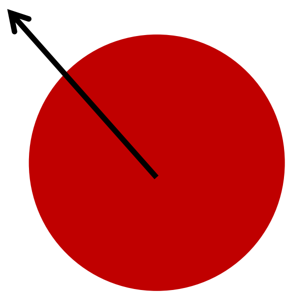
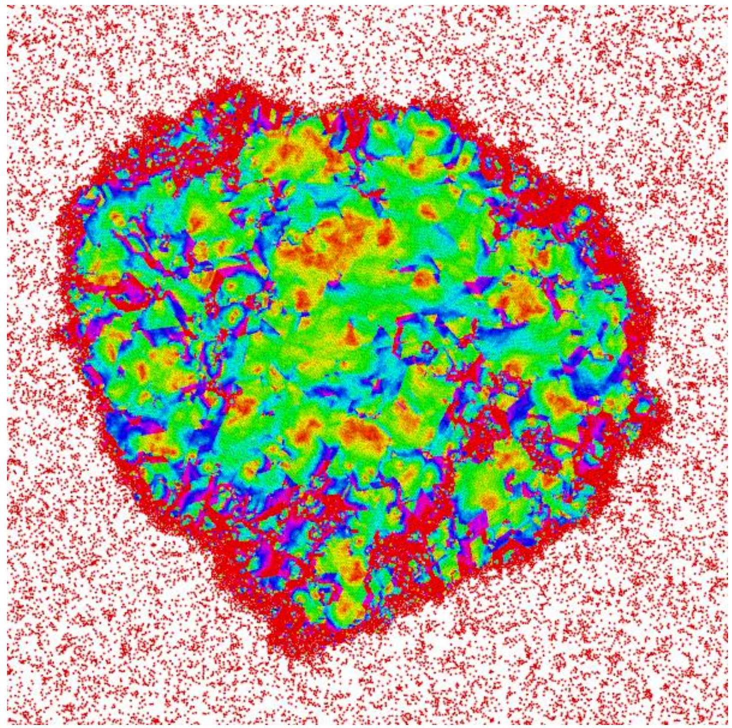
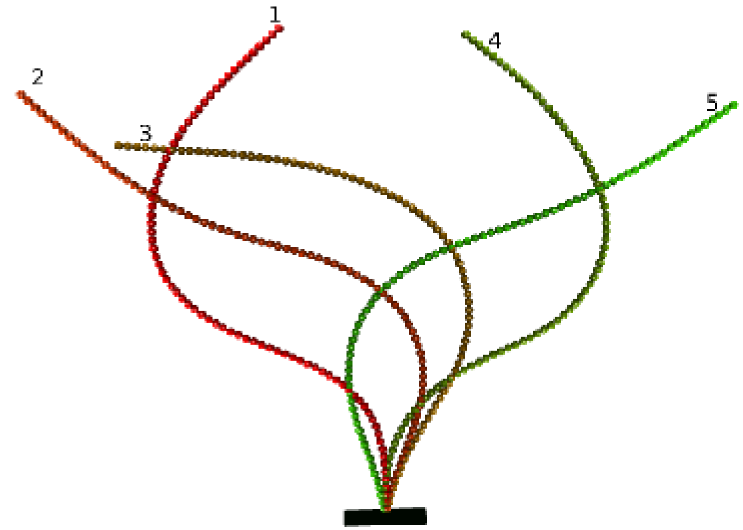
The Secret Life of Self-Propelled Spheres







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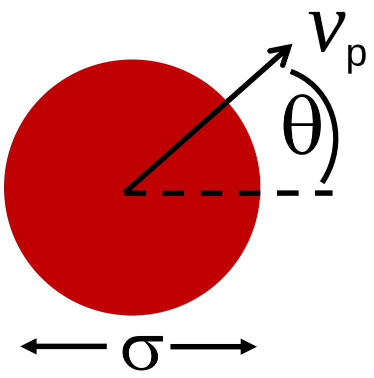
Simulations of Self-Propelled Spheres

Gabe Redner, Aparna Baskaran

- (nearly) hard spheres (WCA potential)
- smooth (no alignment interactions)
- 2D, periodic boundary conditions
- Propulsion velocity $\mathbf{v}_i = v_{\mathrm{p}}(\cos\theta_i, \sin\theta_i)$
- Overdamped Brownian dynamics



$$\dot{\mathbf{r}}_i = \mathbf{v}_i + D\beta\mathbf{F}_i + \sqrt{2D}\boldsymbol{\eta}_i^T$$

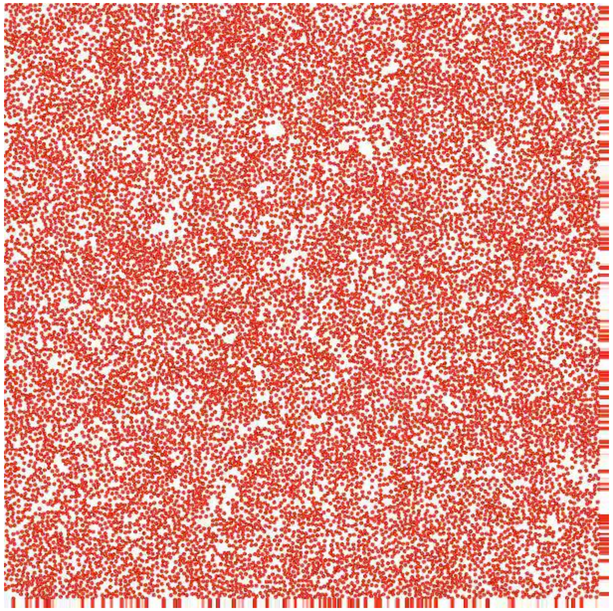
$$\dot{\theta}_i = \sqrt{2D_{\mathrm{r}}}\eta_i^R$$

- neglect hydrodynamic interactions (dense quasi-2D system)

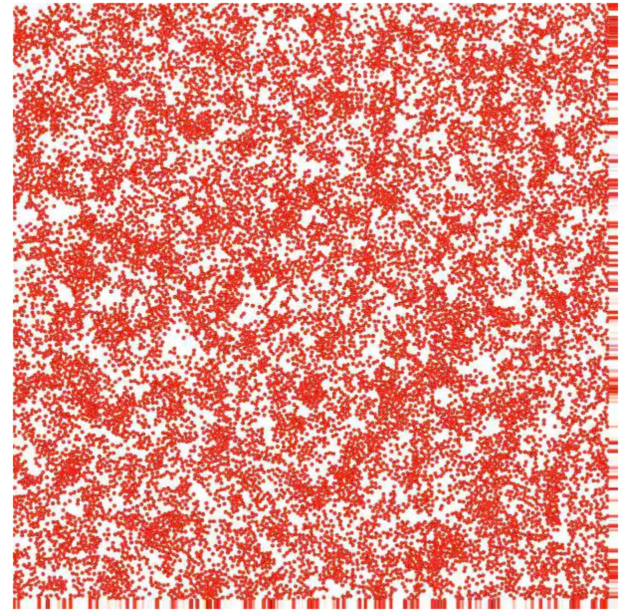
Parameters: density (ρ), Pe = $v_{\mathrm{p}}\sigma/D$

