Collective dynamics of active matter:
from self-propelled particles to migrating cell layers

M. Cristina Marchetti
Syracuse University

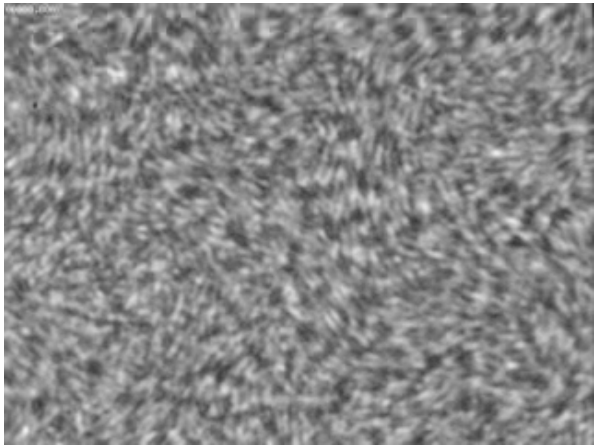
JAKS 2012 Bangalore

- Brief introduction to active matter: examples on a broad range of scales
- Active matter at high density: clustering and glassy states

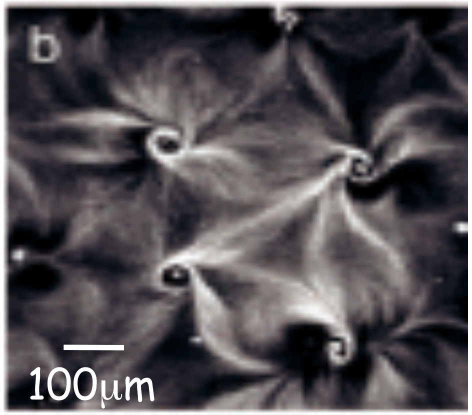
"Active" Matter

- Assembly of interacting self-driven units that consume energy and collectively generate motion or mechanical stress → examples on many scales
  - Bacterial suspensions
  - Biopolymers & motors in cell cytoskeleton
  - Vibrated granular rods
  - Flocks of birds
  - ...

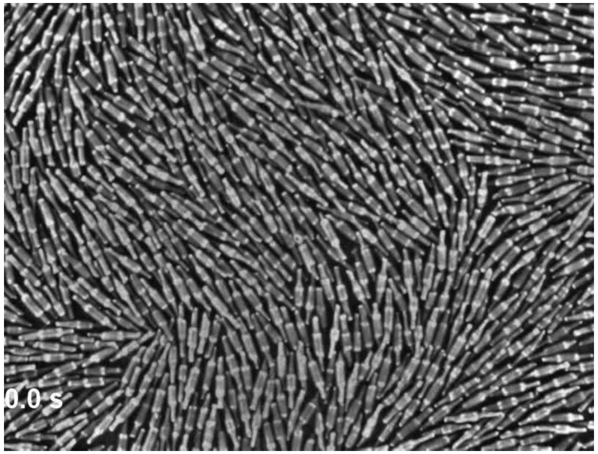
- Self-organization
- Directed, coherent motion
- Noneq. phase transitions



Bacterial turbulence (salmonella ~2 μm length) Berg lab, Harvard



Vortices & Asters in cytoskeletal extracts, Surrey et al, Science 2001



Vibrated granular rods (~5mm length), Narayan et al, Science 2007

On a different scale: groups of insects, fish, birds, …

StarFlag Collaboration

Irene Giardina et al, Rome

What do these systems have in common?

- Nonequilibrium systems where the drive acts on each unit, not applied at the boundary.
- Dynamic self-assembly: onset of “flocking” (= coordinated motion at large scales in a variety of spatio-temporal patterns) in the presence of noise.
- Active particle are often elongated and can order in states with orientational → “living liquid crystals”

Recent years: much progress in classifying the **generic behavior of active fluids** using ideas and tools of condensed matter physics and a combination of numerics & continuum theory

The beginning: Vicsek Model, 1995

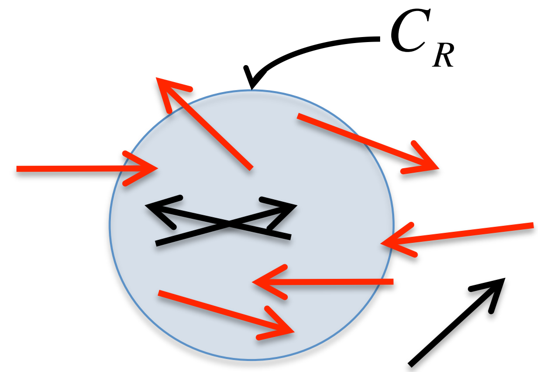
(but see C. Reynolds ~1987)

- N **point particles**, **fixed speed v_0**
- noisy aligning rules

$$\theta_i^{t+\Delta t} = \left\langle \theta_i^t \right\rangle_{C_R} + noise$$

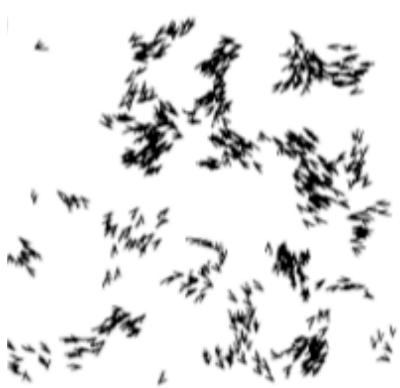
$$\vec{r}_i^{\,t+\Delta t} = \vec{r}_i^{\,t} + \mathrm{v}_0 \left(\cos\theta_i^t, \sin\theta_i^t\right)$$

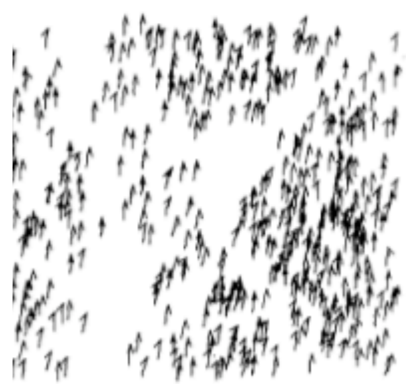
$$\left\langle \theta_i^t \right\rangle_{C_R} = \frac{1}{n_R} \sum_{j \in C_R} \theta_i^t$$



Flocking transition: from **disordered (v=0)** to **ordered moving (v≠0)** phase tuned by noise/density

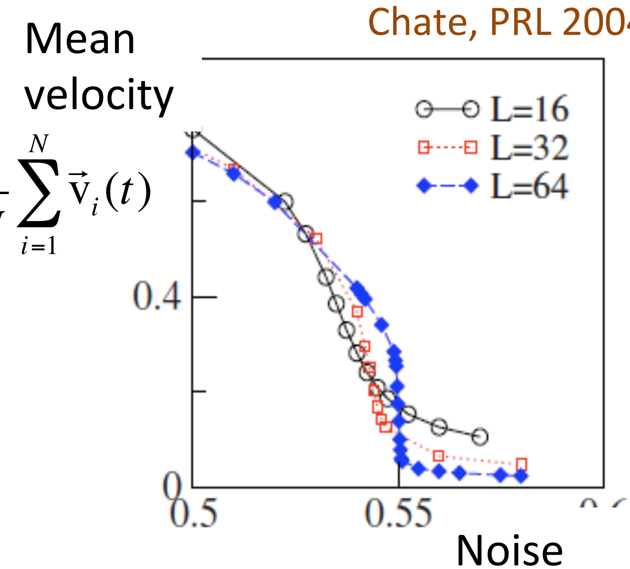
Spontaneously broken symmetry in 2d!





