Phase separation, jamming and glassy dynamics in dense active matter

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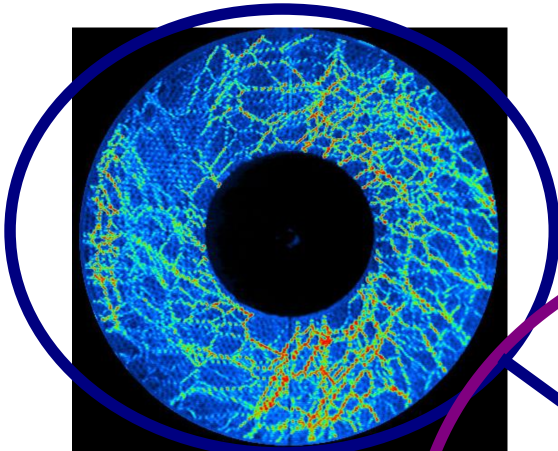
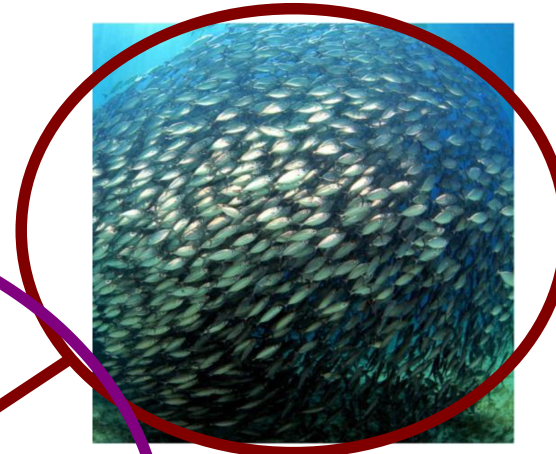
Granular materials



Behringer group, Duke

Solid, passive

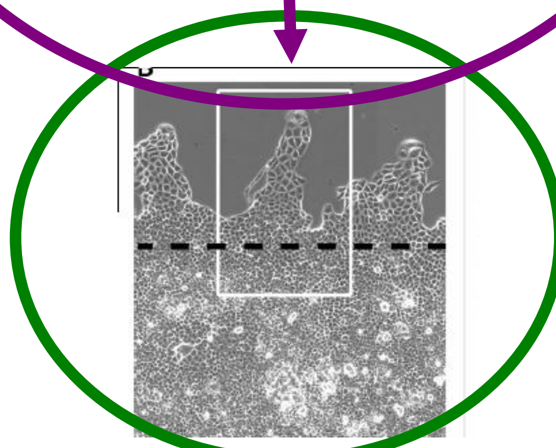
Active matter



Active, liquid phase

Dense active matter

new dynamical and mechanical properties

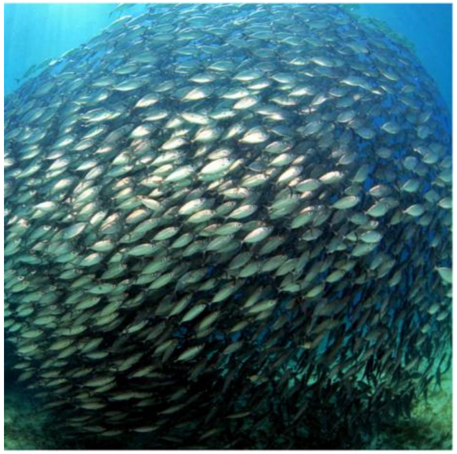


Relevant for:

Self-propelled particles

Cell monolayers, tissues

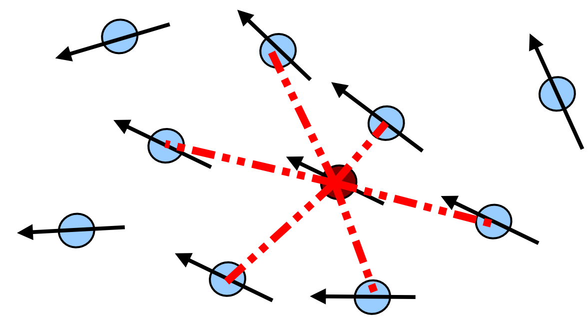
Bacteria



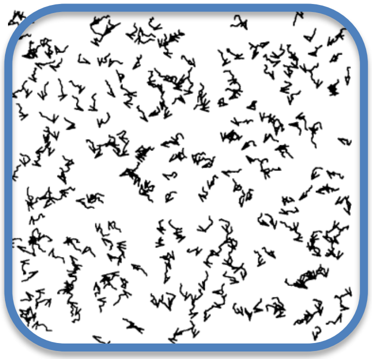
Self-propelled particles

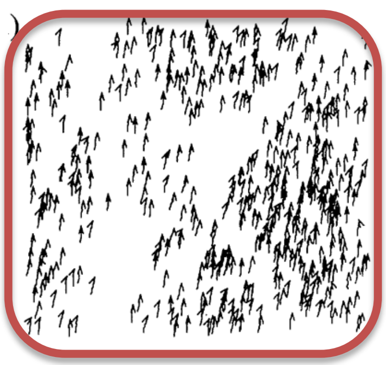
T. Vicsek et al., PRL 75, 1226 (1995)
H. Chate et al., Eur. Phys. J. B 64, 451–456 (2008)

- Self-propelled point particles with constant velocity
- Particles align with their neighbors – various mechanisms



Transition to a polar flocking state





Our Model:

- Incorporate self-propulsion as a force
- Obtain density-dependent velocity

$$\zeta \dot{r}_i = v_0 \hat{n}_i + \mu \sum_j F_{ij}$$

Fully overdamped

Self-propulsion

Short-range forces: Volume exclusion

1. Polar alignment

Active Jamming

S. Henkes, Y.Fily and M. C. Marchetti, PRE 84, 040301(R) (2011)

2. Non-aligning dynamics

Cluster formation

Y. Fily and M. C. Marchetti, PRL 108, 235702 (2012)

3. Non-aligning dynamics

Full phase diagram, glasses

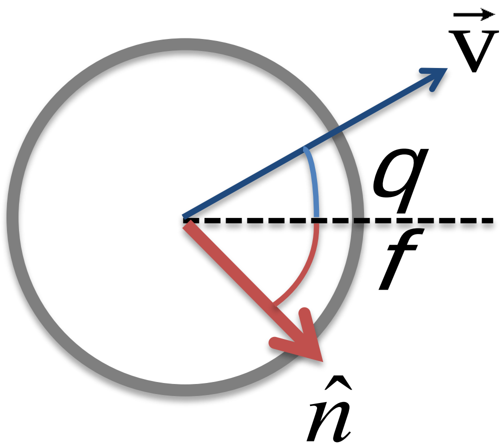
Y. Fily, S. Henkes and M. C. Marchetti, arXiv.1309.3714

1. Polar alignment

Active Jamming

S. Henkes, Y.Fily and M. C. Marchetti, PRE 84, 040301(R) (2011)

Alignment mechanism



adapted from B. Szabó et al., PRE 74, 061908 (2006)

