Self-organization in a Persistent Active Liquid

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Collaborators

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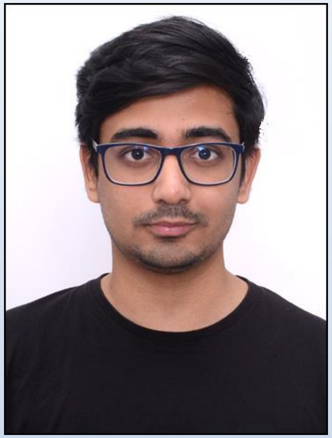

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Active matter (System of self-propelled objects)

An object that can convert stored or ambient energy into systematic motion.

Bacteria

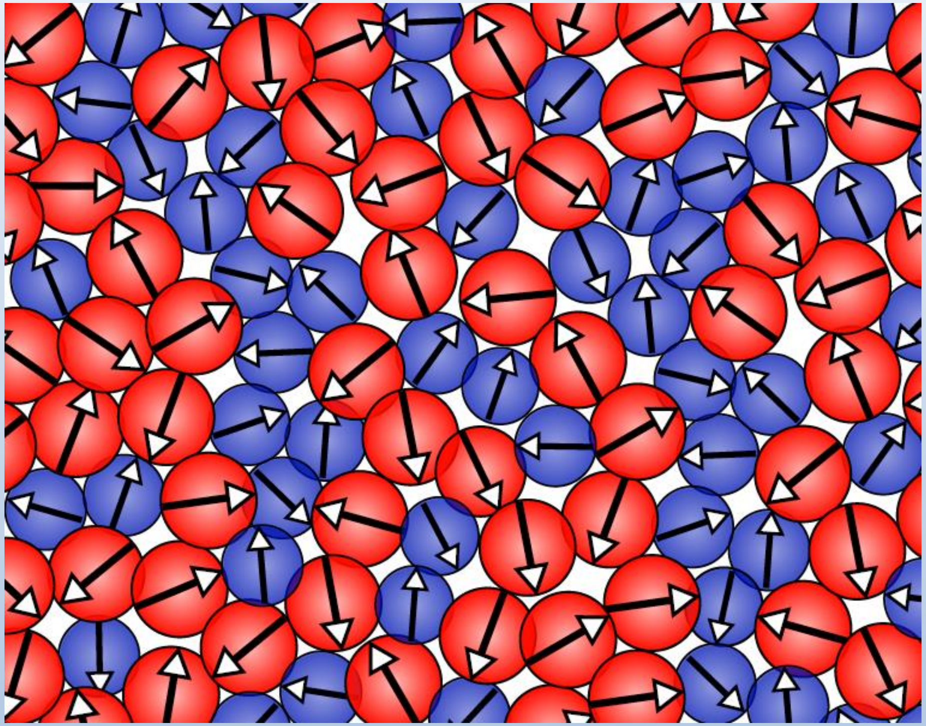
School of fish

Flock of birds

Synthetic Active Matter: Janus colloids, vibrated granular matter

Complex non-equilibrium collective behaviour

Dense systems of active particles



Glassy behaviour and jamming

Motivation:

Glassy behaviour and jamming are observed in many experiments on dense active matter

Biological systems:

- Bacterial cytoplasm
- Cytoskeleton - molecular motor complex
- Epithelial layers of cells (embryogenesis, wound healing, asthma, metastasis of cancer cells, etc.)

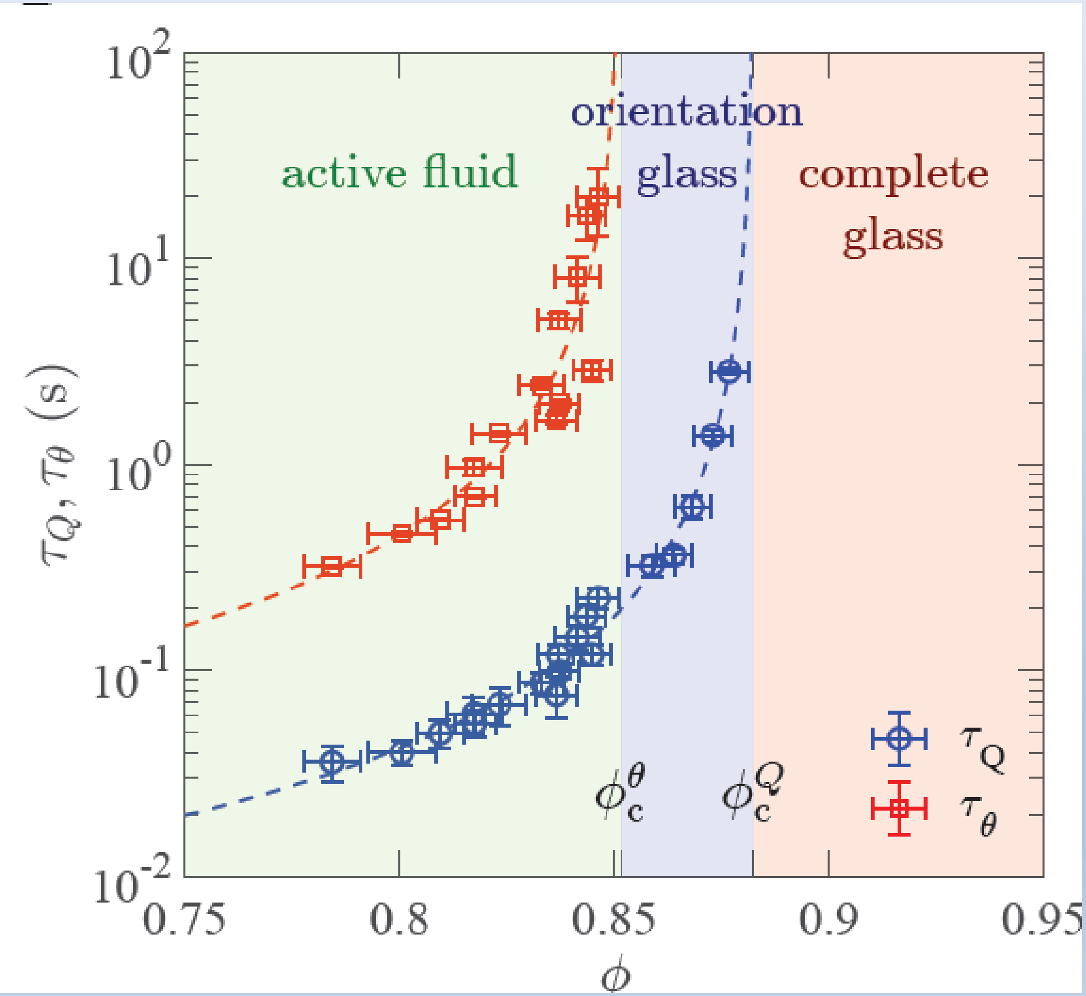
Artificial active matter:

- Janus colloids
- Vibrated granular matter

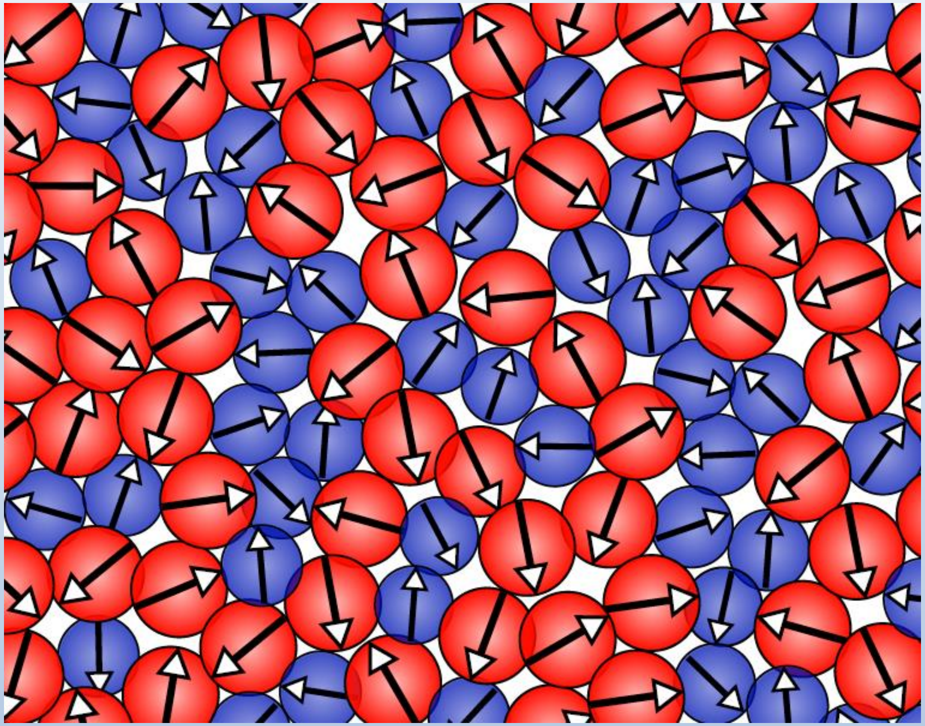
Emergence of bacterial glass

PNAS Nexus (2024)

Hisay Lama,[a] Masahiro J. Yamamoto,[b,a] Yujiro Furuta,[c,d] Takuro Shimaya[a,d] and Kazumasa A. Takeuchi[a,d,*]



Models of dense systems of active particles



- Active forces on different particles act in different directions.
- The direction of the active force on a given particle changes in time.
- The active force is characterized by two parameters: the typical **magnitude** of the force and the **persistence time**.