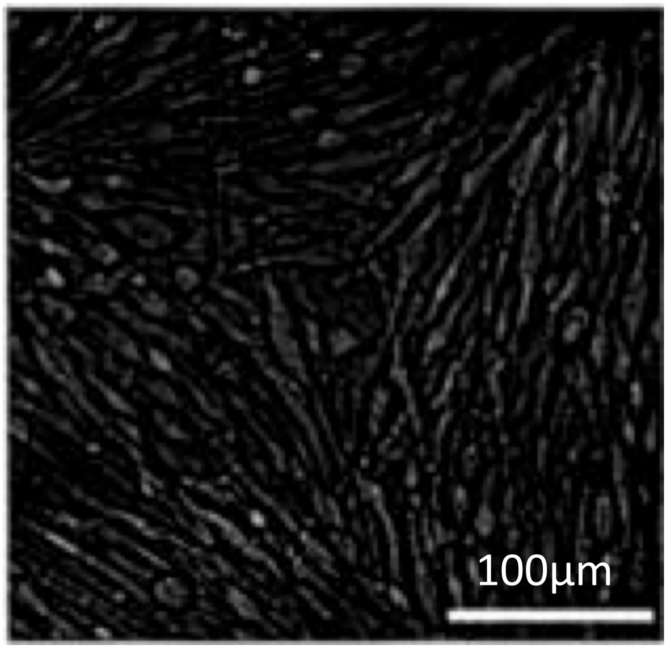
Gregoire & Chate, PRL 2004

$$\vec{\mathrm{v}} = \frac{1}{N} \sum_{i=1}^{N} \vec{\mathrm{v}}_i(t)$$



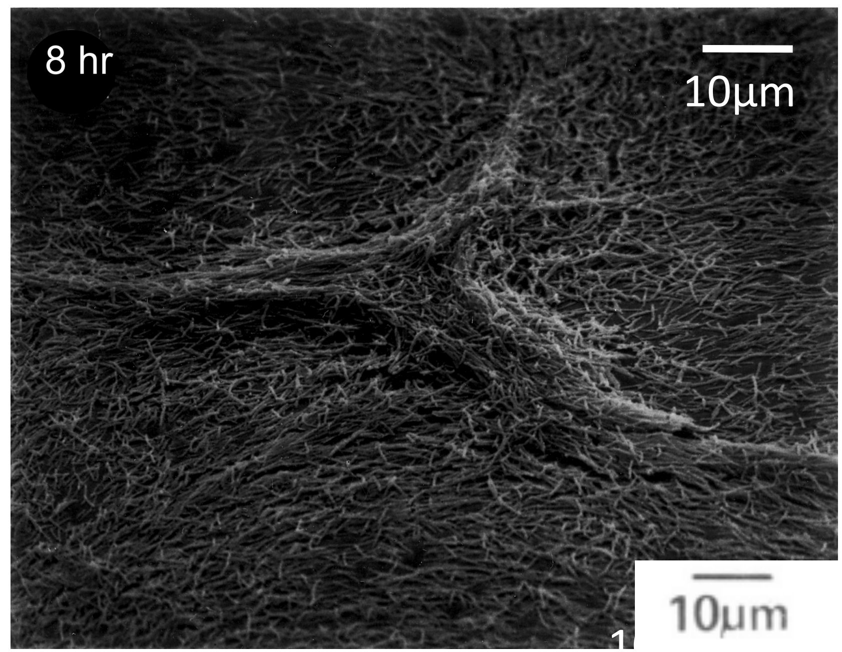
Active systems at high density:

``traffic jams"



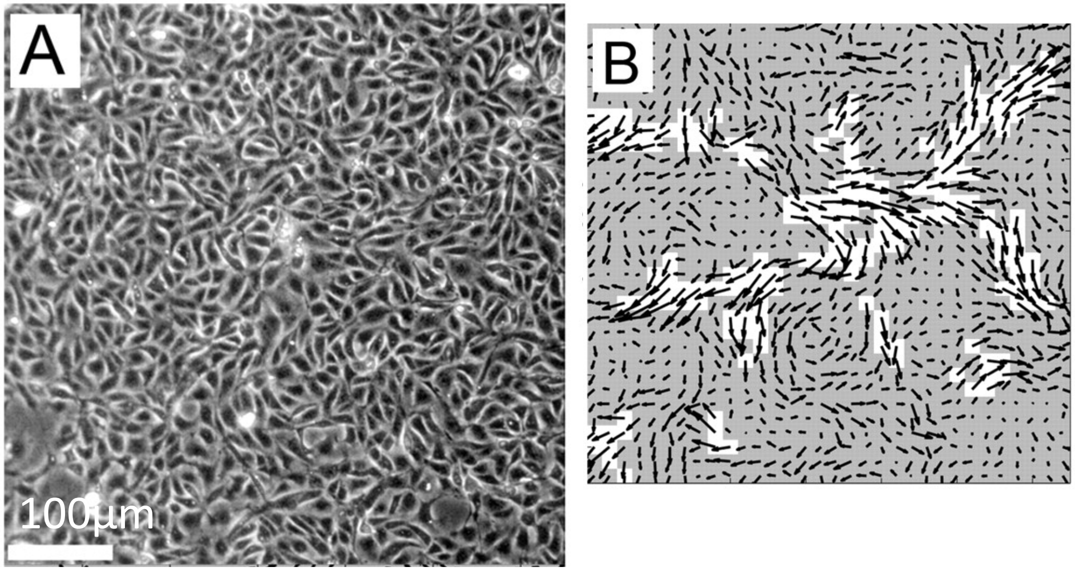
Melanocytes, Kemkemer et al., EPJE 2000

Myxobacteria aggregate formed 8 hours after a solution is deposited onto an agar substrate (Kuner & Kaiser 1982)

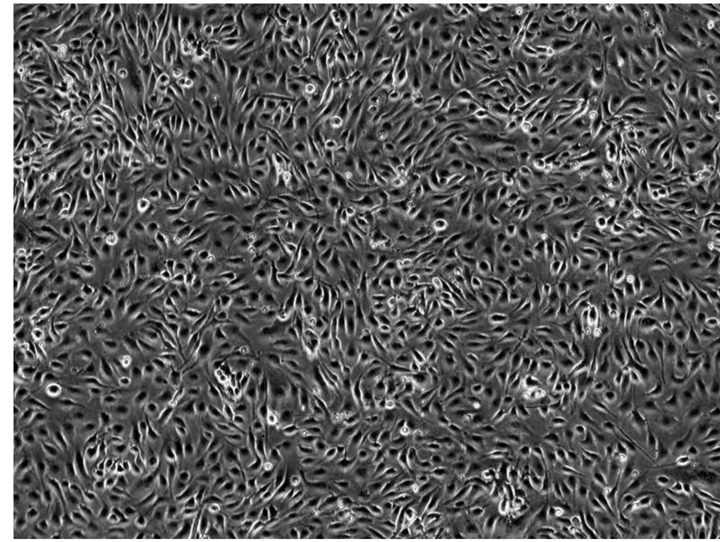


Glass-like dynamics of collective cell migration

Angelini *et al*. PNAS 2011

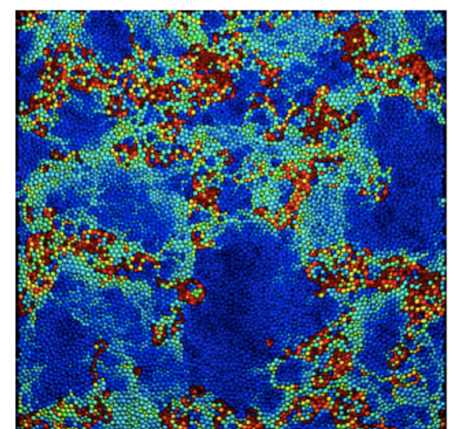


Szabó *et al*, Phys. Biol. 2010
v_{avg} 35 µm/h



- Suppression of diffusive motion with increasing cell density
- Dynamics controlled by dynamical heterogeneities (correlated groups of fast/slow cells) characteristic of glassy systems.