$$\dot{f} = \frac{1}{t}(q - f) + h$$

$$\langle h(t)h(t')\rangle = 2n_r d(t - t')$$

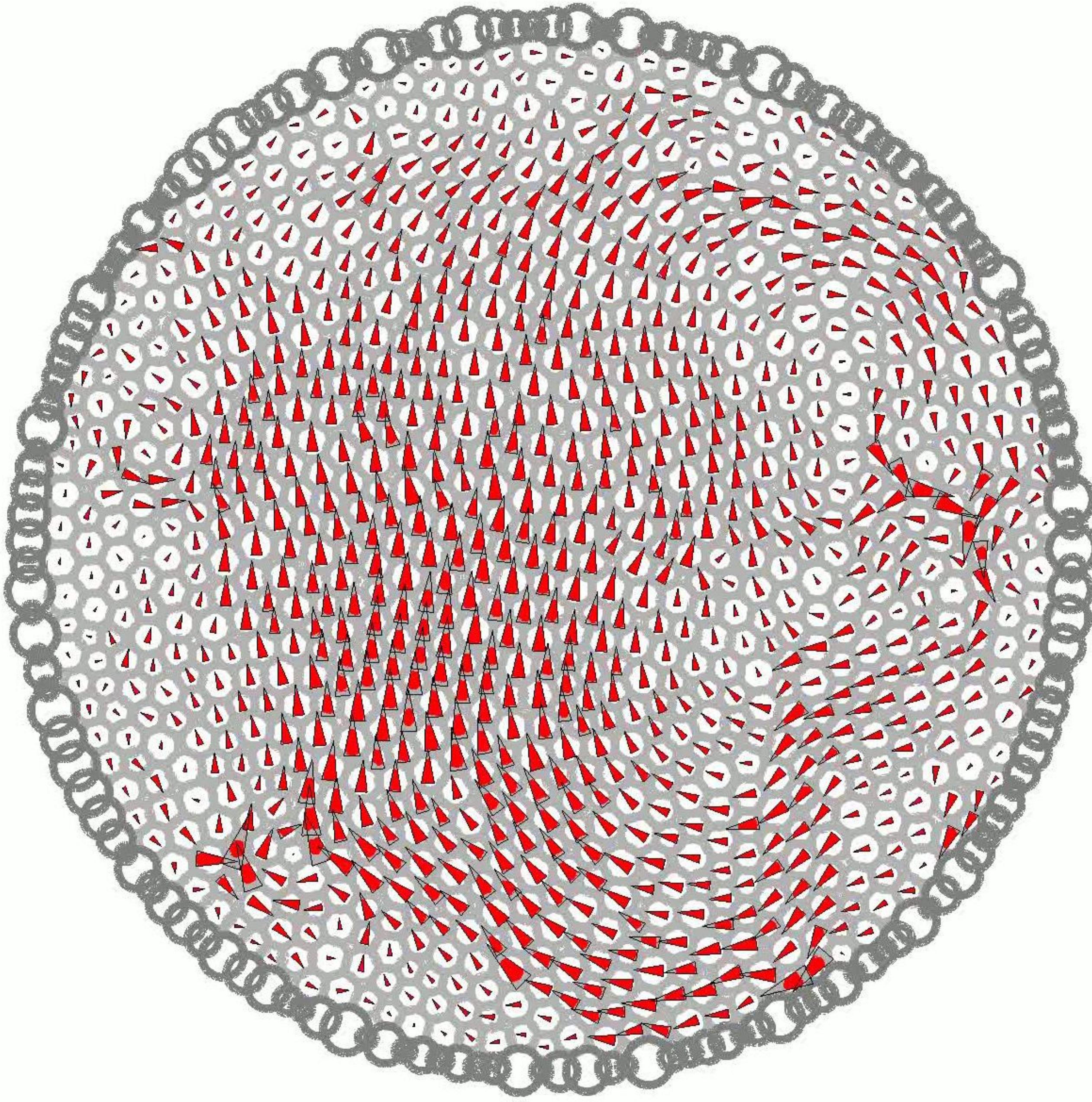
Coupling between polarity and motility with lag time τ $_d$

Additional Ingredients:

- Confinement to disable globally aligned state
- Polydispersity and harmonic potential: The passive limit is the granular Jamming transition

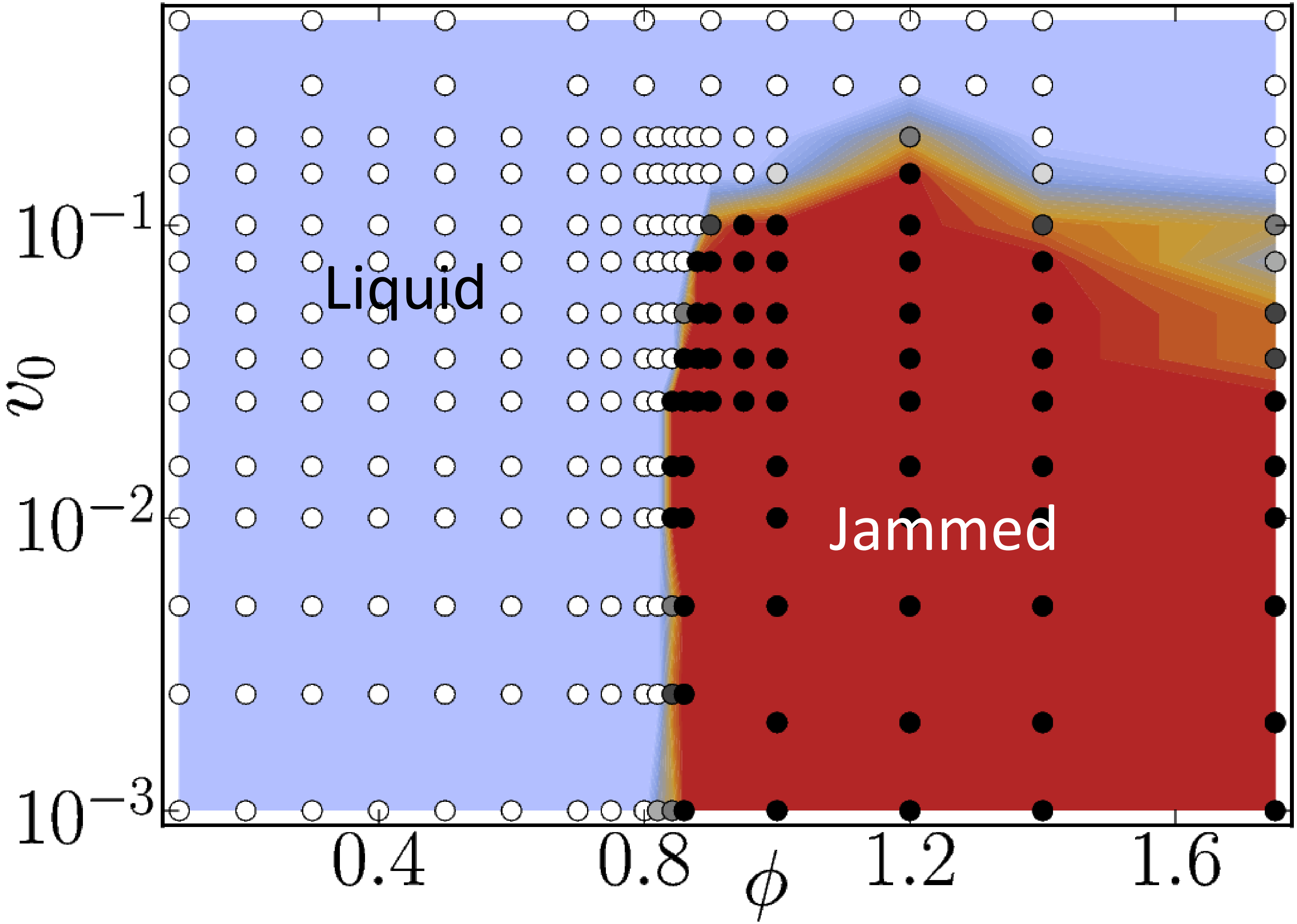
$$V_{ij} = \frac{k}{2}\left(r_{ij} - (R_i + R_j)\right)^2$$

