Binary mixtures of active and passive particles on a frictional substrate

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Equilibrium binary mixtures

Pure active systems on a frictional substrate

Our system: governing equations

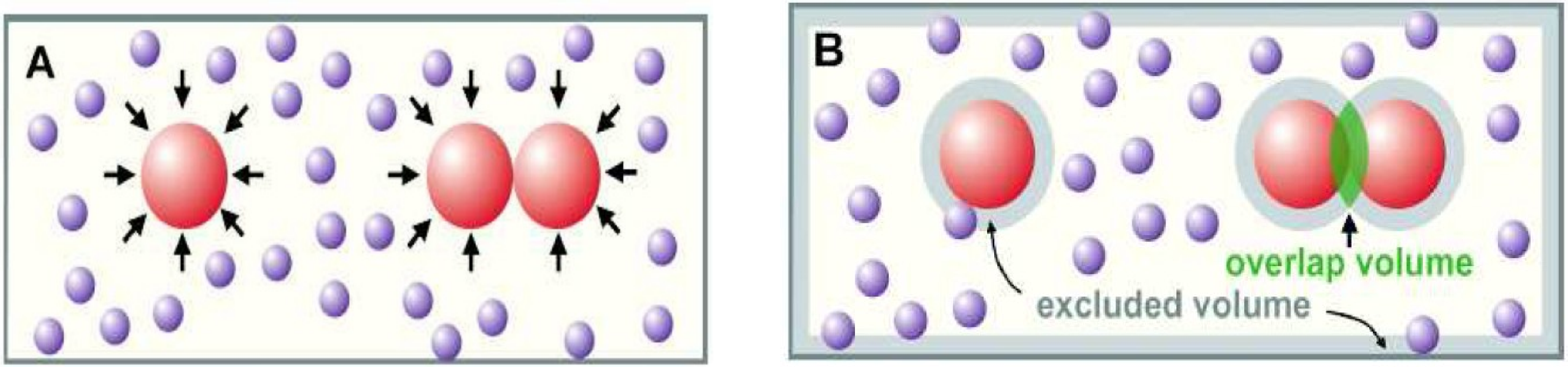
What we are interested in knowing and measuring?

Results

Conclusions

Equilibrium binary mixtures

- Phase separate even for purely repulsive interactions
- Binary mixture of hard spheres - effective attraction due to depletion
- Dense hard sphere mixtures phase separate for size ratios > 5 [T. Biben, Hansen (PRL) 1991].
- First order phase transition [D. Frenkel and Ard A. Louis, PRL (1992)] .



Purely repulsive self-propelled particles

- At large densities, a system of self-propelled particles interacting solely via steric repulsion, phase separate into a concentrated fluid or liquid phase and a gas-like dilute phase [Tailleur and Cates, 2008; Fily and Marchetti, 2012; Fily et al., 2014]

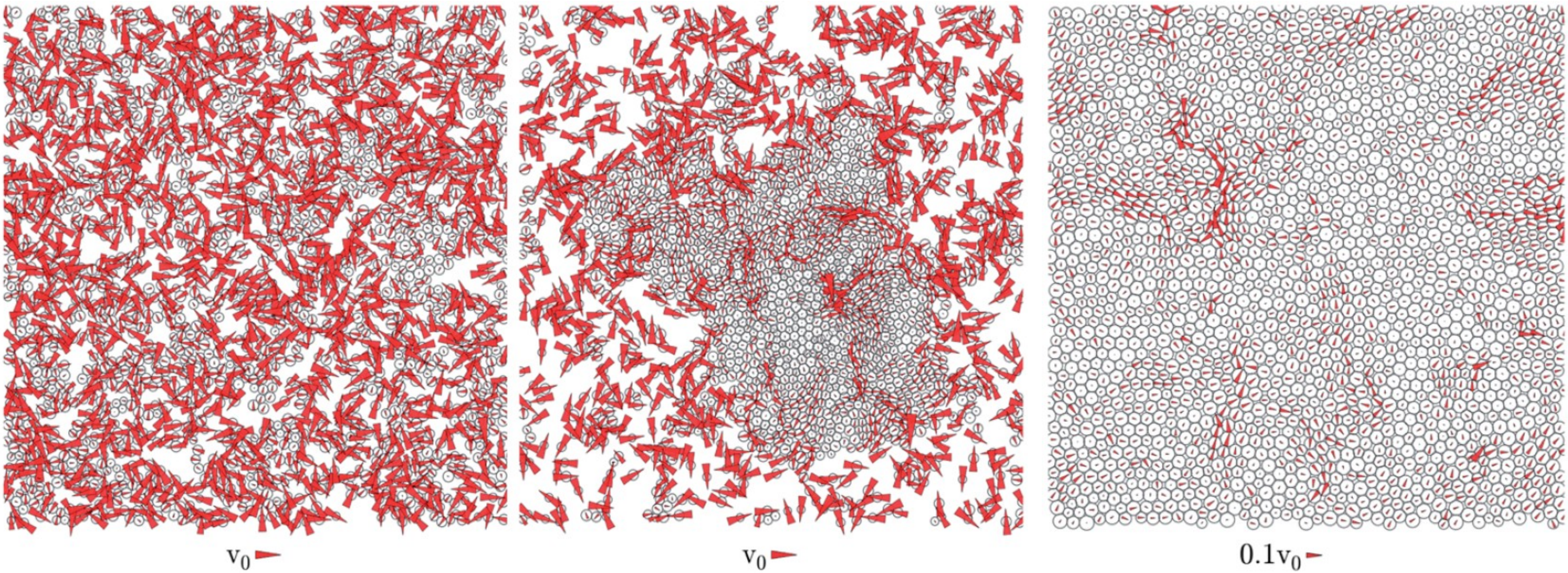
- Mechanism – motility induced phase separation

- Self-propelled discs on a 2D substrate [Fily et al , 2014] distinct regimes:

  homogenous fluid phase

  phase separated fluid

  frozen phase



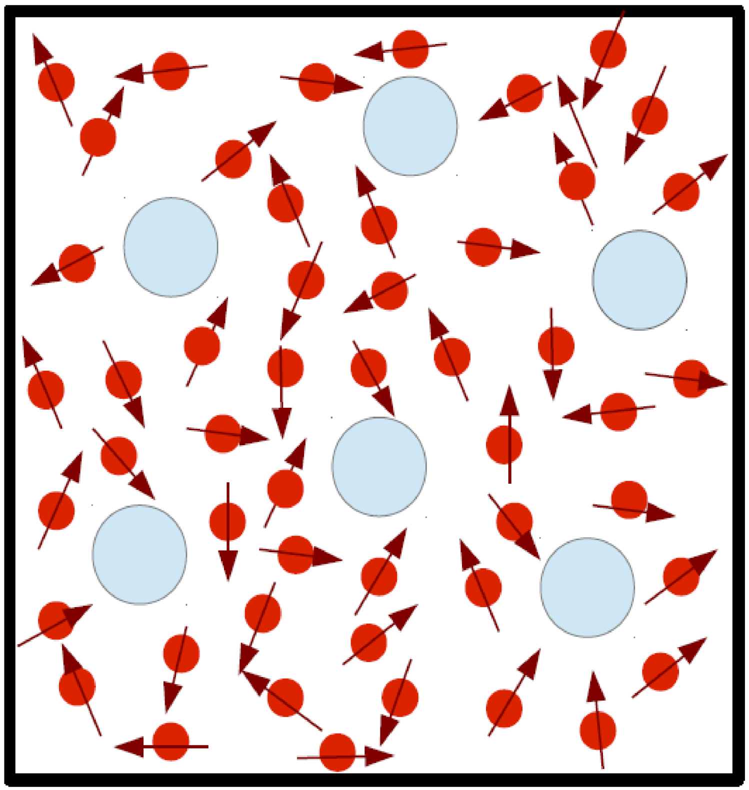
ϕ_s =0.5

ϕ_s =0.9

Fily et al. , Soft Matter, 10, 2014.

