Active dumbbells

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Work in collaboration with

D. Loi & S. Mossa (2007-2009) and

G. Gonnella, G.-L. Laghezza, A. Lamura, A. Mossa & A. Suma (2013-2015)

Kyoto, Japan, August 2015

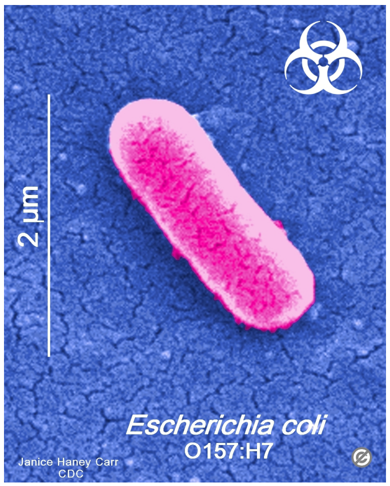
Motivation & goals

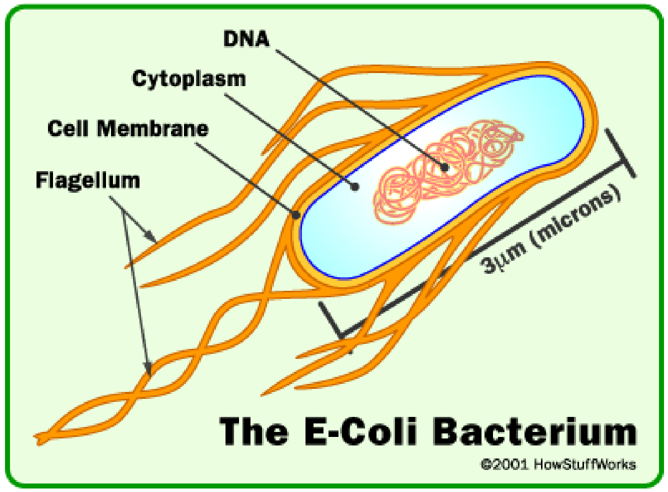
Active dumbbell system

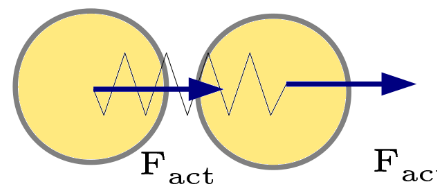
- Reason for working with this model
- Main properties of the model - phase diagram
- Translational and rotational collective motion
- Dynamics of tracers in complex environments revisited.
- Effective temperatures out of equilibrium

Active dumbbell

Diatomic molecule - toy model for bacteria







Escherichia coli - Pictures borrowed from internet.

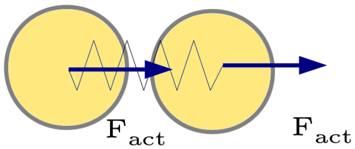
Bacteria colony

Active matter

Rabani, Ariel and Be'er 13

Active dumbbells

Diatomic molecule



Two spherical atoms with diameter $\sigma_{\rm d}$ and mass $m_{\rm d}$

Massless spring modelled by a finite extensible non-linear elastic force between the atoms $\mathbf{F}_{\rm fene} = -\dfrac{k\mathbf{r}}{1 - r^2/r_0^2}$ with an additional repulsive contribution (WCA) to avoid colloidal overlapping.

Polar active force along the main molecular axis $\mathbf{F}_{\rm act} = F_{\rm act}\,\hat{\mathbf{n}}$.

Purely repulsive interaction between colloids in different molecules.

Langevin modelling of the interaction with the embedding fluid:

isotropic viscous forces, $-\gamma \mathbf{v}_i$, and independent noises, η_i, on the beads.

Directional motion (active) and effective torque (noise)

Active dumbbells

Control parameters

Number of dumbbells N and box volume S in two dimensions:

packing fraction $\boxed{\phi = \frac{\pi\sigma_{\rm d}^2 N}{2S}}$

Energy scales:

Active force work $F_{\rm act}\sigma_{\rm d}$

thermal energy k_BT

Péclet number $\boxed{\text{Pe} = \frac{2F_{\rm act}\sigma_{\rm d}}{k_BT}}$

Active force $F_{\rm act}\sigma_{\rm d}/\gamma$

viscous force $\gamma\sigma_{\rm d}^2/m_{\rm d}$

Reynolds number $\boxed{\text{Re} = \frac{m_{\rm d}F_{\rm act}}{\sigma_{\rm d}\gamma^2}}$.

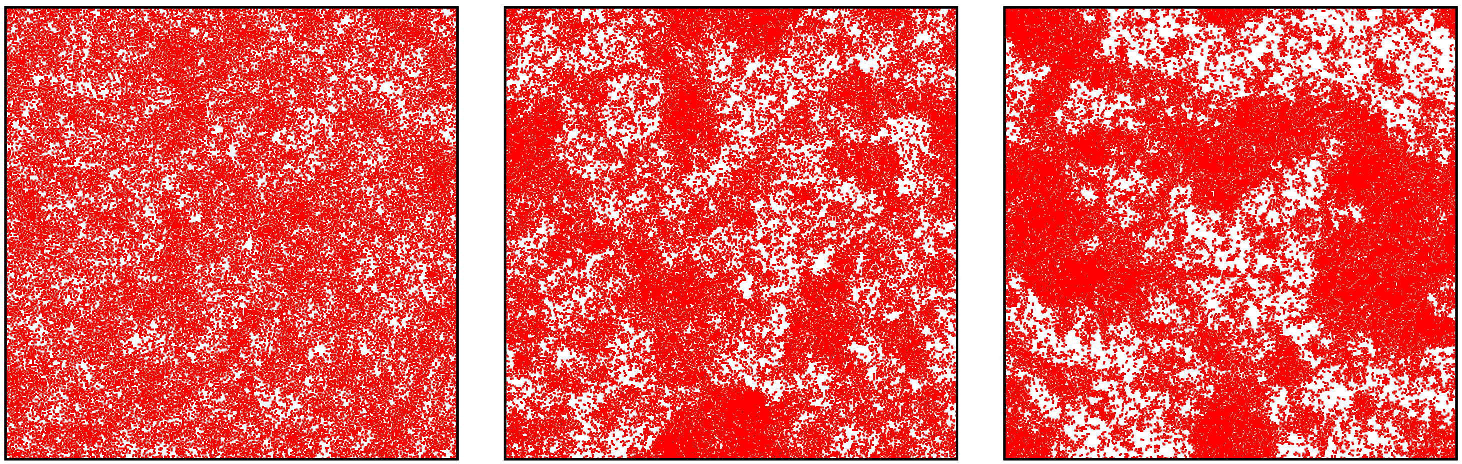
We keep the parameters in the harmonic (fene) and Lennard-Jones (repulsive) potential fixed. Stiff molecule limit: vibrations frozen.

We study the ϕ, $F_{\rm act}$ and k_BT dependencies. Pe $\in [0,40]$, Re $< 10^{-2}$