Model of Active Matter

65:35 mixture of particles in two dimensions, interacting via Lennard-Jones potentials with parameters same as those in the Kob-Andersen model. Dimensionless number density=1.2

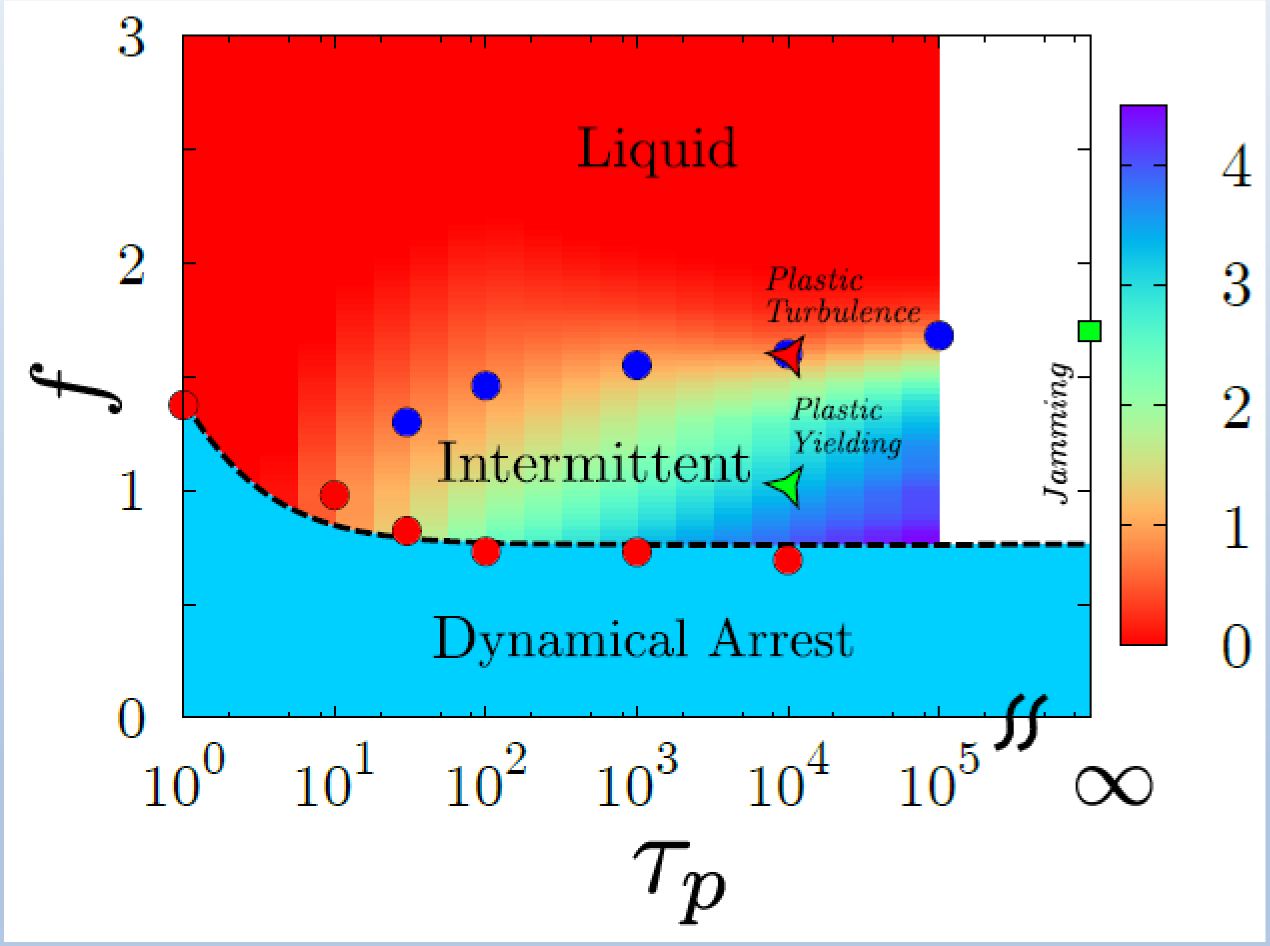
Athermal dynamics, with self-propulsion force of magnitude f acting along different directions for different particles

The direction of the force undergoes rotational diffusion

$$m\ddot{\mathbf{x}}_i = -\gamma\dot{\mathbf{x}}_i + \sum_{i\neq j=1}^{N} \mathbf{f}_{ij} + f\mathbf{n}_i$$

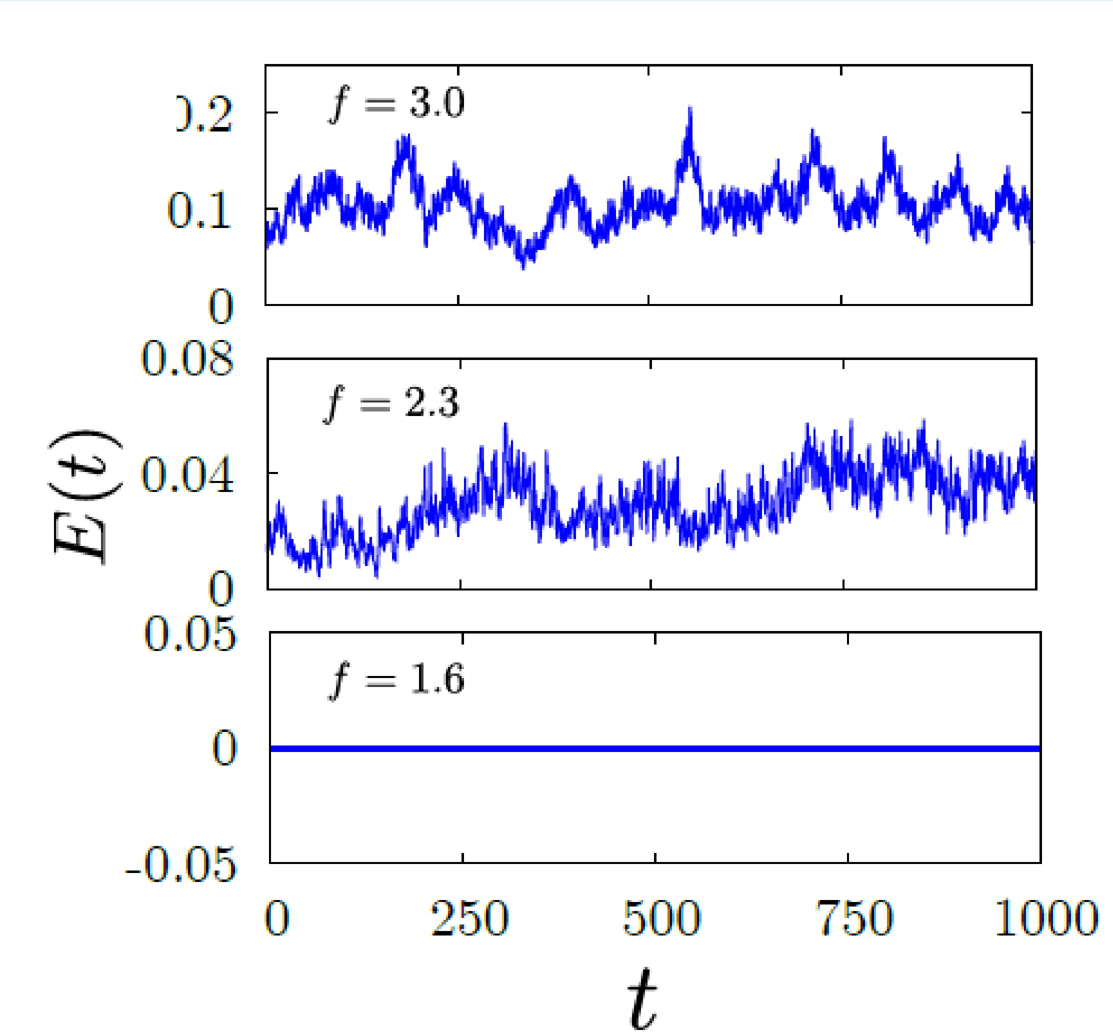
$$\dot{\theta}_i = \xi_i \, . \quad \langle \xi_i(t)\xi_j(t')\rangle = 2\tau_p^{-1}\delta_{ij}\delta(t-t')$$

