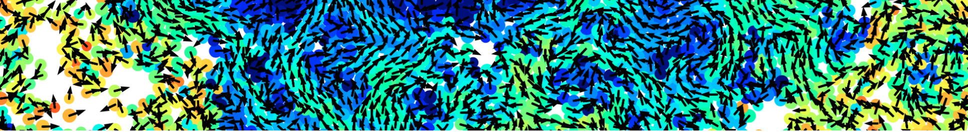

Simple model of active particles

Yann-Edwin Keta

supervised by Joerg Rottler

9/13/18

yketa/active_particles   yketa/UBC_2018_Wiki

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THE UNIVERSITY OF BRITISH COLUMBIA

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1. What is active matter?
2. Model
3. Observations
   - Motility-induced phase separation
   - Displacement correlations and cooperativities
   - Shear strain correlations
4. Conclusion

Non-equilibrium systems

Three general classes:[1]

- Systems relaxing towards equilibrium.

Example

Thermal system adapting to its thermostat, glasses.

[1] Michael E Cates and Julien Tailleur. "Motility-induced phase separation". In: *Annu. Rev. Condens. Matter Phys.* 6.1 (2015), pp. 219–244.

Non-equilibrium systems

Three general classes:[1]

- Systems relaxing towards equilibrium.
- Systems with boundary conditions imposing steady currents.

Example

Sheared liquid, metal rod between two thermostats.

[1] Michael E Cates and Julien Tailleur. "Motility-induced phase separation". In: *Annu. Rev. Condens. Matter Phys.* 6.1 (2015), pp. 219–244.

Non-equilibrium systems

Three general classes:[1]

- Systems relaxing towards equilibrium.
- Systems with boundary conditions imposing steady currents.
- Active matter.

[1] Michael E Cates and Julien Tailleur. "Motility-induced phase separation". In: *Annu. Rev. Condens. Matter Phys.* 6.1 (2015), pp. 219–244.

Active matter

Definition

System composed of self-driven units, *active particles*, each capable of converting stored or ambient free energy into systematic movement.[a]

[a] M Cristina Marchetti et al. "Hydrodynamics of soft active matter". In: *Reviews of Modern Physics* 85.3 (2013), p. 1143.

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Example

Cell tissues, swarms of bacteria, schools of fish, flocks of birds.

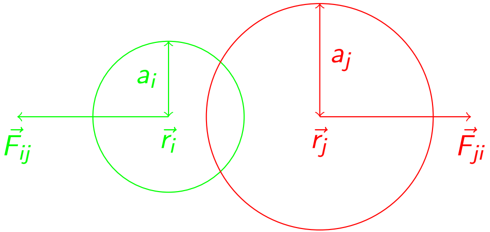
Model system

- 2D disks with packing fraction ϕ and 20% polydispersity.

Yaouen Fily, Silke Henkes, and M Cristina Marchetti. "Freezing and phase separation of self-propelled disks". In: *Soft matter* 10.13 (2014), pp. 2132–2140

Model system

- 2D disks with packing fraction ϕ and 20% polydispersity.
- Purely repulsive interparticle harmonic potential.



$$\vec{F}_{ij} = \begin{cases} k(a_i + a_j - |\vec{r}_i - \vec{r}_j|)\hat{r}_{ij} & \text{if } a_i + a_j \geq |\vec{r}_i - \vec{r}_j| \\ 0 & \text{otherwise} \end{cases}$$

Yaouen Fily, Silke Henkes, and M Cristina Marchetti. "Freezing and phase separation of self-propelled disks". In: *Soft matter* 10.13 (2014), pp. 2132–2140

Model system

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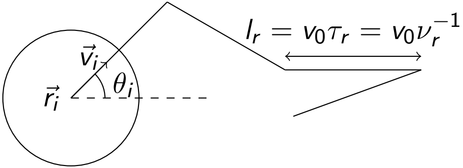
- Particle self-propulsion and Brownian dynamics.

$$\frac{d\vec{r}_i}{dt} = \vec{v}_i + \sum_{j \neq i} \vec{F}_{ij} = v_0 \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} + \sum_{j \neq i} \vec{F}_{ij}$$



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$\rightarrow$ Péclet number: $\text{Pe} = \dfrac{\tilde{v}}{\tilde{\nu}_r} = \tilde{v}\tau_r \equiv$ dimensionless distance travelled before its orientation decorrelates.