The System

- Assymetric mixture of active and passive particles.
- Active particles have constant self-propulsion speed v_1
- Orientation changes randomly over a time scale $\tau = \nu_r^{-1}$
- No translational noise in both species
- All interactions soft and repulsive



Governing equations

- Equations of motion of active particles

$$\partial_t \mathbf{r}_i = v_1 \hat{\boldsymbol{\nu}}_i + \mu_1 \sum_{i \neq j} \mathbf{F}_{ij}^1 \,, \;\; \partial_t \theta_i = \eta_i^r(t) \,.$$

- $\hat{\boldsymbol{\nu}}_i = (cos\theta_i, sin\theta_i)\,, < \eta_i^r(t)\eta_j^r(t') >= 2\nu_r \delta_{ij}\delta(t - t').$
- Equation of motion of passive particles

$$\partial_t \mathbf{r}_i = \mu_2 \sum_{i \neq j} \mathbf{F}_{ij}^2 \,.$$

- Particles are athermal.
- $\mathbf{F}_{ij} = F_{ij}\hat{\mathbf{r}}_{ij}$ with $F_{ij} = k(\sigma_i + \sigma_j - r_{ij})$ if $r_{ij} \leq \sigma_i + \sigma_j$ and $F_{ij} = 0$ otherwise where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$.

Length and time scales

Time scales

- ν_r^{-1} - time over which orientation of active velocity changes
- μk^{-1} - elastic time scale
- σ_1/v_1 - time taken by an active particle to travel 1 radius

Lengths

- σ_1 radius of active particle
- average distance between particles $= (L^2/N)^{1/2}$

* angular Peclet number

  $Pe = v_1/\sigma_1\nu_1$

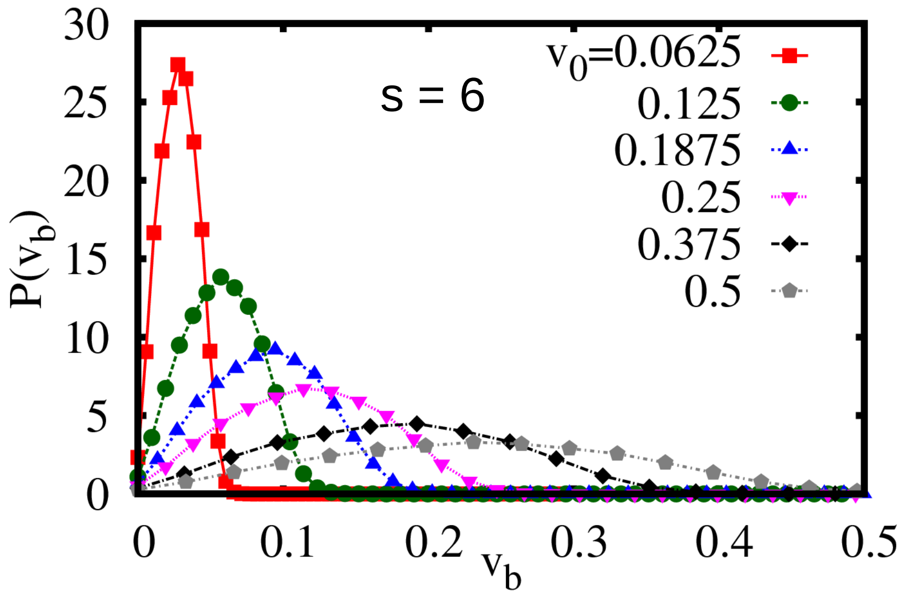
* activity $v_0 = v1/(\sigma_1\mu k)$
* asymmetry in size: $s = \sigma_2/\sigma_1$

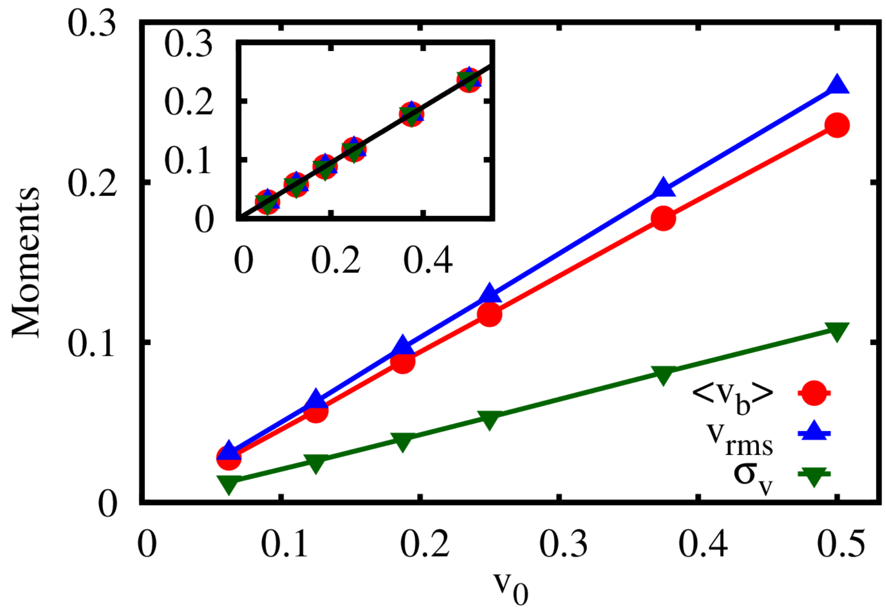
Dilute phase: dynamics of passive particles

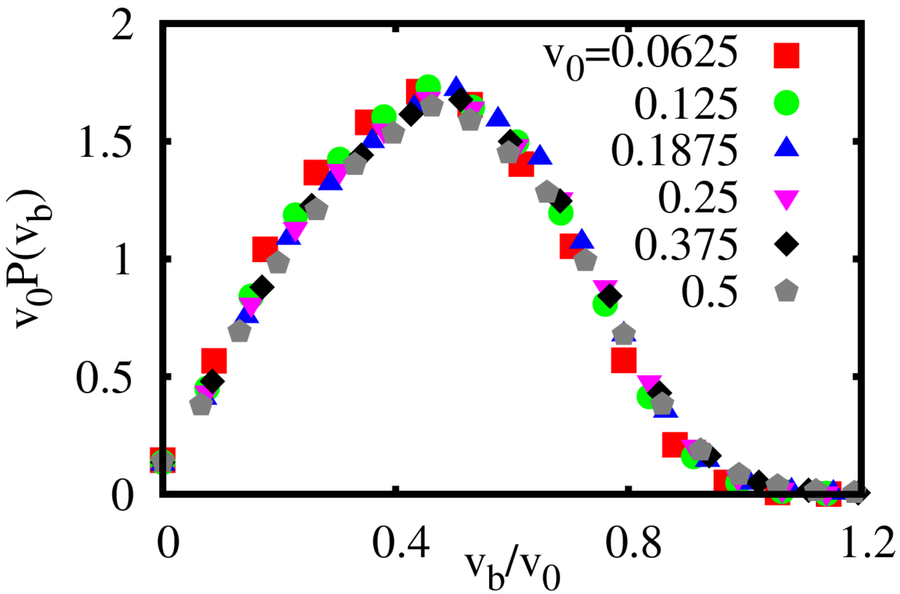
- Velocity distributions:

  $\phi_b = 0.1$, $\phi_s = 0.1$

- Scale with activity







Diffusivity

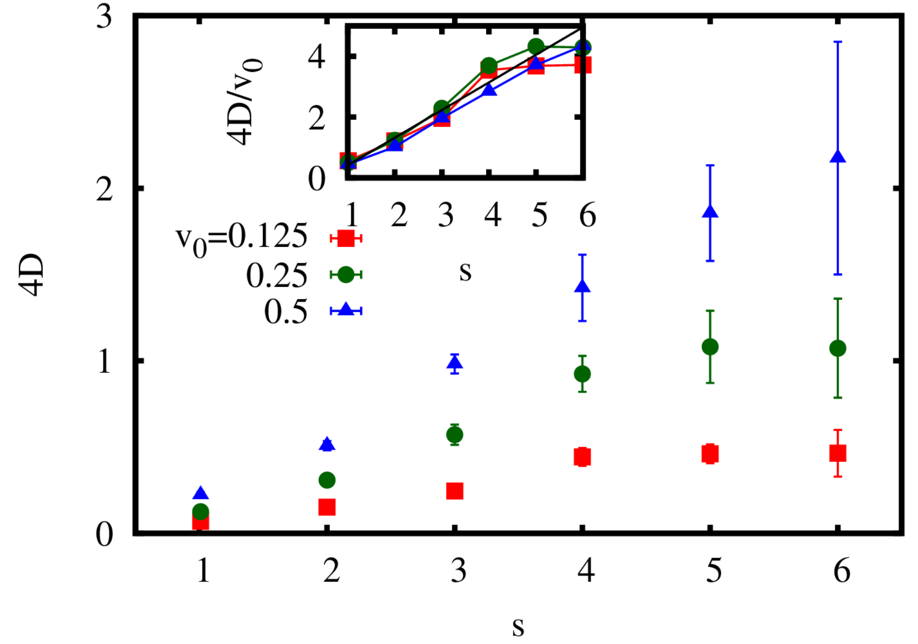
- Mean square displacement

  initial ballistic regime

  diffusive regime -long times

  $\varphi_b = 0.1$
- D scales with activity
- D increases linearly with size
- D decreases beyond a critical

  size ratio s.

