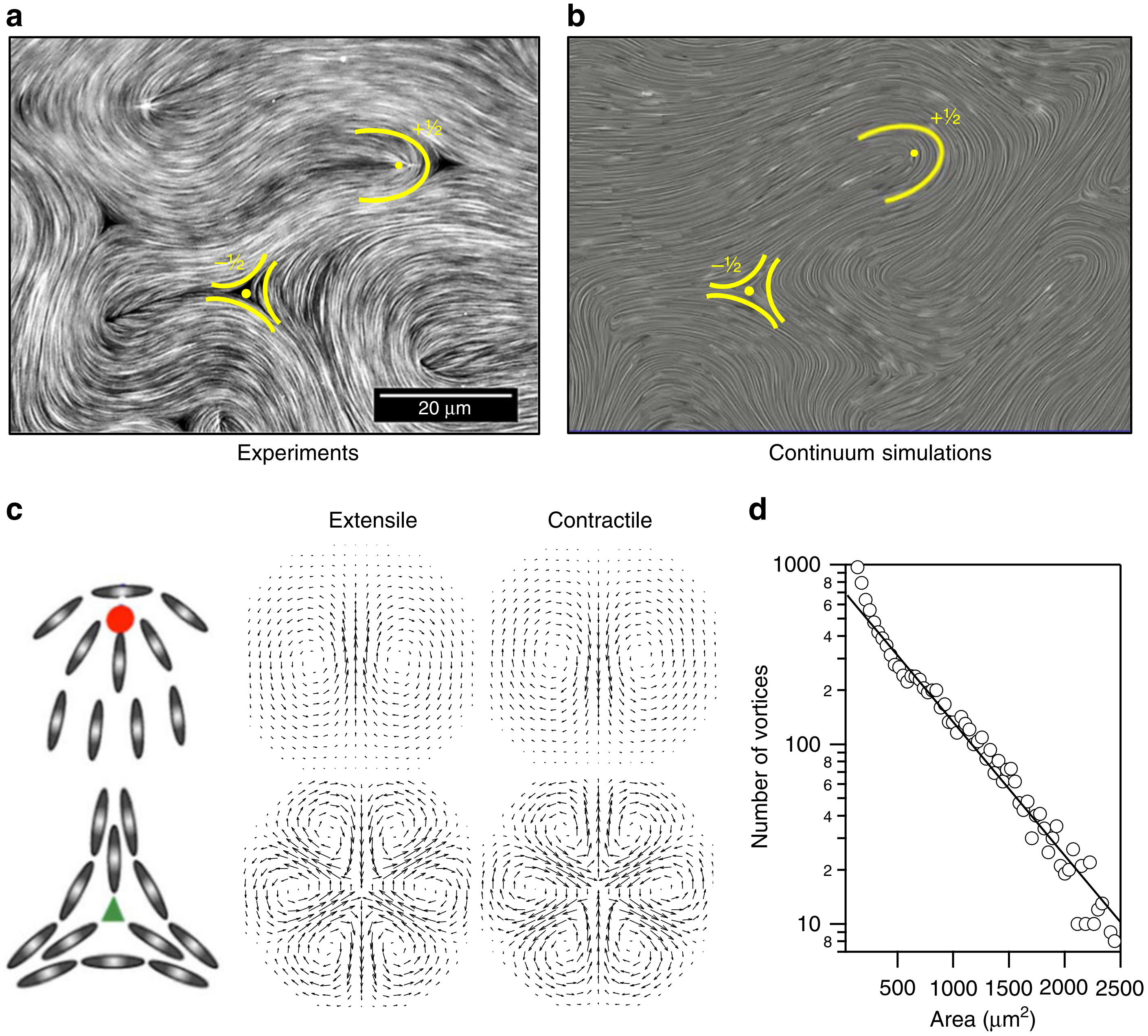


REVIEW ARTICLE

DOI: 10.1038/s41467-018-05666-8 OPEN

Active nematics

Amin Doostmohammadi[1], Jordi Ignés-Mullol[2], Julia M. Yeomans[1] & Francesc Sagués[2]



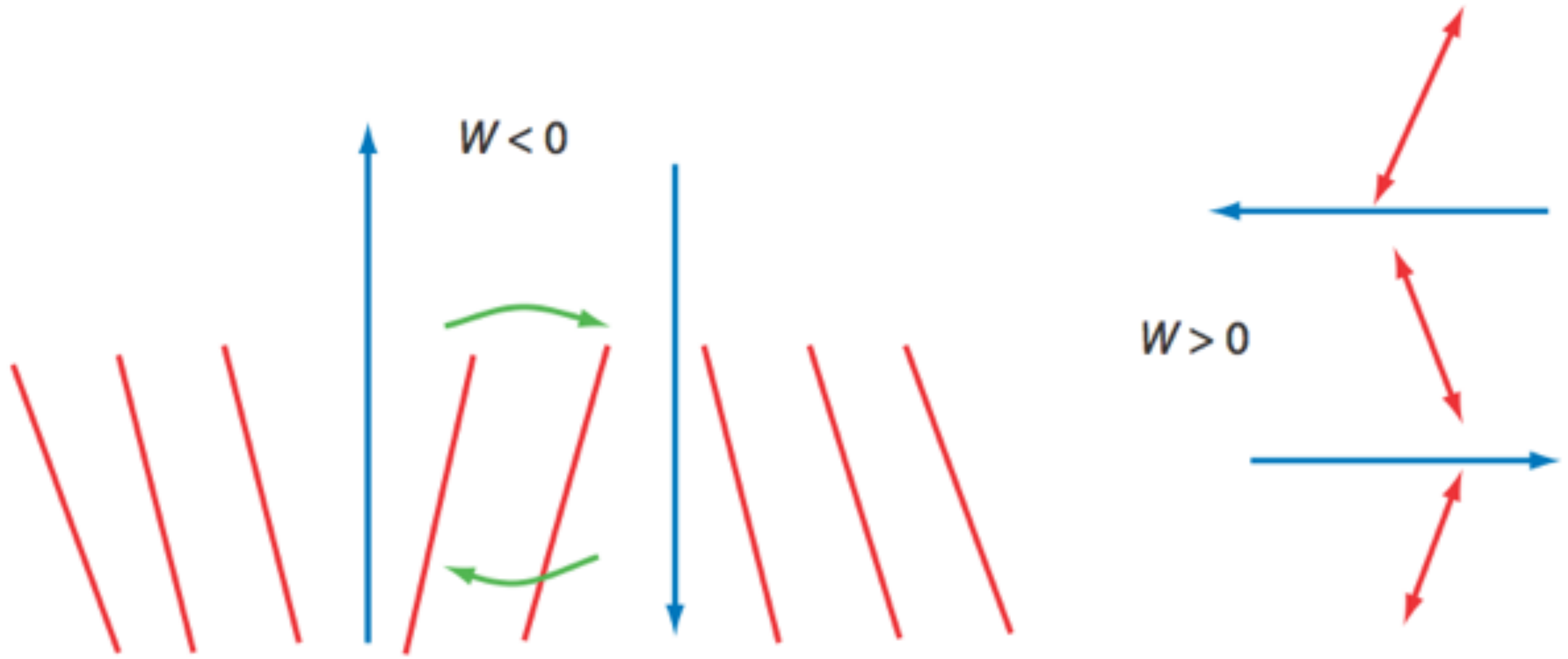
Experiments

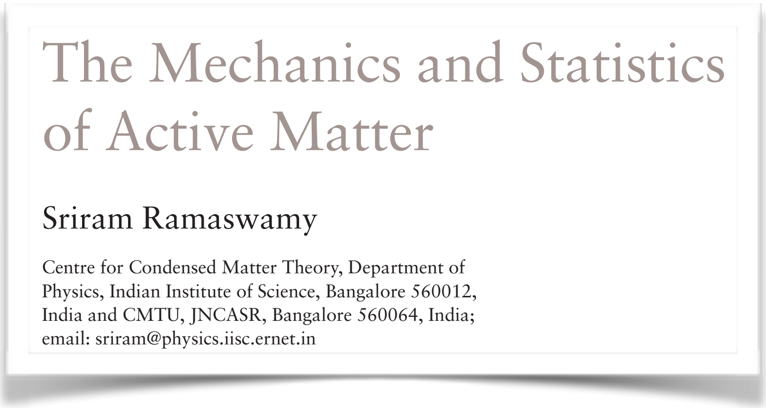
Continuum simulations

Fig. 1 Active nematic turbulence. **a** Fluorescence confocal microscopy micrograph of the active nematic in contact with an oil of 0.05 Pa s (see Supplementary Movie 1 where positive defects are tracked). **b** Snapshot of the time evolution from solving the continuum equations of motion, showing active turbulence. A comet-like, +1/2, and a trefoil-like, −1/2 defect are highlighted in each case. **c** Particle alignment and velocity fields around ±1/2 topological defects in extensile and contractile active systems. **d** Experimental distribution of vortex sizes in an active nematic in the regime of active turbulence, adapted from data in ref. [15], Nature Publishing Group. The solid line is an exponential fit to the data

INSTABILITY OF ACTIVE NEMATICS

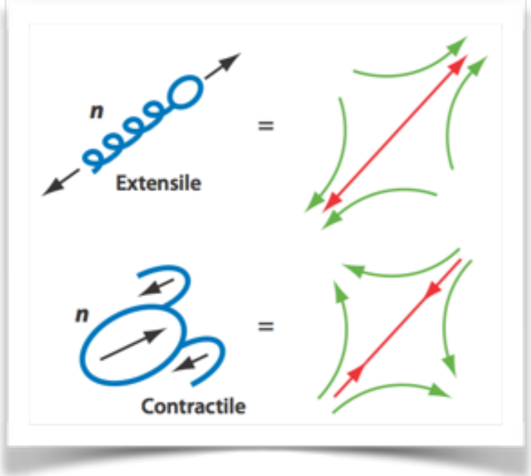
Active nematics exhibit a fundamental hydrodynamic instability




The Mechanics and Statistics of Active Matter

Sriram Ramaswamy

Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India and CMTU, JNCASR, Bangalore 560064, India;
email: sriram@physics.iisc.ernet.in



There are two unstable modes:

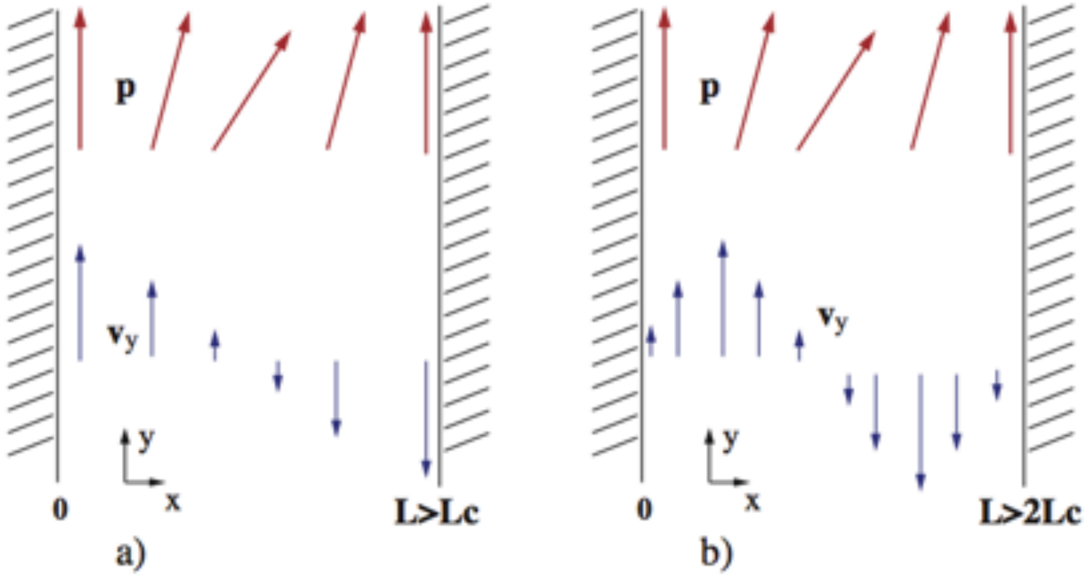
- *extensile* materials are unstable to **bend**
- *contractile* materials are unstable to **splay**

Aditi Simha, Ramaswamy, Phys. Rev. Lett. **89**, 058101 (2002)

EUROPHYSICS LETTERS 1 May 2005
Europhys. Lett., **70** (3), pp. 404–410 (2005)
DOI: 10.1209/epl/i2004-10501-2

Spontaneous flow transition in active polar gels

R. Voituriez[1], J. F. Joanny[1] and J. Prost[1,2]
[1] *Physicochimie Curie (CNRS-UMR168), Institut Curie, Section de Recherche 26 rue d'Ulm, 75248 Paris Cedex 05, France*
[2] *ESPCI - 10 rue Vauquelin, 75231 Paris Cedex 05, France*



The fundamental instability converts to a ***threshold*** for a spontaneous flow transition; the threshold depends on the *width* of the channel

In quasi-1d geometry it is associated with a ***splay*** deformation of the director field

$$\mathbf{n} = \cos\big(\theta(z)\big)\,\mathbf{e}_x + \sin\big(\theta(z)\big)\,\mathbf{e}_z$$


EUROPHYSICS LETTERS 1 May 2005
Europhys. Lett., **70** (3), pp. 404–410 (2005)
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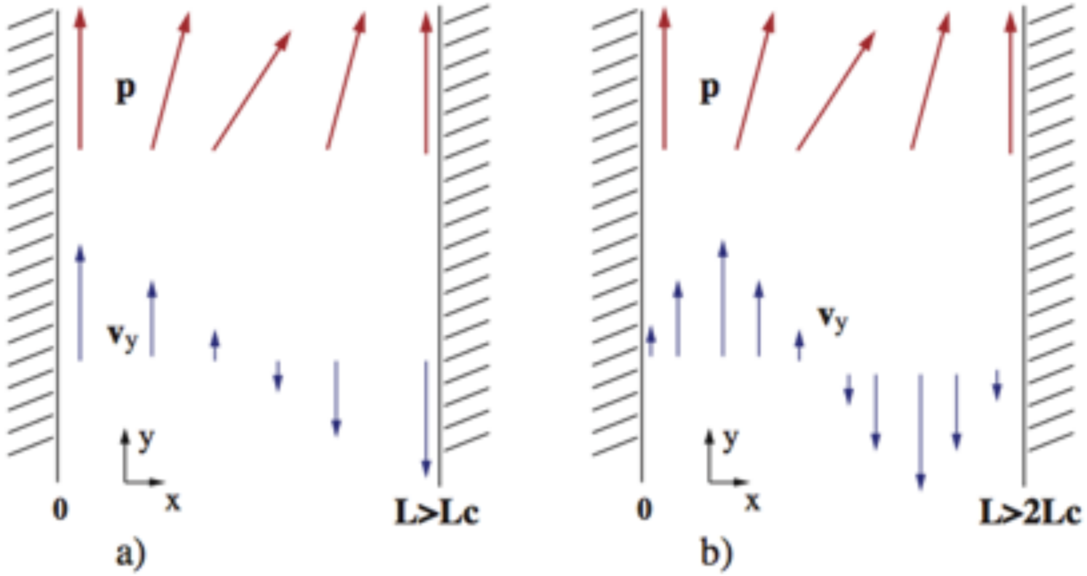

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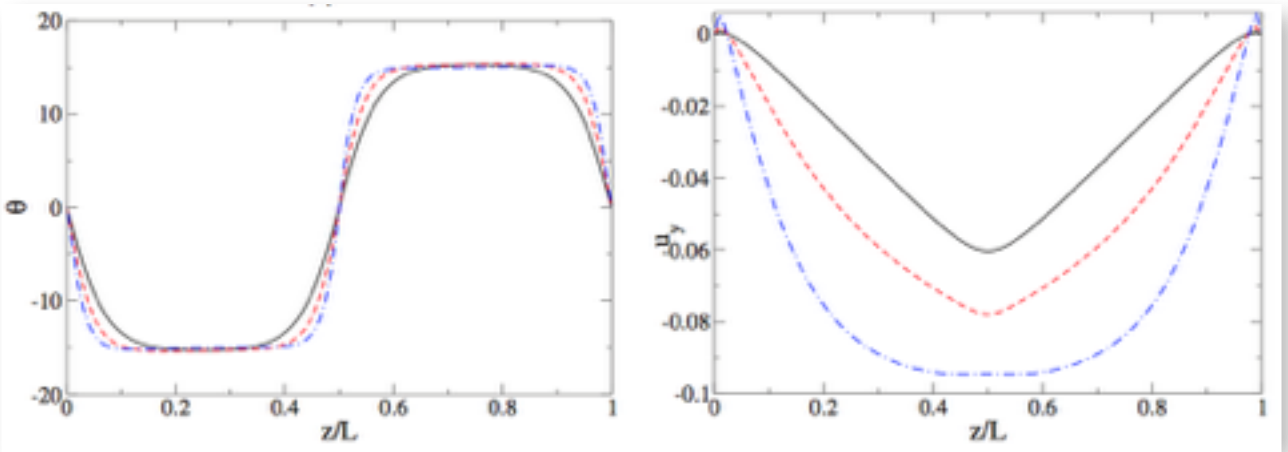
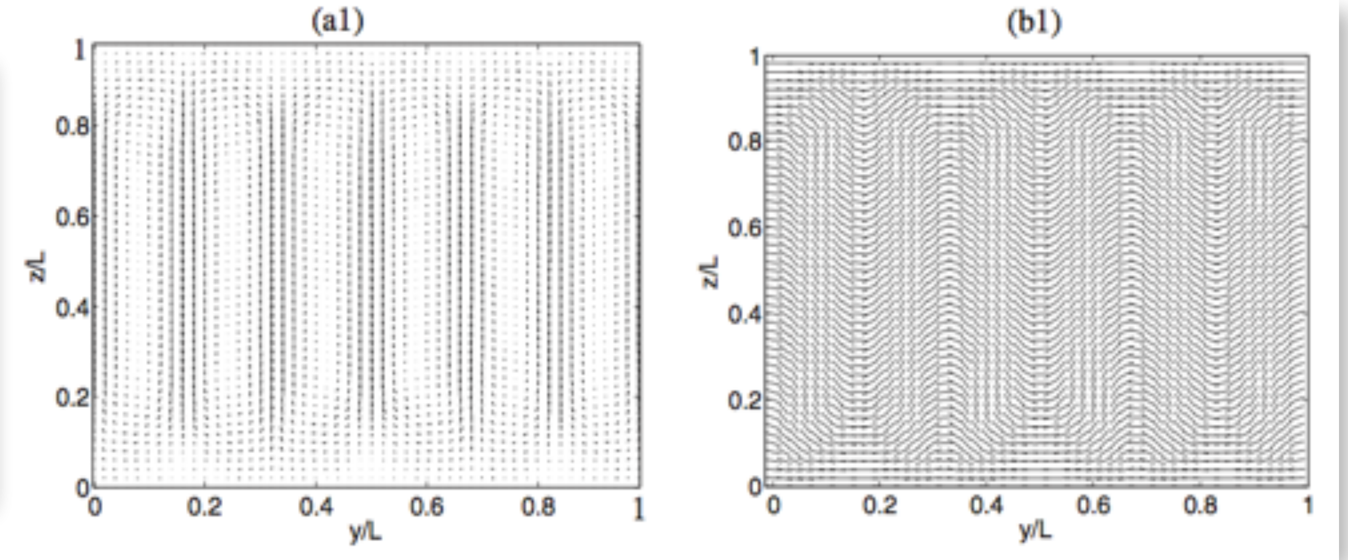
$$\mathbf{n} = \cos\big(\theta(z)\big)\,\mathbf{e}_x + \sin\big(\theta(z)\big)\,\mathbf{e}_z$$

This is confirmed in numerical simulations; although the symmetry of the resultant director profile and flow is different

