Active and Driven Soft Matter

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Boulder School 2009

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Lectures 1 & 2

Lecture 1 - Introduction

- What are active systems?
- Hydrodynamics: symmetries, conservation laws and broken symmetries
- Tutorial: phenomenological hydrodynamics of a fluid

Lecture 2 - Hydrodynamics of "living liquid crystals"

- Tutorial: hydrodynamics of nematic liquid crystals
- Active Hydrodynamics: active stresses, nematic vs polar order
- Spontaneous flow in active films
- Asters, vortices and spirals

Lectures 3 & 4

Lecture 3 - From microdynamics to hydrodynamics: SP rods on a substrate

- Tutorial: Langevin, Fokker-Planck and Smoluchowski dynamics
- Hydrodynamics of SP hard rods
- Instabilities, persistent diffusion, and enhanced order

Lecture 4 - Hydrodynamics of bacterial suspensions

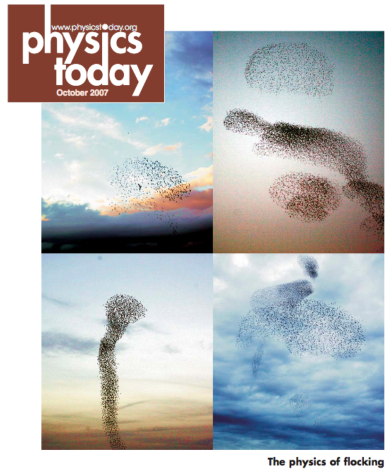
- The simplest "swimmer": pullers vs pushers
- Hydrodynamic interactions
- Instabilities and other results
- Outlook

Today's Lecture

- A tour through living and non-living active systems
- Hydrodynamics as an effective field theory: symmetries, conservation laws and broken symmetries
- Tutorial: hydrodynamics as a generic field theory - isotropic fluid

What is active matter?

- Collection of interacting self-driven units with emergent behavior at large scales
- Energy input that maintains the system out of equilibrium is on each unit, not at boundaries
- Robust behavior in the presence of noise (generally nonthermal)
- Orientable units $\rightarrow$ states with orientational order



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Examples from Living & Non-Living World

- Bacterial suspensions
- *In vitro* mixtures of cytoskeletal filaments and motor proteins
- Cell cytoskeleton
- Layers of vibrated granular rods
- Nanoparticles propelled by catalytically self-generated forces
- Collections of robots

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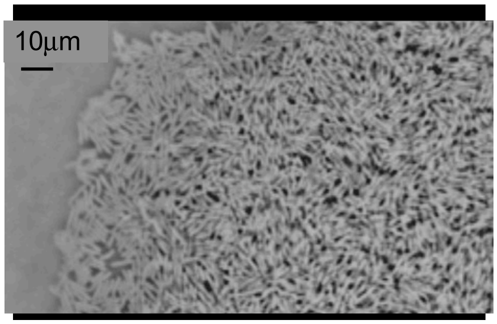
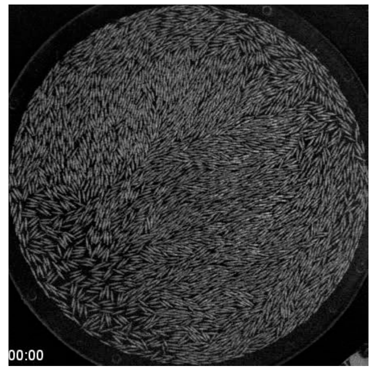
Vortex patterns on all scales



E-coli from Wiebel's lab, Wisconsin-Madison



A layer of vibrated granular rods (L=4.6mm), Narayan et al. Science 2007

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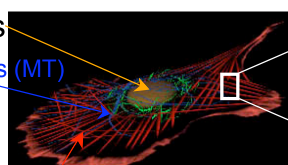
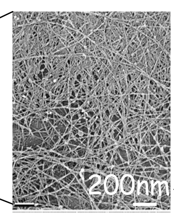
Cell cytoskeleton: polymer network that serves as skeleton and muscle to the cell - controls motility & mechanical properties

nucleus

Microtubules (MT)