Yaouen Fily, Silke Henkes, and M Cristina Marchetti. "Freezing and phase separation of self-propelled disks". In: *Soft matter* 10.13 (2014), pp. 2132–2140

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Spontaneous phase separation

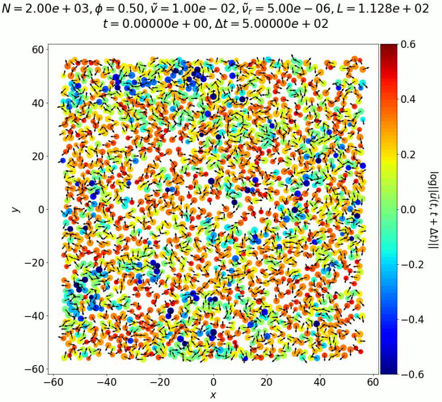

Figure: *(Movie)* Spontaneous phase separation in our active system. $\vec{u}(t, t+\Delta t) \equiv$ particle displacement between times t and $t + \Delta t$.

Motility-induced phase separation

Definition

Phase separated state arising in systems of motile particles which speed decreases sufficiently steeply with increasing local density. A dilute active gas coexists with a dense liquid of substantially reduced motility.

Michael E Cates and Julien Tailleur. "Motility-induced phase separation". In: *Annu. Rev. Condens. Matter Phys.* 6.1 (2015), pp. 219–244

Phase diagram at fixed $\tilde{\nu}_r$

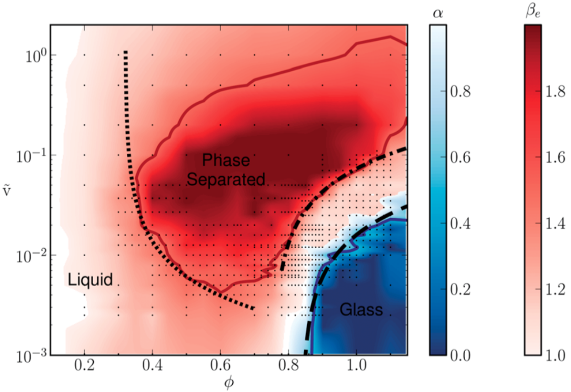

Figure: Phase diagram for $\tilde{\nu}_r = 5 \cdot 10^{-4}$.[2]

[2] Yaouen Fily, Silke Henkes, and M Cristina Marchetti. "Freezing and phase separation of self-propelled disks". In: *Soft matter* 10.13 (2014), pp. 2132–2140.

Local density distribution with varying $\tilde{v}$

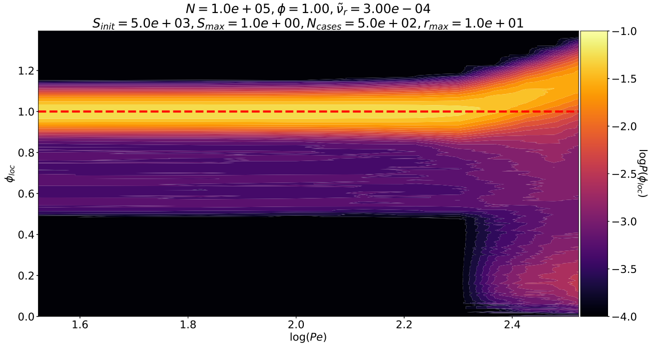

Figure: Histogram of local density ϕ_{loc} with varying self-propulsion velocity $\tilde{v}$, at packing fraction $\phi = 1.00$ and rotation diffusion constant $\tilde{\nu}_r = 3 \cdot 10^{-4}$.

Displacement map at low activity

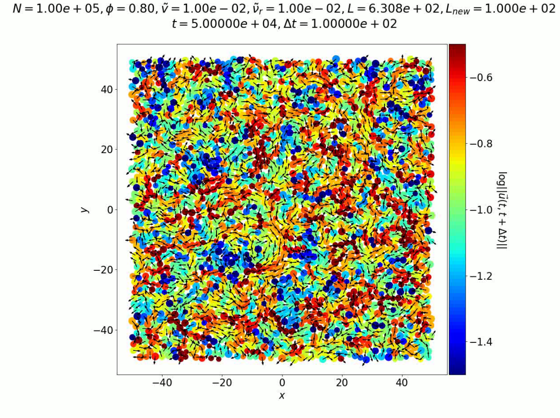

Figure: *(Movie)* Displacement maps at low activity ($\tilde{\nu}_r = 1 \cdot 10^{-2}$) with $\Delta t = \tau_r$. $\vec{u}(t, t + \Delta t) \equiv$ particle displacement between times t and $t + \Delta t$.

