Diffusion, fluctuations and phase separation in an active dumbbell system

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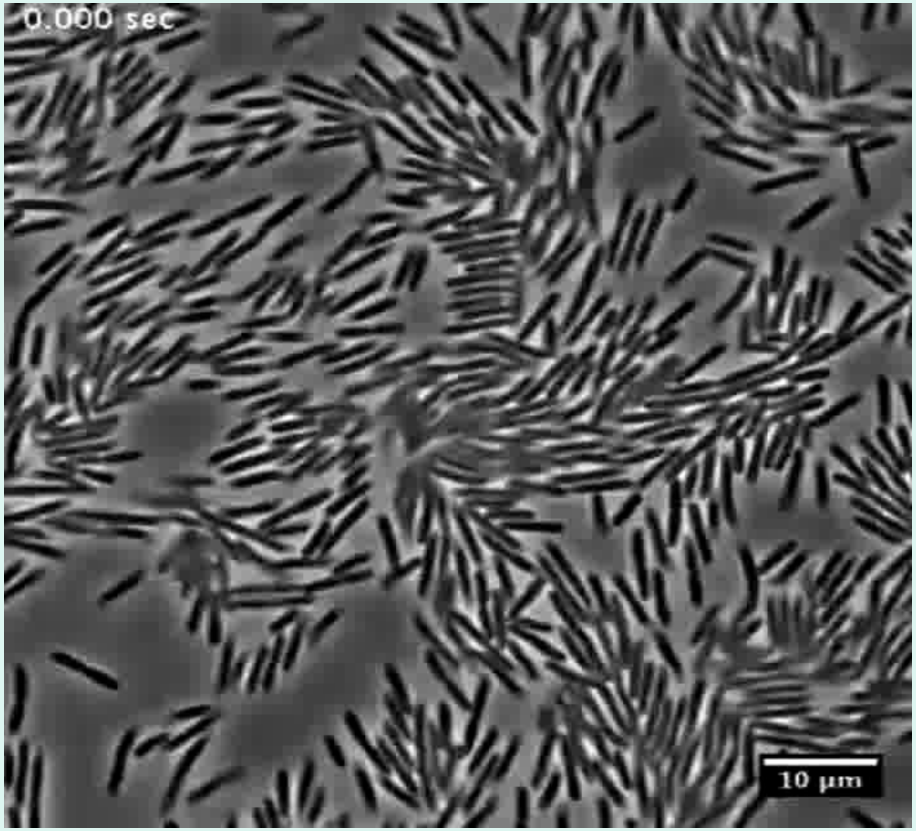
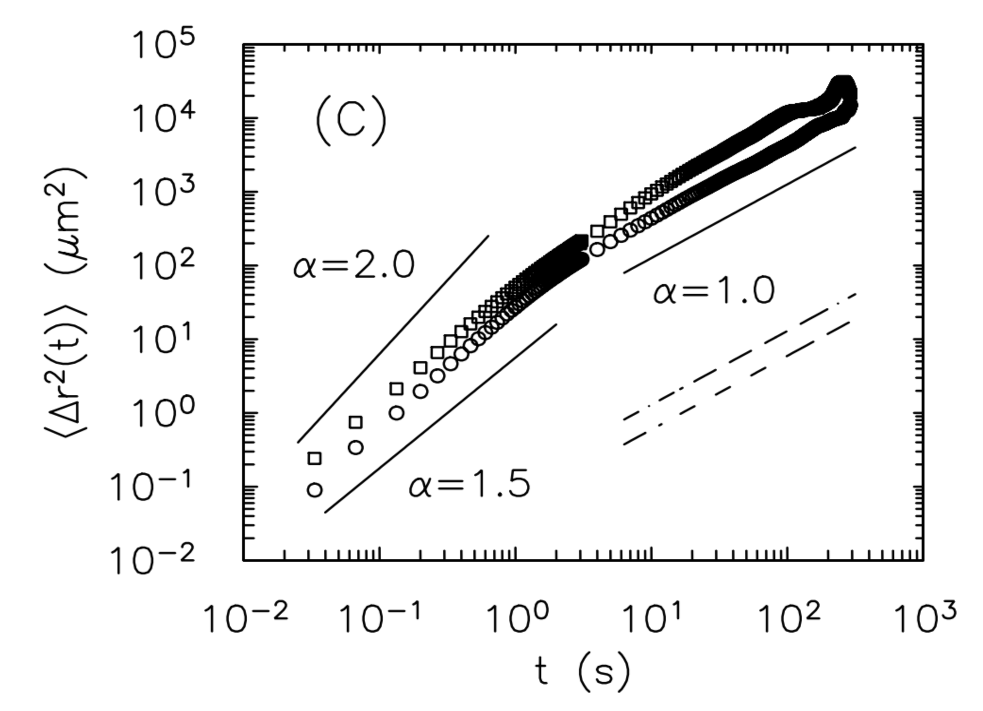
Cluster formation in bacteria colonies



A dense group of E. coli swims in the roughly two dimensional space at an air water interface. Their collective motion is significantly different from their motion as single cells.
Under these conditions they behave more like an active fluid, hence changing the way that nutrients are shared within the group...

Video courtesy Matthew Copeland, University of Wisconsin, Madison

Unusual diffusive behavior of tracers coupled to self-propelled particles



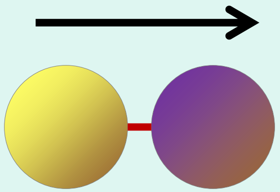
This shows the effect of bacterial motion on micron-scale beads in a freely suspended soap film. Given the sizes of bacteria and beads, the geometry of the experiment is quasi-two-dimensional. Large positional fluctuations are observed for beads as large as 10 mm in diameter, and the measured mean-square displacements indicate superdiffusion in short times and normal diffusion in long times.

Libchaber&Wu, PRL 2000

Motivations

- How the dynamic behavior depends on self-propulsion?
- Does self-propulsion induce phase separation? Is that affected by the shape of the particles?
- How to characterize the kinetics of   clusters?
- Active systems exist in nonequilibrium conditions: Can they be described by an effective temperature?
- How do fluctuations behave?