Hedges,
PNAS 2009
Supercooled
fluid mixture



Today's talk:

active systems at high density → solid-like and glassy states

Local crowding (Peruani, 2006 & 2011; Baskaran & MCM, 2008; Yang et al. 2010) and biochemical signaling (Tailleur & Cates, 2008; Cates et al 2010) can slow down activity. Not captured by Vicsek models with fixed SP speed.

Can active systems self-organize in solid-like states in the presence of a continuous energy input?

Two models: SP & steric effects (2d)

- Self-propelled disks with no alignment: phase separation and giant density fluctuations

Yaouen Fily

- SP disks with alignment as a model for glassy cell layers

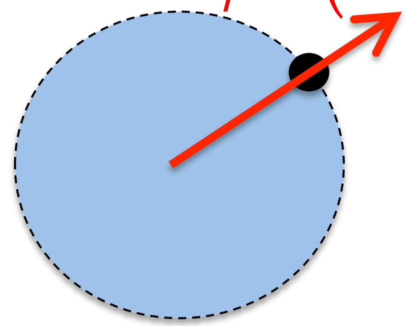
Silke Henkes

SP particles with no alignment

(Y. Fily & MCM arXiv:1201.4847)

- Soft repulsive disks
- SP speed v_0 along axis $\hat{n}$
- Orientational noise D_R

$$\hat{n}_i = \left(\cos\varphi_i, \sin\varphi_i\right)$$



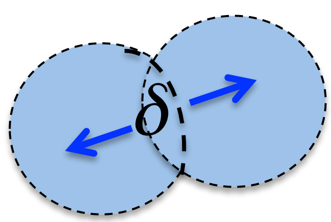
$$\vec{v}_i = v_0 \hat{n}_i + \mu \sum_{j \neq i} \vec{f}_{ij}$$

$$\dot{\theta}_i = \eta_i(t) \qquad \left\langle \eta_i(t) \eta_j(t') \right\rangle = 2D_R \delta_{ij} \delta(t - t')$$

Parameters & time scales

$$\begin{cases} \phi = \dfrac{N\pi a^2}{L^2} & \text{packing fraction} \\ D_R^{-1} & \text{inverse noise strength} \\ a/v_0 & \\ (\mu k)^{-1} & \text{interaction strength} \end{cases}$$

f_{ij} pair repulsive forces $\sim k\delta$



δ= overlap

No alignment rule, no steric alignment
→ no flocking state at any density

See also Bialke' et al arXiv:1112.5281v1

Sharp change of scaling of number fluctuations at $\varphi=\varphi_c\approx 0.4$

Thermal systems $\Delta N = \sqrt{\langle N^2\rangle - \langle N\rangle^2} \sim N^{1/2}$

Orientationally ordered state (polar & nematic) of active systems: (Simha 2002, Chate' 2006, Narayan 2007)

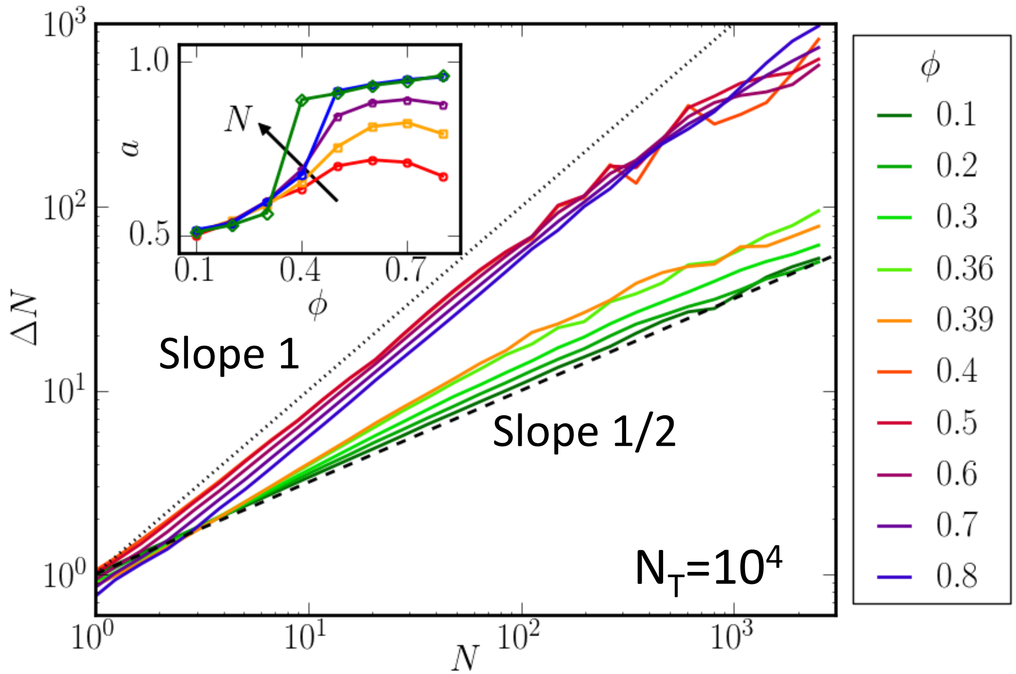
$\Delta N \sim N^a$

$a = 1 \quad d = 2$

SP disks no alignment:

$\Delta N \sim N^a$

$a \sim 0.95 \pm 0.05$

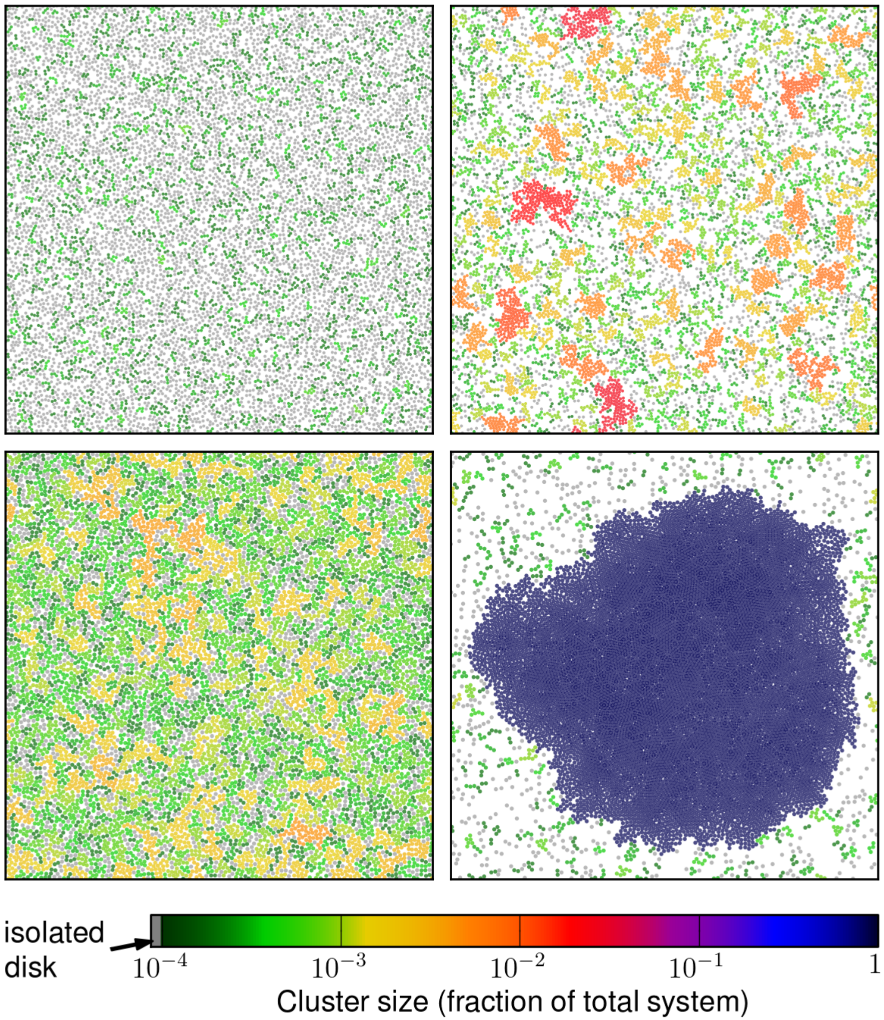


Phase separation at $\varphi=\varphi_c\approx 0.4$

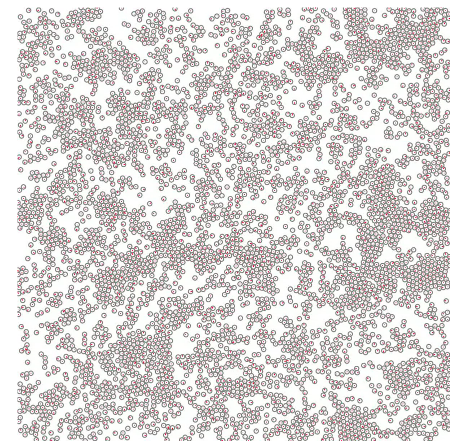
Thermal disks　　SP disks

φ=0.39

φ=0.7

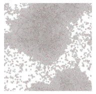


$\varphi_{cp}=0.91$



$$\mu k\delta \sim v_0 \rightarrow \delta_0 \sim v_0 / \mu k$$

$$k_B T_{equiv} \sim k\delta_0^2$$



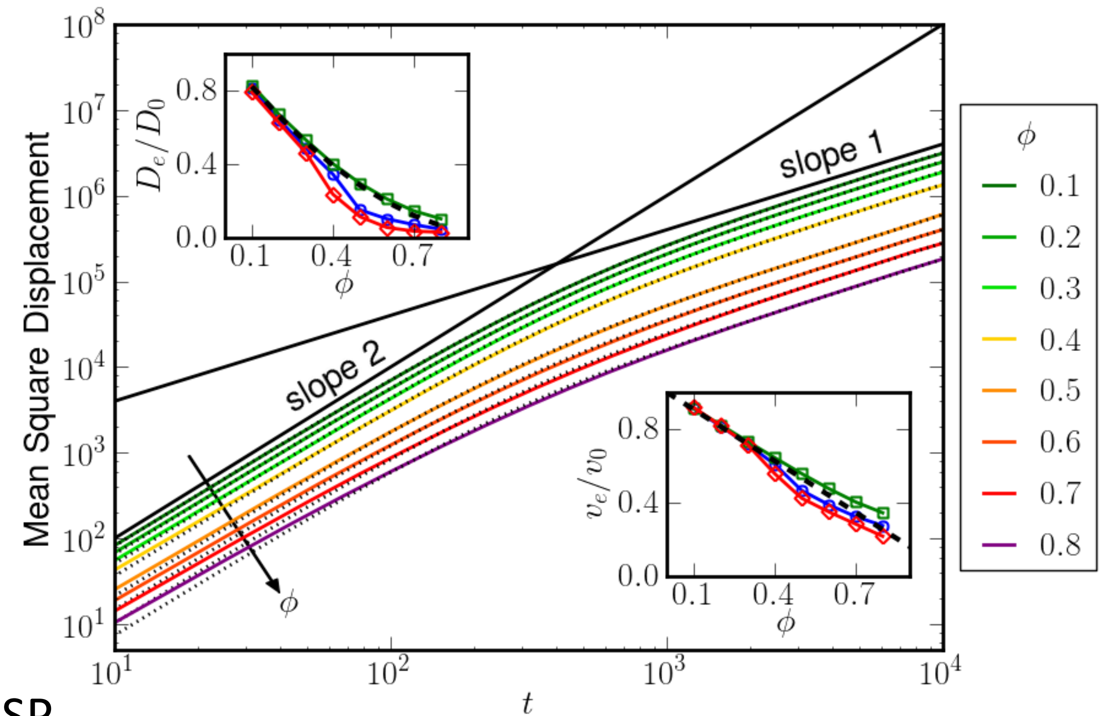
Mean Square Displacement

A single SP disk performs a persistent random walk (PRW):

$t << D_R^{-1} \quad \left\langle \left[\Delta\vec{r}(t)\right]^2 \right\rangle \sim v_0^2 t^2$ ballistic

$t >> D_R^{-1} \quad \left\langle \left[\Delta\vec{r}(t)\right]^2 \right\rangle \sim 4Dt$ diffusive

$$D = \frac{v_0^2}{2D_R}$$



Inset: v_0=0.5, v_0=1, v_0=2

Moderately dense suspension of SP disks: the MSD can be fitted by PRW form with

$$v_0 \rightarrow v_{eff}(\phi) = v_0(1-\lambda\phi)$$
$$D \rightarrow D_{eff}(\phi) = \frac{\left[v_{eff}(\phi)\right]^2}{2D_R}$$

See Tailleur & Cates, PRL 2008
Cates et al, PNAS 2010

Effective continuum model

(see also Farrell, Marenduzzo, Tailleur & MCM, arXiv:1202.0749)

- ✧Conserved density ρ
- ✧Polarization density $\vec{p}(\vec{r},\, t) = \sum_i \hat{n}_i \;\delta(\vec{r} - \vec{r}_i)$, mean orientation
- ✧Interactions replaced by mean-field local speed $v_0 \rightarrow v_{eff}(\rho) = v_0(1-\lambda\rho)$

$$\partial_t \rho = -\vec{\nabla} \cdot \left[\mathrm{v}_{eff} \vec{p} - D \vec{\nabla} \rho \right]$$

$$\partial_t \vec{p} = -D_R \vec{p} - \vec{\nabla}(\mathrm{v}_{eff} \rho) + K \nabla^2 \vec{p} + \vec{f}$$