$$\mathrm{Pe} = \sigma v_{\mathrm{p}} / D$$

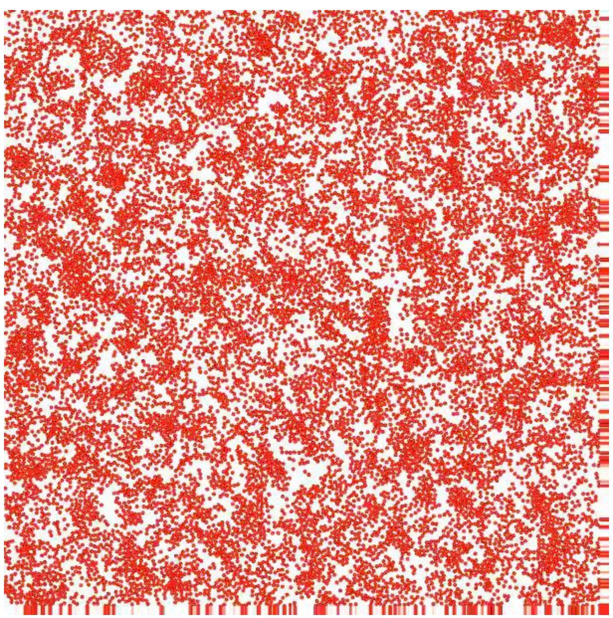
Pe=10



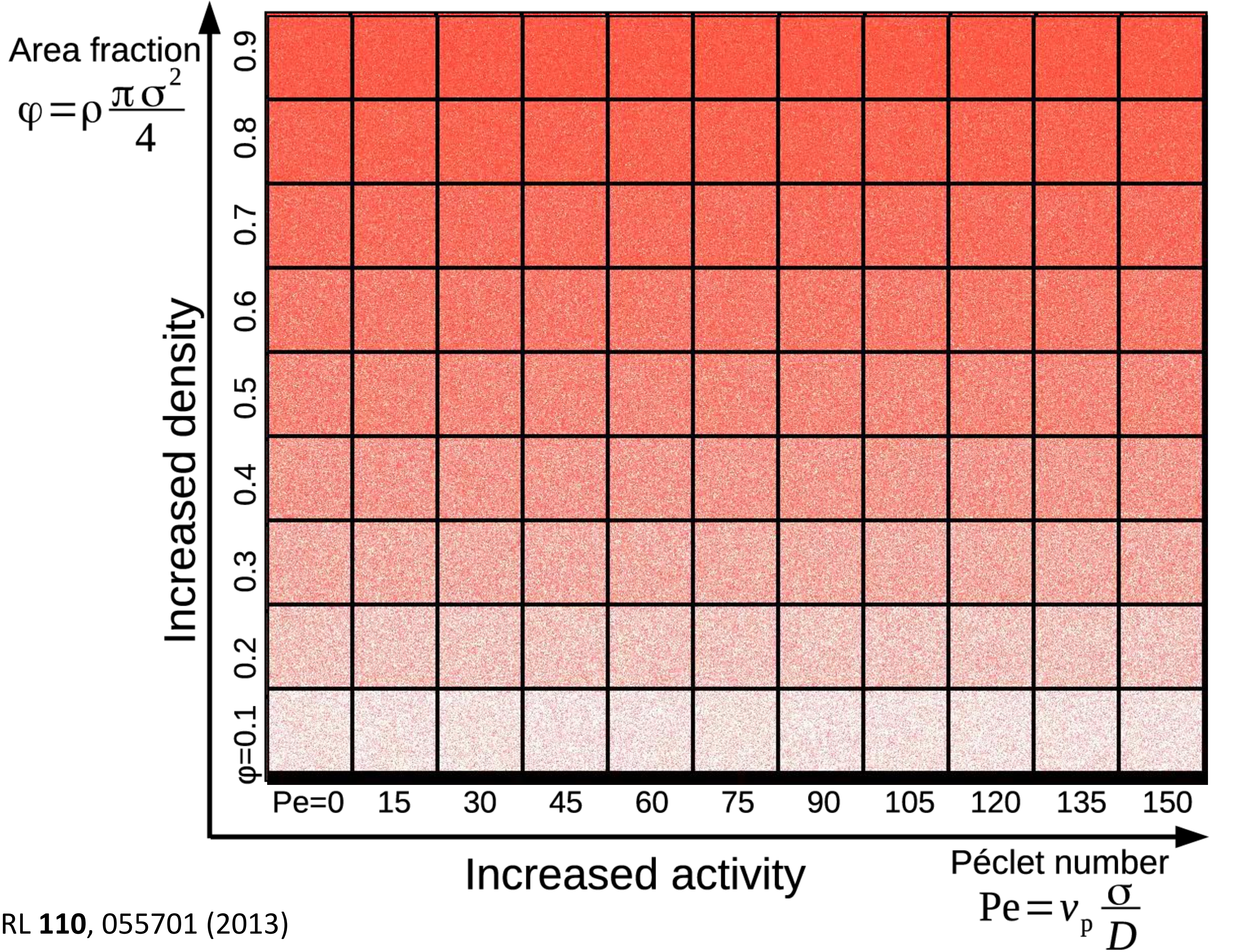
Pe=60



Pe=80

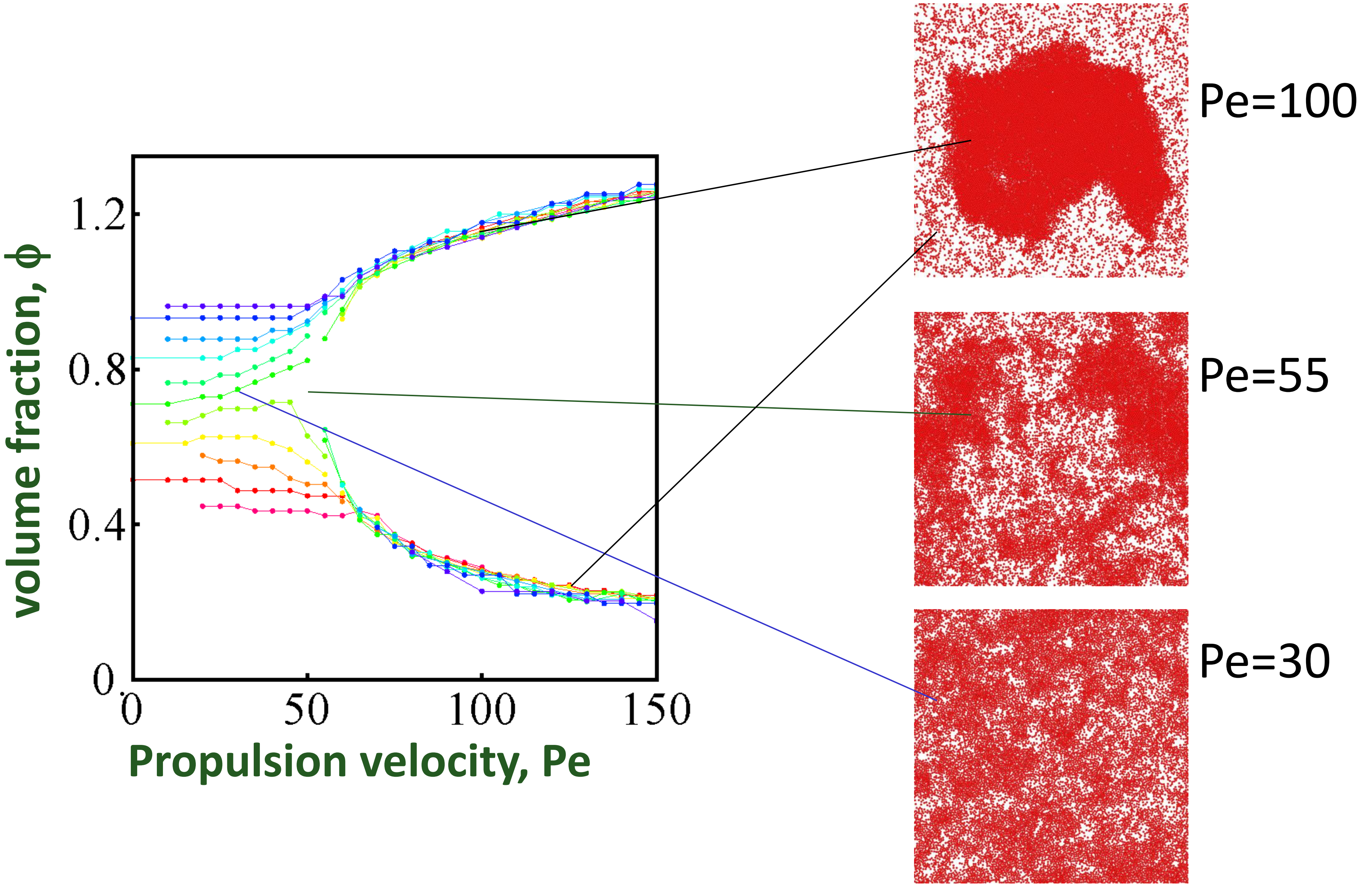


Redner, MFH, and Baskaran PRL (2013)
see also:
Fily and Marchetti, PRL (2012)
Tailleur and Cates, PRL (2008).
A. G. Thompson et al. J Stat Mech (2011).
Bialke, Lowen, Speck, EPL 103, 30008 (2013).
Cates and Tailleur, EPL 101, 20010 (2013).
J. Stenhammar et al. PRL 111, 145702 (2013).
Redner, Baskaran, and MFH, PRE (2013).
T. Speck et al. arXiv:1312.7242(2013)
Fily, Henkes, and Marchetti, Soft Matter (2014).
J. Stenhammar et al. Soft Matter 10, 1489 (2014).
R. Wittkowski et al. arXiv:1311.1256 (2014)



