Fast and Slow Liquid Phases in a System of Self-propelled Particles

Chandan Dasgupta
Department of Physics
Indian Institute of Science
Bangalore, India

Collaborators

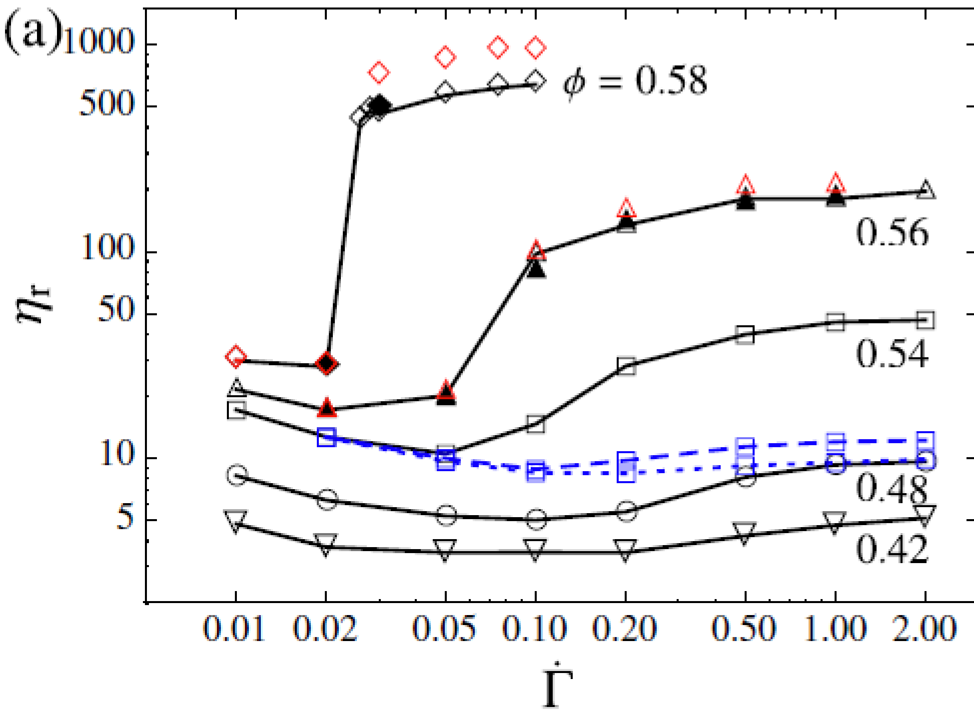
Rituparno Mandal (NCBS, Bangalore)

Pranab Jyoti Bhuyan (IISc, Bangalore)

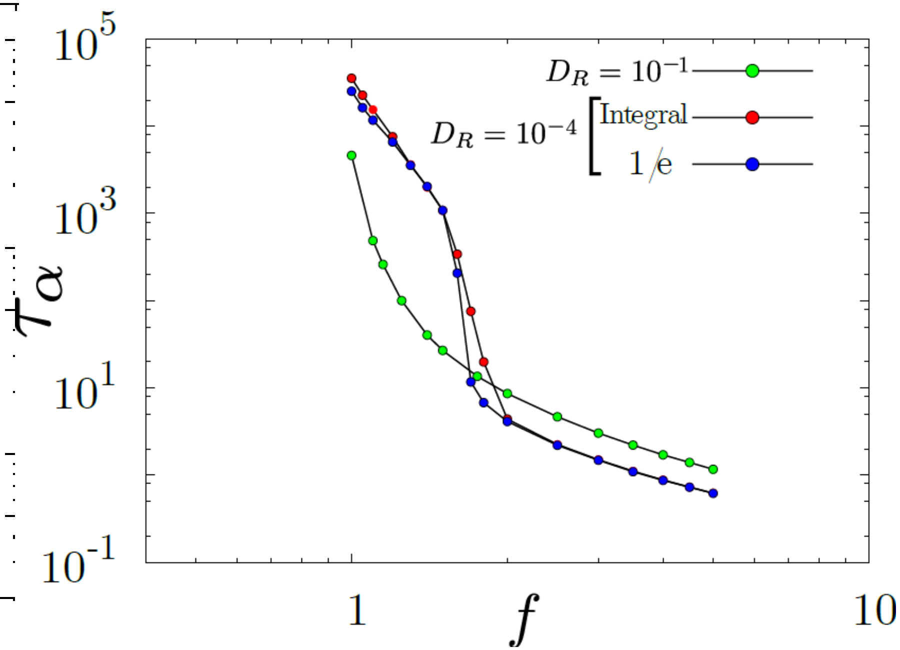
Pinaki Chaudhuri (IMSc, Chennai)

Madan Rao (NCBS, Bangalore)

Saroj Nandi, Nir Gov (Weizmann Institute)



Discontinuous Shear Thickening
[Seto *et al.* Phys Rev Lett 2013]



Transition from Fast Liquid to Slow Liquid in a 2D Active System

1. Nonequilibrium liquid-to-liquid transition with a "discontinuous" change in dynamics

Charactrization of the slow and fast liquid phases and the transition between them. Characteristic length and time scales.

2. Are the effects of the "internal" active forces on an amorphous glassy state similar to those of an external force ?

Shear-induced melting of a glass ⇔ Activity-induced fluidization of a dense system of active particles ?

Active matter (System of self-propelled objects)