Active dumbbells

Phase segregation

Fixed packing fraction ϕ and fixed activity $F_{\rm act}$, vary $k_B T$



$k_B T = 0.01$ $\quad$ $k_B T = 0.003$ $\quad$ $k_B T = 0.001$

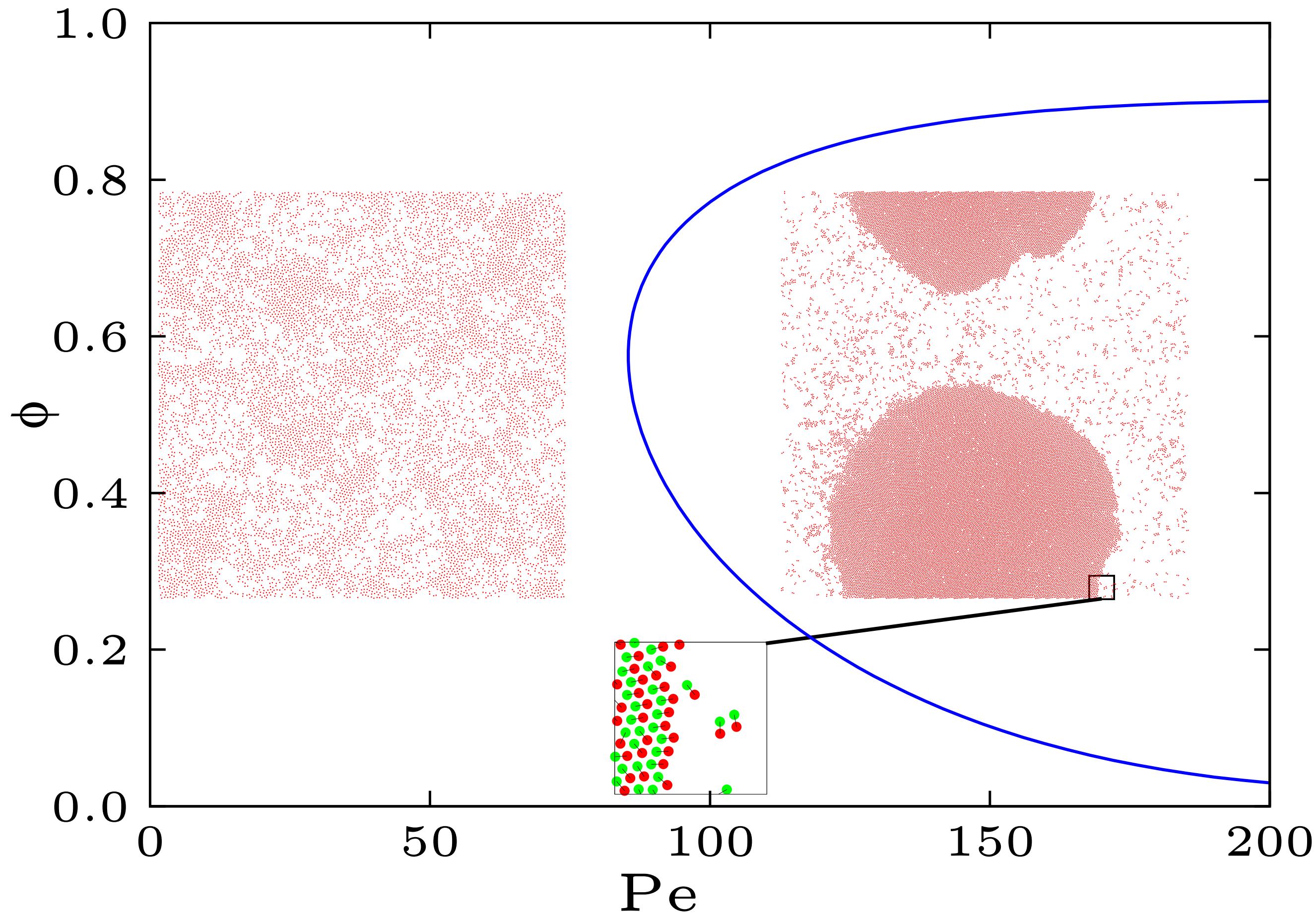
Mixed $\quad$ Large density fluctuations $\quad$ Segregation

$$\mathrm{Pe} = \frac{2F_{\rm act}\sigma_{\rm d}}{k_B T} \text{ increases} \rightarrow$$

Gonnella, Lamura & Suma 13

Active dumbbells

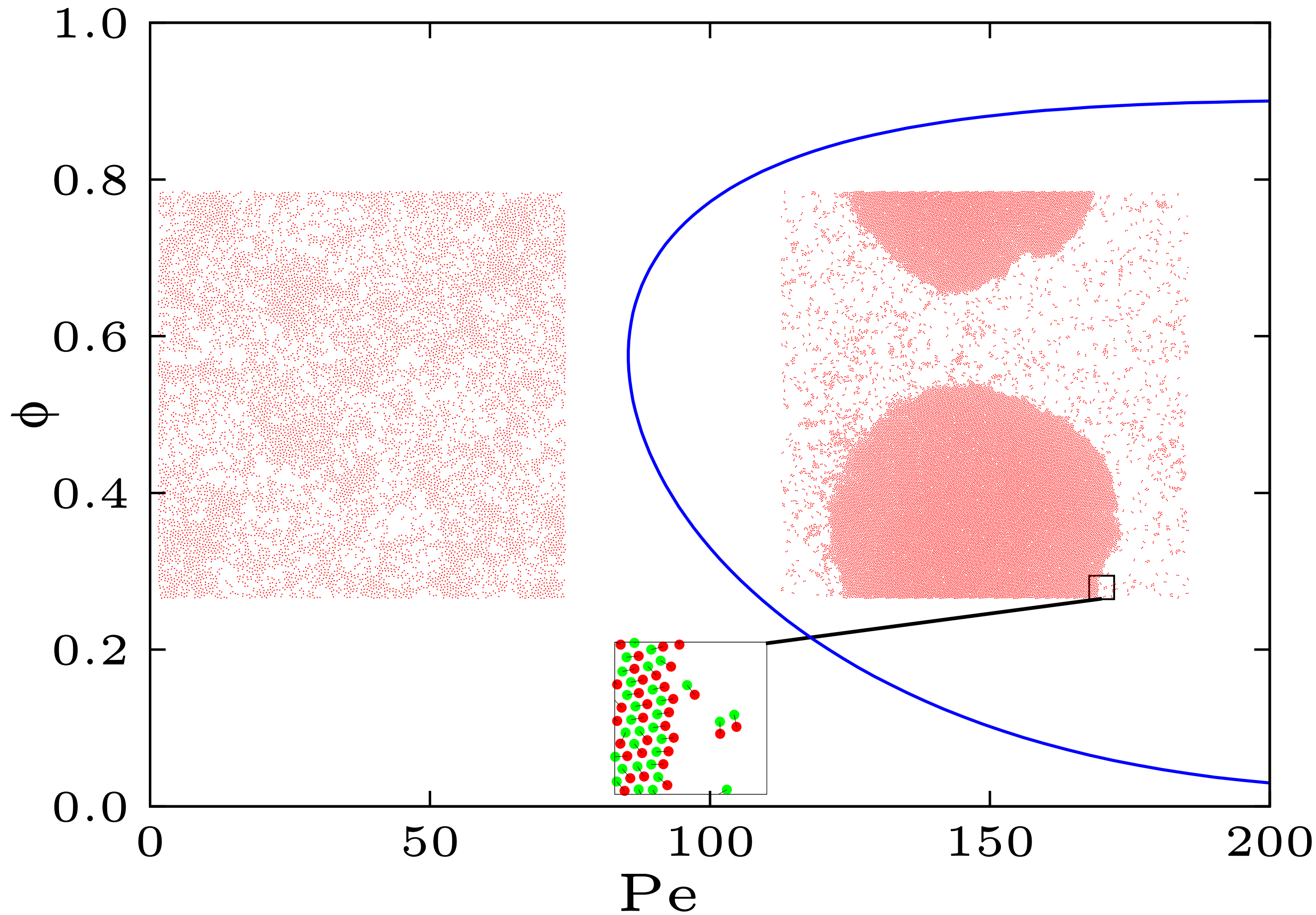
Phase diagram : from the distribution of local dumbbell density



Mechanism for aggregation: note the head-tail alignment in the cluster.

Active dumbbells

Phase diagram



Focus on the dynamics in the homogeneous phase ; vary ϕ and Pe.

Single molecule limit

Active force switched-on, $F_{\mathrm{act}} \neq 0$

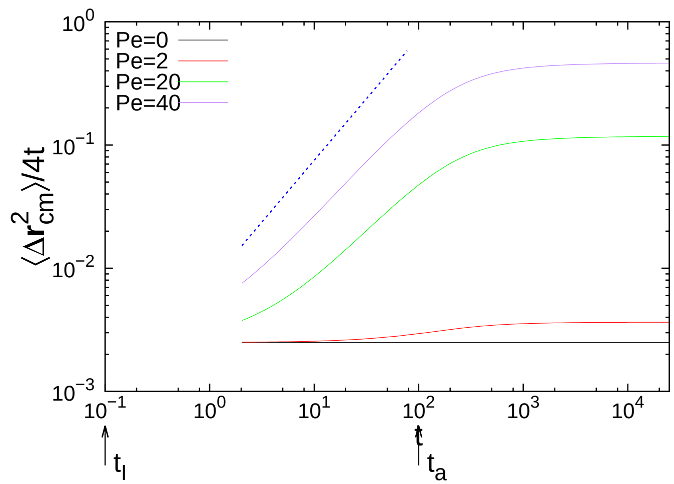
ballistic $\longrightarrow$ diffusive $\longrightarrow$ ballistic $\longrightarrow$ diffusive

- The dynamics is accelerated by F_{act} and a new ballistic regime in the centre-of-mass translational motion appears at $t^* = 16 t_a/\mathrm{Pe}^2$

- Ballistic to diffusive crossover of the cm motion at $t_a = \gamma\sigma_{\mathrm{d}}^2/(2k_BT)$

  Note that $t_a \to \infty$ at $k_BT \to 0$.