Isotropic state $\rho=\rho_0$, $\mathbf{p}=0$ linearly unstable at $\phi=\phi^*=1/(2\lambda)$

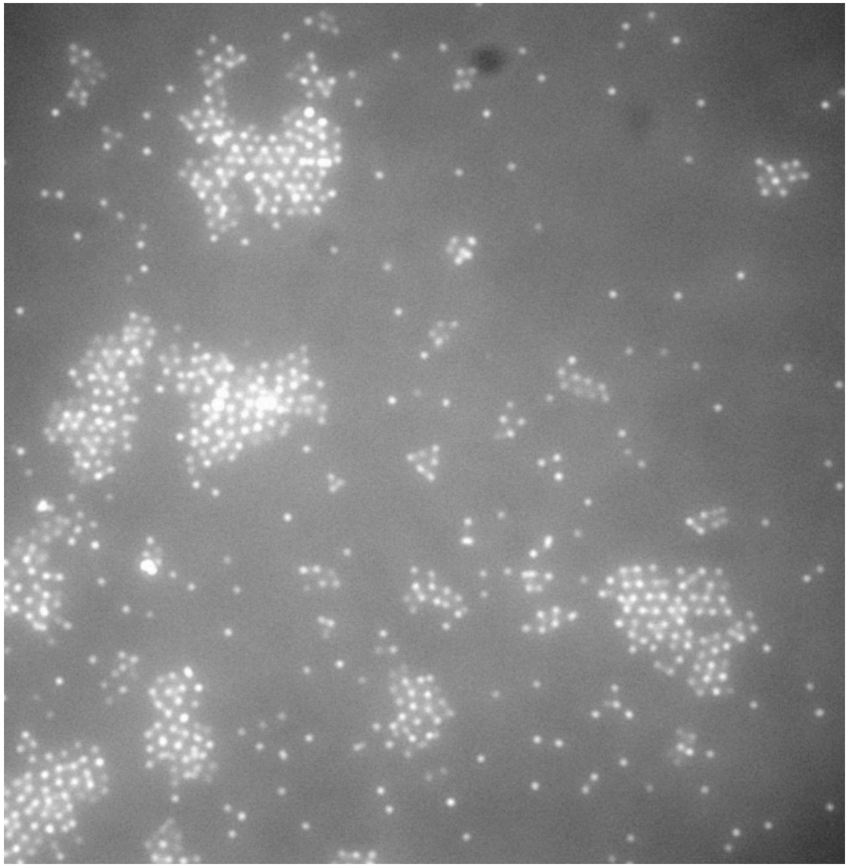
$$\mathcal{D} = D + \frac{\mathrm{v}_{eff}}{D_R}\left(\mathrm{v}_{eff} + \rho_0 \frac{d\mathrm{v}_{eff}}{d\rho} \right)$$

Effective diffusivity vanishes at $\phi=\phi^*\approx 0.45$ (for D=0) signaling phase separation (Cates et al, 2010)

SP particles, no alignment: Summary

- Data suggestive of gas-cluster transition at ϕ=0. 4 well below close packing arising solely from steric effects and self propulsion
- Formation of large "frozen" stationary cluster: SP systems cannot be described by an effective temperature (Tailleur & Cates, 2008; Bialke' et al, 2011)
- Compare to very recent experiments in SP colloids (Bocquet, Lyon) and in myxobacteria (Peruani et al)

L. Bocquet, Lyon



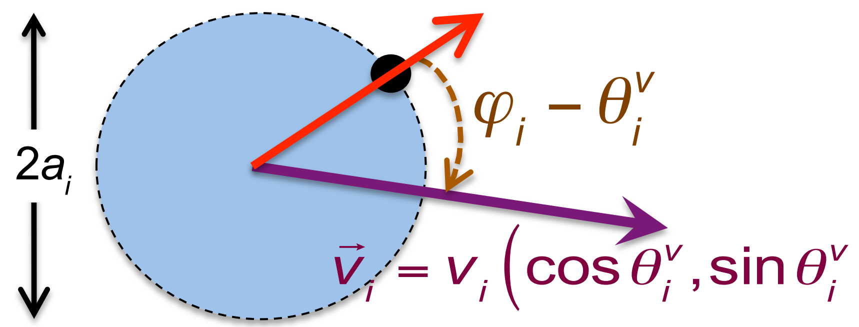
Add alignment → Agent-Based Model of Collective Cell Migration

Henkes, Fily & MCM, PRE 2011

New ingredients:

- **Alignment rule***
- **polydispersity**
- SP represents cell polarization

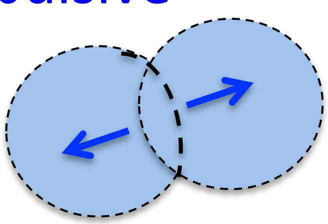
$$\hat{n}_i = \left(\cos\varphi_i, \sin\varphi_i\right)$$



$$\vec{v}_i = \dot{\vec{r}}_i = v_0\hat{n}_i + \mu\sum_j \vec{f}_{ij}$$

$$\dot{\varphi}_i = \frac{1}{\tau}\left(\theta_i^v - \varphi_i\right) + \eta_i(t) \qquad \left\langle \eta_i(t)\eta_j(t')\right\rangle = \sigma^2\delta_{ij}\delta(t-t')$$

f_{ij} pair repulsive forces:

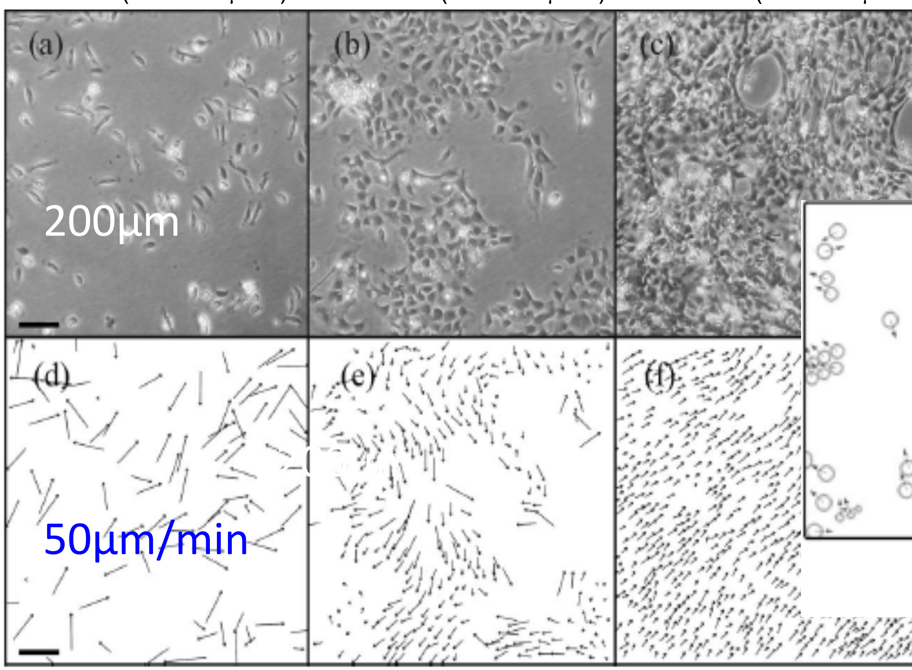


*Szabó et al, PRE 74, 06918 (2006)