High Density: Jammed / Glassy State

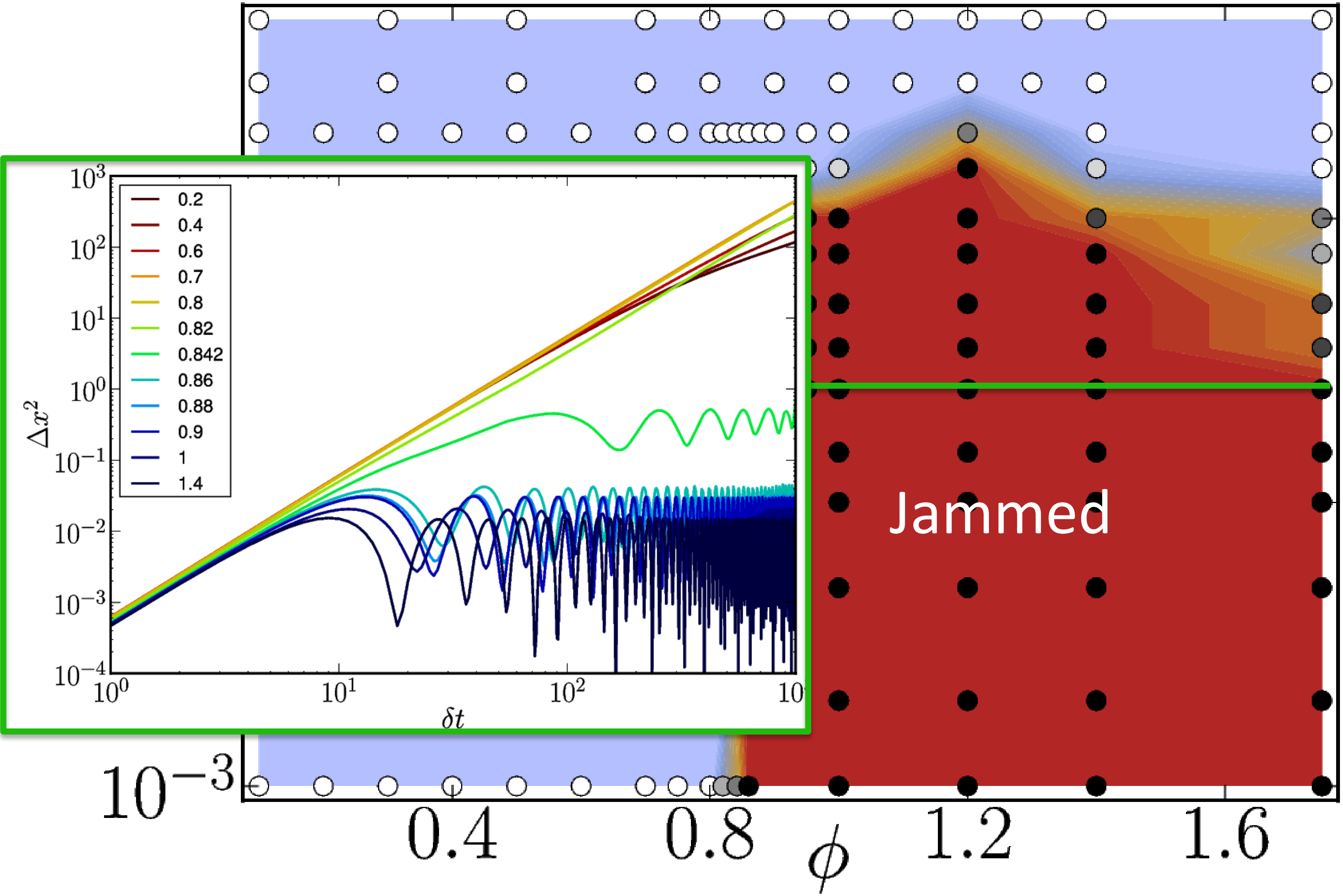


$\Phi=0.95$
$v_0=0.025$
$2\nu_r=0.01$

Phase Diagram



Phase Diagram



Dynamics in the jammed phase

Linearize the equations of motion around the mean jammed state:

$$\delta \mathbf{r}_i = v_0 \hat{\mathbf{n}}_i + \sum_j \mathbf{F}_{ij} \qquad M_{ij} \delta r_j$$

$$\dot{\phi} = \frac{1}{\tau}(\theta - \phi) + \eta \qquad M_{ij} = H_{ij} = \frac{\partial^2 V}{\partial r_i \partial r_j} \quad i \neq j$$

Hessian matrix

Decompose the positions and the polar angle in the normal modes of the dynamical matrix:

$$\delta \mathbf{r}_i = \sum_\nu a_\nu(t) \boldsymbol{\xi}_i^\nu \, , \qquad \hat{\mathbf{n}}_i = \sum_\nu b_\nu(t) \boldsymbol{\xi}_i^\nu \, .$$

Obtain harmonic oscillator equations for the displacements

$$\ddot{a}_\nu + \frac{1}{\tau}\left[1 - \frac{v_0\Delta}{v_{rms}} + \mu\tau\omega_\nu^2\right]\dot{a}_\nu + \frac{\mu}{\tau}\omega_\nu^2 a_\nu = 0.$$

effective intertia introduced by the angular coupling

F

$$v_{rms}^2 = \frac{1}{N}\sum_\nu [\dot{a}_\nu(t)]^2$$

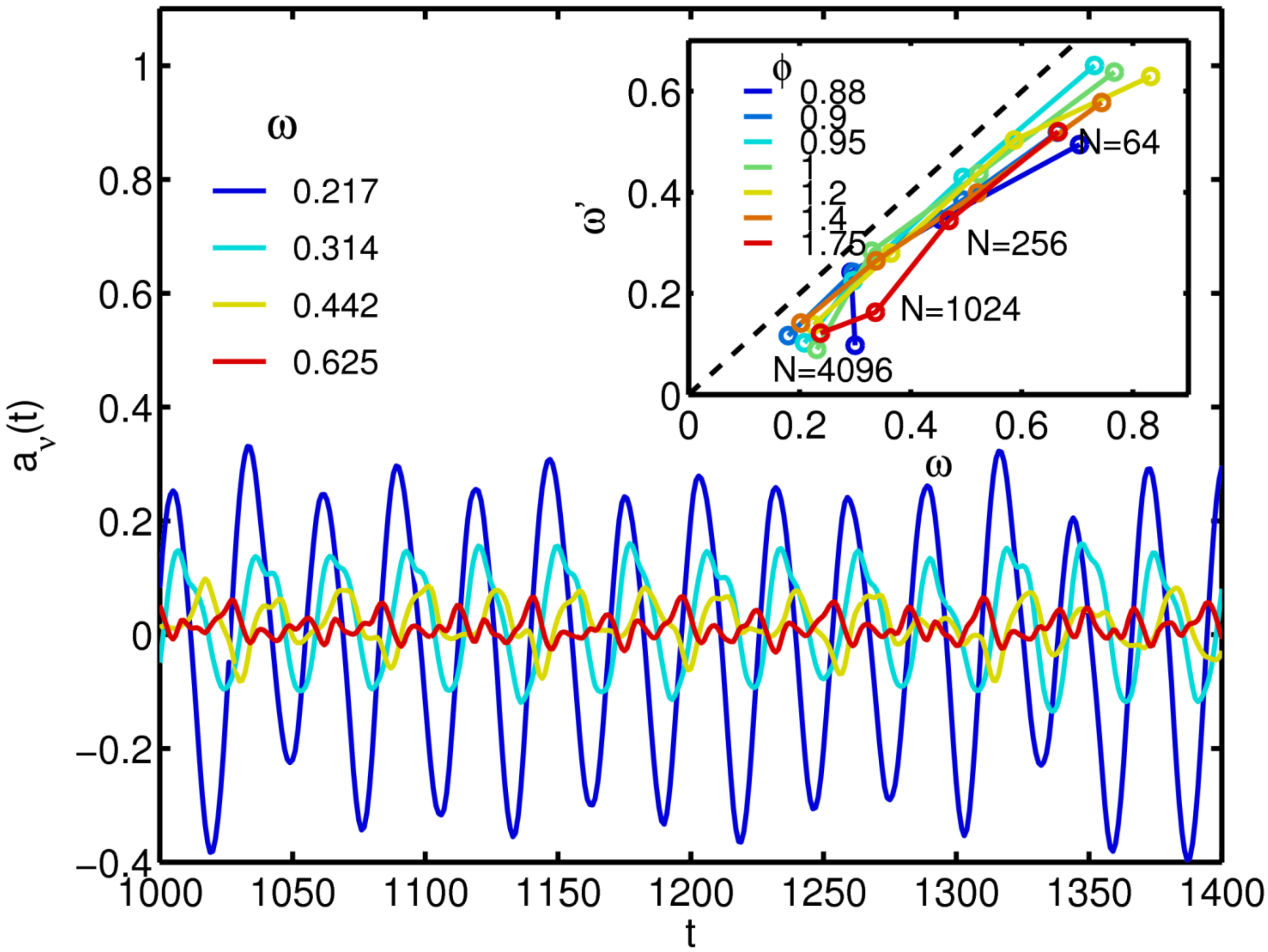
$$D = e^{-s^2 t^2/2}$$

Friction term increasing quadratically with mode frequencies.

