Lecture 2 – Collective effects in dense active systems: phase separation, jamming & glassy states

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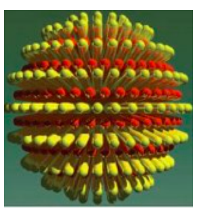
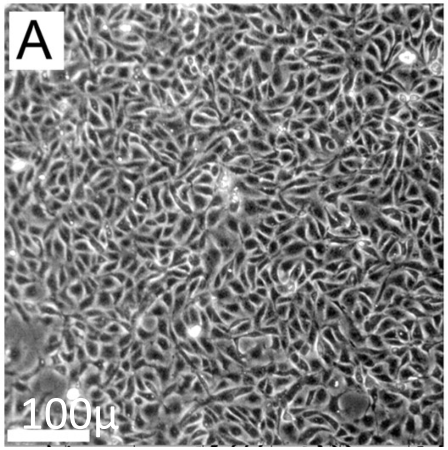


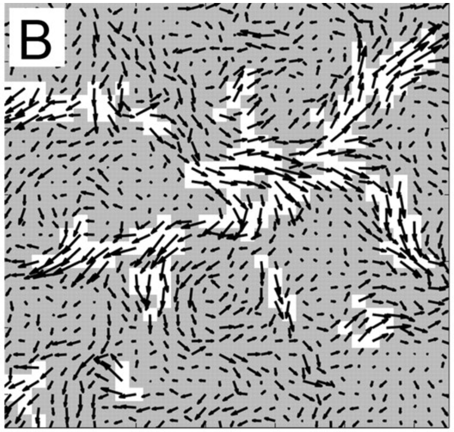
Soft Matter Program @SU

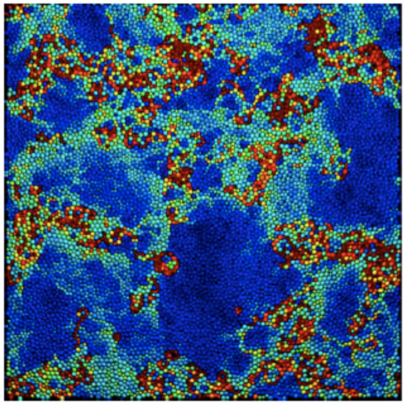
SYRACUSE BIOMATERIALS INSTITUTE

GIST, Korea, July 2014

Glass-like dynamics of collective cell migration



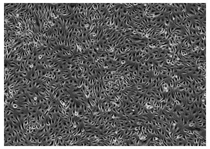




Hedges, 2009
supercooled fluid mixture

Angelini *et al*. 2011: MDCK epithelial cells, v_{avg} 35 μm/h

Szabó *et al*, 2010
BAEC endothelial cells →

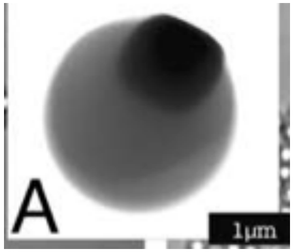


- Suppression of diffusive motion with increasing cell density
- Dynamics controlled by dynamical heterogeneities