Add **polydispersion** as size variation is needed to yield glass in 2d repulsive soft disks
→ passive limit is the granular jamming transition

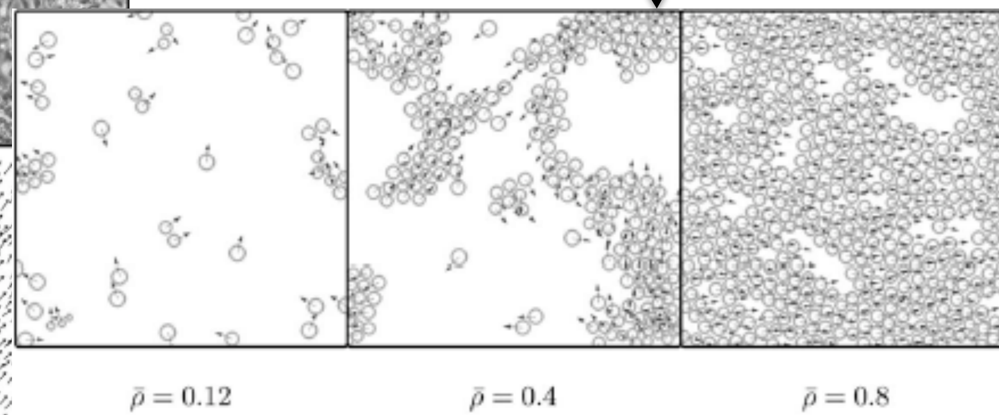
Szabó et al. (2006): **Open system & Periodic Boundary Conditions** → transition to flocking state with increasing cell density

$1.8\ cells / (100x100 \mu m^2)$ $5.3\ cells / (100x100 \mu m^2)$ $14.7\ cells / (100x100 \mu m^2)$



goldfish keratocytes

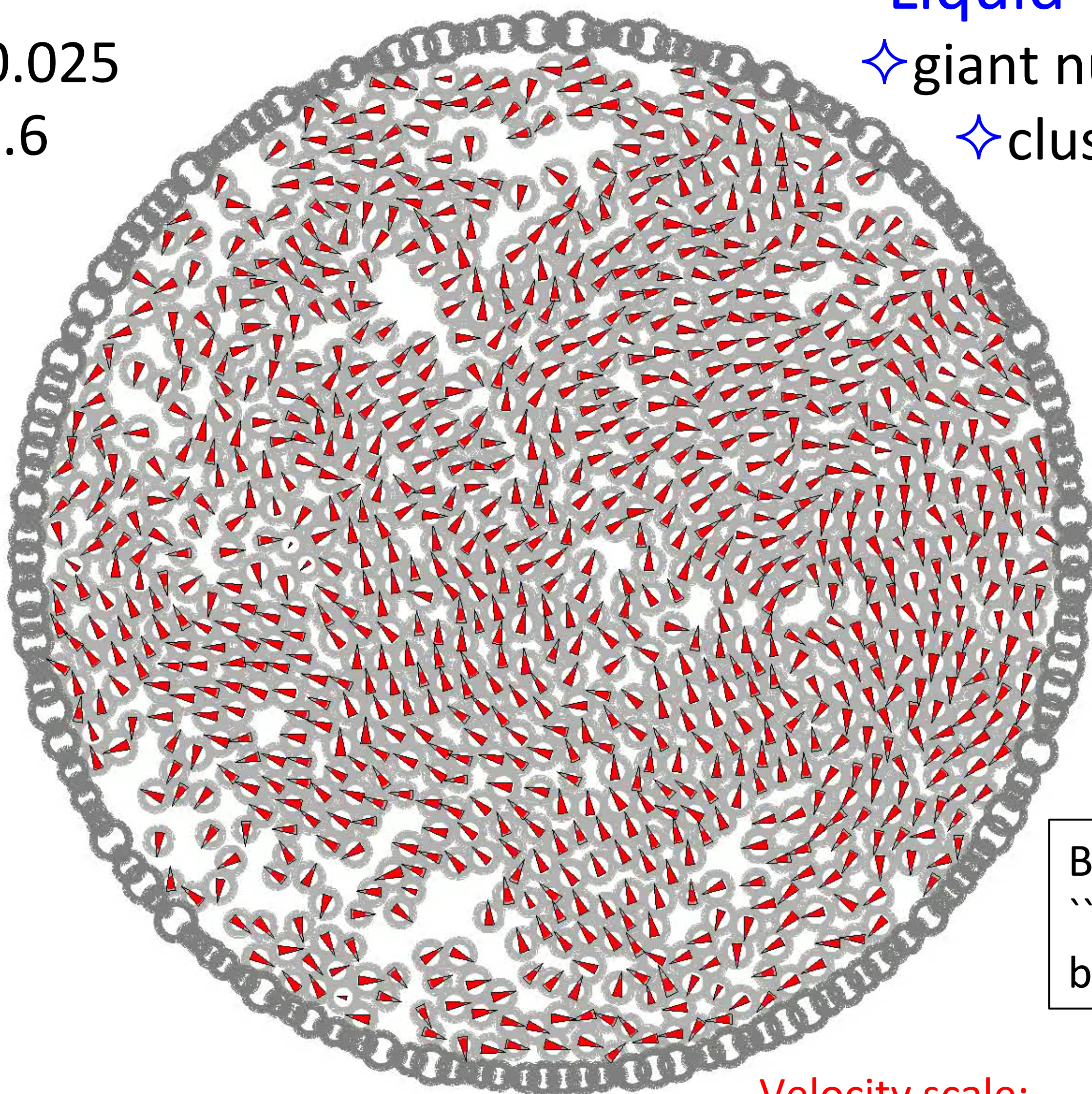
numerical model (includes short-range attraction)



Our model:

- Polydispersion
- Confinement to disable global translation

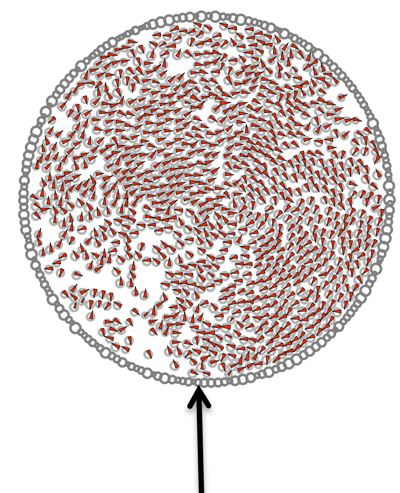
v_0=0.025
φ=0.6



“Liquid” state:

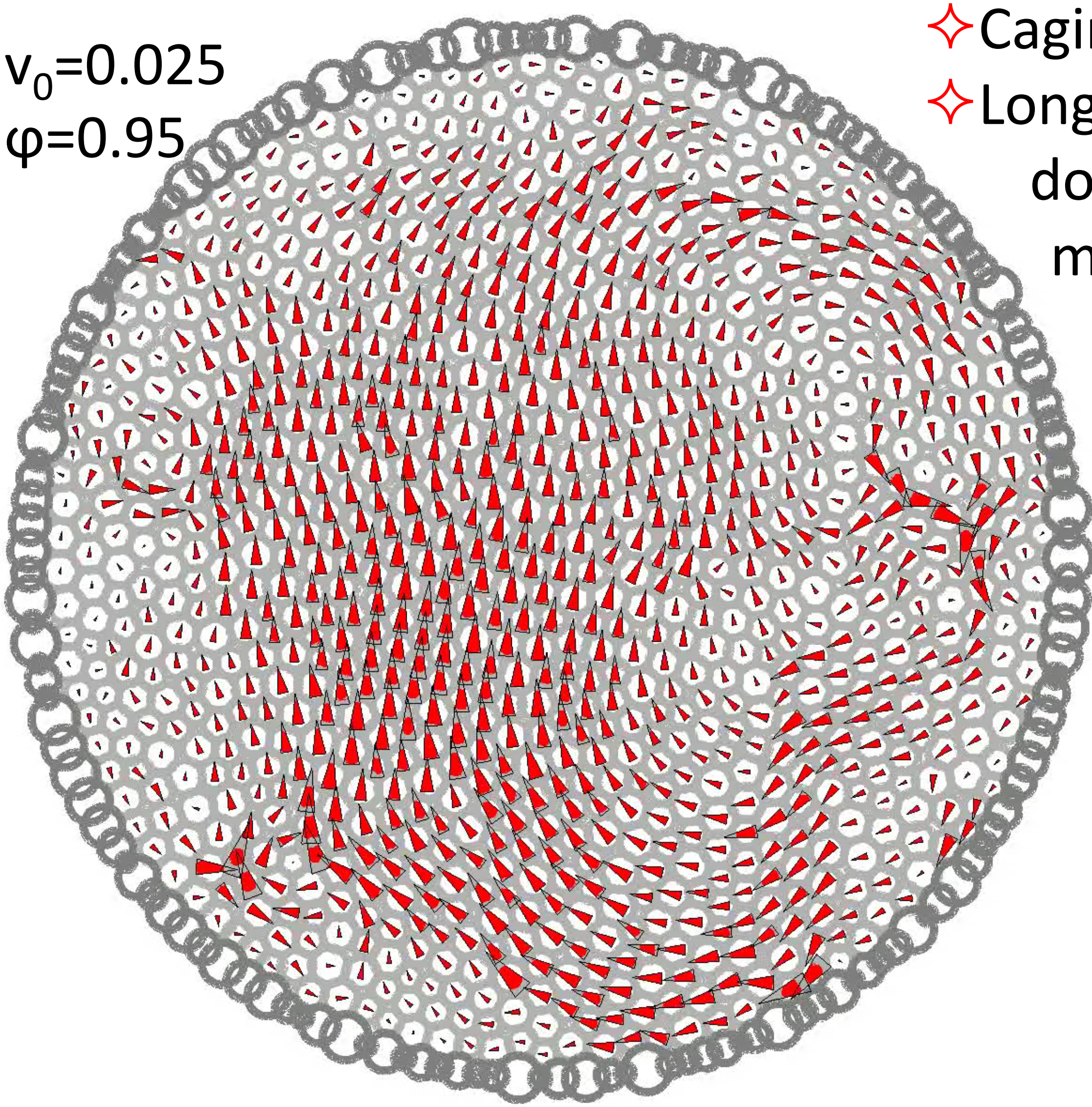
✧giant number fluctuations

✧clustering yields ballistic MSD at all times



BC: row of soft spheres ``glued” to the box boundary

Velocity scale:
red arrow=diameter → v=v_0



"Glass" or "jammed" state:

- ✧Caging and oscillations
- ✧Long time dynamics dominated by low frequency modes of jammed soft disks

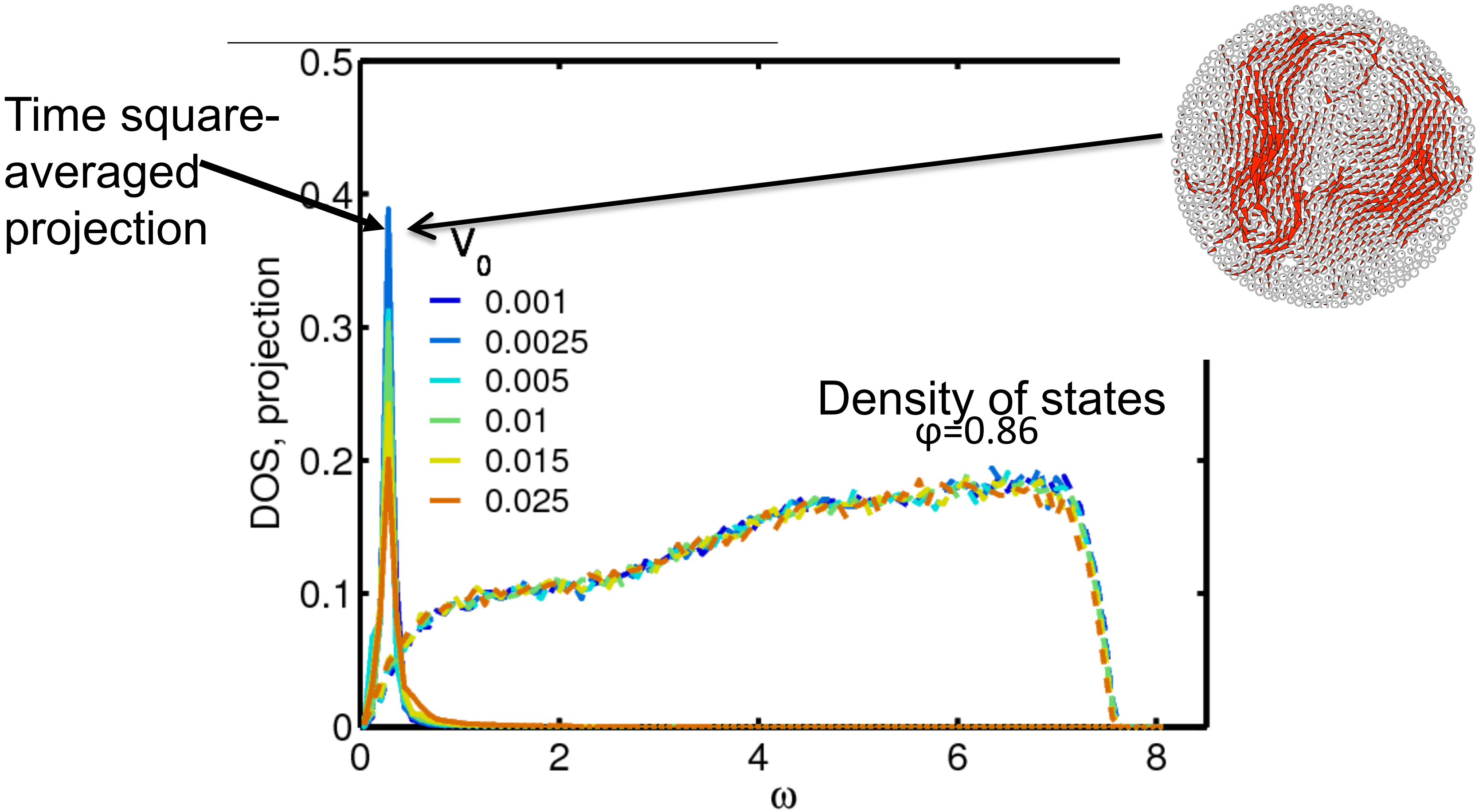
What are these oscillations?