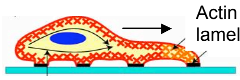


actin cytoskeleton



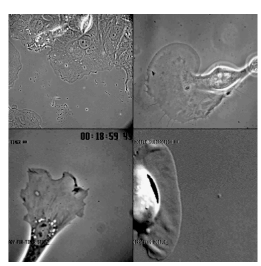
Borisy & Svitkina

fish keratocyte



Actin lamellipodium

Fragment of lamellipodia can move on their own in the absence of cell body. (Verkhovsky et al. 1996)



V. Small, Vienna

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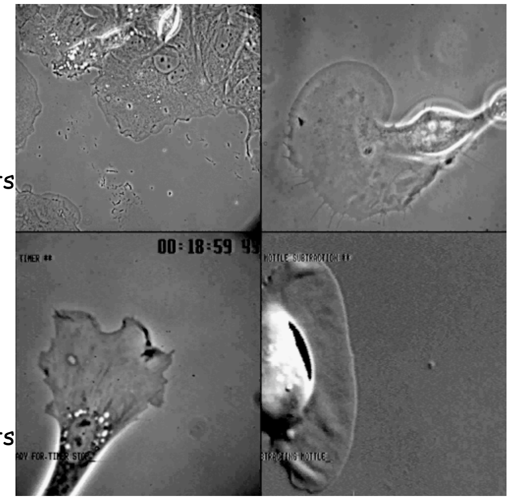
In vivo: active cytoskeleton controls cell motility

mouse
fibroblasts
(3h)

mouse
melanoma
(20min)



chick
fibroblasts
(2h)

trout
keratocyte
(4min)
v=15μm/min

V. Small, IMBA, Vienna.

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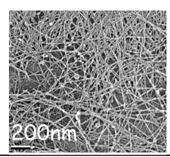
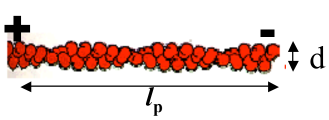
Ingredients of cytoskeleton: filaments & crosslinkers



Stiff filamentary proteins:
- F-actin: d ~ 6nm, l_p ~ 10μm
- MT : d ~ 20nm, l_p ~ 1mm

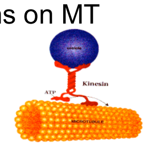
Polarity & Treadmilling



Crosslinkers: motor proteins, stationary linkers, [capping proteins], [severing proteins]

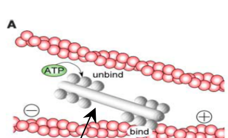
Motor proteins hydrolyze ATP to “walk” in a given direction on polar filaments:

- kinesins and dyneins on MT
- myosin on F-actin



Motor clusters crosslink filaments and drive filament sliding & contraction

→ **Active crosslinkers**



myosin II

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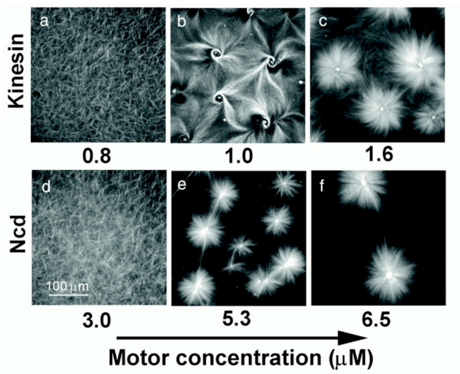
In vitro: activity drives pattern formation

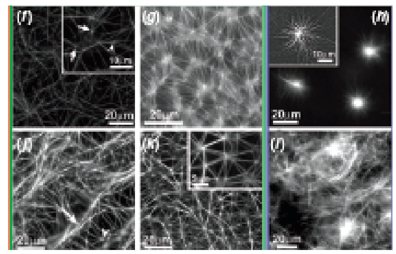
extracts of cytoskeletal filaments and motor proteins

Microtubules & kinesins



T. Surrey et al, Science **292**, 5519 (2001)

Actin, myosin II & fascin



Backouche et al., Phys. Biol. **3**, 264 (2006)

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Long-Lived Giant Number Fluctuations in a Swarming Granular Nematic