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

Bacteria

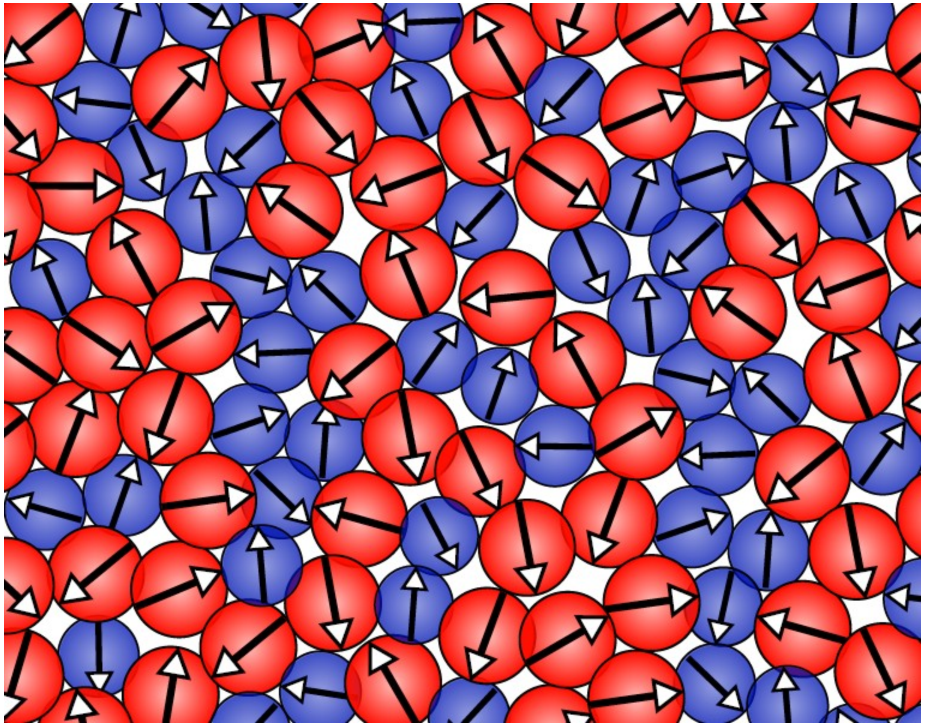
School of fish

Flock of birds

Motor proteins in cells

Interesting collective behavior

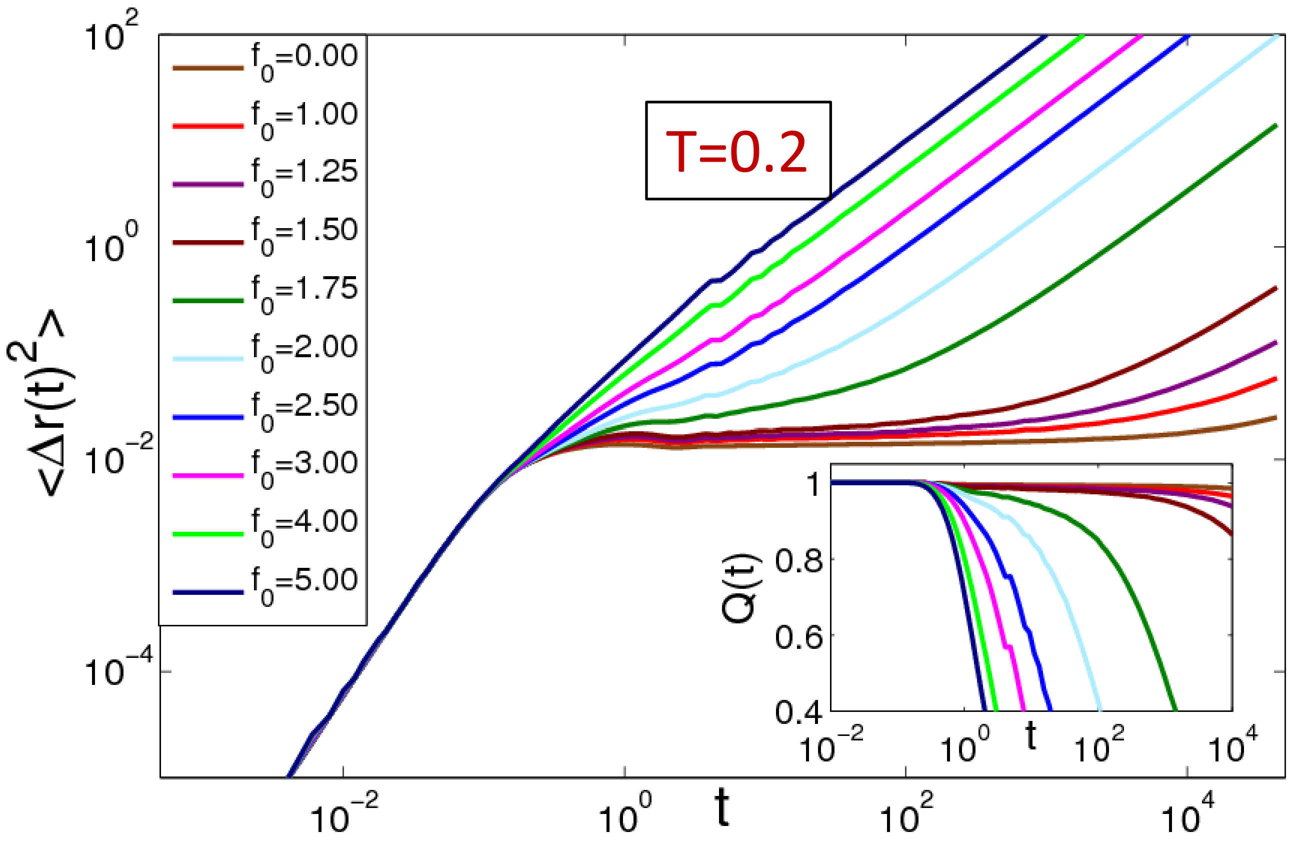
Dense system of active particles



- 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**.

Kob-Andersen Model with Activity

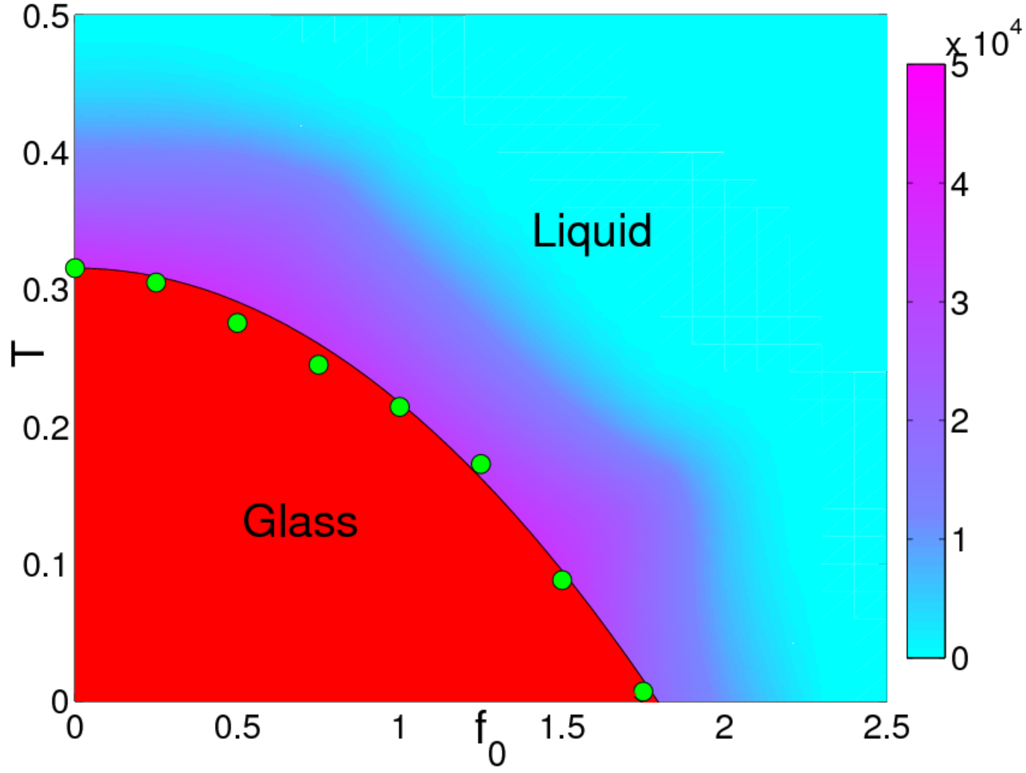
Mean-square displacement and overlap function



Short persistence time

Figure 6 : MSD for the active Kob-Andersen model for different values of the self-propulsion force f_0 for $T = 0.2$, $\rho_a = 1.0$ and $\tau_p = 4.0$. Inset: Plots of the overlap function $Q(t)$

“Phase diagram” in the temperature – activity plane



Short persistence time

Green circles: T_{VFT} obtained from VFT fits of the temperature dependence of the relaxation time

Solid line: from heuristic description in terms of an “active temperature”.