Oscillation frequency set by mode frequency and alignment timescale

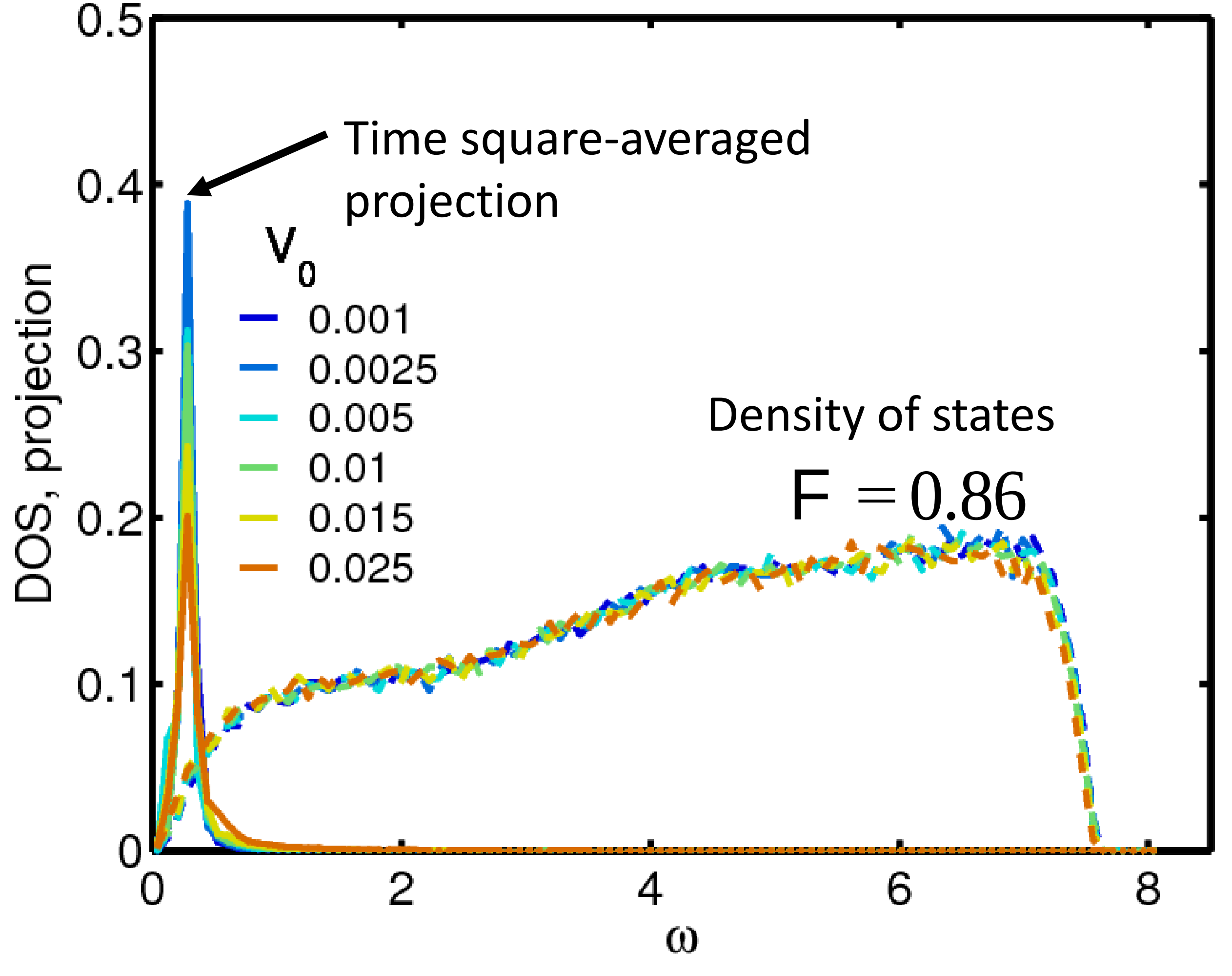
W_n Mode frequencies

Numerical mode projection coefficients



Idea: The energy of the system cascades down to the lowest energy mode.