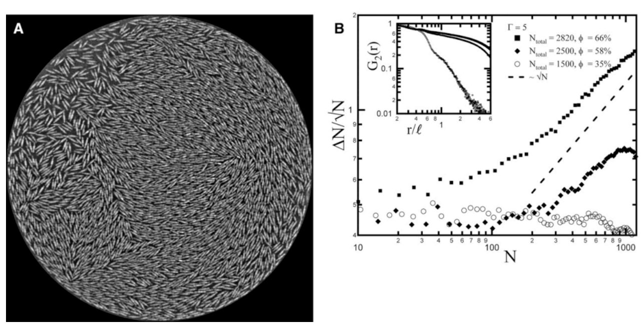
Vijay Narayan, Sriram Ramaswamy, Narayanan Menon

Science **317**, 105 (2007)

Science AAAS

Fluctuations in # particles expected to satisfy central limit theorem $\sqrt{\Delta N} = \sqrt{\langle N^2\rangle - \langle N\rangle^2} \sim \sqrt{\langle N\rangle} \Rightarrow \frac{\sqrt{\Delta N}}{\langle N\rangle} \sim \frac{1}{\sqrt{\langle N\rangle}}$

Active rod nematic $\sqrt{\Delta N} \sim \sqrt{\langle N\rangle}$!



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Collective behavior of active matter

- Emergent behavior qualitatively different from that of the individual constituents
- Onset of directed large-scale motion (relation to cell motility?)
- Athermal order-disorder transitions: LRO in 2d
- Pattern formation on various scales
- Novel correlations (giant number fluctuations seen in vibrated layers of granular rods)
- Unusual mechanical and rheological properties: cells stiffen when stresses and adapt their mechanical properties to the environment

$\rightarrow$ **"living liquid crystals"**

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Today's Lecture

- A tour through living and non-living active systems
- Hydrodynamics as an effective field theory: symmetries, conservation laws and broken symmetries
- Tutorial: hydrodynamics as a generic field theory - isotropic fluid

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Goal of Theoretical Work

Use the tools and ideas of (soft) condensed matter physics (hydrodynamics and broken symmetries) to develop an effective theory describing the behavior of active matter:

- Characterization of phases & ordered structures
- Role of noise
- Rheological and mechanical properties
- What is the role of physical interactions vs biochemical or chemotactic ones?
- Can we think of motility as a "material property" and of the onset of motion as a nonequilibrium phase transition?

Understanding the microscopic mechanisms responsible for collective behavior

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Theoretical work can be grouped into three classes:

Rule-based models (Vicsek, 1995)

Numerical simulations

Symmetry-based **phenomenological hydrodynamics**
•Toner & Tu (1998)
•Ramaswamy et al (2002)
•Kruse, Joanny, Julicher, Prost & Sekimoto (2004)

Lectures 1 & 2

Microscopic derivation of hydrodynamics for specific models
•Liverpool & MCM (2003)
•Baskaran & MCM (2008)
•Aranson et al. (2005)

Lectures 3 & 4

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Coarse-graining and hydrodynamics

Coarse-grained description of phases and dynamics of systems of many interacting degrees of freedom (liquids, solids, liquid crystals) in terms of few macroscopic fields: $\underset{\sim 10^{23}}{\{\vec{r}_i, \vec{p}_i\}} \rightarrow \underset{<10}{\{\rho, \vec{g}, \varepsilon, \ldots\}}$

cf. field theories in particles physics, hard CM, cosmology

Two Routes:

- Phenomenology: based on symmetries, generic, but with undetermined parameters
- Derivation from microscopic models: approximations needed, model-dependent expression for various parameters

Interplay between the two approaches crucial for full understanding

First step: identify the hydrodynamic fields as "slow variables", with relaxation rates $\omega(k) \to 0$ when $k \to 0$ (Martin, Parodi, Pershan, PRA 6, 2401 (1972))

Two classes of hydrodynamic fields:

- densities of **conserved variables**: # particles, momentum , energy
- **broken symmetry fields** in systems with spatial order

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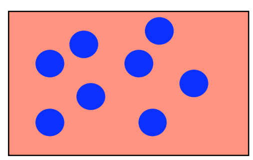
Conserved fields

Example: colloidal fluid = large (~μm) particles in a solvent



$\rightarrow$ only one conserved field: density $\rho(r,t)$

Fluctuations form equilibrium $\delta\rho(r,t) = \delta\rho(r,t) - \rho_0$ occur at finite T with probability ~ exp(-F/kT)