Role of crowding and steric effects vs activity

Active Colloids

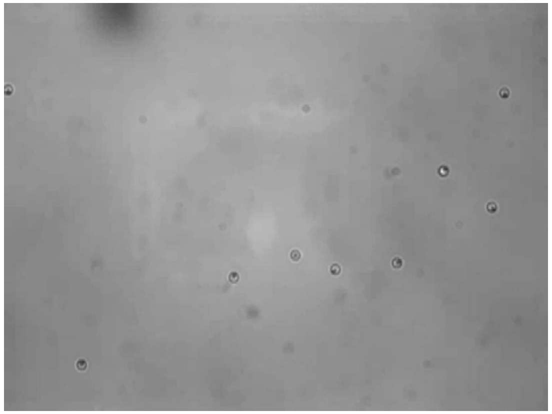
Palacci et al, Science2013

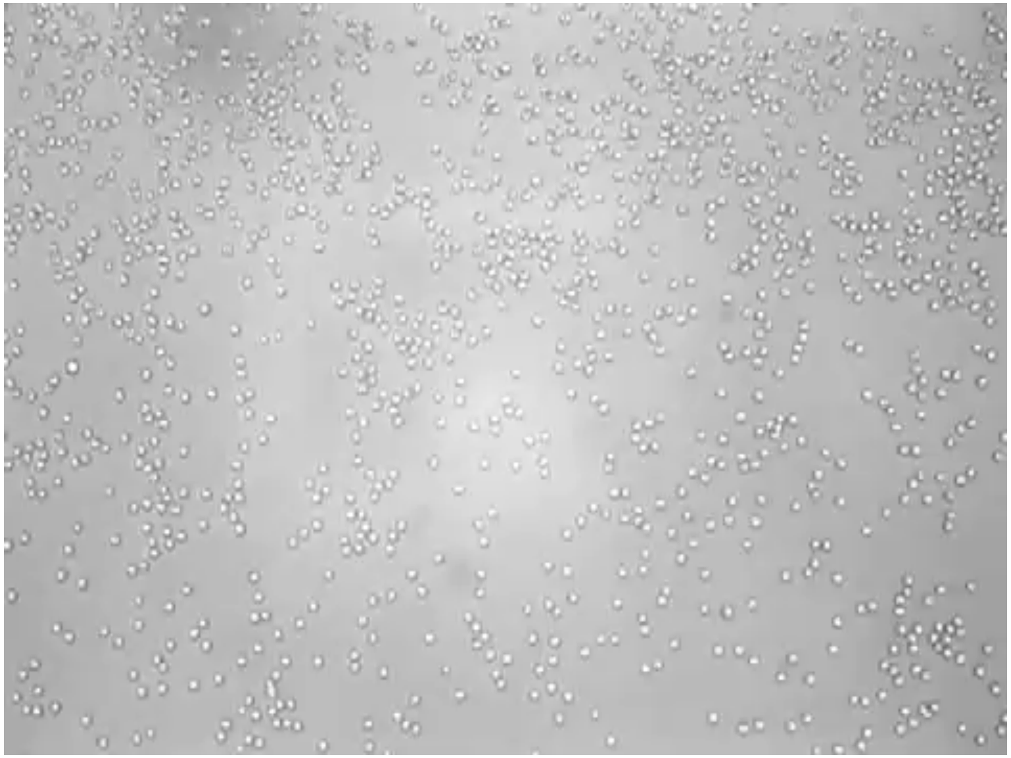


$2D$

$L = 600nm$

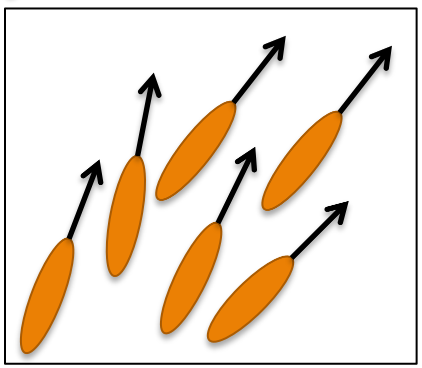
$v_0 = 15\mu m / s$





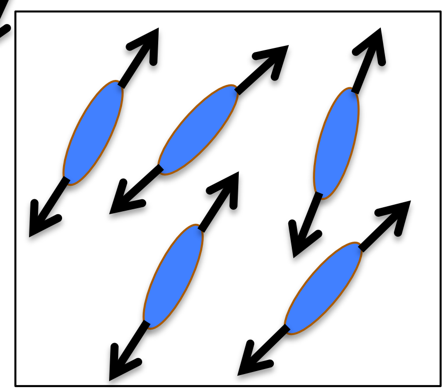
Active Particles & Types of Order

Polar (head≠tail): bacteria, birds, fish, …

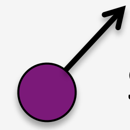


``Ferromagnetic'' order: a moving state or flock

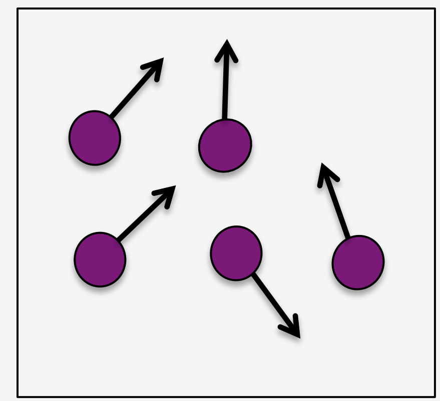
Apolar: melanocytes, vibrated grains, …



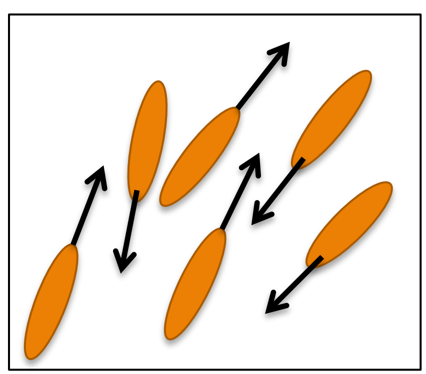
Nematic order: no mean motion



Spherical: colloids



No orientational order (unless imposed by aligning rules), but surprising collective behavior



Nematic order of polar particles

Self-propelled repulsive soft colloids:

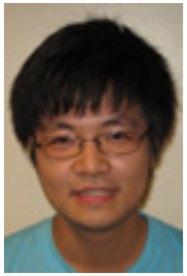
a simple model to explore the interplay of self-propulsion and crowding in active systems. Possible relevance to collective cell migration, wound healing and cell sorting.

- Self-propelled disks with **no alignment →active colloids**

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

Silke Henkes
Aberdeen, UK

Yaouen Fily,
Brndeis



Xingbo Yang,
Syracuse

Self-Propelled particles + repulsive interactions

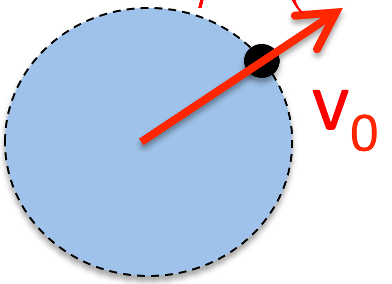
- Repulsive disks of radius a
- SP speed v_0 along axis $\hat{\mathbf{n}}_\mathbf{i}$
- Orientational noise D_r

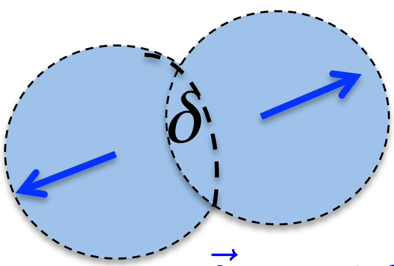
Fily & MCM PRL 108, 235702 (2012)
Fily, Henkes & MCM, Soft Matter 10, 2132 (2014)

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

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

$$\hat{n}_i = (\cos\theta_i, \sin\theta_i)$$





$\vec{f}_{ij} \sim k\delta$: spring-like pair repulsive forces $\propto$ overlap δ

$$\phi = \frac{N \pi a^2}{L^2}$$ packing fraction

See also:
Redner et al PRL 110, 055701 (2013);
Cates & Tailleur *EPL* **101** 20010 (2013);
Buttinoni et al PRL 110, 238301 (2013)

Single Active Particle

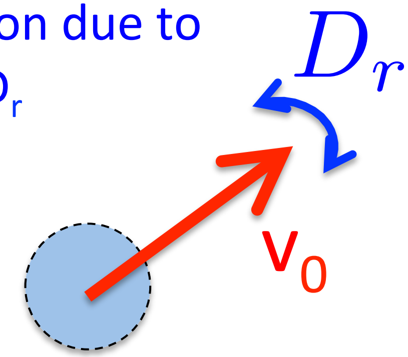
Brownian particle:
random walk (RW)

$$\langle[\mathbf{r}(t)-\mathbf{r}(0)]^2\rangle = 2Dt$$

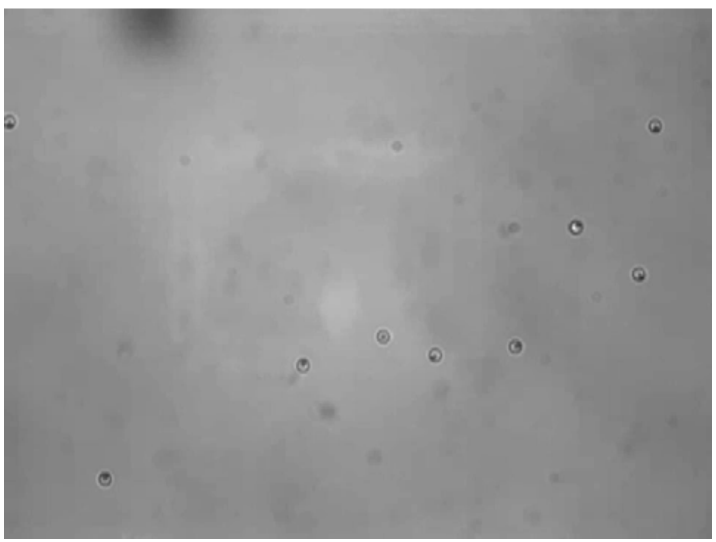
$$D = \frac{k_B T}{\zeta}$$

Active particle: persistent RW

- Ballistic `runs' at speed v_0
- Change of direction due to rotational noise D_r