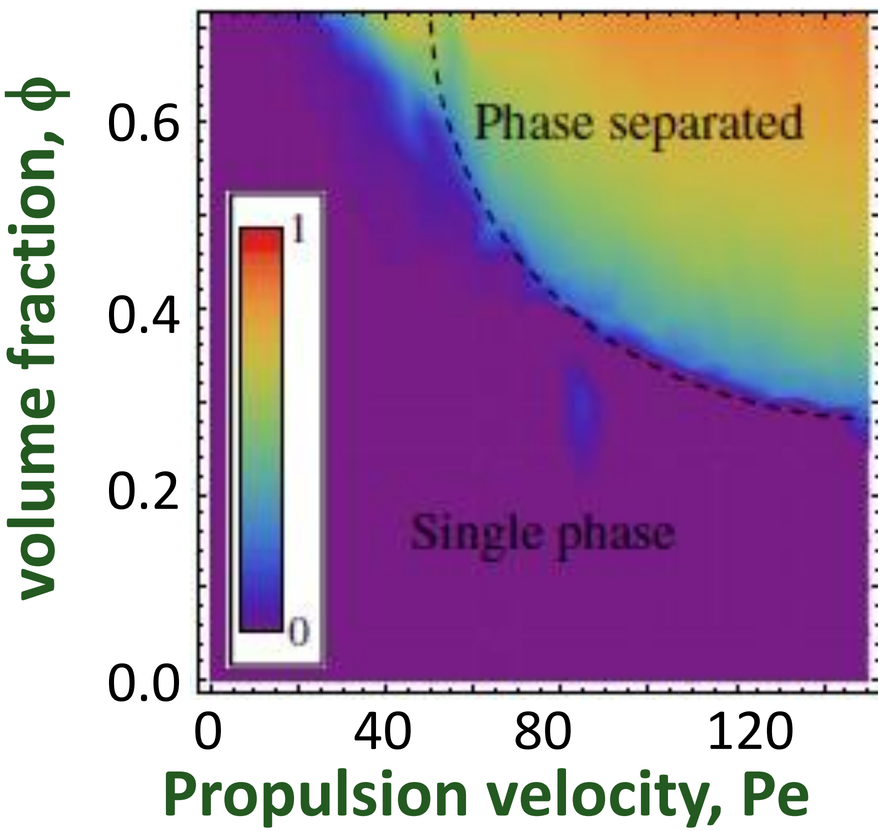
PRL **110**, 055701 (2013)

Phase Coexistence

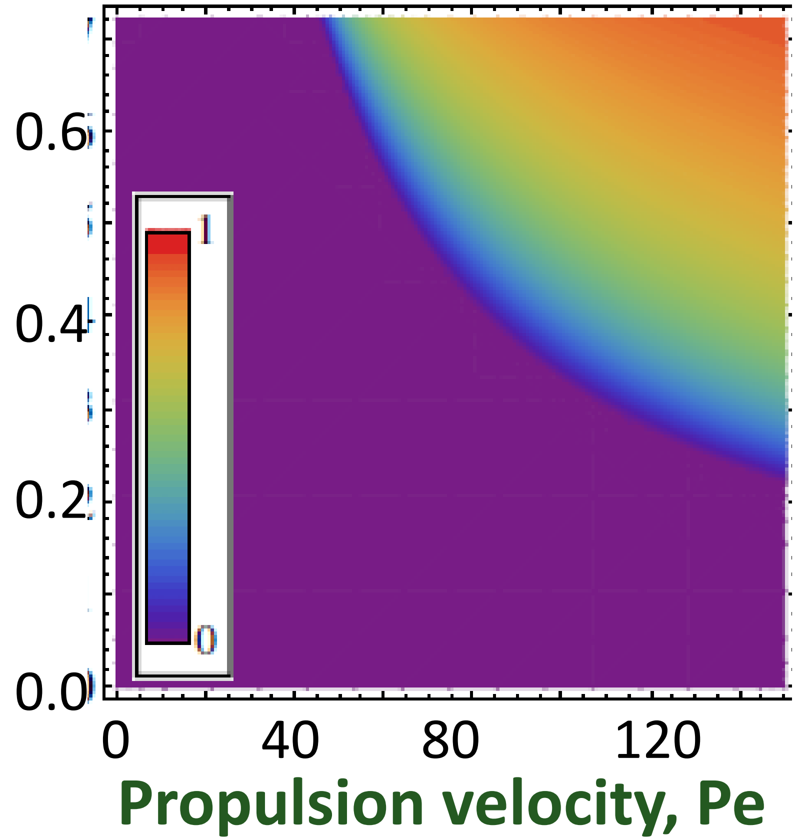


fraction in clusters

simulation

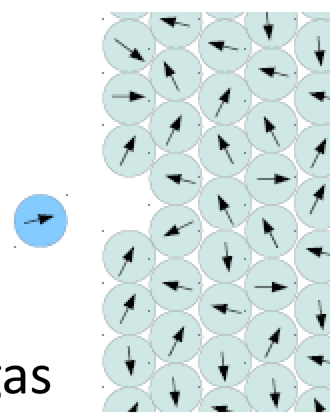


theory



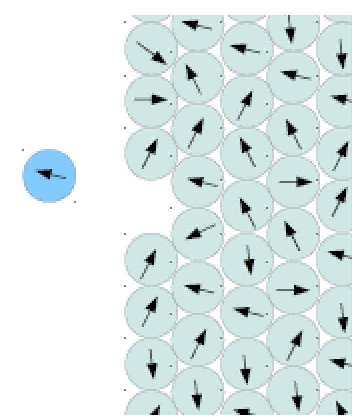
$$k_{\mathrm{on}} = \frac{\rho_{\mathrm{gas}} v_{\mathrm{p}}}{\pi}$$

ρ_{gas} = density in gas



$$k_{\mathrm{off}} = \frac{\kappa D_{\mathrm{r}}}{\sigma}$$

κ= fit parameter



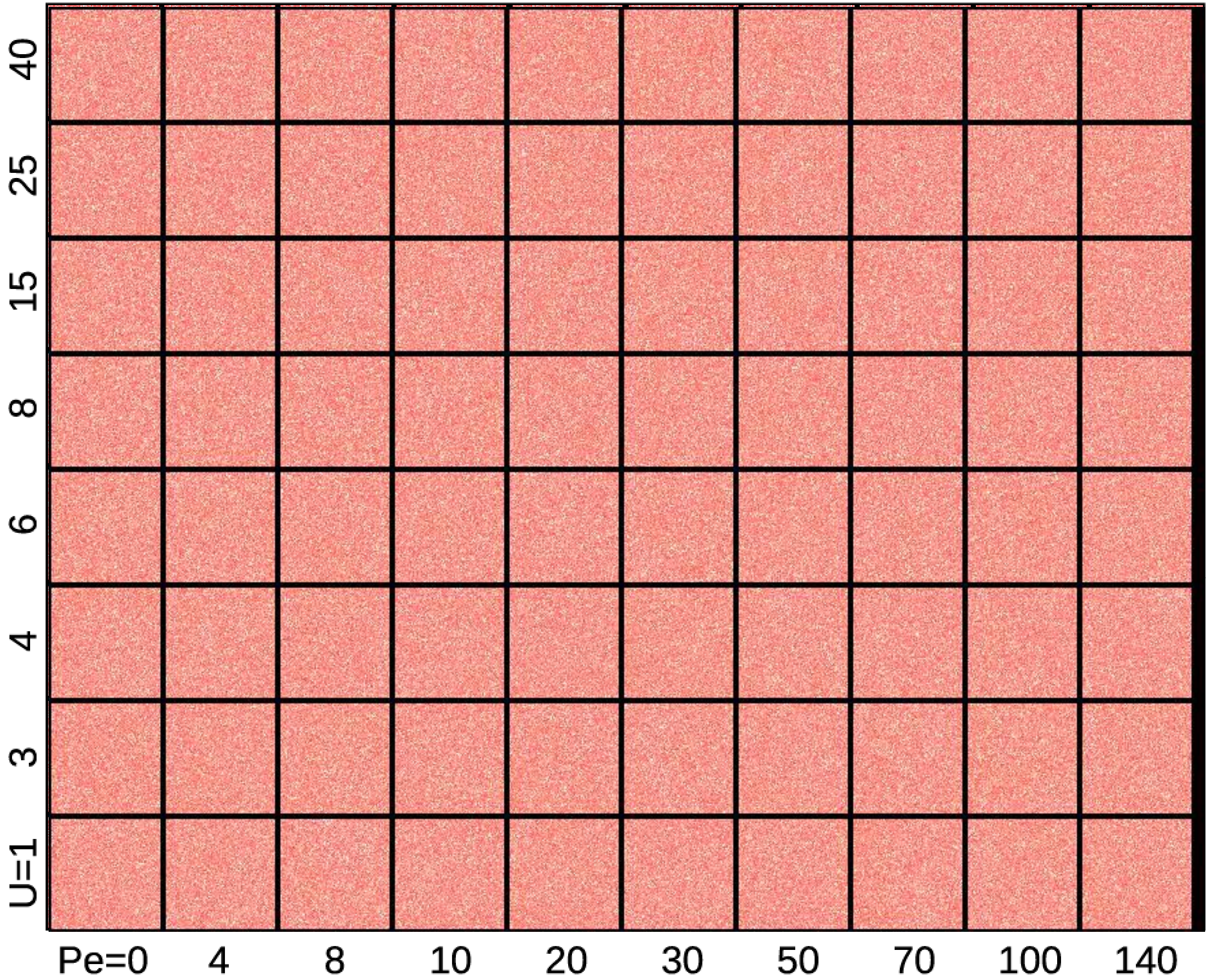
Adding Attractions (Lennard-Jones)

attraction strength

$$U = \frac{\epsilon}{k_B T}$$

re-entrance!

