Active Matter

Lectures for the 2011 ICTP School on Mathematics and Physics of Soft and Biological Matter

Lecture 2

M. Cristina Marchetti

Syracuse University

Coarse-graining and hydrodynamics

Much progress in the understanding of phases and dynamics of systems of many interacting degrees of freedom (liquids, solids, liquid crystals) has been obtained via a coarse-grained description in terms of few macroscopic fields:

$$\underset{\sim 10^{23}}{\left\{\vec{r}_i, \vec{p}_i\right\}} \quad \rightarrow \quad \underset{<10}{\left\{\rho, \vec{g}, \varepsilon, \; ...\right\}}$$

cf. field theories in particles physics, hard condensed matter, cosmology

Can an effective continuum theory or hydrodynamics of active systems describe bacteria, vibrated rods, birds, cell cytokeleton and more?

First: a quick review of hydrodynamics as an effective field theory

Hydrodynamics as an effective field theory

Two Routes:

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

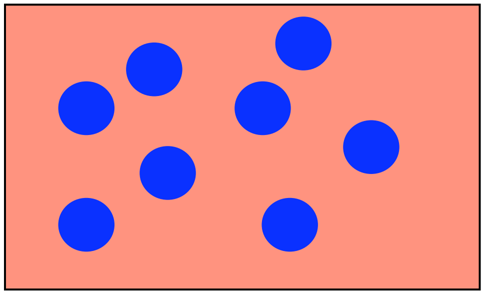
Interplay between the two approaches crucial for full understanding

First step: identify the hydrodynamic fields as "slow variables", with relaxation rates that vanish at large wavelength (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

Conserved field



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

→ only one conserved field: density $\rho(\vec{r},t)$

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

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

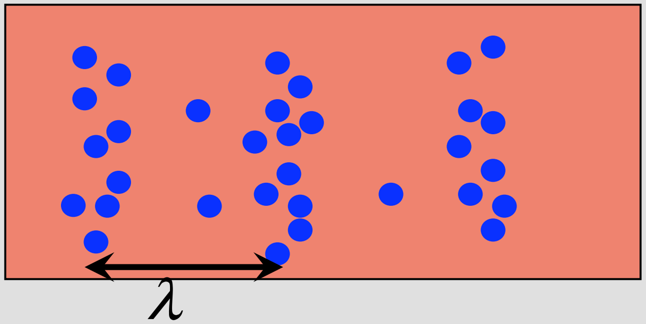
$$\partial_t \delta\rho = -\vec{\nabla}\cdot\vec{j}$$

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

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

diffusion

Periodic density modulation of wavelength $\lambda = 2\pi / k$



Homogeneity is restored in a time $1/\omega(k)$ that diverges as k→0 or

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

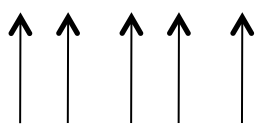
$$\delta\rho_k(t) = \delta\rho_k e^{-\omega(k)t} \qquad \omega(k) = Dk^2$$

hydrodynamic mode

Broken symmetry field: magnetic system

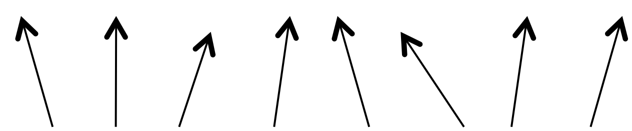
Order parameter: magnetization $\vec{M}(\vec{x},t)=\left\langle \sum_{\alpha}\vec{S}_{\alpha}\delta\left(\vec{x}-\vec{x}_{\alpha}(t)\right)\right\rangle$

The magnitude of M in the ordered state is determined by T and materials properties.
The energy does not depend on the direction of M. When the system magnetizes rotational symmetry is broken spontaneously.



broken symmetry field: $\hat{m}=\frac{\vec{M}}{\left|\vec{M}\right|}$

A uniform twist of $\hat{m}$ costs no energy; long wavelength fluctuations have finite stiffness.
→ spin wave excitations: low energy Goldstone/hydrodynamic modes with relaxation rate that vanishes when k→0



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 coarse-grained free energy (equilibrium) or directly a set of hydrodynamic equations (nonequilibrium).
5. 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