- The diffusion constant is $D_A = k_BT/(2\gamma)\,(1 + \mathrm{Pe}^2)$



$$\langle [\mathbf{r}_{\mathrm{cm}}(t+t_0) - \mathbf{r}_{\mathrm{cm}}(t_0)]^2 \rangle$$

Single molecule limit

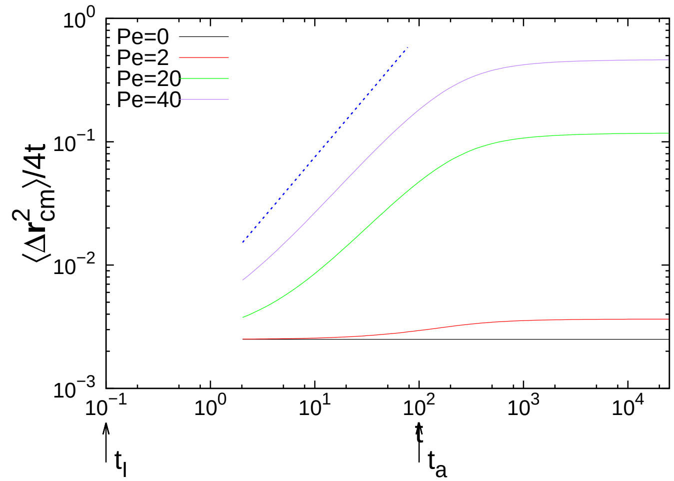
Active force switched on, $F_{\rm act} \neq 0$

- The dynamics is accelerated by $F_{\rm act}$ and a new ballistic regime in the centre-of-mass translational motion appears at $t^* = 16 t_a/\mathrm{Pe}^2$

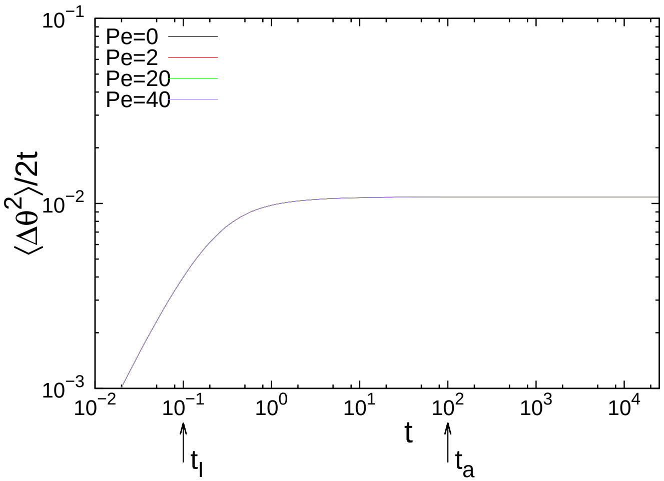
- Ballistic to diffusive crossover of the cm motion at $t_a = \gamma \sigma_{\rm d}^2/(2 k_B T)$

  Note that $t_a \to \infty$ at $k_B T \to 0$.

- The rotational motion is not affected by the longitudinal active force.



$$\langle [\mathbf{r}_{\rm cm}(t+t_0) - \mathbf{r}_{\rm cm}(t_0)]^2 \rangle$$

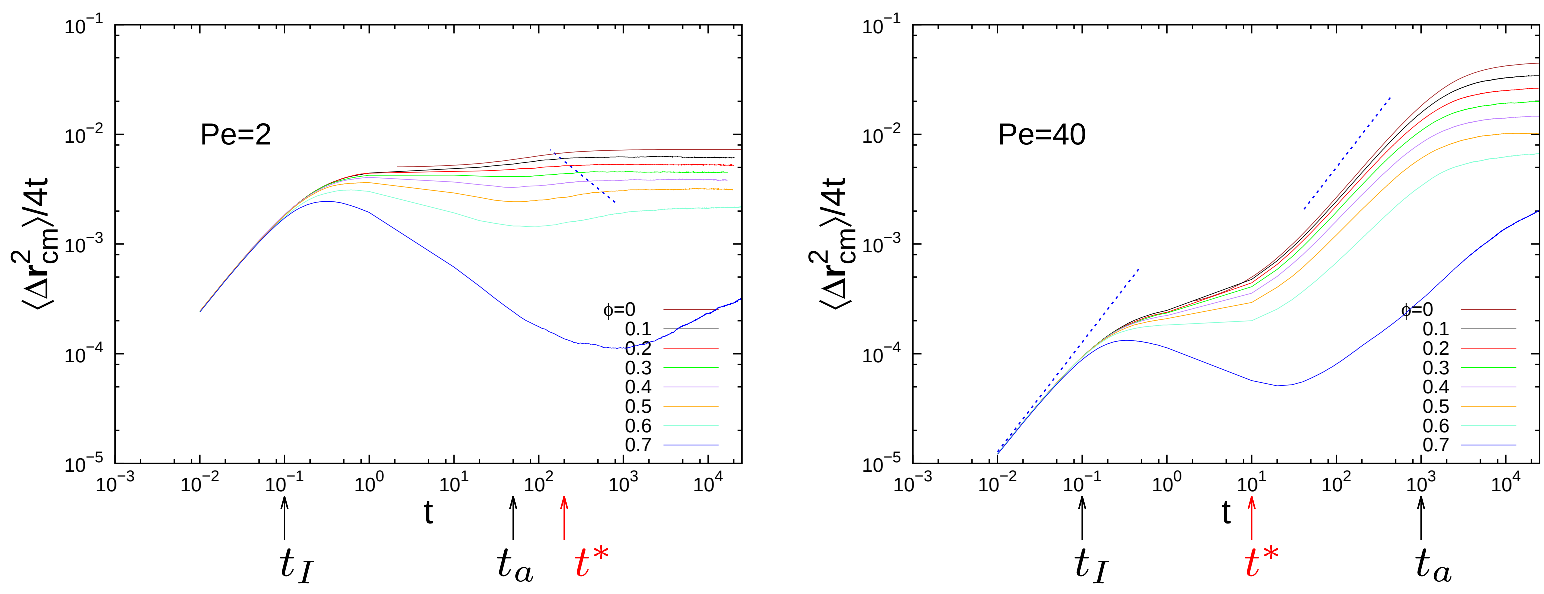


$$\langle [\theta(t+t_0) - \theta(t_0)]^2 \rangle$$

Finite density system

Centre-of-mass mean-square displacement

$$\langle \Delta \mathbf{r}_{\rm cm}^2 \rangle = \langle [\mathbf{r}_{\rm cm}(t + t_0) - \mathbf{r}_{\rm cm}(t_0)]^2 \rangle$$