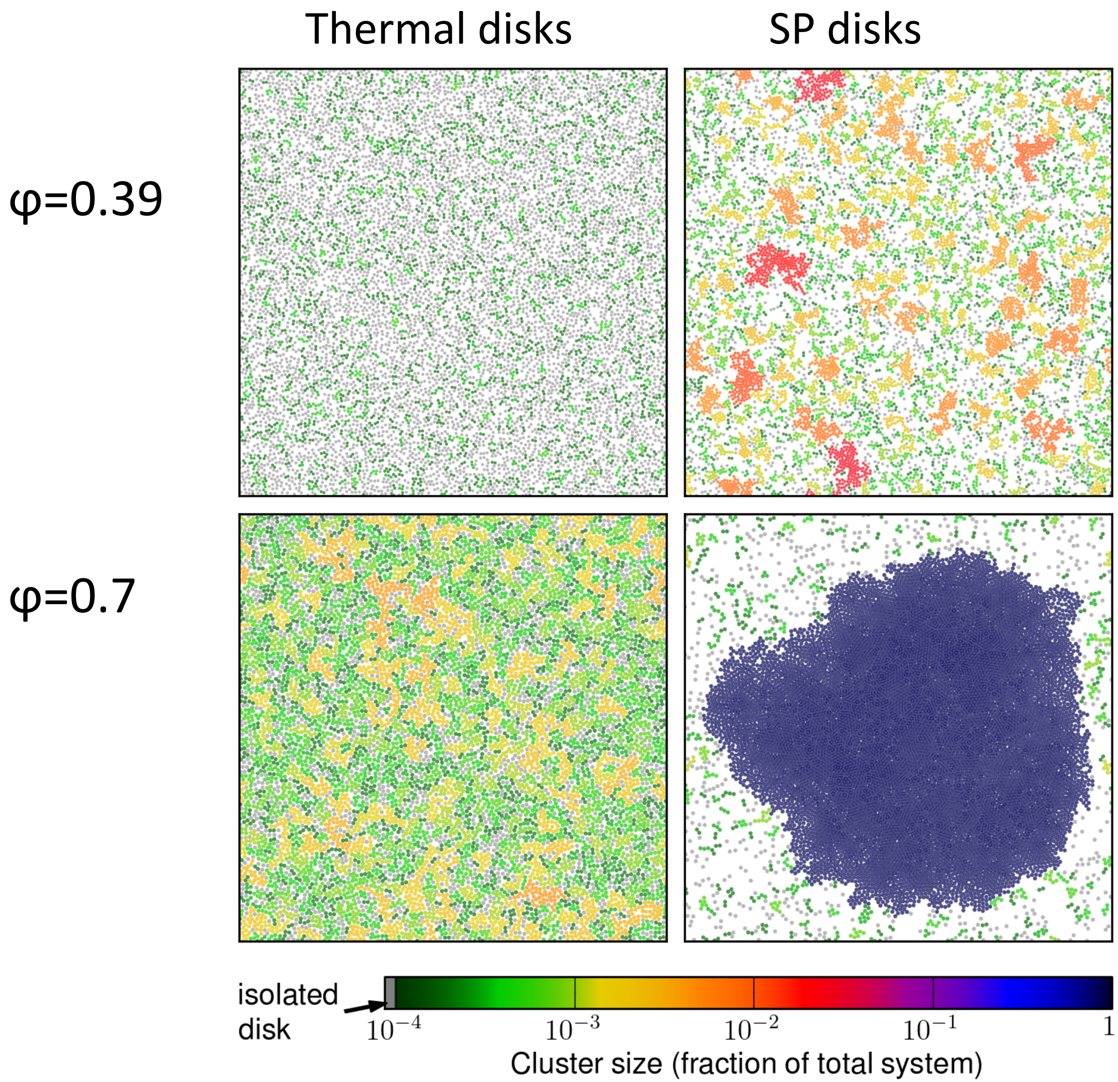


$$D_{eff} = \frac{v_0^2}{2D_r}$$



Light-activated colloids (cf E. coli)
Palacci et al 2013 $v_0 = 15\mu m/s$

Athermal Phase Separation with **no Attraction**



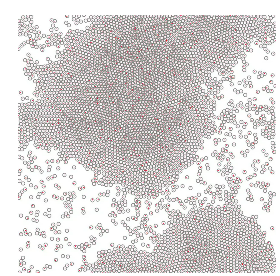
$$\left.\begin{array}{l} N_T = 10^4 \\ v_0 = 1 \\ D_r = 5\times10^{-3} \end{array}\right\} \quad \varphi_c \approx 0.4$$

$$\varphi_{RCP} \simeq 0.842$$

Thermal disks:

$$\mu k\delta \sim v_0 \rightarrow \delta_0 \sim {}^{v_0}\!/_{\mu k}$$

$$k_B T_{equiv} \sim k\delta_0^2 \sim 0.1$$



``Self-Trapping”

One particle in one dimension: Schnitzer, PRE 48, 2553 (1993)

If the SP speed is v(x) is position-dependent particles accumulate in region of small v(x)

steady state → $\rho(x) = \rho_0 \frac{\mathrm{v}(0)}{\mathrm{v}(x)}$ $\neq$ Brownian diffusion $\rho = \text{constant}$

many particles:

$$v(x) \to v(\rho(x))$$

→ ``self-trapping”

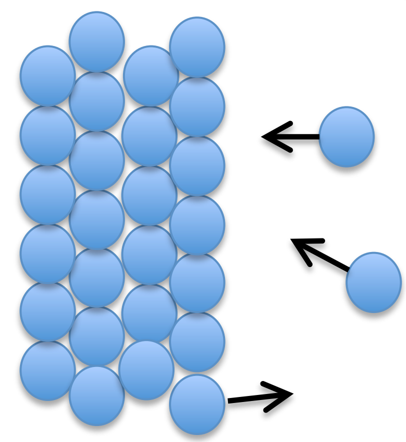
Tailleur & Cates, PRL 2008

Kinetic argument:

small D_r: active pressure overcomes steric repulsion

Redner et al, 2013

$$p_a \sim v_0^2 \rho_{gas}$$



Crowding suppresses motility

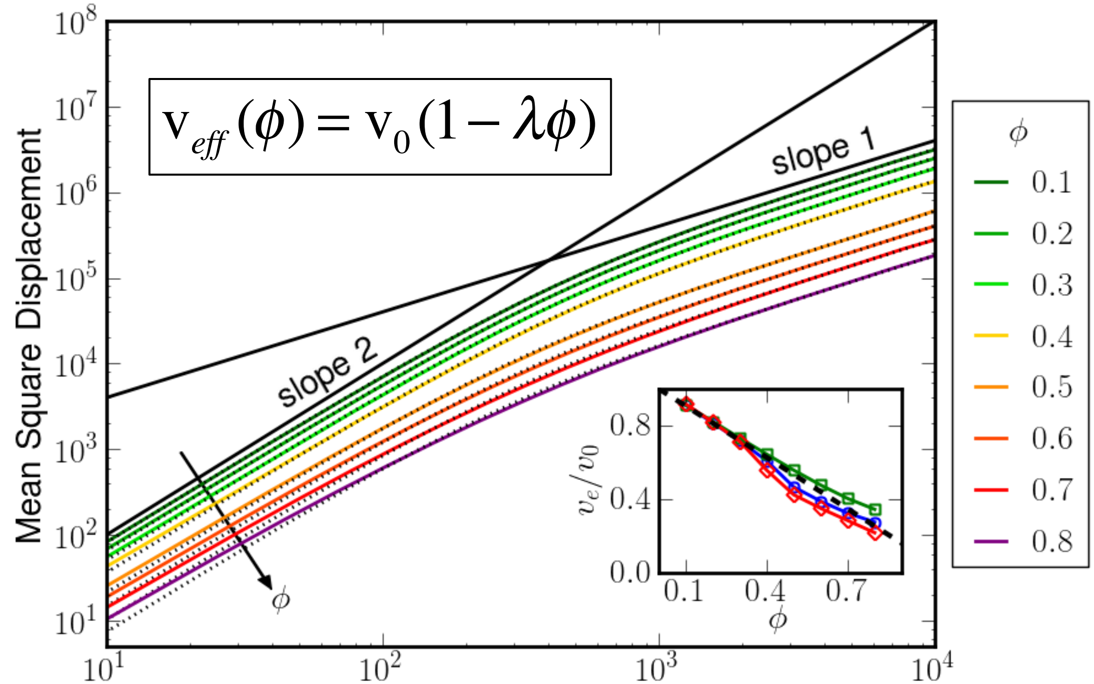
Persistent random walk (PRW) of single SP disk

$$\langle[\Delta\mathbf{r}(t)]^2\rangle = 4\frac{v_0^2}{2D_r}\left[t + \frac{1}{D_r}\left(e^{-D_r t} - 1\right)\right]$$

$$\sim 4Dt \qquad D = \frac{v_0^2}{2D_r}$$

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

$$V_0 \longrightarrow V_{eff}(\phi)$$



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

Expect effective (mean-field) model to apply if rotational correlation time $1/D_r$ > mean free time between collisions.