The decay of fluctuations in time is controlled by a conservation law

$$\partial_t \delta\rho = -\vec{\nabla} \cdot \vec{j}$$

$$\vec{j} = -D\, \vec{\nabla} \delta\rho$$

$$\boxed{\rightarrow \quad \frac{\partial \delta\rho}{\partial t} = D\nabla^2 \delta\rho}$$

diffusion

$$\delta\rho(\vec{r},t) = \sum_{\vec{k}} \delta\rho_k(t) e^{i\vec{k}\cdot\vec{r}}$$

$$\delta\rho_k(t) = \delta\rho_k e^{-\omega(k)t}$$

$$\omega(k) = Dk^2$$

hydrodynamic mode

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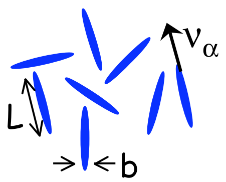
Broken symmetry fields → example of Nematic Liquid Crystals

Liquid of rod-like molecules: upon increasing density (or lowering T) the molecules order in a phase with long-range **orientational order** (Onsager 1949)



$$\rho_N \sim \frac{1}{v_{ex}} \sim \frac{1}{L^2 b}$$

Isotropic liquid: orientational symmetry

Nematic liquid: broken orientational symmetry

Competition of translational & rotational entropy

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Entropy at work

Elephant seals on the California coast - courtesy of Arshad Kudrolli

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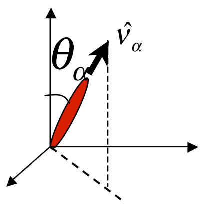
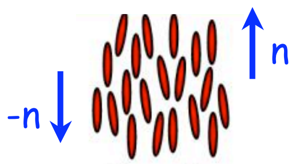
Ordered state



rods have no head/tail $\rightarrow$ $<\sum_\alpha \cos\theta_\alpha>=0$

order parameter: $Q_{ij}=<\sum_\alpha(\hat{v}_{\alpha i}\hat{v}_{\alpha j}-\frac{1}{3}\delta_{ij})>$



$\boxed{Q_{ij}=S(n_i n_j-\frac{1}{3}\delta_{ij})}$

director n (|n|=1) is broken symmetry field

n $\rightarrow$ -n is a symmetry of ordered state

Fluctuations $\delta n_k=n_k-n_0$ of wavelength $\lambda=2\pi/k$ cost no energy when $k\rightarrow 0$ and decay via a "slow" mode $\delta n_k(t) \sim \exp[-\omega(k)t]$, with $\omega(k\rightarrow 0)=0$.

The broken symmetry fields are hydrodynamic fields.

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Constructing a hydrodynamic theory

1. Identify hydrodynamic variables (conserved densities and broken symmetry fields). The hydrodynamic equations must contain only these variables and their gradients.
2. Identify symmetries.
3. Identify conservation laws.
4. Construct constitutive equations for the fluxes as functions of the hydrodynamic fields and their gradients:
   a) Rule out any term explicitly forbidden by symmetry or conservation laws
   b) Since one is interested in large scales and slow variation, keep terms to leading order in the gradients of the hydrodynamic fields

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Tutorial 1: isotropic fluid

1. Conserved densities: density ρ
   momentum $\vec{g} = \rho \vec{\mathrm{v}}$
   (energy)
2. Symmetries: rotational invariance, space & time translational invariance ,Galileian invariance
3. Conservation laws: $\partial_t \rho = -\vec{\nabla} \cdot \vec{g}$ $\quad \partial_t g_i = -\partial_j \pi_{ij}$
4. Constitutive equation for the fluxes:
   density flux $\vec{g} = \rho \vec{\mathrm{v}}$
   momentum flux $\pi_{\mathrm{ij}} = \pi_{\mathrm{ij}}(\rho, \vec{g}, \varepsilon, \nabla \rho, ...)$

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Entropy production: fluxes & forces