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



3. Non-aligning dynamics

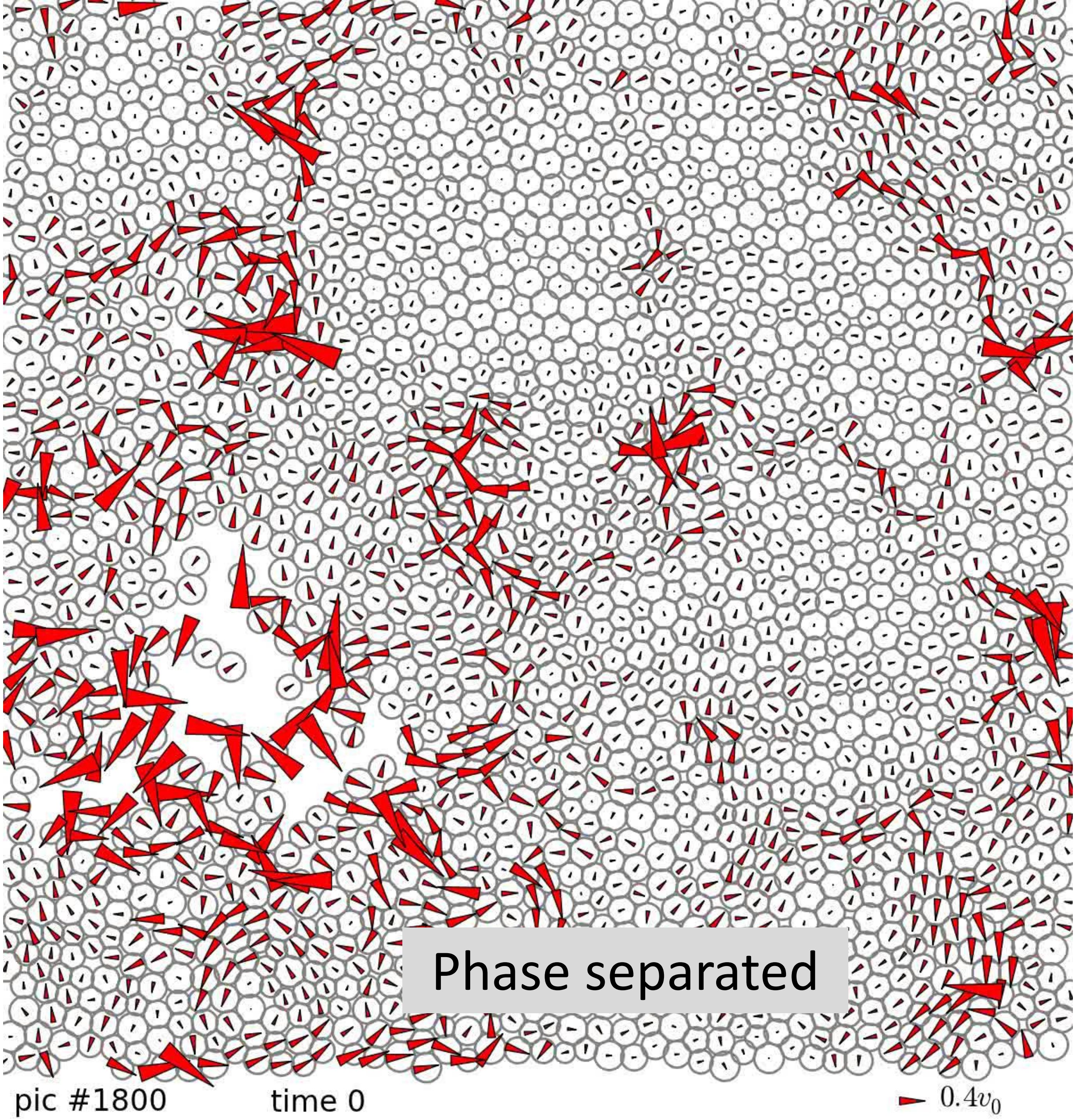
Full phase diagram, glasses

Y. Fily, S. Henkes and M. C. Marchetti, in preparation

$V_0 = 0.5$

$t = 100$

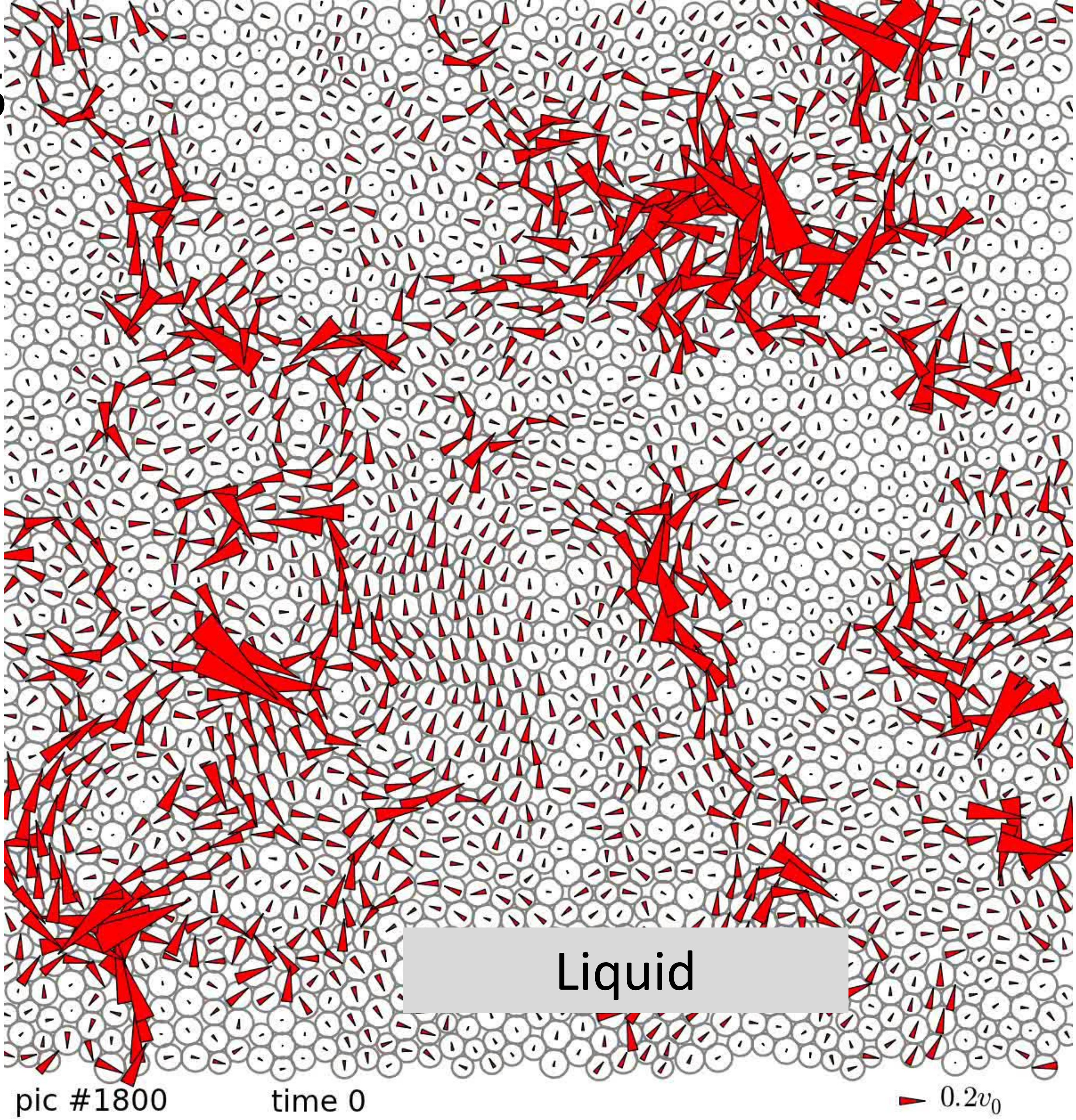
$F = 0.9$



$V_0 = 0.25$

$t = 100$

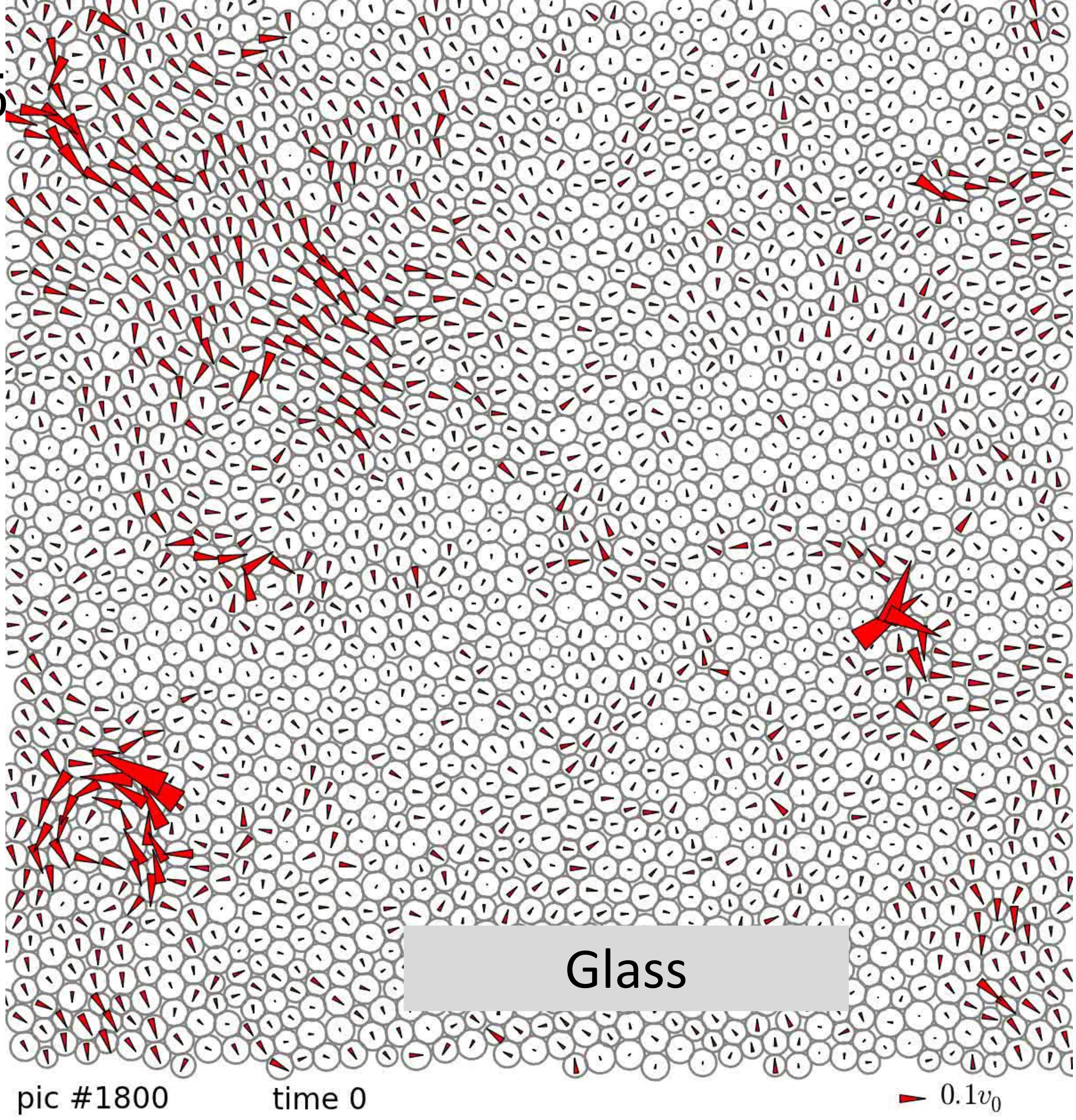
F $= 0.9$



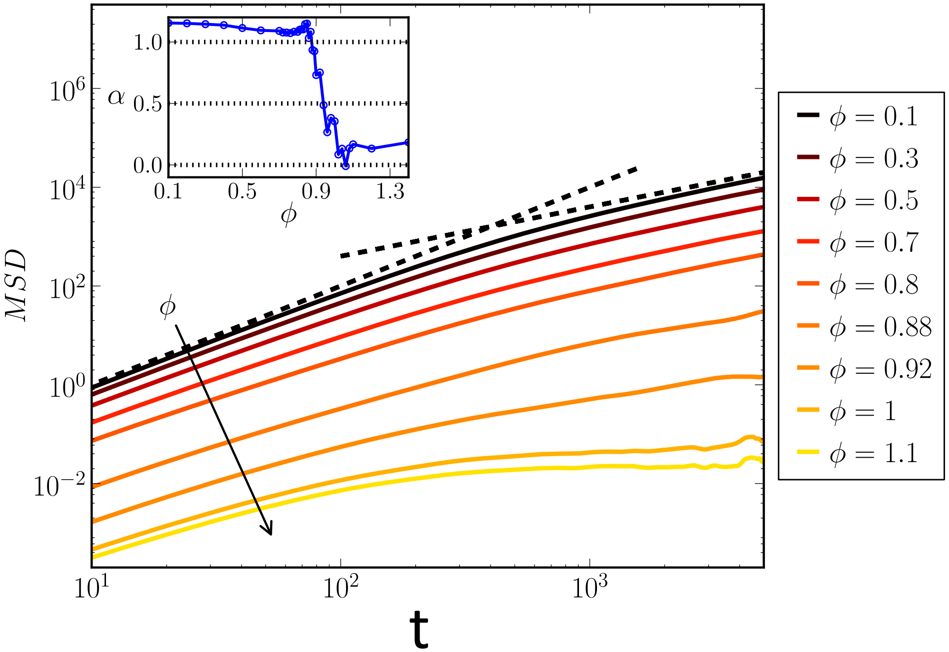
Liquid

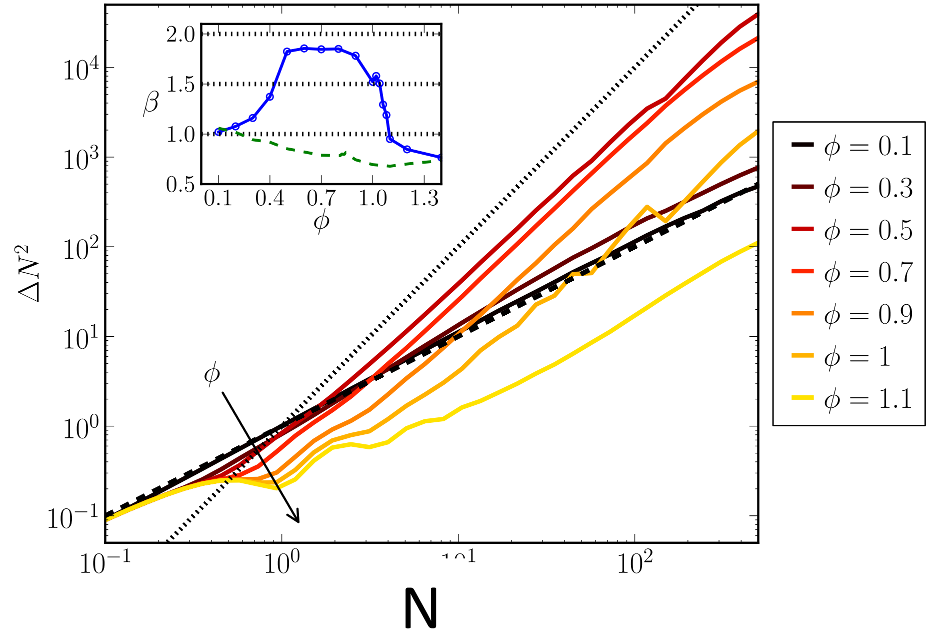