Effective continuum model

(Fily & MCM, PRL 2012; Farrell, MCM, Marenduzzo & Tailleur PRL 2012)

✧density ρ

✧mean orientation (polarization) ***p*** ,

$$\partial_t \rho = -\nabla \cdot [v_{eff}(\rho)\mathbf{p}] + D\nabla^2 \rho$$

$$\partial_t \mathbf{p} = -D_r \mathbf{p} - \frac{1}{2}\nabla \cdot [v_{eff}(\rho)\rho)] + K\nabla^2 \mathbf{p}$$

convection
diffusion
relaxation

For t>>1/D_R can be recast as a diffusion equation with effective diffusivity $\mathcal{D}_{eff}$ that changes sign above φ*

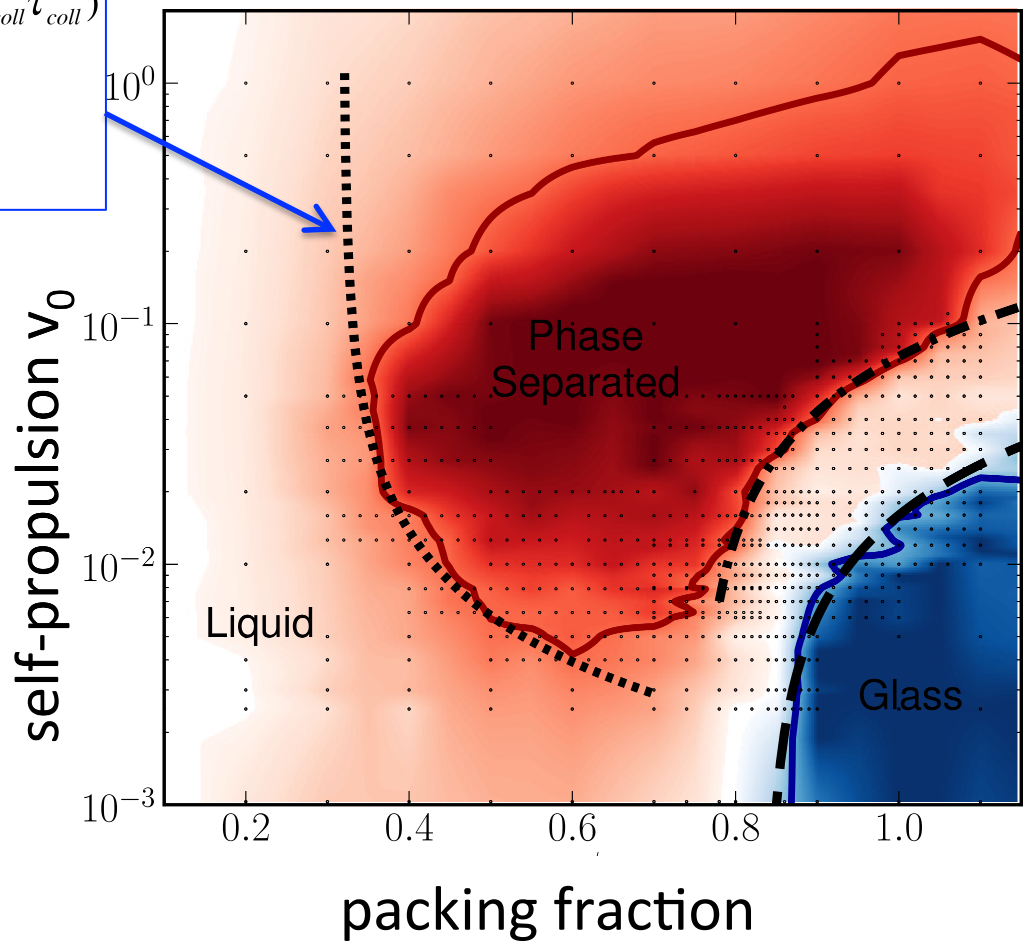
$$\partial_t \rho = \vec{\nabla} \cdot \left[\mathcal{D}_{eff}(\rho) \vec{\nabla} \rho \right]$$

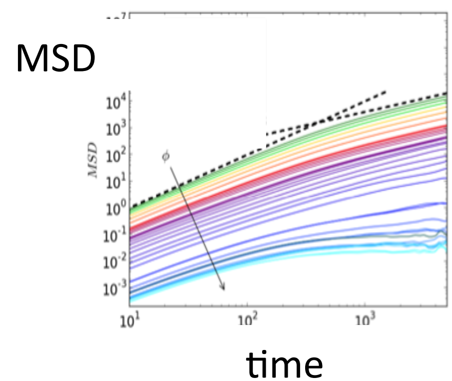
$$\mathcal{D}_{eff} = D + \frac{\mathrm{v}_{eff}^2}{2D_R}\left(1 + \frac{d \ln \mathrm{v}_{eff}}{d \ln \rho}\right) < 0 \quad \text{for} \quad \varphi \geq \varphi^*(\mathrm{v}_0, \lambda, D_r)$$