Phase diagram in the self-propulsion force vs. persistence time plane

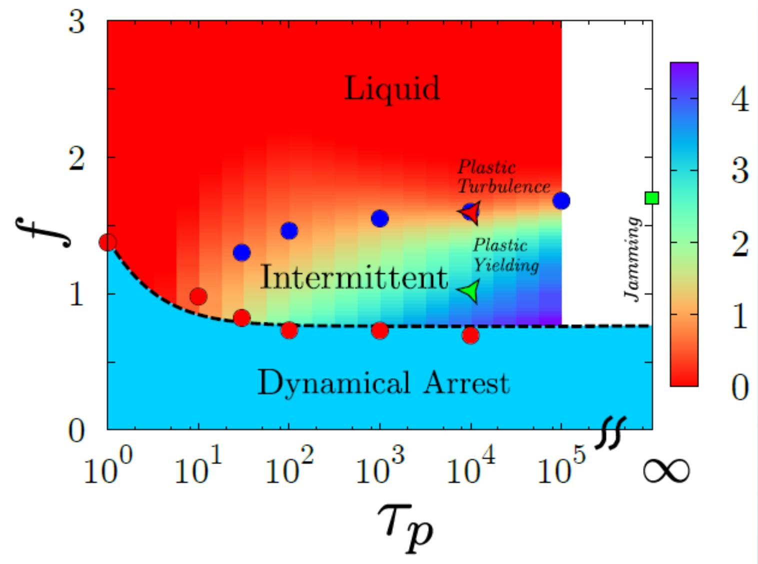


R. Mandal *et al.*, Nat. Comm. **11**, 2581 (2020)

Infinite persistence time



Average kinetic energy vs. time



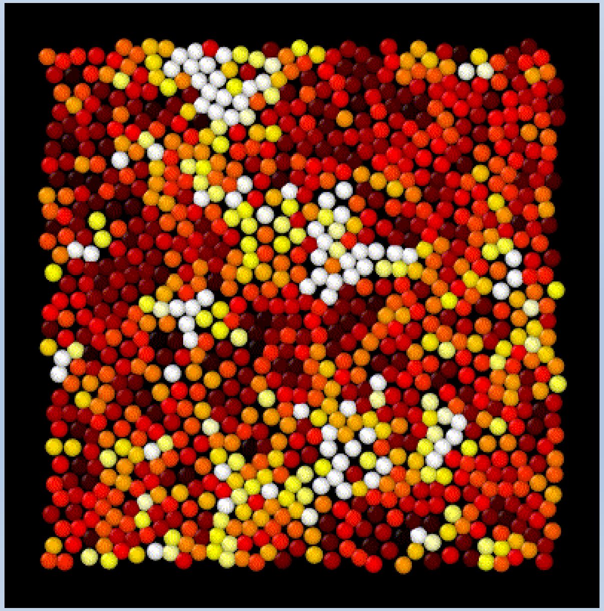
A jammed state is reached as *f* is decreased below a threshold value

Nat. Comm. 2020

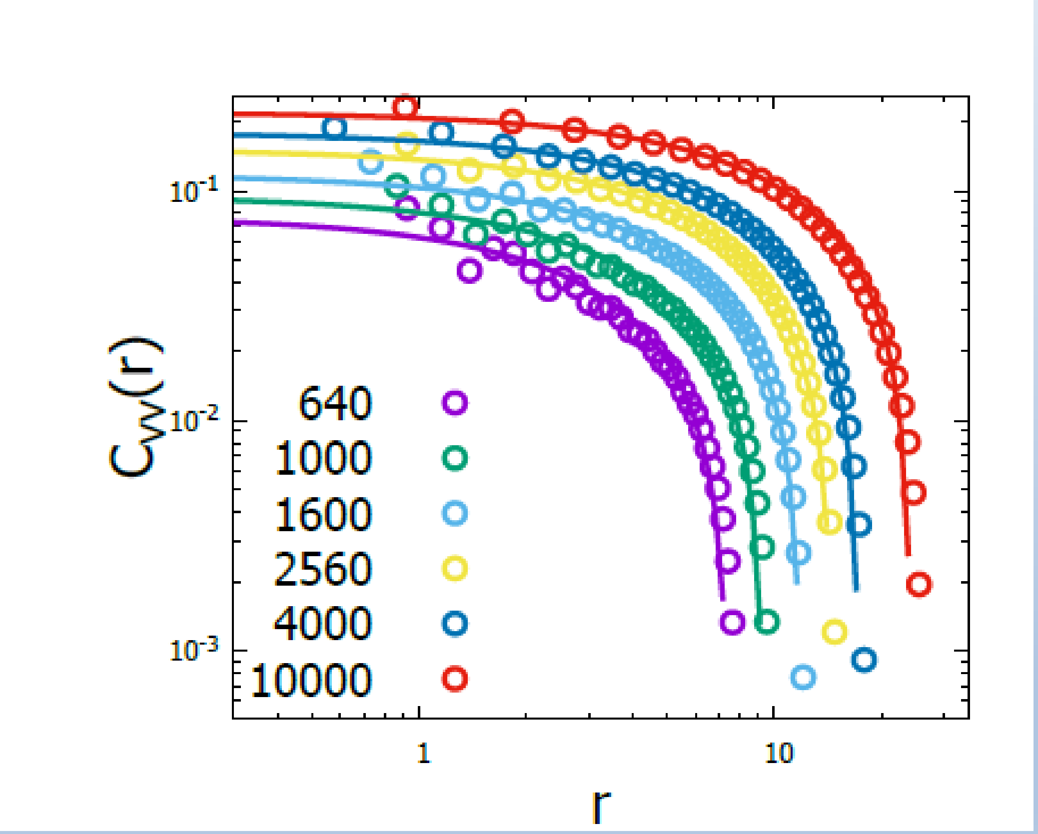
See also Liao and Xu, Soft Matter (2018), Yang *et al*, Phys. Rev. E (2022)

Infinite persistence time: Self-propulsion forces on different particles are in different directions, but they do not change with time.

Properties of the liquid state at f=3.0

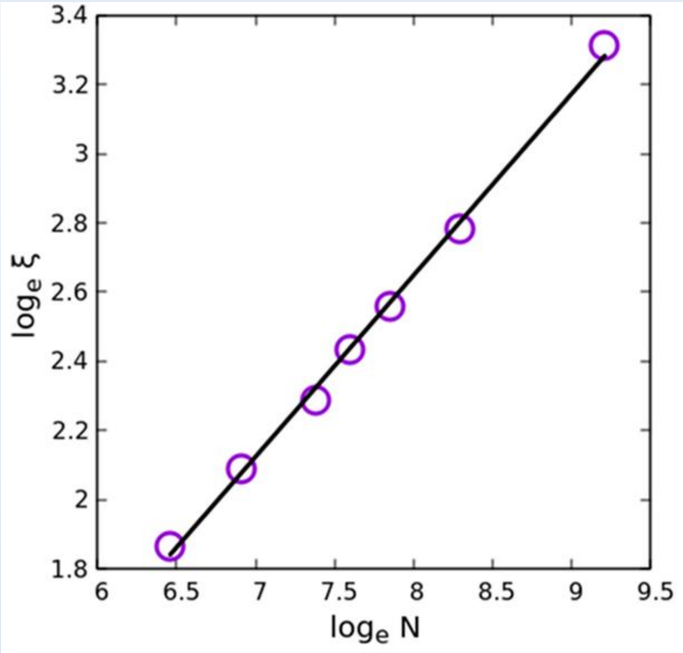


Particle velocities show strong spatial correlation



Correlation length increases with system size.

Correlation length is proportional to the system size

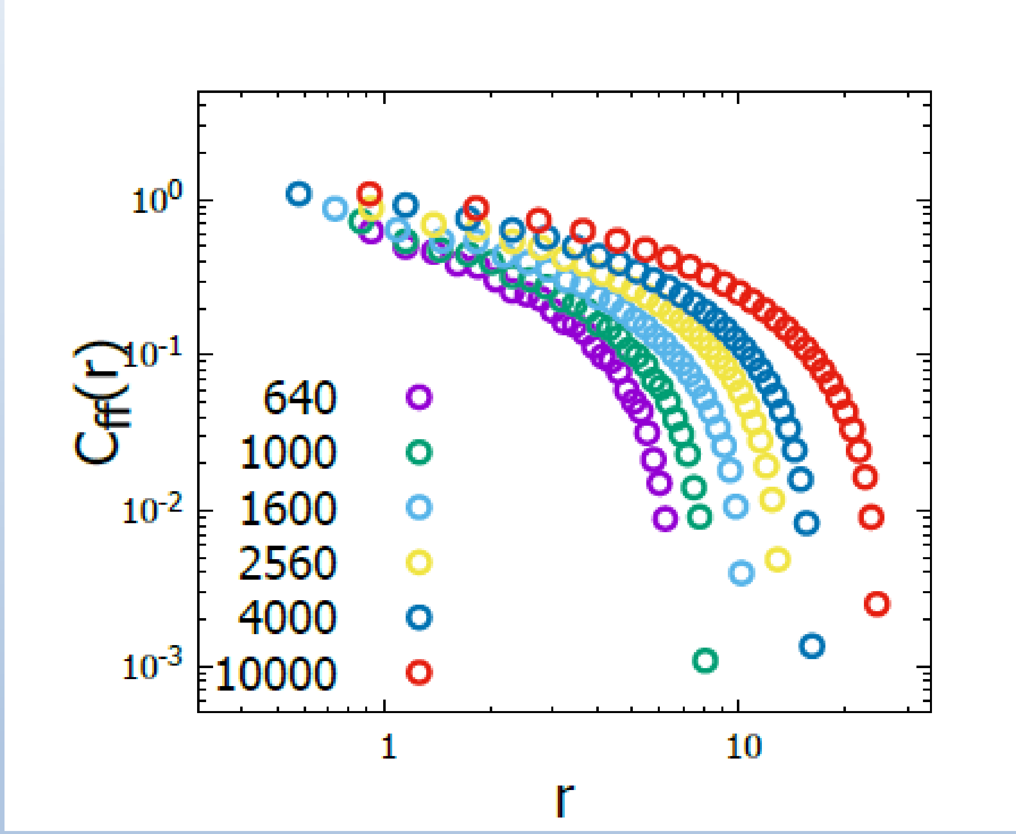


Yang *et al*, Phys. Rev. E **106**, L012601 (2022); Henkes *et al,* Nat. Commun**. 11**, 1405 (2020); Caprini and Marconi, Phys. Rev. Res. **2**, 033518 (2020); Szamel and Flenner, EPL **133**, 60002 (2021).