Long Persistence Times

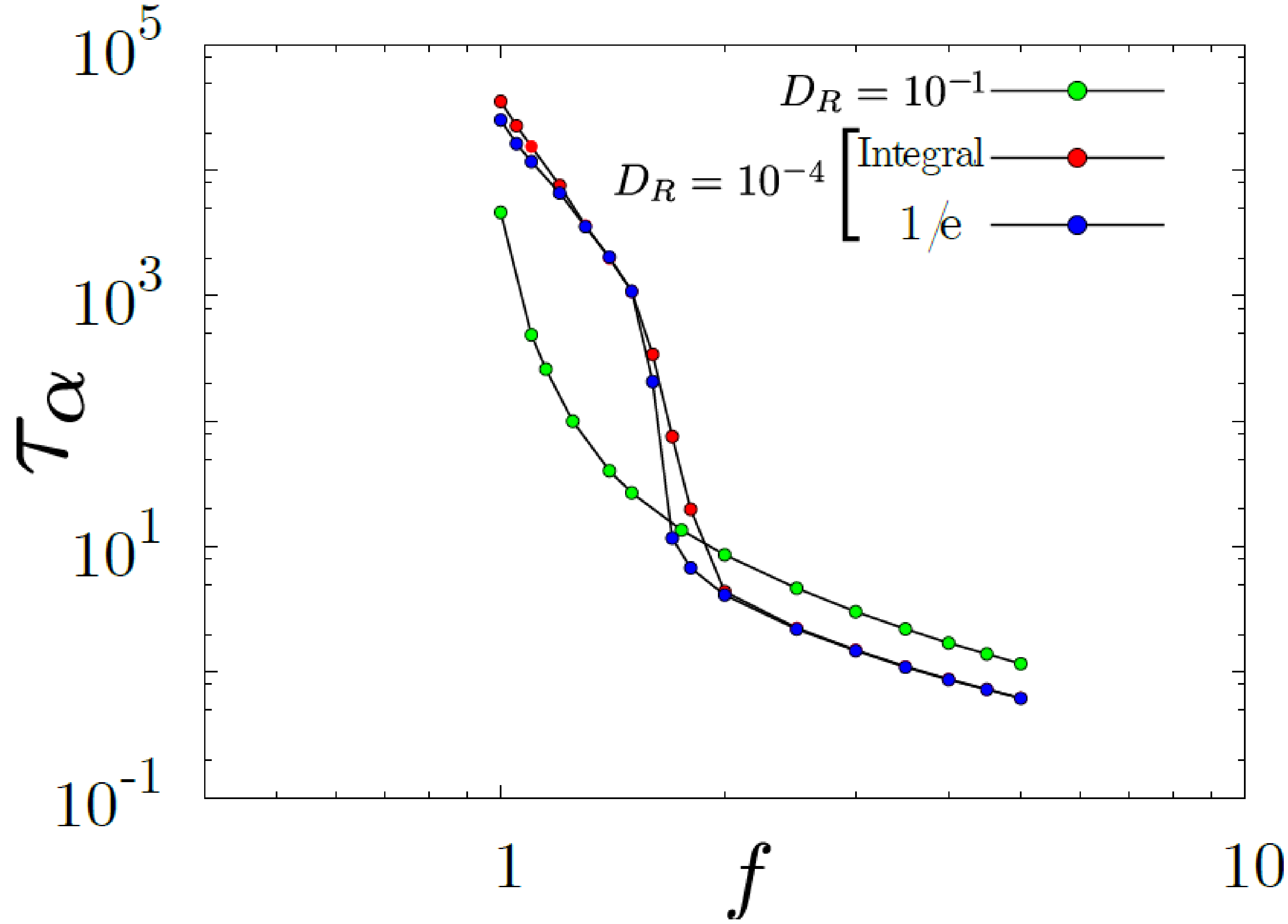
Model

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

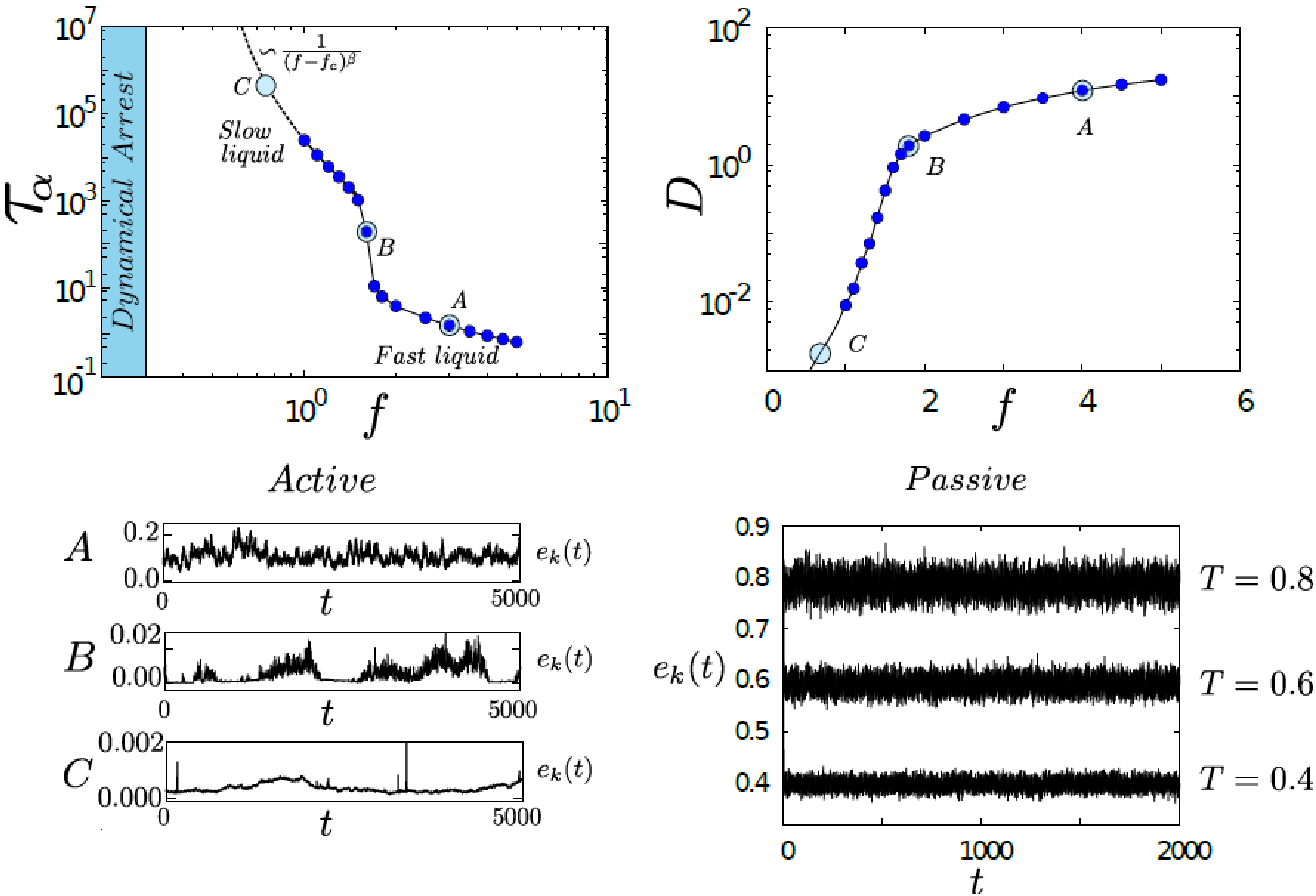
Athermal dynamics, with self-propulsion force of magnitude f acting along a specified direction $\mathbf{n}_i$ associated with particle i

$$m\dot{\mathbf{v}}_i = -\gamma \mathbf{v}_i + \sum_{j \in \mathbb{NN}} \mathbf{f}_{ij} + f\mathbf{n}_i$$

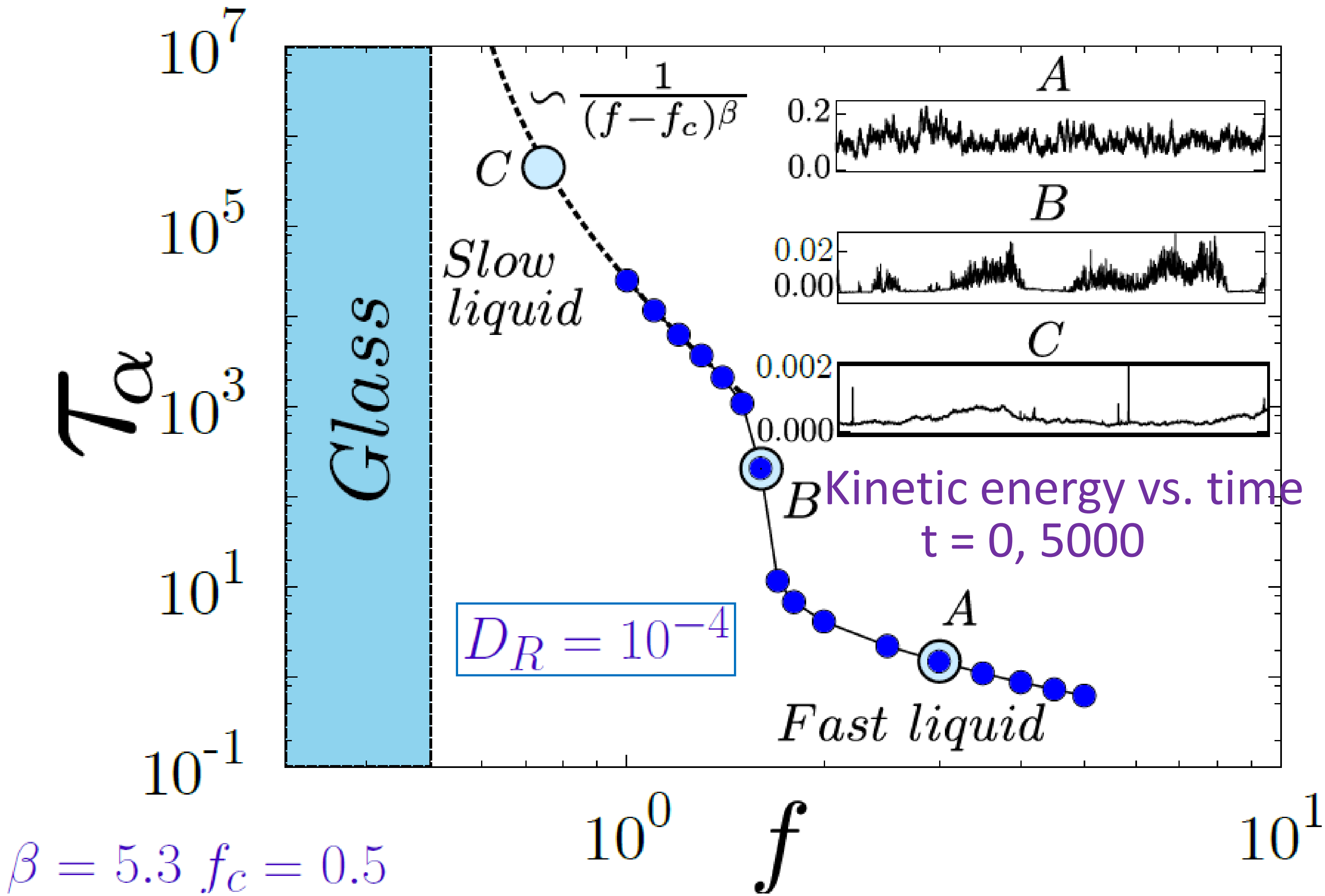
The vector $\mathbf{n}_i$ undergoes rotational diffusion with diffusion constant D_R .



Alpha relaxation time calculated from the overlap function Q(t)



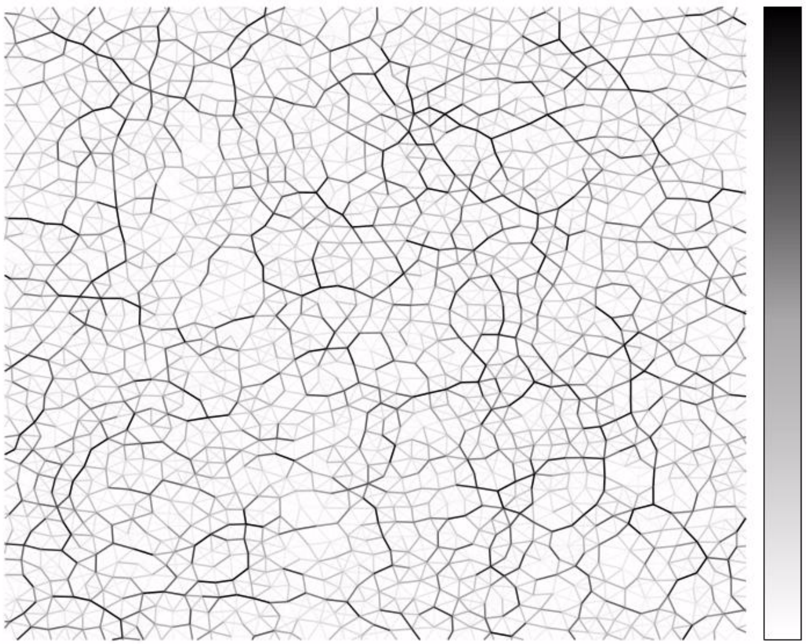
τ_α
10^7
10^5
10^3
10^1
10^{-1}
Dynamical Arrest
$\sim \frac{1}{(f-f_c)^\beta}$
C
Slow liquid
B
A
Fast liquid
10^0
f
10^1
D
10^2
10^0
10^{-2}
C
B
A
0
2
4
6
f
Active
Passive
A
0.2
0.0
$e_k(t)$
0
t
5000
B
0.02
0.00
$e_k(t)$
0
t
5000
C
0.002
0.000
$e_k(t)$
0
t
5000
0.9
0.8
0.7
0.6
0.5
0.4
$e_k(t)$
$T = 0.8$
$T = 0.6$
$T = 0.4$
0
1000
2000
t