$V_0 = 0.05$
$t = 100$

$F = 0.9$



Characterize using MSD and number fluctuation exponents

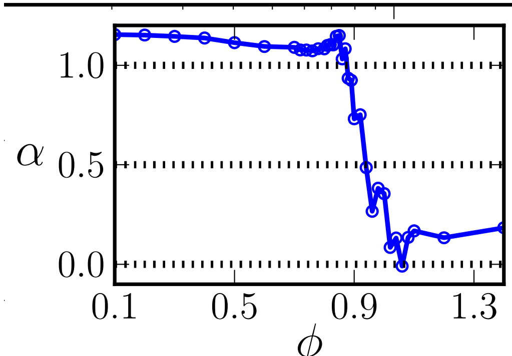




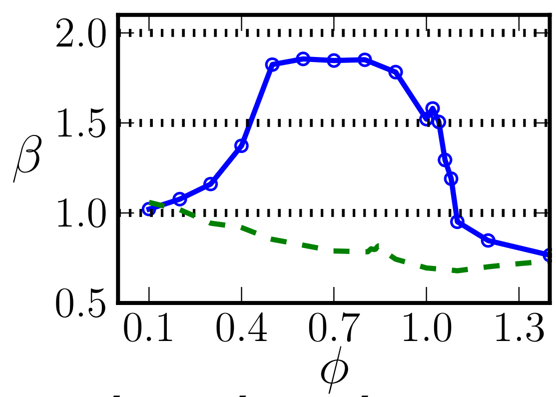
Long-time exponent α:

1 for diffusion

0 for a glass



Exponent β:



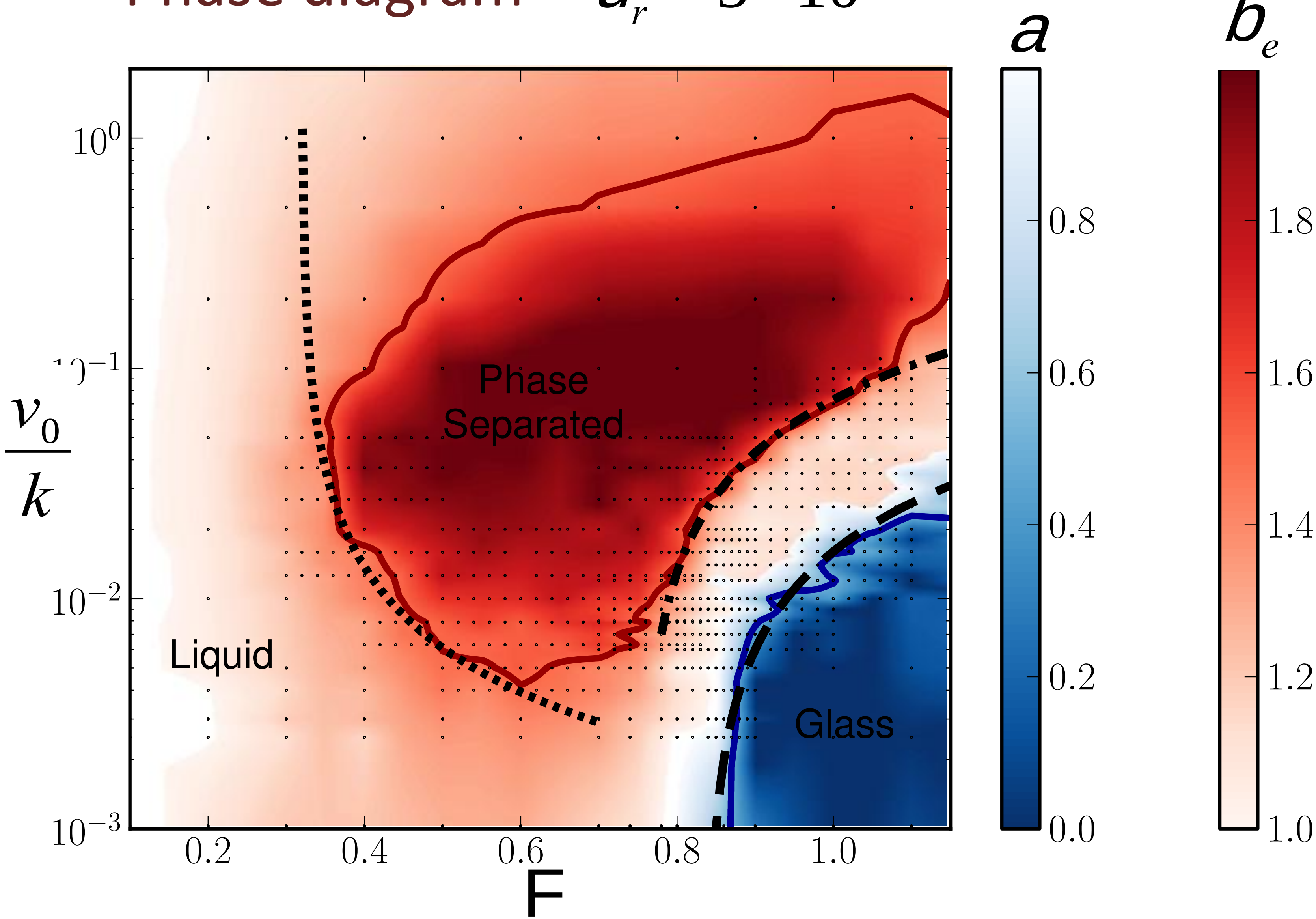
=1 for standard fluctuations

>1 for cluster formation

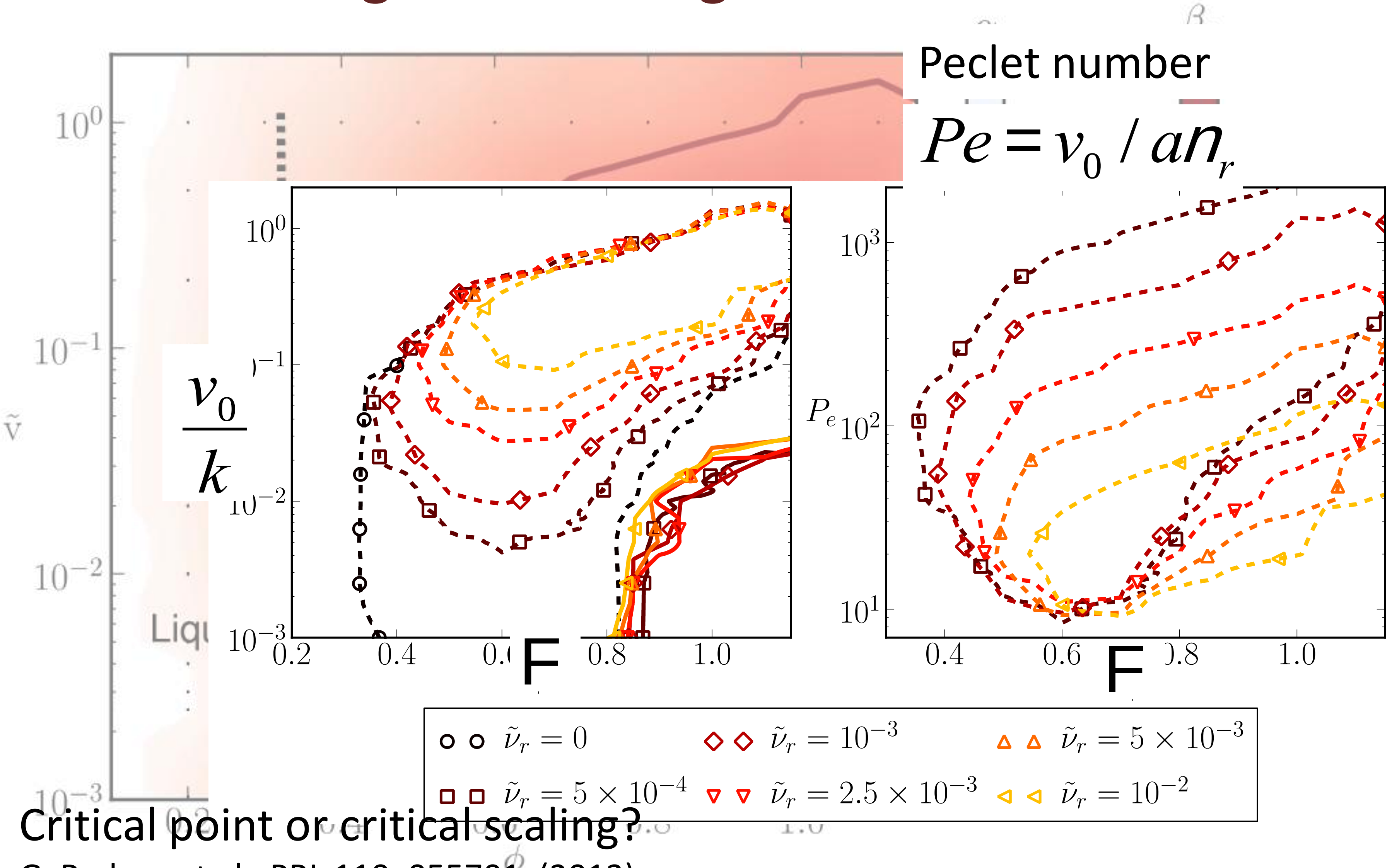
<1 for glassy packings (hyperuniform fluctuations)