Example: 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: $\partial_t \rho = -\vec{\nabla} \cdot \vec{g}$ $\qquad$ $\partial_t g_i = -\partial_j \pi_{ij}$
4. Constitutive equation for the fluxes:

density flux $\vec{g} = \rho\vec{\mathrm{v}}$

momentum flux $$\pi_{\mathrm{ij}} = \rho \mathrm{v}_i \mathrm{v}_j - \overbrace{\sigma_{\mathrm{ij}}(\rho, \vec{g}, \varepsilon, \underbrace{\nabla\rho, \vec{\nabla}\vec{\mathrm{v}}, \ldots}_{\text{driving forces}})}^{\text{stress tensor}}$$

Constitutive Eqs & Hydrodynamics

$$R \equiv T\frac{dS}{dt} = -\int_{\vec{r}} \sum \text{flux} \times \text{force} \qquad \text{"rate of entropy production"}$$

Reversible process R=0

Irreversible process R>0

flux=(flux)$^{\text{rev}}$+ (flux)$^{\text{diss}}$

Crucial role of parity under time reversal

$$\sigma_{ij} = \sigma_{ij}^{r} + \sigma_{ij}^{d} \qquad \text{stress tensor}$$

$$\sigma_{ij}^{r} = -p\delta_{ij} \qquad \sigma_{ij}^{d} = 2\eta(\mathrm{v}_{ij} - \tfrac{1}{3}\delta_{ij}\mathrm{v}_{kk}) + \eta_b\delta_{ij}\mathrm{v}_{kk}$$

$$\mathrm{v}_{ij} = \frac{1}{2}\left(\partial_i \mathrm{v}_j + \partial_j \mathrm{v}_i\right)$$

Hydrodynamic Equations:

$$\partial_t \rho = -\vec{\nabla} \cdot (\rho\vec{\mathrm{v}})$$

$$\rho(\partial_t + \vec{\mathrm{v}} \cdot \vec{\nabla})\vec{\mathrm{v}} = -\vec{\nabla}p + \eta\nabla^2\vec{\mathrm{v}} + (\eta_{\mathrm{b}} - \tfrac{2}{3}\eta)\vec{\nabla}(\vec{\nabla} \cdot \vec{\mathrm{v}})$$

Navier-Stokes equation

Examples of hydrodynamics of active particles on a substrate

1. Hydrodynamics as a phenomenological theory based on symmetries and conservation laws: continuum theory of Vicsek model → polar particles with polar interactions[1] (Toner & Tu, 1995 & 1998; Ramaswamy et al, 2003-08; Bertin et al., 2006 & 2009; Mishra et al 2010; Ihle 2011)
2. Derivation of hydrodynamics from a microscopic model of SP hard rods: polar particles with apolar interactions[2] (Baskaran & Marchetti, 2008 & 2010; Peruani et al. 2006, Ginelli et al 2010; Yang et al 2010)
3. [Not covered in the lecture: active nematic → apolar active particles with apolar interactions (Ramaswamy et al 2003; Chate' et al 2006; Mishra & Ramaswamy 2006)

1. Toner, Tu & Ramaswamy, Ann. Phys. 318, 170 (2005)
2. Baskaran & MCM, PRE 77, 011920 (2008); PRL 101, 268101 (2008)

Question

- The Vicsek model with an explicit alignment rule yields “flocking”, i.e., collective coherent motion at large scales

- Can we obtain flocking in models with only “physical interactions”?
  - Excluded volume
  - [Medium mediated interactions]

Continuum Effective Theory of Vicsek Model

Phenomenology:Toner & Tu, 1995 & 1998

Slow Variables:

- Conserved: concentration ρ
- Broken symmetry: P – dual role: order parameter/current v_0P

$$\partial_t \rho = -\vec{\nabla}\cdot(v_0\vec{P} - D\vec{\nabla}\rho + noise)$$

alignment

$$\partial_t \vec{P} + \lambda_1\left(\vec{P}\cdot\vec{\nabla}\right)\vec{P} + \lambda_2\left(\vec{\nabla}\cdot\vec{P}\right)\vec{P} = -\left[\alpha(\rho) + \beta P^2\right]\vec{P} - \vec{\nabla}\pi(\rho,|\vec{P}|) + K\nabla^2\vec{P} + \vec{f}$$

pressure

noise

advection
breaking of Galileian
invariance

homogeneous
states

$$\left\langle f^i_{\vec{x},t}\ f^j_{\vec{x}',t'}\right\rangle = 2\Delta\delta_{ij}\delta_{\vec{x},\vec{x}'}\delta_{t,t'}$$

$$\pi(\rho,P) = w\rho + \lambda_3 P^2/2 + \ldots$$

Microscopic derivations of the continuum equations have been carried out by explicit coarse-graining of Vicsek model → yield parameter values (Bertin et al, 2003, 2009; Ihle, 2010) $\rightarrow \alpha(\rho,\Delta) \sim \rho_c(\Delta) - \rho$

Most of the terms in the equation for P can be obtained in terms of derivatives of the free energy of a polar (ferroelectric) liquid crystal

$$F=\int_{\vec r}\left[\frac{\alpha}{2}\vec P^2+\frac{\beta}{4}\vec P^4+\frac{C}{2}\delta\rho^2+\frac{K}{2}\left(\vec\nabla\cdot\vec P\right)^2-w\left(\vec\nabla\cdot\vec P\right)\delta\rho+w'P^2\left(\vec\nabla\cdot\vec P\right)\right]$$

$$\partial_t\vec P+\lambda_1\left(\vec P\cdot\vec\nabla\right)\vec P=-\frac{1}{\gamma}\frac{\delta F}{\delta\vec P}+\vec f$$

Let γ=1

$$\frac{\delta F}{\delta\vec P}=\alpha\vec P+\beta P^2\vec P-K\nabla^2\vec P-w\vec\nabla\delta\rho-w'\vec\nabla P^2+2w'\vec P\left(\vec\nabla\cdot\vec P\right)$$

$$w'\to\lambda_3/2$$

$$2w'\to\lambda_2$$

Terms in blue are unique to polar systems, not present in nematic

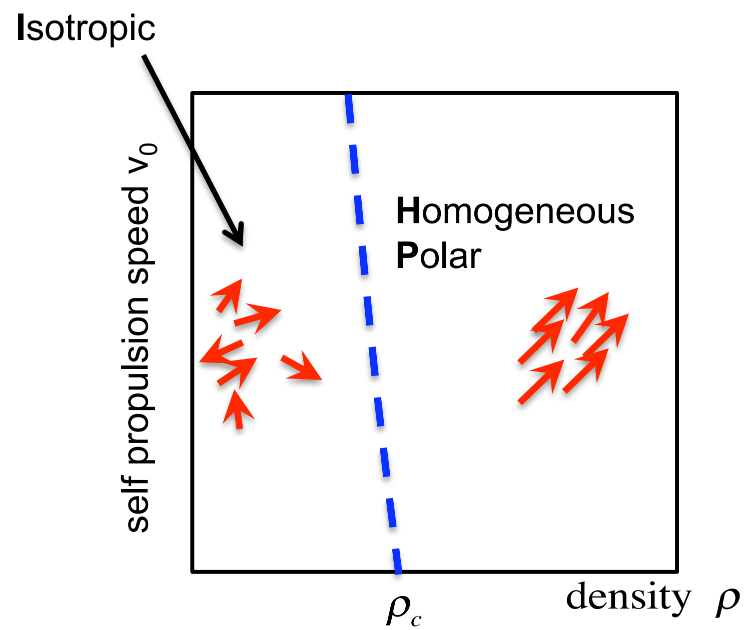
Term in red is intrinsically nonequilibrium and cannot be obtained from a free energy