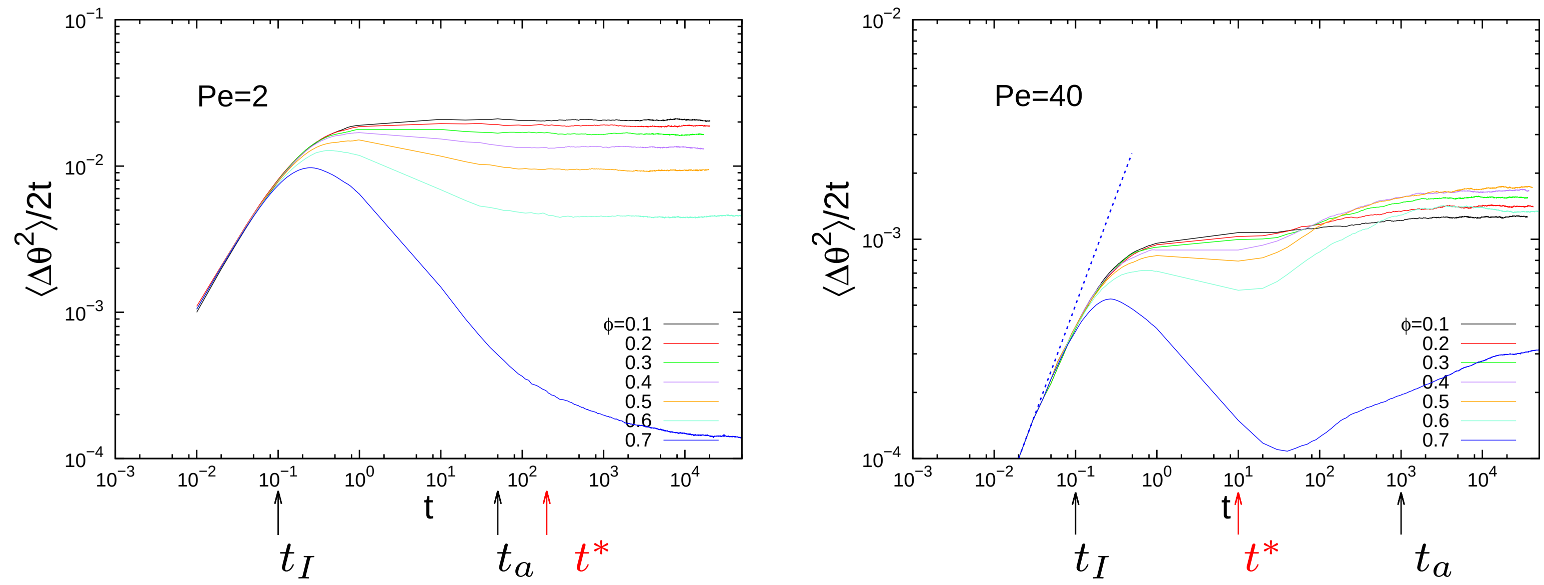


Pe and ϕ effect

Finite density system

Angular mean-square displacement

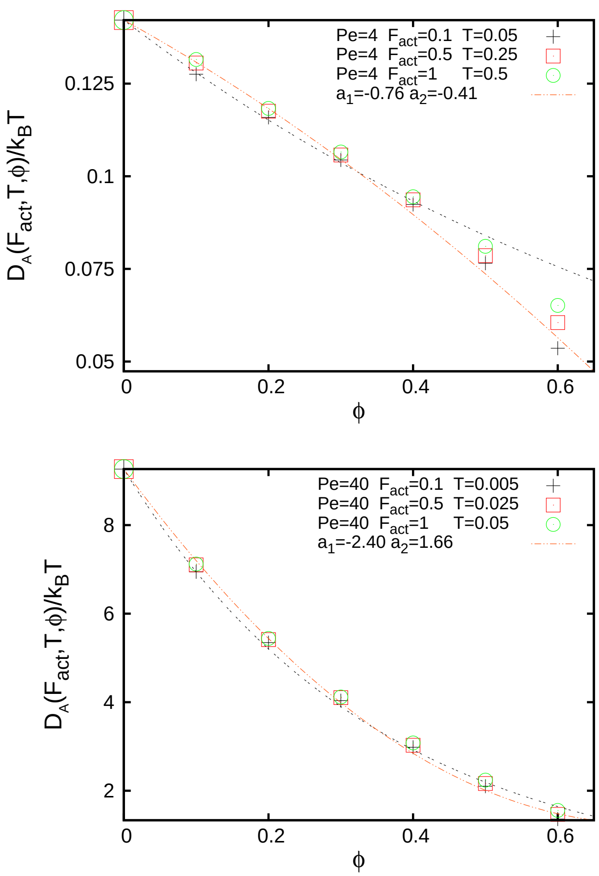
$$\langle \Delta\theta^2 \rangle = \langle [\theta(t+t_0) - \theta(t_0)]^2 \rangle$$



Pe and ϕ effect

Diffusion constants

$$\langle \Delta \mathbf{r}_{\rm cm}^2 \rangle \simeq 2dD_A t$$



$$\frac{D_A}{k_B T} = f_A(\text{Pe}, \phi)$$

Translational diffusion

diminishes at

increasing density

at all Pe

increases at

increasing Pe

at fixed ϕ

Proposals for ϕ, Pe dependence

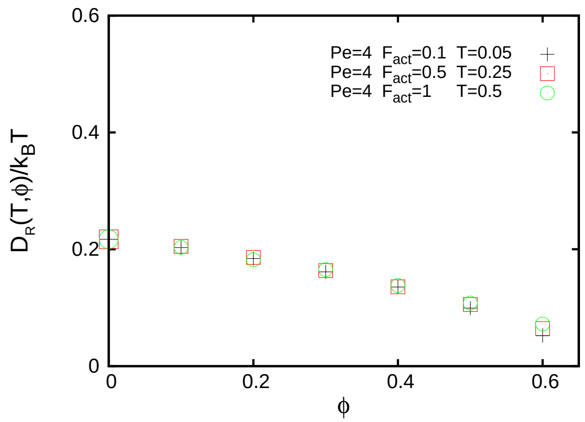
Similar to what observed for

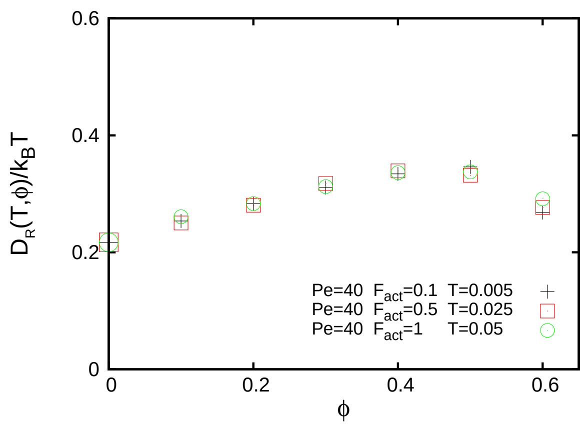
e.g., Janus particles in H_2O_2

Zheng ***et al*** **13**

Diffusion constants

$$\langle \Delta\theta^2 \rangle \simeq 2 D_R t$$





Rotational diffusion

enhanced at

increasing density

for large Pe

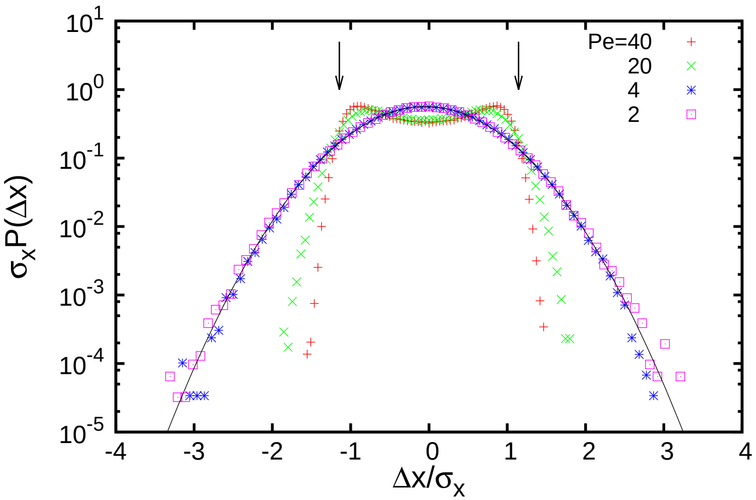
Incipient clusters

$$\frac{D_R}{k_B T} = f_R(\text{Pe}, \phi)$$

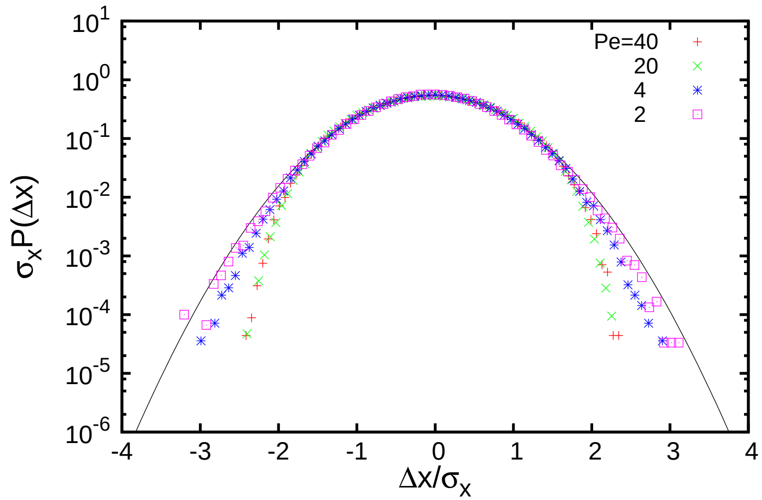
Fluctuations

Translational motion in the active-force driven regimes

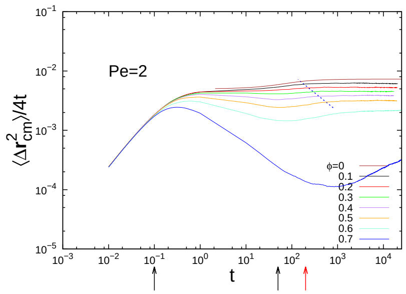
$$p(\Delta x) = p(x_{\rm cm}(t+t_0) - x_{\rm cm}(t_0))$$