$$\xi \propto \sqrt{\tau_p}$$

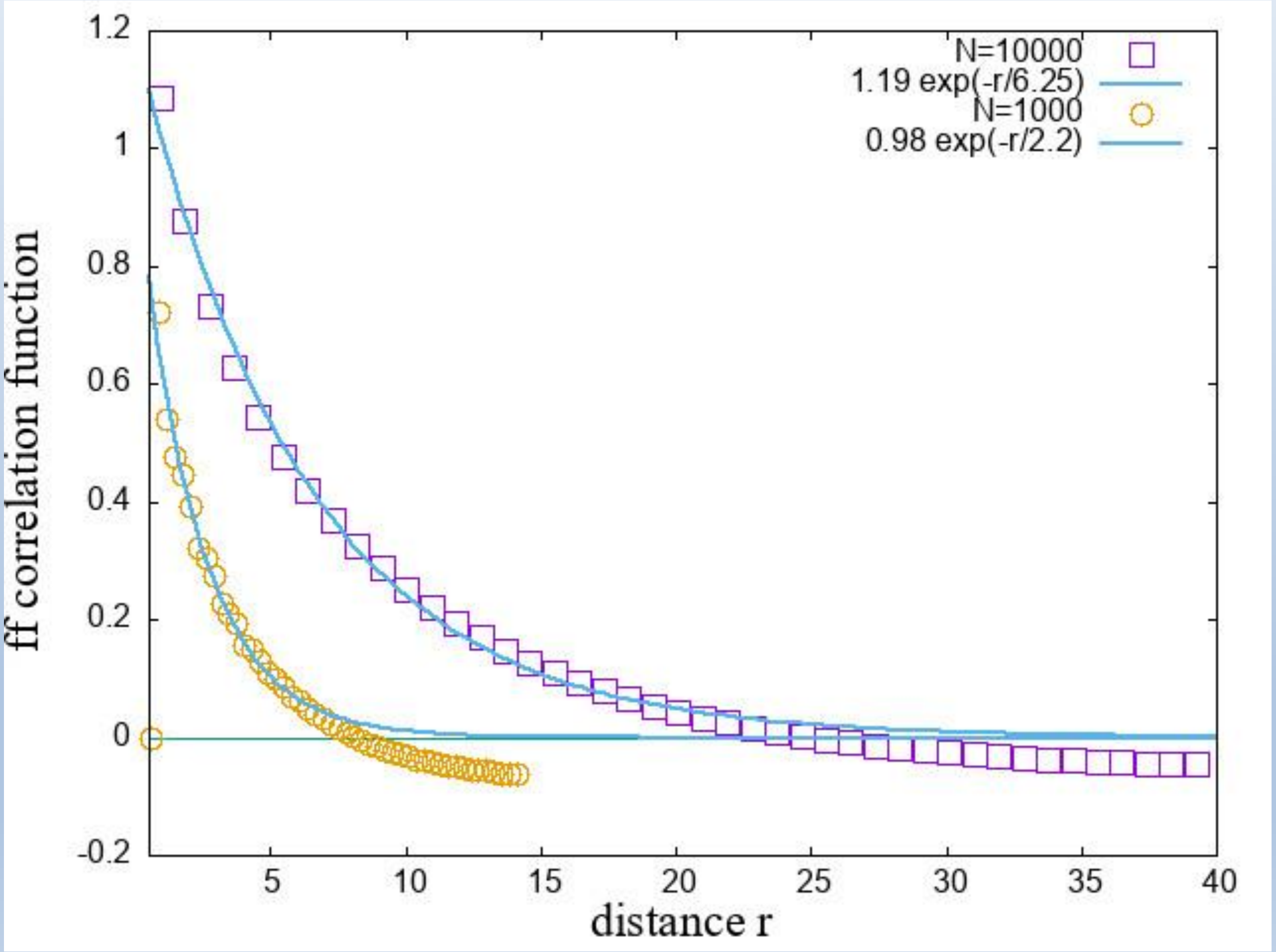
The liquid state is "**critical**" in the sense that the correlation length associated with particle velocities diverges in the thermodynamic limit.

Self-propulsion forces also exhibit strong spatial correlation

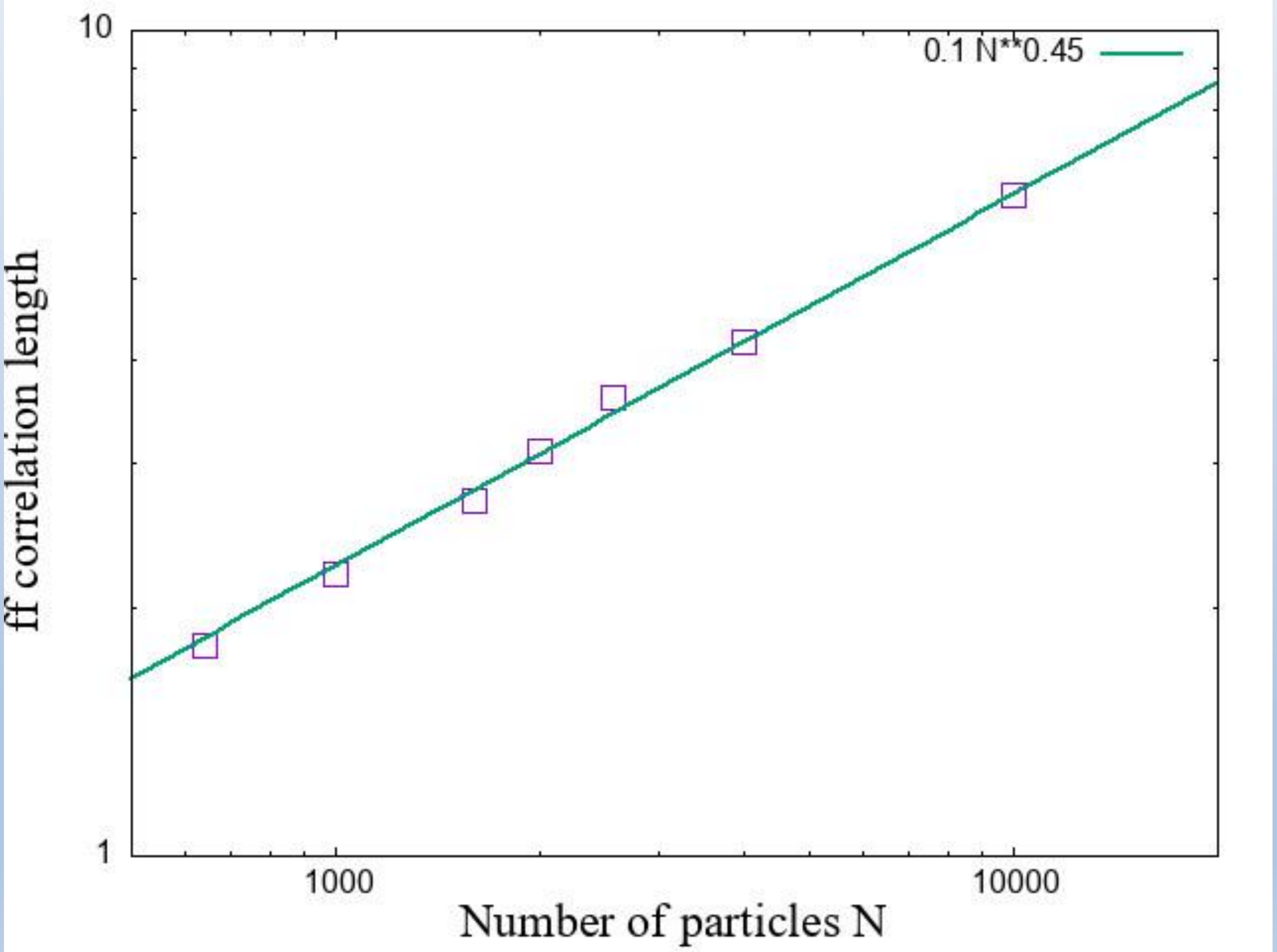


Correlation length is proportional to the system size.