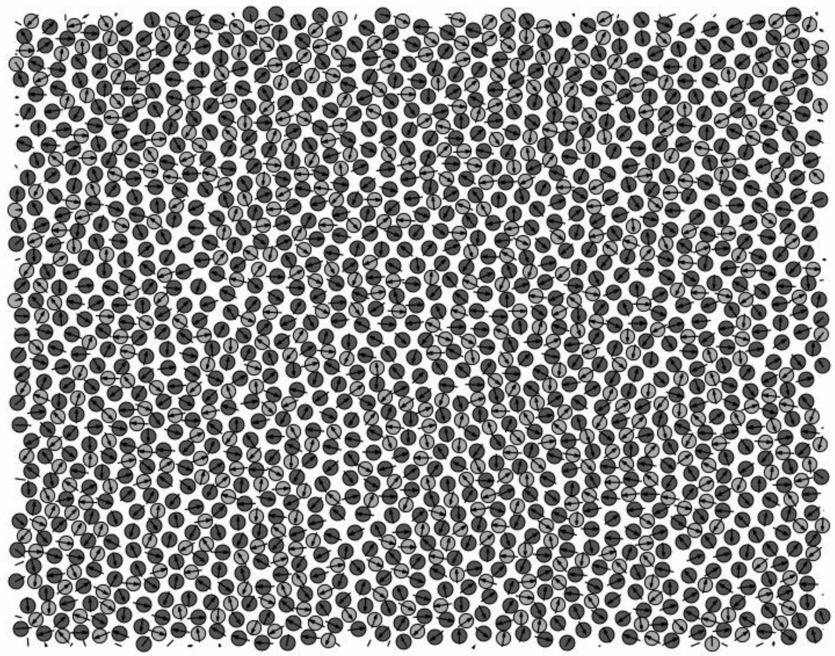
Phase diagram

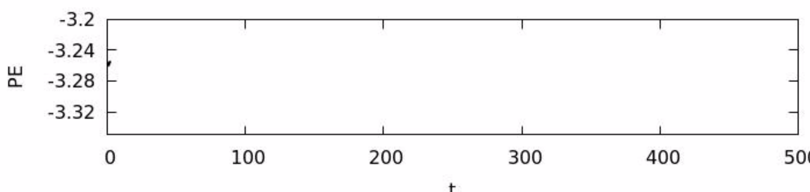
Dynamics in the "fast liquid" phase [f = 3.0]

"Force chains"

