Aggregation & Segregation of Confined Active Particles

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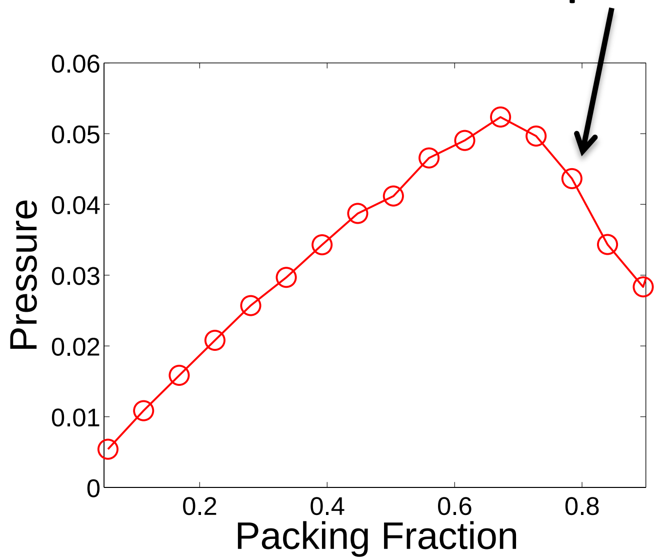
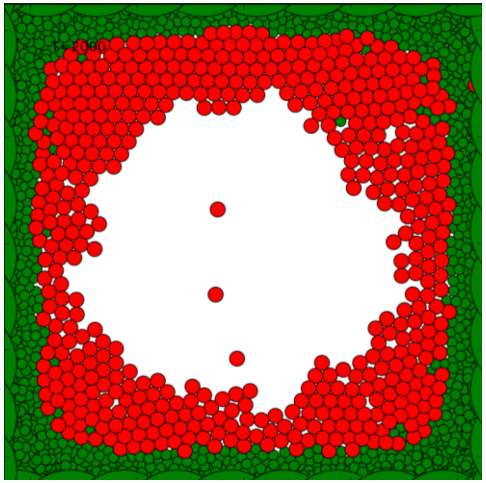
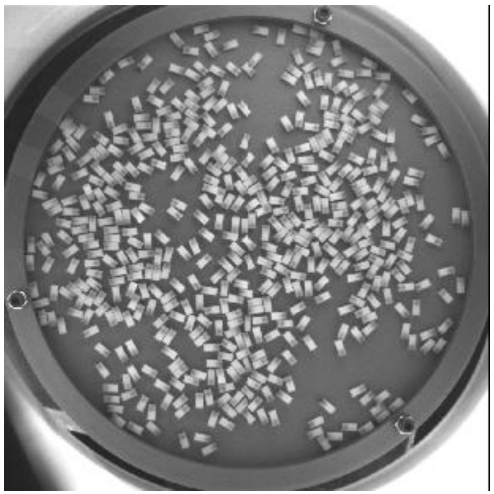
- Aggregation at wall
- Critical speed required for aggregation
- Non-monotonic pressure



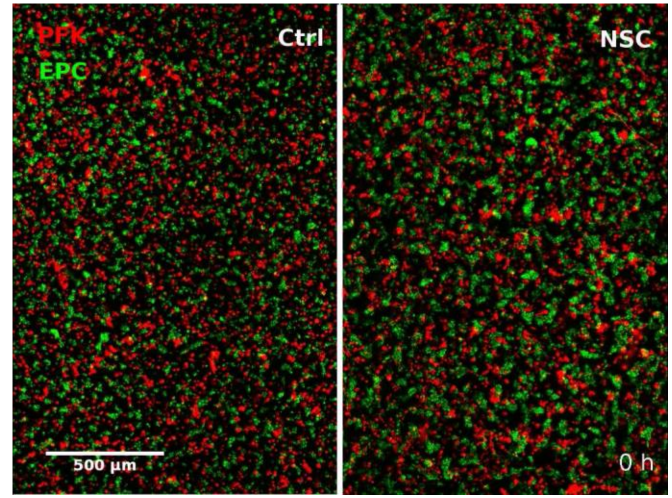


- Segregation without adhesion

Confined Active Matter



Kudrolli et al. (PRL 2008):
Vibrated granular rods



Méhes et al. (PLoS one 2012):
Cell sorting in co-cultures

Models of segregation:

S. R. McCandlish et al, Soft Matter (2012)

Belmonte et al. PRL (2008)

What happens to confined self-propelled particles without alignment and attraction?

Model of Self-Propelled Particle

Over-damped equations of motion

$$\partial_t \vec{r}_i = v_0 \vec{u}_i + \mu \sum_j \vec{F}_{ij}$$

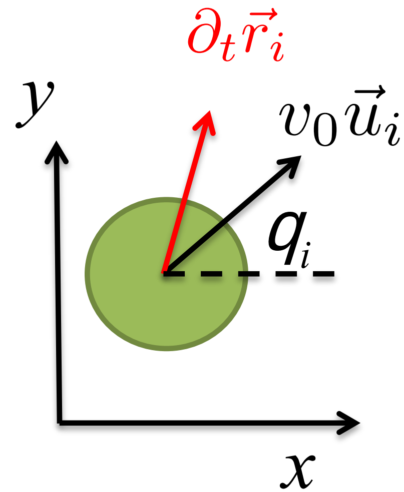
v_0 : Active velocity

$$\partial_t \theta_i = \eta_i(t)$$

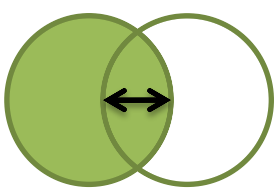
μ : Mobility

$$\langle \eta_i(t)\eta_j(t') \rangle = 2D_r \delta_{ij} \delta(t - t')$$

D_r : Rotational diffusion rate



Harmonic potential interaction



$$\vec{F}_{ij} = -k \delta \hat{r}_{ij}$$

δ: Overlap

Persistent random walker:

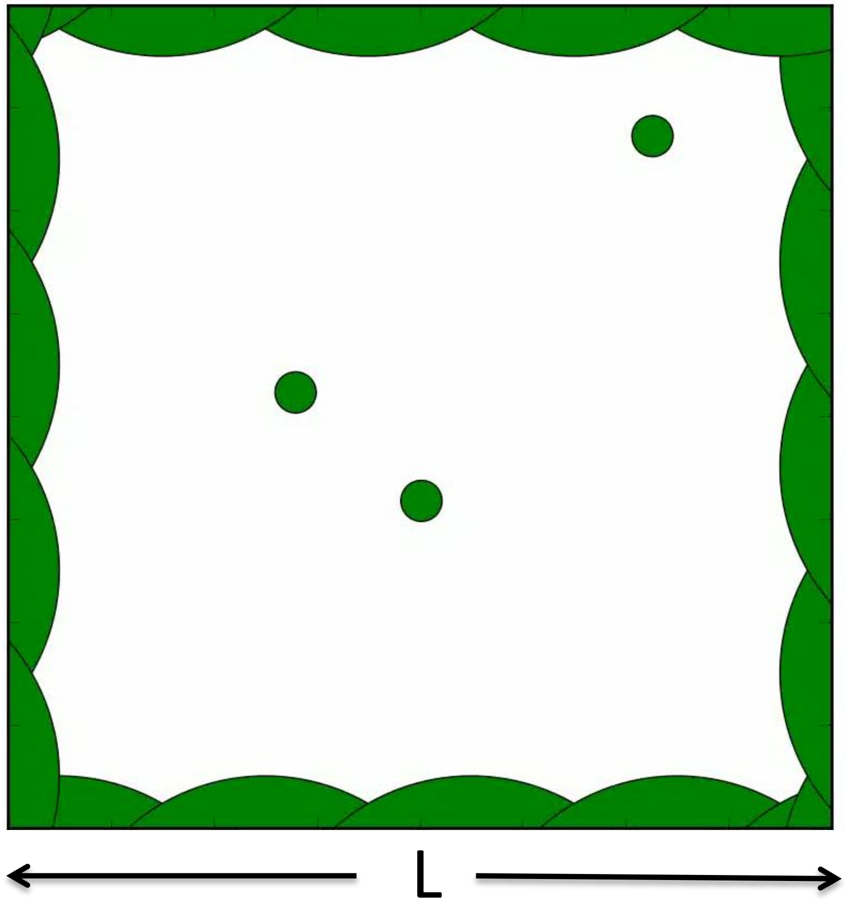
Short-time ballistic motion with v_0

Long-time diffusion with $D = \frac{v_0^2}{2D_r}$

Szabo et al 2006; Peruani et al 2006; Chaté et al 2008; Henkes et al, 2011;
Fily et al 2012; Redner et al 2013; S. A. Mallory et al 2013; …

Confinement in 2D Box

Immobile particles are glued to the wall to confine the system.



Control parameters:

v_0 : Active velocity

D_r : Rotational diffusion rate (time^{-1})