Equal-time spatial correlation of the self-propulsion force



The length scale associated with active force correlations is proportional to system size

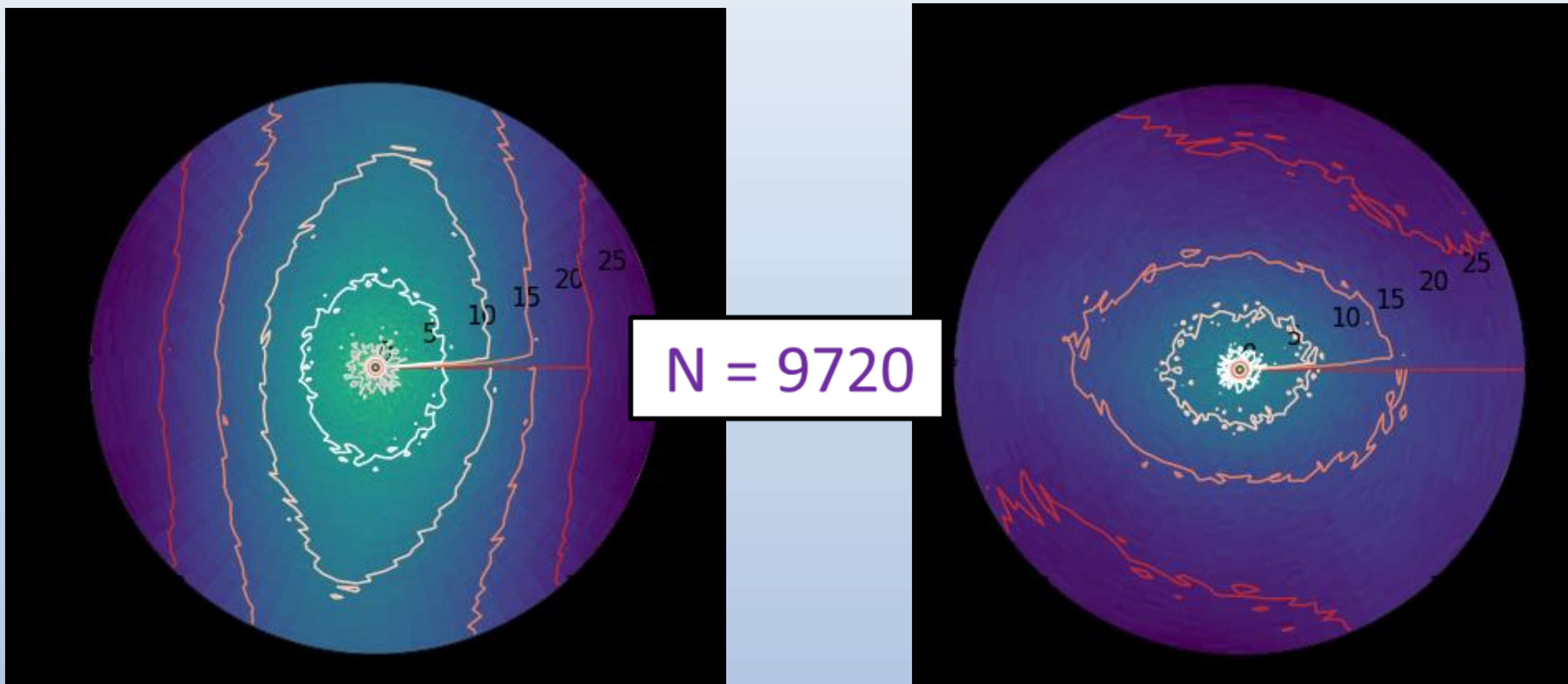


Self-organization of velocities and self-propulsion forces

Self-propulsion forces and particle velocities have random directions in the initial state.

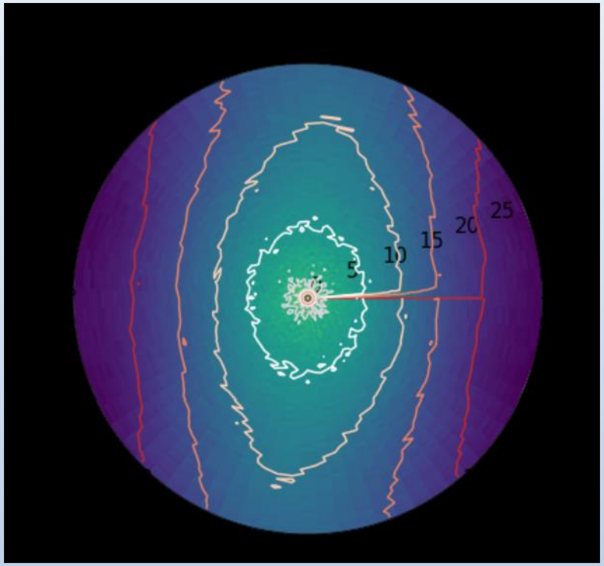
The particles **self-organize** into a steady state in which particles with similar directions of the self-propulsion forces come close to one another and move together. The length scales of spatial correlations of the velocity and the self-propulsion force are proportional to the system size.

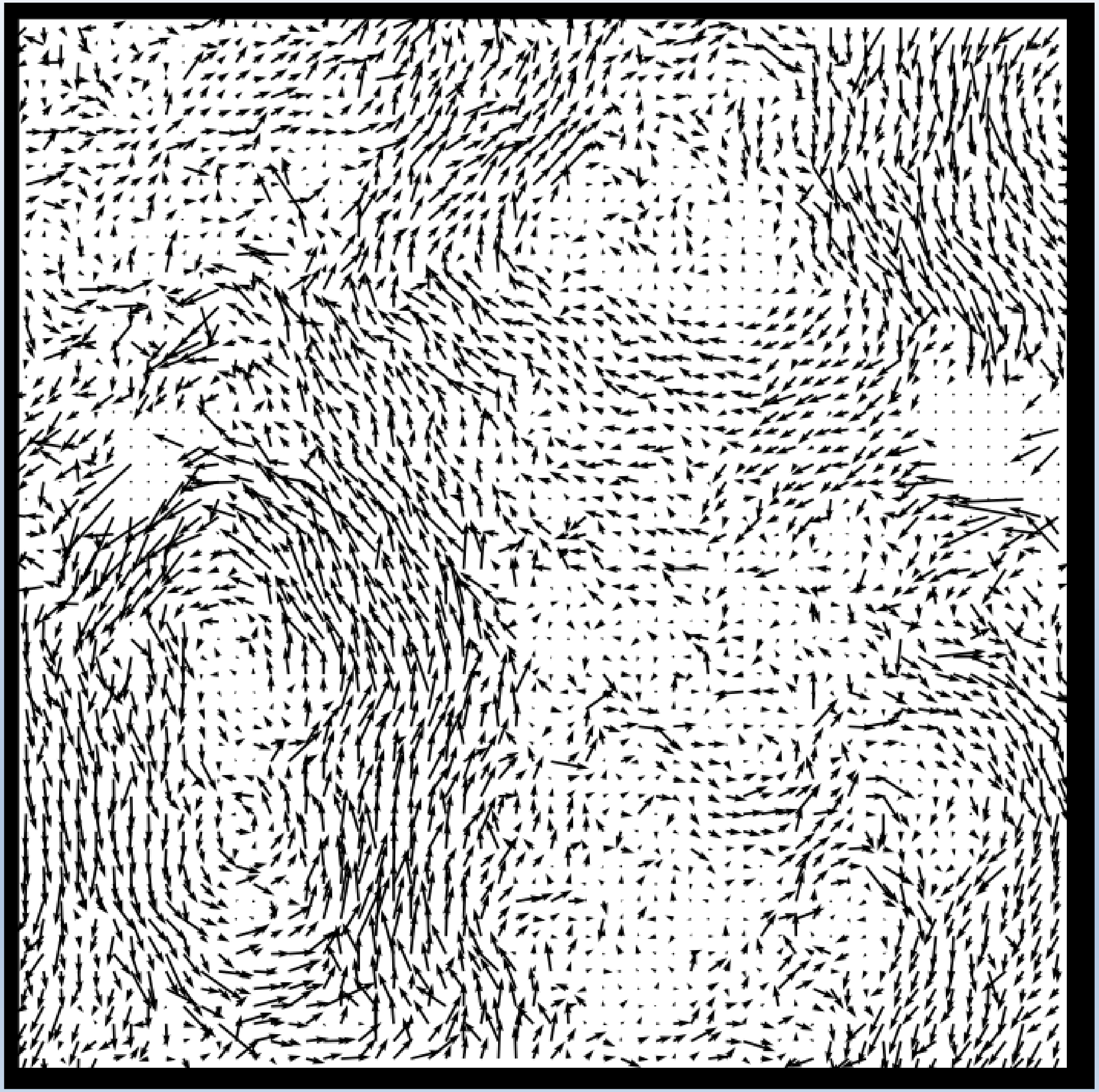
Anisotropy of the velocity correlation function



Colour plots of C_vv(**r**) in the steady state in two different runs.
The colour indicates the value of the correlation function.
Contours of constant values of the correlation function are shown.

Map of coarse-grained velocity





Uniaxial Anisotropy

Let θ_i be the angle made by the velocity of particle i with the x-axis.