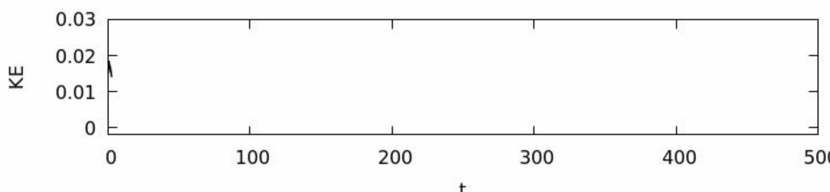


Particle positions



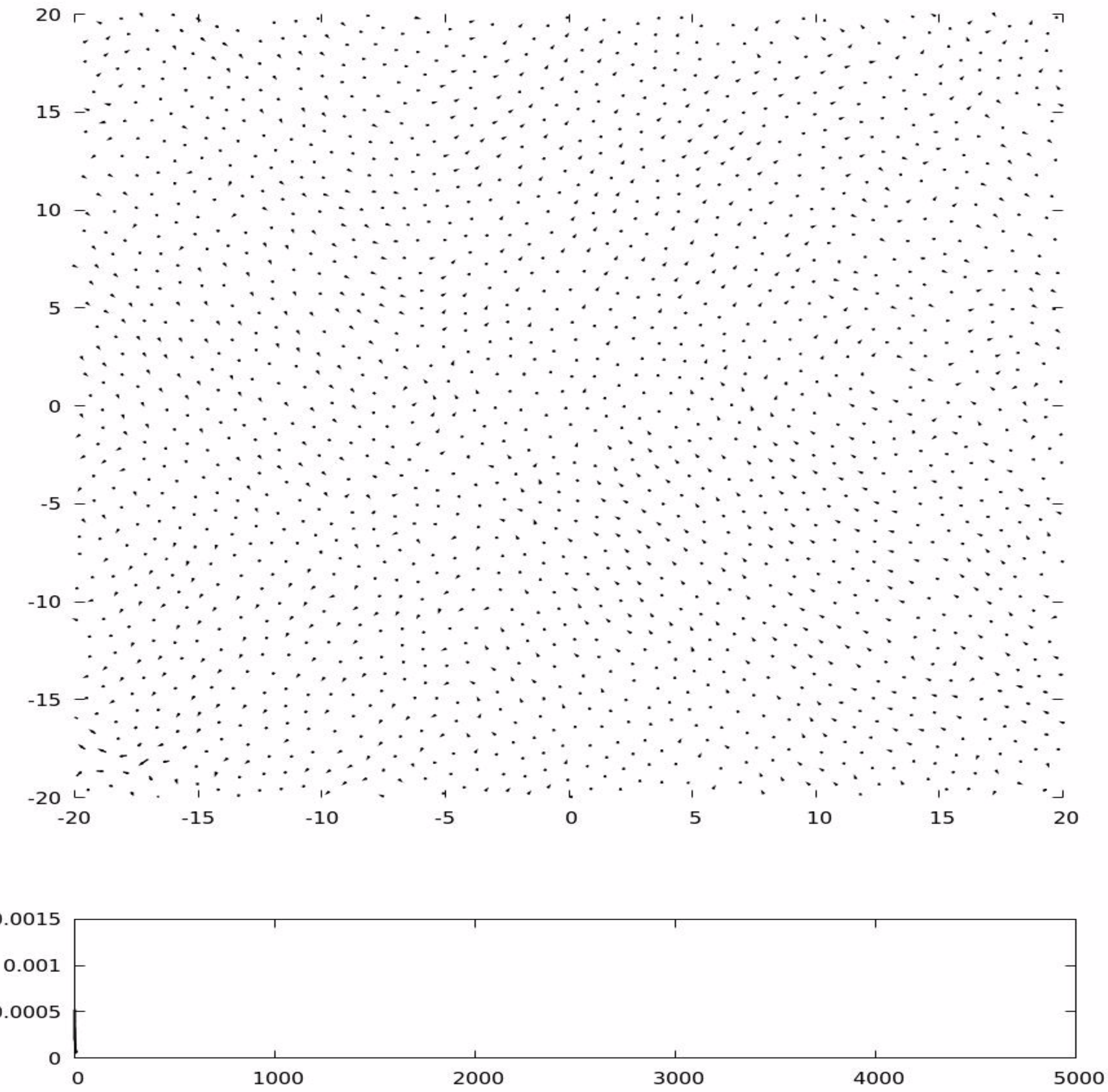


Potential energy

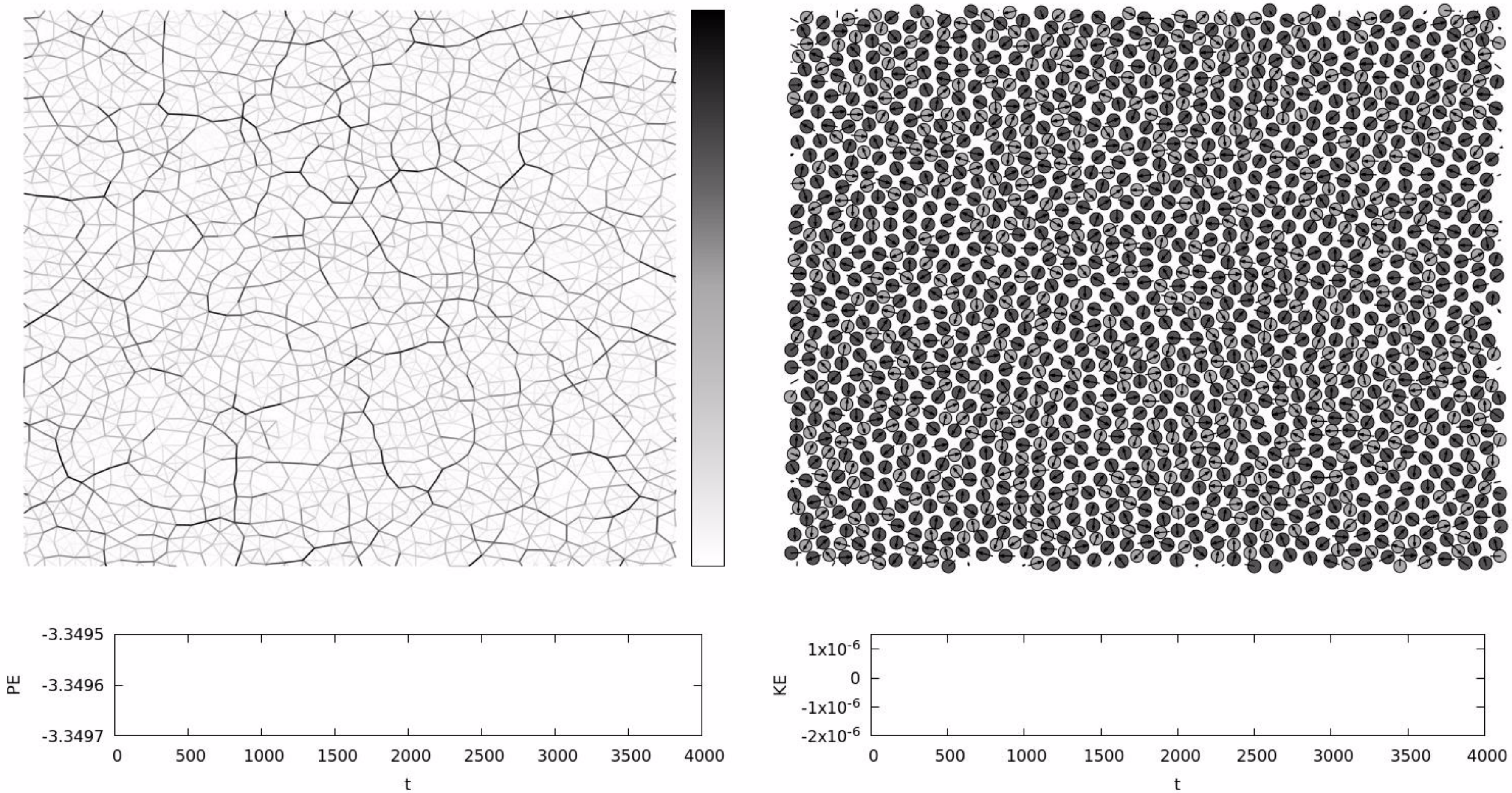


Kinetic energy

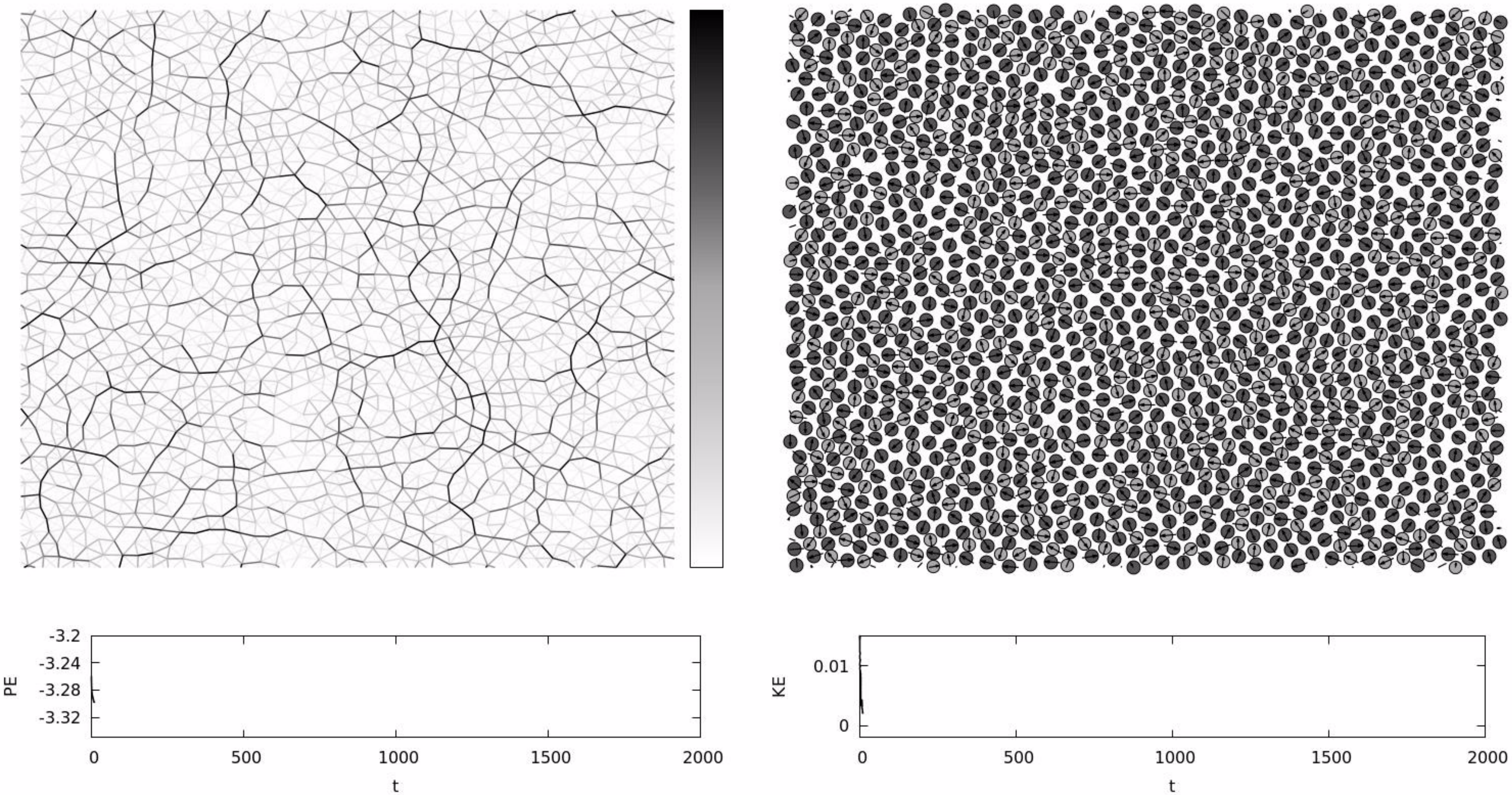
Dynamics in the "slow liquid" phase [f = 1.0]



Dynamics in the “glass” phase [f = 0.2]

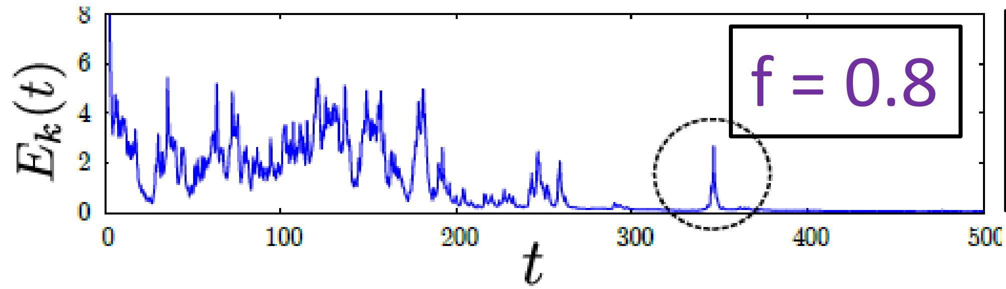


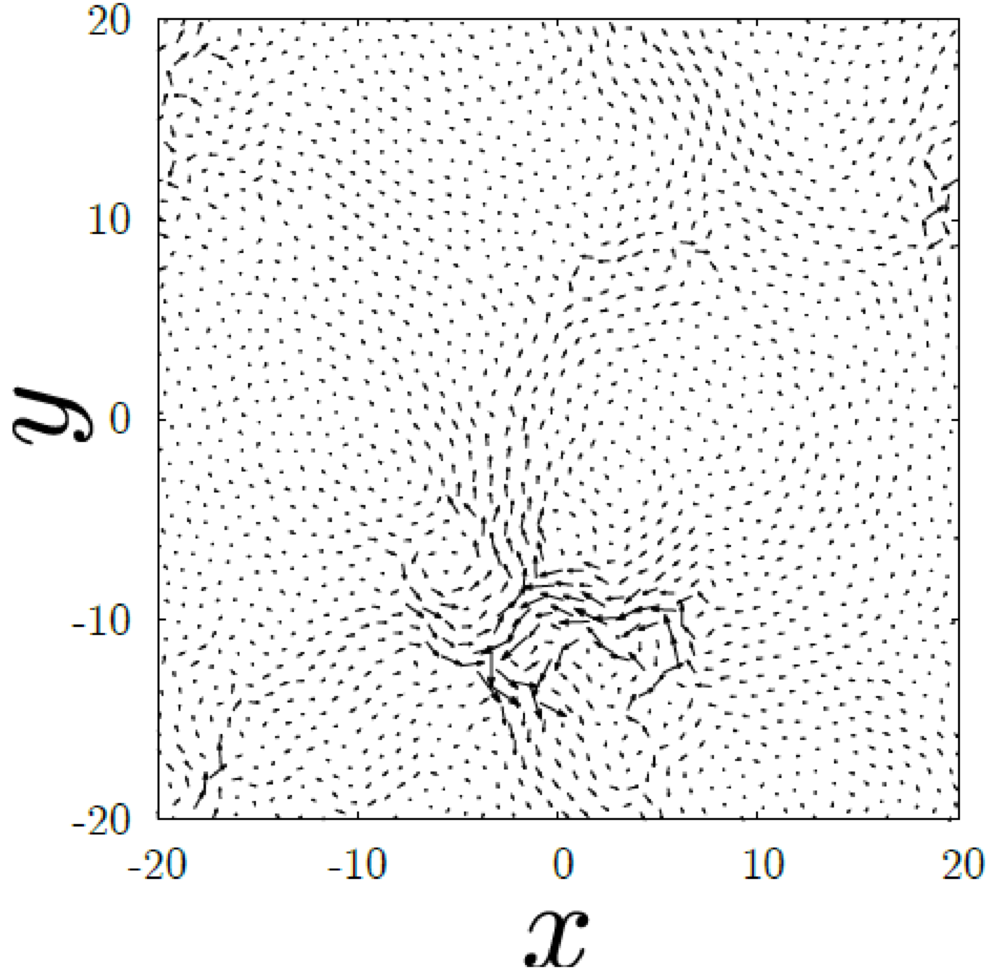
Dynamics in the intermediate phase [f = 1.4]