Displacement map at high activity

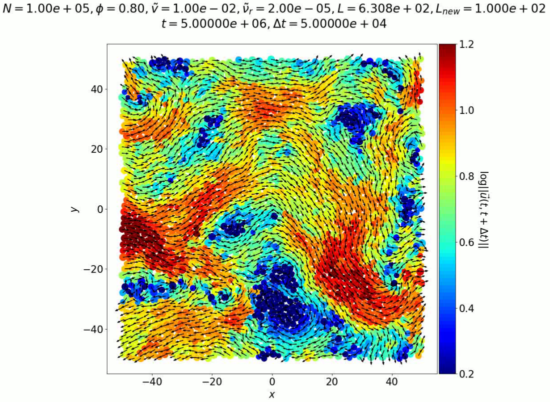

Figure: *(Movie)* Displacement maps at high activity ($\tilde{\nu}_r = 2 \cdot 10^{-5}$) with $\Delta t = \tau_r$.
$\vec{u}(t, t + \Delta t) \equiv$ particle displacement between times t and $t + \Delta t$.

Displacement correlation

$\vec{u}(\vec{r}, t, t + \Delta t) \equiv$ displacement of particle at position $\vec{r}$ between times t and $t + \Delta t$

$$C_{uu}(\Delta\vec{r}, \Delta t) = \langle \vec{u}(\vec{r} + \Delta\vec{r}, t, t + \Delta t) \cdot \vec{u}(\vec{r}, t, t + \Delta t) \rangle_{\vec{r}, t}$$

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$$C_{uu}(\Delta\vec{r}, \Delta t) \xrightarrow[\text{isotropy}]{} C_{uu}(\Delta r, \Delta t)$$

Displacement cooperativity

$$\chi(\Delta t) = \frac{1}{L^2} \int dr\ 2\pi r\ C_{uu}(r, \Delta t)$$

with L the characteristic length of the system.

Definition

$\chi \equiv$ average proportion of particles acting as coherently moving neighbours $\rightarrow$ measure of dynamic heterogeneity.

Adam Wysocki, Roland G Winkler, and Gerhard Gompper. "Cooperative motion of active Brownian spheres in three-dimensional dense suspensions". In: *EPL (Europhysics Letters)* 105.4 (2014), p. 48004

Burkhard Doliwa and Andreas Heuer. "Cooperativity and spatial correlations near the glass transition: Computer simulation results for hard spheres and disks". In: *Physical Review E* 61.6 (2000), p. 6898

Displacement cooperativity with varying $\tilde{\nu}_r$

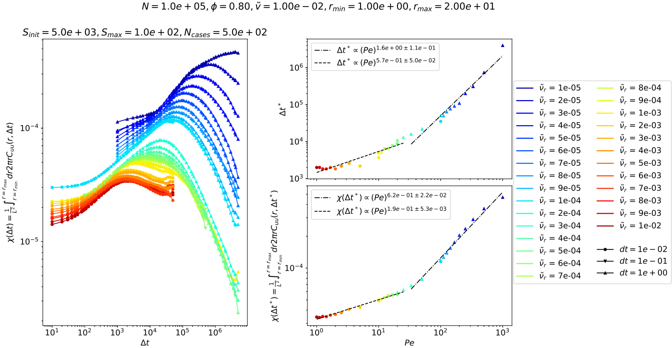

Figure: Comparison of displacement cooperativities $\chi(\Delta t)$, times of maximum cooperativity Δt^* and maximum cooperativities $\chi(\Delta t^*)$, at packing fraction $\phi = 0.80$ and self-propulsion velocity $\tilde{v} = 1 \cdot 10^{-2}$.

- $\rightarrow$ Clear change of $\Delta t^*(\text{Pe})$ and $\chi(\Delta t^*, \text{Pe})$ slopes at MIPS.
- $\rightarrow$ $(\tau_r \nearrow \Leftrightarrow \text{Pe} \nearrow) \Rightarrow \Delta t^* \nearrow, \ \chi(\Delta t^*) \nearrow$

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Linearised shear strain

$$\vec{u}(\vec{r}, t, t+\Delta t) = \begin{pmatrix} u_x(\vec{r}, t, t+\Delta t) \\ u_y(\vec{r}, t, t+\Delta t) \end{pmatrix} \equiv \text{displacement of particle at}$$

position $\vec{r}$ between times t and $t + \Delta t$

Accumulated shear strain at position $\vec{r}$ between times t and $t + \Delta t$

$$\varepsilon_{xy}(\vec{r}, t, t+\Delta t) = \frac{1}{2}\left(\frac{\partial}{\partial x} u_y(\vec{r}, t, t+\Delta t) + \frac{\partial}{\partial y} u_x(\vec{r}, t, t+\Delta t)\right)$$