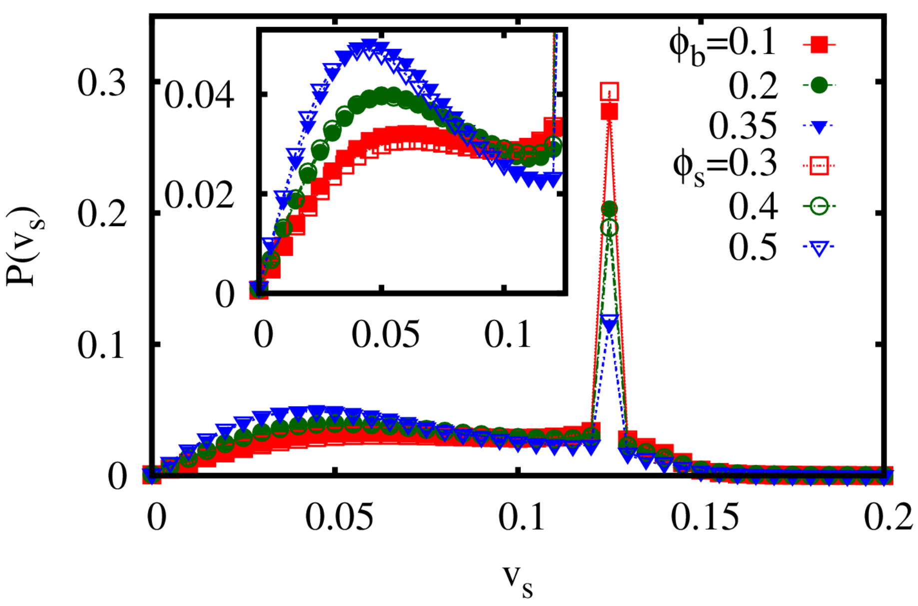


Dense mixtures

Velocity distribution of active particles

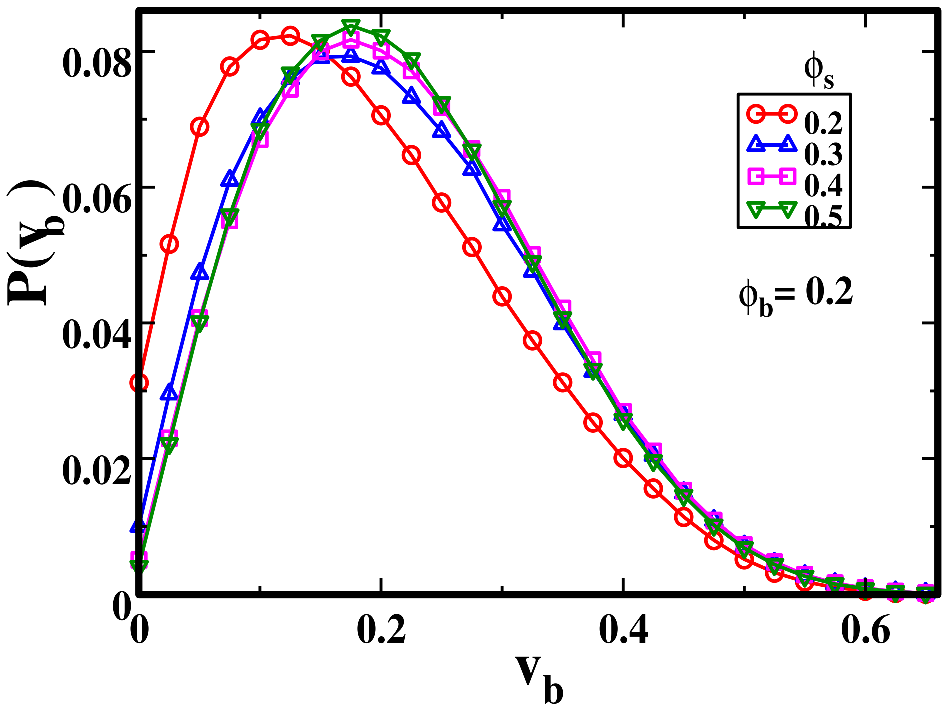
- Peaked at the self propulsion speed
- Particles slower as ϕ_s inreases
- Small hump at low velocities

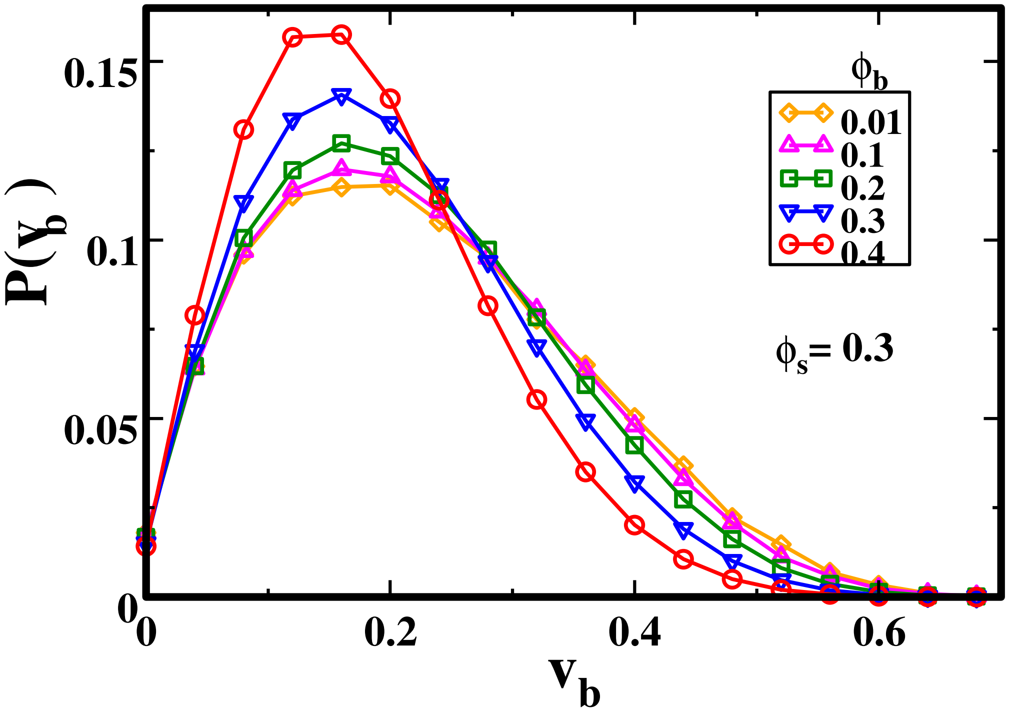
s = 5



ϕ_s	ϕ_b	ϕ_s^{eff}
0.3	0.1	0.333
0.3	0.2	0.375
0.3	0.35	0.4615
0.3	0.076	0.325
0.4	0.076	0.433
0.5	0.076	0.541

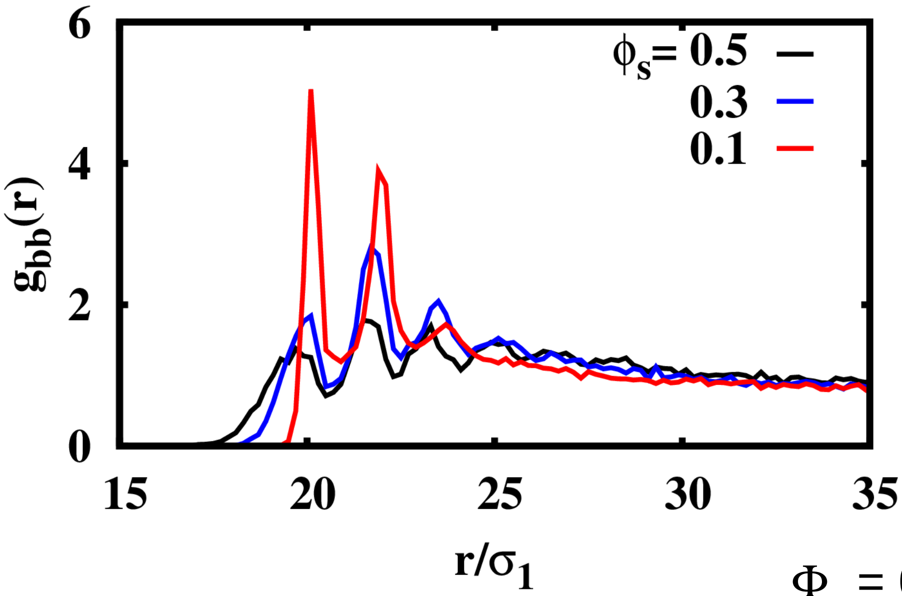
Velocity distribution of passive particles