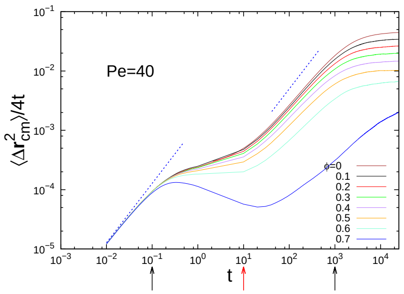


$t^* < t < t_a$



$t_a < t$





$$\phi = 0.1$$

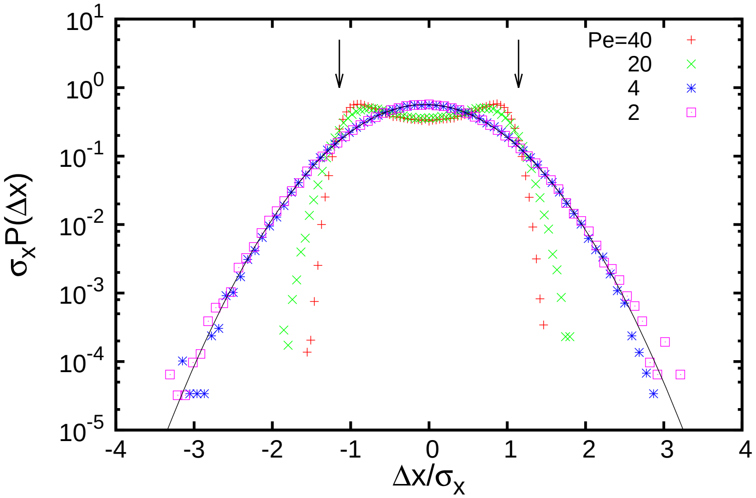
$$\sigma_x = \langle \Delta x^2 \rangle^{1/2}$$

Non-Gaussian at high Pe

Fluctuations

Translational motion in the active-force driven regimes

$$p(\Delta x) = p(x_{\rm cm}(t+t_0) - x_{\rm cm}(t_0))$$



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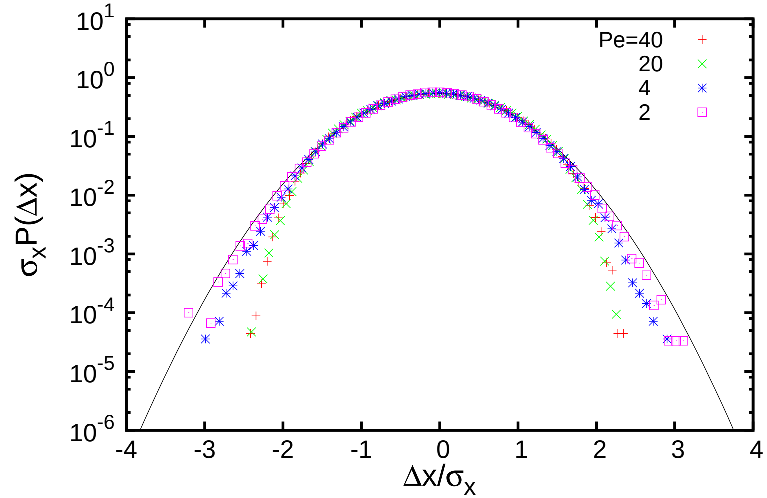
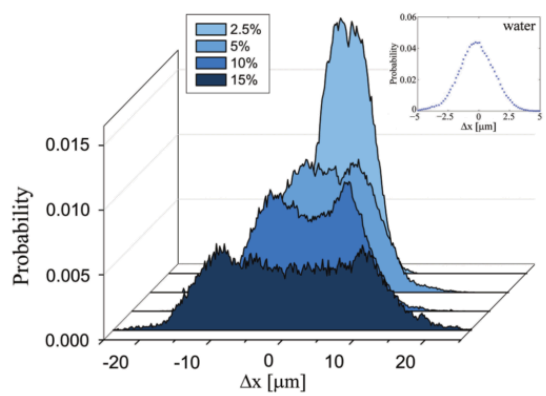


$t_a < t$



Janus particles in H_2O_2

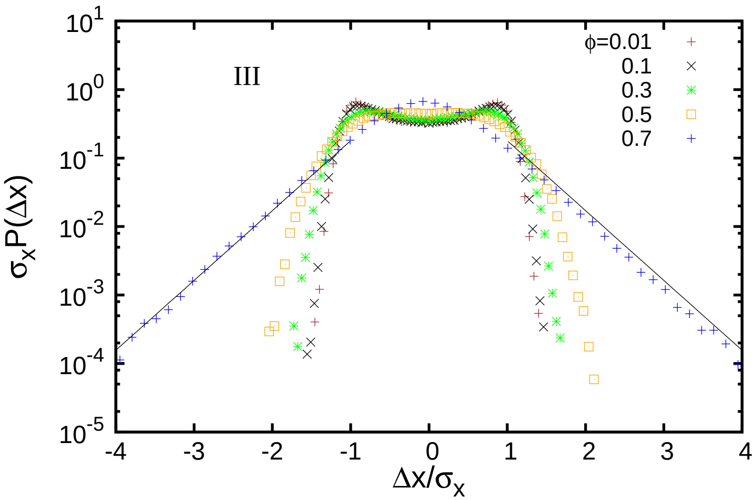
Same double peak at high Pe

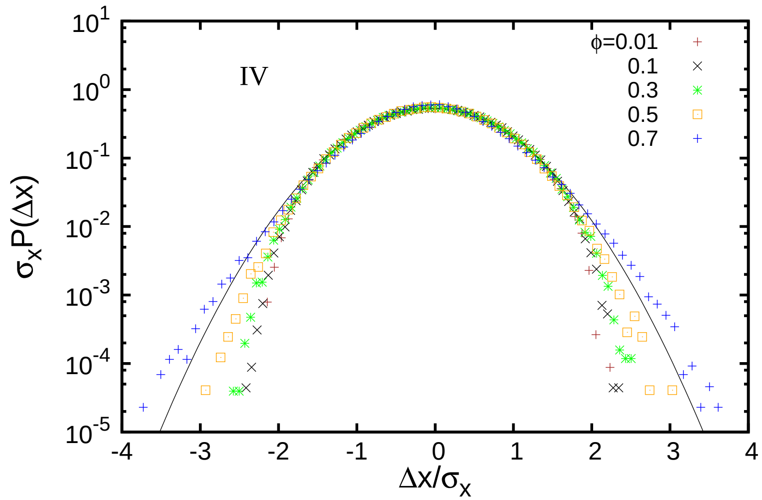
Zheng *et al.* **13**

Fluctuations

Translational motion in the active-force driven regimes

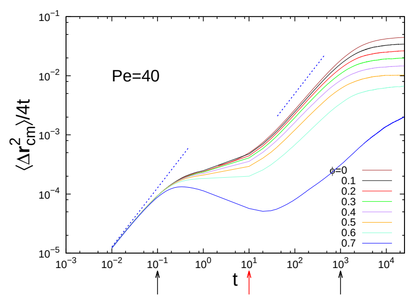
$$p(\Delta x) = p(x_{\rm cm}(t+t_0) - x_{\rm cm}(t_0))$$