Area fraction
$\rho = 0.4$



Pe = $\sigma v_0 / D$

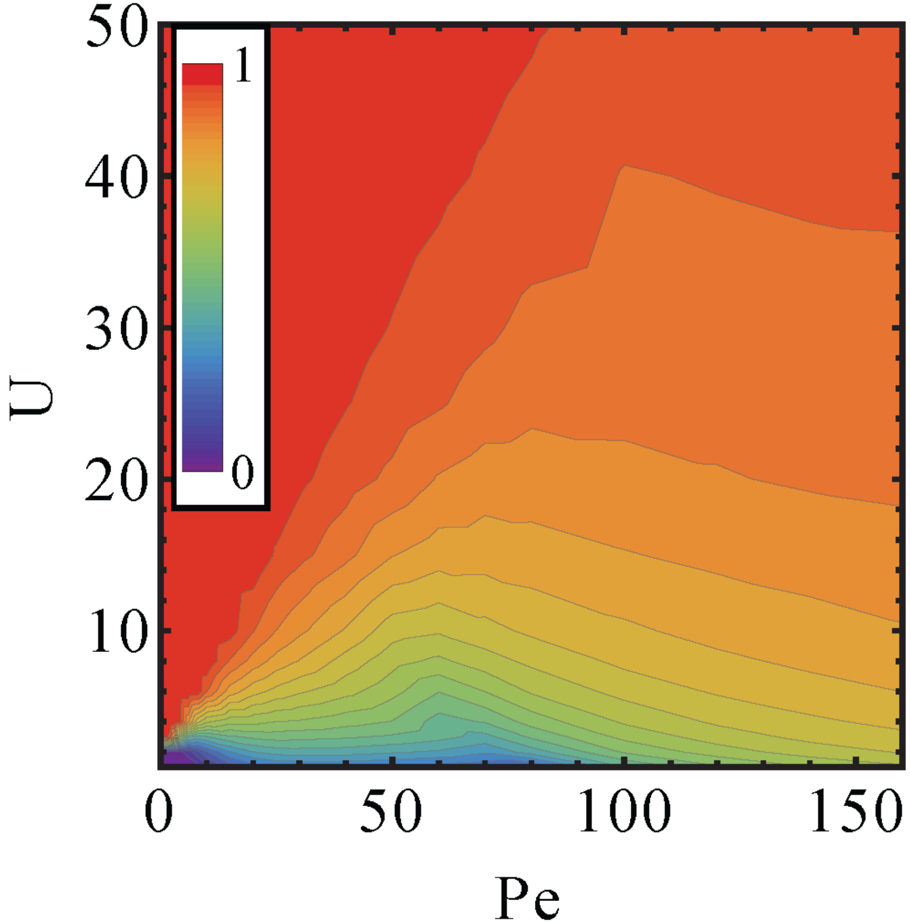
increasing activity →

PRE **88**, 012305 (2013)

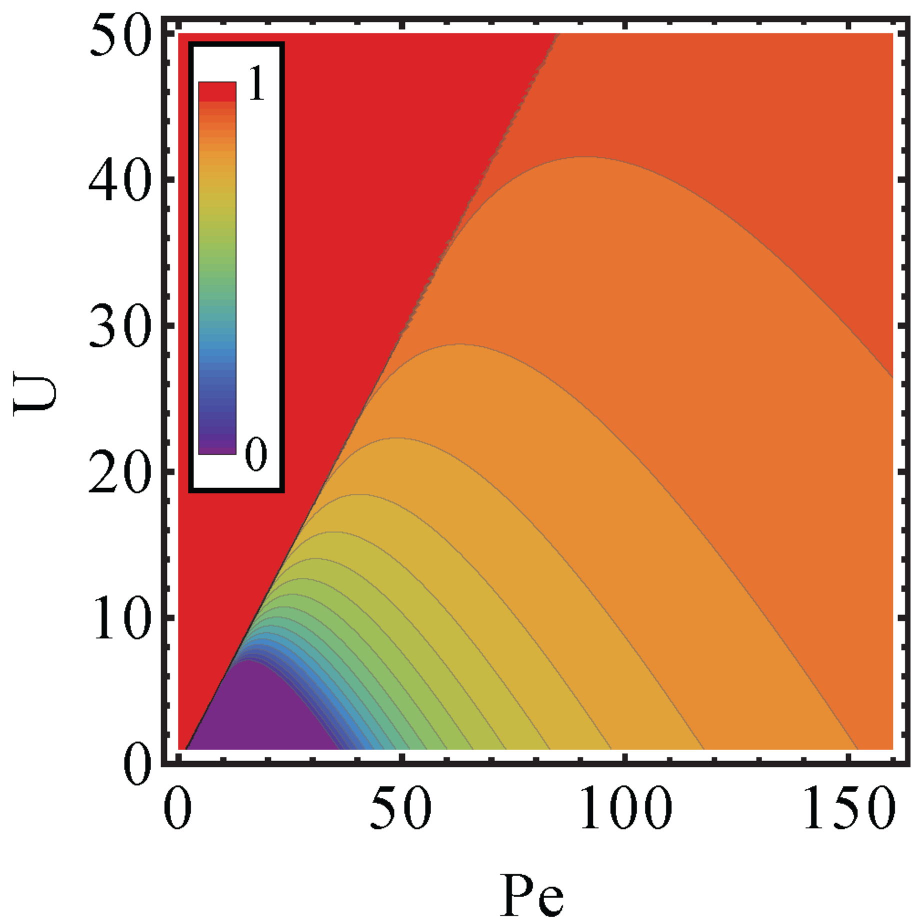
Re-Entrant Phase Separation

fraction of particles in dense phase

simulations



theory



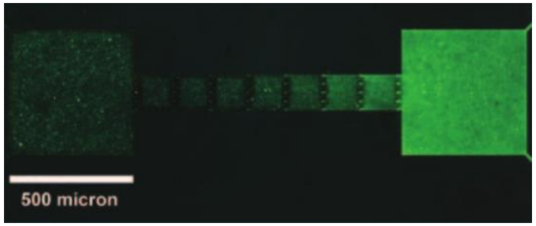
PRE **88**, 012305 (2013)

Boundary Effects on Active Particles

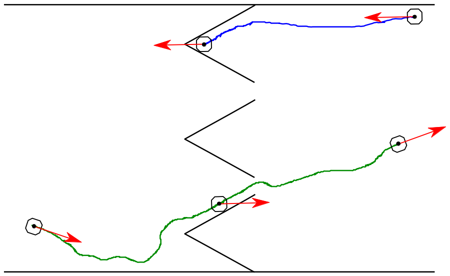
Yaouen Fily, Aparna Baskaran

- Particles accumulate near walls
- Patterned walls lead to new behaviors

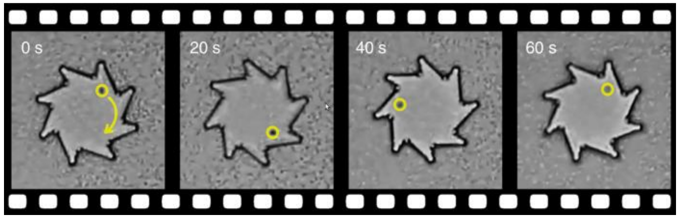
Funnels direct bacteria



(Galajda J. Bacteriol. 2007)



Bacteria-powered micro-gear



(Di Leonardo PNAS 2010)

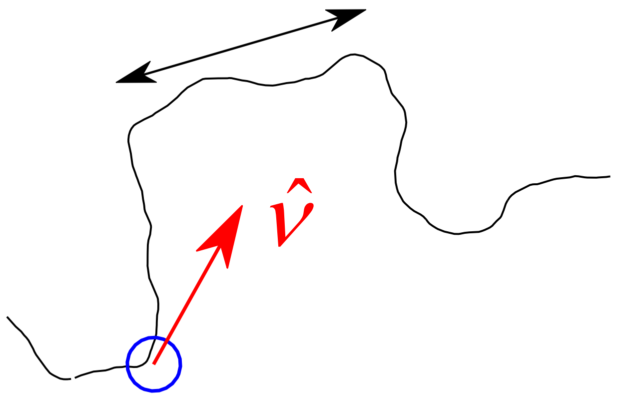
General theory for effect of boundary shape?

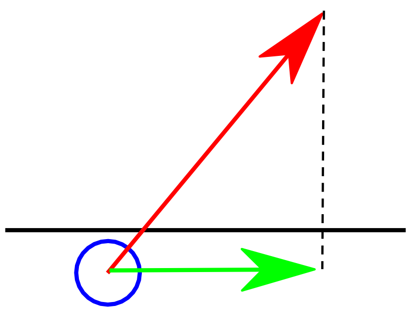
- Particle density generated by arbitrary wall shape.
- Wall shape that yields arbitrary particle density.
- Pressure on the wall.