ϕ : Packing fraction

$$= \frac{\text{active particle area}}{\text{accessible area}}$$

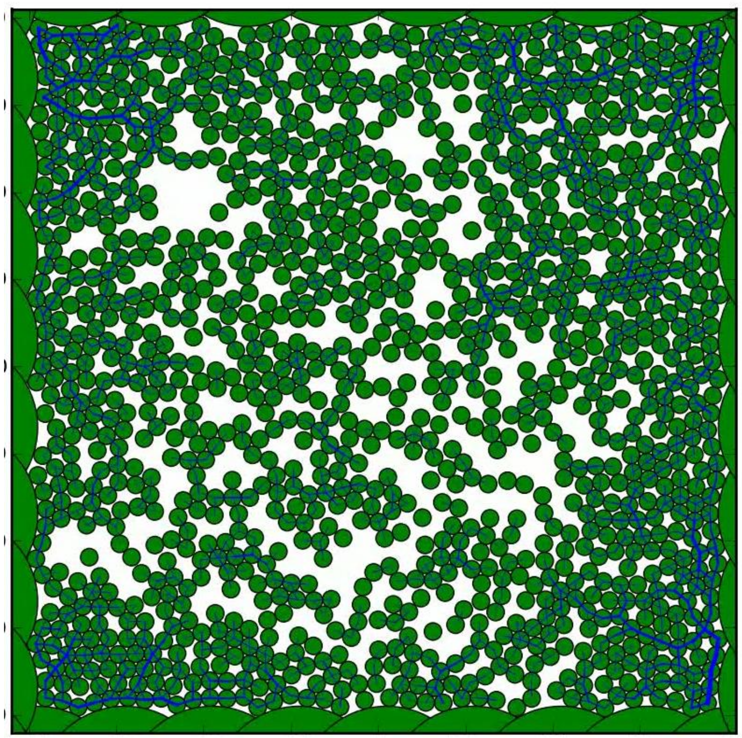
ρ : Number density

$$= \frac{\text{\# of active particles}}{\text{accessible area}}$$

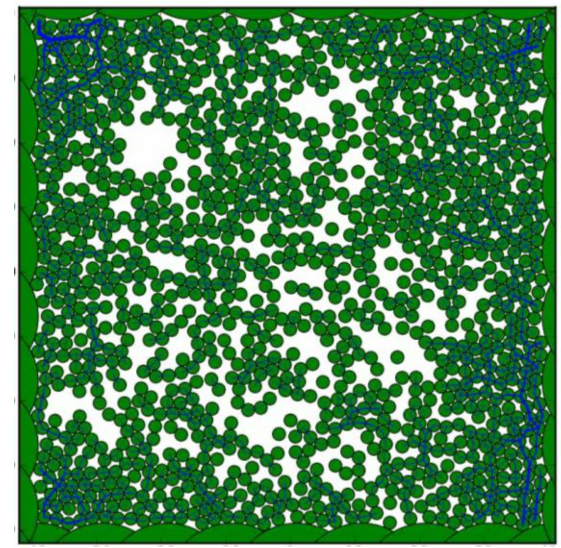
L : System size

Confined Monodisperse System

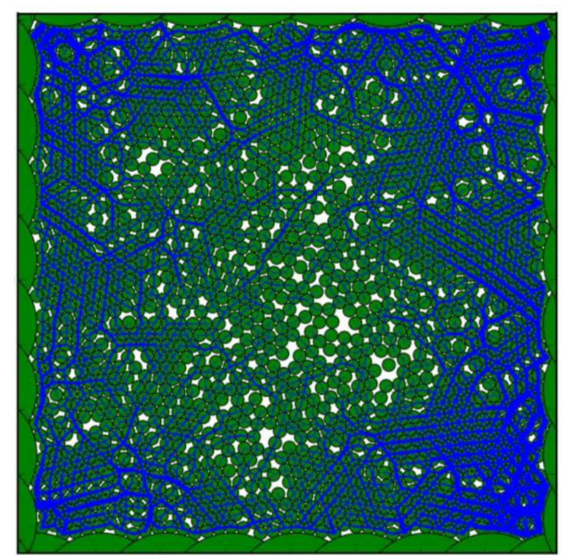
Small rotational diffusion rate



Increase Rotational diffusion



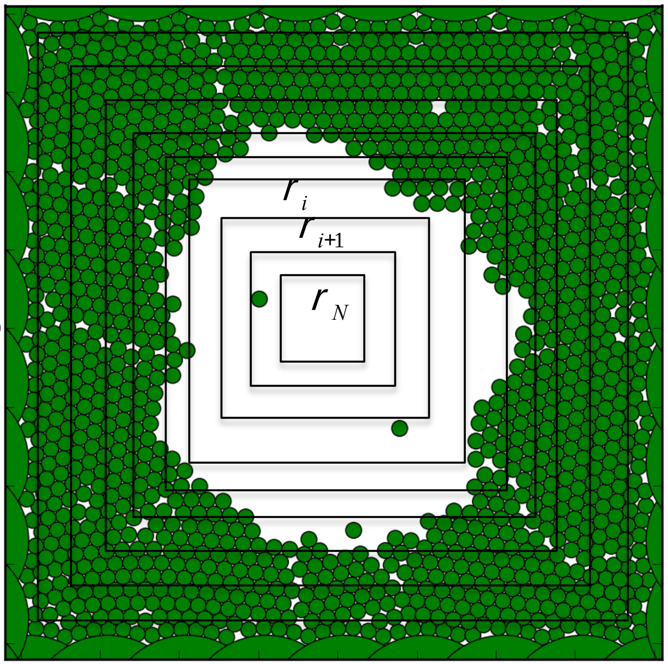
Increase Packing fraction



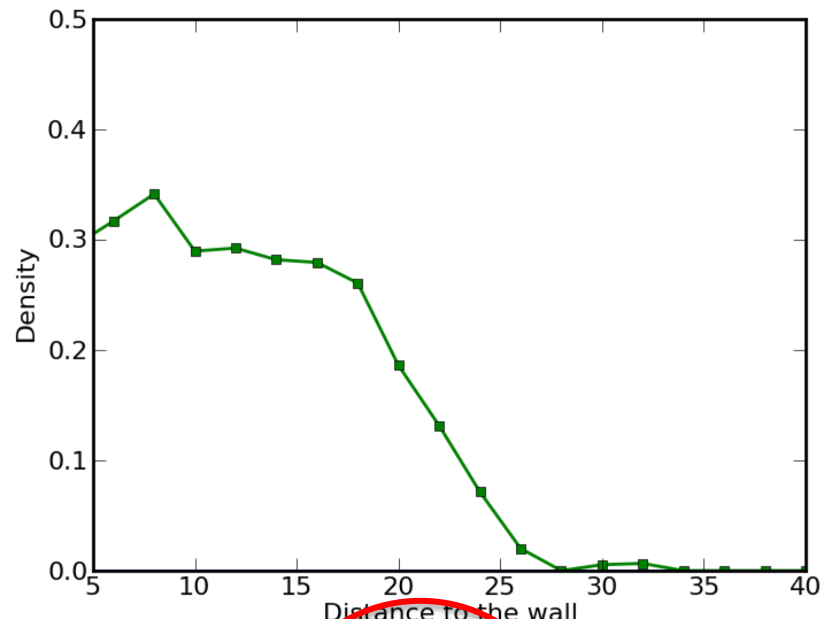
1. Aggregation
2. Inhomogeneous forces

Quantification of aggregation

Divide the system into nested square strips:

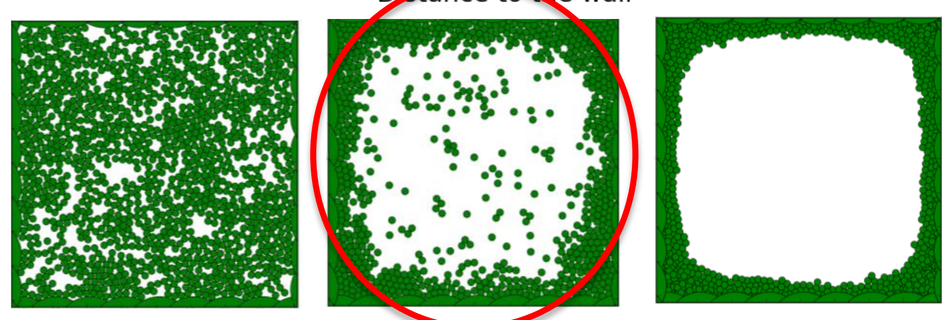


Density vs. Distance:



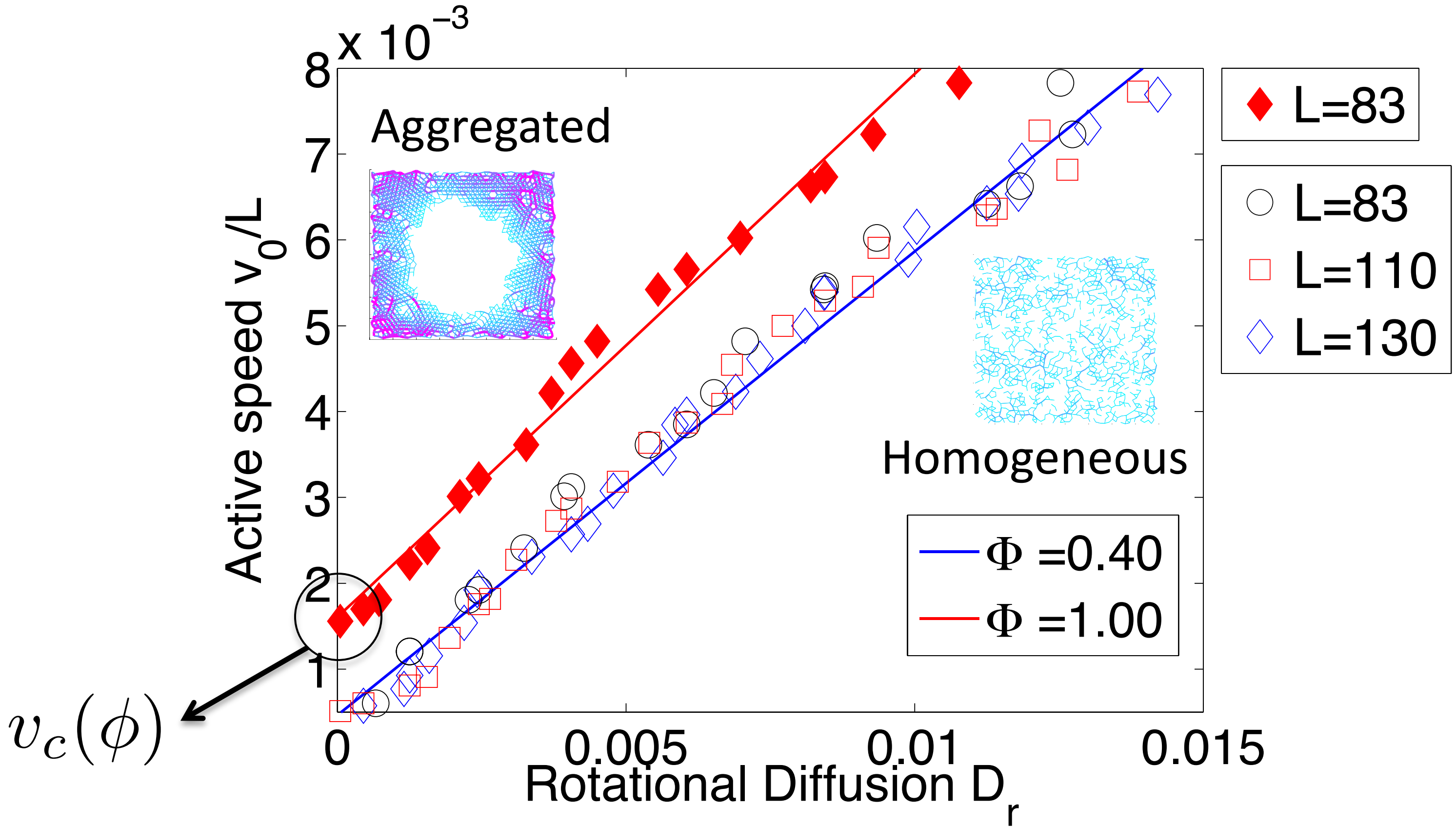
Define Gini coefficient:

$$Gini = \frac{1}{2N^2 |\bar{r}|} \sum_i \sum_j |r_i - r_j|$$



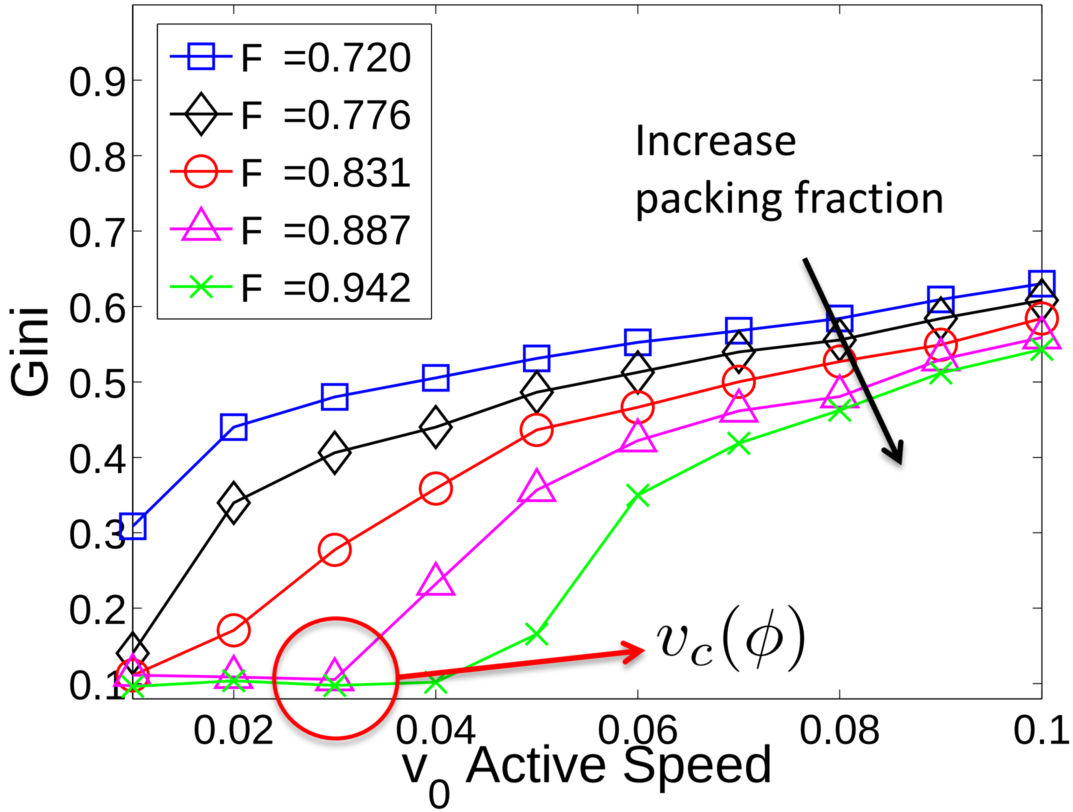
$Gini \sim 0$ $\quad$ $Gini = 0.5$ $\quad$ $Gini \sim 1$

Phase Diagram



- Low packing fraction (single particle behavior):
  Time to cross system ~ $L/v_0 \sim D_r^{-1}$
- High packing fraction (collective behavior):
  Critical active velocity $v_c(\phi)$ required for aggregation

Critical Velocity



- $v_c(\phi)$ kicks in around packing fraction 0.85, close to jamming (Donev et al. 2004).
- A finite velocity threshold is required to overcome the yield stress.

Two ways to calculate pressure

1. Force per unit length on the wall.

(S. A. Mallory et al. have calculated pressure on the wall at low packing fraction for a confined active system. http://arxiv.org/abs/1310.0826)

2. Irving-Kirkwood pressure:

$$\sigma_{\alpha\beta}^{IK} = \sigma_{\alpha\beta}^{\text{int}} + \sigma_{\alpha\beta}^{act}$$

$$\sigma_{\alpha\beta}^{\text{int}} = \frac{1}{L^2}\left\langle \sum_{i \neq j} F_{ij}^{\alpha} r_{ij}^{\beta} \right\rangle$$

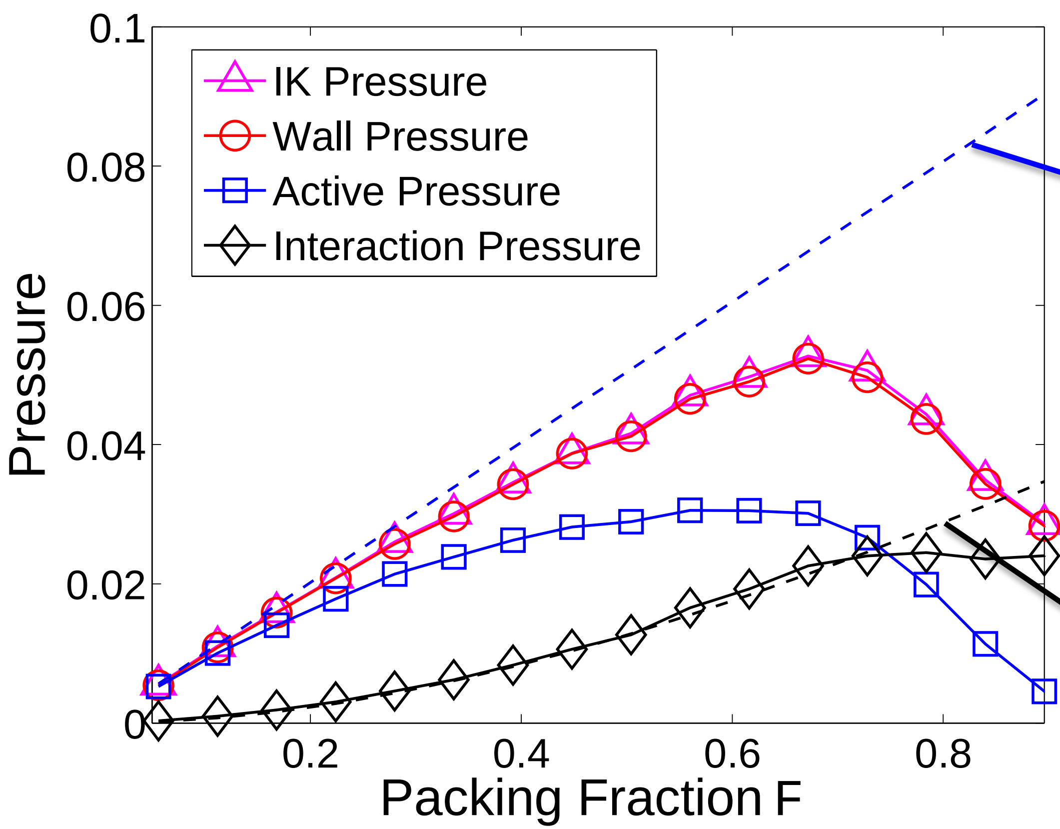
$$\sigma_{\alpha\beta}^{act} = \frac{1}{L^2}\left\langle \sum_{i} F_{iact}^{\alpha} r_{i}^{\beta} \right\rangle$$