Rolls form in quasi-2d geometry

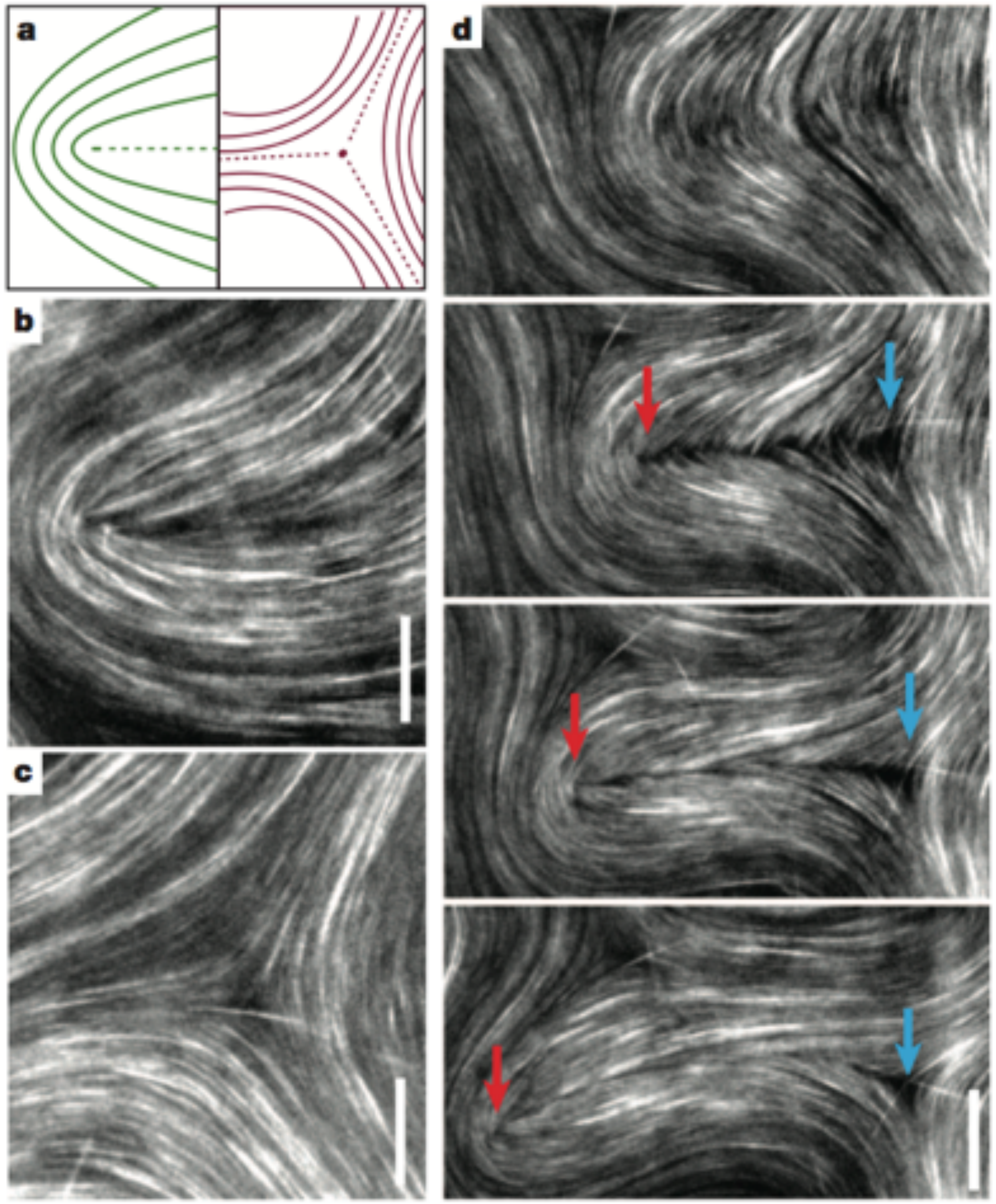


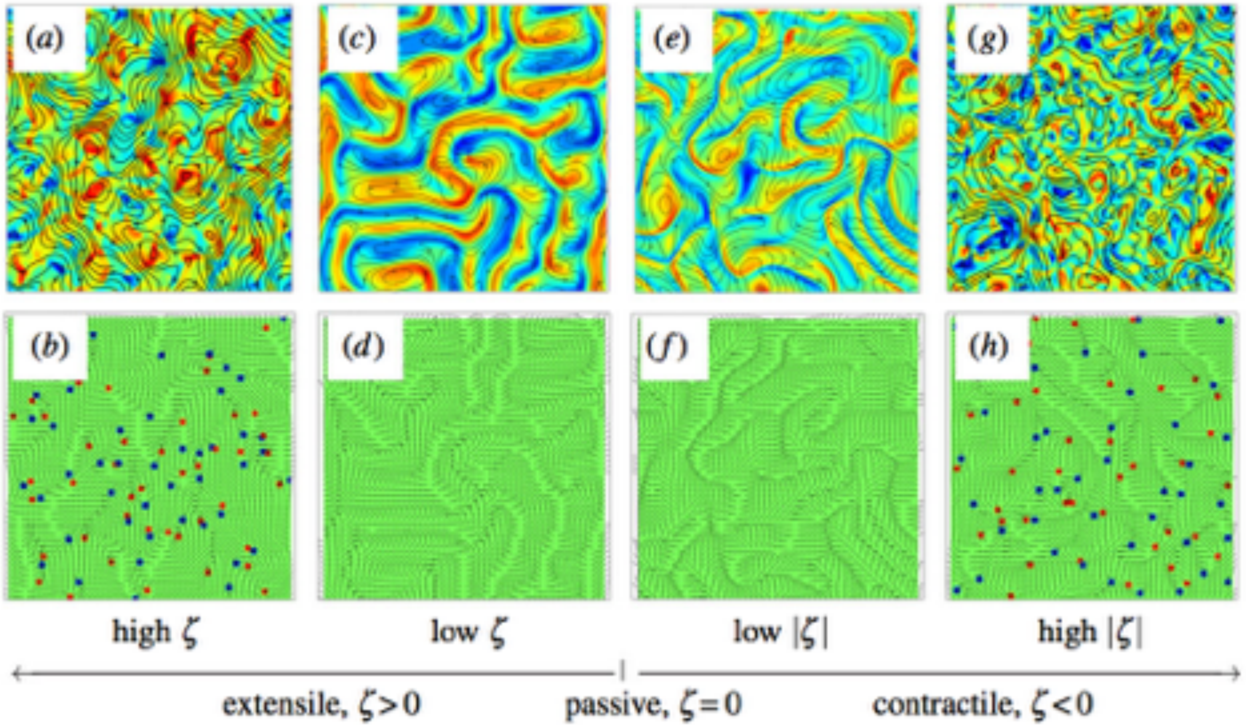


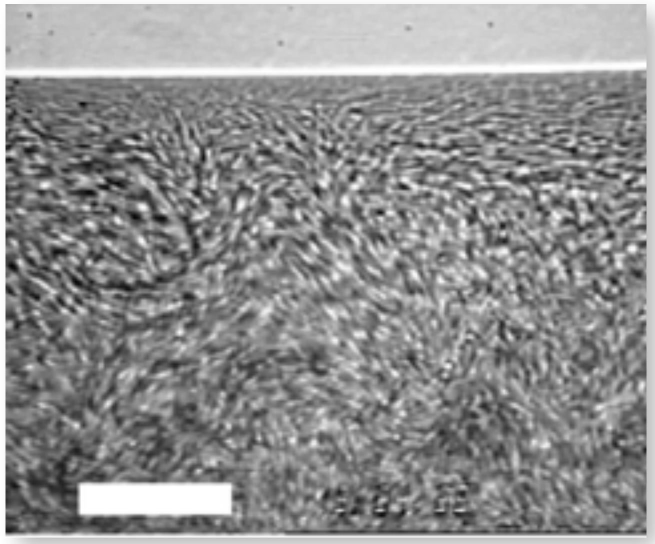
Marenduzzo, Orlandini, Cates & Yeomans, Phys. Rev. E **76**, 031921 (2007)

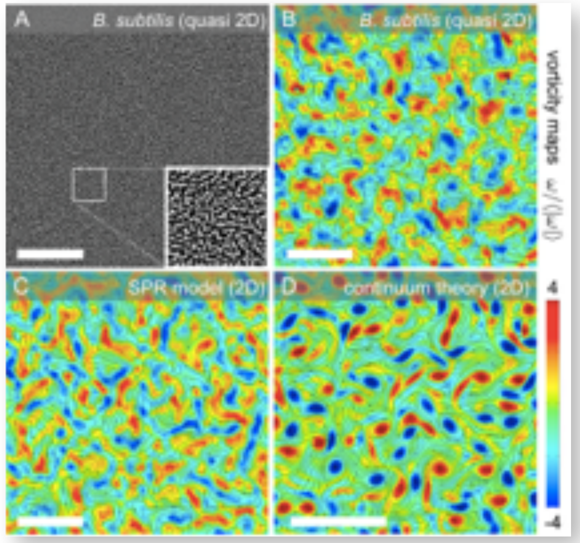
ACTIVE TURBULENCE

The instability leads to the production of defects; their proliferation creates a ‘turbulent’ state

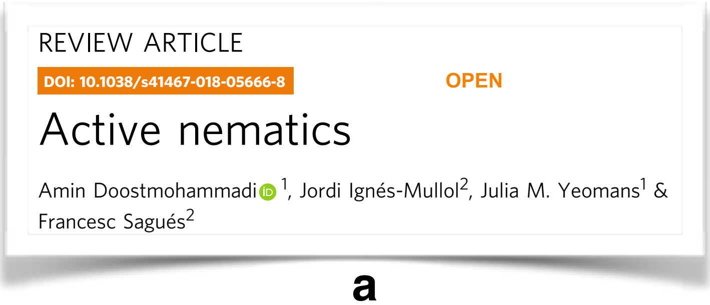








Sanchez *et al.*, Nature **491**, 431 (2012)
Dombrowski *et al.*, Phys. Rev. Lett. **93**, 098103 (2004)
Wensink *et al.*, Proc. Natl. Acad. Sci. USA **109**, 14308 (2012)
Thampi, Golestanian & Yeomans, EPL **105**, 18001 (2014)



REVIEW ARTICLE

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OPEN

Active nematics

Amin Doostmohammadi[1], Jordi Ignés-Mullol[2], Julia M. Yeomans[1] &
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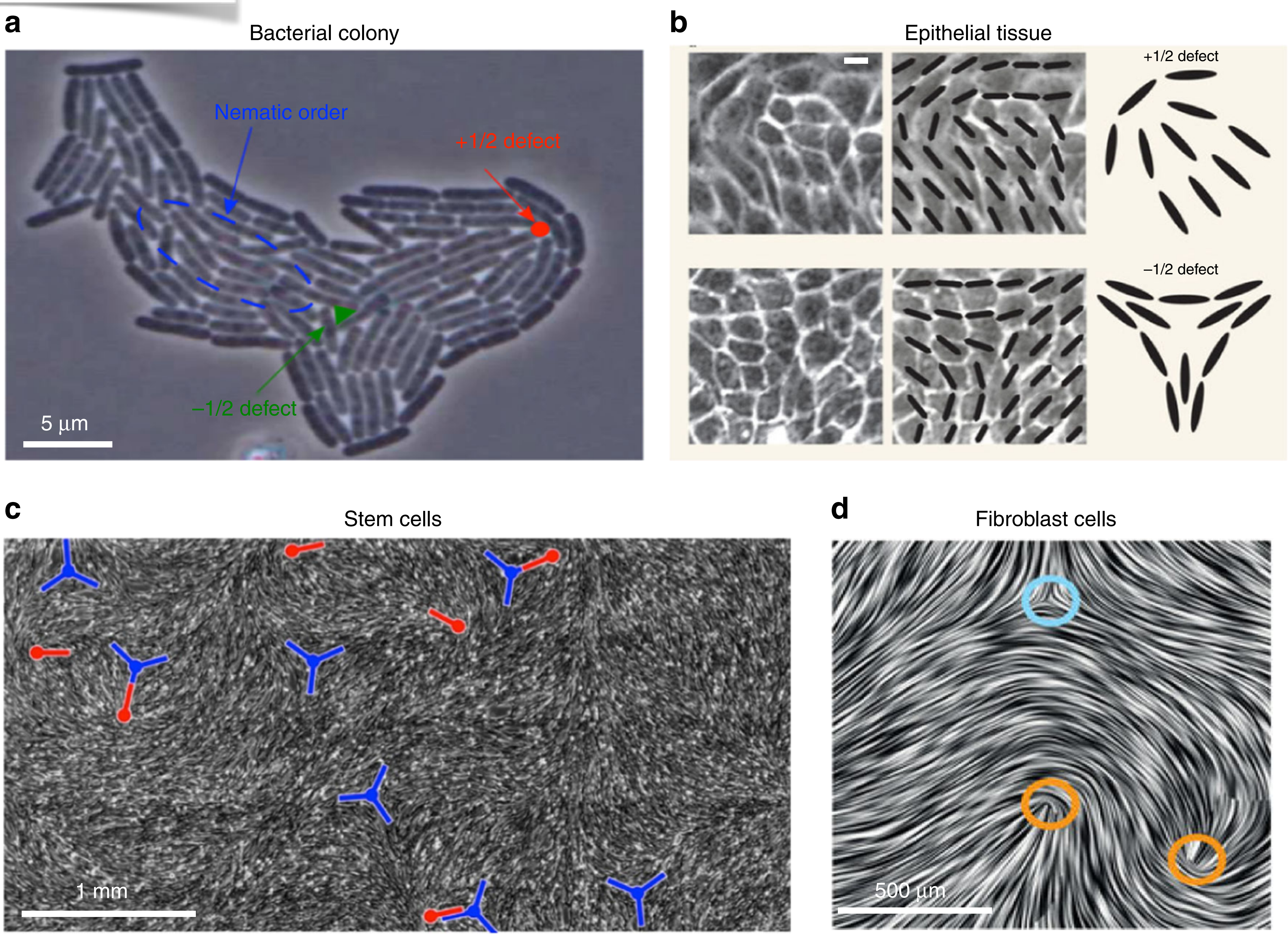
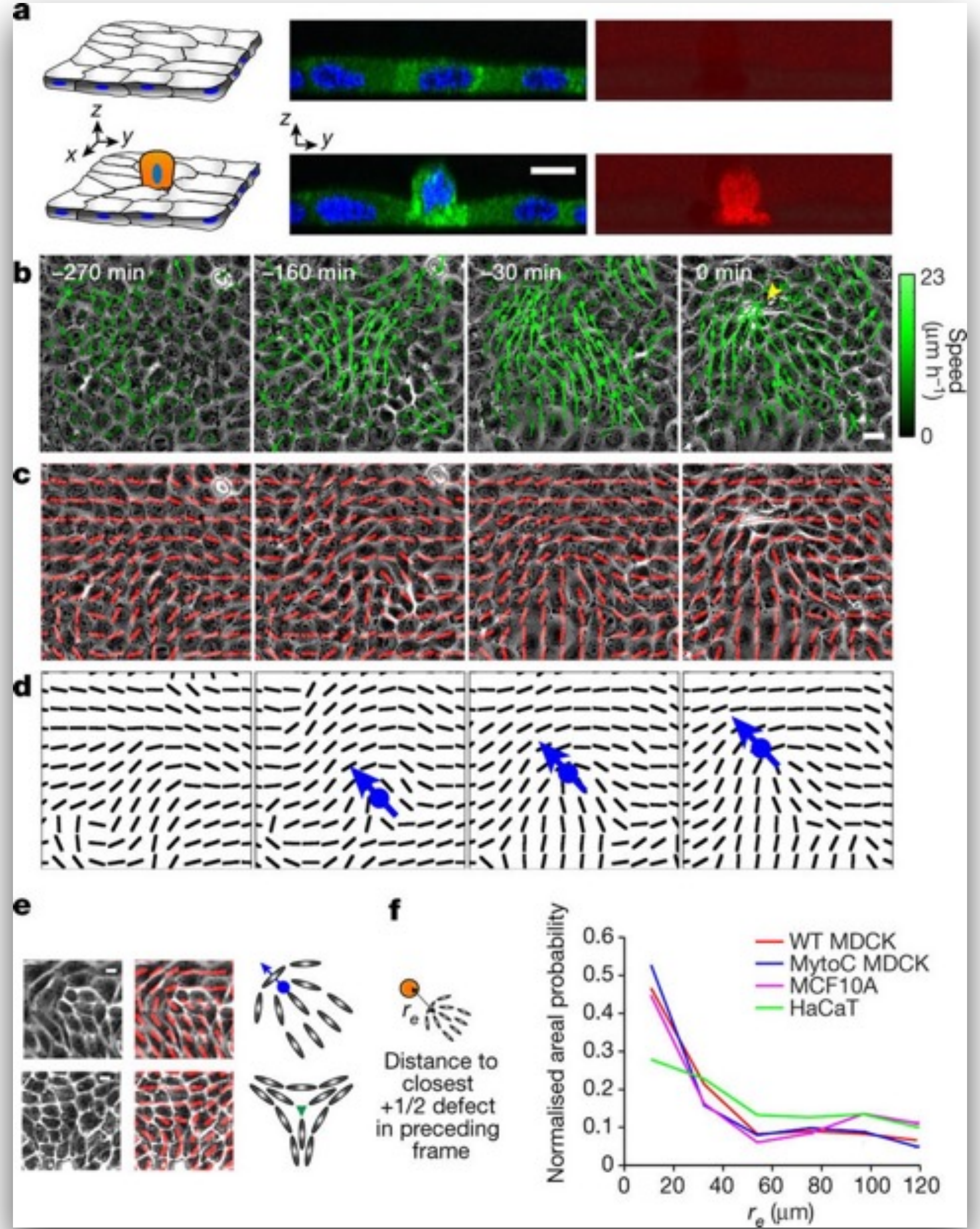
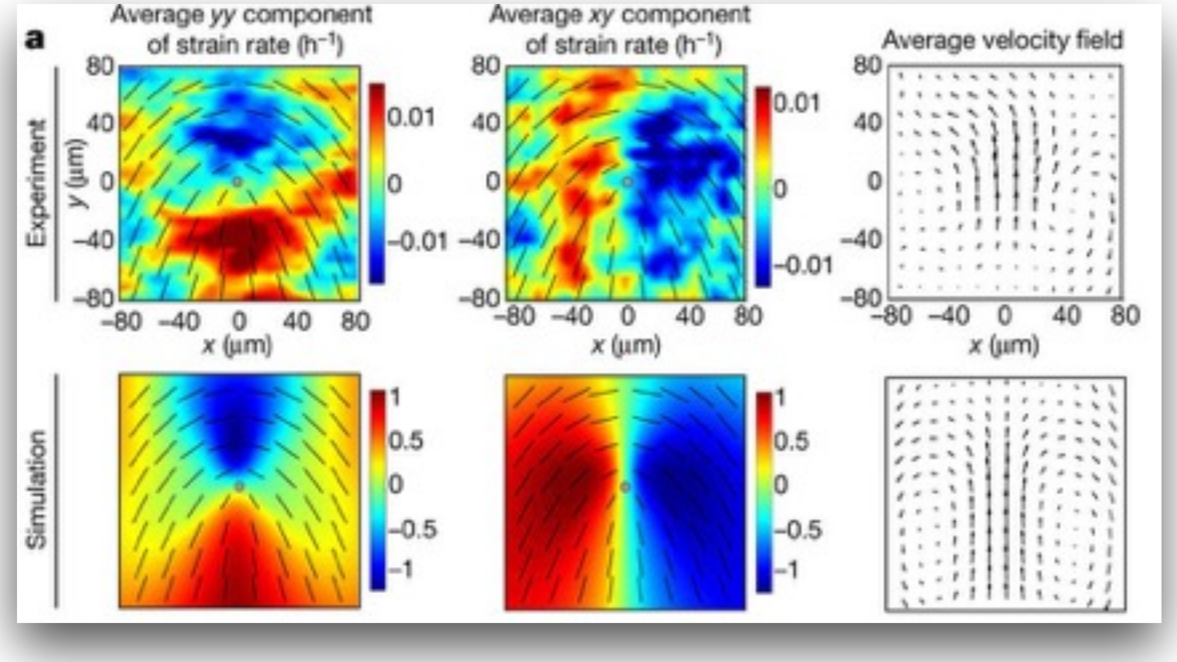