Assume local thermodynamics and calculate rate of entropy production (isothermal processes)

$$F = \int_{\vec{r}} \left(\frac{g^2}{2\rho} + f_0(\rho) \right) \qquad \dot{F} = \frac{d}{dt}(U - TS) = -T\dot{S}$$

$$R \equiv T\frac{dS}{dt} = -\int_{\vec{r}} \left[(\vec{g} - \rho\vec{v}) \cdot \vec{\nabla}\frac{\mu}{m} + \left(\pi_{ij} - \rho v_i v_j - \delta_{ij} p \right) \partial_i v_j \right]$$

$$R = -\int_{\vec{r}} \sum \text{flux} \times \text{force}$$

Hyd. field	Flux	Force
ρ	$\vec{g}$	$\vec{\nabla}\mu$
$\vec{g}$	π_{ij}	$\partial_i v_j$

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Constitutive Eqs & Hydrodynamics

$$R \equiv T\frac{dS}{dt} = -\int_{\vec{r}} \left[(\vec{g} - \rho\vec{v}) \cdot \vec{\nabla}\frac{\mu}{m} + \left(\pi_{ij} - \rho v_i v_j - \delta_{ij} p \right) \partial_i v_j \right] = -\int_{\vec{r}} \sum \text{flux} \times \text{force}$$

Reversible process R=0

Irreversible process R>0

flux=(flux)^{rev}+ (flux)^{diss}

Crucial role of parity under time reversal

$\vec{g} = \rho\vec{v}$ $\qquad \pi_{ij} = -\rho v_i v_j - \sigma_{ij}$ $\qquad \sigma_{ij}$ stress tensor

$\vec{g}^d = 0$ $\qquad \sigma^r_{ij} = -p\delta_{ij}$ $\qquad \sigma^d_{ij} = 2\eta(u_{ij} - \tfrac{1}{3}\delta_{ij}u_{kk}) + \eta_b\delta_{ij}u_{kk}$

$$u_{ij} = \frac{1}{2}\left(\partial_i v_j + \partial_j v_i \right)$$

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Hydrodynamic Equations

$$\boxed{\begin{aligned}&\partial_t \rho = -\vec{\nabla}\cdot(\rho\vec{v})\\ &\rho(\partial_t + \vec{v}\cdot\vec{\nabla})\vec{v} = -\vec{\nabla}p + \eta\nabla^2\vec{v} + (\eta_b - \tfrac{2}{3}\eta)\vec{\nabla}(\vec{\nabla}\cdot\vec{v})\end{aligned}}$$

Navier-Stokes equation

In the context of active systems two approximations will often be relevant:

- incompressible fluid $\rho = \text{constant} \Rightarrow \vec{\nabla}\cdot\vec{v}=0$
- flow at low Reynolds number $\rho\left(\partial_t\vec{v} + \vec{v}\cdot\vec{\nabla}\vec{v}\right) = \vec{\nabla}\cdot\vec{\sigma} \quad \Rightarrow \vec{\nabla}\cdot\vec{\sigma}$

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Low Reynolds number hydrodynamics

Navier-Stokes eqn of fluid flow:

$$\underbrace{\rho\left(\partial_t\vec{v} + \vec{v}\cdot\vec{\nabla}\vec{v}\right)}_{\substack{\text{accelaration/inertial forces}\\ \sim\rho v^2/L}} = \vec{\nabla}\cdot\vec{\sigma} = -\vec{\nabla}p + \underbrace{\eta\,\nabla^2\vec{v}}_{\substack{\text{viscous force}\\ \sim\eta v/L^2}}$$

$$\mathrm{Re} = \frac{\text{inertial force}}{\text{viscous force}} \sim \frac{v\rho L}{\eta}$$

- $\mathrm{Re} \ll 1$ Stokes flow: $\vec{\nabla}\cdot\vec{\sigma} = 0$
- $\mathrm{Re} \gg 1$ turbulent flow

bacteria*:
L ~ microns
v ~ 10 microns/sec
Re~10^{-4}-10^{-5}

To keep in mind: yet we saw that bacterial suspensions (Re<<1) and overdamped systems (Re=0) exhibit swirling "turbulent" motion

*E. M. Purcell, Am. J. Phys. 45, **3** (1977)

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Summary

- A tour through living and non-living active systems
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- Tutorial: hydrodynamics as a generic field theory - isotropic fluid

Next

- Hydrodynamics of active systems

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