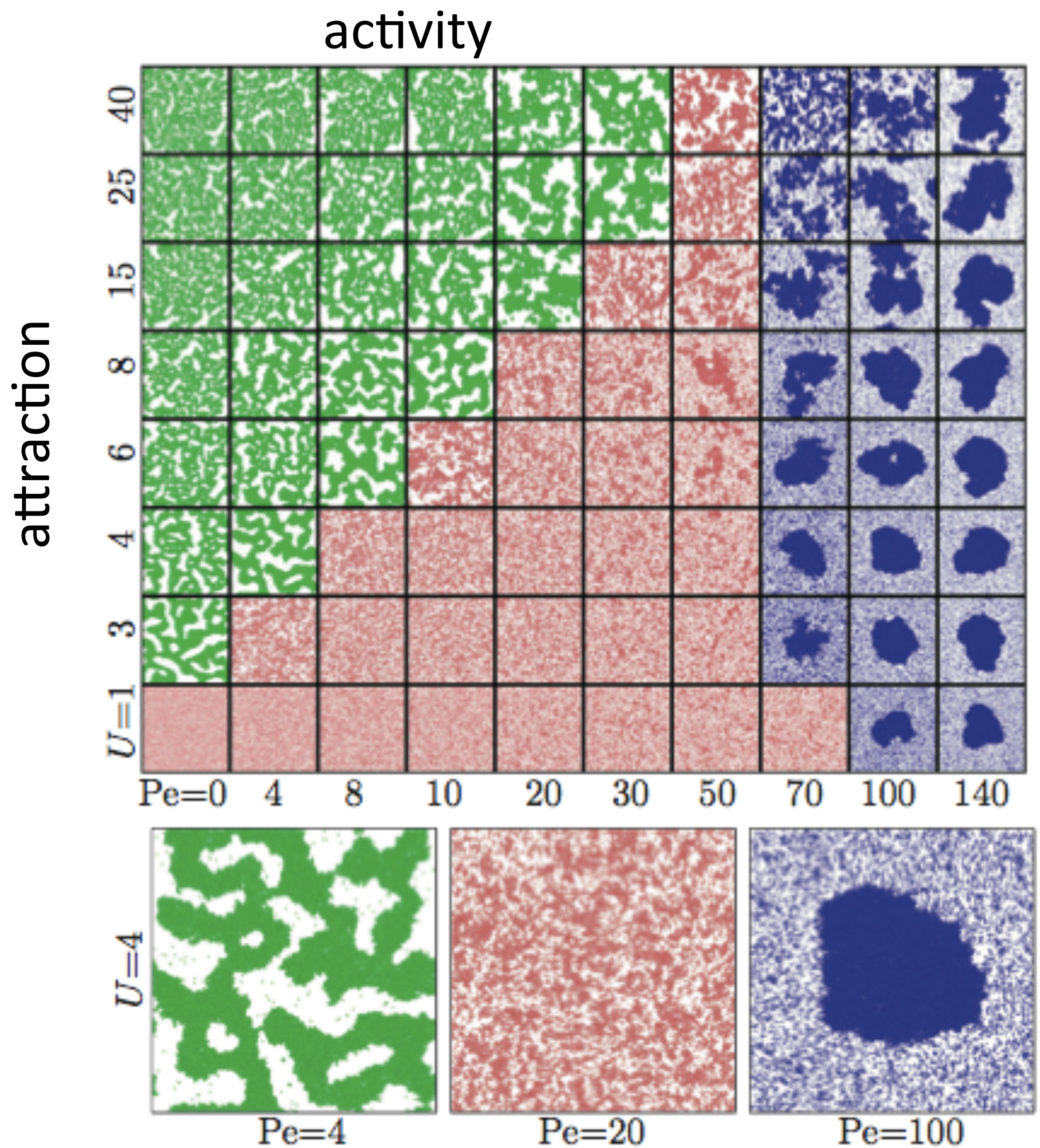
→ spinodal

Spinodal line from MFT with

$$v(\rho) = v_0(1 - f_{coll}\tau_{coll})$$
$$f_{coll} = 2a\rho v_0$$
$$\frac{1}{\tau_{coll}} = \frac{v_0}{a} + D_r$$



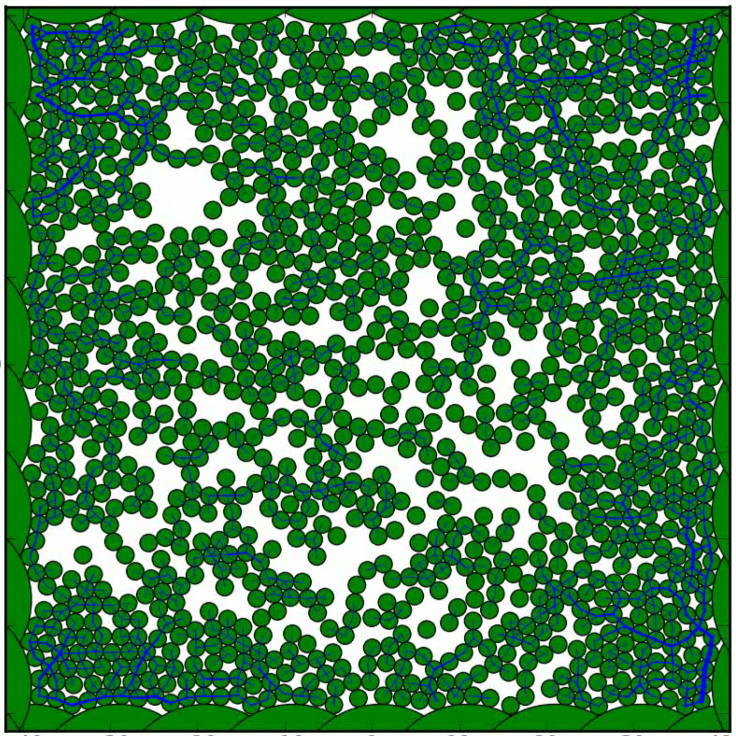




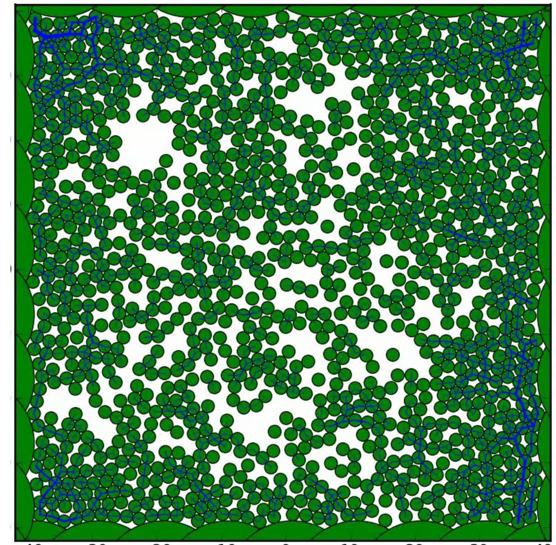
Redner, Baskaran &
Hagan, PRE 3013

Confined Active Colloids

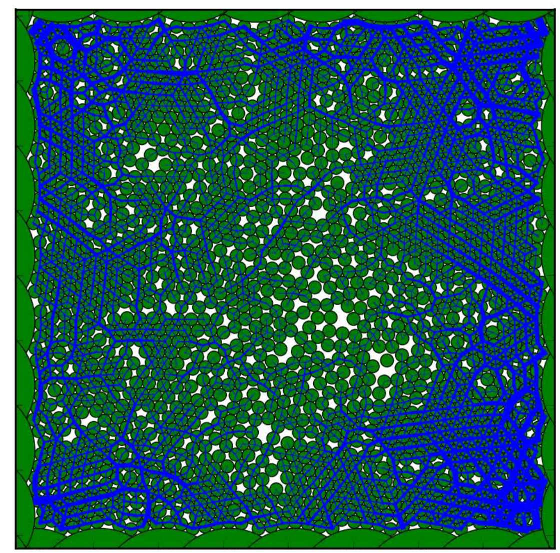
Small rotational diffusion rate



Increase Rotational diffusion



Increase Packing fraction



1. Wall aggregation
2. Inhomogeneous forces

Two ways to calculate pressure

1. Force per unit length on the wall.

2. Irving-Kirkwood pressure:

$$\sigma^{IK}_{\alpha\beta} = \sigma^{int}_{\alpha\beta} + \sigma^{act}_{\alpha\beta}$$

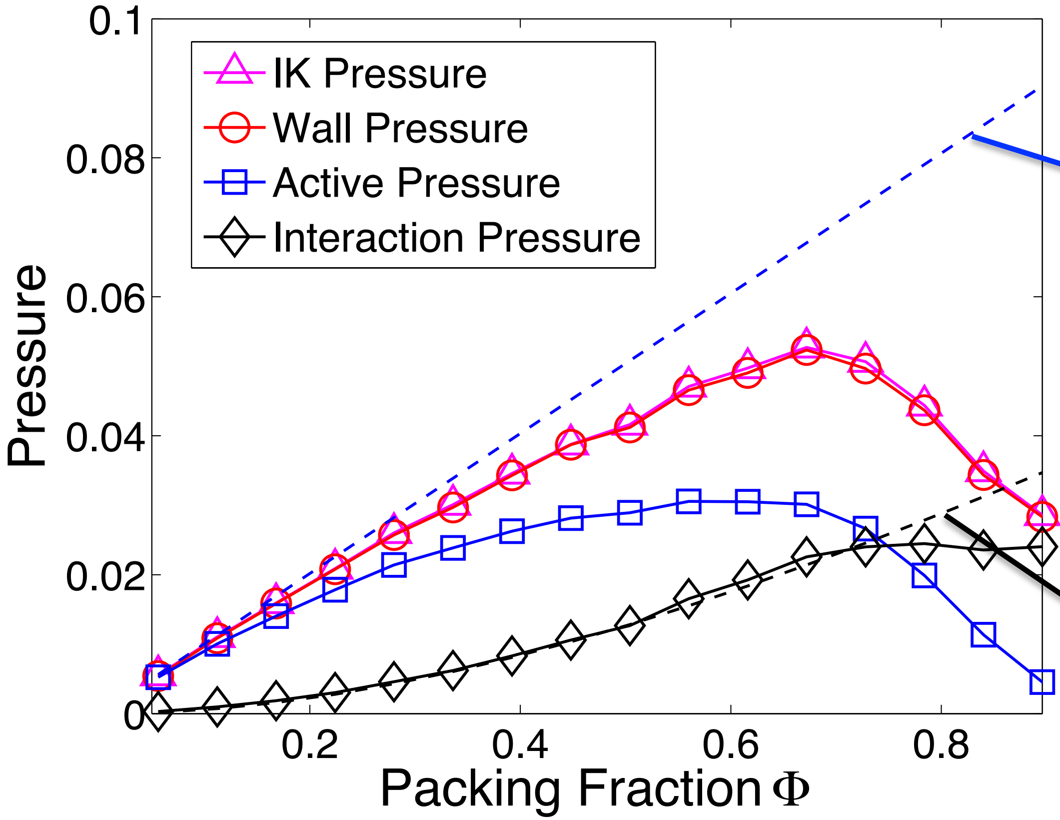
$$\sigma^{\text{int}}_{\alpha\beta} = \frac{1}{L^2}\left\langle \sum_{i\neq j} F^{\alpha}_{ij} r^{\beta}_{ij} \right\rangle$$