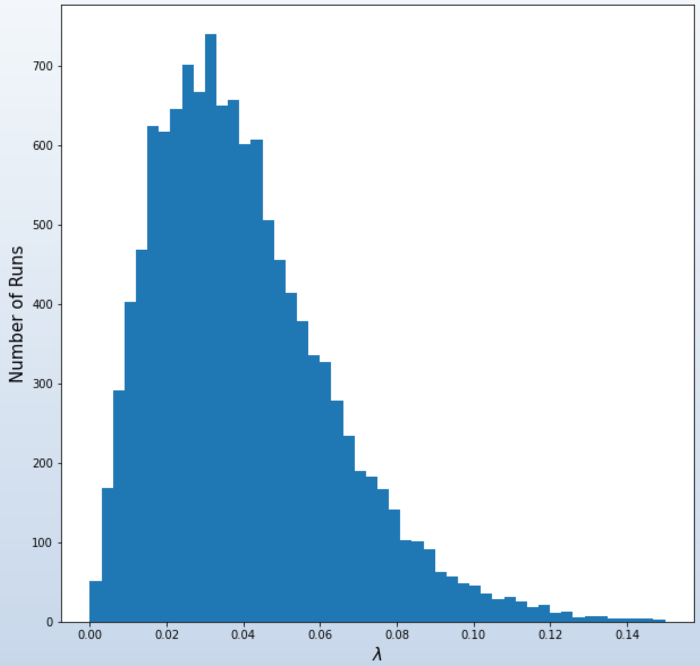
Consider the 2×2 matrix $\mathbf{M}$ with

$$M_{11} = \frac{1}{N}\sum_{i=1}^{N} \cos^2\theta_i - \frac{1}{2},$$

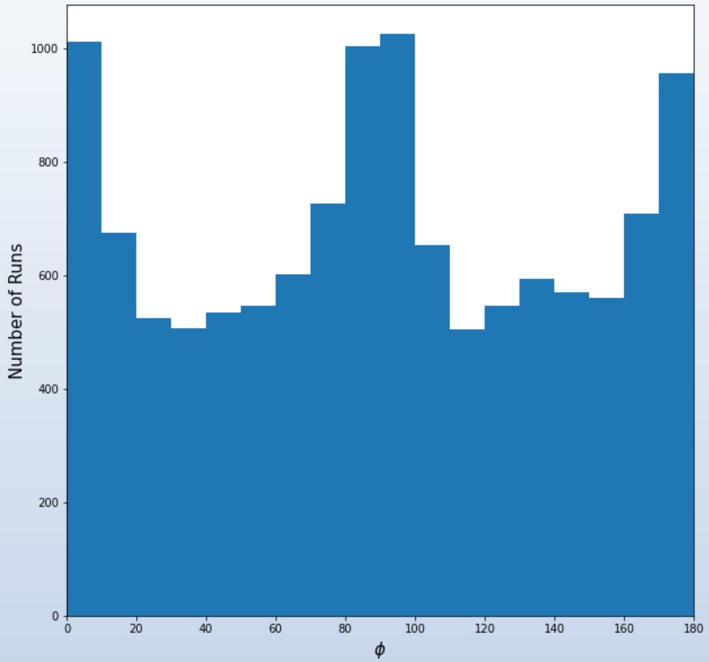
$$M_{22} = \frac{1}{N}\sum_{i=1}^{N} \sin^2\theta_i - \frac{1}{2},$$

$$M_{12} = M_{21} = \frac{1}{N}\sum_{i=1}^{N} \sin\theta_i \cos\theta_1 .$$

The positive eigenvalue λ of $\mathbf{M}$ denotes the degree of anisotropy and the corresponding eigenvector $(\cos\phi, \sin\phi)^T$ gives the angle of the preferred direction with the x-axis.



Distribution of λ

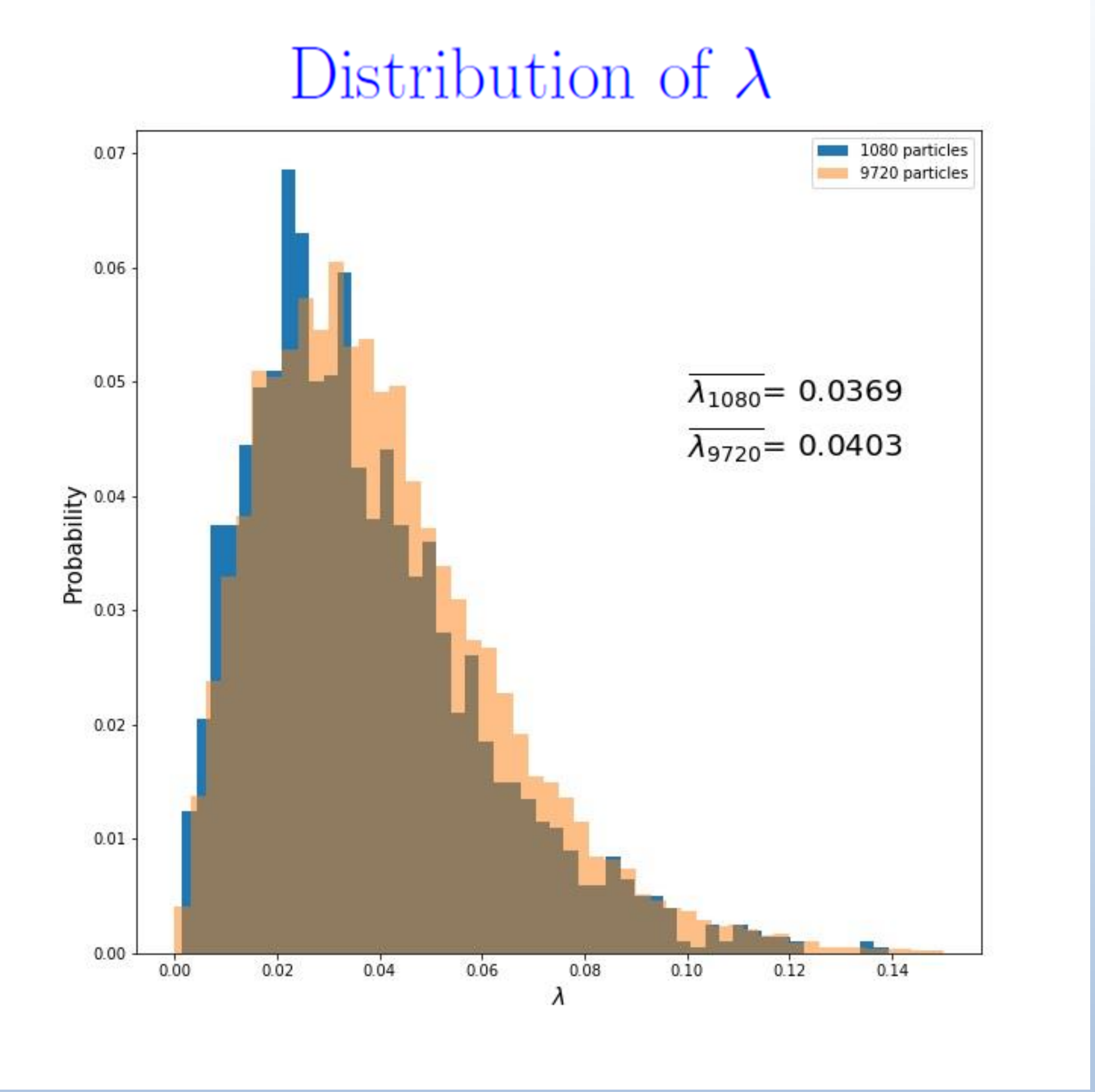


Distribution of ϕ

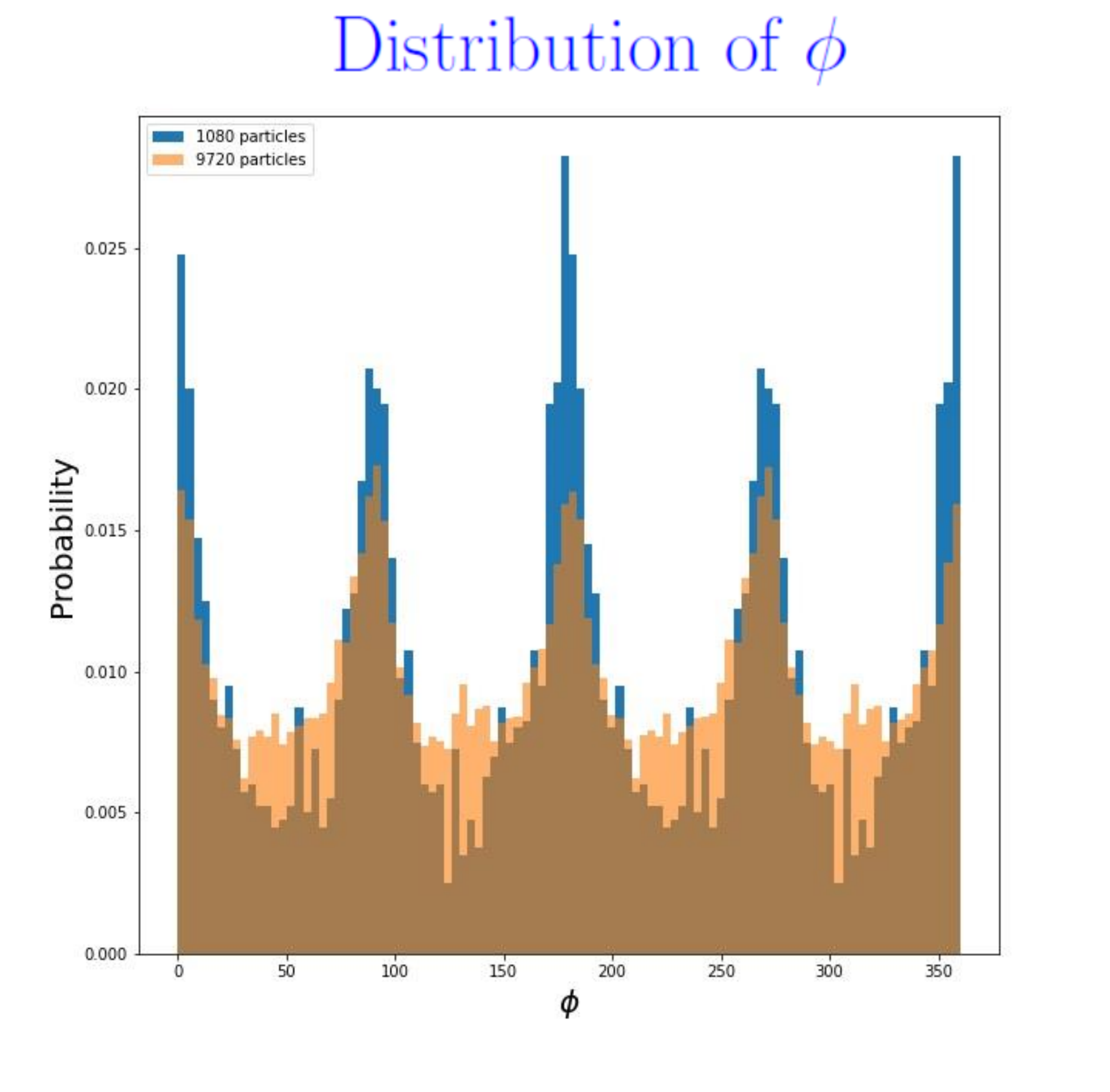
The particles form two large streams that flow in opposite directions.