Active dumbbells



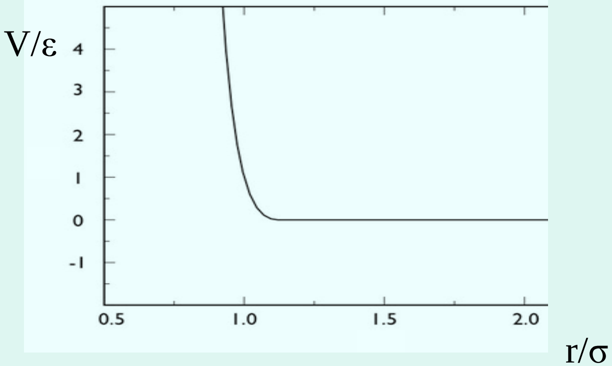
$$m_d \ddot{\mathbf{r}}_i(t) = -\gamma \dot{\mathbf{r}}_i(t) - \partial_i U + \sqrt{2TK_B\gamma}\eta_i + \mathbf{F}_{\text{act}\,i}$$

γ friction felt by each particle

η uncorrelated gaussian noise with zero average and unit variance

U includes the repulsive Weeks-Chandler-Anderson potential between each particle and the FENE potential for the two colloids of each dumbbell

$$F_{fene}(\vec{r}) = \frac{k\vec{r}}{1 - \frac{\vec{r}^2}{r_0^2}}$$



$\mathbf{F}_{\text{act}\,i}$ active force on each particle, constant in magnitude and directed along the main direction of the dumbbell

Dimensionless relevant numbers

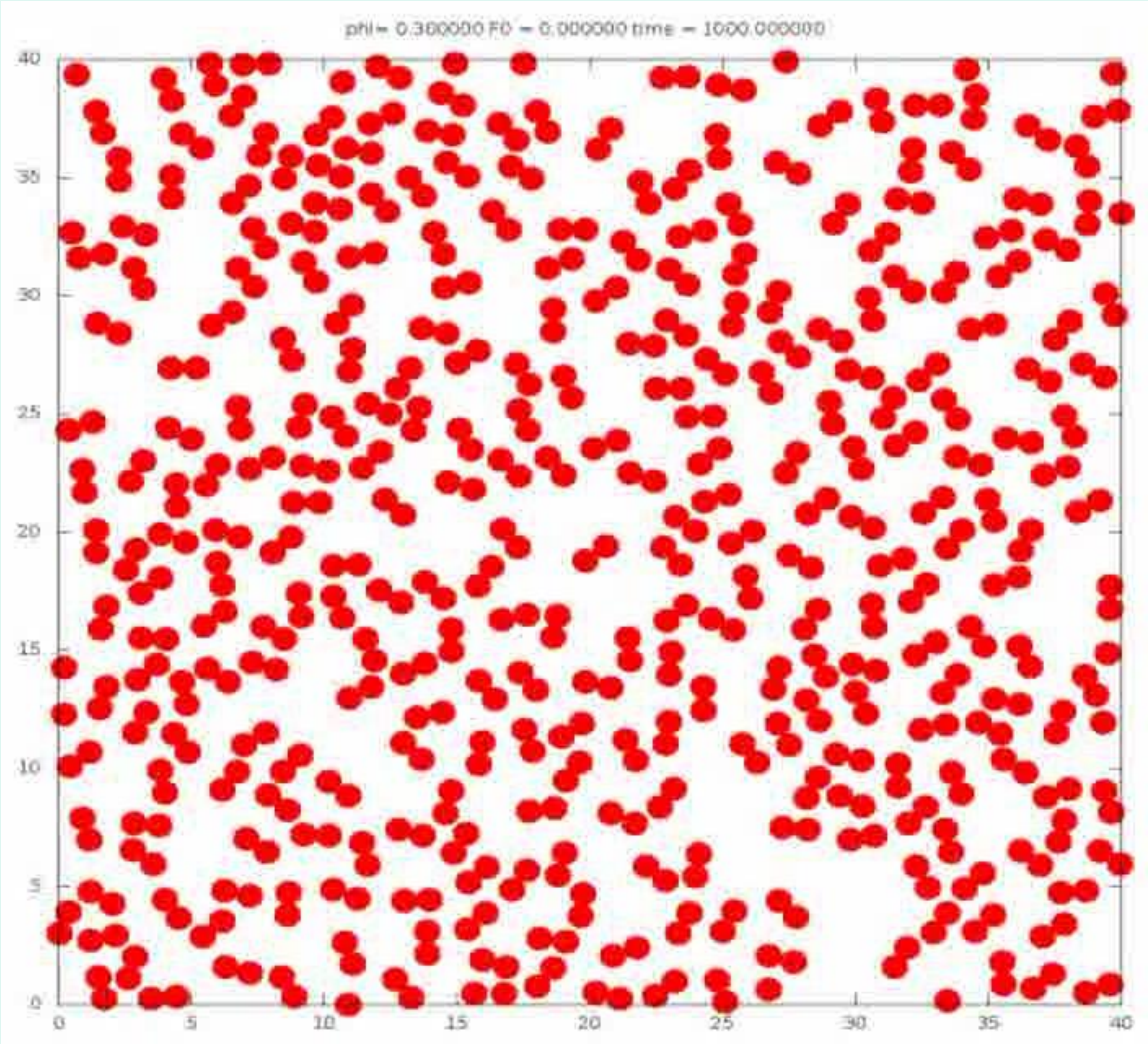
$$\mathrm{Pe} = \frac{Lv}{D} \Longrightarrow \mathrm{Pe}_{\mathrm{act}} = \frac{2\sigma_{\mathrm{d}} F_{\mathrm{act}}}{k_B T} \approx 100$$

$$\mathrm{Re} = \frac{Lv}{\nu} \Longrightarrow \mathrm{Re}_{\mathrm{act}} = \frac{m F_{\mathrm{act}}}{\sigma_{\mathrm{d}} \gamma^2} \approx 0.01$$