Homogeneous Steady States

$$\rho = \rho_0 = \text{constant}$$

$$\left[\alpha(\rho) + \beta P^2\right]\vec{P} = 0$$

$$\alpha(\rho) \sim \rho_c - \rho$$



MF model yields continuous transition at $\alpha = 0$

$\alpha > 0$

Isotropic state P_0=0

$\alpha < 0$

Polarized flocking/ moving state $P_0 = \pm\sqrt{-\alpha / \beta}$

Properties of Ordered Phase: Linearized theory

$$\rho = \rho_0 + \delta\rho$$

$$\vec{P} = \vec{P}_0 + \delta\vec{P}$$

$$\partial_t \rho = -v_0 \vec{\nabla} \cdot \vec{P}$$

$$\partial_t \vec{P} + \lambda_1 \left(\vec{P}\cdot\vec{\nabla}\right)\vec{P} + \ldots = -\left[\alpha(\rho) + \beta P^2\right]\vec{P} - \vec{\nabla}\pi(\rho) + K\nabla^2\vec{P} + \vec{f}$$

Variations in local ordering tendency

$$\alpha(\rho) = \alpha_0 + \alpha'\delta\rho$$

$$\vec{\nabla}\pi(\rho) \simeq v_1 \vec{\nabla}\delta\rho$$

1) Ordered & disordered state support **traveling density (sound) waves** (Baskaran & MCM, 2008) $\omega = \pm q_{\|}\sqrt{v_0 v_1}$

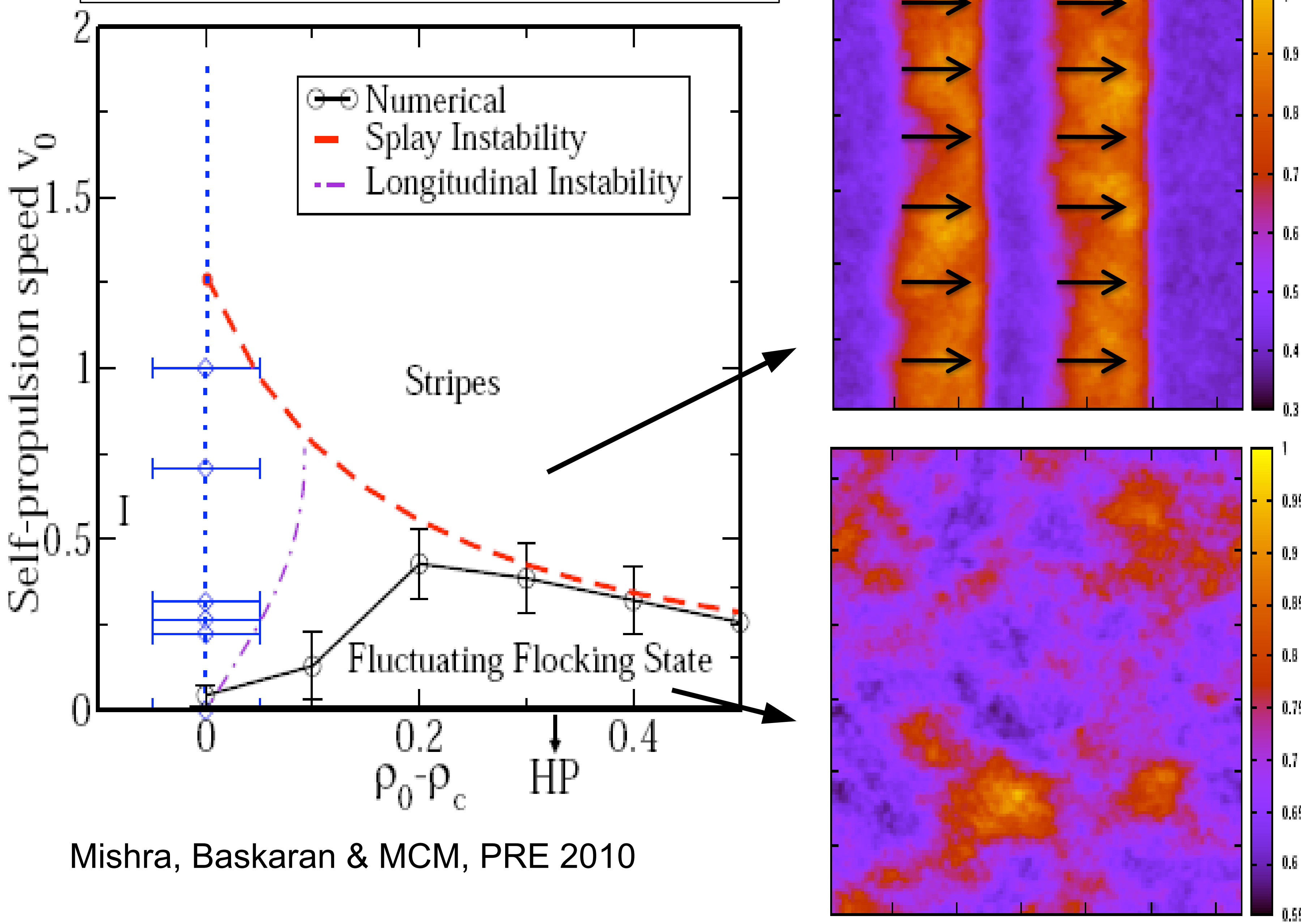
2) **Giant number fluctuations** near onset of putative continuous transition (Toner & Tu 1995; Ramaswamy & Simha, EPL 2003; Narayan et al, Science 2007) Chate et al, 2008: a=0.8 (2d)