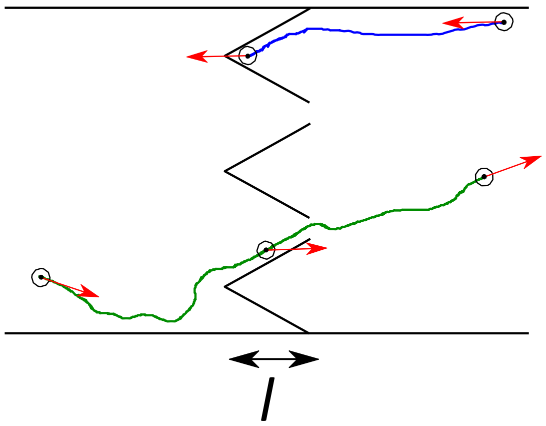
Model

non-interacting, non-aligning self-propelled spheres in a convex container

persistence length (v_p/D_r)



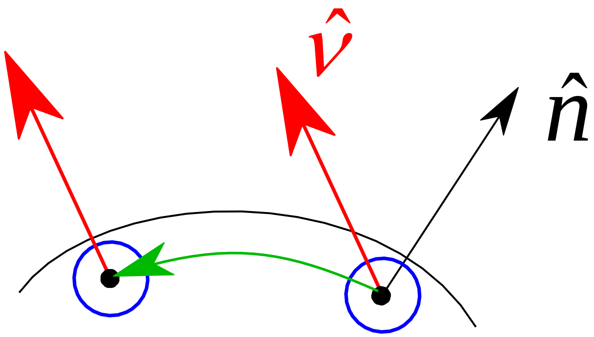




- propulsion velocity v_p along $\hat{\nu}$
- angular diffusion (diffusion constant D_r)
- wall force
- dramatic boundary effects when $l \ll v_p/D_r$

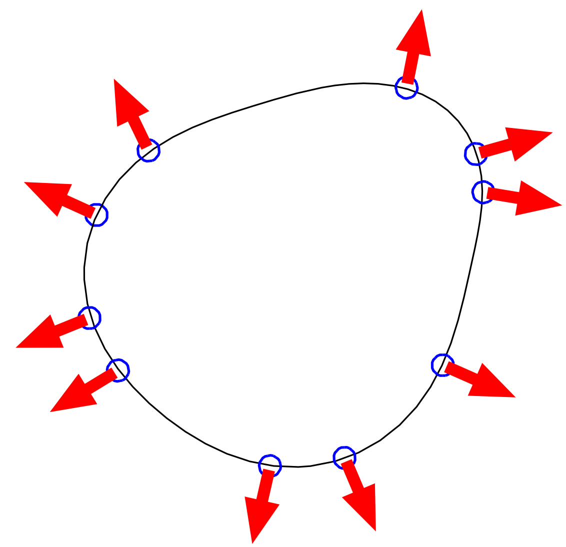
  [Wan PRL (2008), Tailleur EPL (2009)]

Dynamics at the Wall



$\hat{n}$ = normal to wall

$\hat{\nu}$ = particle orientation



particle moves until $\hat{n}$ aligns with $\hat{\nu}$

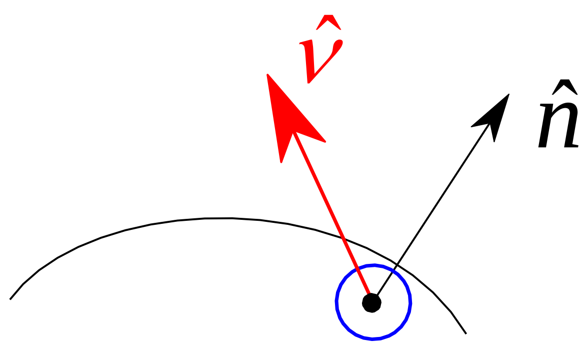
→ $\hat{\nu} = \hat{n}$

particle never leaves boundary

requires small noise: $R << v_p/D_r$ strong confinement

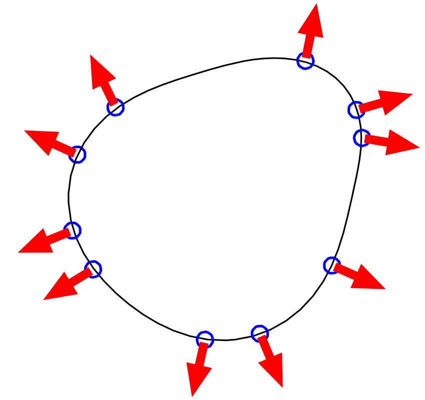
boxsize persistence length

Particle Density on the Boundary



strong confinement

$\hat{v} \approx \hat{n}$



angular dynamics is purely diffusive

$$\rho(\hat{v}) = \text{constant} \quad \rightarrow \quad \rho(\hat{n}) = \text{constant}$$

$$\rho(s) \propto \left| \frac{d\hat{n}}{ds} \right| \equiv \text{curvature}$$

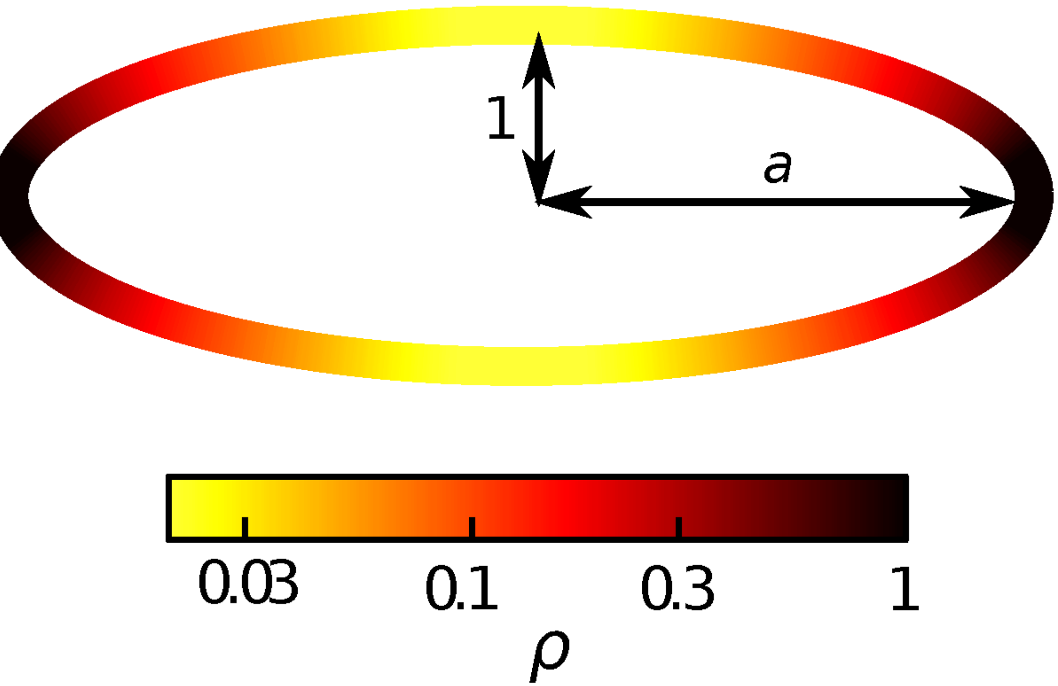
(requires convexity)