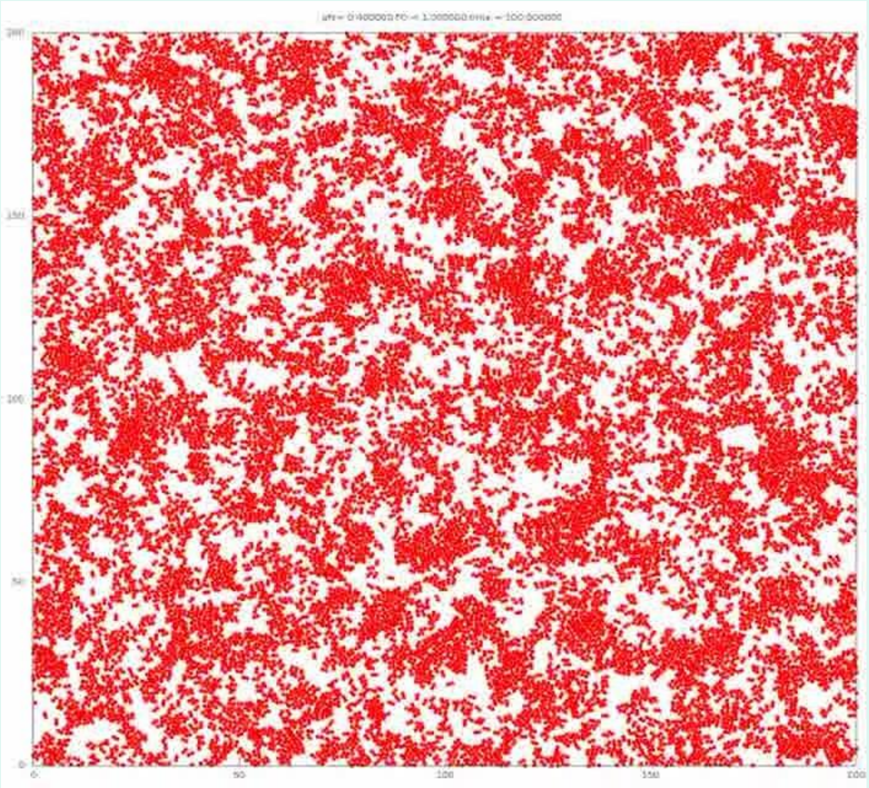
$$\phi = \frac{N\pi\sigma^2}{2A}$$

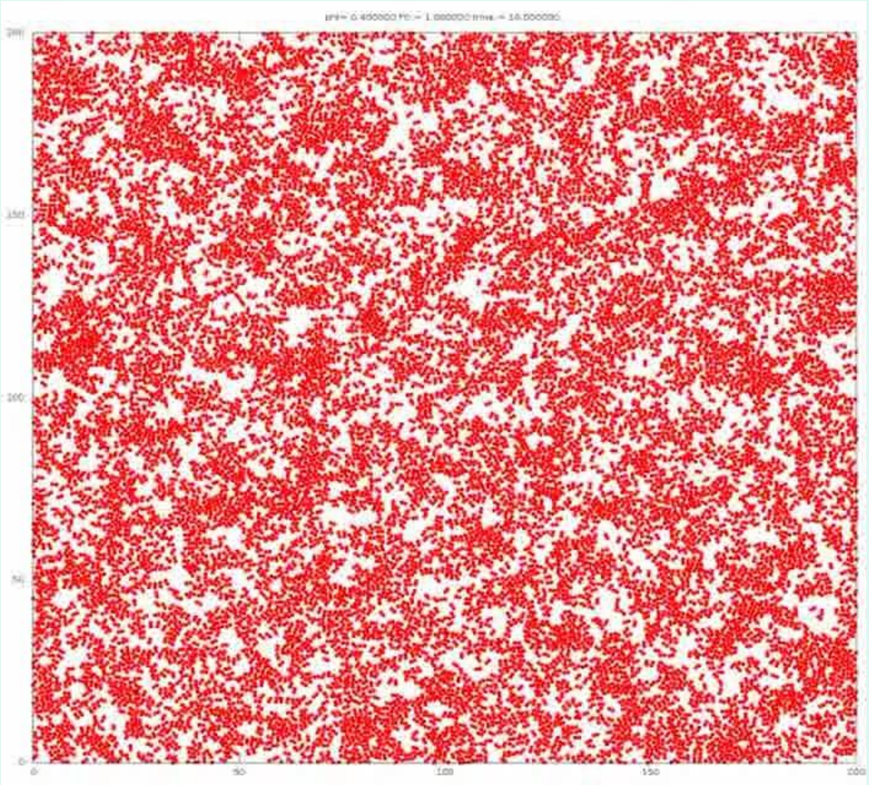
σ Diameter of each colloid in a dumbbell