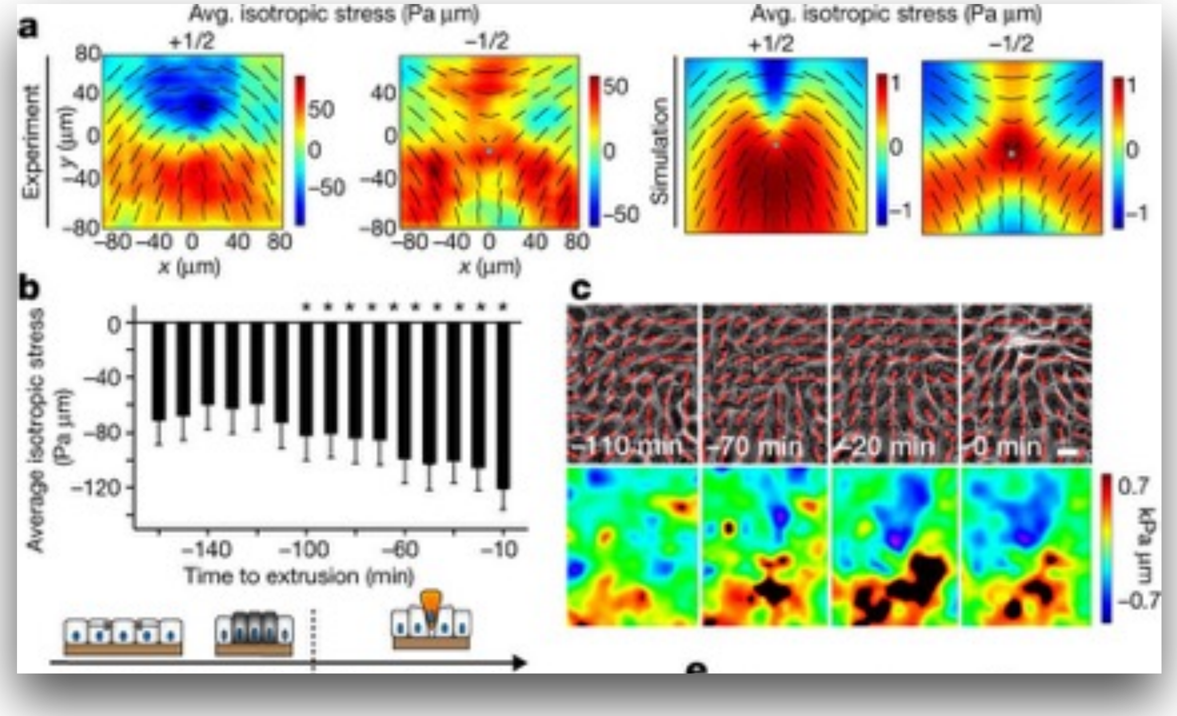
Fig. 4 Active nematic defects in biological systems. **a** Growing colony of *E. coli* bacteria[99] (Copyright (2014) by the American Physical Society). The motion of +1/2 defects towards the growing interface can lead to shape changes of the colony. **b** Epithelial tissue of Madine-Darby canine kidney (MDCK) cells. Scale bar is 10 μm[32] (Nature Publishing Group). Strong correlations between the position of +1/2 defects and cell death and extrusion have been reported. **c** Monolayer of neural progenitor stem cells[100] (Nature Publishing Group). Cells are depleted from −1/2 defects (blue, trefoil symbols) and accumulate at +1/2 ones (red, comet-like symbols). **d** Dense monolayer of mouse fibroblast cells[57] (Nature Publishing Group) showing −1/2 and +1/2 topological defects marked by blue and orange circles, respectively

Topological defects in epithelia govern cell death and extrusion

Thuan Beng Saw[1,2]*, Amin Doostmohammadi[3]*, Vincent Nier[4], Leyla Kocgozlu[1], Sumesh Thampi[3,5], Yusuke Toyama[1,6,7], Philippe Marcq[4], Chwee Teck Lim[1,2], Julia M. Yeomans[3] & Benoit Ladoux[1,8]



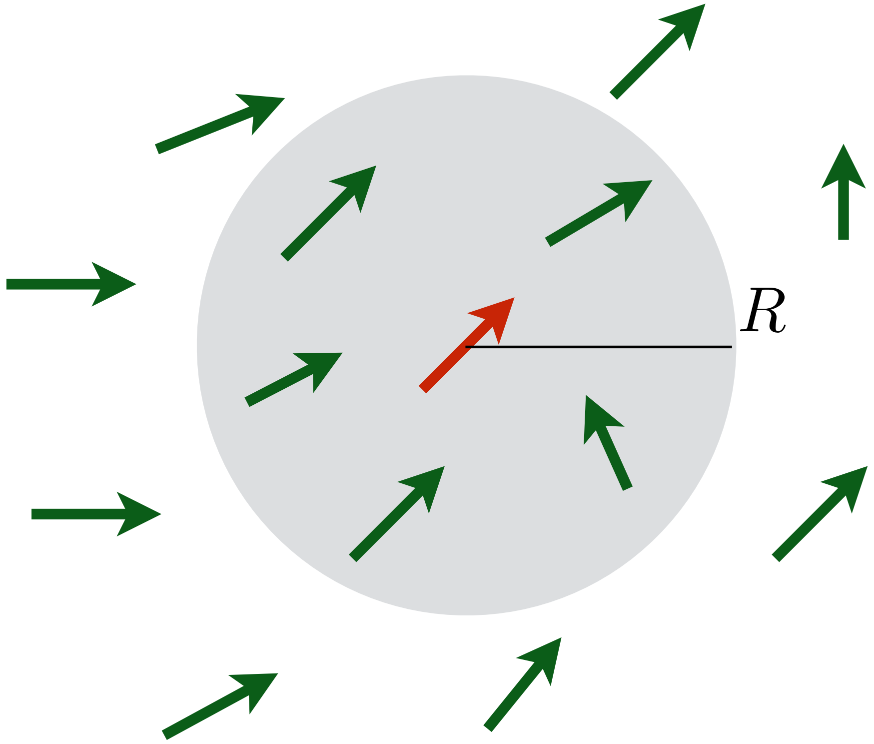




Videos from Beng Saw *et al*.

Vicsek Model

Birds (or boids) fly with some speed and **align** with their neighbours, subject to **noise**



step 1: propagation

$$\mathbf{x}_i(t+\delta t) = \mathbf{x}_i(t) + \mathbf{v}_i(t)\,\delta t$$

step 2: alignment

$$\mathbf{v}_i = v_0\big[\cos\theta_i\,\mathbf{e}_x + \sin\theta_i\,\mathbf{e}_y\big]$$

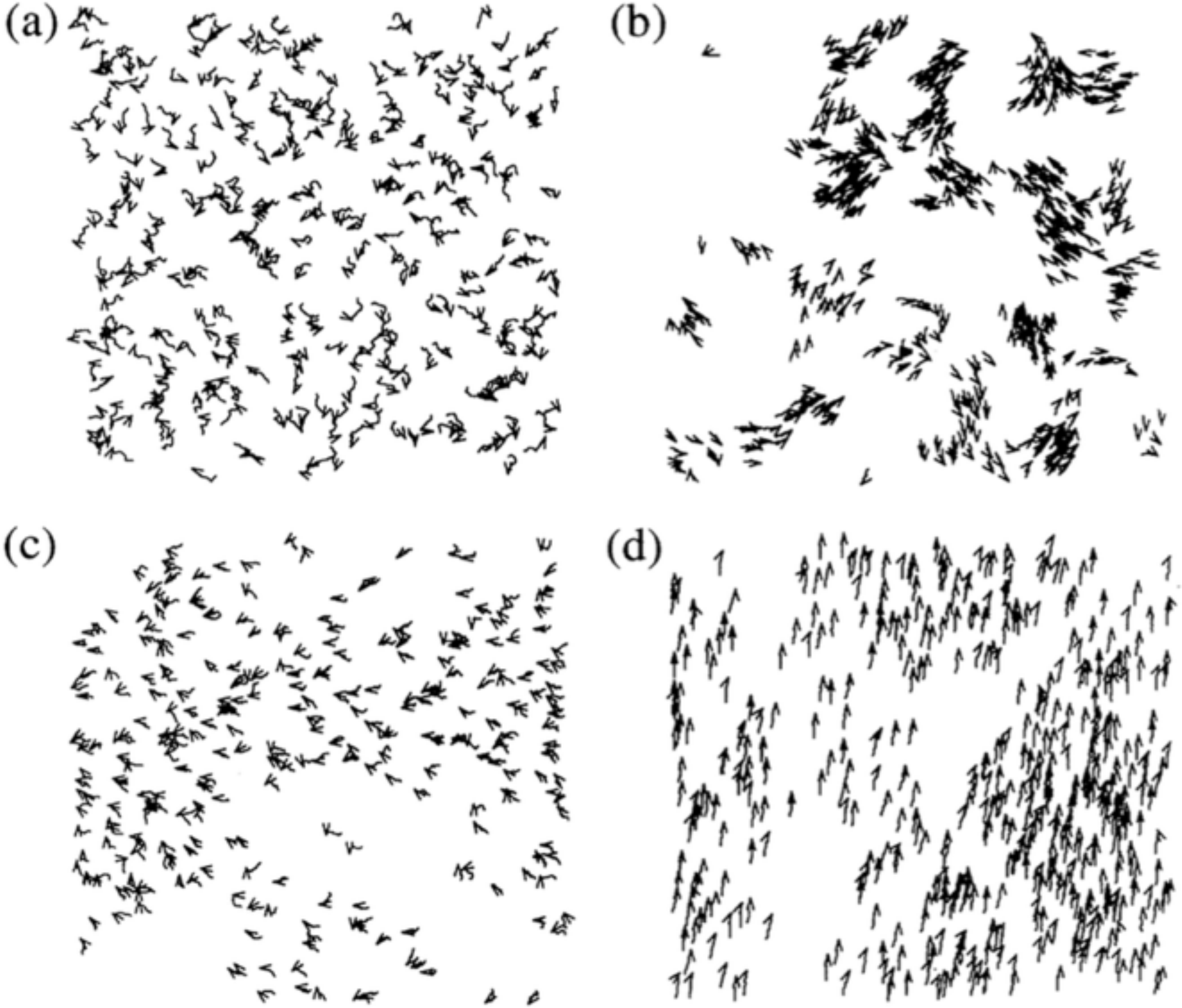
$$\theta_i(t+\delta t) = \big\langle\theta_j(t)\big\rangle_{|\mathbf{x}_i-\mathbf{x}_j|<R} + \xi_i(t) \qquad \xi_i(t)\in[-\eta,\eta]$$

uniform random variable

angular noise

Relevant variables:	flying speed	v_0	*unimportant*
	interaction range	R	*unimportant*
	number density	$\rho = N/L^2$	
	noise strength	η	

Vicsek Model



low density
high noise

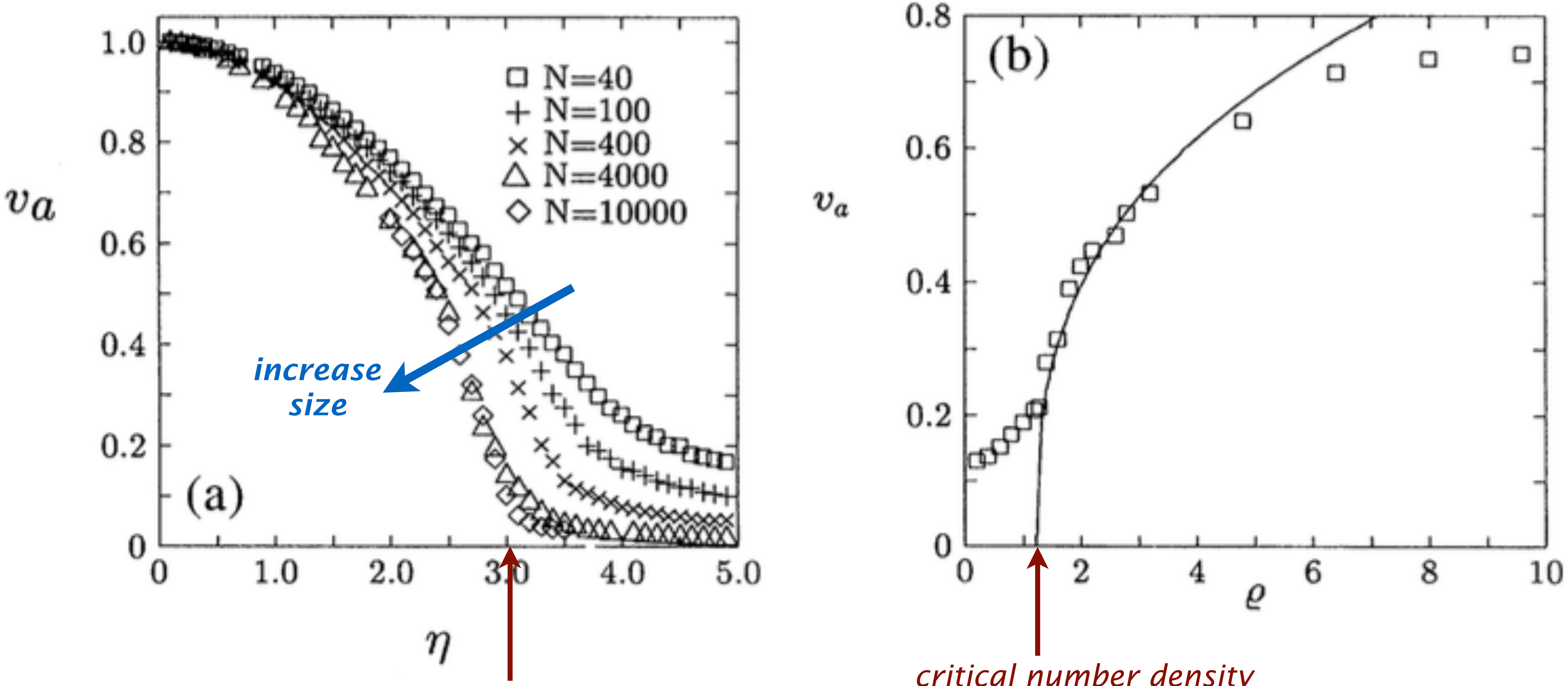
low density
low noise

high density
high noise

high density
low noise

Vicsek Model

Look for a ‘flocking transition’ as we vary the relevant parameters



increase size

critical noise strength

critical number density

Reminiscent of a continuous transition with finite size effects

Vicsek Model

It took over 10 years to discover that this paradigm is not quite correct

The general consensus now is that the transition is ***discontinuous***

(a) order parameter

(b) Binder cumulant

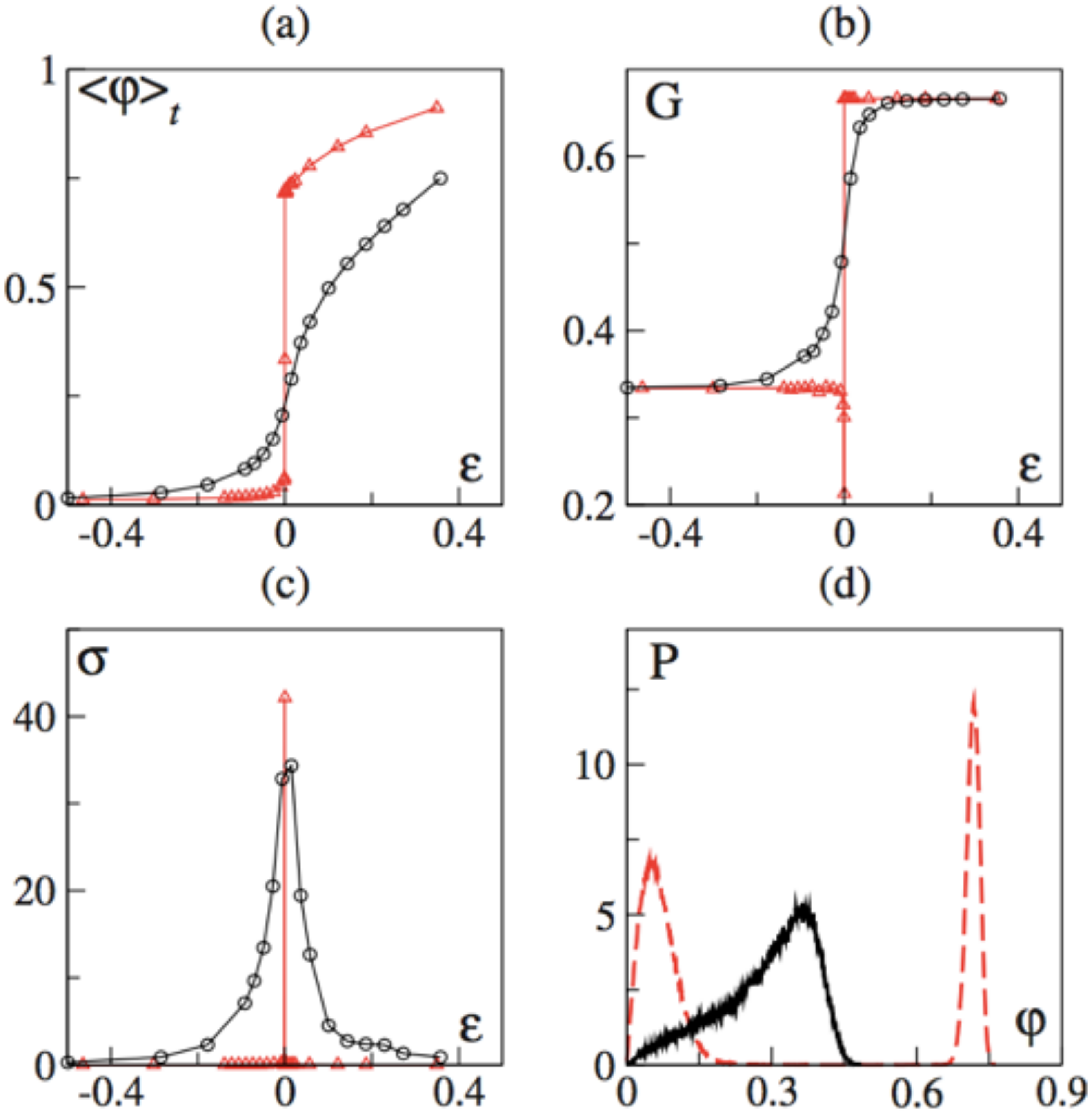
$$G(\eta, L) = 1 - \frac{\langle U^4(t) \rangle_t}{3\langle U^2(t) \rangle_t^2}$$

(c) variance

(d) probability distribution

black circles: angular noise

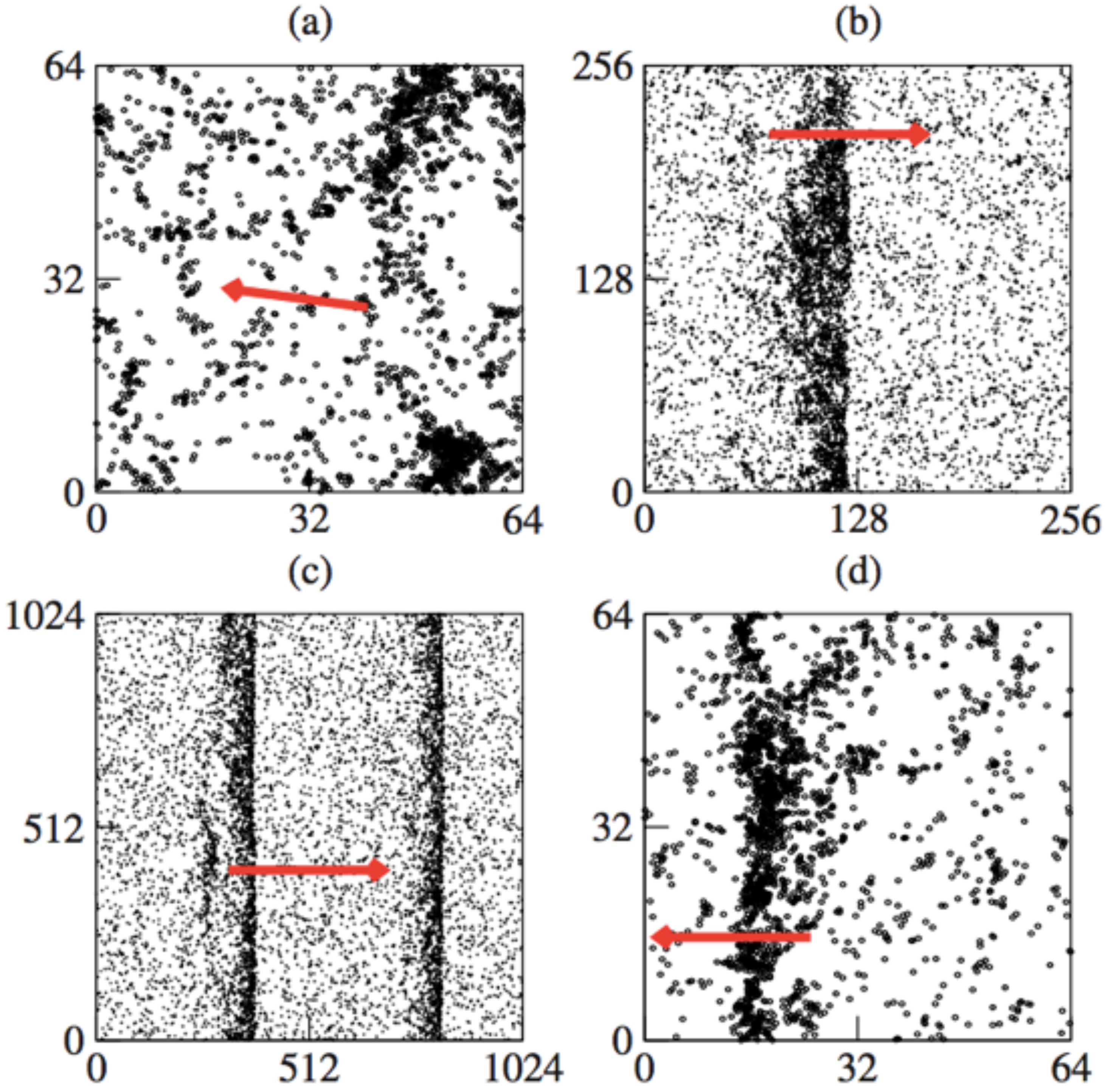
red triangles: vectorial noise



Chaté *et al.*, Phys Rev E **77**, 046113 (2008)