$t^* < t < t_a$

$t_a < t$



Pe = 40

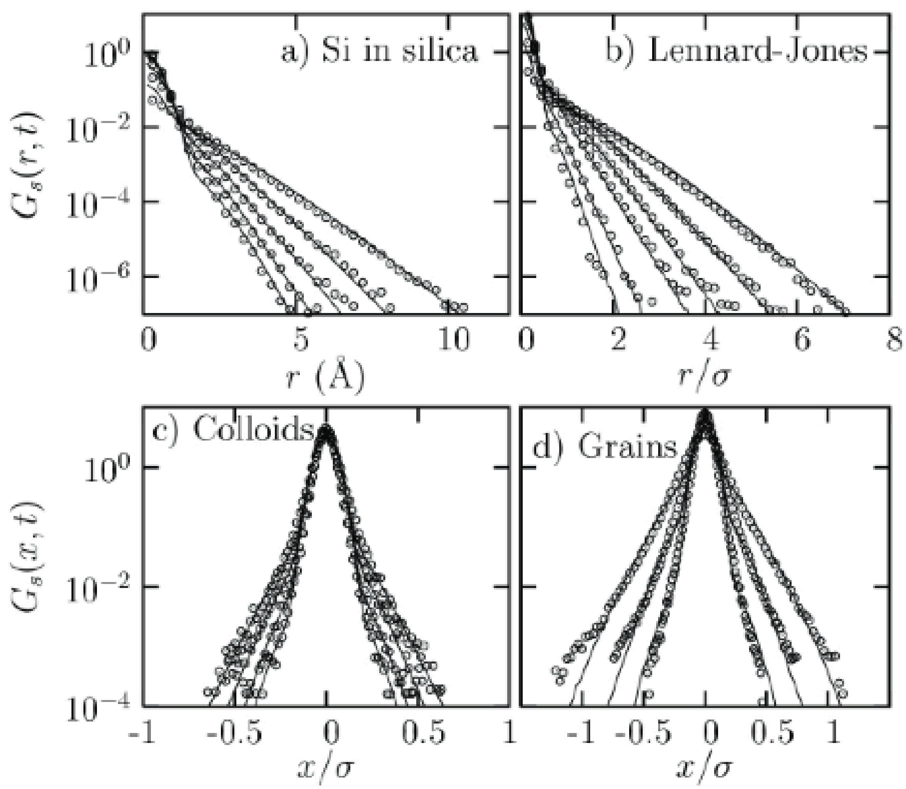
$\sigma_x = \langle \Delta x^2 \rangle^{1/2}$

Non-Gaussian & exponentail tails in III

Fluctuations

Translational motion in super-cooled liquids and granular matter

$$G_s(r) = N^{-1} \sum_{i=1}^{N} \langle \delta(r - |\vec{r}_i(t+t_0) - \vec{r}_i(t_0)|) \rangle$$



van Hove correlation function

delay-time shorter than the

structural relaxation time $t < t_\alpha$

$\sigma = \langle \Delta \mathbf{r}^2 \rangle^{1/2}$

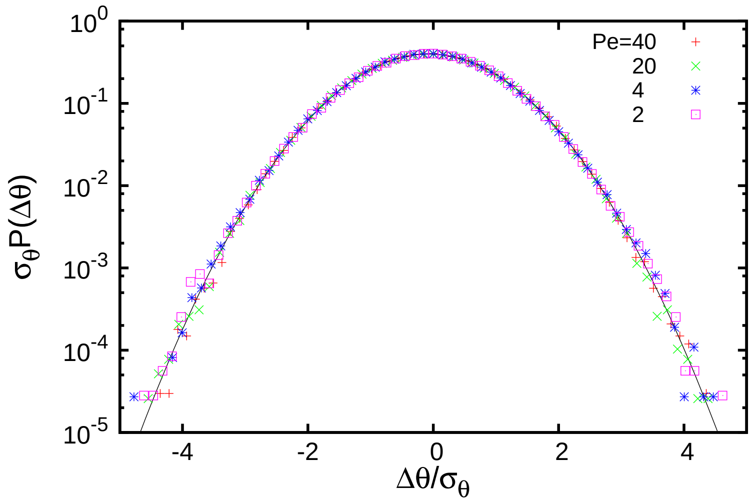
Exponential tails

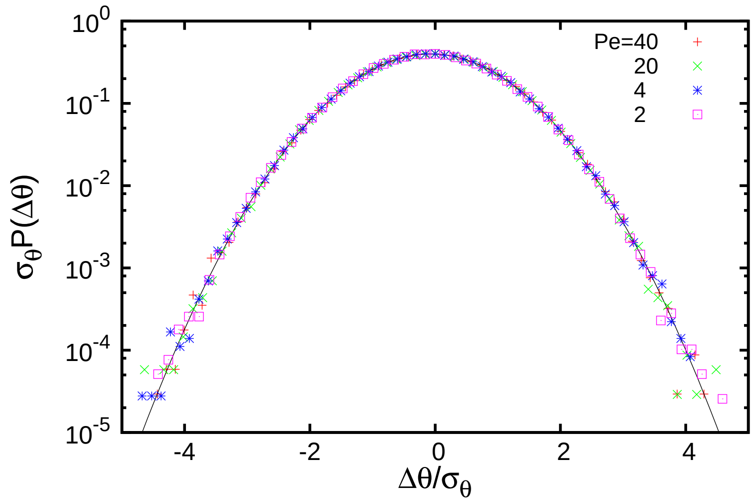
Chaudhuri, Berthier & Kob 07

Fluctuations

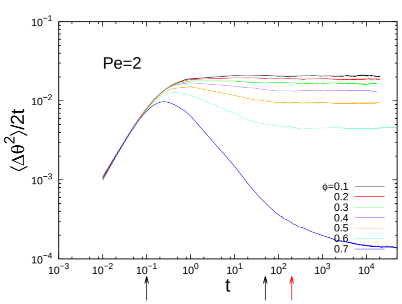
Rotational motion in the active-force driven regimes

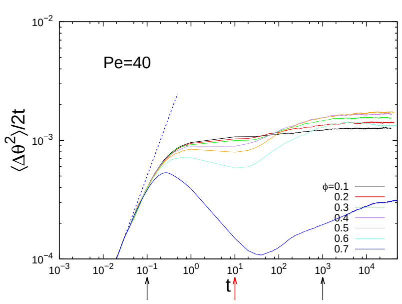
$$p(\Delta\theta) = p(\theta(t+t_0) - \theta(t_0))$$





$$t^* < t < t_a \qquad\qquad t_a < t$$





$$\phi = 0.1$$ Low density

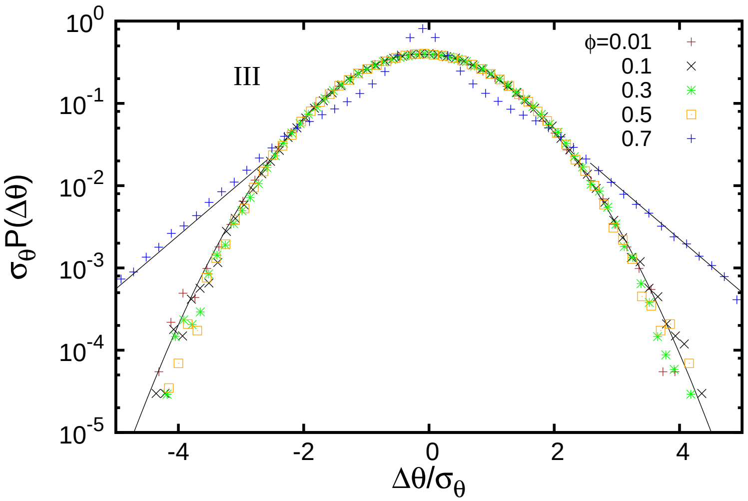
$$\sigma_\theta = \langle \Delta\theta^2 \rangle^{1/2}$$