In absence of activity

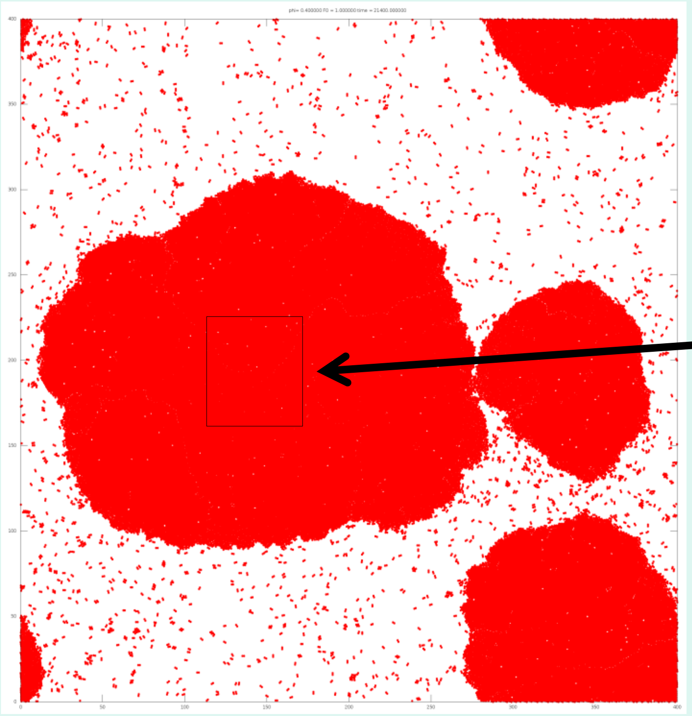


With activity at different temperatures

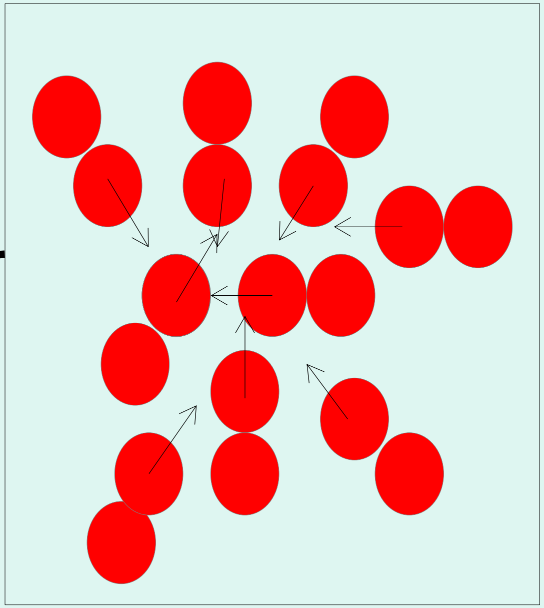




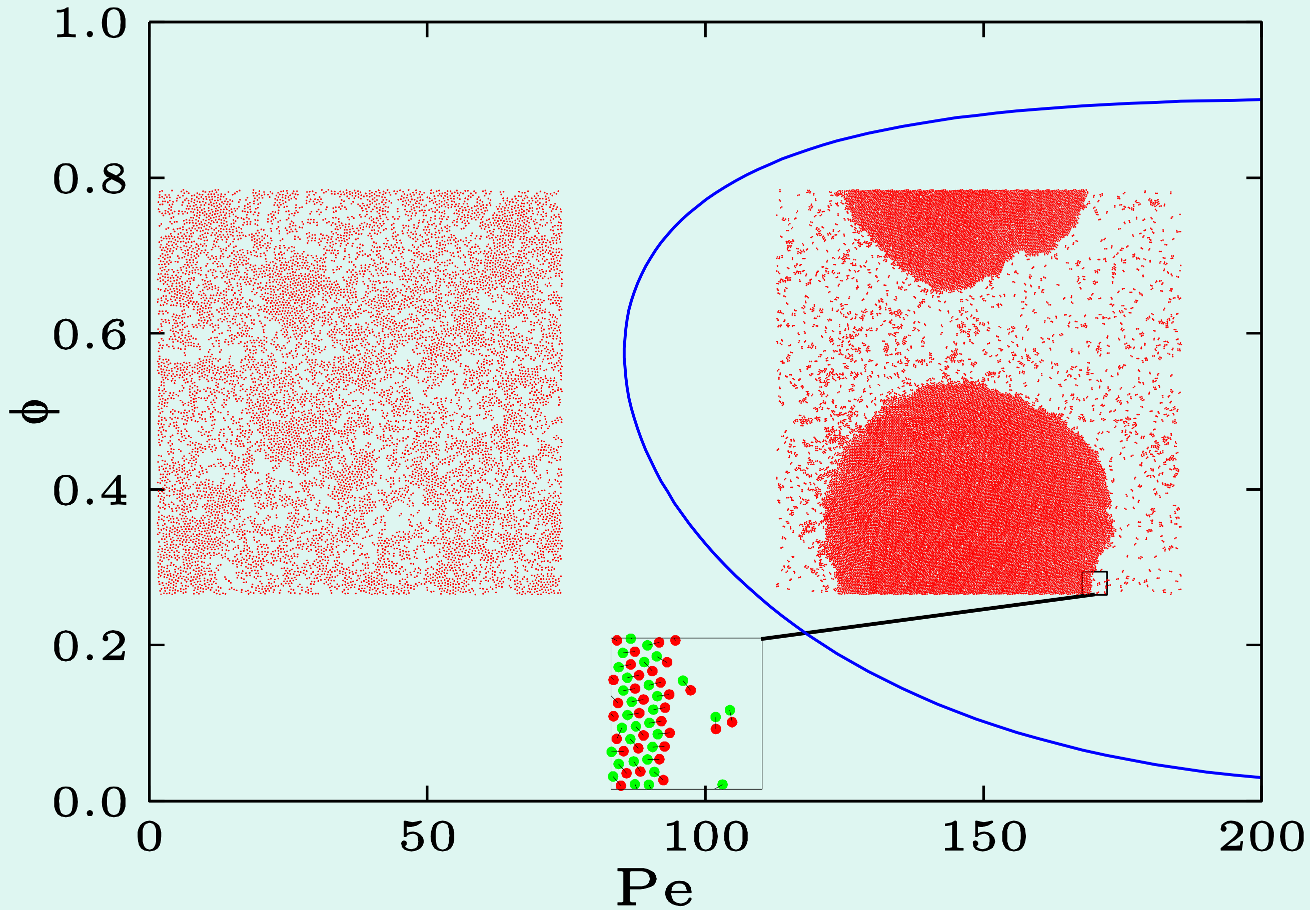
Phase transition



Mechanism of aggregation



Phase diagram



Dynamics in the homogeneous phase: diffusion and fluctuations

Diffusion: single dumbbell

Center of mass position:

$$2m_{\rm d}\ddot{\mathbf{r}}_{\rm cm}(t) = -2\gamma\dot{\mathbf{r}}_{\rm cm}(t) + 2\mathbf{F}_{\rm act}(t) + \xi(t)$$

$$\langle \xi_a(t)\xi_b(t')\rangle = 4\gamma k_B T\, \delta_{ab}\delta(t-t')$$

Relative position:

$$m_{\rm d}\ddot{\mathbf{r}}(t) = \gamma\dot{\mathbf{r}}(t) + 2\mathbf{F}_{\rm int}(t) + \zeta(t)$$

$$\langle \zeta_a(t)\zeta_b(t')\rangle = 4\gamma k_B T\, \delta_{ab}\delta(t-t')$$

Elongation and rotation:

$$\begin{aligned} \gamma\dot{r} &= 2F_{\rm int} + \zeta_x \cos\theta + \zeta_y \sin\theta \,, \\ \gamma r\dot{\theta} &= -\zeta_x \sin\theta + \zeta_y \cos\theta \,. \end{aligned}$$

$$r \approx \sigma_{\rm d} \quad \to \quad \langle\theta^2\rangle = \theta_0^2 + 2D_R t, \qquad D_R = \frac{2k_BT}{\gamma\sigma_{\rm d}^2}$$

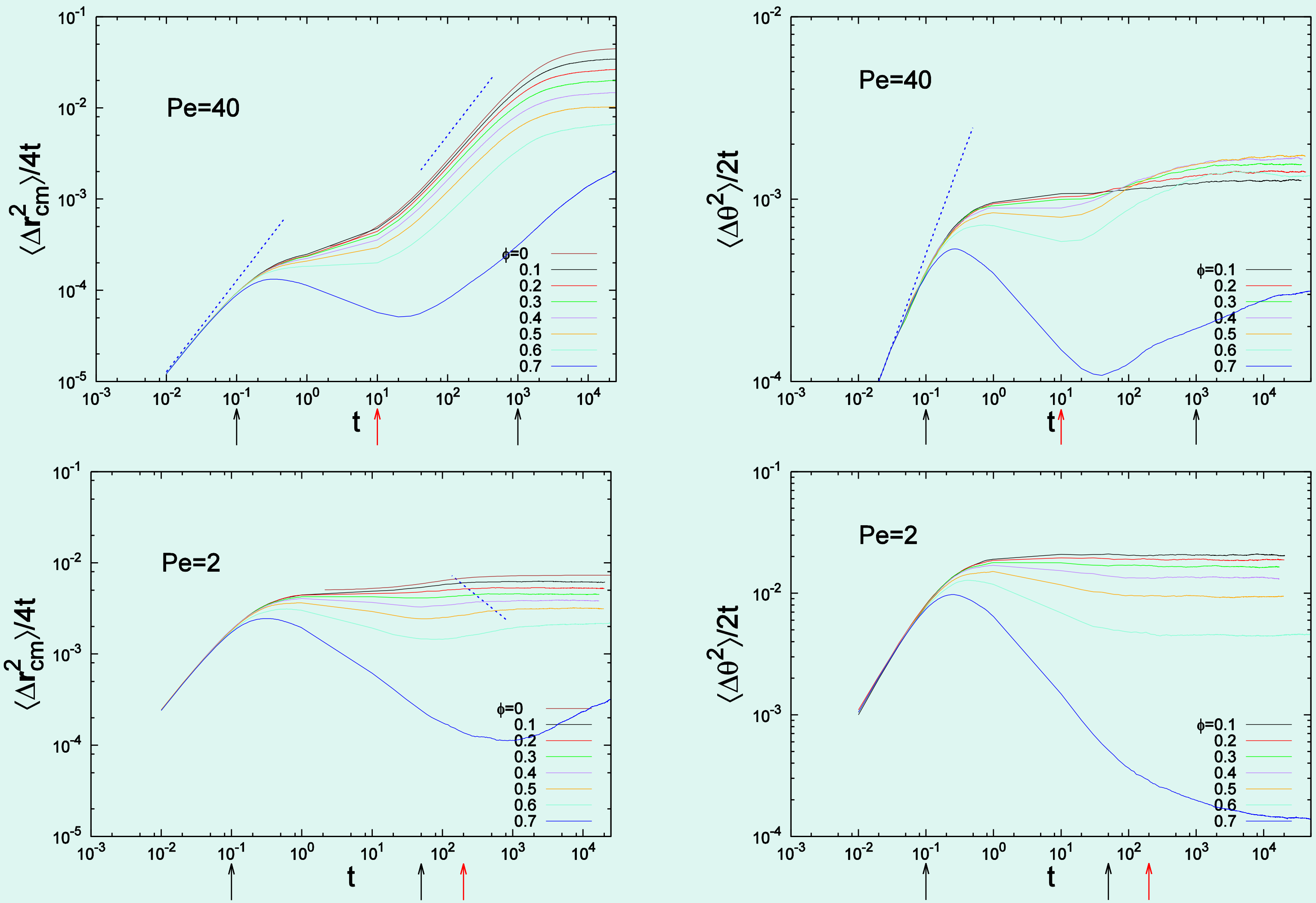
Translations:

$$\langle\triangle\mathbf{r}_{\rm cm}^2\rangle(t) = 4D_{\rm cm}^{\rm pd}\; t + \left(\frac{F_{\rm act}}{\gamma}\right)^2 \frac{2}{D_R}\left(t - \frac{1-e^{-D_R t}}{D_R}\right)\; , D_{\rm cm}^{\rm pd} = \frac{k_BT}{2\gamma}$$