The streams are preferentially oriented in the x or y direction

True symmetry breaking or finite size effect?



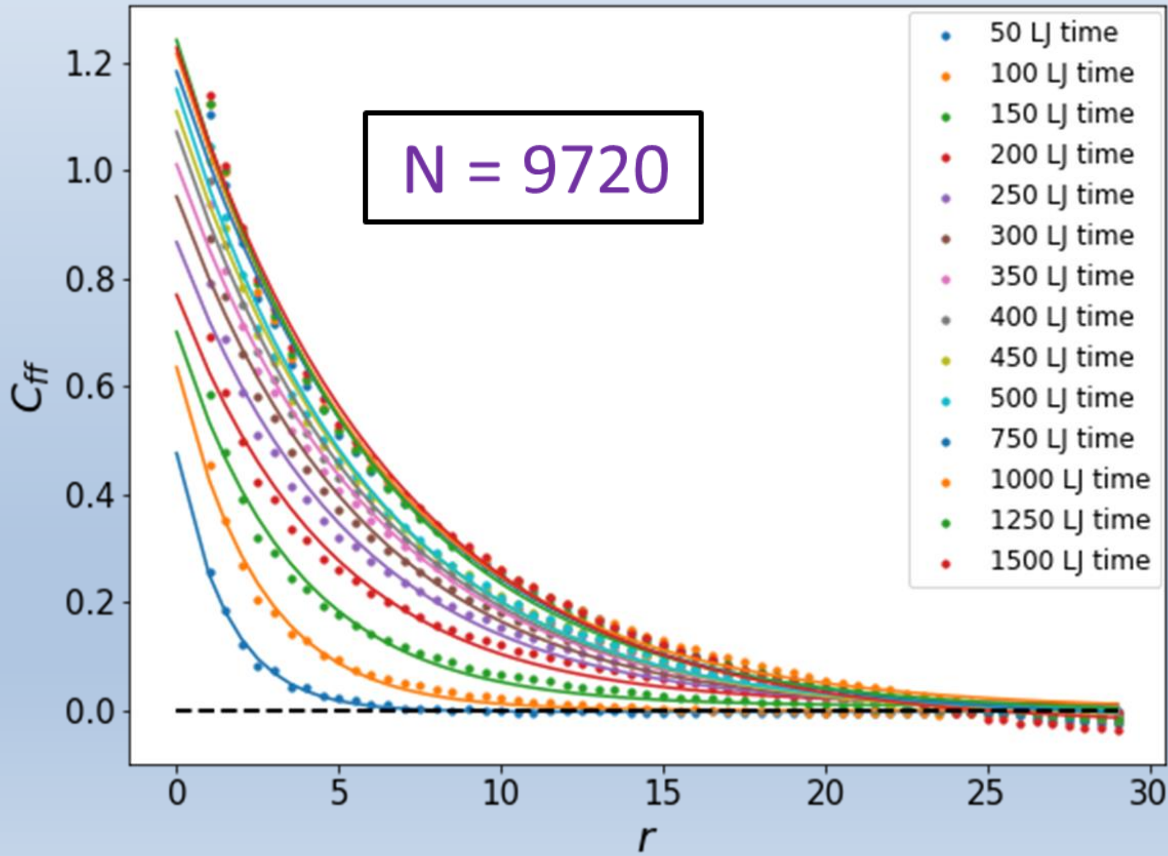
Distribution shifts to larger values as the system size is increased



Heights of peaks in the x and y directions decrease with increasing system size

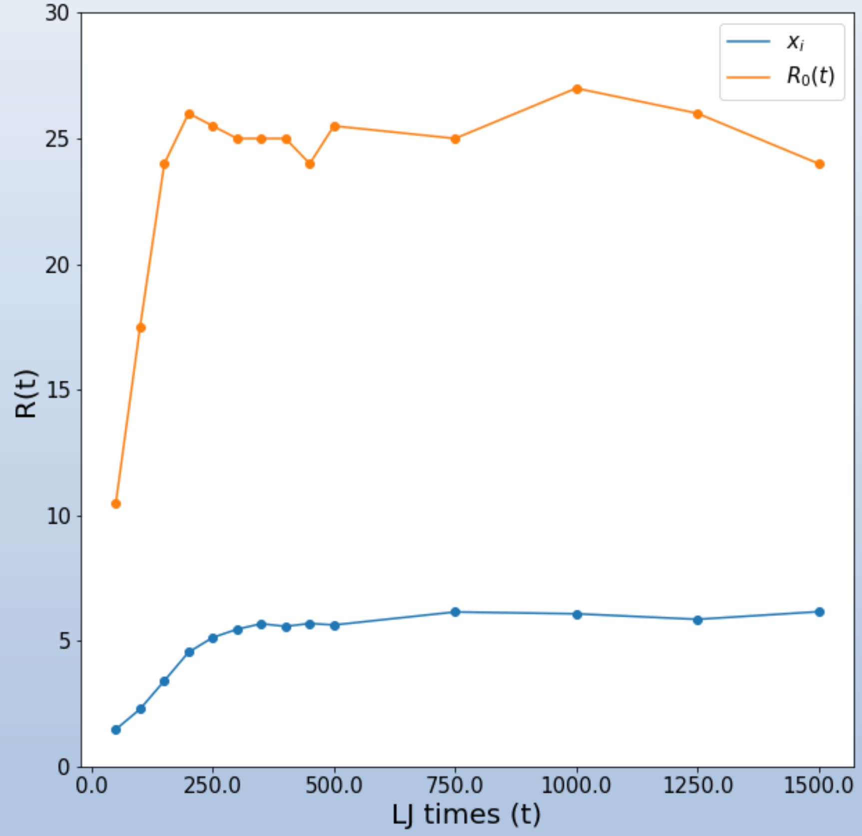
The process of the growth of correlations with time is analogous to the formation and coarsening of ordered domains after a quench from a high-temperature disordered slate to a temperature below the ordering temperature.

Growth of correlations with time



Growth of the length scale of correlations

N = 9720



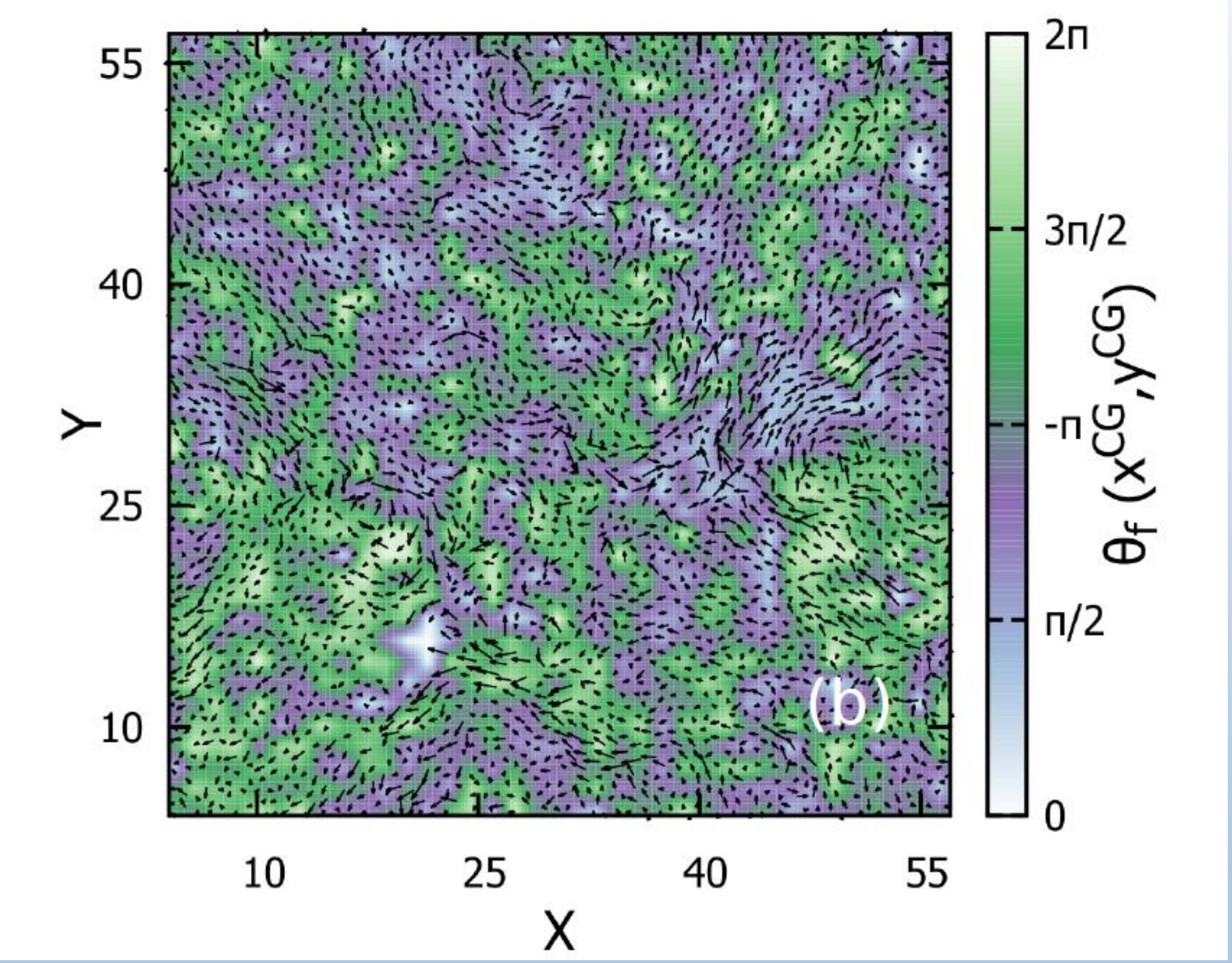
The growth of the length scale is qualitatively different from that in a two-dimensional conserved XY model.