$$\sigma^{act}_{\alpha\beta} = \frac{1}{L^2}\left\langle \sum_{i} F^{\alpha}_{iact} r^{\beta}_{i} \right\rangle$$

$\Rightarrow$

$$P_{act} = \sigma^{act}_{\alpha\alpha} / 2$$
$$P_{\text{int}} = \sigma^{\text{int}}_{\alpha\alpha} / 2$$
$$P_{IK} = \sigma^{IK}_{\alpha\alpha} / 2$$

Non-monotonic Pressure



$$D_r^{-1} >> L / \mathrm{v}_0$$

Ideal active gas pressure:

$$P_{act} = \frac{\rho \mathrm{v}_0^2}{2\mu D_r}\left[1 - \exp(-\frac{D_r L}{2\mathrm{v}_0})\right]$$

$$\xrightarrow{D_r^{-1} >> L / \mathrm{v}_0} P_{act} \sim \rho \frac{\mathrm{v}_0 L}{4\mu} \quad *$$

(S. A. Mallory et al. 2013)

* Knudsen gas

Interaction pressure:

$$P_{\mathrm{int}} = c\left(\frac{L\mathrm{v}_0}{16R}\phi^2 - \frac{L\mathrm{v}_0}{48R}\phi^3\right)$$

c is a fitting parameter and chosen to be 1.2 here.

Agent-Based Model of Collective Cell Migration

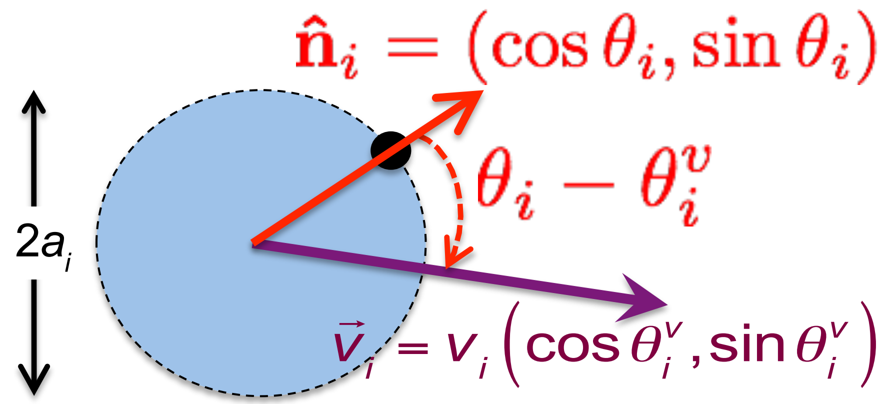
Henkes, Fily & MCM, PRE 2011

New ingredients:

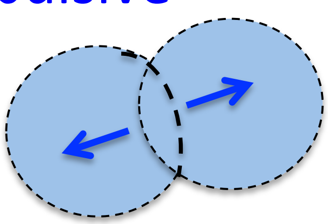
- **Alignment rule***
- SP represents cell polarization

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

$$\dot{\theta}_i = \frac{1}{\tau}(\theta_i^v - \theta_i) + \eta_i(t)$$



f_{ij} pair repulsive forces:



*Szabó et al, PRE 74, 06918 (2006)

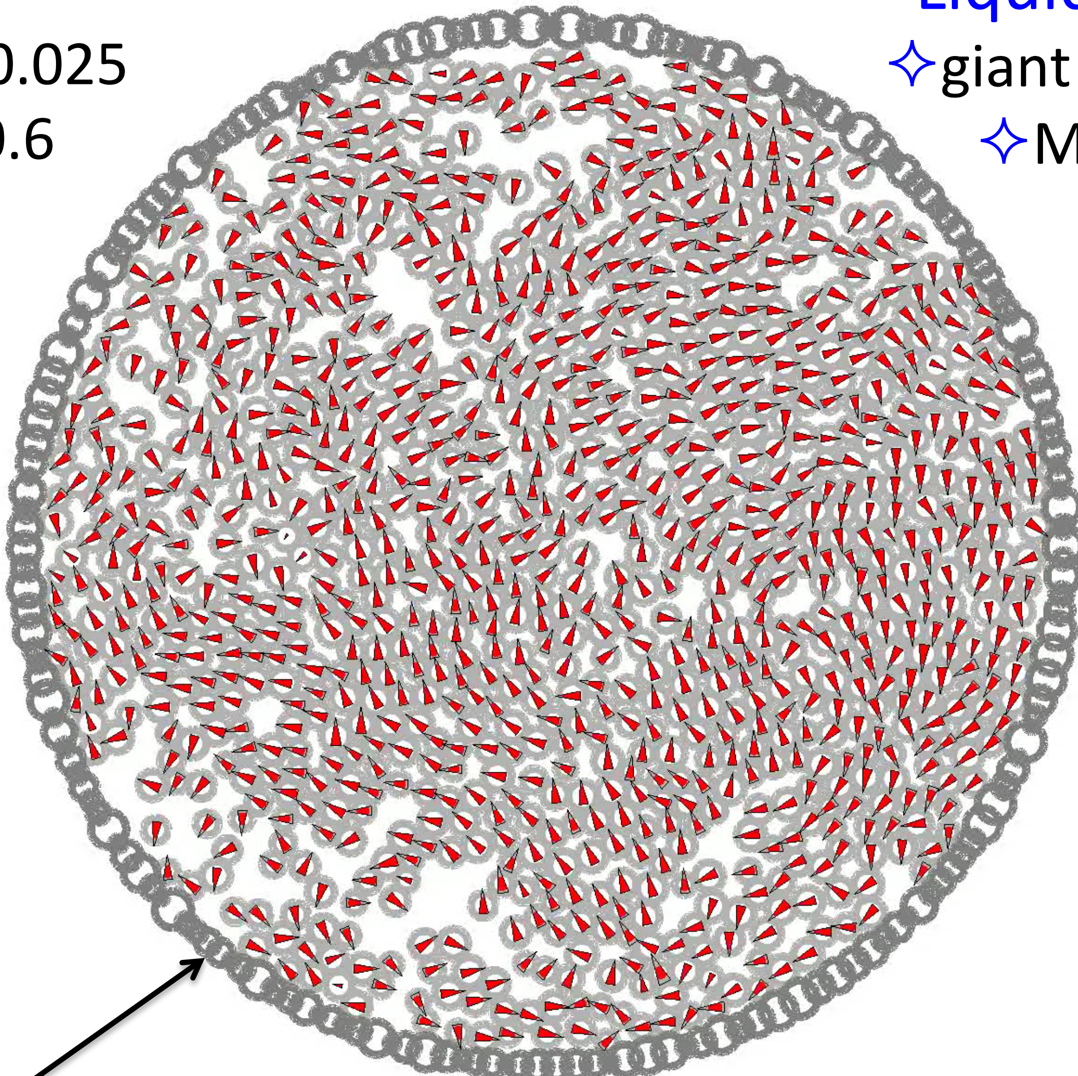
- Add **polydispersion** as size variation is needed to yield glass in 2d repulsive soft disks → passive limit is the granular jamming transition
- Add **confinement** to disable global translation