$$\sqrt{\left\langle (\Delta N)^2 \right\rangle} \sim N^a$$

$a = 1/2 + 1/d$

3) **Ordered state is linearly unstable** near MF transition
Characteristic longitudinal length scale ~ $(K/\alpha)^{1/2}$
(Gregoire et al, 2009; Mishra, Baskaran & MCM, 2010)

Numerical Solution of Continuum Eqs.



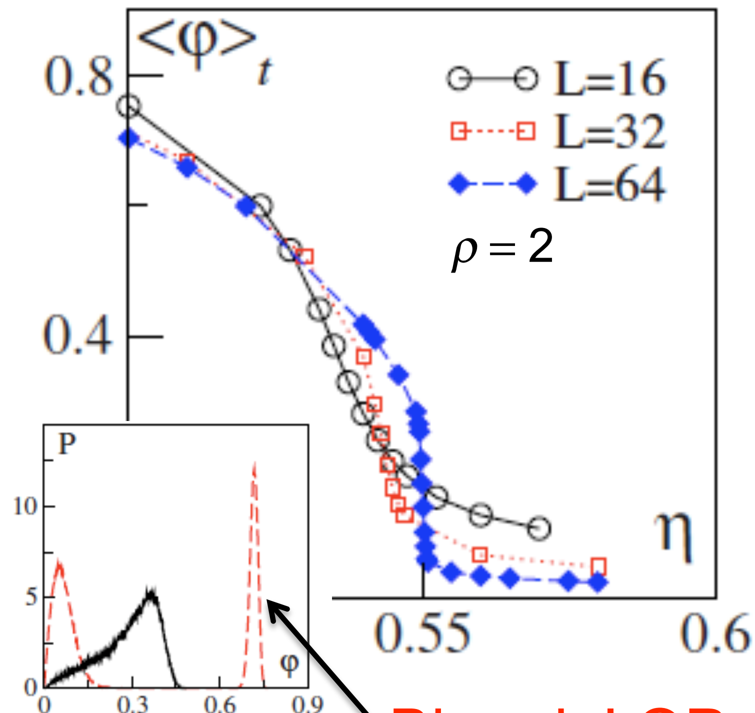
Mishra, Baskaran & MCM, PRE 2010

Vicsek model: numerics

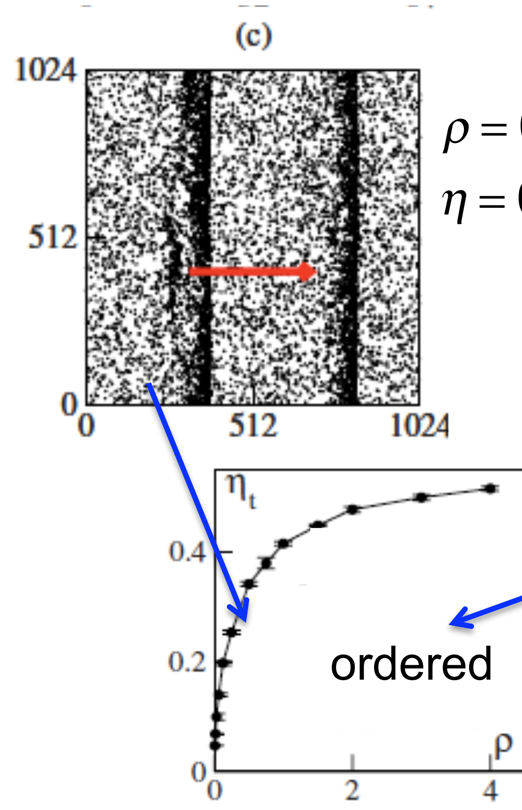
Gregoire & Chate, PRL 2004
Chate et al PRE 2008