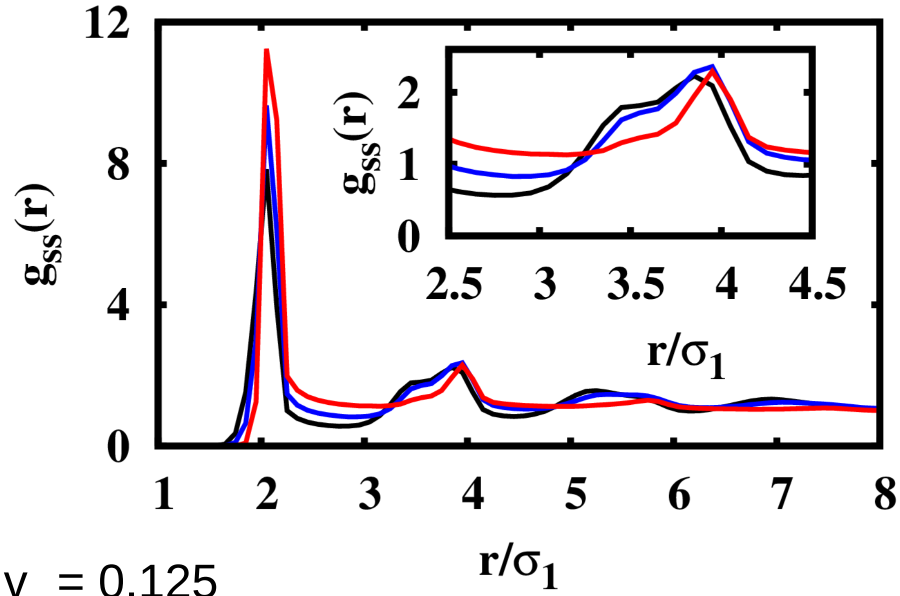




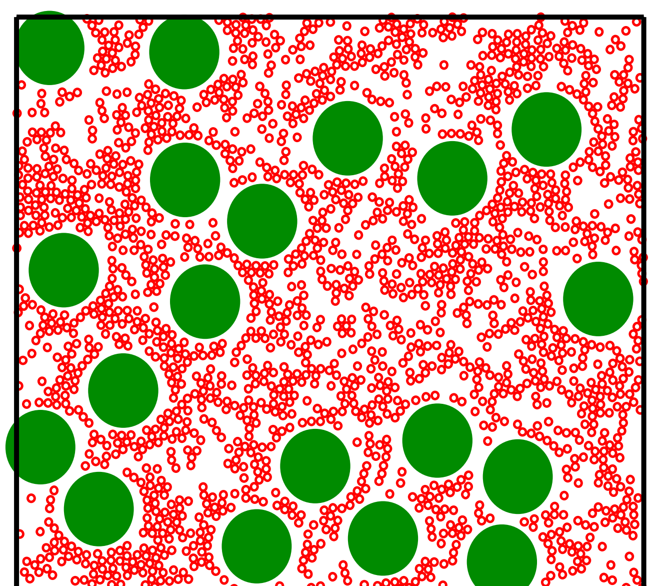
Effective interactions

- Radial distribution functions between pairs of particles



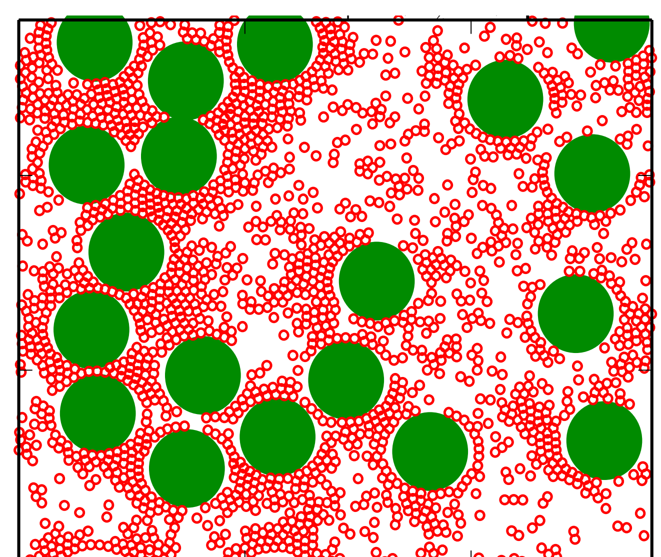


$\Phi_b = 0.3$, $v_0 = 0.125$



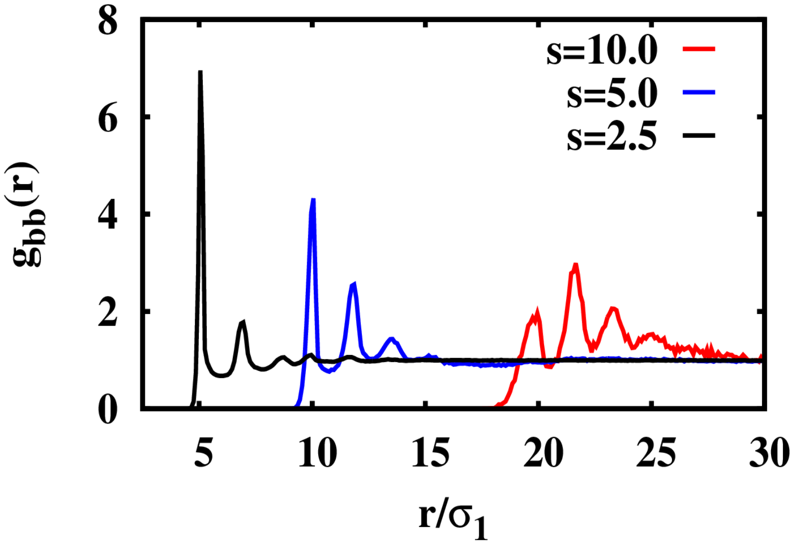
s = 10

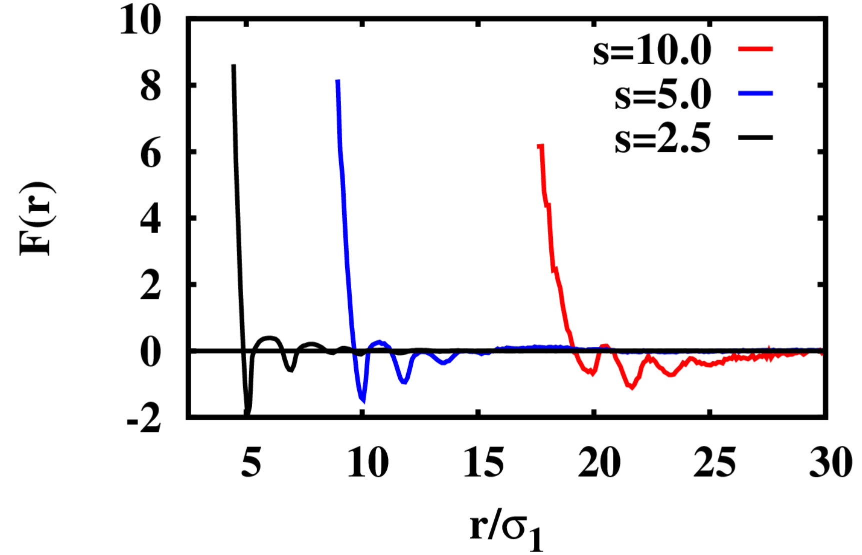
$\phi_b = \phi_s = 0.3$