$$P_{act} = \sigma_{\alpha\alpha}^{act} / 2$$

$$P_{\text{int}} = \sigma_{\alpha\alpha}^{\text{int}} / 2$$

$$P_{IK} = \sigma_{\alpha\alpha}^{IK} / 2$$

Non-monotonic Pressure



$$D_r^{-1} >> L / v_0$$

Ideal active gas pressure:

$$P_{act} = \frac{r v_0^2}{2 m D_r}\left[1 - \exp\left(-\frac{D_r L}{2 v_0}\right)\right]$$

$$\xrightarrow{D_r^{-1} >> L / v_0} P_{act} \sim r \frac{v_0 L}{4 m}$$

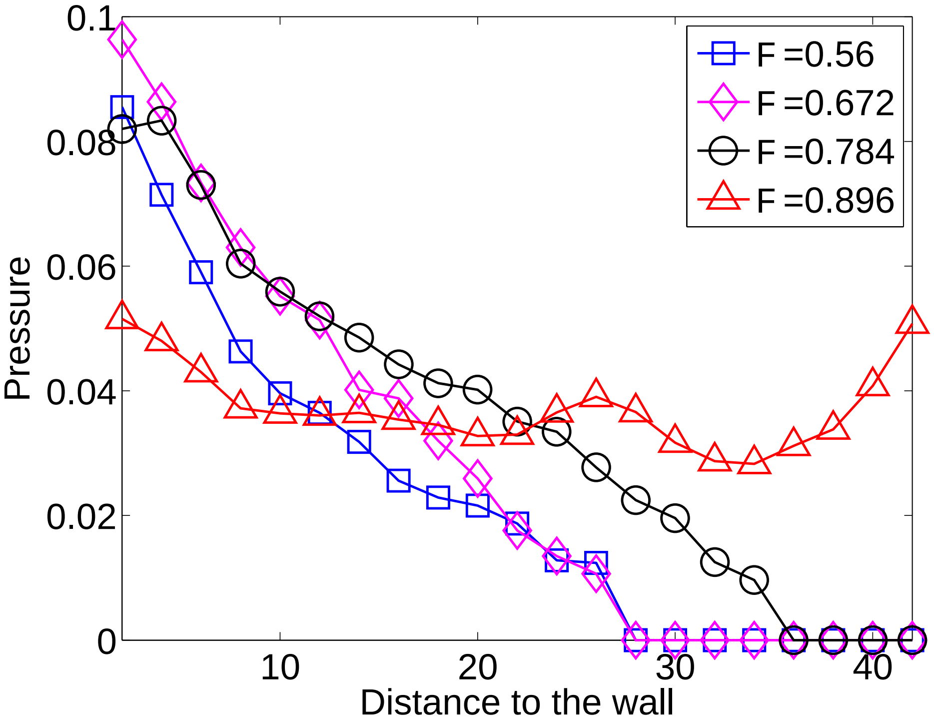
(S. A. Mallory et al. 2013)

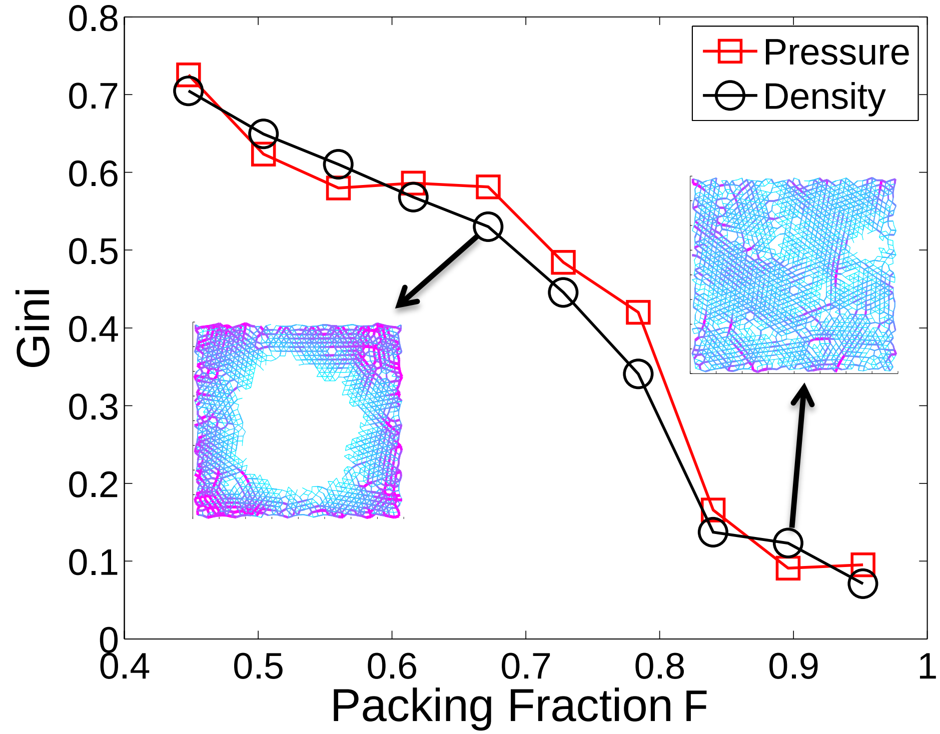
Interaction pressure:

$$P_{int} = c\left(\frac{L v_0}{16R} f^2 - \frac{L v_0}{48R} f^3\right)$$

c is a fitting parameter and chosen to be 1.2 here.

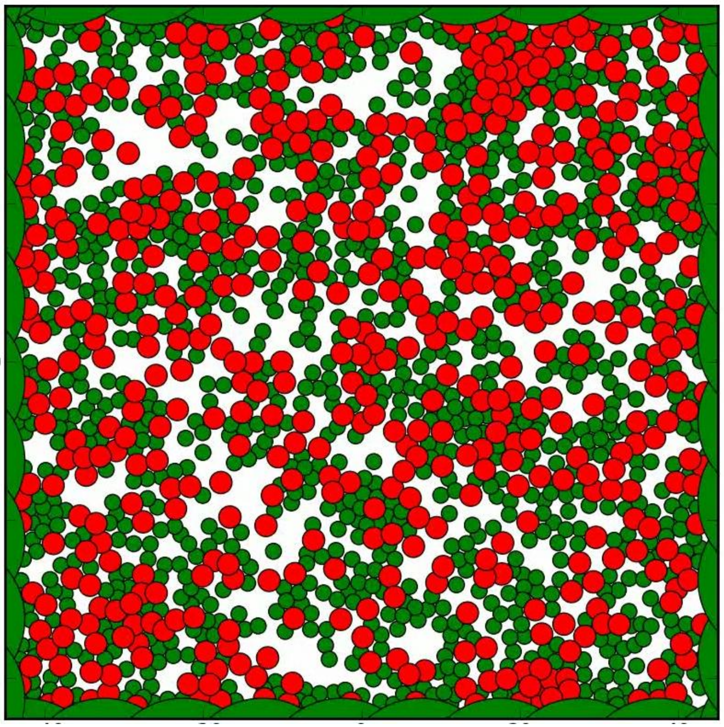
Inhomogeneous pressure

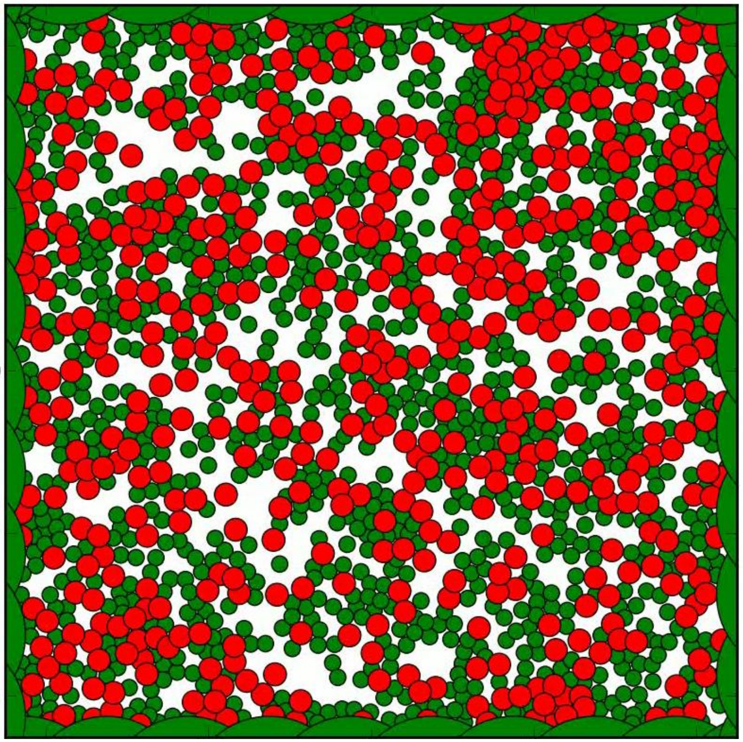




- Strong density gradient yields strong pressure gradient.
- Speculation: caging effect at large packing fraction diminishes the pressure gradient, resulting in a decrease of pressure.
- Wide precursor to jamming.