$$b_e = b - (b_{T\to 0} - 1)$$

Phase diagram $u_r = 5 \times 10^{-4}$



Phase diagram - scaling



Critical point or critical scaling?

G. Redner et al., PRL 110, 055701 (2013)

J. Bialke et al., arXiv1307:4908

Low density (right) clustering transition phase boundary

$$D(\rho) = D_e + \frac{v_e}{2\nu_r}\left(v_e + \rho\frac{dv_e}{d\rho}\right)$$

Estimate v_e using binary collisions only:

$$v_e = v_0(1 - \nu\tau)$$

ν: collision frequency

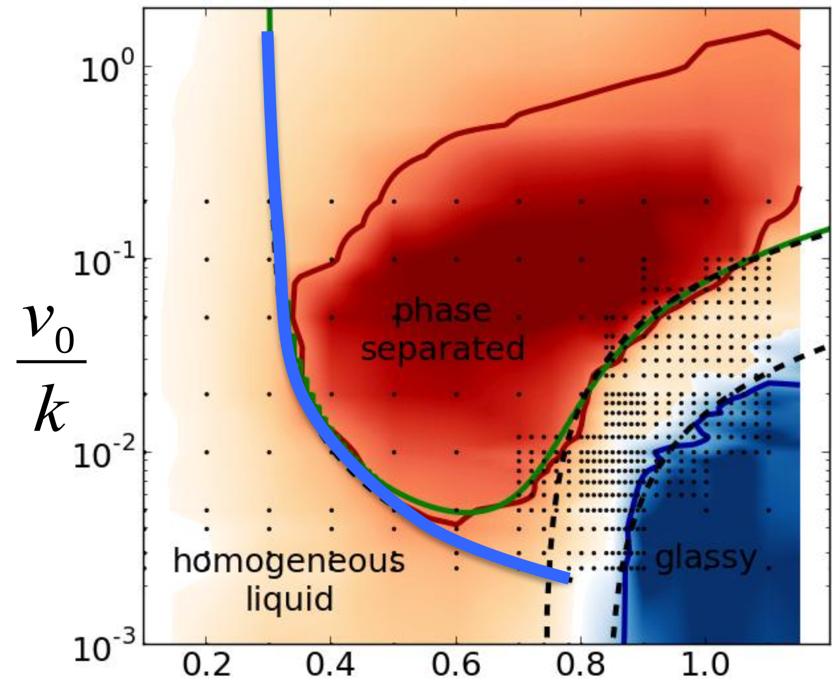
$$\nu = 2 a v_0 \rho$$

τ: collision delay

$$\tau^{-1} = \tau_1^{-1} + \tau_2^{-1}$$

$$\tau_1 \approx a/v_0, \qquad \tau_2 \approx 1/2\nu_r$$

move around — reorientation time



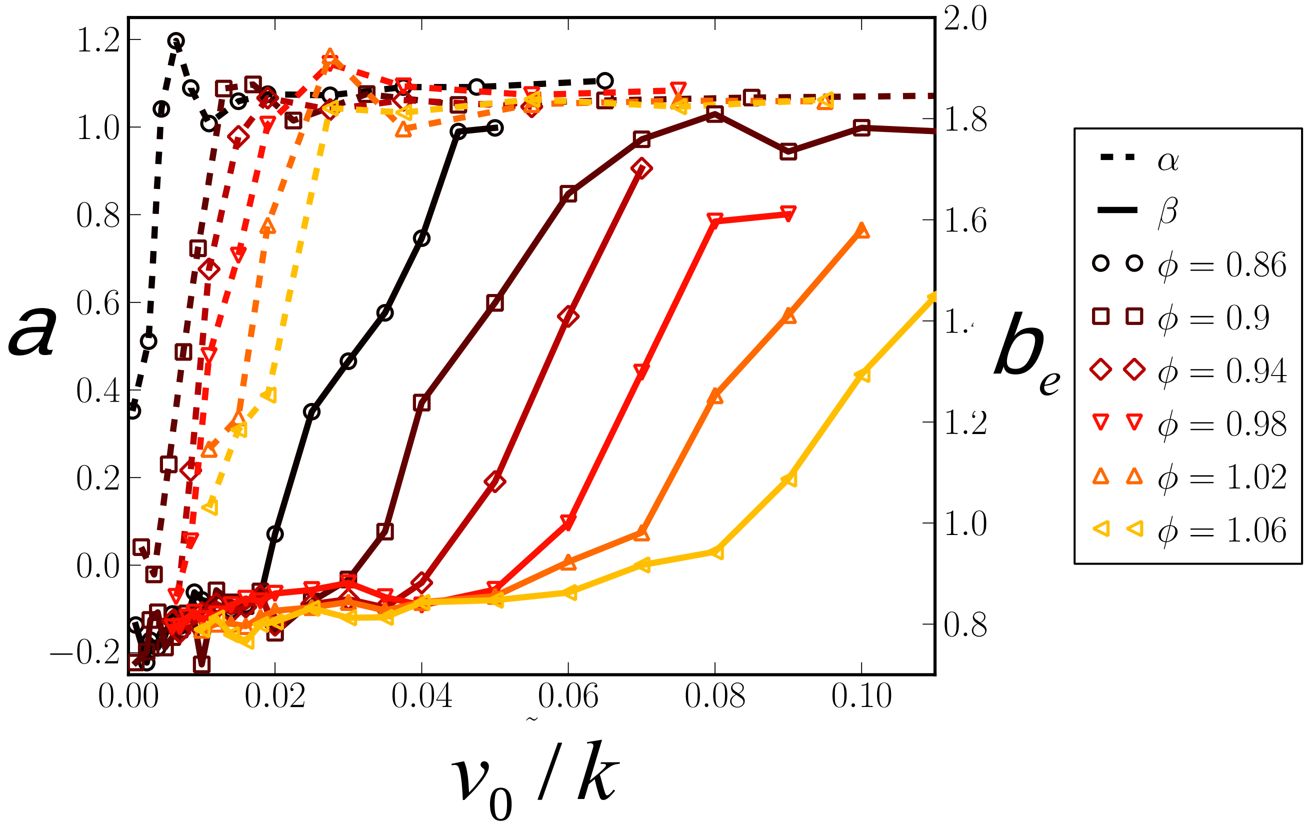
$$v_e = v_0(1 - \Phi/\Phi^*)$$

$$\Phi^* = \gamma_1 + \frac{\gamma_2 a}{2 v_0 \nu_r} = \gamma_1 + \gamma_2/Pe$$

$$\gamma_1 = 0.32, \quad \gamma_2 = 2.2$$

see also: G.S. Redner et al., PRL 110, 055701 (2013)