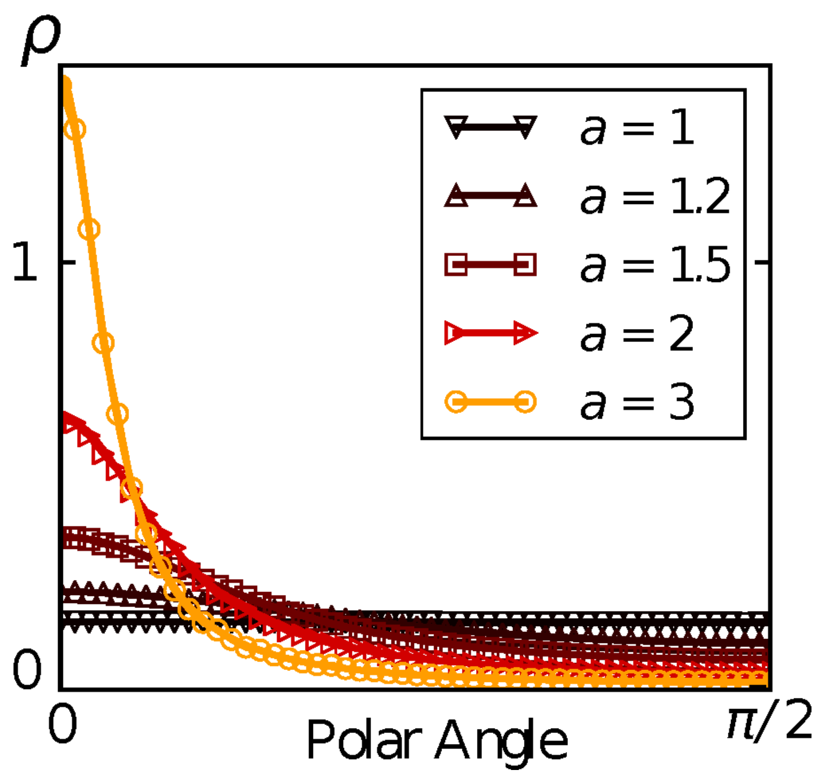
s = arclength along the boundary

Proper derivation → arXiv:1402.5583

Simulations

Elliptical containers





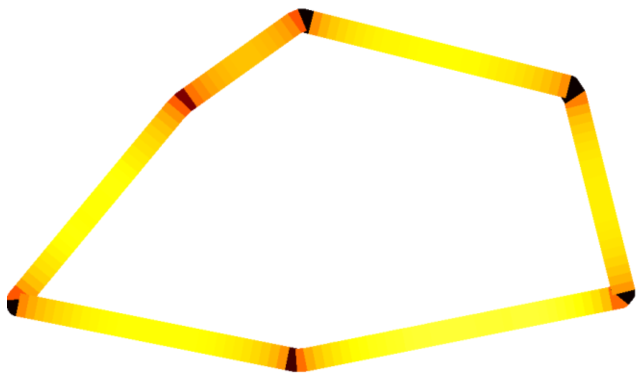
$D_r = 10^{-3}$

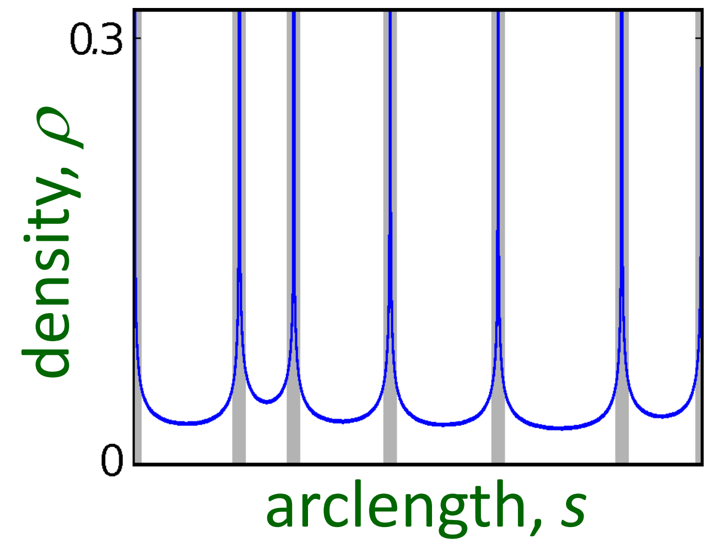
$v_p = 1$

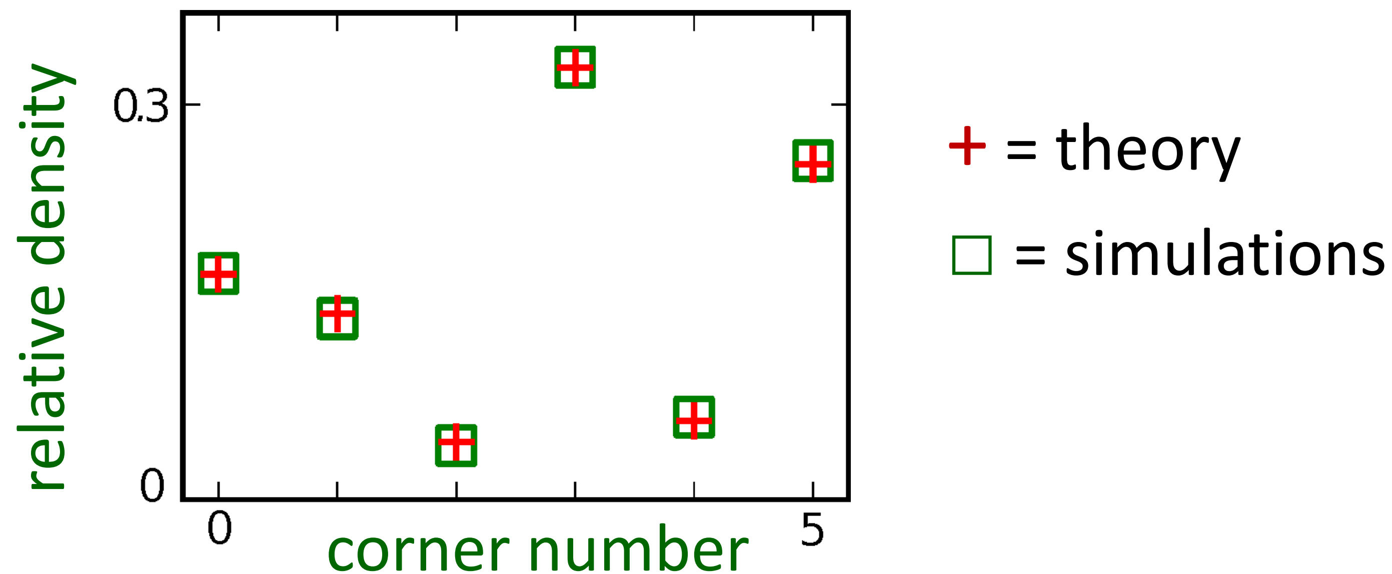
strong confinement $\frac{RD_r}{v_p} \ll 1$

Simulations

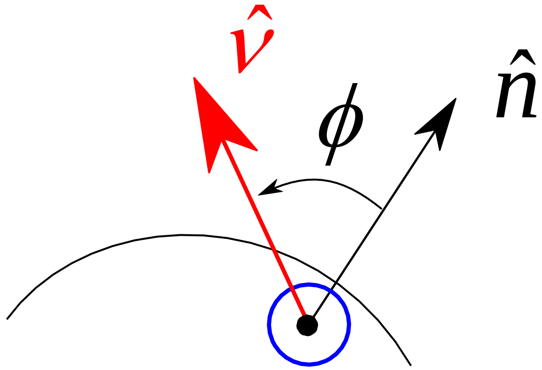
Polygonal containers







Pressure



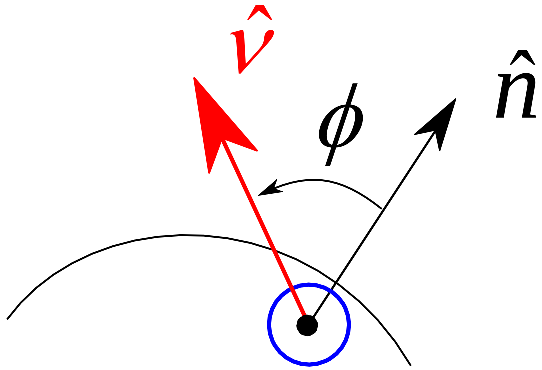
$$\text{pressure} = \rho \frac{v_p}{\mu} \langle \hat{v} \cdot \hat{n} \rangle$$

wall force

μ = mobility

$$\phi = 0 \;\Rightarrow\; \hat{v} = \hat{n} \;\Rightarrow\; \text{pressure} \propto \text{density} \propto \text{curvature}$$