Projection of shear strain correlation

$$C_{\varepsilon_{xy}\varepsilon_{xy}}(\Delta\vec{r}, \Delta t) = \langle \varepsilon_{xy}(\vec{r} + \Delta\vec{r}, t, t + \Delta t)\varepsilon_{xy}(\vec{r}, t, t + \Delta t)\rangle_{\vec{r},t}$$

Bernd Illing et al. "Strain pattern in supercooled liquids". In: *Physical review letters* 117.20 (2016), p. 208002

Projection of shear strain correlation

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$$C_4^4(\Delta r,\Delta t) = \frac{1}{\pi}\int_0^{2\pi} d\theta \;\cos(4\theta)\; C_{\varepsilon_{xy}\varepsilon_{xy}}(\Delta\vec{r}\equiv(\Delta r,\theta),\Delta t)$$

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$$\propto \frac{1}{\Delta r^2} \qquad \text{(elastic medium)}$$

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Shear strain map at high activity (real space method)

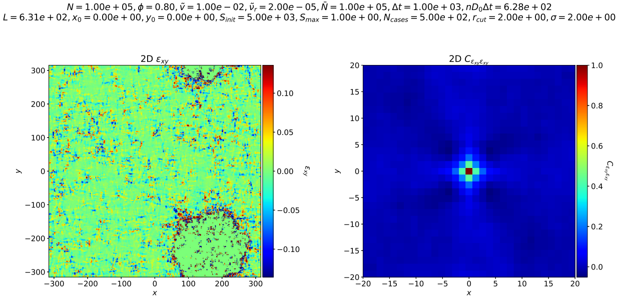

Figure: Shear strain map $\varepsilon_{xy}(\vec{r}, t, t+\Delta t)$ and corresponding shear strain correlations $C_{\varepsilon_{xy}\varepsilon_{xy}}(\Delta\vec{r}, \Delta t)$, at packing fraction $\phi = 0.80$, self-propulsion velocity $\tilde{v} = 1 \cdot 10^{-2}$ and rotation diffusion constant $\tilde{\nu}_r = 2 \cdot 10^{-5}$.

$\rightarrow$ Highest strain values at phase interface.

$\rightarrow$ Quadropular symmetry of shear strain correlations.

Collective mean square displacements

$$\vec{u}(\vec{r}, t, t + \Delta t) \xrightarrow[\text{Fourier transform}]{} \tilde{\vec{u}}(\vec{k}, t, t + \Delta t)$$

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F Leonforte et al. "Continuum limit of amorphous elastic bodies. iii. three-dimensional systems". In: *Physical Review B* 72.22 (2005), p. 224206

Collective mean square displacements

$$\vec{u}(\vec{r}, t, t+\Delta t) \xrightarrow[\text{Fourier transform}]{} \tilde{\vec{u}}(\vec{k}, t, t+\Delta t)$$

$$C^{\perp}(\vec{k}, \Delta t) = \left\langle ||\tilde{\vec{u}}_{\perp}(\vec{k}, t, t+\Delta t)||^2 \right\rangle$$

$$C^{||}(\vec{k}, \Delta t) = \left\langle ||\tilde{\vec{u}}_{||}(\vec{k}, t, t+\Delta t)||^2 \right\rangle$$

respectivement the transversal and longitudinal collective mean square displacements (CMSD).

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CMSD and shear strain correlations

$$C_{\varepsilon_{xy}\varepsilon_{xy}}(\Delta\vec{r},\Delta t) = \mathcal{F}^{-1}\Big\{ -\frac{k_x^2 k_y^2}{k^2}\Big(C^{\perp}(\vec{k},\Delta t) - C^{||}(\vec{k},\Delta t)\Big) + \frac{k^2}{4}C^{\perp}(\vec{k},\Delta t)\Big\}(\Delta\vec{r})$$

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$$\begin{aligned} C^{||}(\vec{k},\Delta t) &= 0 \\ C^{\perp}(\vec{k},\Delta t) &\propto k^{-2} \end{aligned} \qquad \text{(incompressible glass)}$$