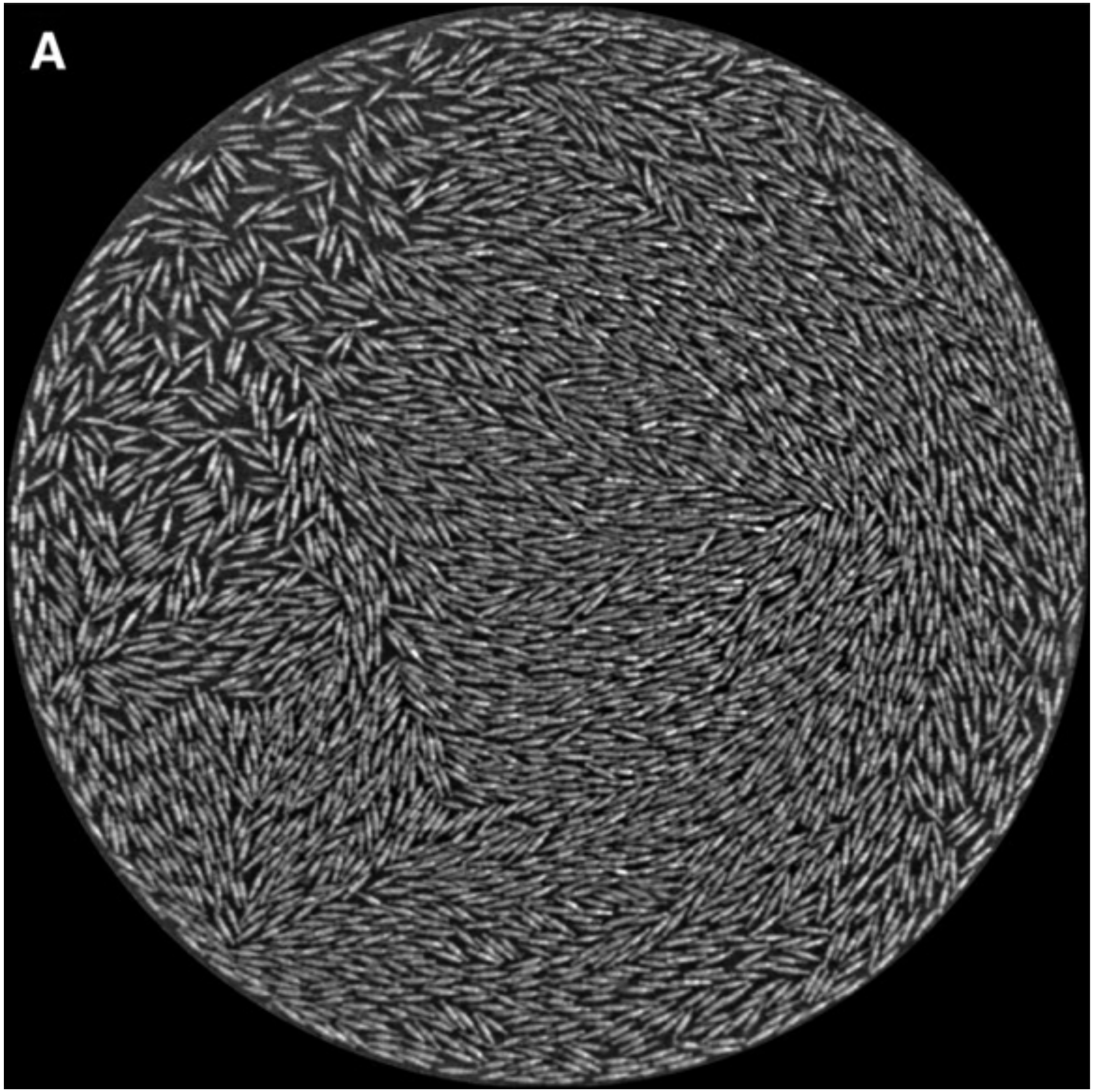
Nature of the Ordered Phase

There are travelling bands of high density and order separated by disordered low density regions



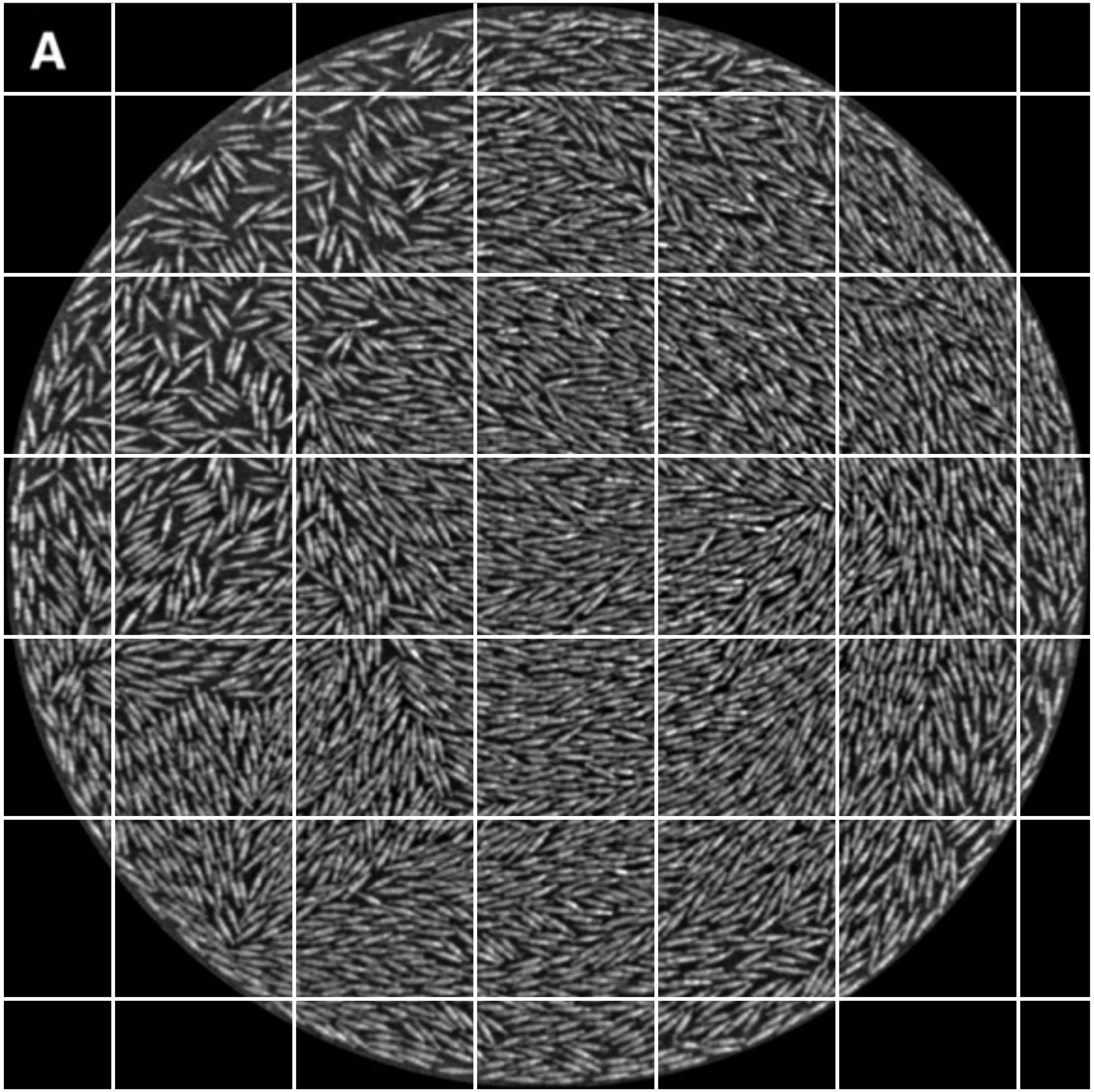
Chaté *et al.*, Phys Rev E **77**, 046113 (2008)

Giant Number Fluctuations



Narayan, Ramaswamy & Menon, *Science* **317**, 105 (2007)

Giant Number Fluctuations



Narayan, Ramaswamy & Menon, *Science* **317**, 105 (2007)

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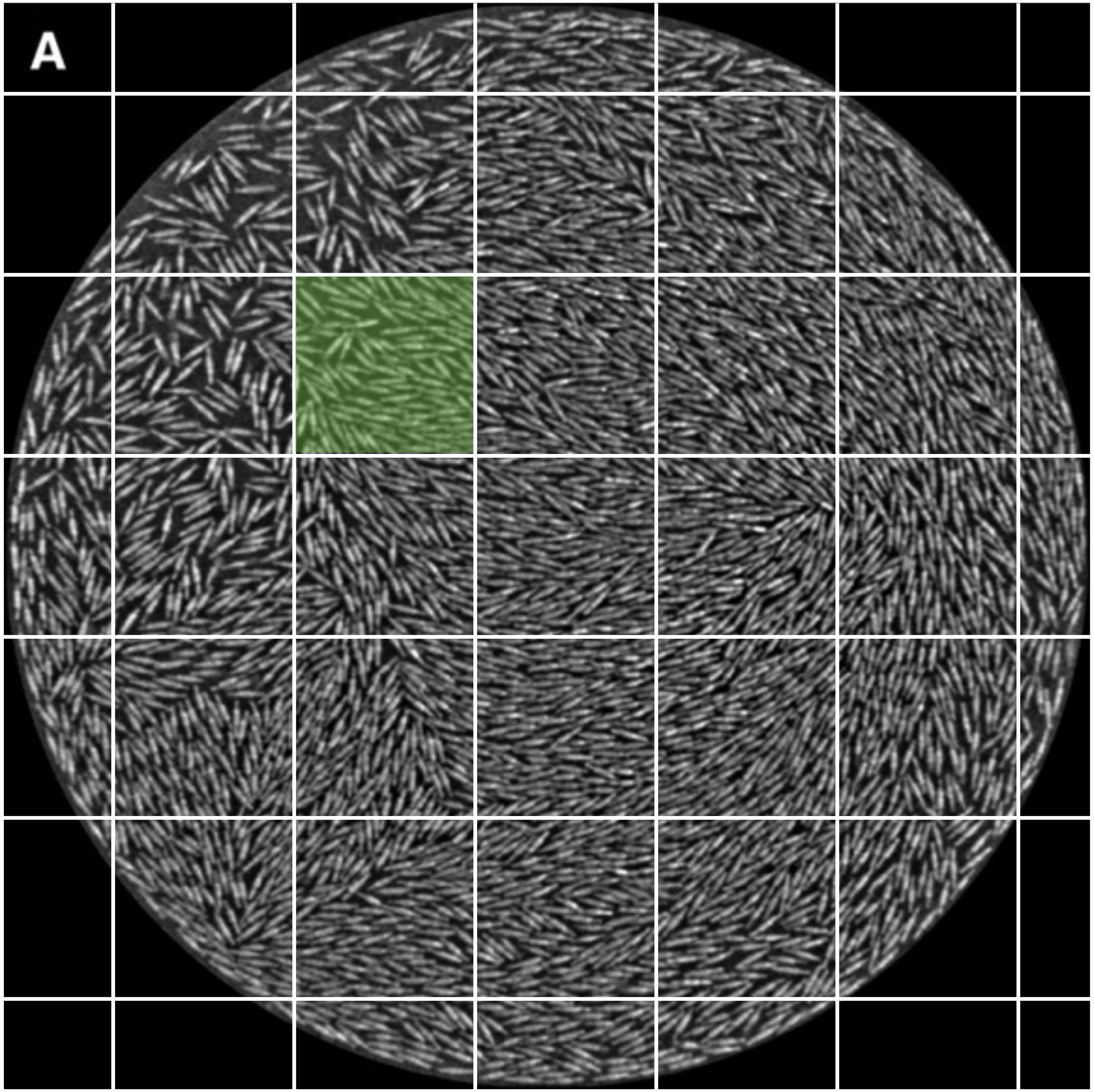

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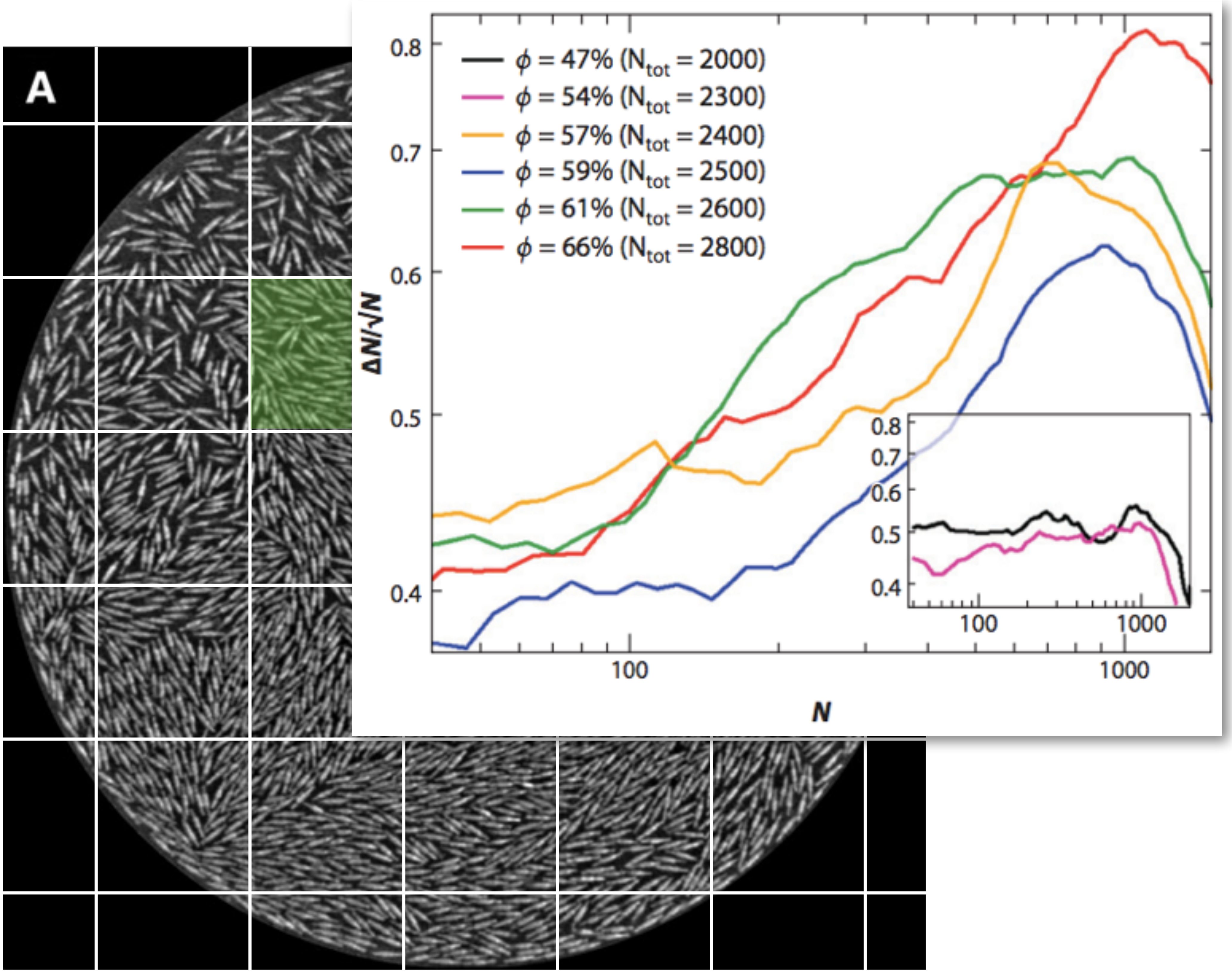

Narayan, Ramaswamy & Menon, *Science* **317**, 105 (2007)