$$\langle \varphi \rangle_t = \frac{\langle v \rangle_t}{v_0}$$

- Discontinuous onset of order
- Coexistence of ordered & disordered states
- Traveling bands



Bimodal OP distribution

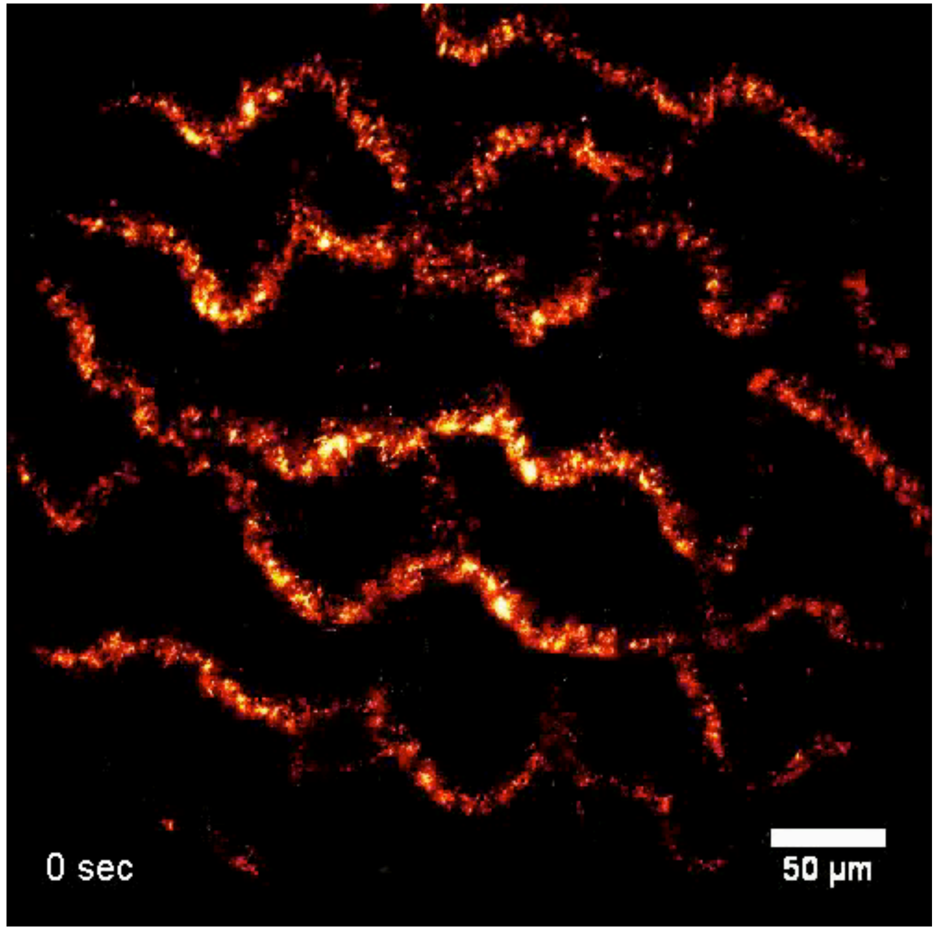


$\rho = 0.5$
$\eta = 0.3$

large fluctuations, intermittency

Actin motility assays at high actin density→ traveling density waves

$\rho_{actin} > 20\ fils / \mu m^2$



V. Schaller et al, Nature **467,** 73 –77 (2010)

http://www.nature.com.libezproxy2.syr.edu/nature/journal/v467/n7311/extref/nature09312-s3.mov

Nex Lecture:

Hydrodynamics of Self-Propelled hard rods: derivation by explicit coarse-graining of a microscopic model.