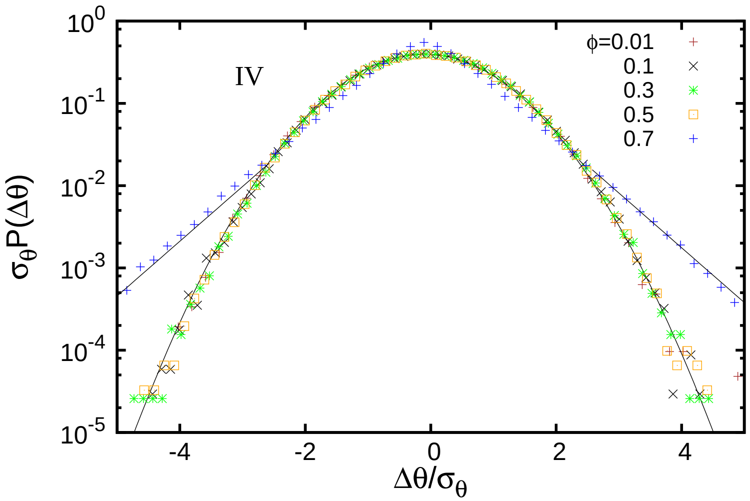
Gaussian

Fluctuations

Rotational motion in the active-force driven regimes

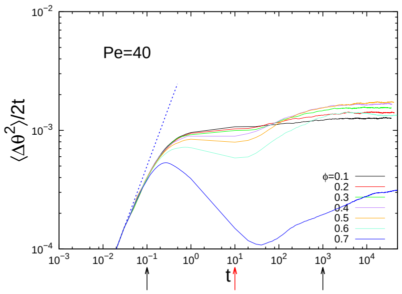
$$p(\Delta\theta) = p(\theta(t+t_0) - \theta(t_0))$$





$t^* < t < t_a$

$t_a < t$



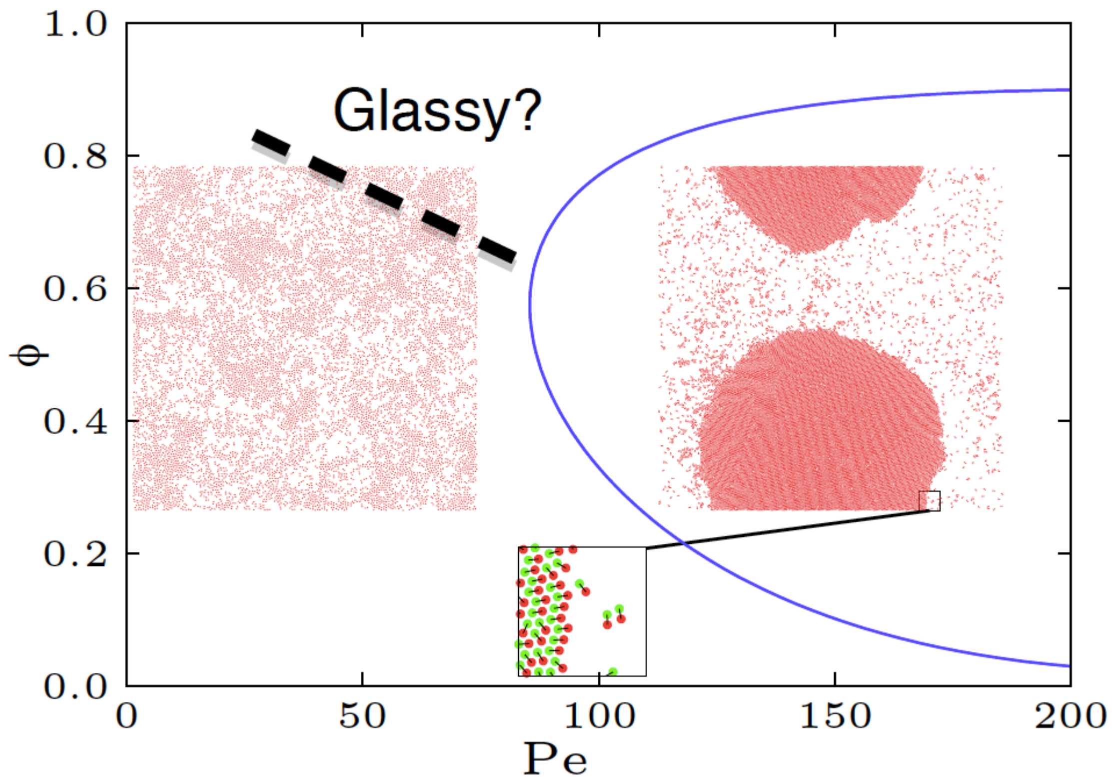
Pe = 40

$\sigma_\theta = \langle \Delta\theta^2 \rangle^{1/2}$

Exponential tails for $\phi \geq 0.7$

Active dumbbells

Phase diagram

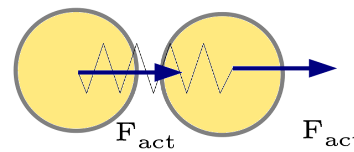


cfr. **Berthier 13 ; Berthier & Levis 14-15** for a different model system

& **Suma** *et al.* work in progress

Active dumbbells

Diatomic molecule



Two spherical atoms with diameter σ_{d} and mass m_{d}

Massless spring modelled by a finite extensible non-linear elastic force between the atoms $\mathbf{F}_{\mathrm{fene}} = -\dfrac{k\mathbf{r}}{1 - r^2/r_0^2}$ with an additional repulsive contribution (WCA) to avoid colloidal overlapping.

Polar active force along the main molecular axis $\mathbf{F}_{\mathrm{act}} = F_{\mathrm{act}}\,\hat{\mathbf{n}}$.

Purely repulsive interaction between colloids in different molecules.

Langevin modelling of the interaction with the embedding fluid:

isotropic viscous forces, $-\gamma\mathbf{v}_i$, and independent noises, η_i, on the beads.

Directional motion (active) and effective torque (noise)

Passive tracers

Spherical particles

Spherical particle with diameter $\sigma_{\rm tr}$ and mass $m_{\rm tr}$

Very low tracer density $\phi_{\rm tr} \ll \phi$

No polar active force $\mathbf{F}^{\rm tr}_{\rm act} = 0$

Purely repulsive interaction between colloids in different molecules & tracers.

Langevin modelling of the interaction with the embedding fluid:

viscous forces, $-\gamma_{\rm tr}\mathbf{v}^{\rm tr}_\alpha$, and independent noises, $\eta^{\rm tr}_\alpha$, on the tracers.

We will distinguish thermal $\gamma_{\rm tr} \neq 0$ from athermal $\gamma_{\rm tr} = 0$ tracers

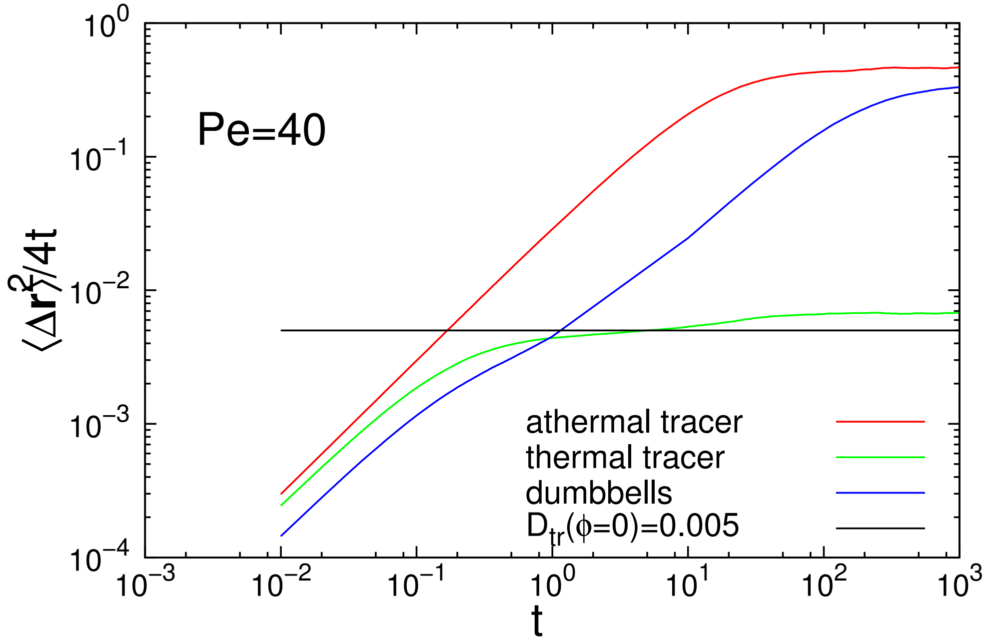
Active dumbbells

Spherical tracers to probe the dynamics of the “active bath"