Mean square displacement: finite density

Single dumbbell: $\text{ballistic} \mapsto \text{diffusive} \mapsto \text{ballistic} \mapsto \text{diffusive}$

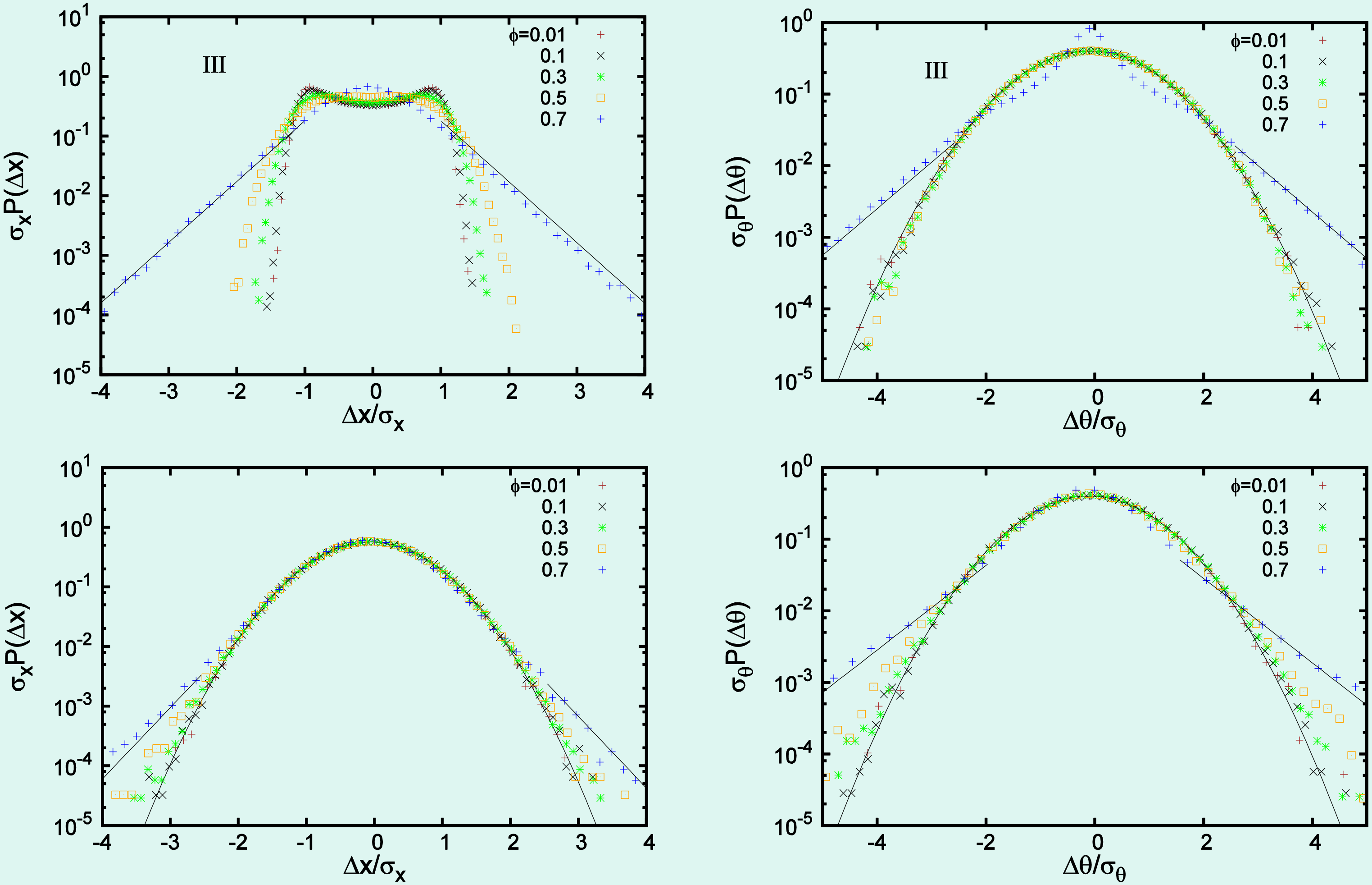
t_I $\qquad t^*$ $\qquad t_a \equiv D_r^{-1}$



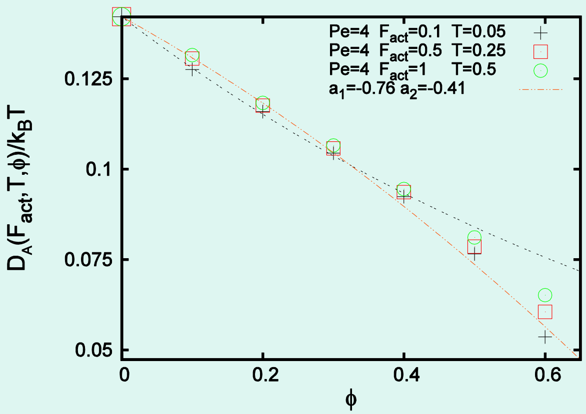
Fluctuations in super- and sub-diffusive regimes