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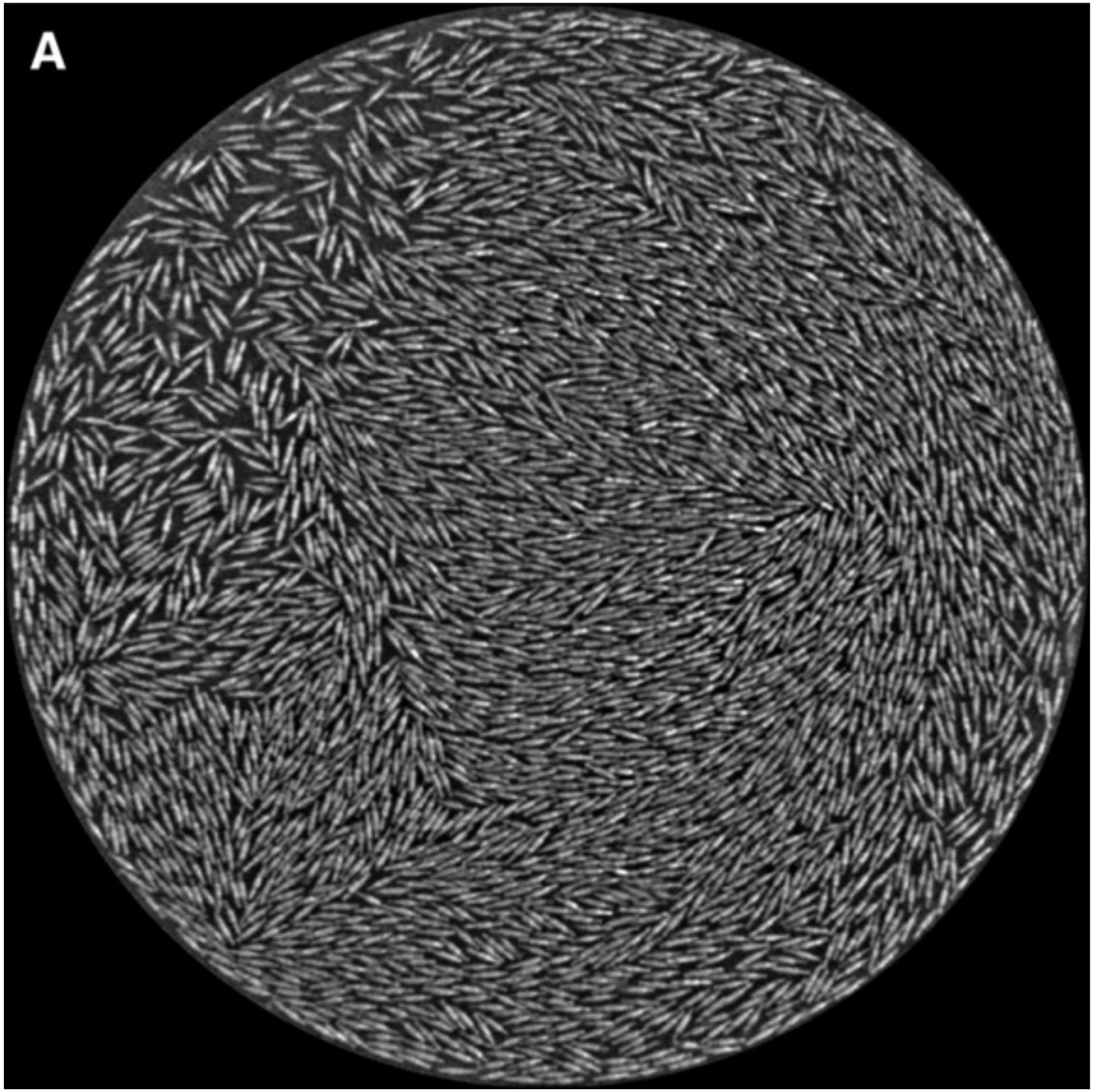
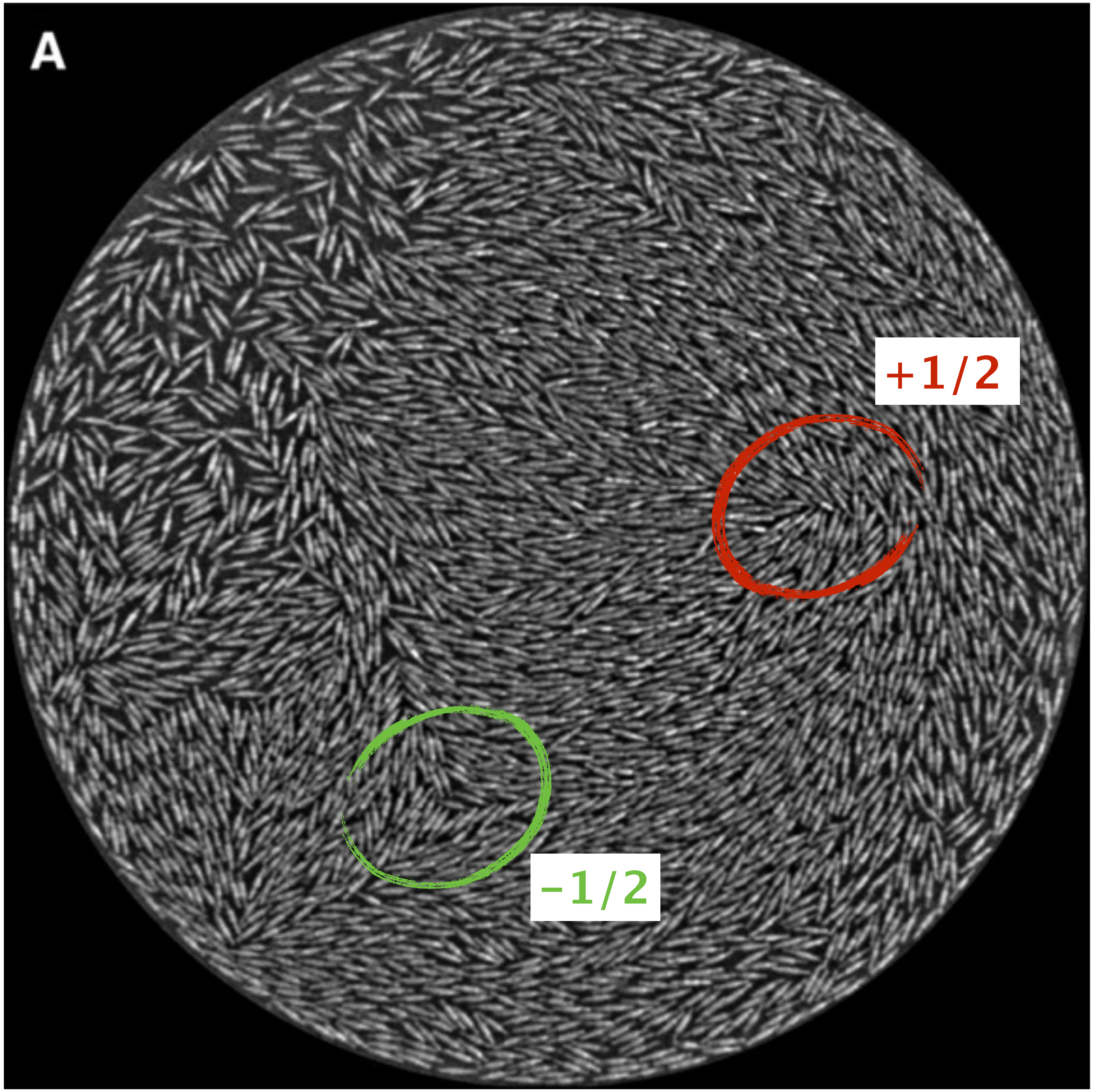


this system is nematic ‼

Narayan, Ramaswamy & Menon, *Science* **317**, 105 (2007)

Giant Number Fluctuations



this system is nematic !!

Narayan, Ramaswamy & Menon, *Science* **317**, 105 (2007)

Active Nematics

As in active polar fluids, it is the active particle current flux that is most interesting

continuity equation $\partial_t \rho = -\nabla \cdot \mathbf{J}$

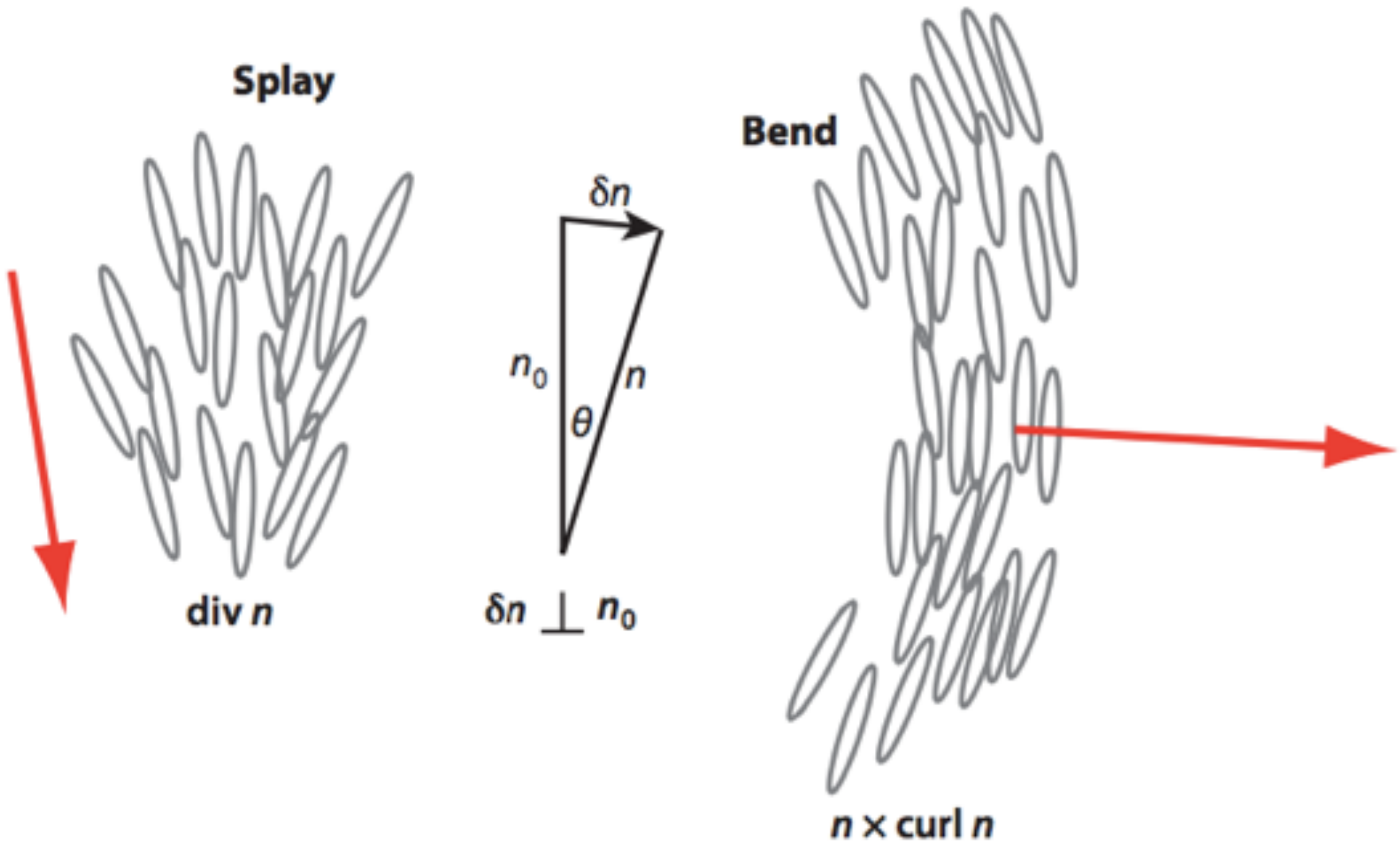
$$\mathbf{J} = -\frac{1}{\gamma_\rho}\nabla\frac{\delta F}{\delta \rho} + \zeta\nabla\cdot\mathbf{Q}$$

active flux

$$\nabla\cdot\mathbf{Q} \sim \mathbf{n}(\nabla\cdot\mathbf{n}) + (\mathbf{n}\cdot\nabla)\mathbf{n}$$

splay *bend*

Gradients in the orientation generate particle currents



$$\mathbf{n} = \sin\theta(x,y)\,\mathbf{e}_x + \cos\theta(x,y)\,\mathbf{e}_y$$

$$\approx \theta\,\mathbf{e}_x + \mathbf{e}_y$$

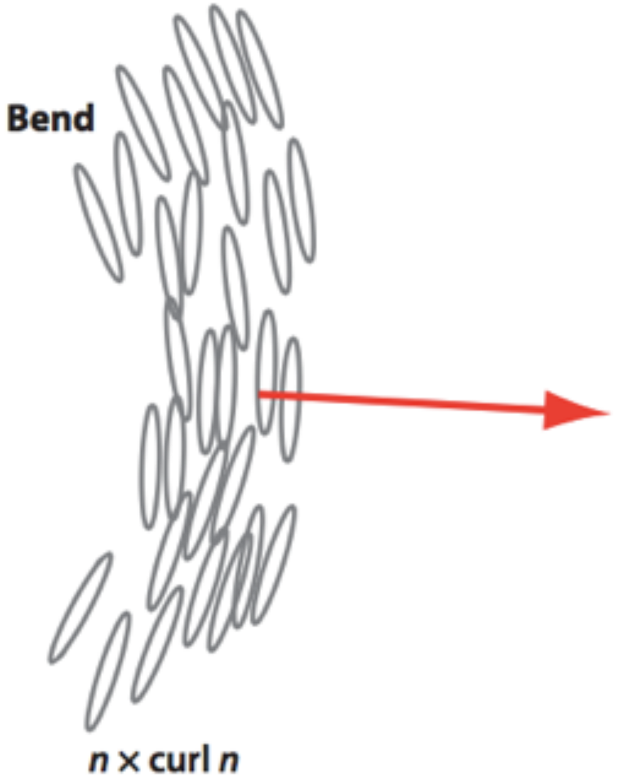
θ small

bend $(\mathbf{n}\cdot\nabla)\mathbf{n} \approx \partial_y\theta\,\mathbf{e}_x$

splay $\mathbf{n}(\nabla\cdot\mathbf{n}) \approx \partial_x\theta\,\mathbf{e}_y$

Giant Number Fluctuations

The active flux drives particle motion, so the diffusive particle flux should have comparable magnitude



scalings

$$\underbrace{-D\nabla\delta\rho}_{\text{diffusive flux}} \quad \sim \quad \underbrace{\zeta\nabla\cdot\mathbf{Q}}_{\text{active flux}}$$

$$-D\partial_x\delta\rho \sim \zeta\partial_y\theta$$

$$\Longrightarrow \quad |\delta\rho|^2 \sim |\theta|^2 \sim \frac{1}{q^2}$$

$$\boxed{\Longrightarrow \quad \delta N \sim N^{1/2+1/d}}$$

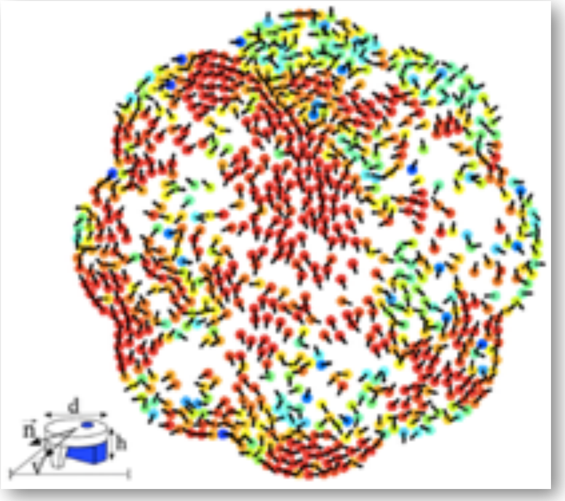
as before

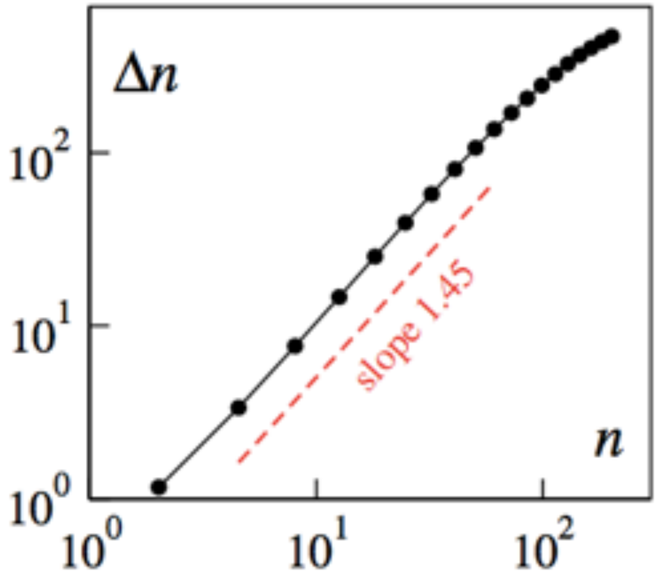
giant number (density) fluctuations are a generic feature of active systems, both polar and nematic

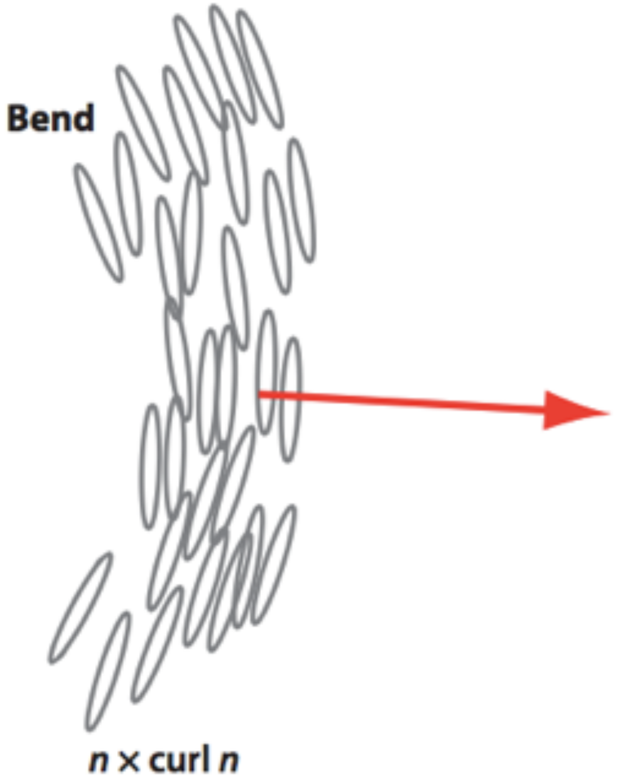
Giant Number Fluctuations

giant number (density) fluctuations are a generic feature of active systems, both polar and nematic

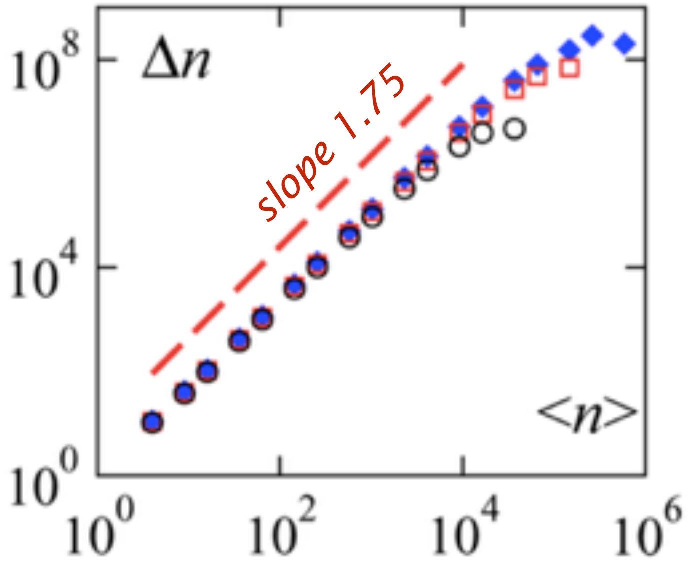
vibrated polar discs

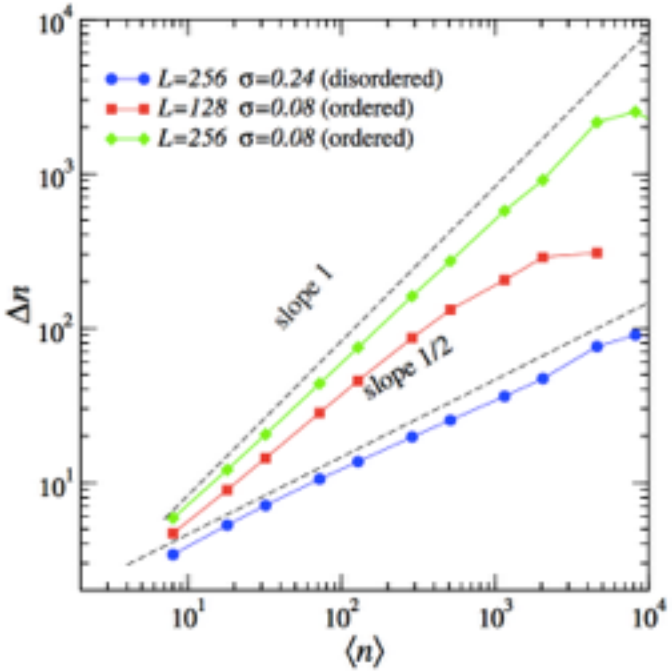






simulations of the metric-free Vicsek model





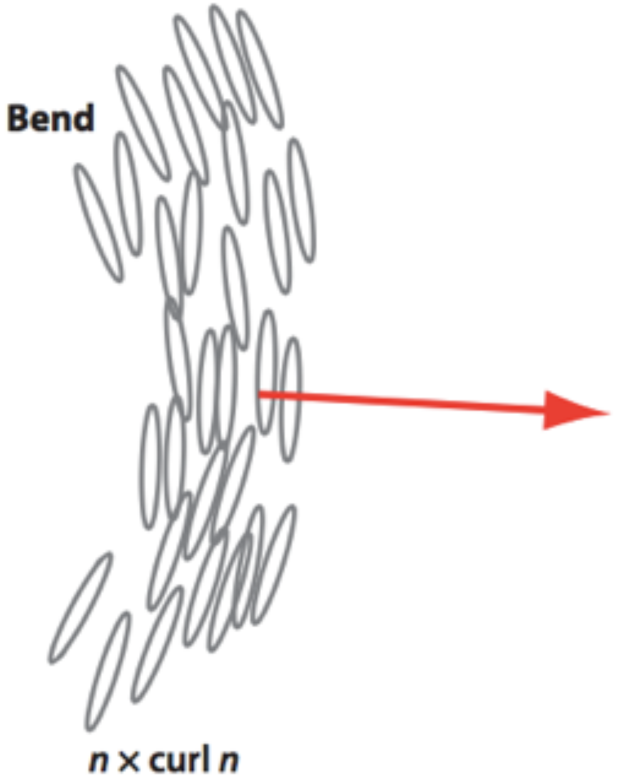
simulations of a 'nematic' Vicsek model

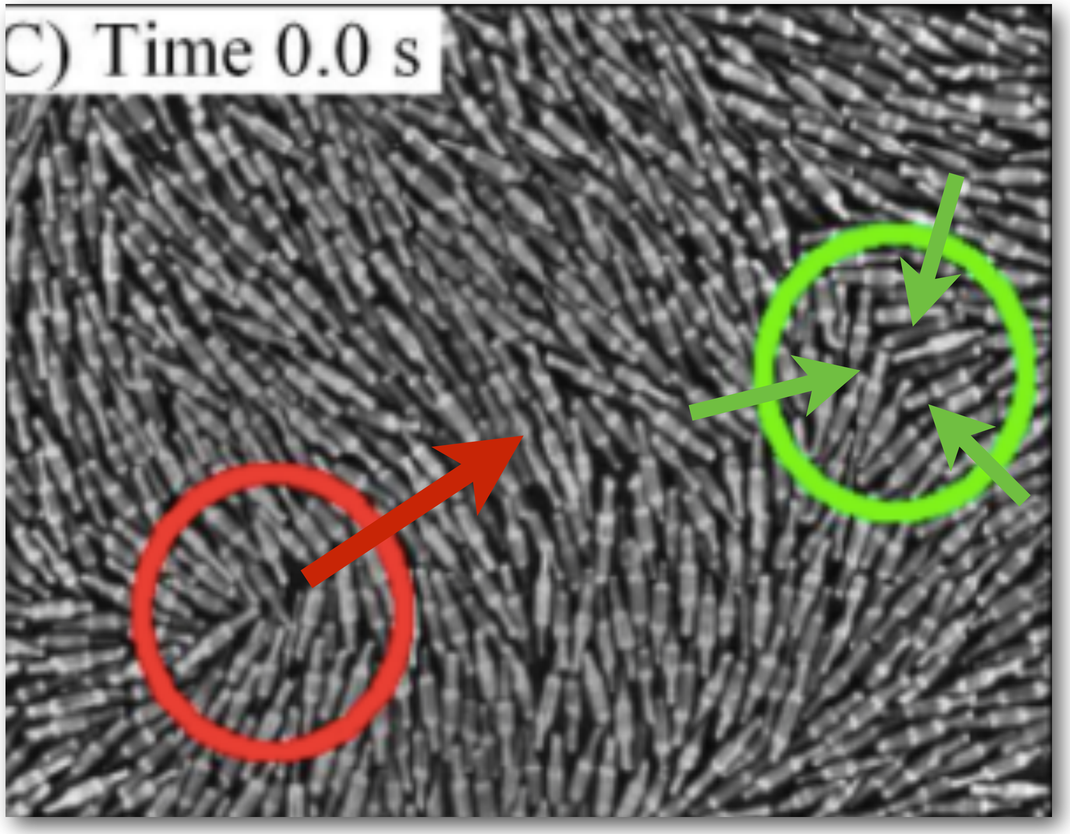
Chaté, Ginelli & Montange, *Phys Rev Lett* **96**, 180602 (2006)
Deseigne, Dauchot & Chaté, *Phys Rev Lett* **105**, 098001 (2010)
Ginelli & Chaté, *Phys Rev Lett* **105**, 168103 (2010)