Gonnella, Laghezza, Lamura, Mossa, Suma & LFC

Passive tracer motion

Thermal *vs.* athermal



$\sigma_{\rm d} = \sigma_{\rm tr}, \; m_{\rm d} = m_{\rm tr}$

thermal

$\gamma_{\rm d} = \gamma_{\rm tr}, \; T_{\rm d} = T_{\rm tr}$

athermal

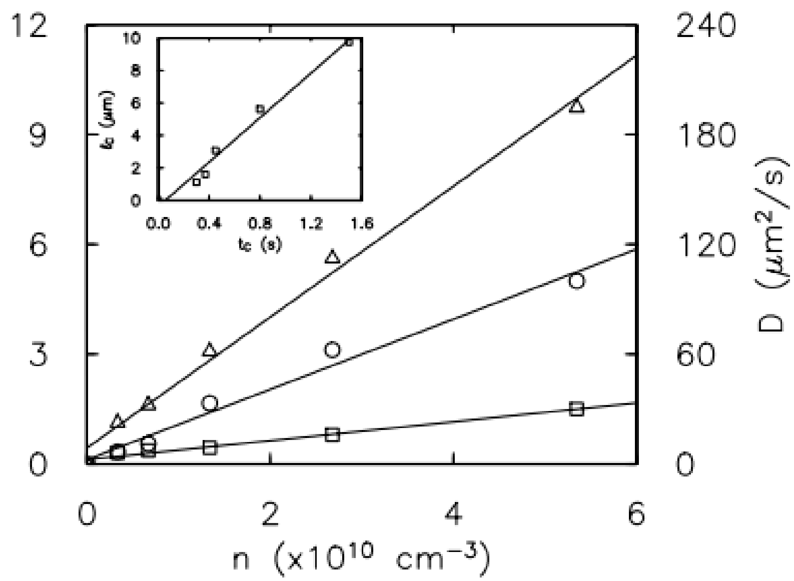
$\gamma_{\rm tr} = 0, \; T_{\rm d} = T_{\rm tr}$

Study of the dependence on $m_{\rm tr}$, ϕ, and other parameters

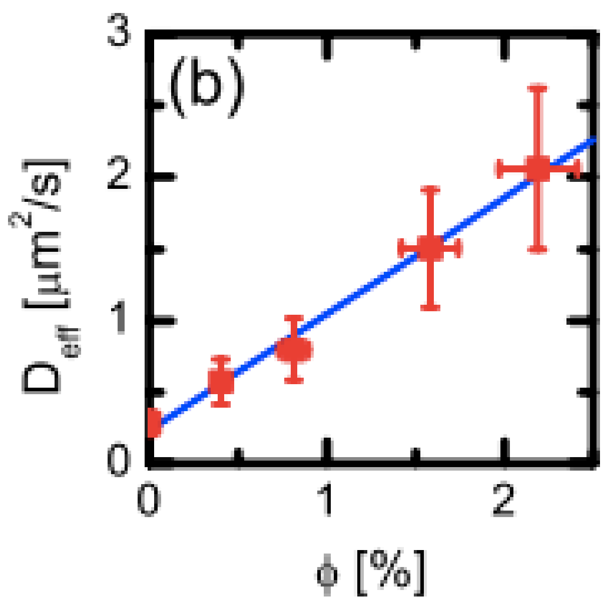
Suma, Gonnella & LFC in preparation

Diffusivity enhancement

Active density dependence of the tracer's diffusion constant



Wu & Libchaber 00 bacteria



Leptos *et al.* **09** algae

Is this captured by this model (with no hydrodynamics) for some parameters ?

Motivation & goals

Active dumbbell system

- Model with persistent activity & segregation
- Translational and rotational collective motion in the homogeneous phase

  Four dynamic regimes even at finite ϕ

  $D/(k_B T)$'s in last diffusive regime depend on Pe, ϕ

  Complex (though simpler than in just passive colloids, cfr. **Tokuyama & Oppenheim 94**) dependence of translational diffusion constant on ϕ

  Enhanced rotational diffusion constant for increasing $\phi < 0.5$

  More complex than Pe^2 corrections at finite ϕ

- Effective temperatures out of equilibrium.

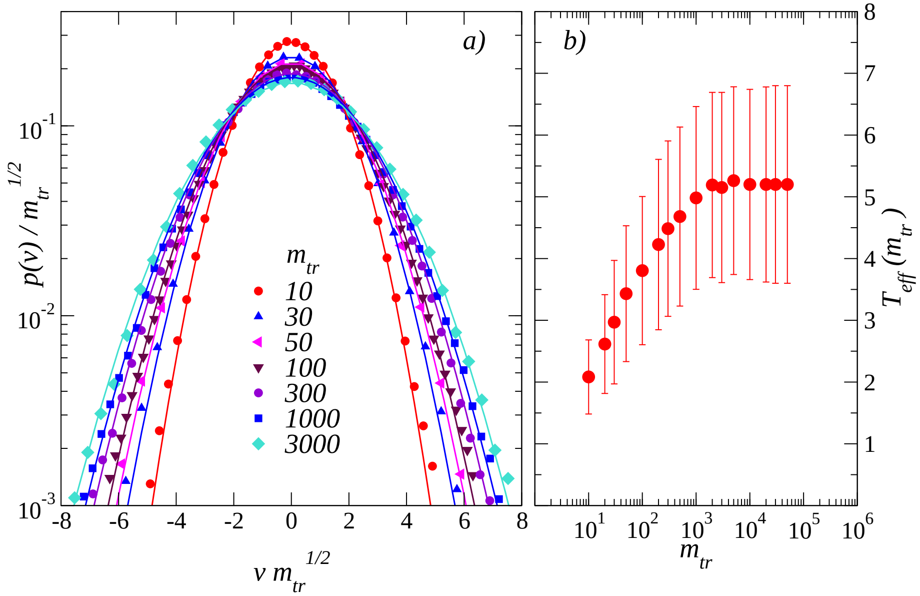
w/ Gonnella, Laghezza, Lamura, Mossa & Suma via FDT

In progress : potential and kinetic tracers coupled to the active dumbbells, always in homogenous phase

(non persistent) Active polymers

Tracer's velocities & effective temperature

Spherical particles with mass m_{tr} that interact with the active matter.

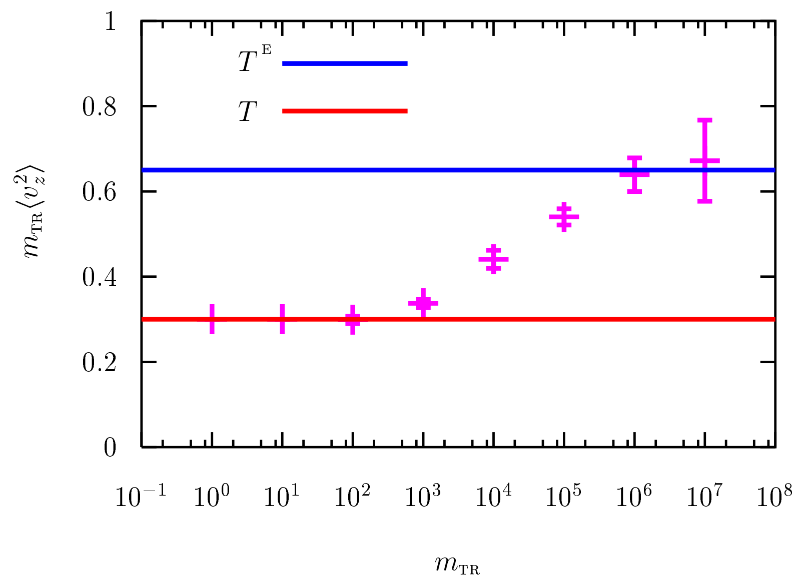


Maxwell pdf of tracers' velocities v at an effective temperature $T_{\rm eff}(m_{tr})$

Loi, Mossa & LFC 07-09

Work in progress

Passive Leannard-Jones system



The kinetic energy of a tracer particle (the thermometer) as a function of its mass ($\tau_0 \propto \sqrt{m_{tr}}$) $\frac{1}{2} m_{tr} \langle\, v_z^2 \rangle = \frac{1}{2} k_B T_{\text{eff}}$.

J-L Barrat & Berthier 00

Same measurement in active dumbbell sample to compare with measurements of T_{eff} from FDT.