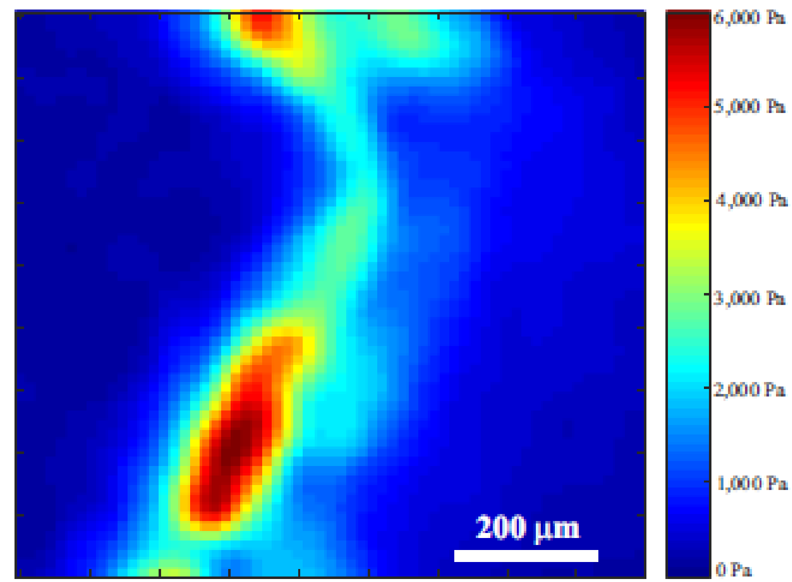


Intermittent behavior

Displacement of particles in an "avalanche"

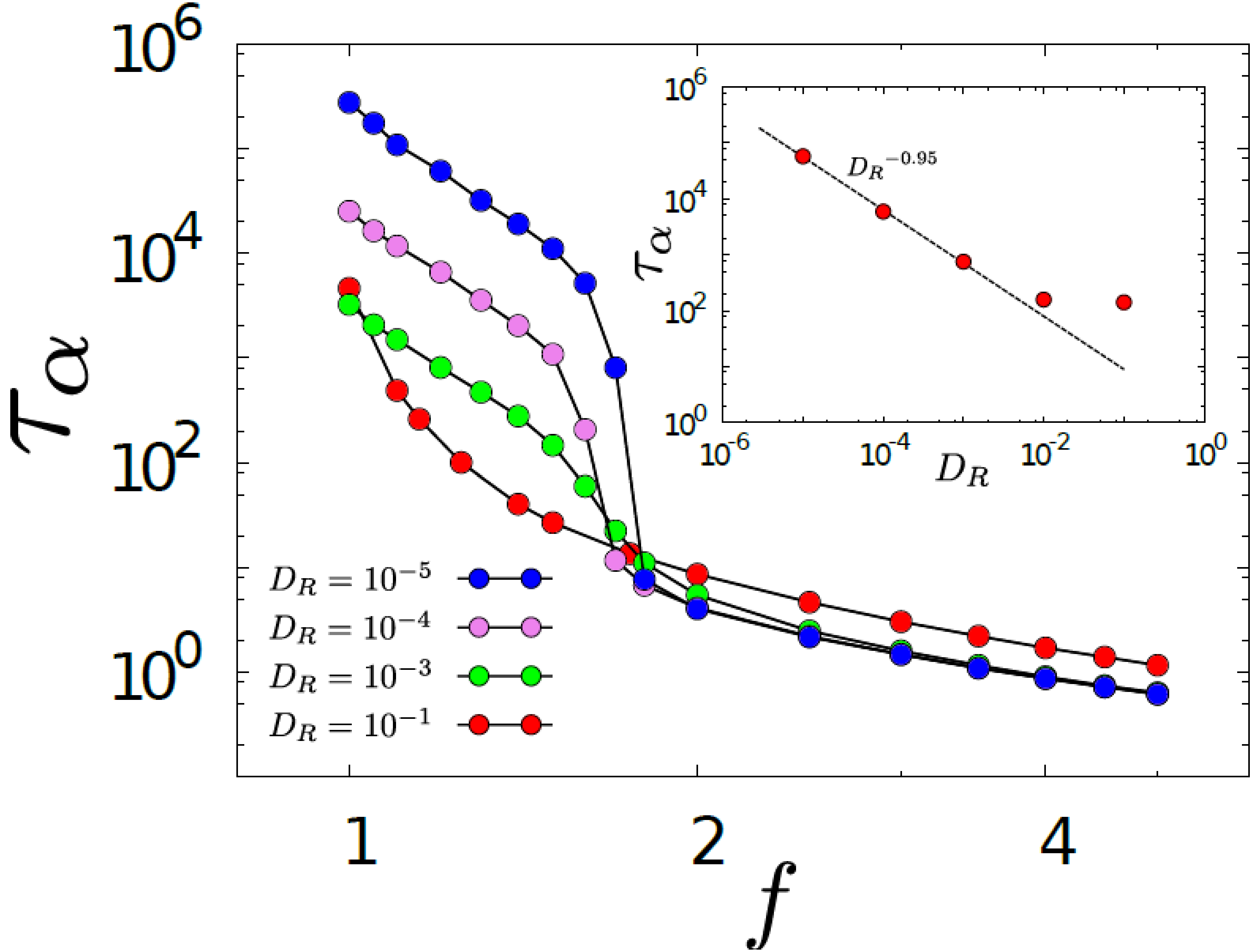






Rathee *et al*, PNAS 2017

Dependence on the value of the persistence time



Transition or crossover between fast and slow liquid phases?

Overlap function (Lacevic *et al.*, 2003)

$Q(t) = \sum_i w(|\mathbf{r}_i(0) - \mathbf{r}_i(t)|)$ where
$w(r) = 1$ if $r \leq a$, $= 0$ otherwise.

Overlap Function $q(t) = \frac{1}{N}\langle Q(t) \rangle$

Self part of the density autocorrelation function

$\rho(\mathbf{r}, t) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i(t))$

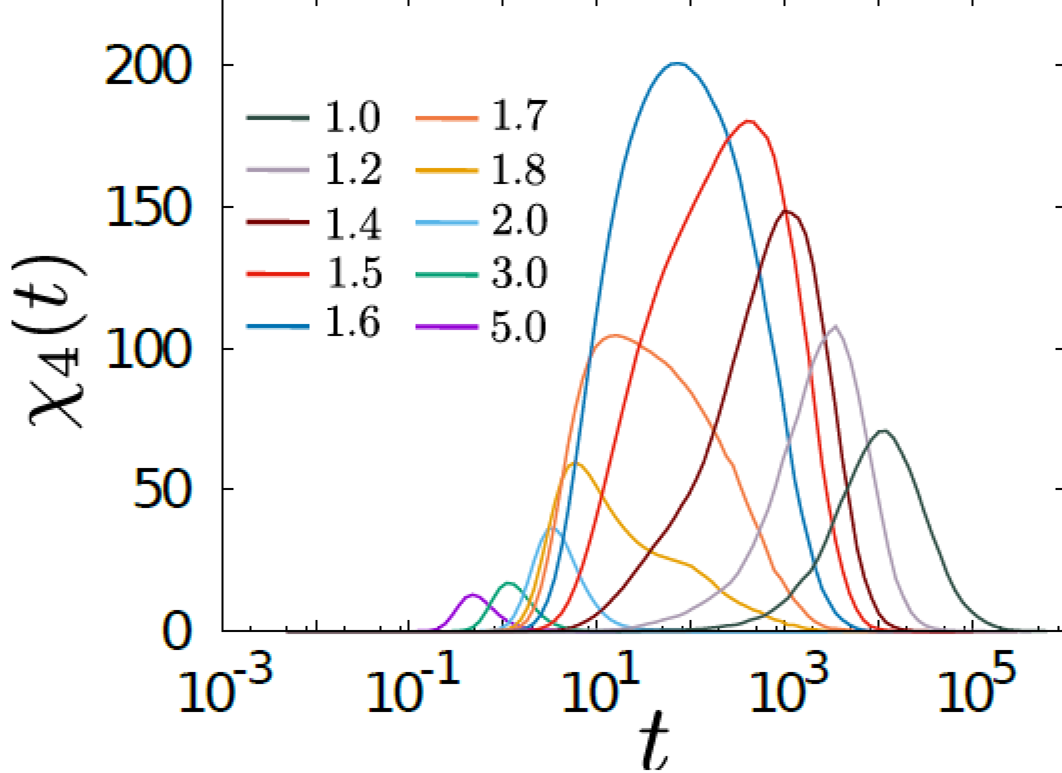
$\rho(\mathbf{r}, 0)\rho(\mathbf{r}, t) = \sum_{i,j} \delta(\mathbf{r} - \mathbf{r}_i(0))\delta(\mathbf{r} - \mathbf{r}_j(t)),$

"Self"-part $(i = j)$:

$\sum_i \delta(\mathbf{r} - \mathbf{r}_i(0))\delta(\mathbf{r}_i(0) - \mathbf{r}_i(t))$