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CMSD at high activity

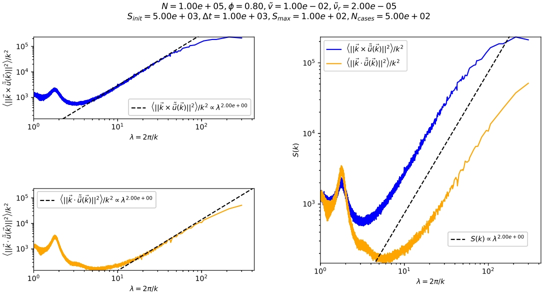


Figure: Transversal and longitudinal CMSD, $C^{\perp}(k, \Delta t) \equiv \left\langle ||\tilde{\vec{u}}_{\perp}(\vec{k}, t, t+\Delta t)||^2 \right\rangle$ and $C^{||}(k, \Delta t) \equiv \left\langle ||\tilde{\vec{u}}_{||}(\vec{k}, t, t+\Delta t)||^2 \right\rangle$, at packing fraction $\phi = 0.80$, self-propulsion velocity $\tilde{v} = 1 \cdot 10^{-2}$ and rotation diffusion constant $\tilde{\nu}_r = 2 \cdot 10^{-5}$.

$\rightarrow$ $C^{||}(k, \Delta t) \neq 0$.

$\rightarrow$ $C^{\perp}(k, \Delta t), C^{||}(k, \Delta t) \propto k^{-2}$ for $\sim$ a decade.

Projected strain correlations from CMSD at high activity

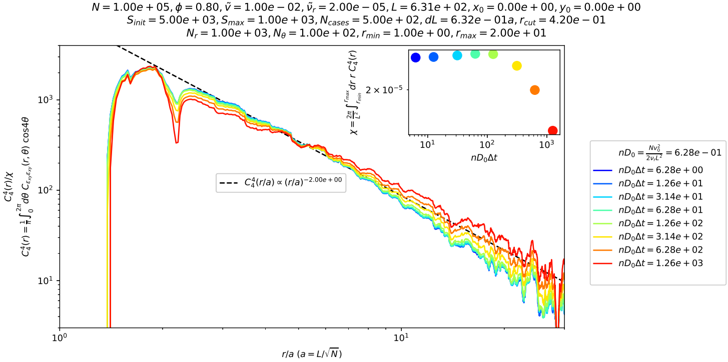
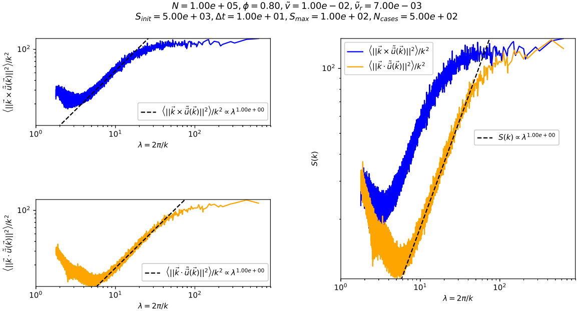


Figure: Shear strain correlations $C_4^4(\Delta r, \Delta t)$ rescaled by its susceptibility, at packing fraction $\phi = 0.80$, self-propulsion velocity $\tilde{v} = 1 \cdot 10^{-2}$ and rotation diffusion constant $\tilde{\nu}_r = 2 \cdot 10^{-5}$.

$\rightarrow$ Algebraic decay over two decades of lag times.

CMSD at low activity



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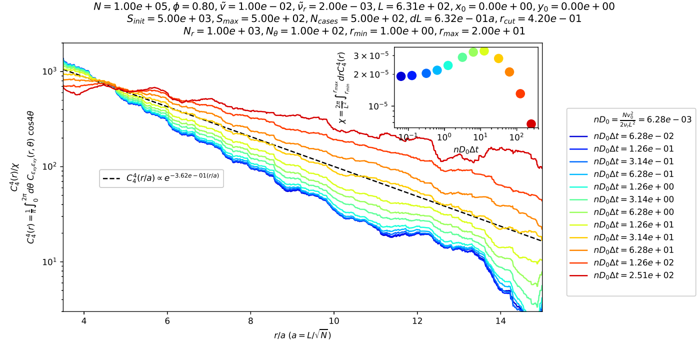
$\rightarrow$ $C^{\perp}(\vec{k}, \Delta t), C^{||}(k, \Delta t) \propto k^{-1}$ for $\sim$ a decade.

Projected strain correlations from CMSD at low activity



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- $\rightarrow$ Exponential decay at all lag times.
- $\rightarrow$ Exponential decay length scale around $2a$ and increasing function of lag time.

Conclusion

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- At fixed self-propulsion velocity, this transition is accompanied by increased cooperativity $\Rightarrow$ increased dynamic heterogeneity.
- Shear strain correlations show algebraic decay for phase-separated systems and exponential decay for homogenous fluid systems.

Outlook

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- Characterise the transition from exponential to algebraic decay in shear strain correlations.