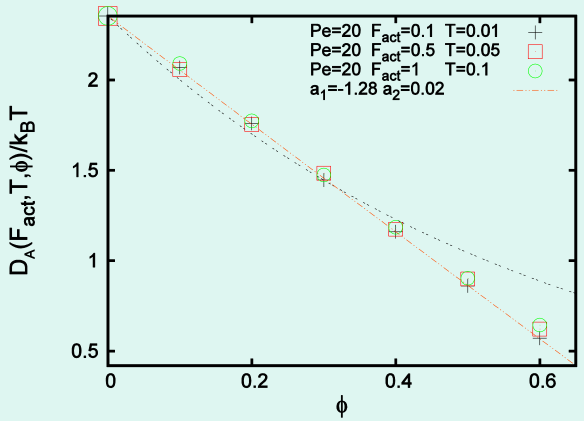
Pe=40

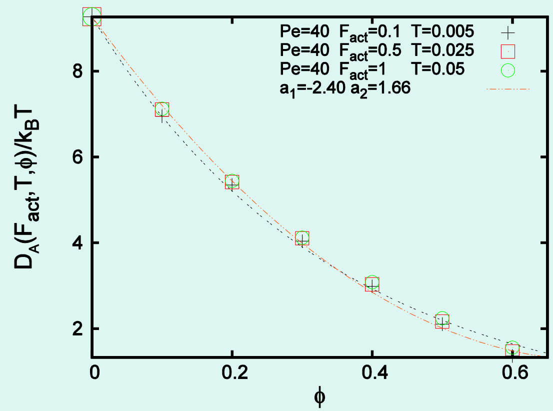
Pe=2

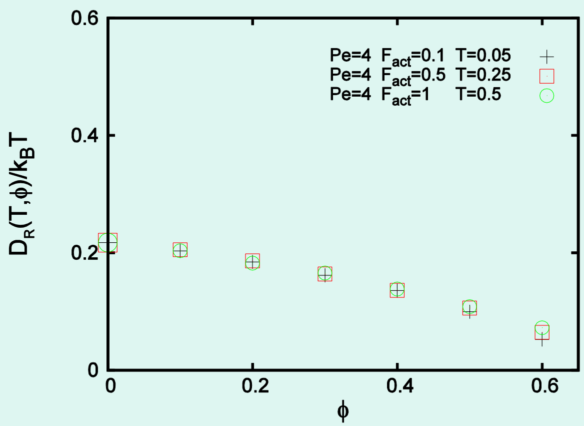


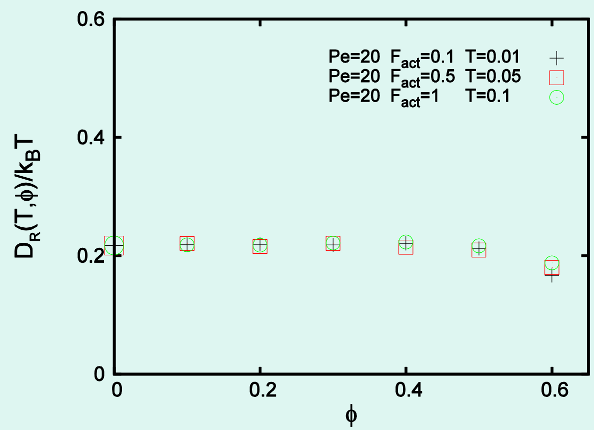
Late diffusive regime

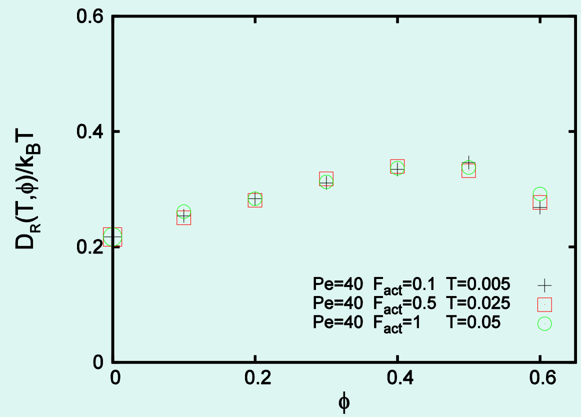




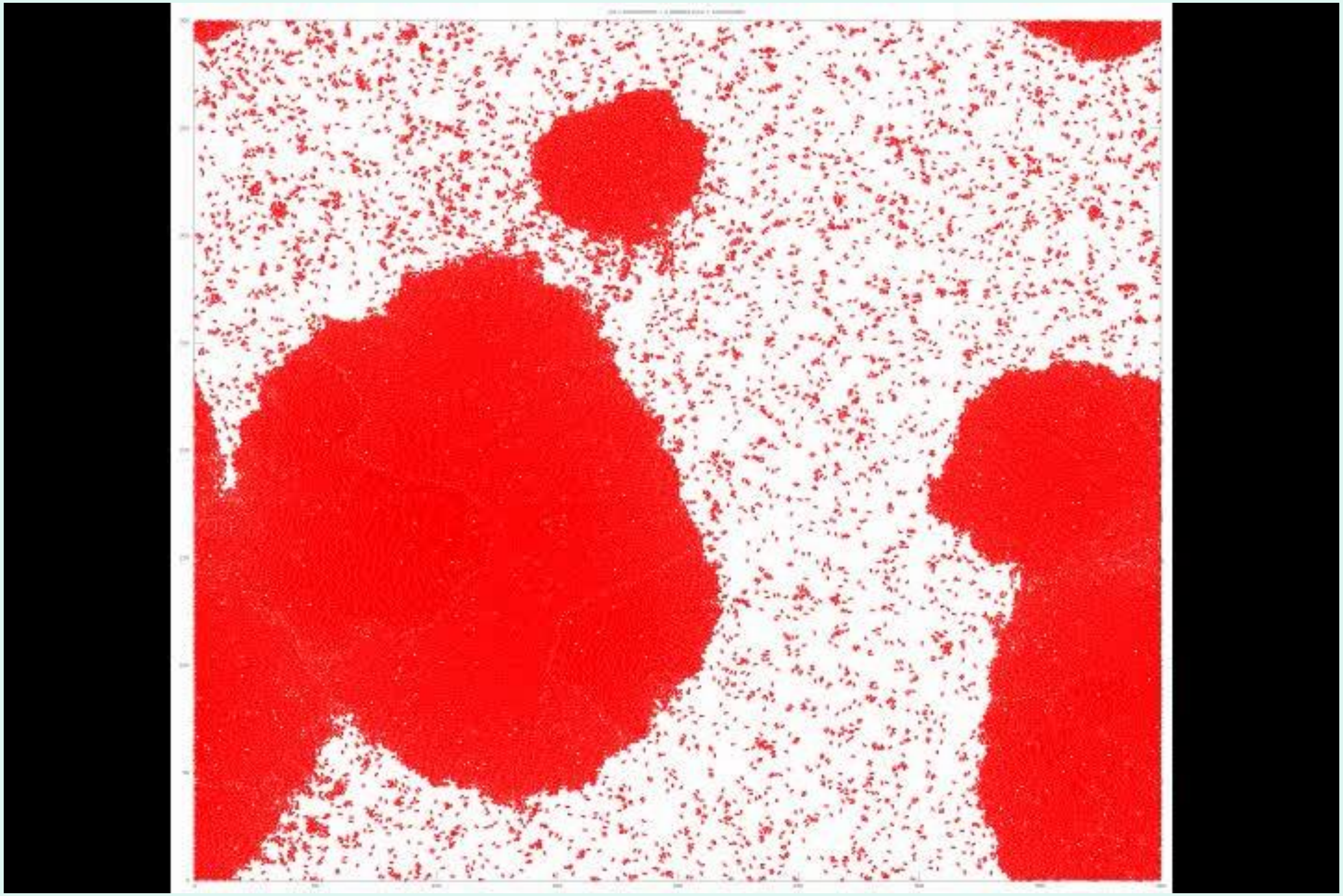








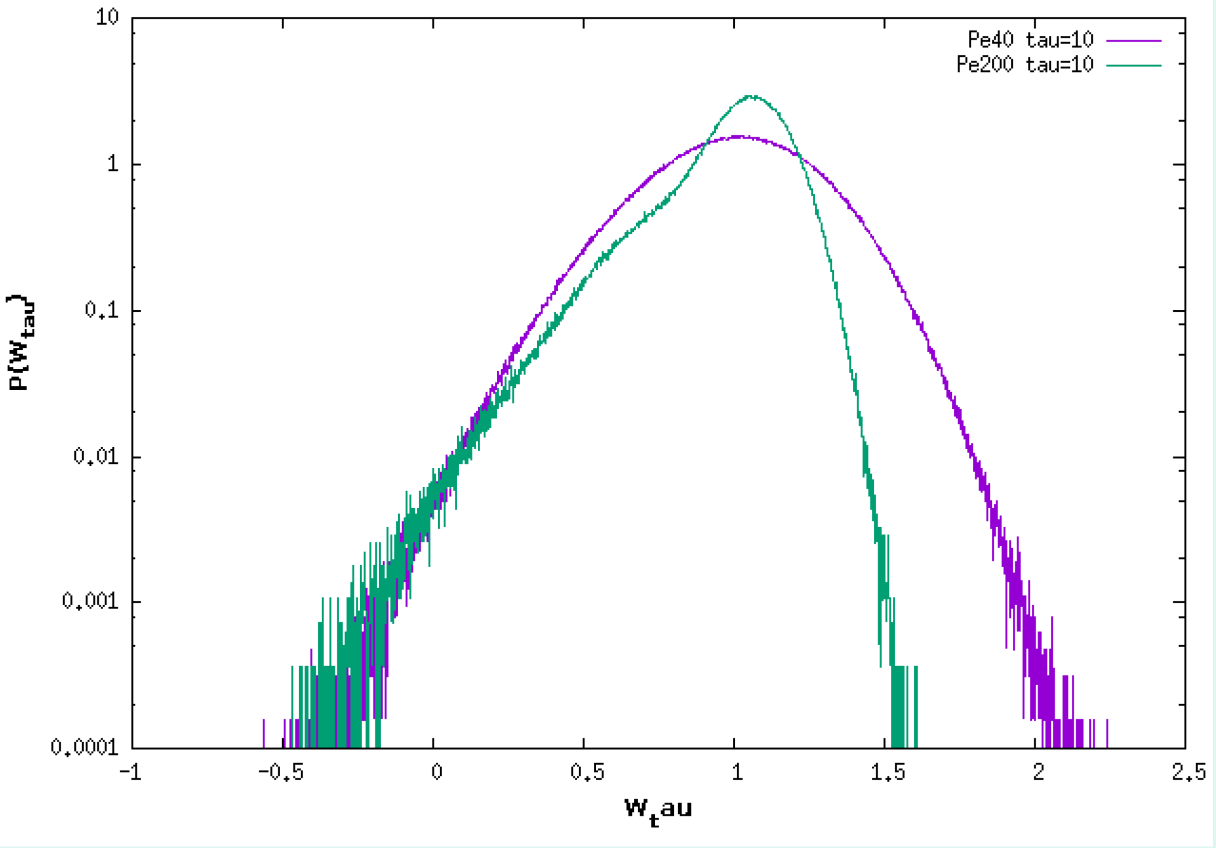
Dynamics of rotating clusters