Segregation without adhesion

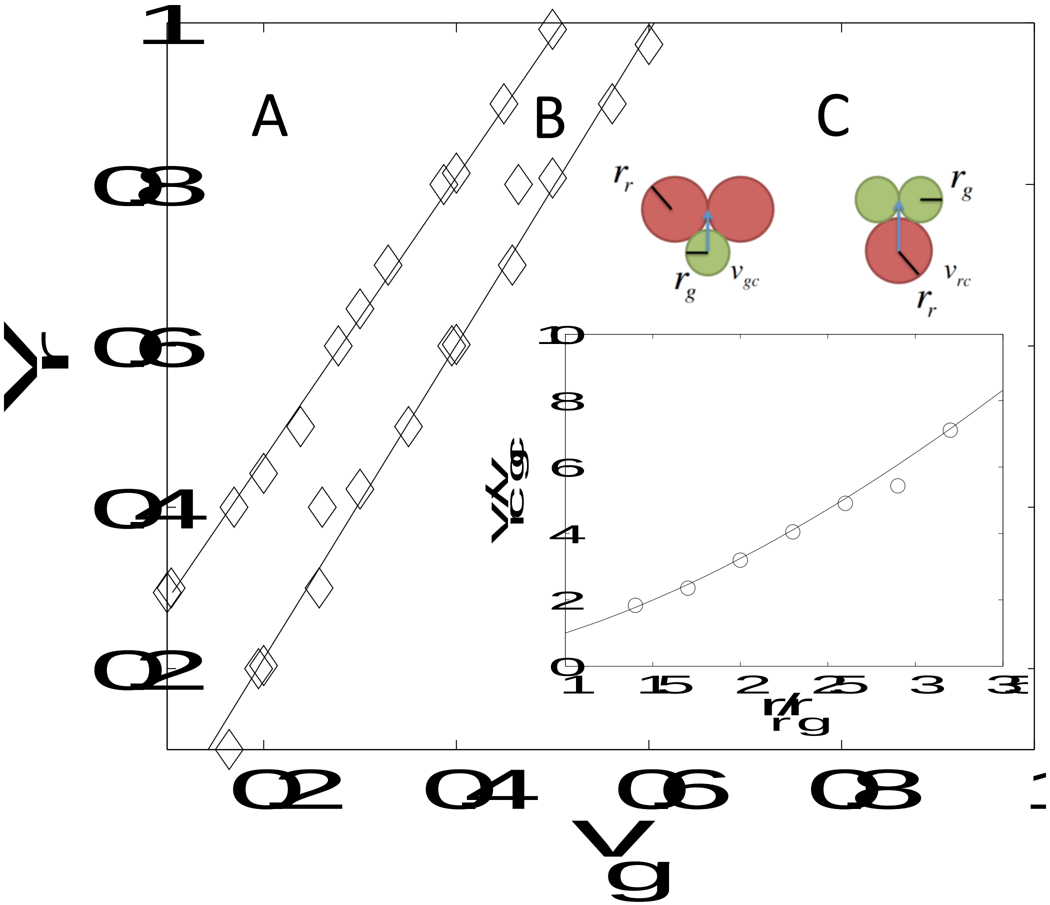


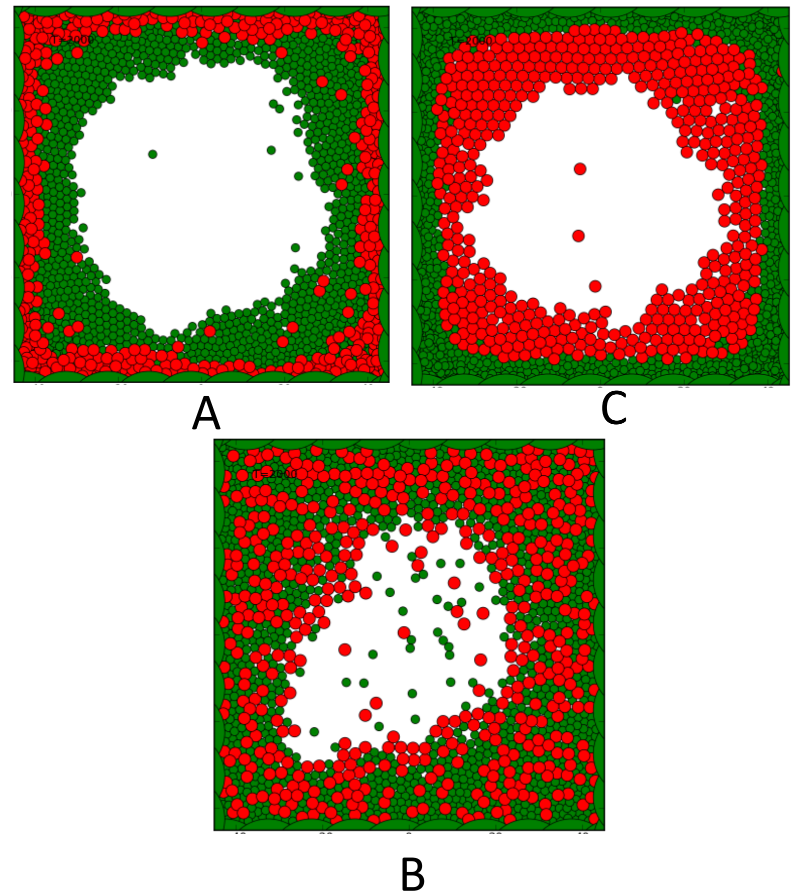


No adhesion, $v_{red} = v_{green}$
radius ratio 1:1.4

No adhesion, $v_{red} = 4v_{green}$
radius ratio 1:1.4

Asymmetry of energy barriers leads to segregation





Conclusions

- SP particles aggregate at the wall in the absence of any attraction or alignment.
- A critical SP velocity is required for aggregation above $f \sim 0.85$, corresponding to jamming.
- The pressure is non-monotonic and starts decreasing before jamming.
- In a mixture, this aggregation effect can be used to achieve segregation without differential adhesion or attraction. It bears possible relevance to morphogenesis.

Acknowledgements

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