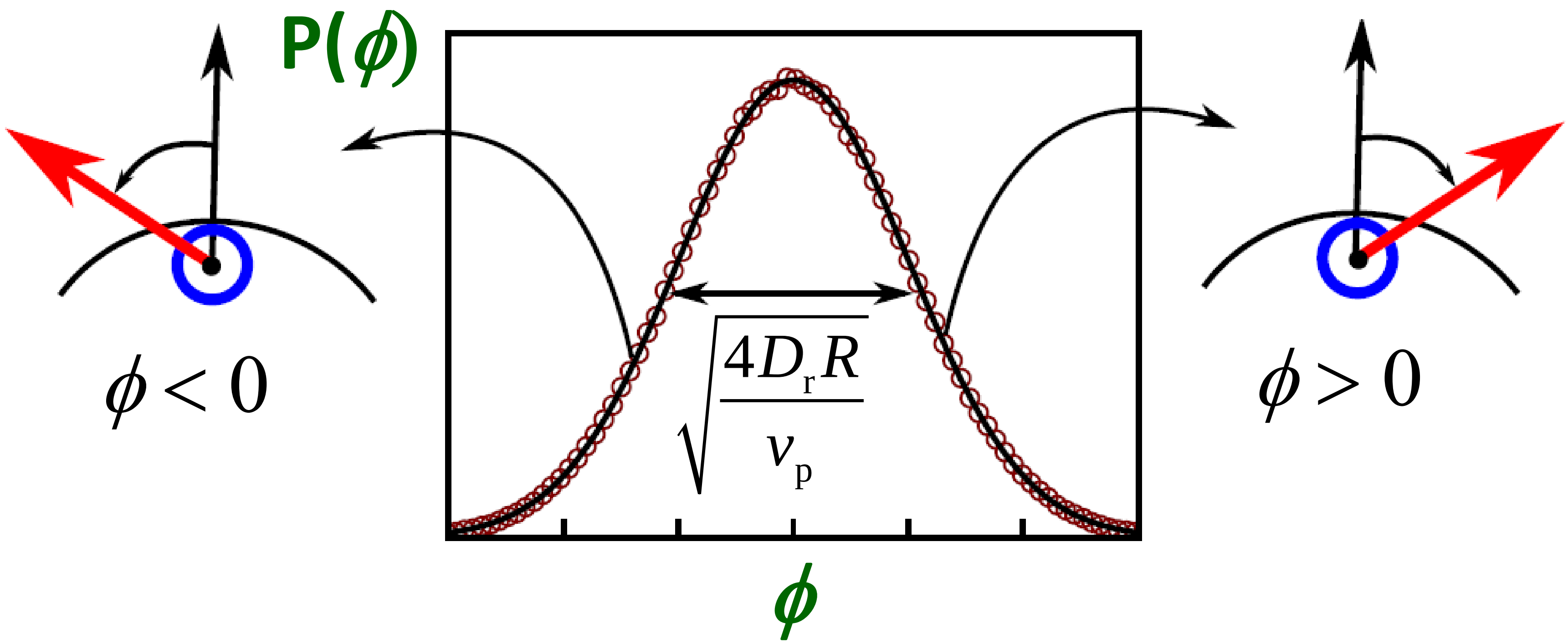
Pressure



slowly varying curvature

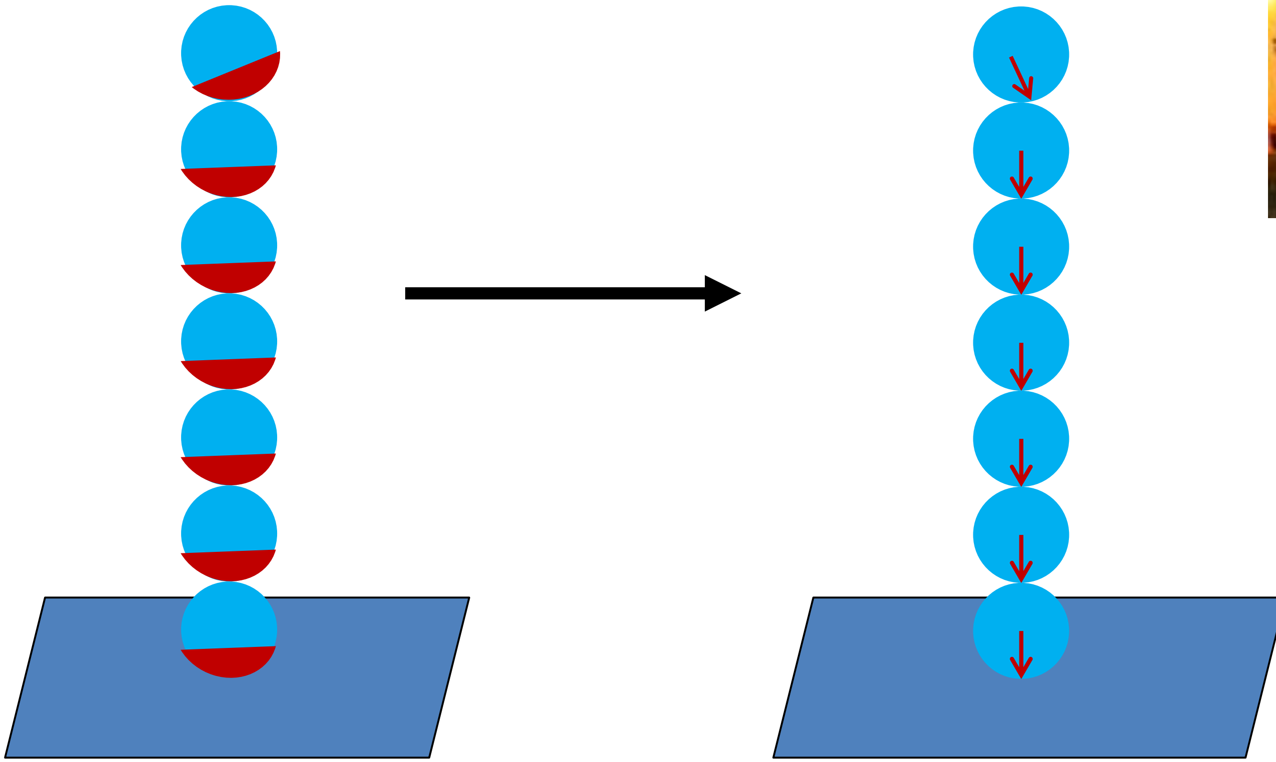
$$\langle \hat{v} \cdot \hat{n} \rangle = \langle \cos\phi \rangle = \exp\left[-\frac{RD_r}{2v_p} \right]$$

explains result in Mallory et al. arXiv:1310.0826



Minimal Model for an Active Filament

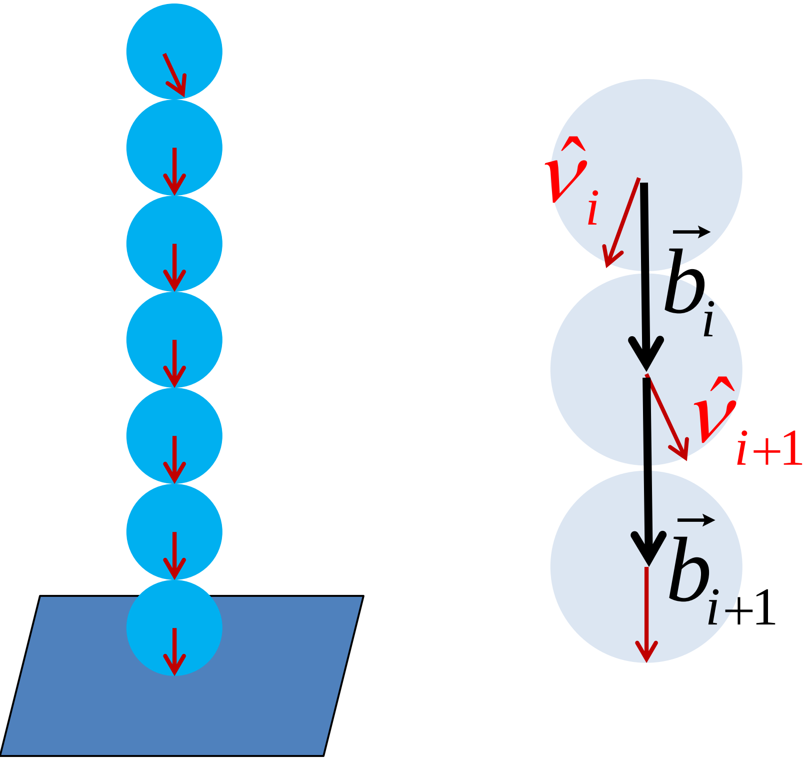
Raghu Chelakkot, Arvind Gopinath, Mahadavan



tethered, self-propelled Janus particles attached to surface

filament of self-propelled spheres

Model



linker stretching

$$U_{\mathrm{s}} = \frac{\kappa_{\mathrm{s}}}{2}\left(|\vec{b}_i| - b_0\right)^2$$

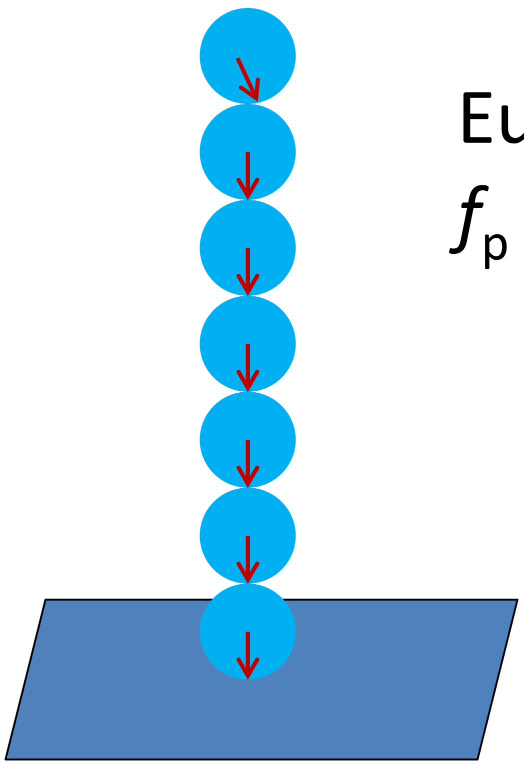
linker bending

$$U_{\mathrm{b}} = \frac{\kappa}{2}\left(\vec{b}_{i+1} - \vec{b}_i\right)^2$$

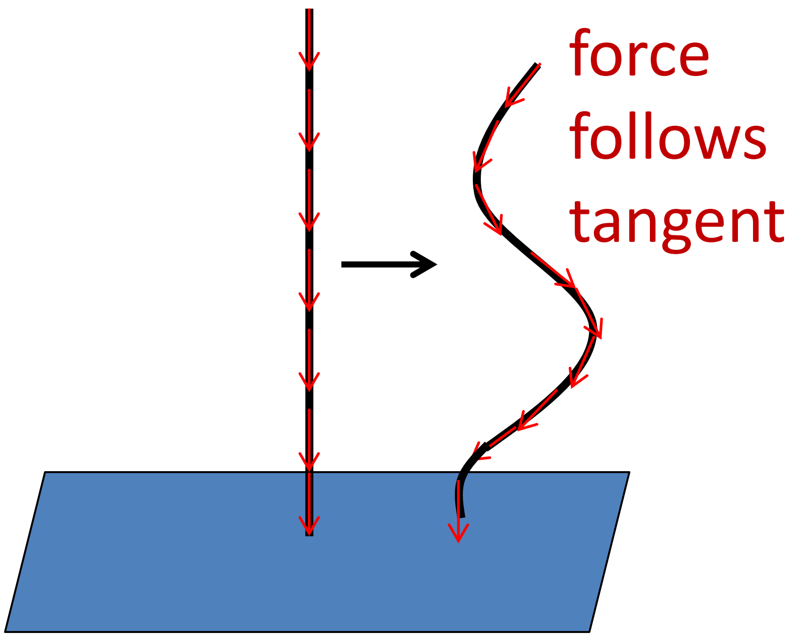
propulsion direction

$$U_{\mathrm{a}} = \frac{\kappa_{\mathrm{a}}}{2}\left(\hat{v}_i - \vec{b}_i\right)^2$$