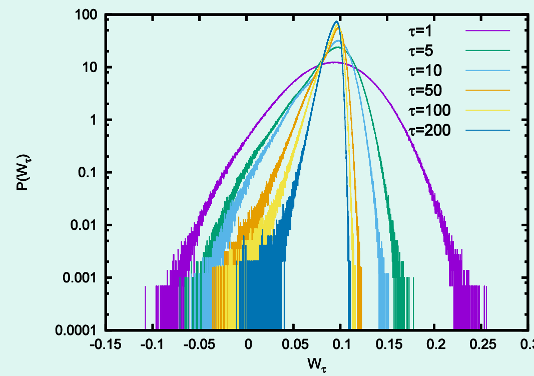


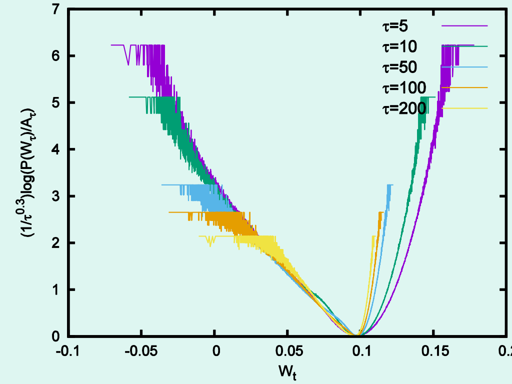
Condensation of fluctuations?

Inspired by exp work on
conical particles in vibrating granular
media by Kumar et al PRL2011

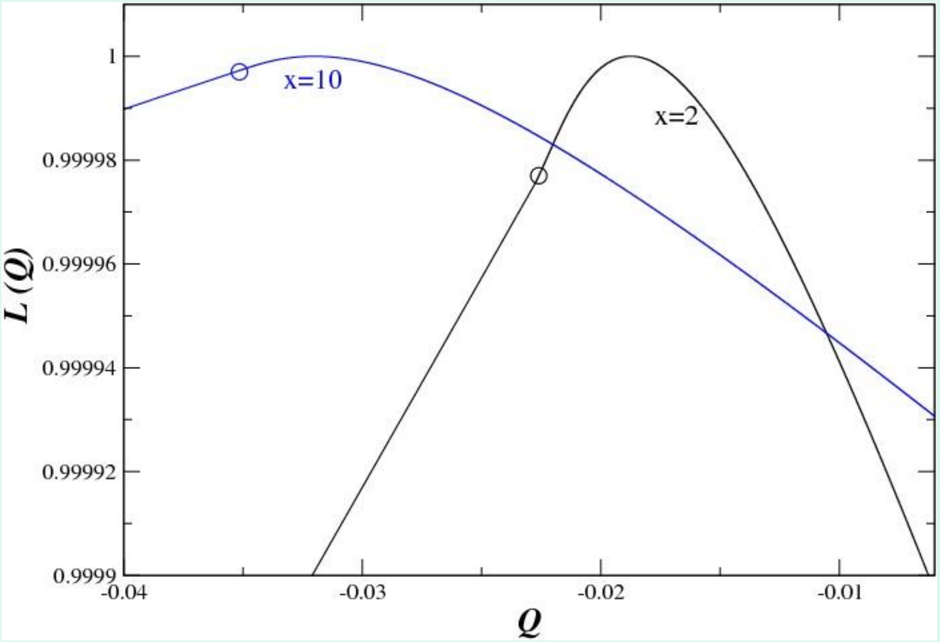
$$W_\tau = \frac{1}{\tau}\int_t^{t+\tau} dt'\,\dot{\mathbf{r}}_{\rm cm}(t')\cdot\mathbf{n}_{\rm dumbbell}(t')$$