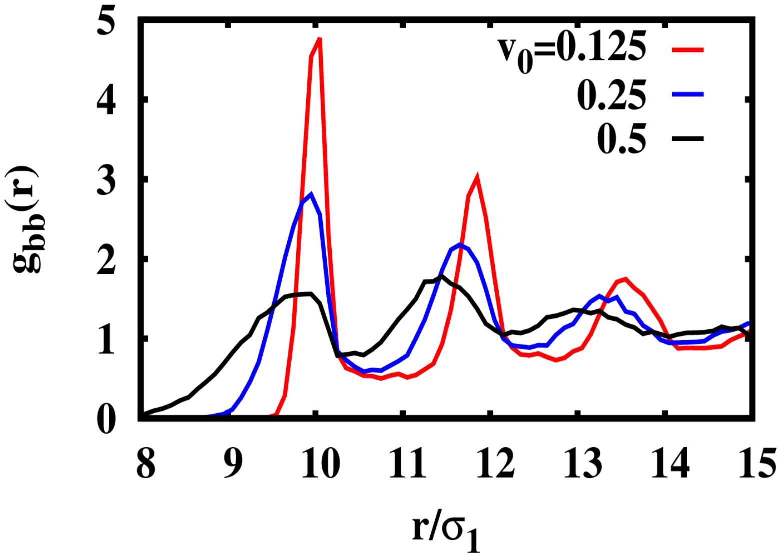


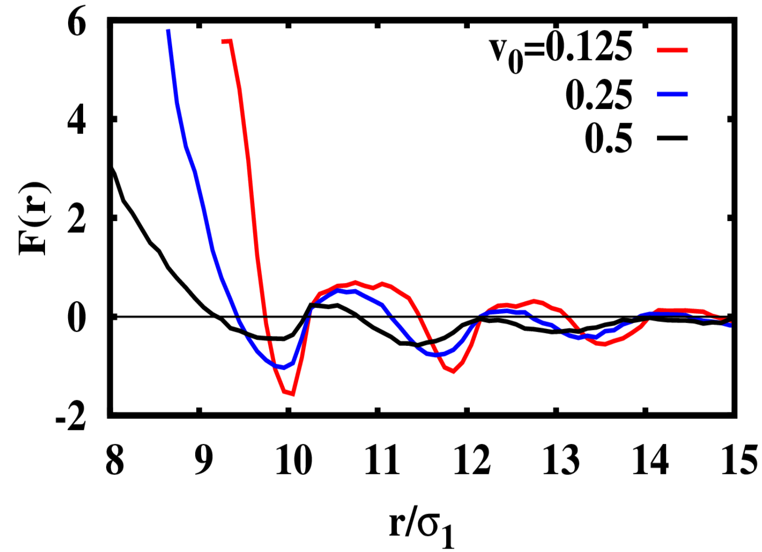
Interaction potential: $F(r) \sim -\,ln\, g_{bb}(r)$

$\phi_b = \phi_s = 0.3$



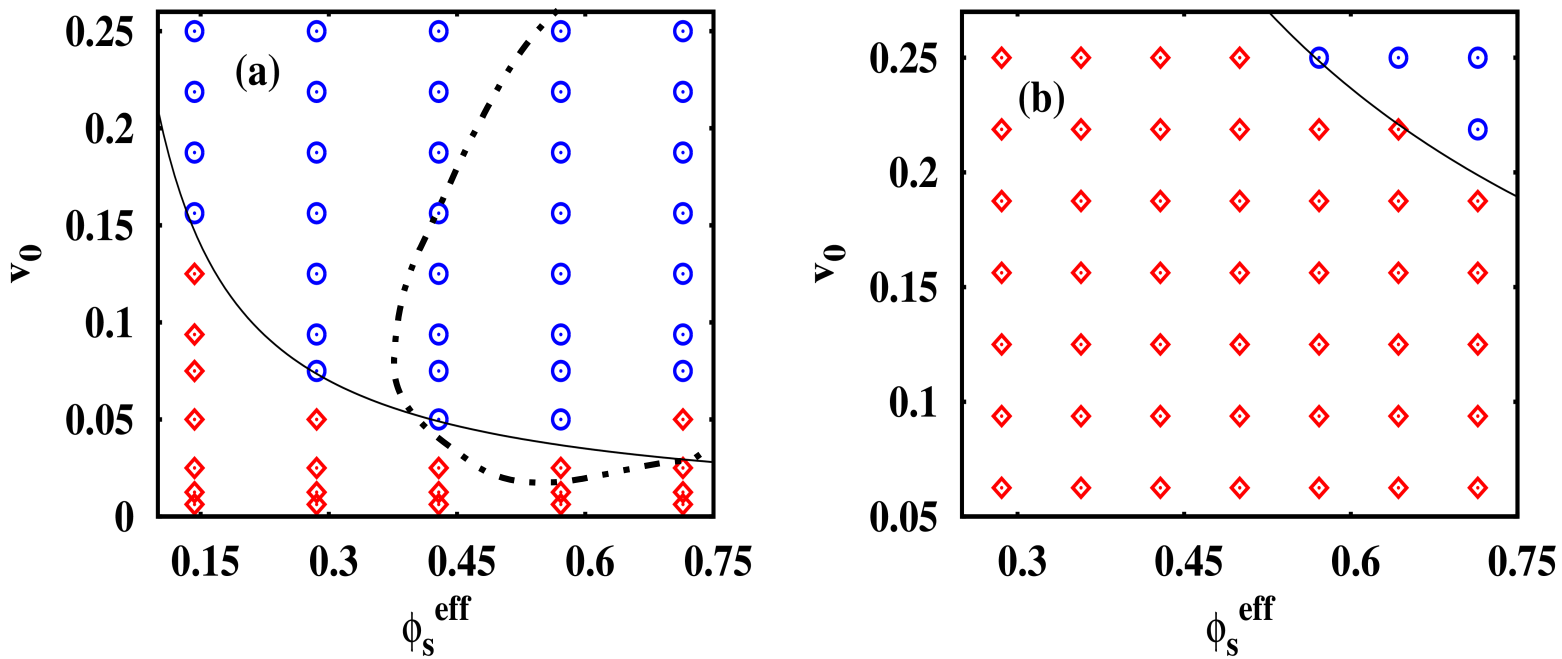






Phase diagram

- Phase 1: active particles aggregate in small not so dense clusters
- Phase 2: active particles aggregate in dense large clusters