Porod's Law is not satisfied, implying rough domain walls.

Summary

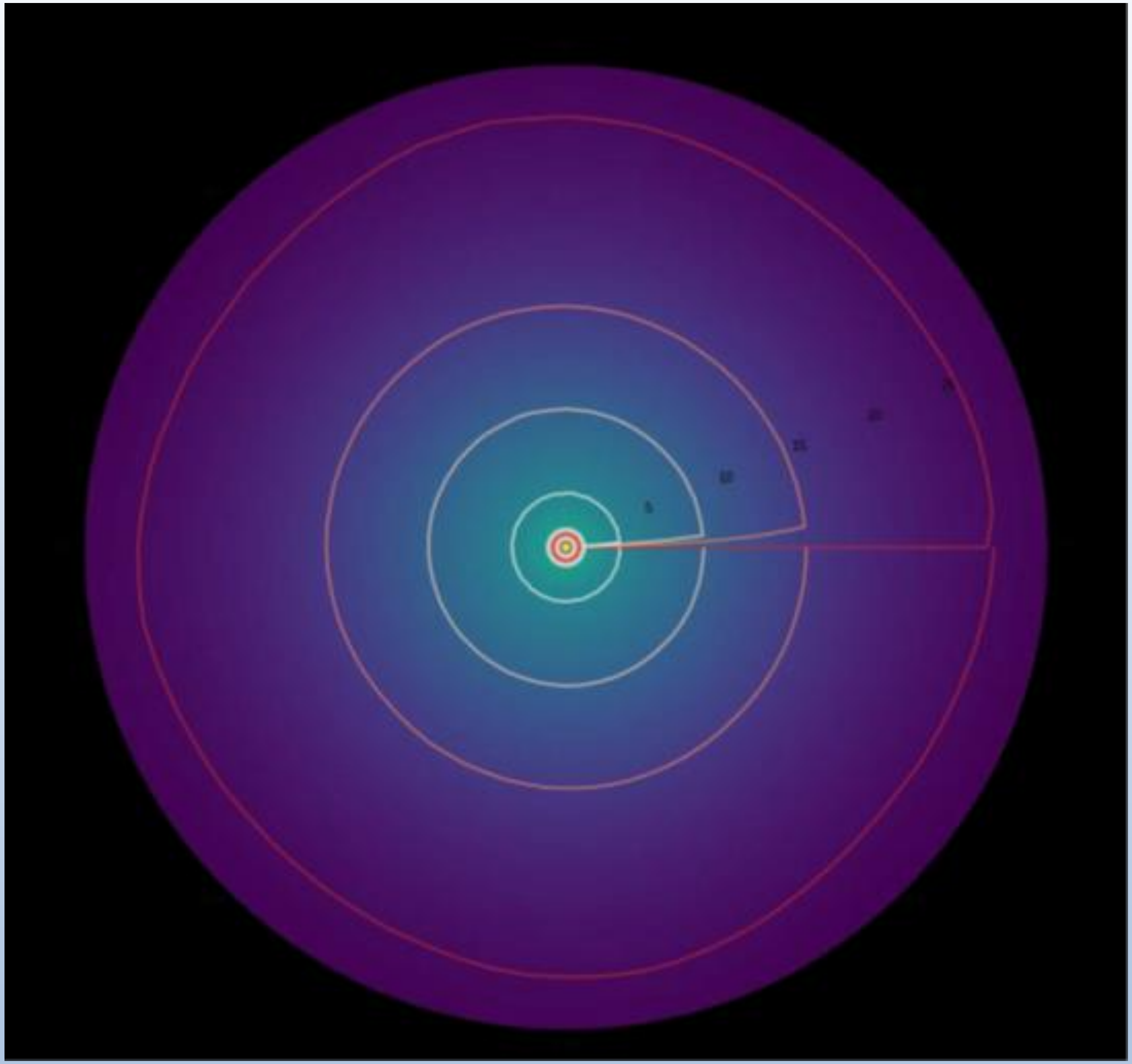
- In a persistent active liquid, the particles self-organize to form a state in which particles with similar directions of the active force come together and continue to move together [“velocity sorting”].
- Length scales of spatial correlations of particle velocities and active forces are proportional to the system size.
- Formation of two large streams flowing in opposite directions.
- Preferred directions of the large-scale flow (?).
- Growth of correlations is qualitatively different from that in the conserved XY model.

Thank you!



Spatial distribution of the angle of the coarse-grained self-propulsion force

N = 9720



Colour plots of C_vv(r) averaged over many configurations in the steady state

Summary

Dense persistent active liquids [dense collections of interacting particles with randomly assigned external forces that do not change with time] are "critical" with long-range velocity correlations and self-organization of active forces.

A theoretical description of this self-organization process is not yet available.

Why is the limit of infinite persistence time interesting?

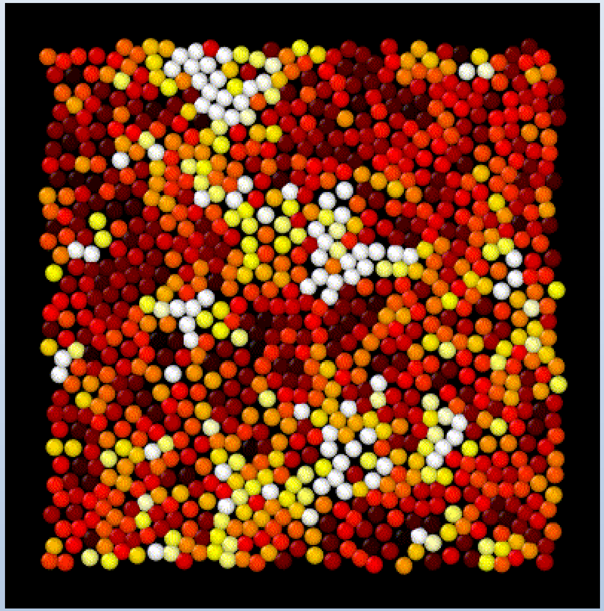
- Jammed states with force balance are possible only in this limit.
- In this limit, it is possible to define a "Hamiltonian" for the system of particles that has the property that every jammed state corresponds to a local minimum of the Hamiltonian.

$$\mathcal{H} = \sum_{i=1}^{N} \sum_{j=i+1}^{N} V(|\mathbf{r}_i - \mathbf{r}_j|) - \sum_{i=1}^{N} \mathbf{f}_i \cdot \mathbf{r}_i .$$

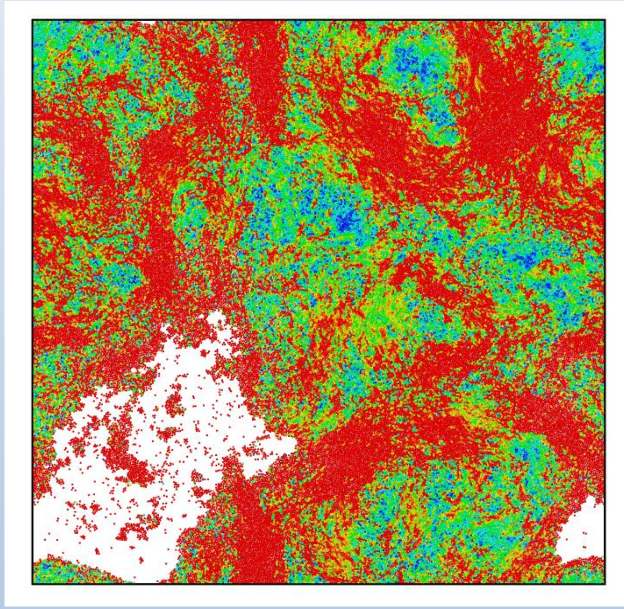
- Results for the properties of liquid and jammed states obtained in this limit may provide some understanding of the properties of the transient "flowing" and "jammed" states found in the intermittent phase for large but finite persistence time.
- The liquid and jammed states exhibit interesting properties in this limit.

Motility-induced Phase Separation?

f=3.0, N=1000



f=3.0, N=100000



Does the presence of voids for large N cutoff the growth of the correlation lengths?