Self-Propulsion of Defects

Distortions in the director are especially strong around topological defects

The active current leads to directed motion of defects in active nematics

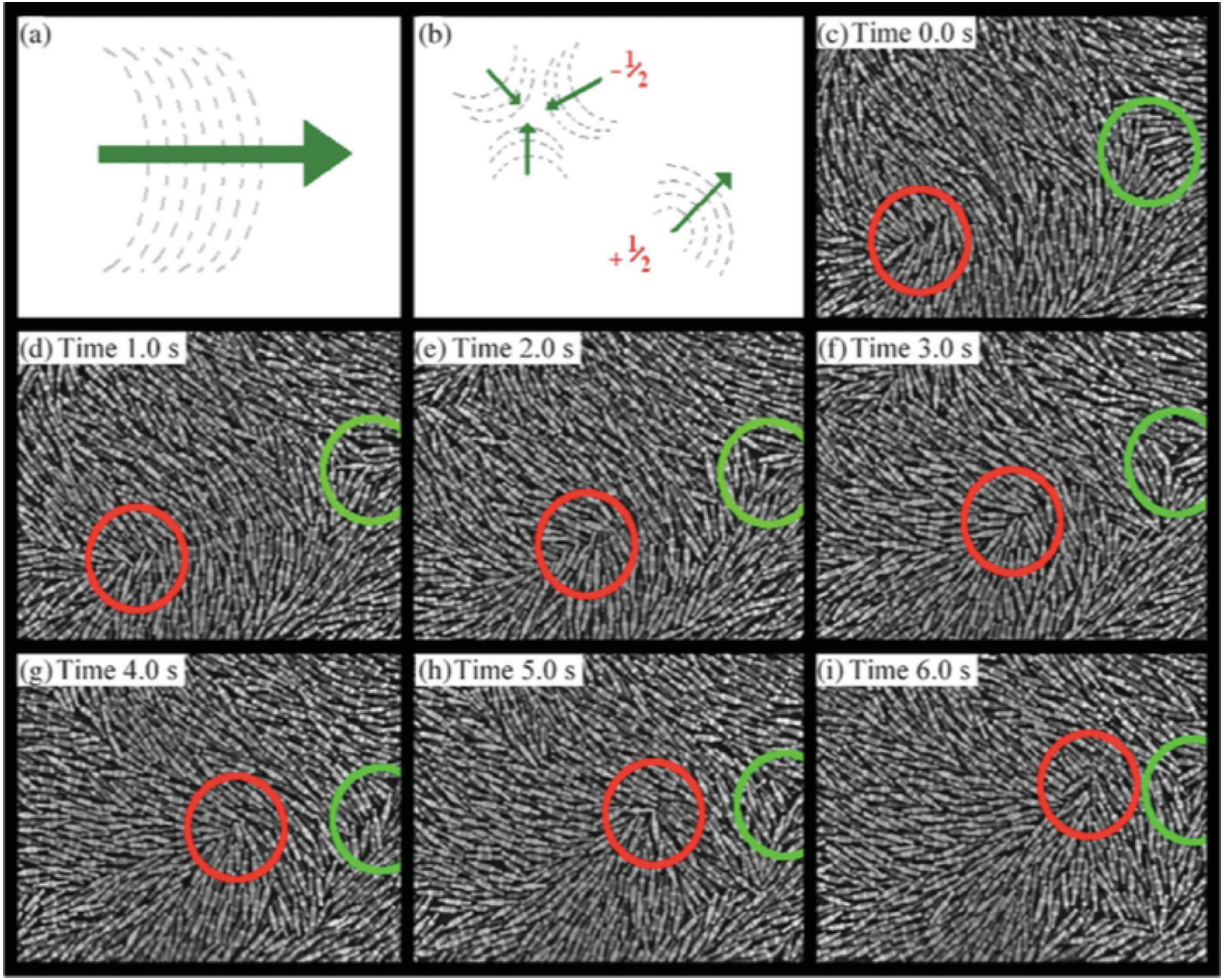




+1/2 defects self-propel in the direction of bend distortions

other defects do not self-propel

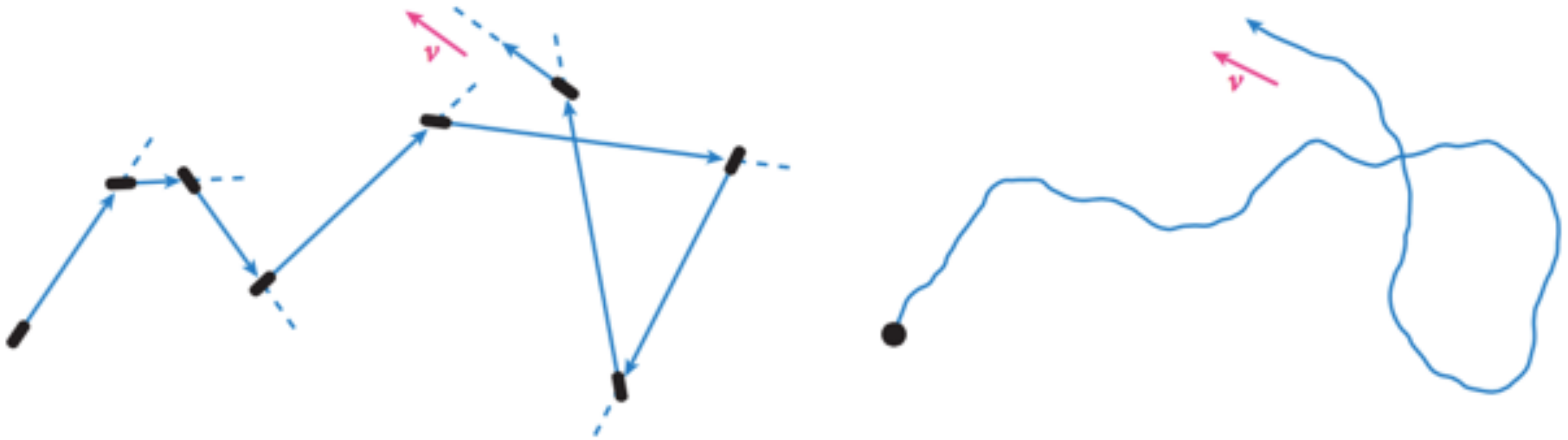
Self-Propulsion of Defects

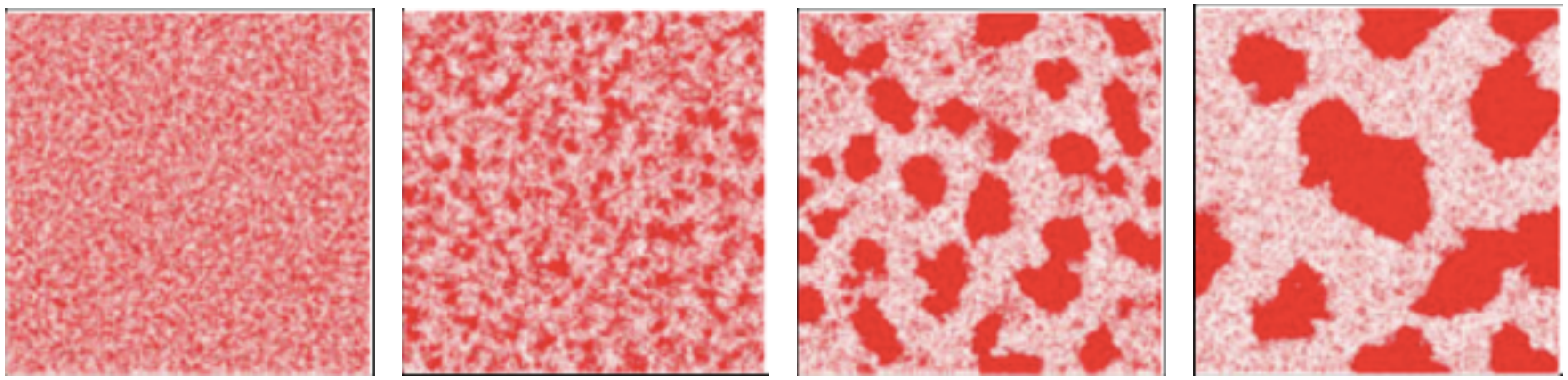


Motility-Induced Phase Separation

Michael E. Cates[1] and Julien Tailleur[2,*]

Annu. Rev. Condens. Matter Phys. **6**, 219–244 (2015)





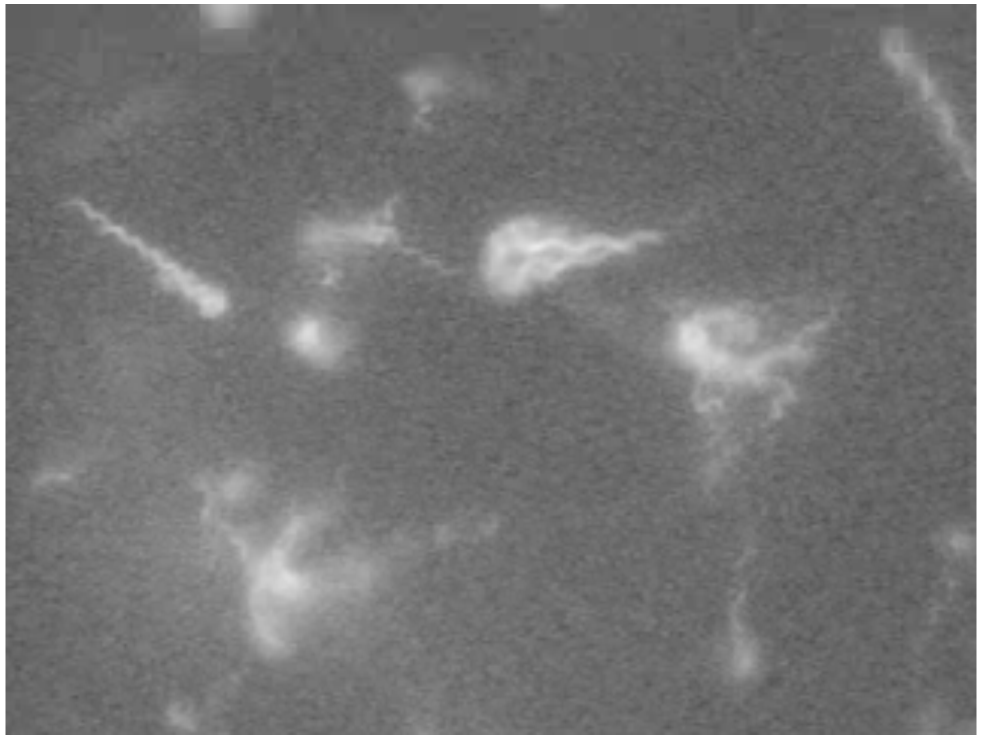
SELF–PROPELLED PARTICLES

Escherichia coli adopt an interesting strategy for exploring the world they live in

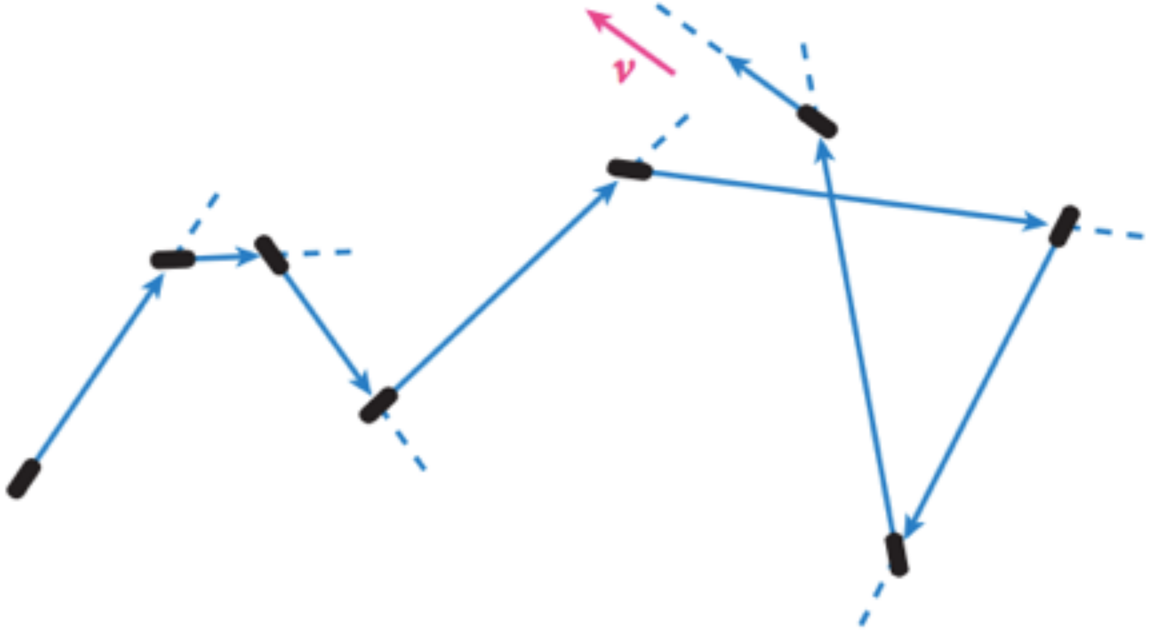
They swim in a directed fashion for some time …

… and then stop, spin around and take off in a new direction

This is called ***run and tumble***



Howard Berg (Harvard)



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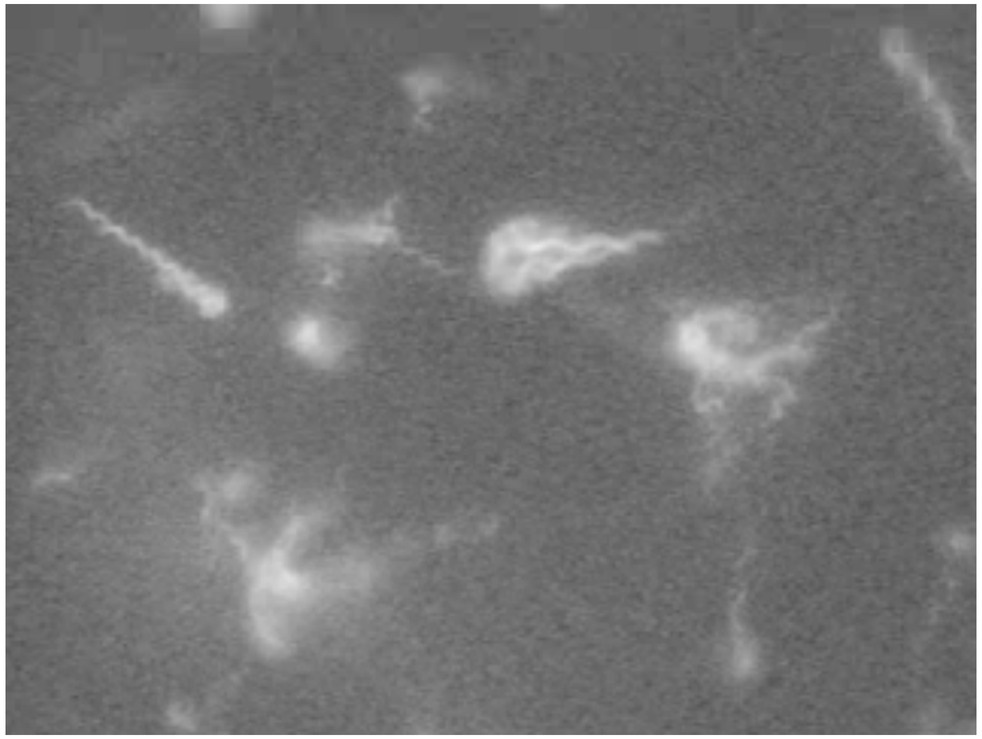

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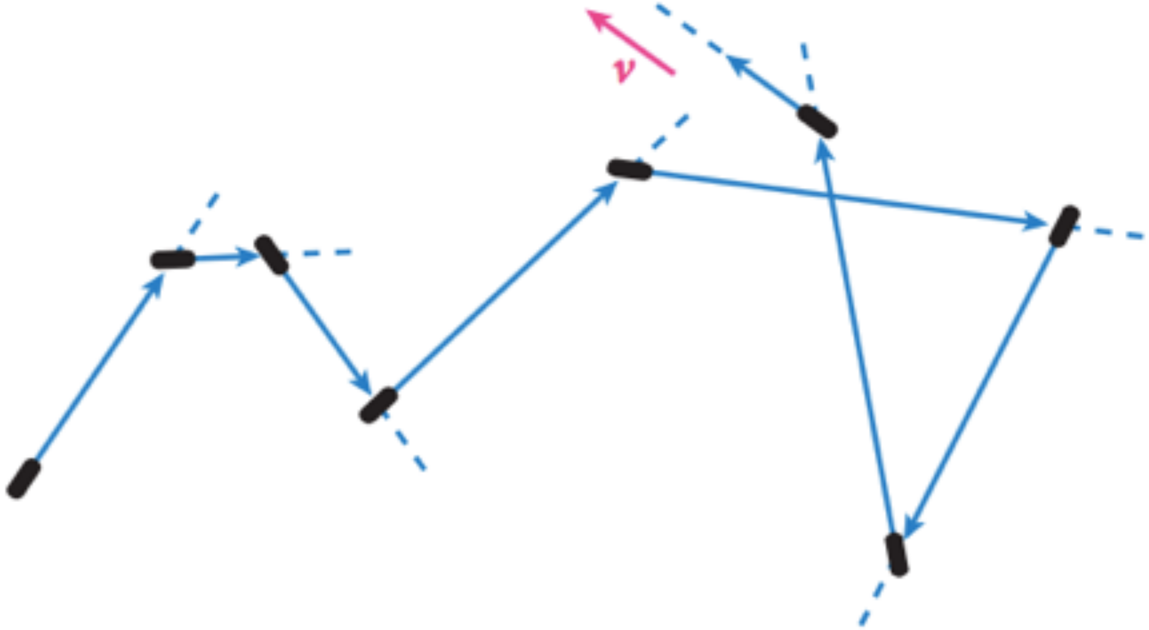
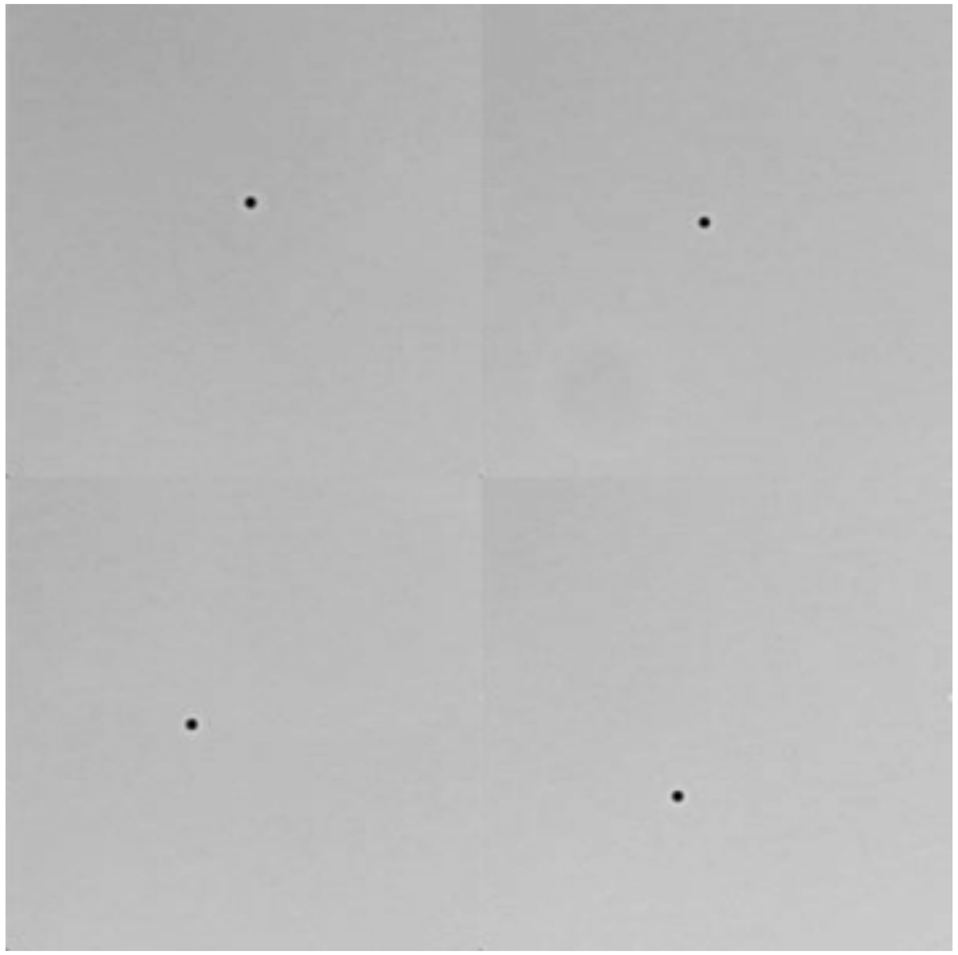