Condensation of energy fluctuations in a quenched ferromagnet

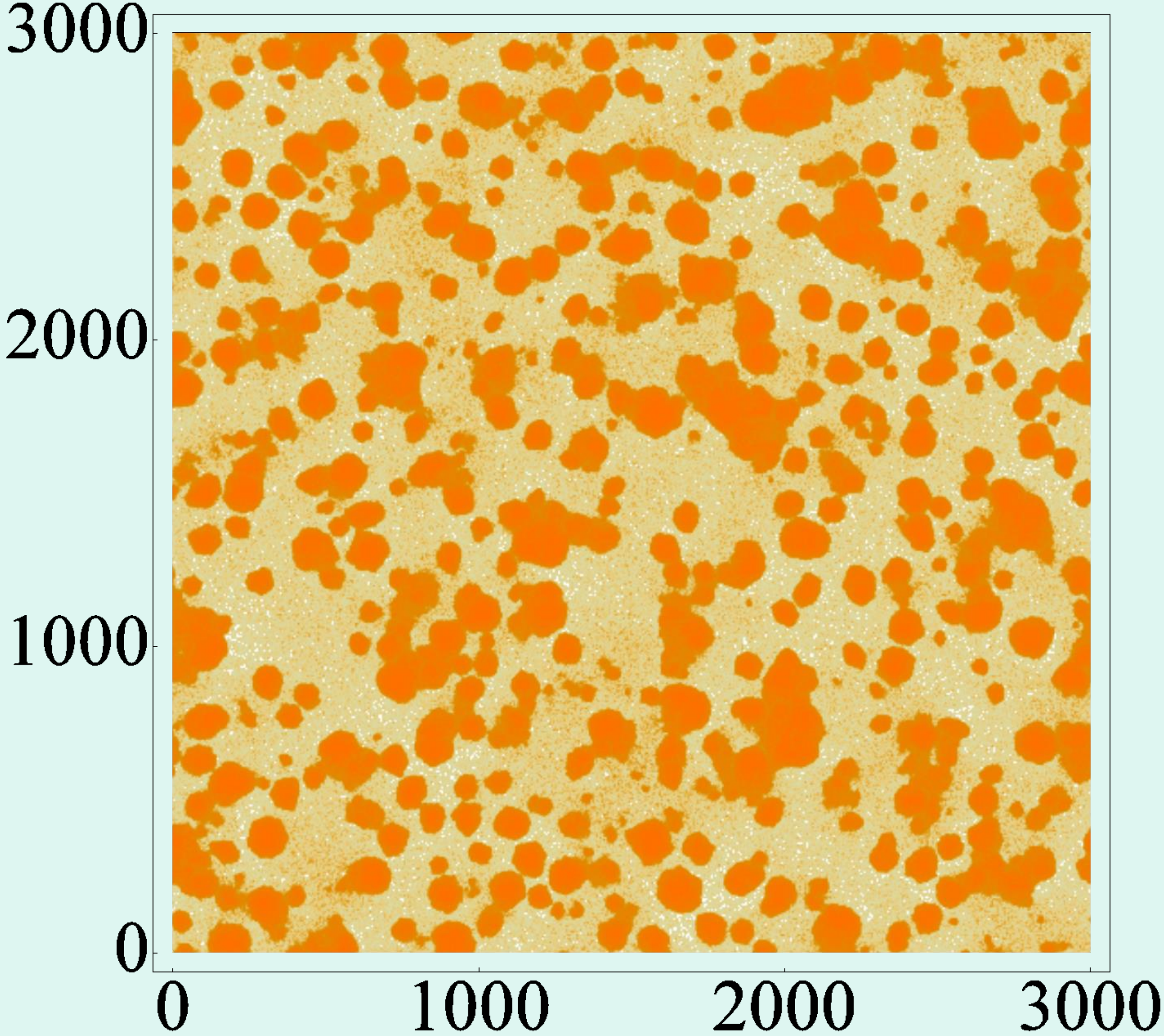


GG&Corberi&Zannetti, JPA2014,PRE2015 etc

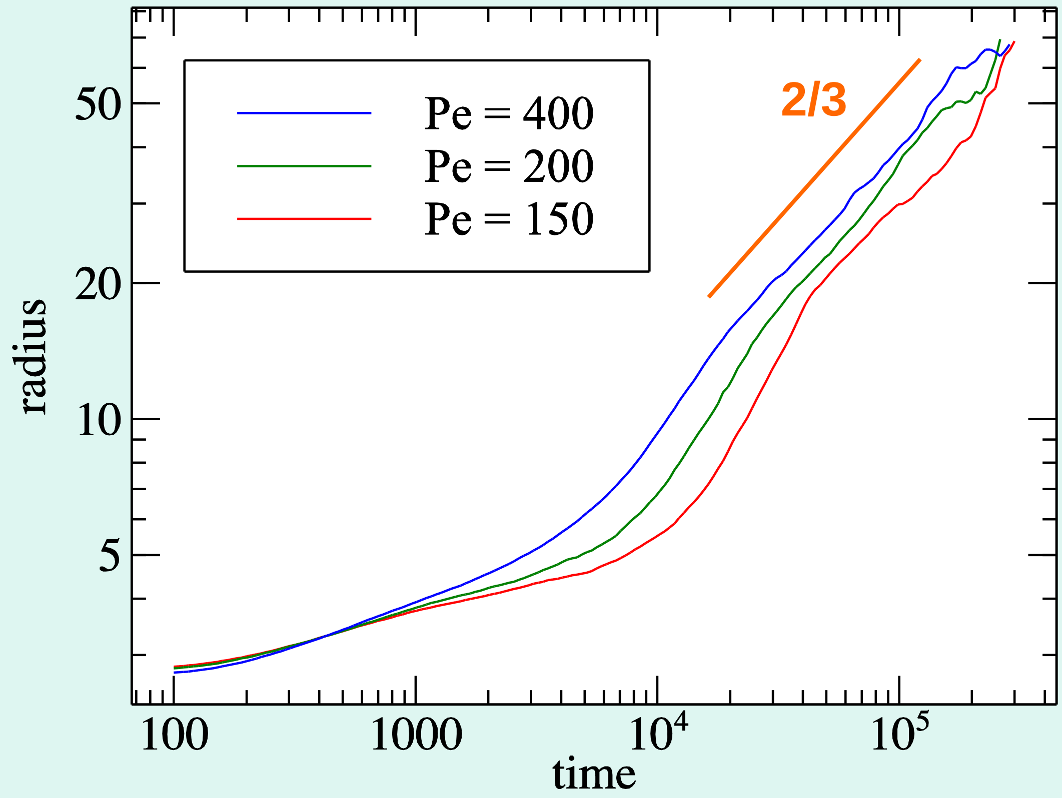
Exact calculations show a discontinuity in the third derivative of the large deviation function

Kinetics of aggregation

Growth kinetics



Growth laws



Conclusions

- Very rich diffusion behavior.
- Rotational diffusion increases with density at large Peclet number. Non-gaussian fluctuations.
- Peculiar behavior of velocity fluctuations. Condensation?
- Motility-induced phase separation is favored by the shape of dumbbells.
- Clusters rotate. Angular velocity is proportional to the inverse of the radius; polarization shows a spiral pattern.

Suma, Gonnella, Marenduzzo & Orlandini EPL 2014
Suma, Cugliandolo, Gonnella, Lamura, Mossa PRE 2014,
Cugliandolo, Gonnella, Suma PRE 2015