Melting and cluster formation



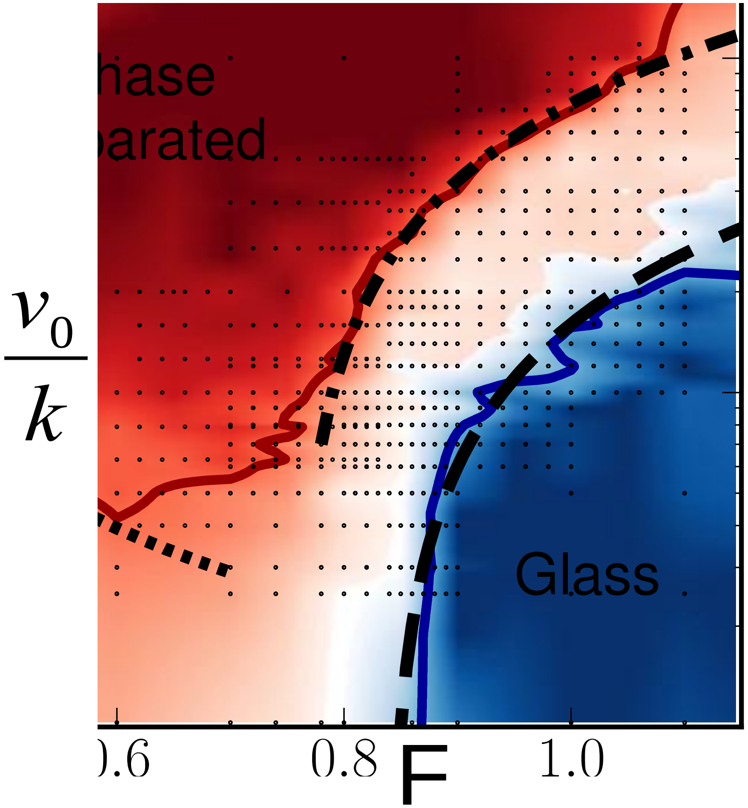
Left: melting transition

Right: clustering transition

Transitions separated by an order of magnitude in driving

Both scale linearly in distance from zero-activity jamming φ-φ_J

See also: J. Bialke et al., PRL 108, 168301 (2012)



A simple scaling criterion

Passive pressure in the solid phase

$$p = p_0\left(\Phi - \Phi_J\right), \quad p_0 = 0.34k$$

Bulk modulus (from O'Hern et al., PRE (2003))

Active pressure of an active particle pushing against its neighbors:

$$p_a \approx v_0 / 2a\mu$$

Pressure balance predicts scaling:

$$\tilde{v}^* = v_0 / a\mu k = u\left(\Phi - \Phi_J\right),$$

$$u^* = 2p_0 / k = 0.68$$

dimensionless parameter

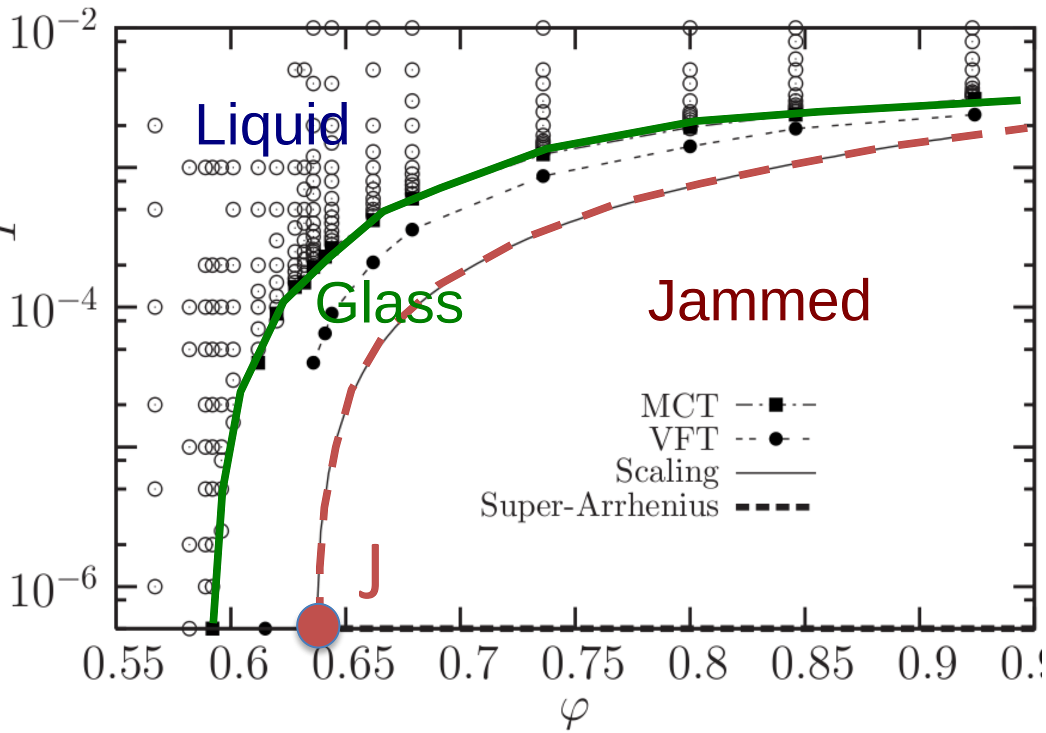
Melting: *u = 0.07*

Resembles simple melting criterion

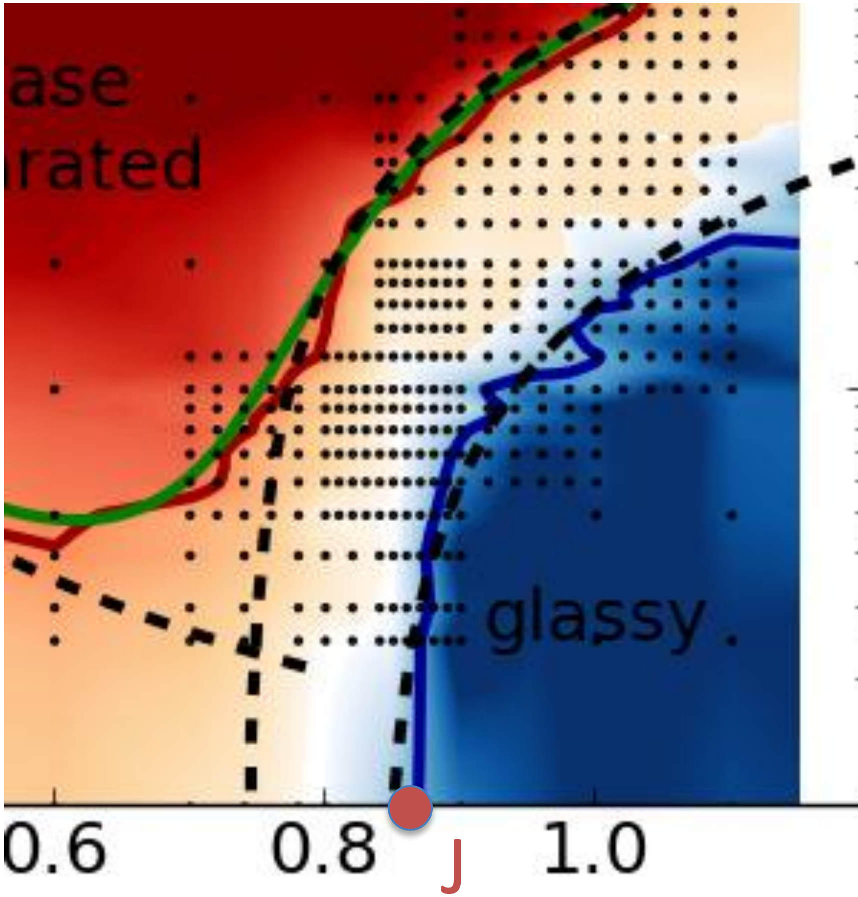
Clustering: *u = 0.7*

Clustering starts at full pressure balance – Maxwell construction for a first order phase transition

Active glasses: shift of the glass transition density



L. Berthier and T. Witten, PRE 80, 021502 (2009)



Importance of reorientation time scale:

- L. Berthier and J. Kurchan, Nature 2013
- L. Berthier, arXiv:1307.0704 (hard spheres)
- R. Ni et al, arXiv 1306.3605 (hard spheres)

Conclusions

- Cluster formation is a generic feature of active systems due to density dependent velocity
- Dynamical arrest / glassy dynamics is generic without alignment, and is possible under confinement for polar alignment
- Novel dynamical phase in the high-density, low velocity limit dominated by the low frequency modes of the underlying packing
- Rich phase space combining alignment mechanisms, cluster formation and glassy dynamics remains to be explored