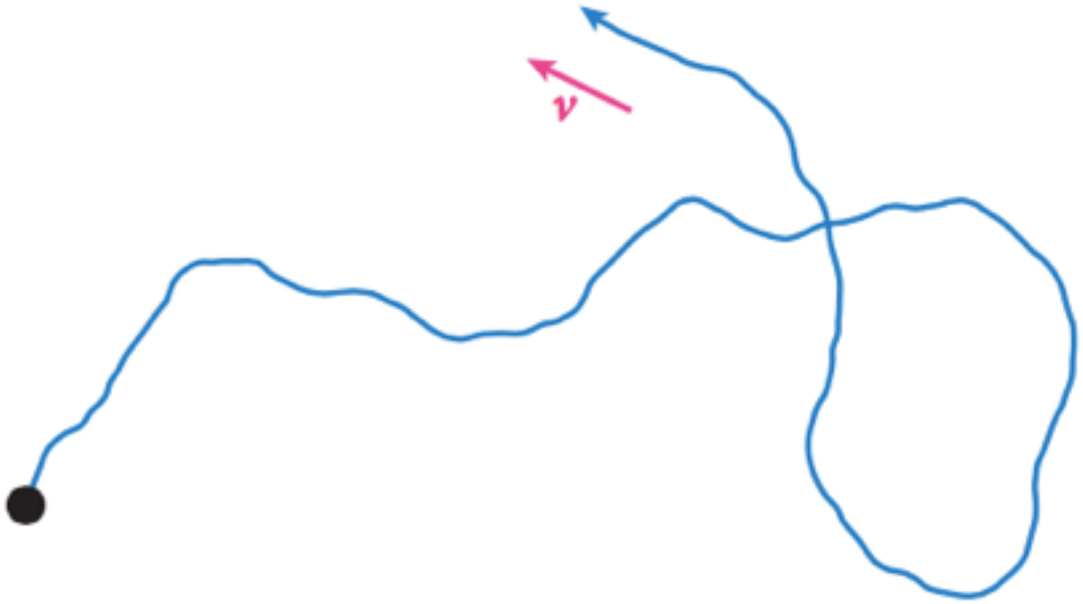
SELF–PROPELLED PARTICLES

It has been known for a long time (Derjaguin) that a colloid in a concentration gradient will move — ***diffusiophoresis***

Catalytic decomposition of hydrogen peroxide by a Janus particle creates an anisotropic concentration field

The colloid moves in this concentration field, that it itself generates — ***self-diffusiophoresis***[†]





Howse *et al.*, *Phys Rev Lett* **99**, 048102 (2007)
Golestanian, *Phys Rev Lett* **102**, 188305 (2009)

[†] This is not purely diffusiophoretic, but also has relevant electrokinetic and electrophoretic aspects

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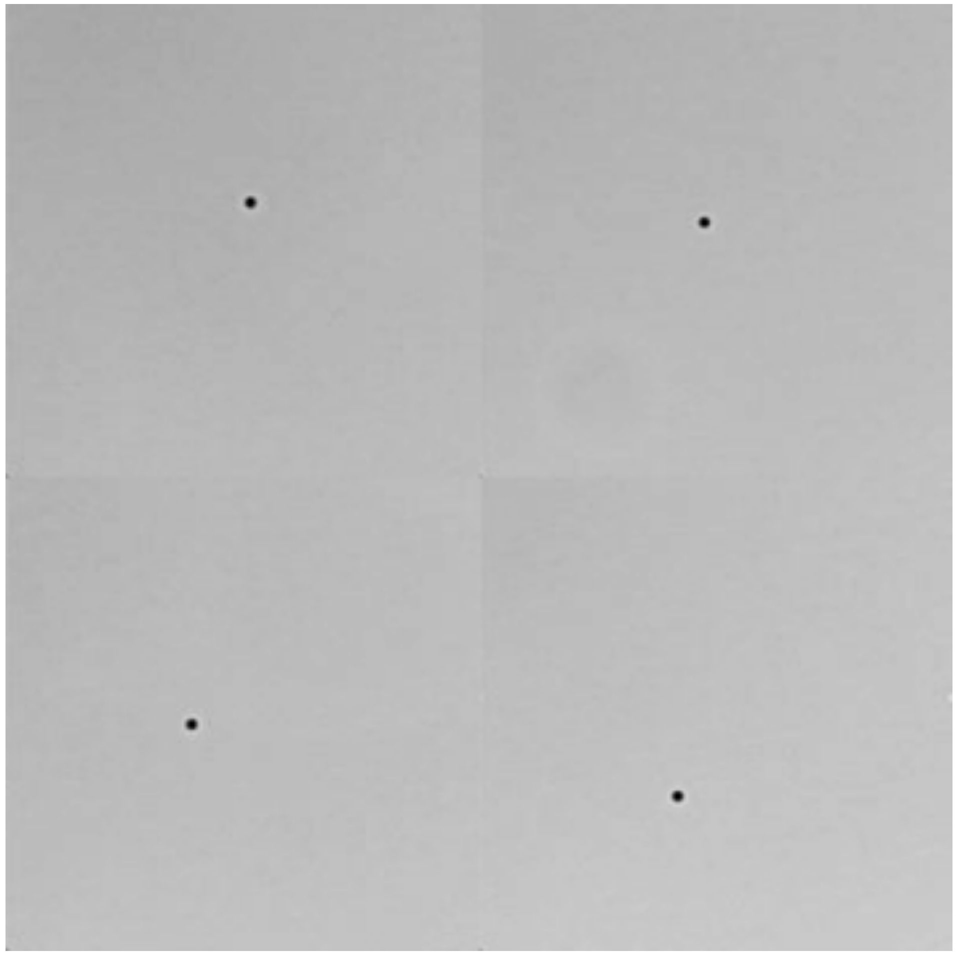

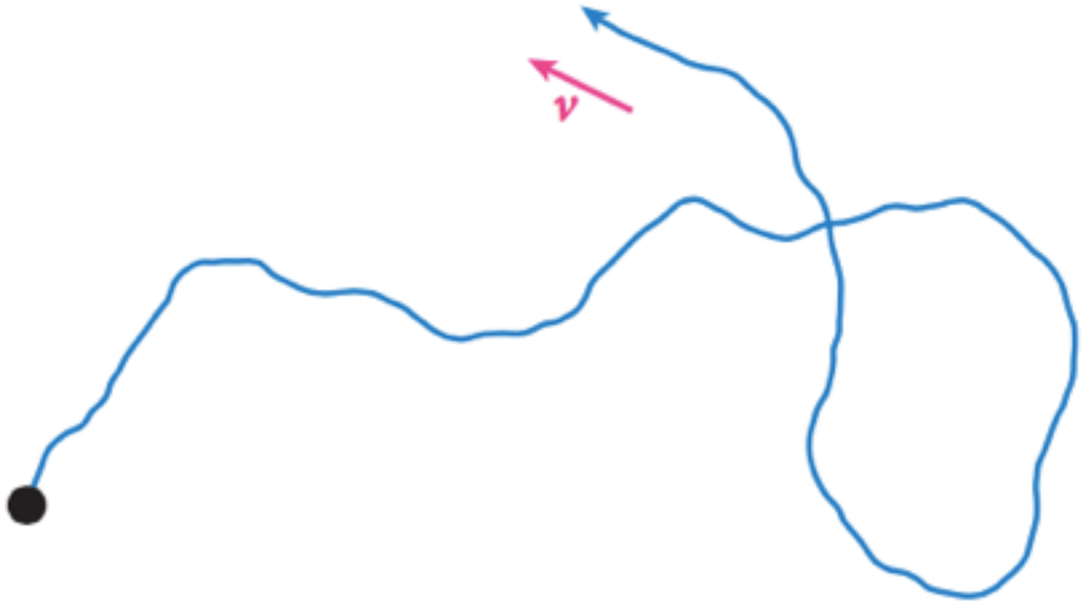

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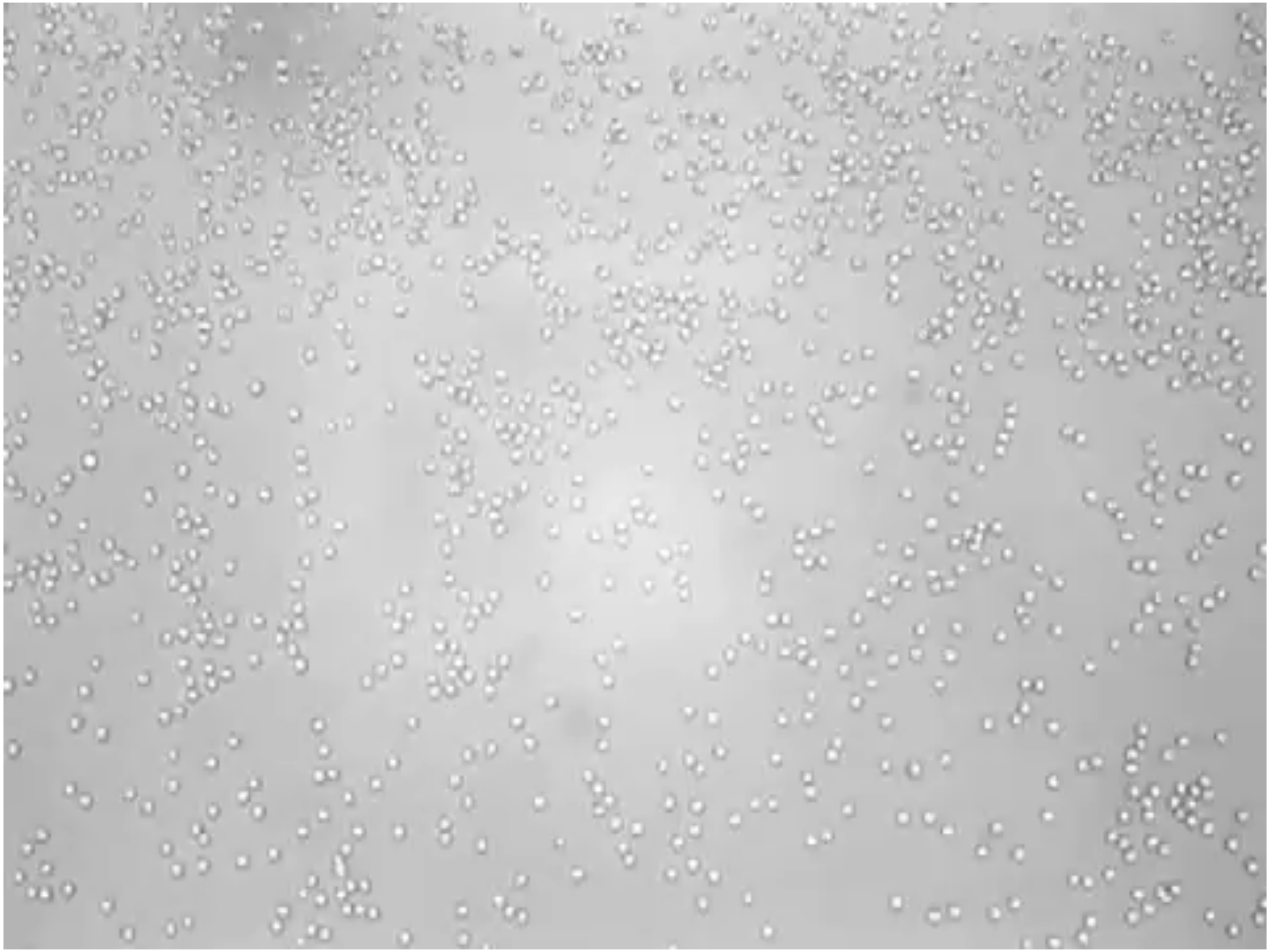
MOTILITY–INDUCED PHASE SEPARATION



Experiments on clustering in self-phoretic colloids provide some evidence in support of the MIPS paradigm

Finite cluster sizes (arrested coarsening) is not currently accounted for by MIPS

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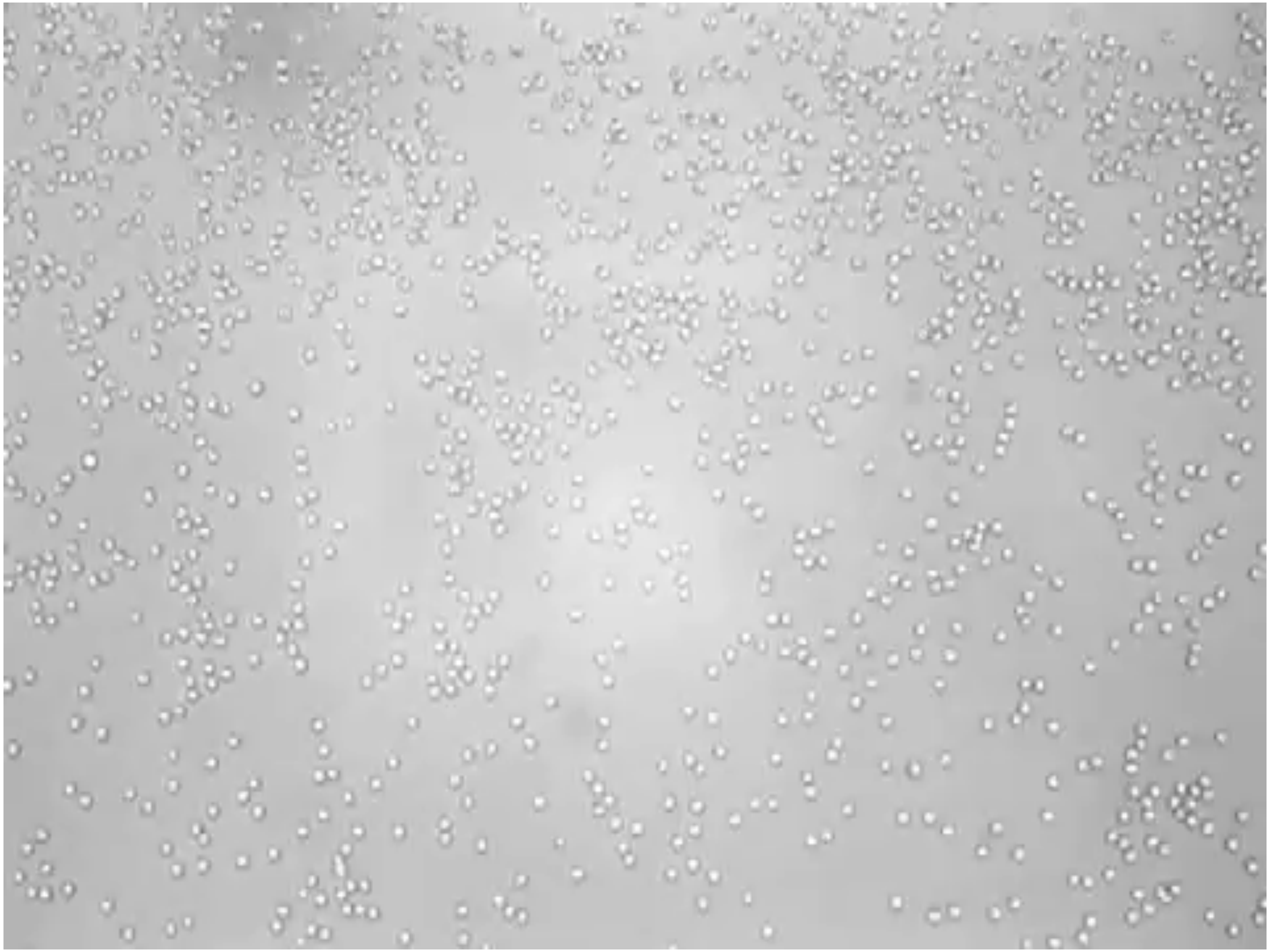

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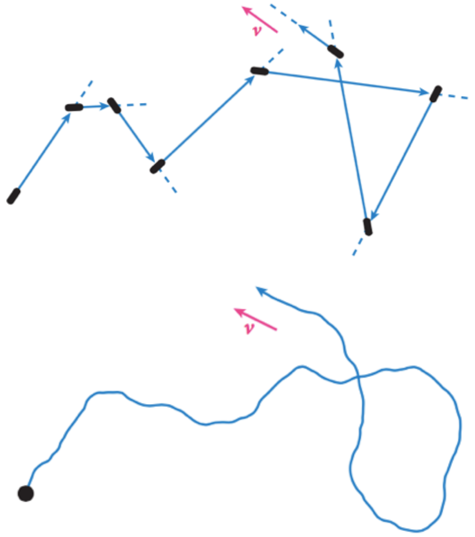
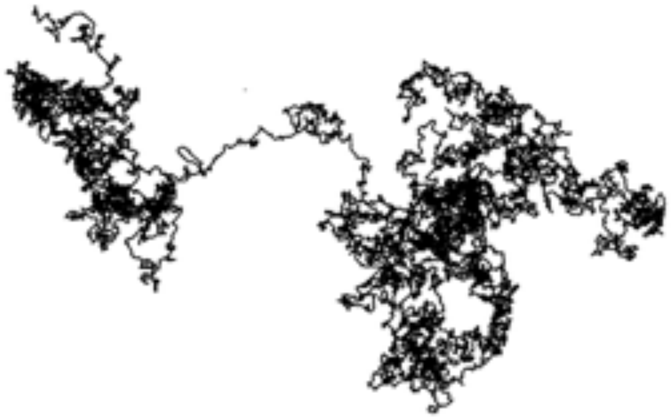
SELF–PROPELLED PARTICLES

At short times the motion is directed, but at long times both of these systems look like they perform random walks

If so, then

(unordered) active system $\overset{!!}{\Longleftrightarrow}$ **passive Brownian particle**





There is, of course, a (significantly) enhanced diffusion constant, but you can work that out

run and tumble $D = \dfrac{v^2}{\alpha d}$

active Brownian particle $D = \dfrac{v^2}{d(d-1)D_r}$

$$D = \frac{v^2 \tau}{d} + D_t$$

$$\tau^{-1} = \alpha + (d-1)D_r$$

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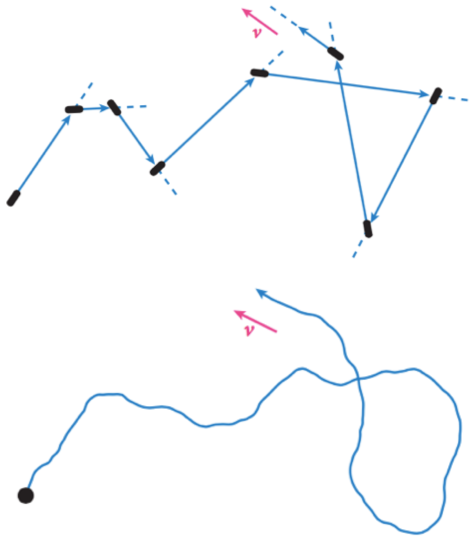
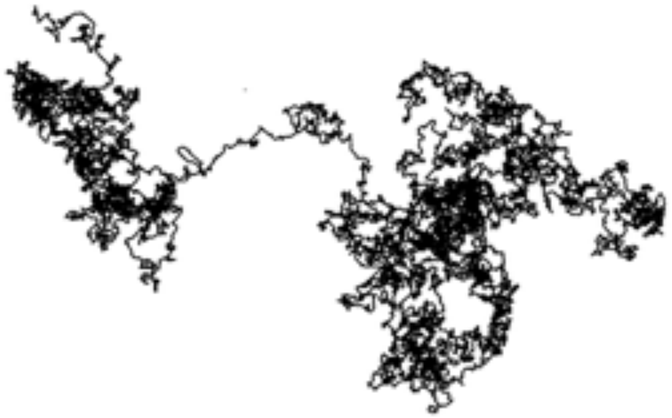




Today we will look at this mapping to an equivalent passive system

A natural question, then, is ***what makes an active system active*** ?