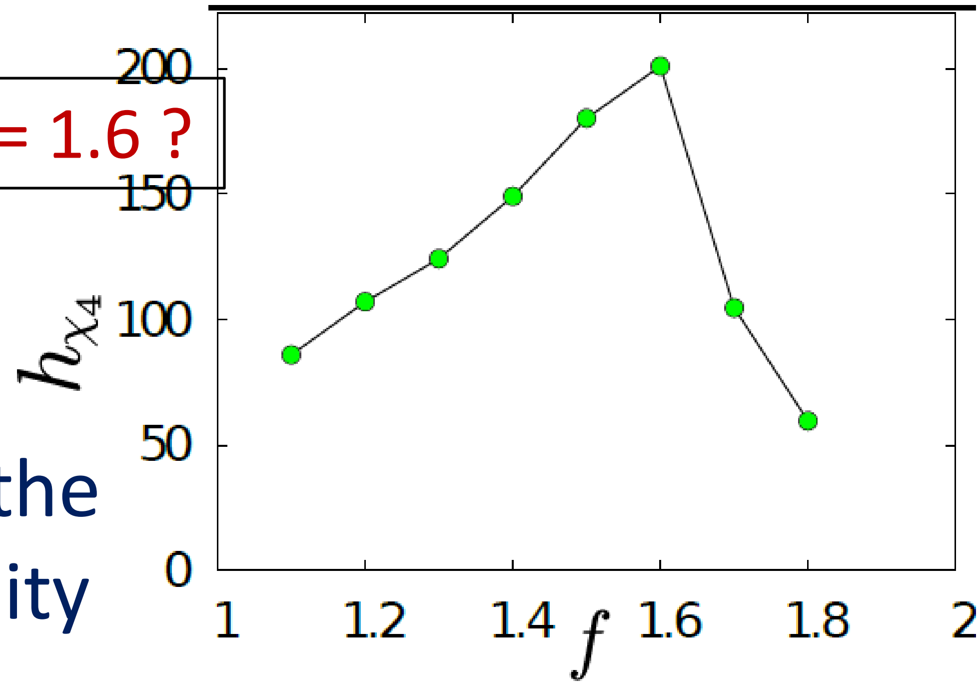
Four-point susceptibility (CD *et al.*, 1991)

$\chi_4(t) = \frac{1}{N}[\langle Q^2(t) \rangle - \langle Q(t) \rangle^2]$

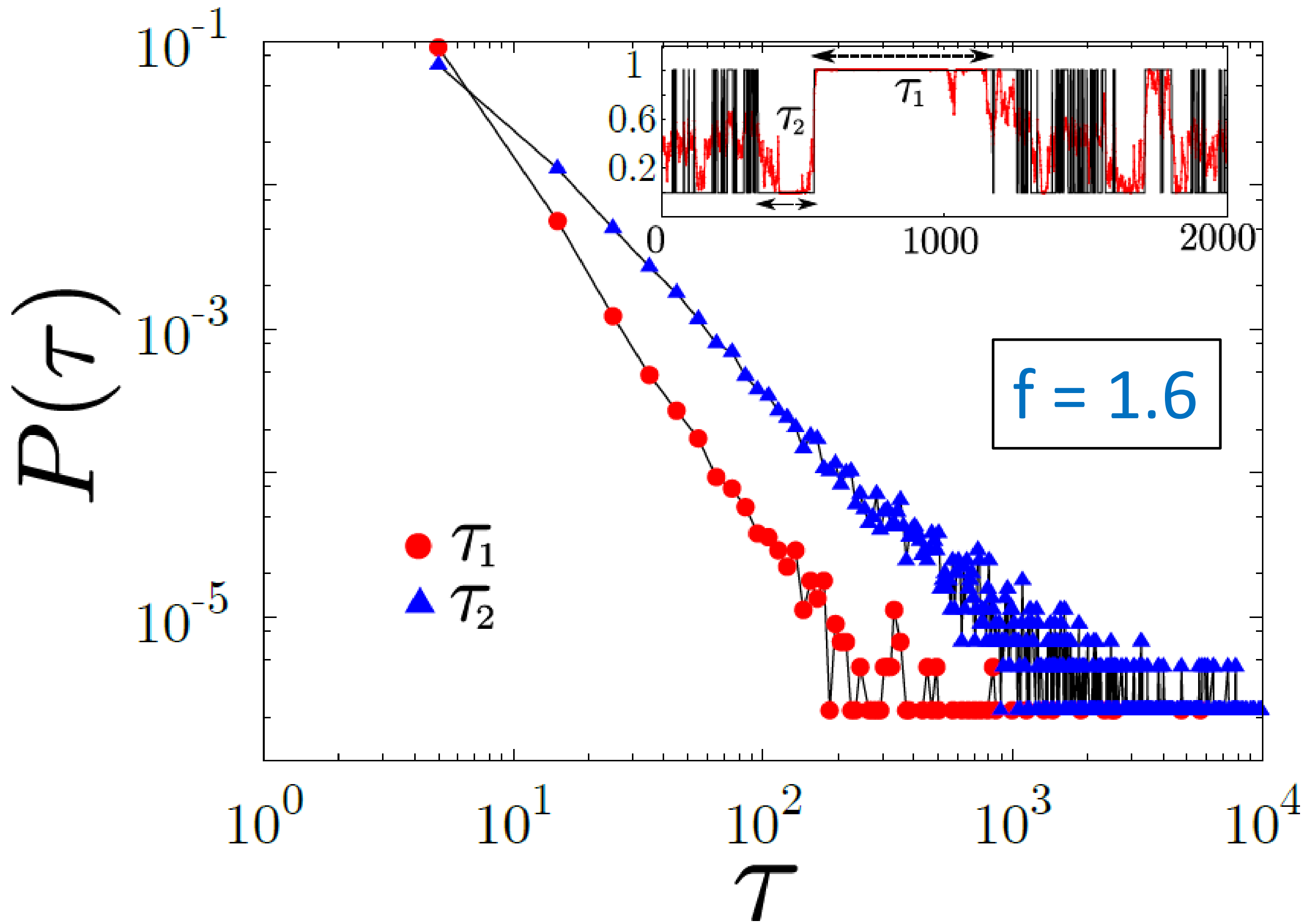


Four-point susceptibility

Transition or crossover near f = 1.6 ?



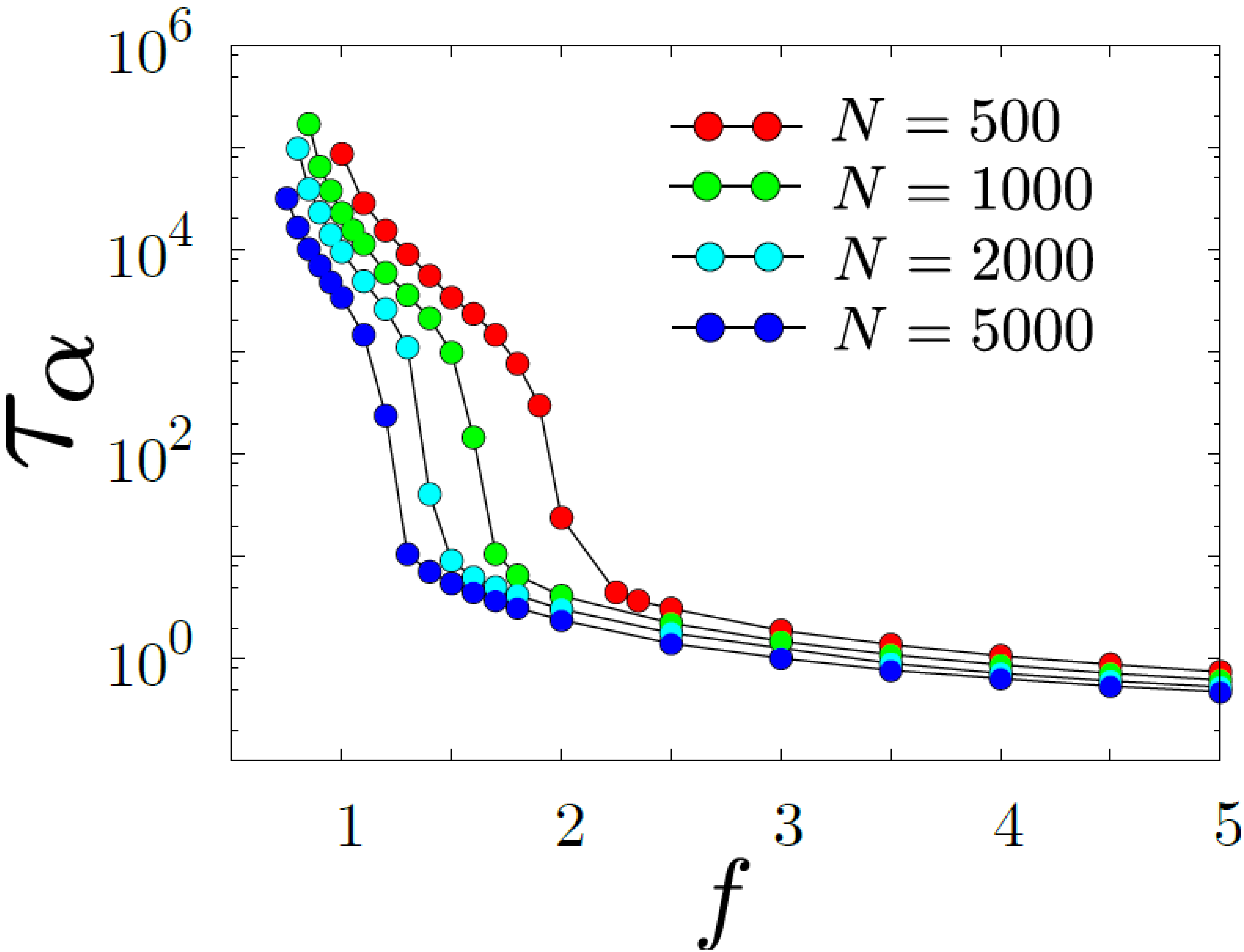
Height of the peak of the four-point susceptibility