s = 10

s = 5

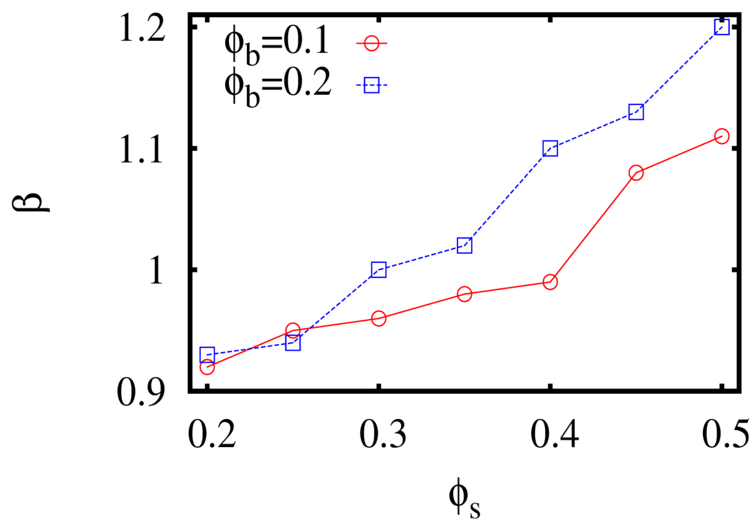
$$v_0 \sim 1/\phi_s$$

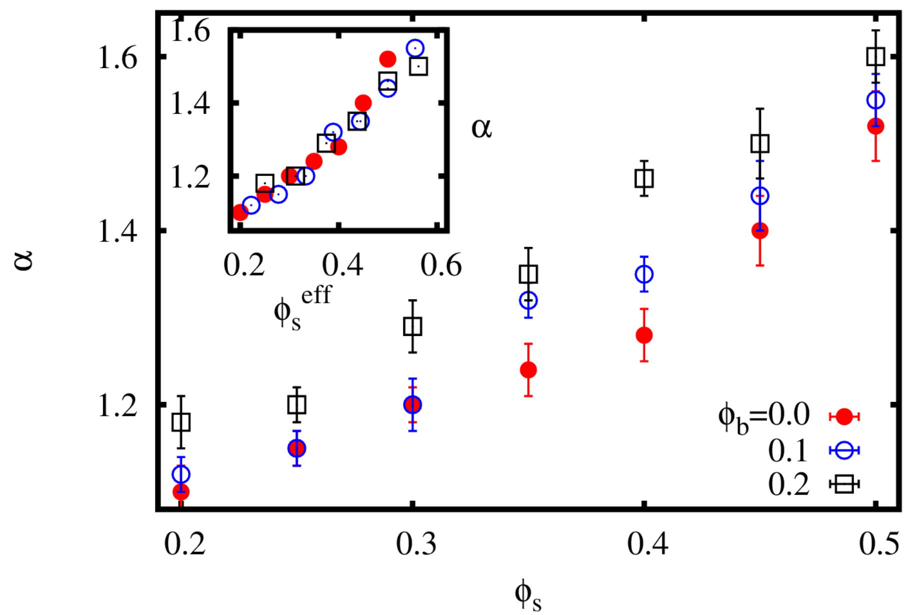
Number fluctuations

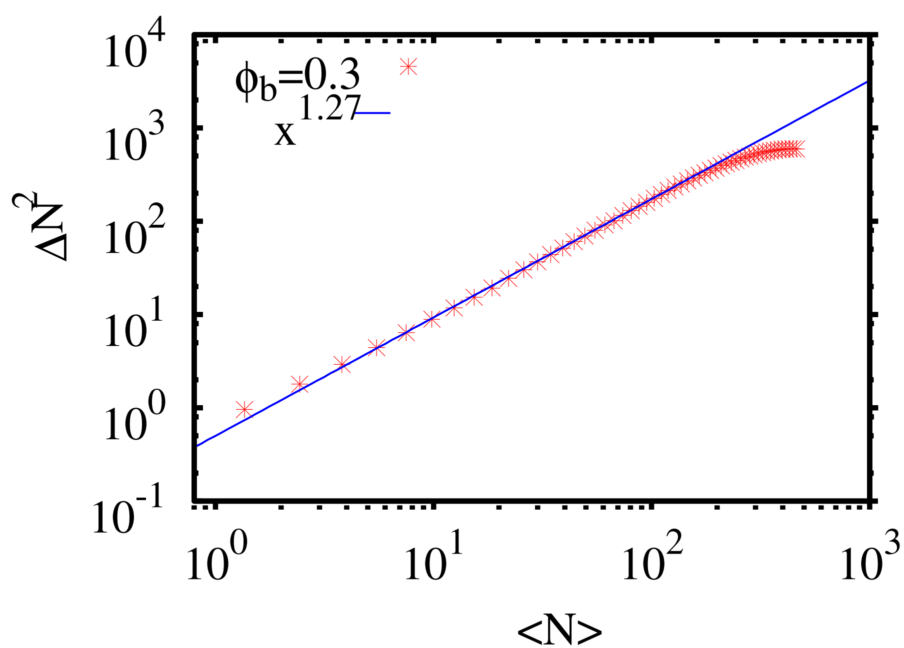
$$\Delta N_s^2 \sim N_s^{\alpha}\ , \quad \Delta N_b^2 \sim N_b^{\beta}\ .$$

α increases with ϕ_s . β > 1 for ϕ_s > 0.4

ϕ_s	ϕ_b	α	β
0.4	0.1	1.35±0.02	1.0±0.01
0.45	0.1	1.44±0.04	1.08±0.02
0.5	0.05	1.53±0.03	1.05±0.02
0.5	0.1	1.55±0.03	1.11±0.02
0.5	0.2	1.55±0.03	1.22±0.03





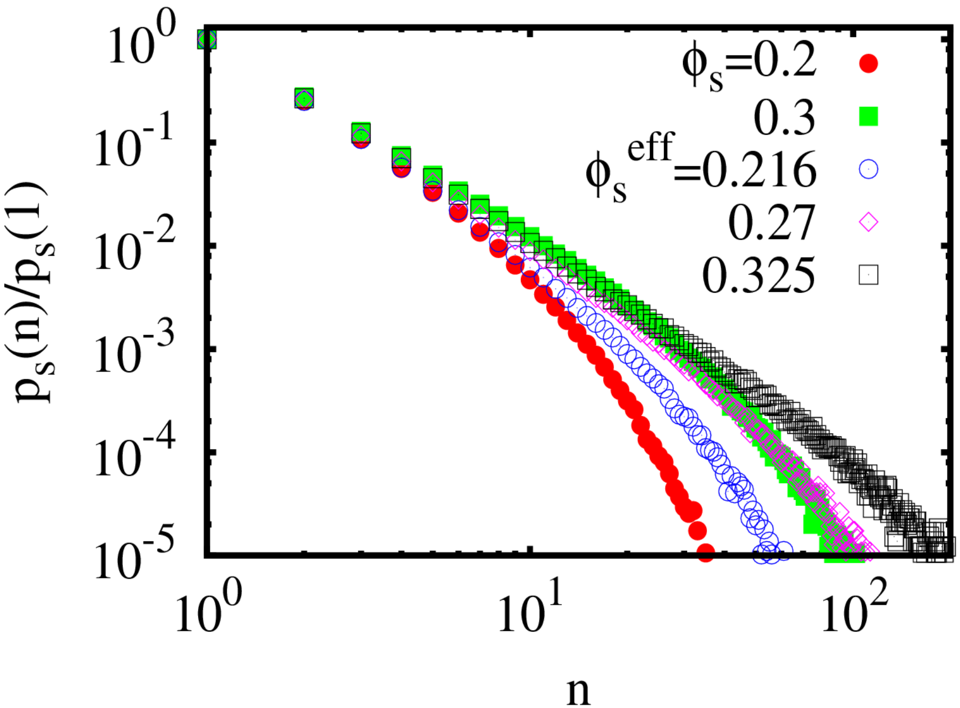


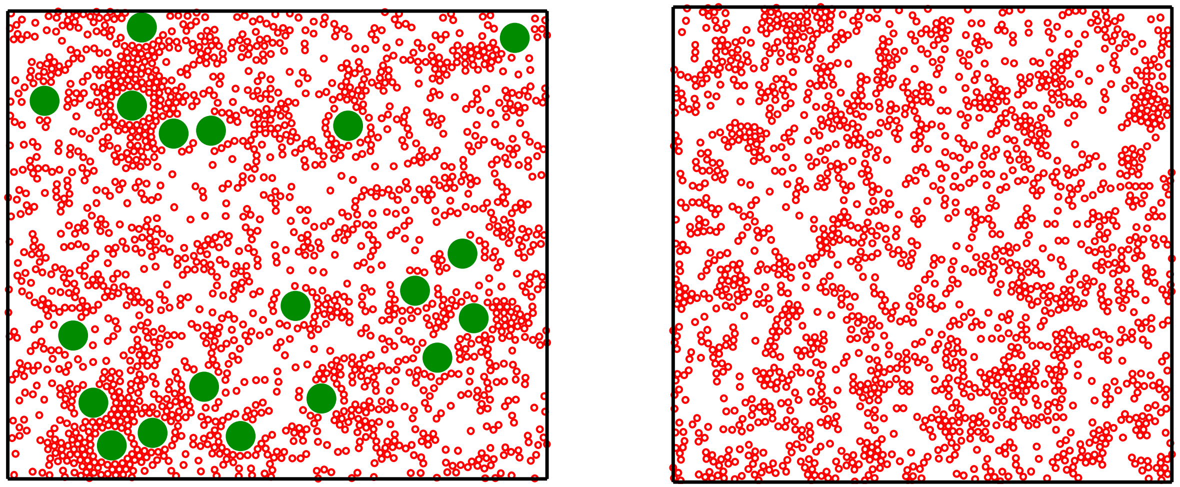
Cluster Formation

- Pure active system: homogenous fluid or phase separated phase

- Passive particles enhance clustering/aggregation of active particles.