MANY BODY EFFECTS — SLOWING DOWN

Things slow down when they become more dense

There is an all too well-known example …

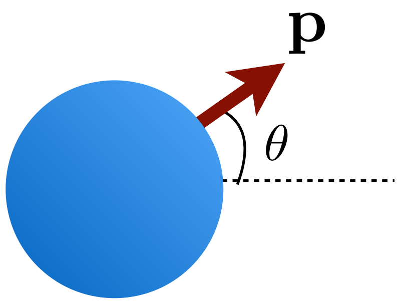
The same happens in active Brownian particle systems

It gives rise to phase separation in a system without attractive interactions, called **MIPS**

This is a *collective phenomenon*, but let's start with something simpler

a single active Brownian particle in an inhomogeneous environment, so that it has a position-dependent swim speed

SIMULATIONS OF ACTIVE BROWNIAN PARTICLES



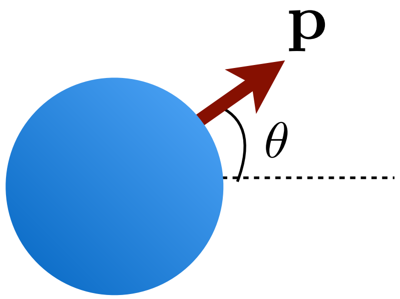
Using molecular dynamics, active Brownian particles can be simulated directly

$$\partial_t \mathbf{r}_i = \frac{D_t}{k_{\mathrm{B}} T} \left(\mathbf{F}_i + F_p \mathbf{p}_i \right) + \sqrt{2 D_t}\, \mathbf{\Lambda} \qquad \partial_t \theta_i = \sqrt{2 D_r}\, \Lambda_\theta$$

Weeks-Chandler-Anderson interactions

Redner *et al.*, *Phys Rev Lett* **110**, 055701 (2013)
Stenhammar *et al.*, *Soft Matter* **10**, 1489 (2014)

SIMULATIONS OF ACTIVE BROWNIAN PARTICLES



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A density dependent swim speed emerges from the simulation

It is well–approximated by a simple linear form $v(\rho) = v_0\big(1 - \rho/\underbrace{\rho^*}_{\approx \text{ close packing density}}\big)$

Redner *et al.*, *Phys Rev Lett* **110**, 055701 (2013)
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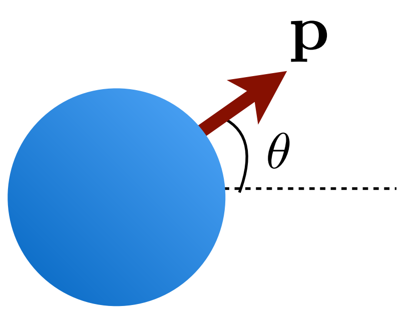

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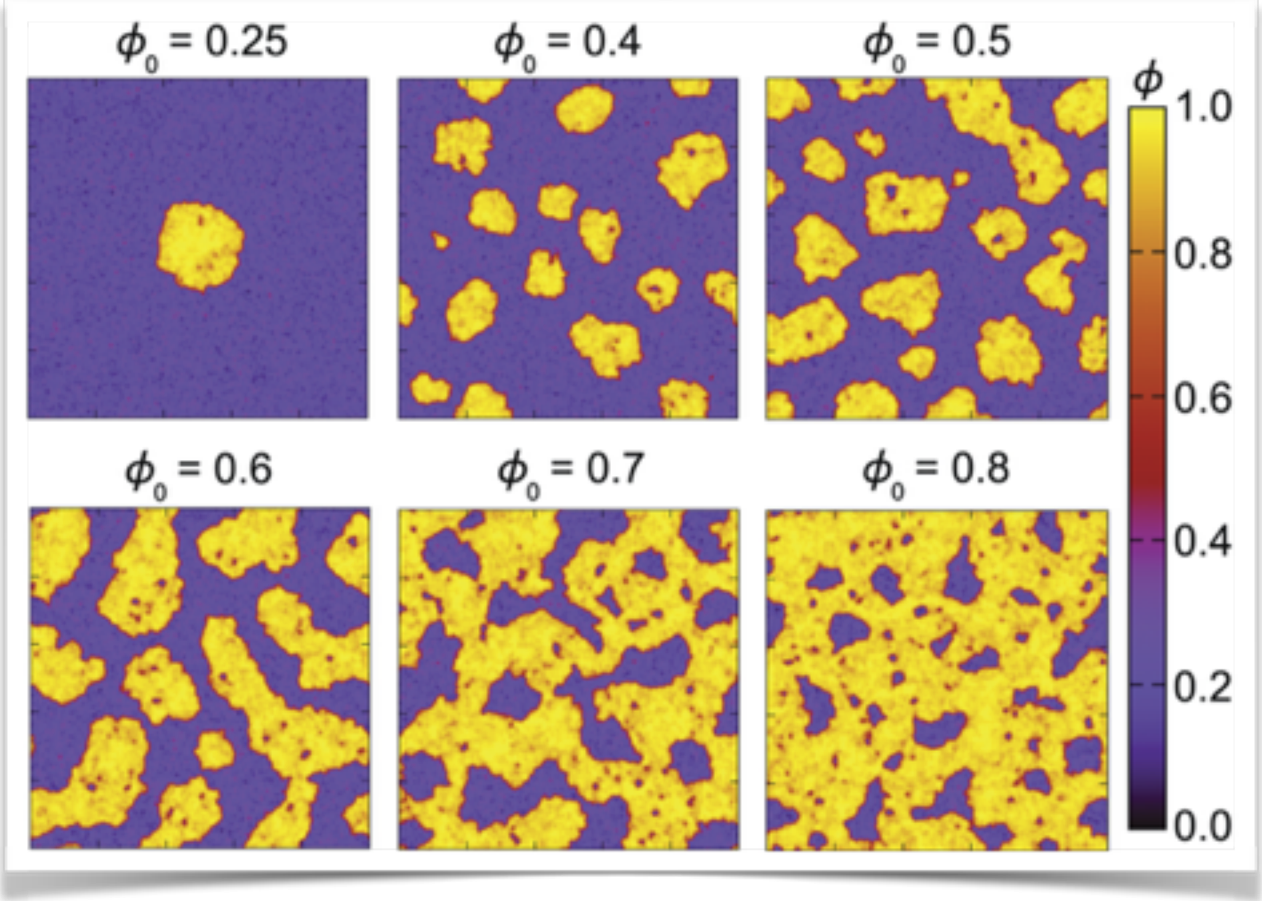
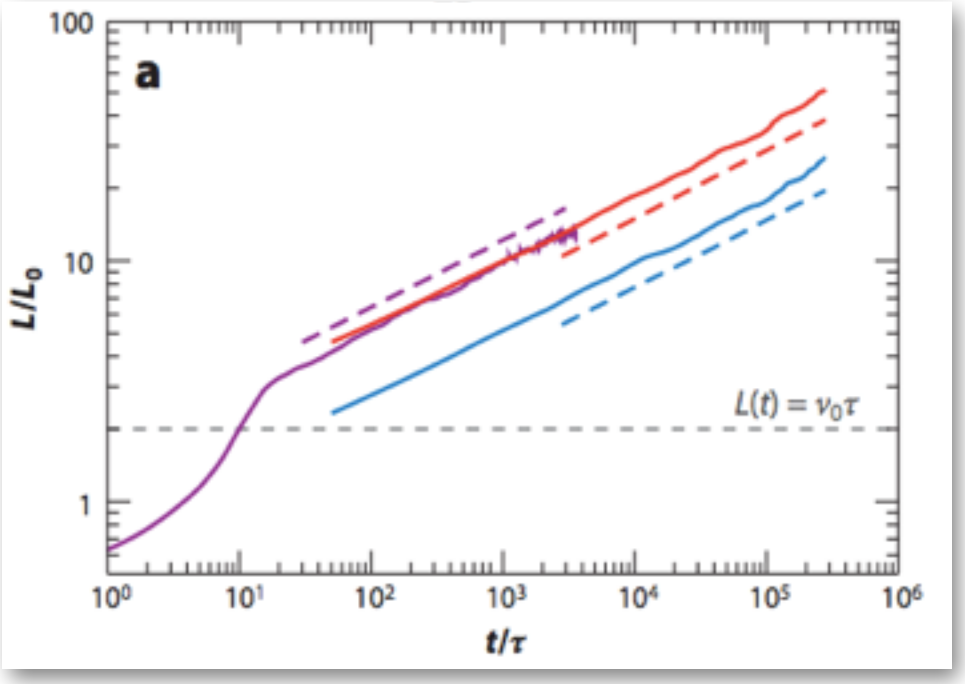




Redner *et al.*, *Phys Rev Lett* **110**, 055701 (2013)
Stenhammar *et al.*, *Soft Matter* **10**, 1489 (2014)

SIMULATIONS OF ACTIVE BROWNIAN PARTICLES

Not all features are captured by the “thermodynamic” theory

Simulations reveal that there is a critical Péclet number for MIPS

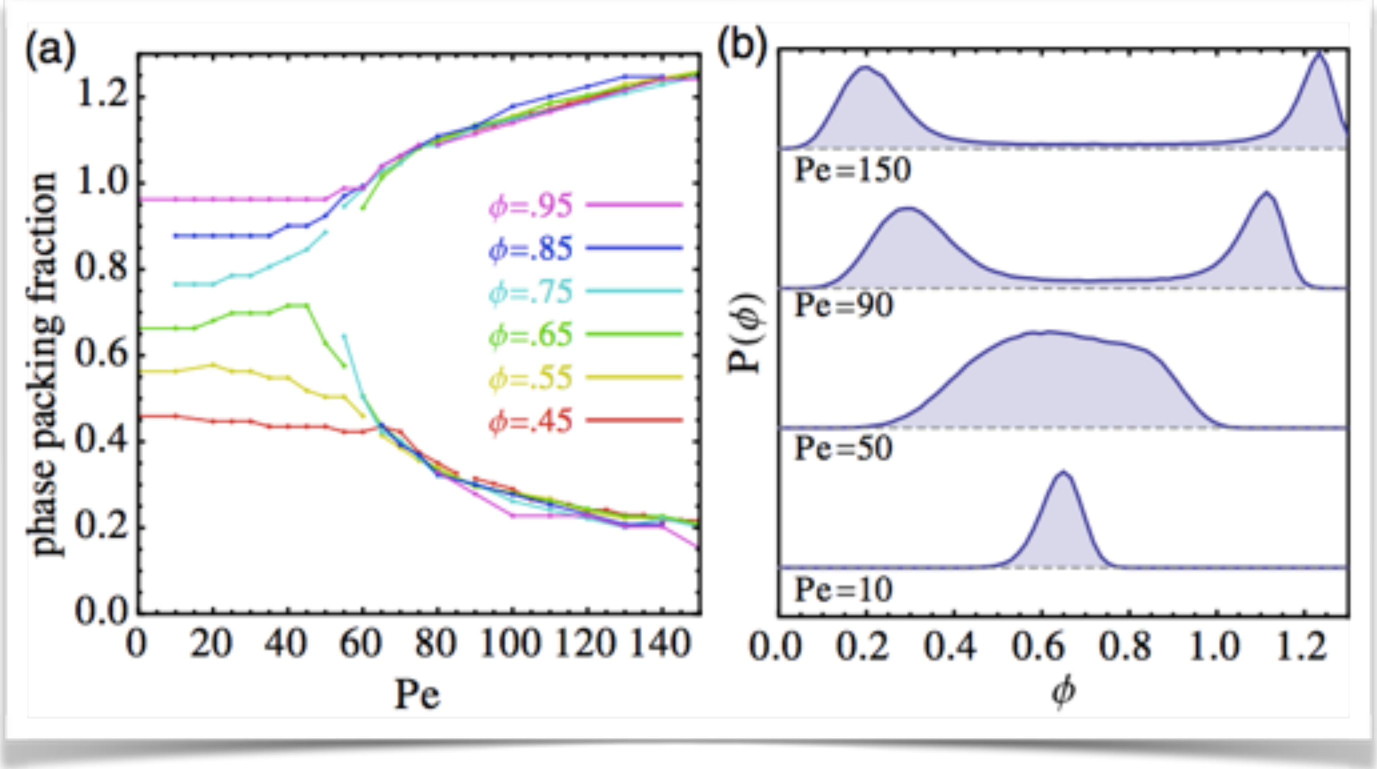
$$\mathrm{Pe} = \frac{3v_0\tau}{\sigma}$$

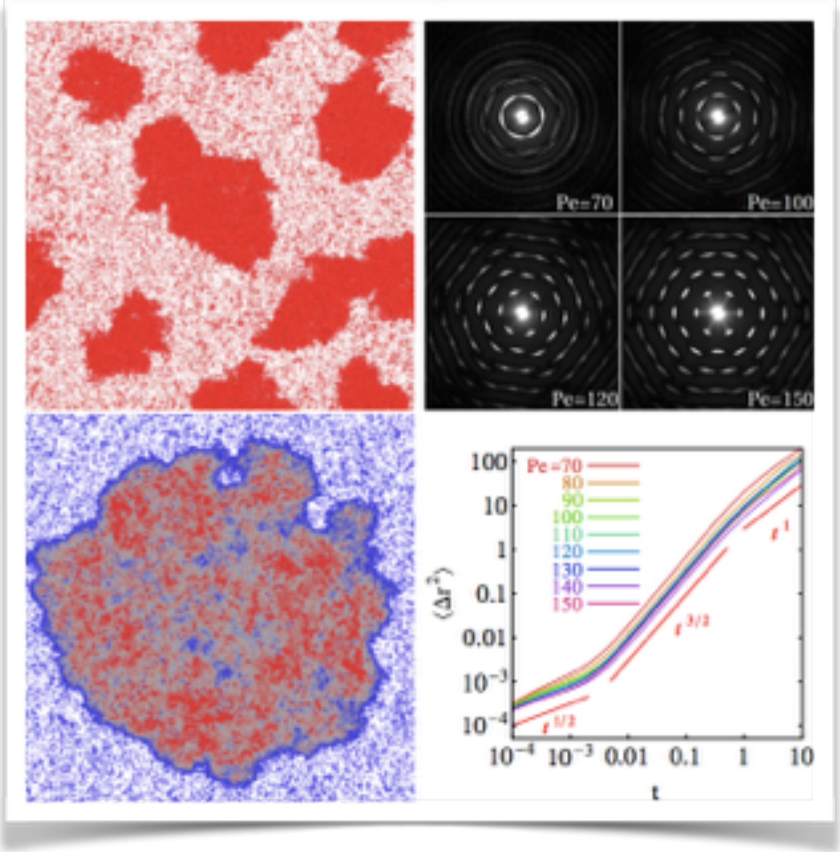
particle size in the WCA potential

It is analogous to an inverse temperature

MIPS is not observed below the critical value

$$\mathrm{Pe} < \mathrm{Pe}_c \simeq \begin{cases} 55 & 2d \\ 125 & 3d \end{cases}$$



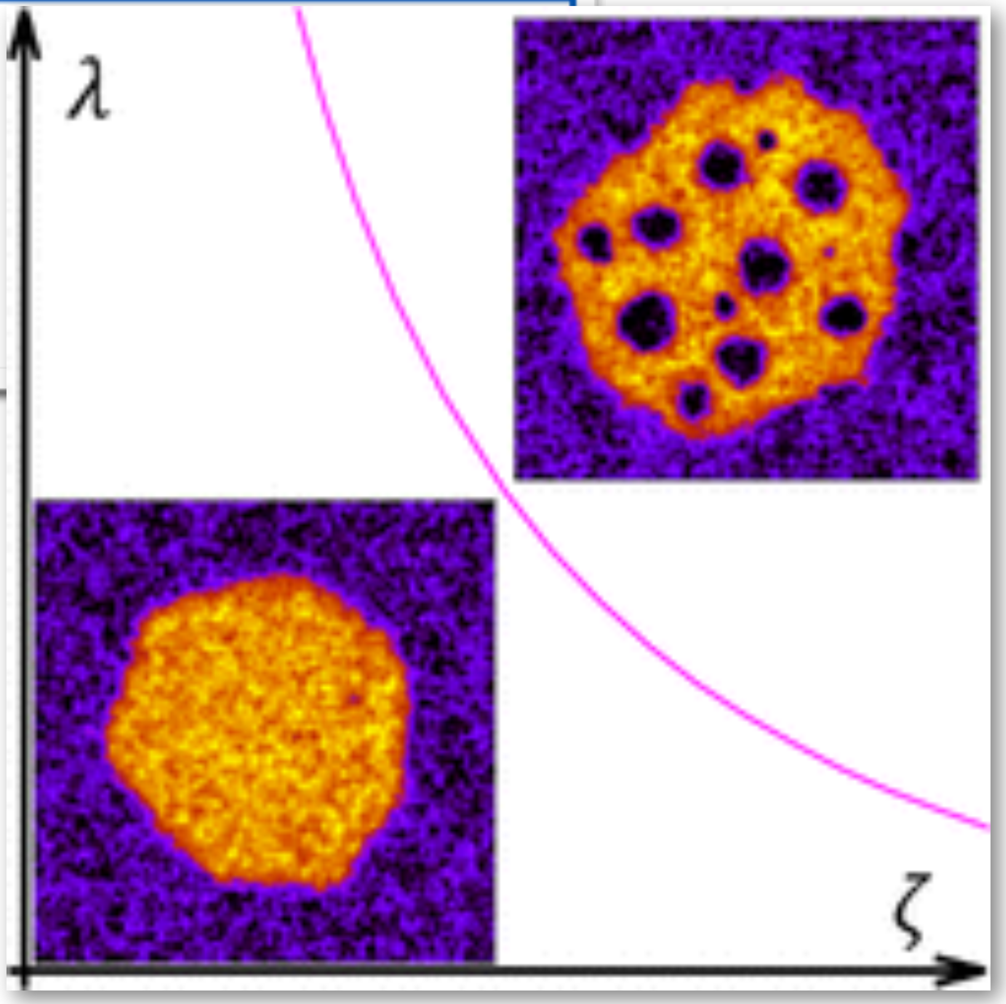


Redner *et al.*, *Phys Rev Lett* **110**, 055701 (2013)
Stenhammar *et al.*, *Soft Matter* **10**, 1489 (2014)


PHYSICAL REVIEW X

Cluster Phases and Bubbly Phase Separation in Active Fluids: Reversal of the Ostwald Process

Elsen Tjhung, Cesare Nardini, and Michael E. Cates
Phys. Rev. X **8**, 031080 – Published 24 September 2018




PHYSICAL REVIEW E
covering statistical, nonlinear, biological, and soft matter physics

Generalized thermodynamics of phase equilibria in scalar active matter

Alexandre P. Solon, Joakim Stenhammar, Michael E. Cates, Yariv Kafri, and Julien Tailleur
Phys. Rev. E **97**, 020602(R) – Published 20 February 2018