“Liquid” state:

✧giant number fluctuations

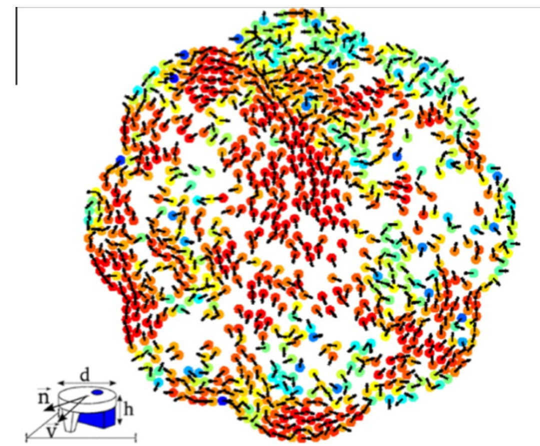
✧MSD ballistic at all times

v_0=0.025
φ=0.6



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

Velocity scale:
red arrow=diameter → $v=v_0$

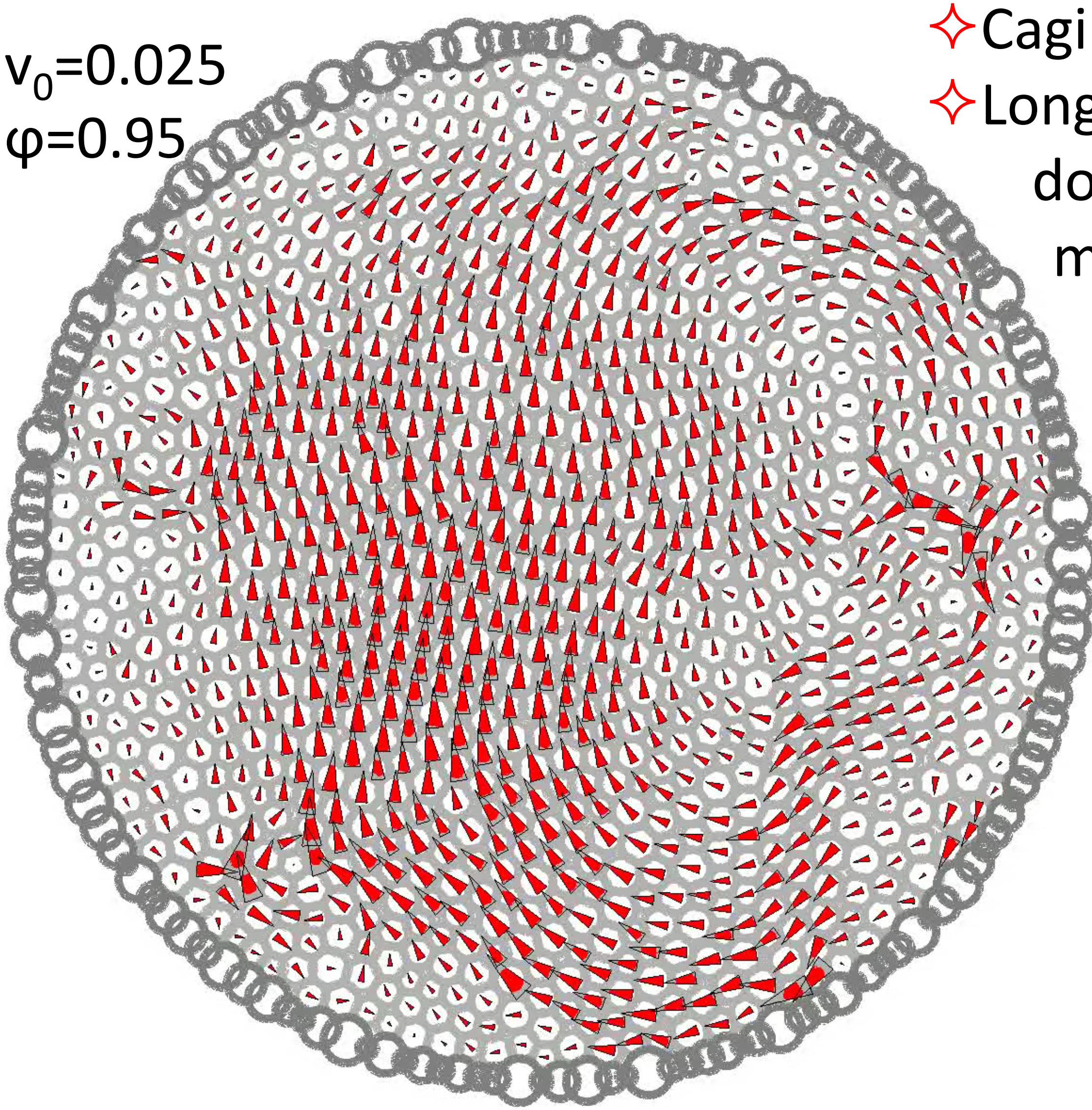


Deseigne et al, PRL2010

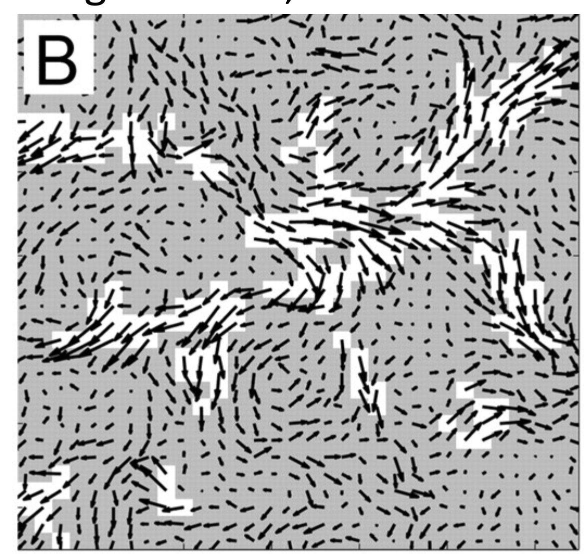
"Glass" or "jammed" state:

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

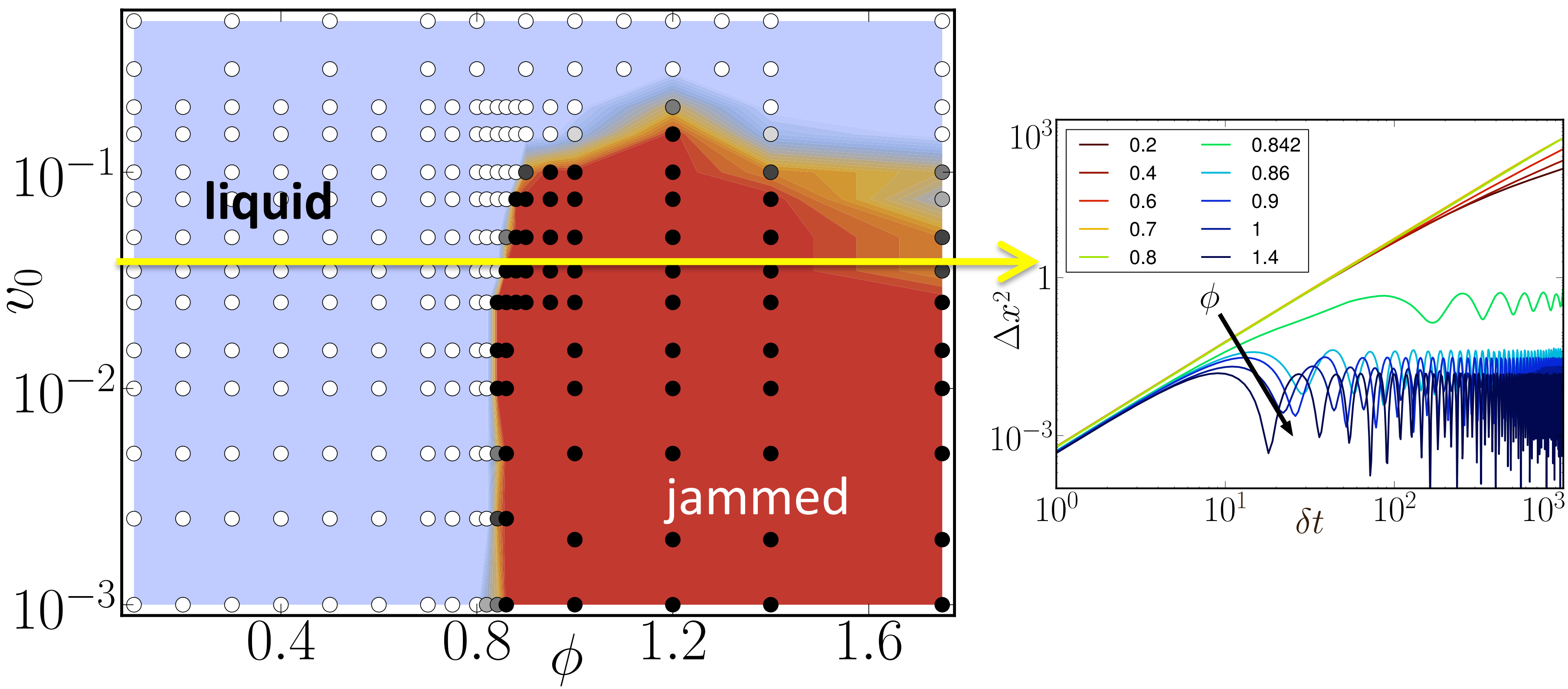
v_0=0.025
φ=0.95



Angelini et al, PNAS 2011



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



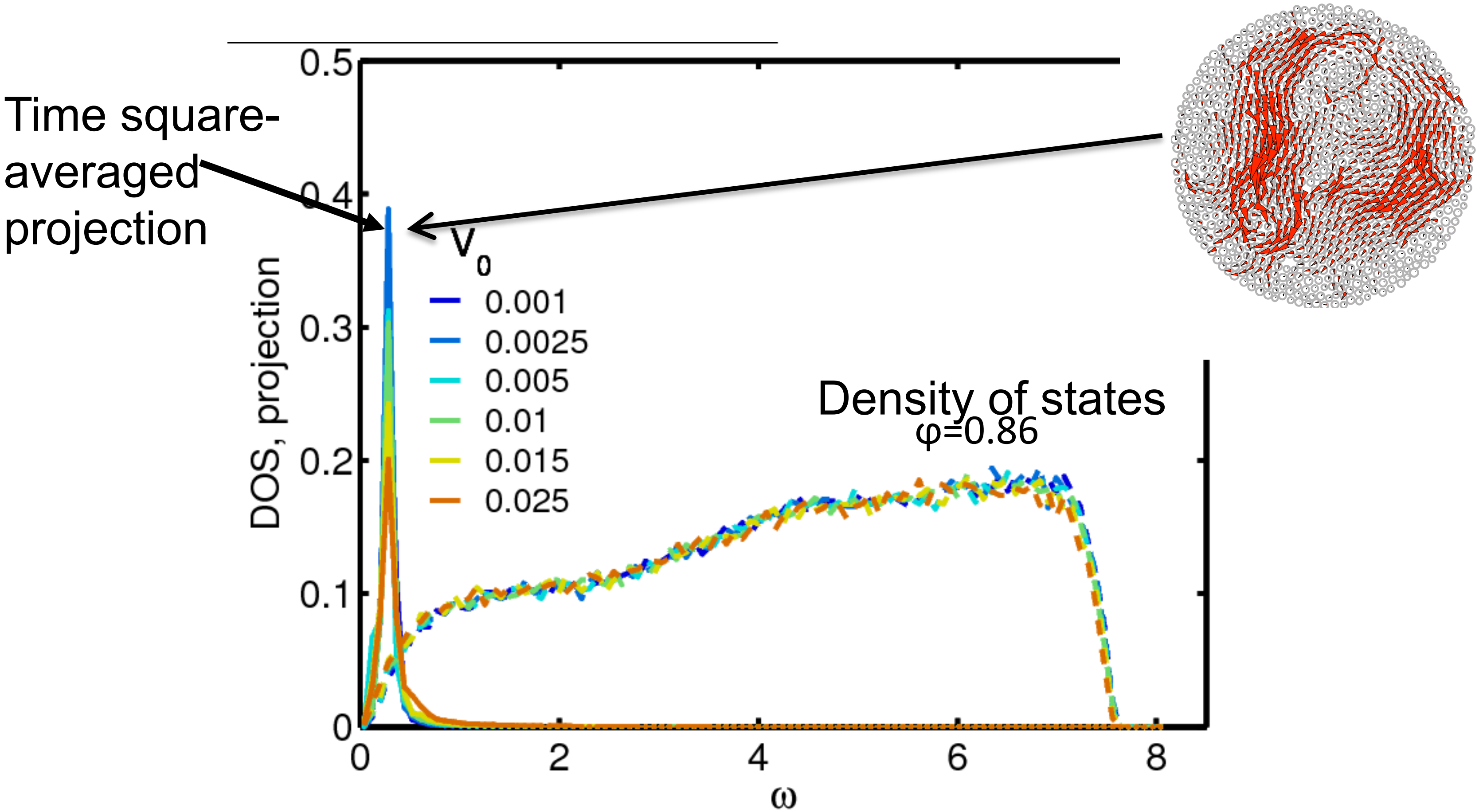
What are these oscillations?

- The system is in a glassy state; 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 ~$1/\omega^2$



Final remarks

- Active systems are nonequilibrium systems where the drive acts on each unit, not applied at the boundary or via an external field.
- They include living and synthetic systems and span many scales.
- Collectives of interacting, active entities (motor-filament complexes, bacteria, cells, synthetic swimmers, birds,…) as a new kind of `Active Matter' with novel states and properties.
- Progress in using active matter paradigm to model behavior of living matter.

MCM, Joanny, Ramaswamy, Liverpool, Prost, Rao & Simha, *Hydrodynamics of Soft Active Matter*, Rev. Mod. Phys. **85**, 1143–1189 (2013)