ϕ_b=0.076 v_0 = 0.125



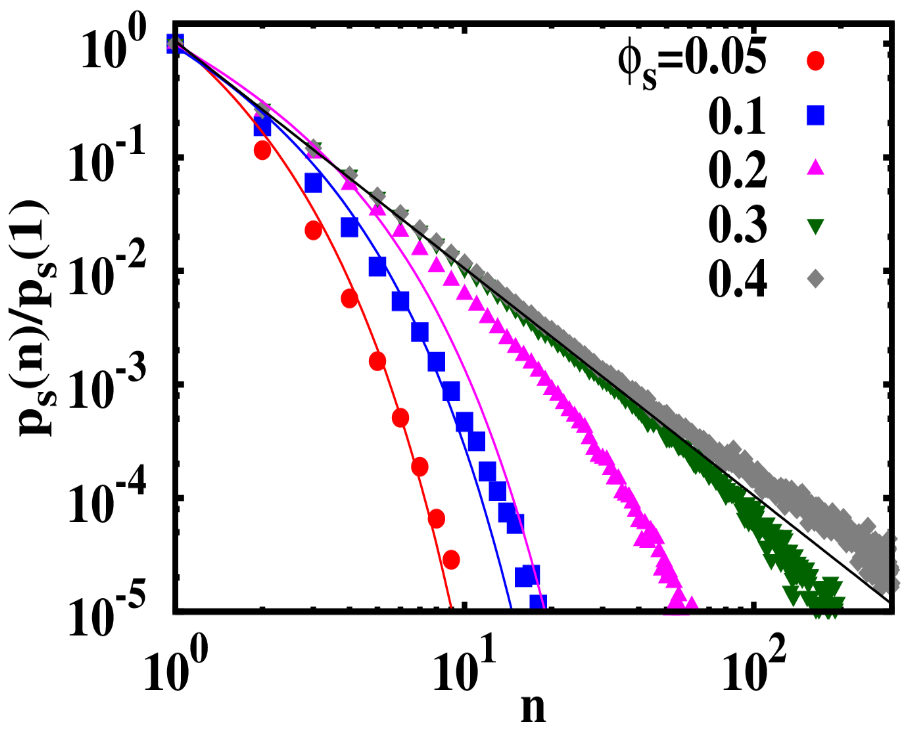


s = 5

ϕ_s = 0.3

Cluster size distribution

- for small ϕ_s, CSD fits to $f(n) = exp(-n/n_0) /n$
- n_0 mean cluster size
- For large ϕ_s, CSD follows a power law
- power law $\sim 1/n^2$

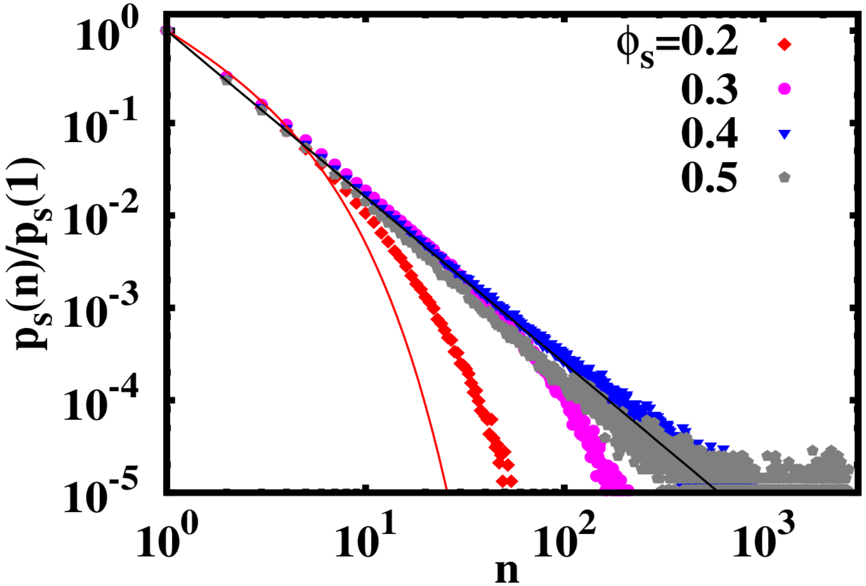


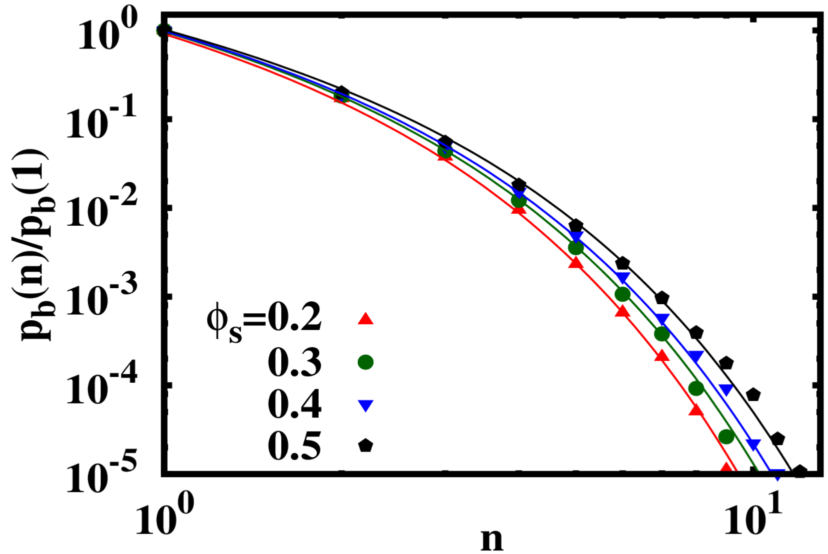
s = 5 , ϕ_b = 0.076

v_0 =0.125

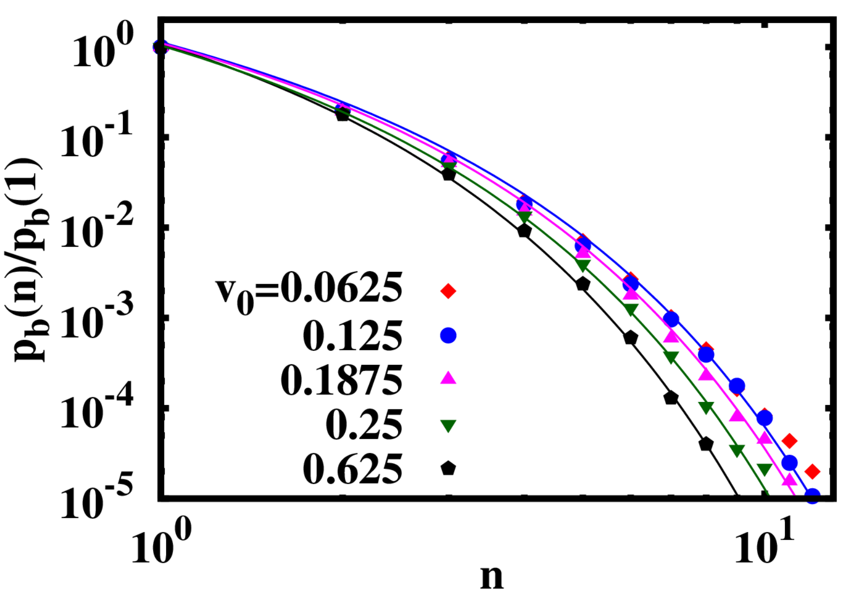
Cluster size distributions: variation with ϕ_s, activity