- The system is in a glassy state; the self-propulsion excites the collective low energy modes of the system.
- Although the dynamics is overdamped, the angular alignment time scale τ provides an effective inertia
- Can study the low frequency modes analytically by expanding around jammed state
- Energy is not distributed by equipartition, but cascades into low energy modes

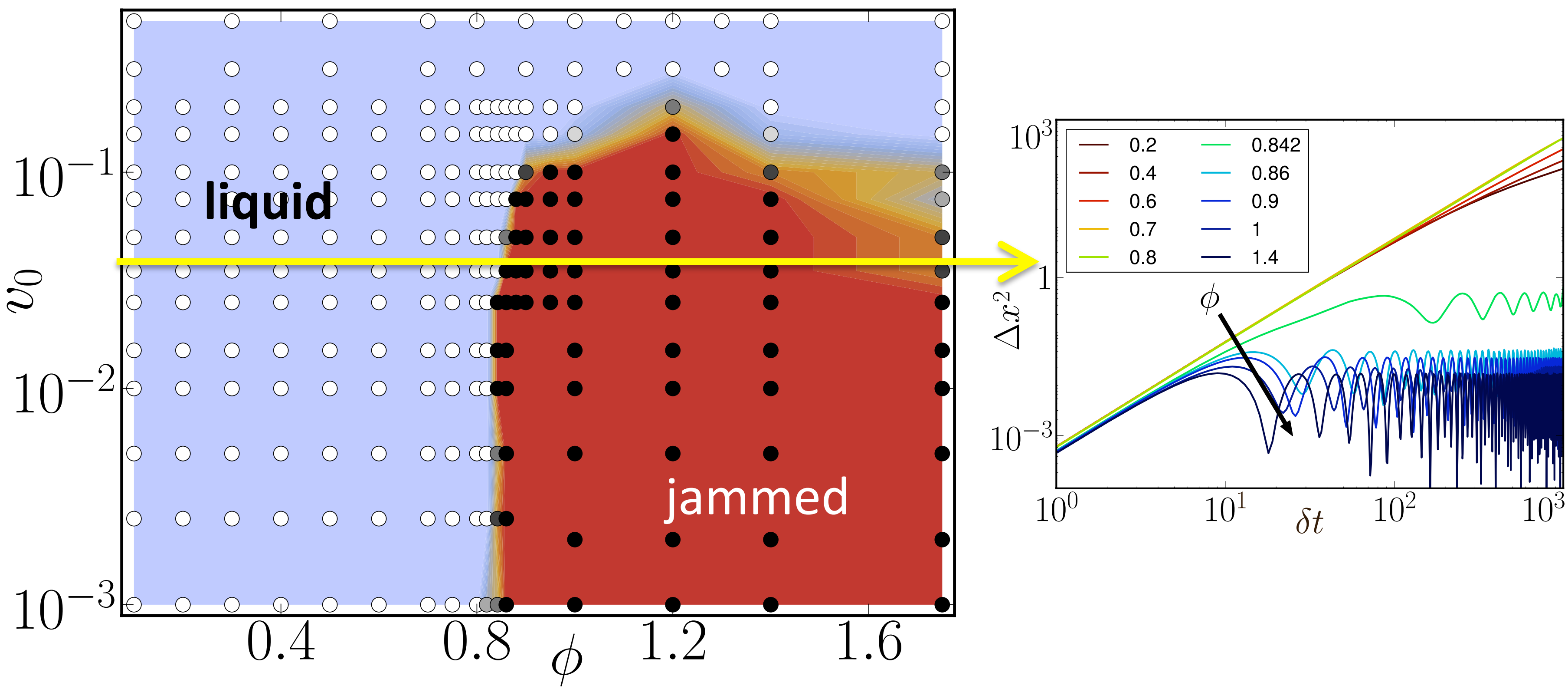
Low-energy "phonons" control the dynamics at long times

Energy is not distributed by equipartition, but cascades into low energy modes

very non-thermal → equipartition would lead to ~$1/\omega^2$



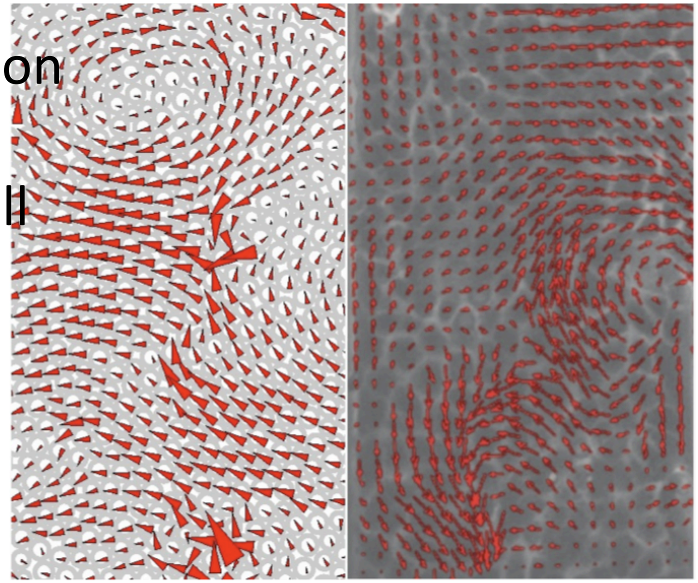
Transition from an active fluid to an active glassy or jammed state with increasing packing fraction φ



Migrating cell model: Summary & Outlook

- Excluded volume interaction yields frustration and glassy dynamics at high density:
  - slowing down of diffusion
  - dynamical heterogeneities
  - collective dynamics dominated by low frequency modes
  - heterogeneous stress distribution
- To explore:
  - Magnitude v_0 & direction of cell polarization determined by environment
  - Role of substrate-mediated contractile cell couplings
  - Role of cell adhesion → wound healing
  - Contrast to thermal glass/jamming transition

Poujade *et al.*, PNAS 2007, wound healing



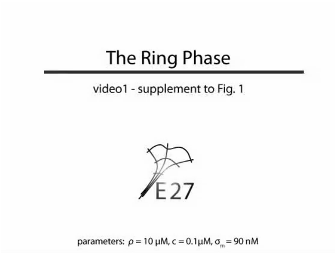
Summary & Questions

- Dense active systems appear highly non-thermal→ no effective temperature
- Are clustering and phase separation a generic properties of systems driven out of equilibrium by an energy input on each particle?
- Are the large frozen clusters a "dynamically frozen" state intermediate between the liquid and the crystal/glass?

Frozen active states in actin motility assay with passive crosslinkers (fascin)

Schaller et al, PNAS Nov 2011

Reichhardt & Reichhardt, PNAS 2011



Thanks to many students, postdocs and collaborators:

- Aphrodite Ahmadi (SU → SUNY Cortland)
- Shiladitya Banerjee (SU)
- Aparna Baskaran (SU → Brandeis)
- Yaouen Fily (SU)
- Luca Giomi (SU → Harvard)
- Gavin Hartnett (SU→Santa Barbara)
- Silke Henkes (SU)
- Tannie Liverpool (Bristol, UK)
- Kristian Mueller-Nedebock (Stellenbosch, SA)
- Shraddha Mishra
- Xingbo Yang (SU)