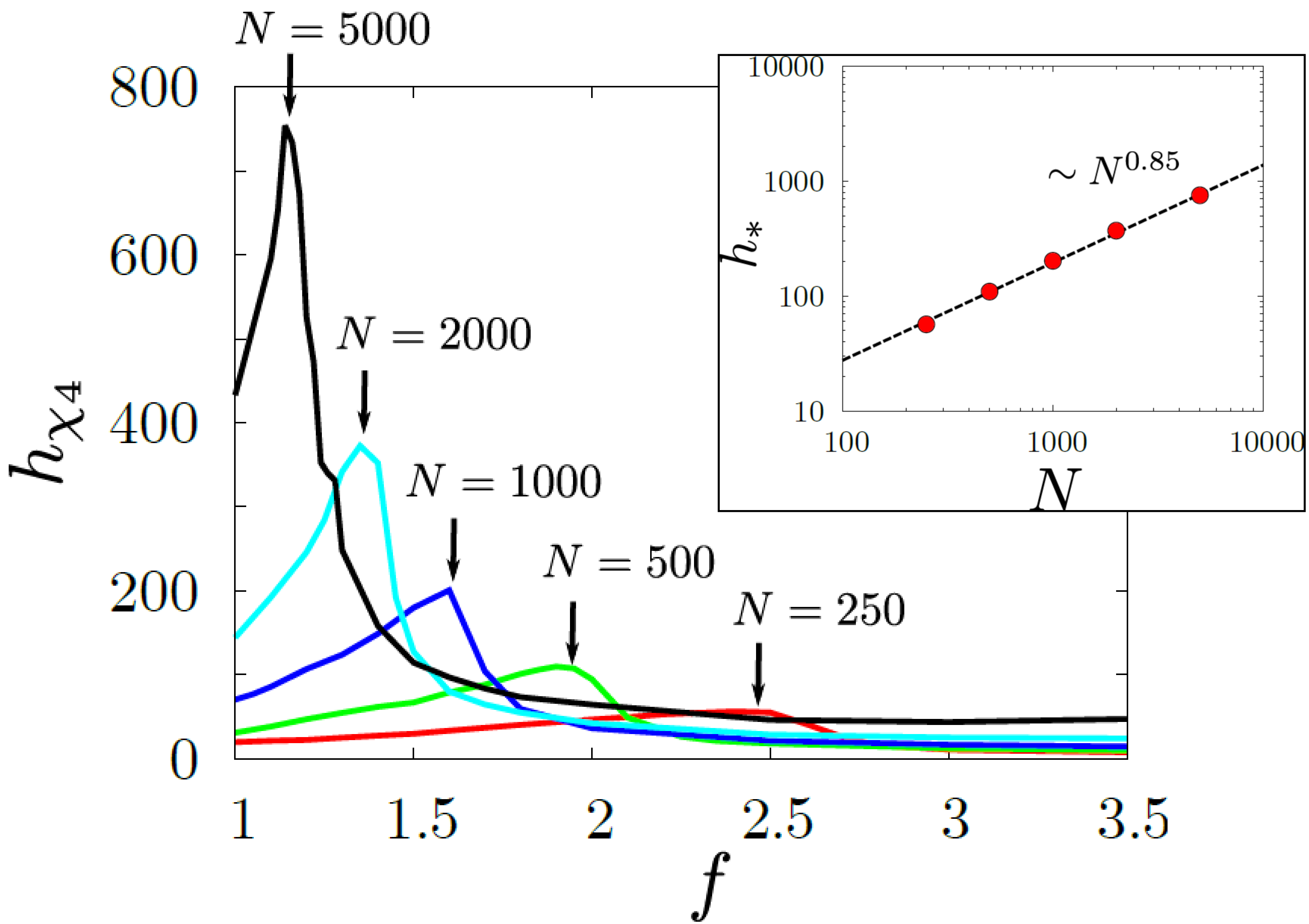
Transition or crossover near f = 1.6 ?

Distributions of time intervals of states with low and high level of rearrangement

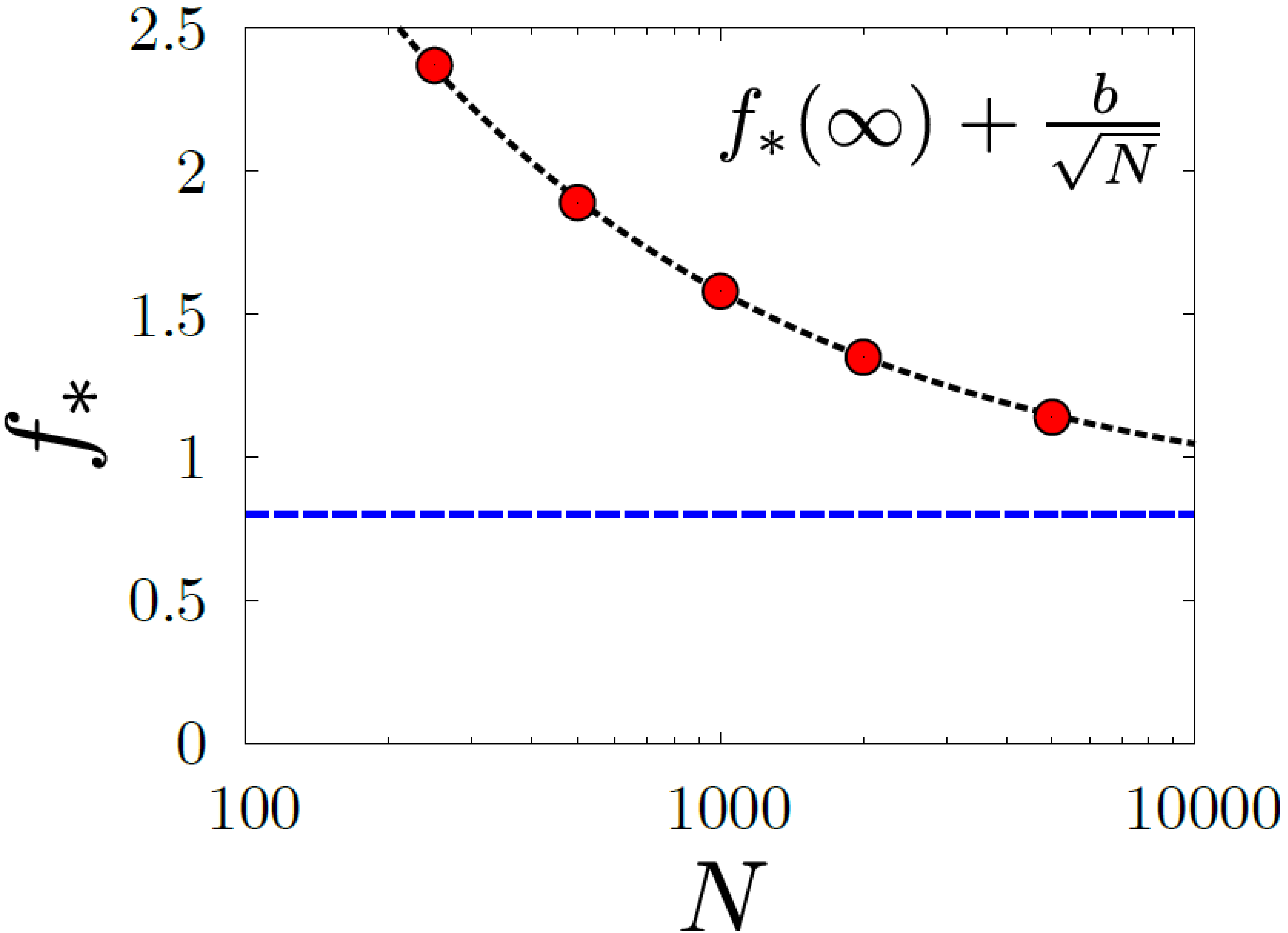
Dependence on System size



Dependence on System size



Dependence on System size



Conclusions:

- An athermal system with self-propulsion forces with **large persistence time** exhibits a transition (crossover?) from a **fast liquid** phase to a **slow liquid** phase as the strength of the active force is decreased.

- The slow liquid phase exhibits **intermittency** with "**avalanches**" separated by quiescent periods.

- The typical time interval between successive avalanches increases as the strength of the active force is decreased, leading to a **glass phase** for small values of the active force.

Similarities with externally driven amorphous materials?

Intermittent aging in metallic glasses

Questions:

External Driving (e.g. Shear): Macroscopic, Asymmetric, Flow.
Internal Driving (Active Systems): Microscopic, Symmetric, No Centre-of -Mass Motion. Do they have similar effects in liquids and amorphous systems?

Discontinuous Shear Thinning?

Discontinuous Shear Thickening (DST) in a system of self-propelled particles with friction?

Growing length and time scales near DST?