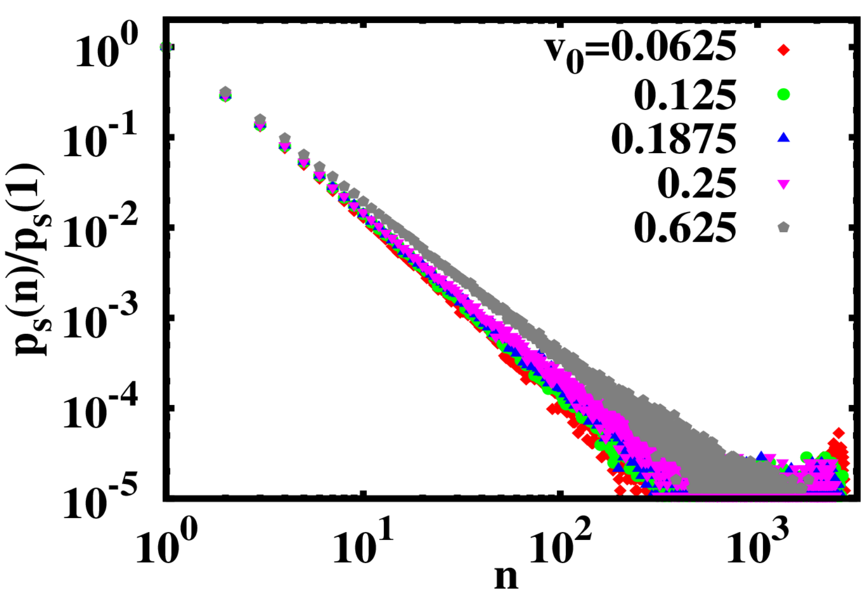
$\phi_b = 0.1$





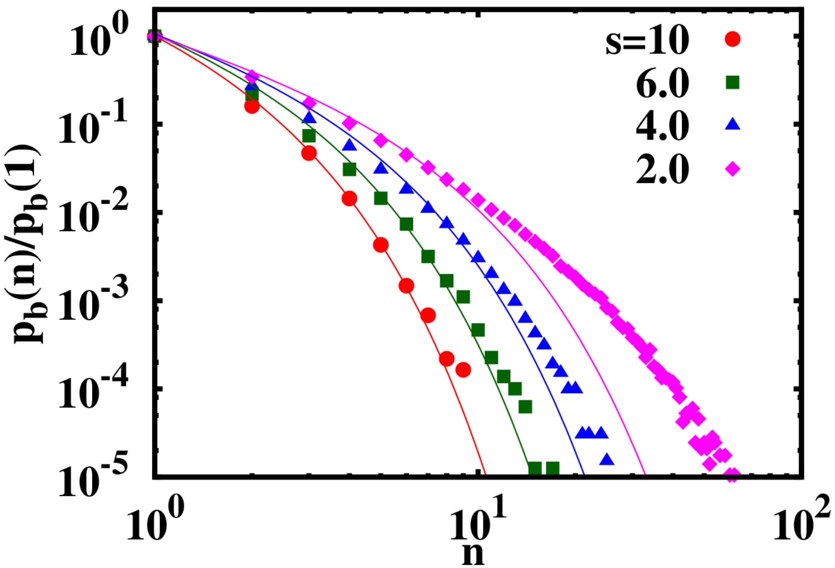
ϕ_b=0.1 , ϕ_s = 0.5

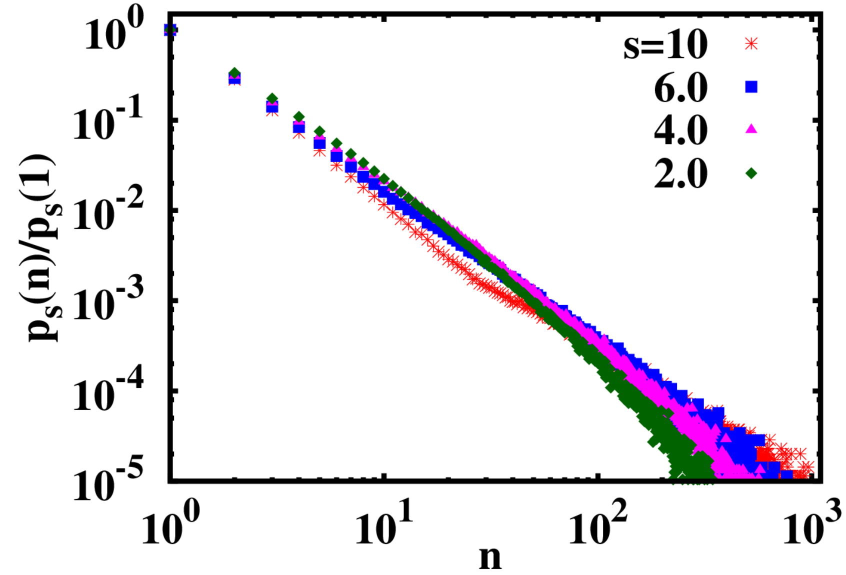


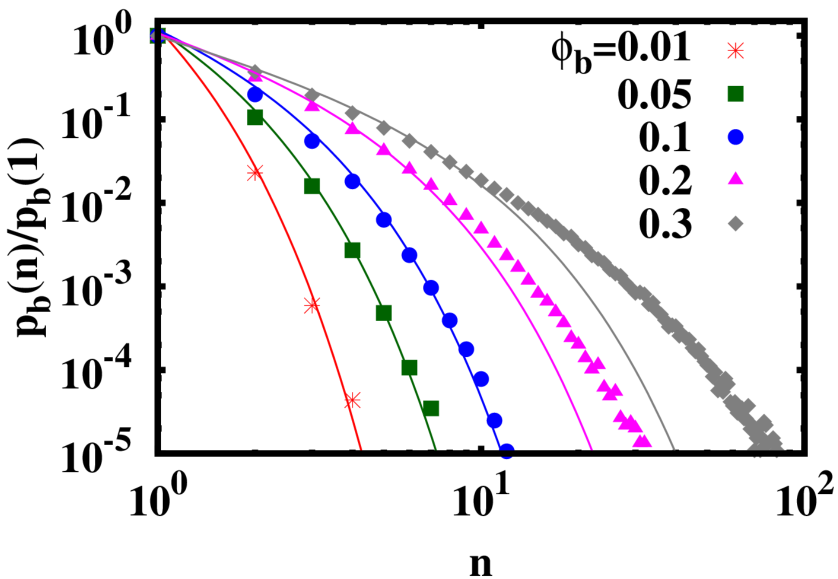


Cluster size distribution: variation with asymmetry

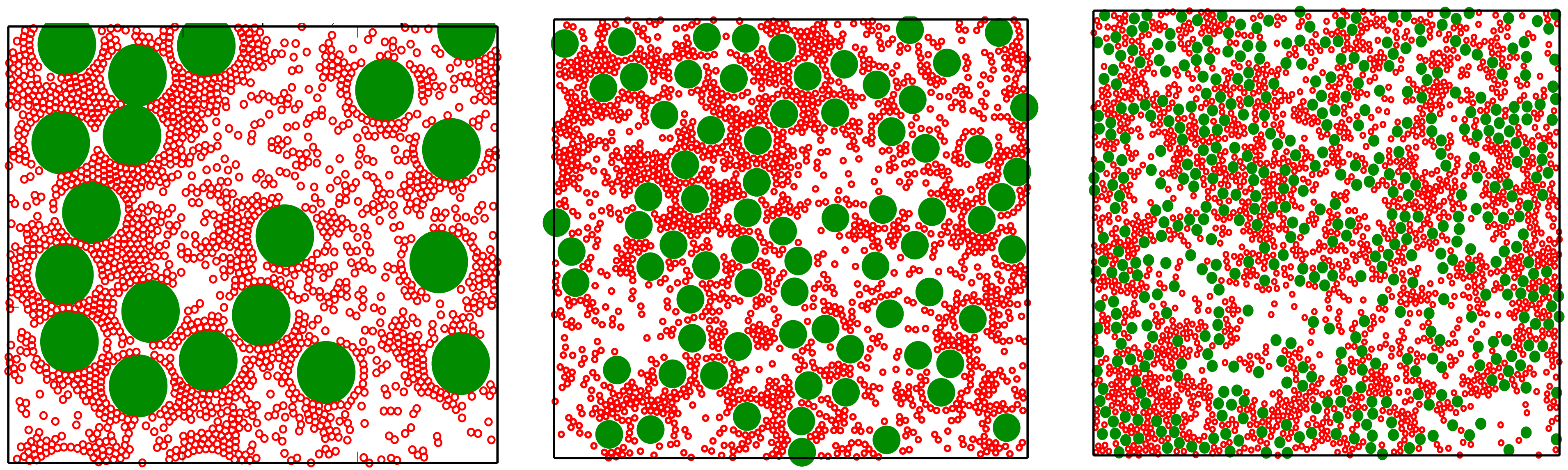
$\phi_b = \phi_s = 0.3$







$\phi_s = 0.5$



s = 10   s = 5   s = 2

$\phi_b = \phi_s = 0.3$ $v_0 = 0.125$

Results

- Dilute mixtures

  Passive particles : velocity distribution scales with activity, diffusivity varies linearly with size, decreases for large sizes

  Active particles: slower in the presence of passive particles, velocity distribution developes a small peak at small v_s for large ϕ_s . Passive particles enhance this peak.

- Dense mixtures

  No phase separation as in equilibrium binary mixtures.

  Active particles hamper clustering of big passive particles

  Motility induced clustering: passive particles enhance aggregation of active particles. Small particles hamper formation of dense clusters, large particles enhance cluster formation, in particular, large dense aggregates.

Thank you