Buckling Due to Active Force



Euler buckling for
$f_p \sim \kappa/L^3$

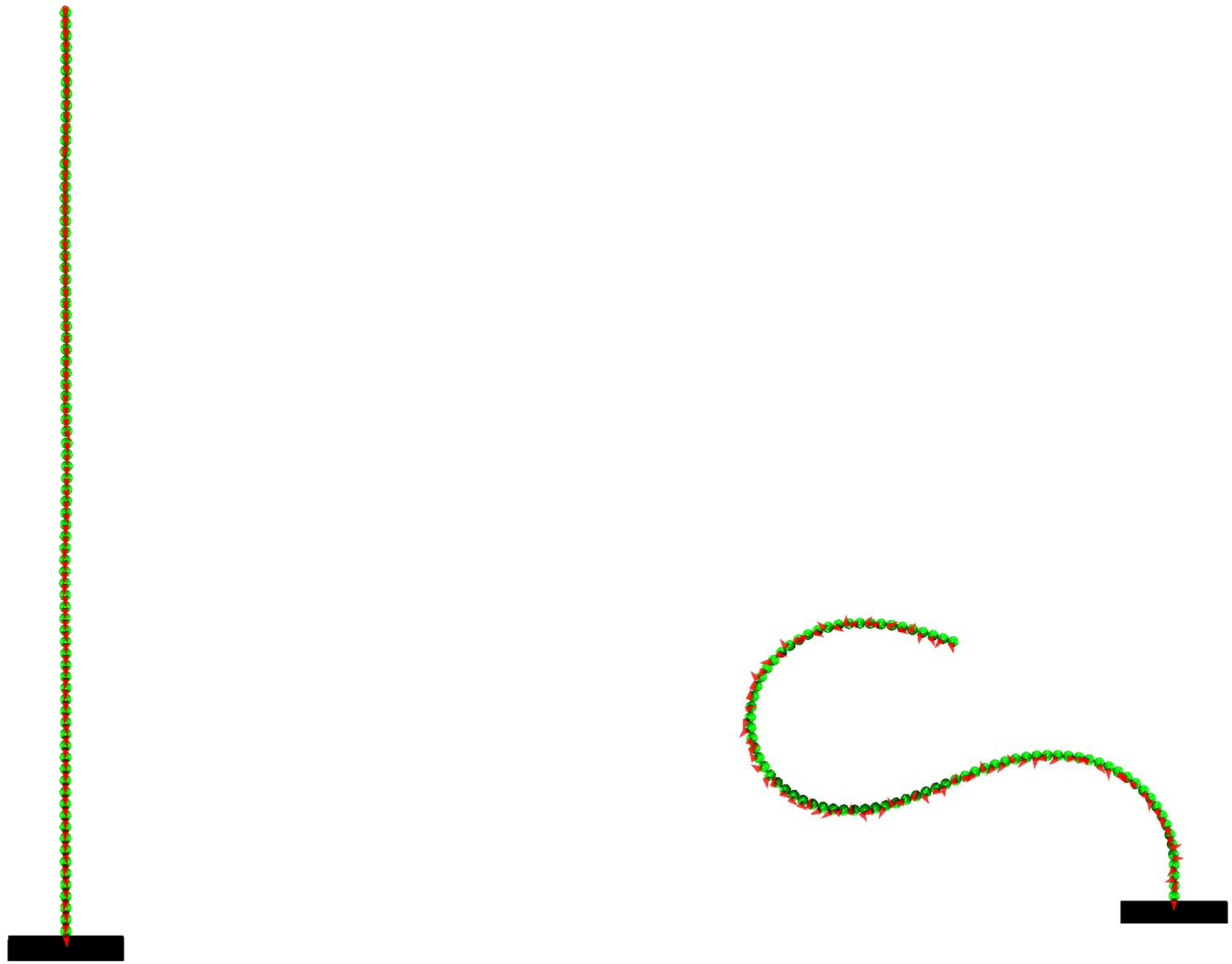


L = filament length (number of spheres)

κ = bending rigidity

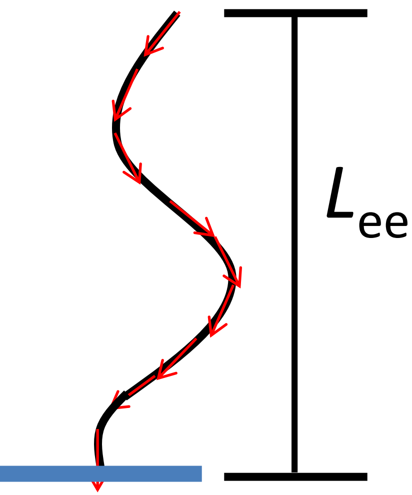
f_p = effective propulsion force per sphere

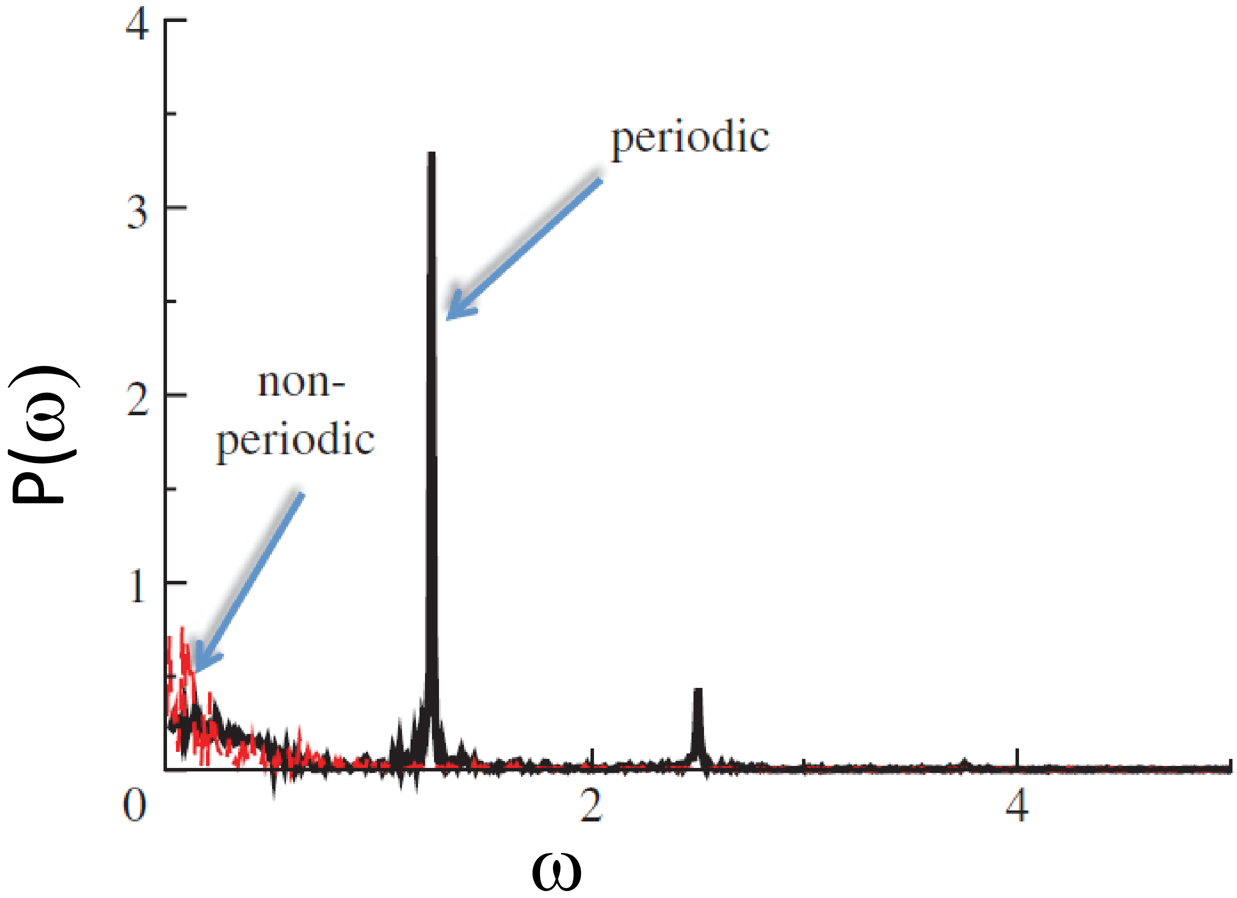
κ_a=20, f_p=20 κ_a=0.5, f_p=20



Periodic Beating

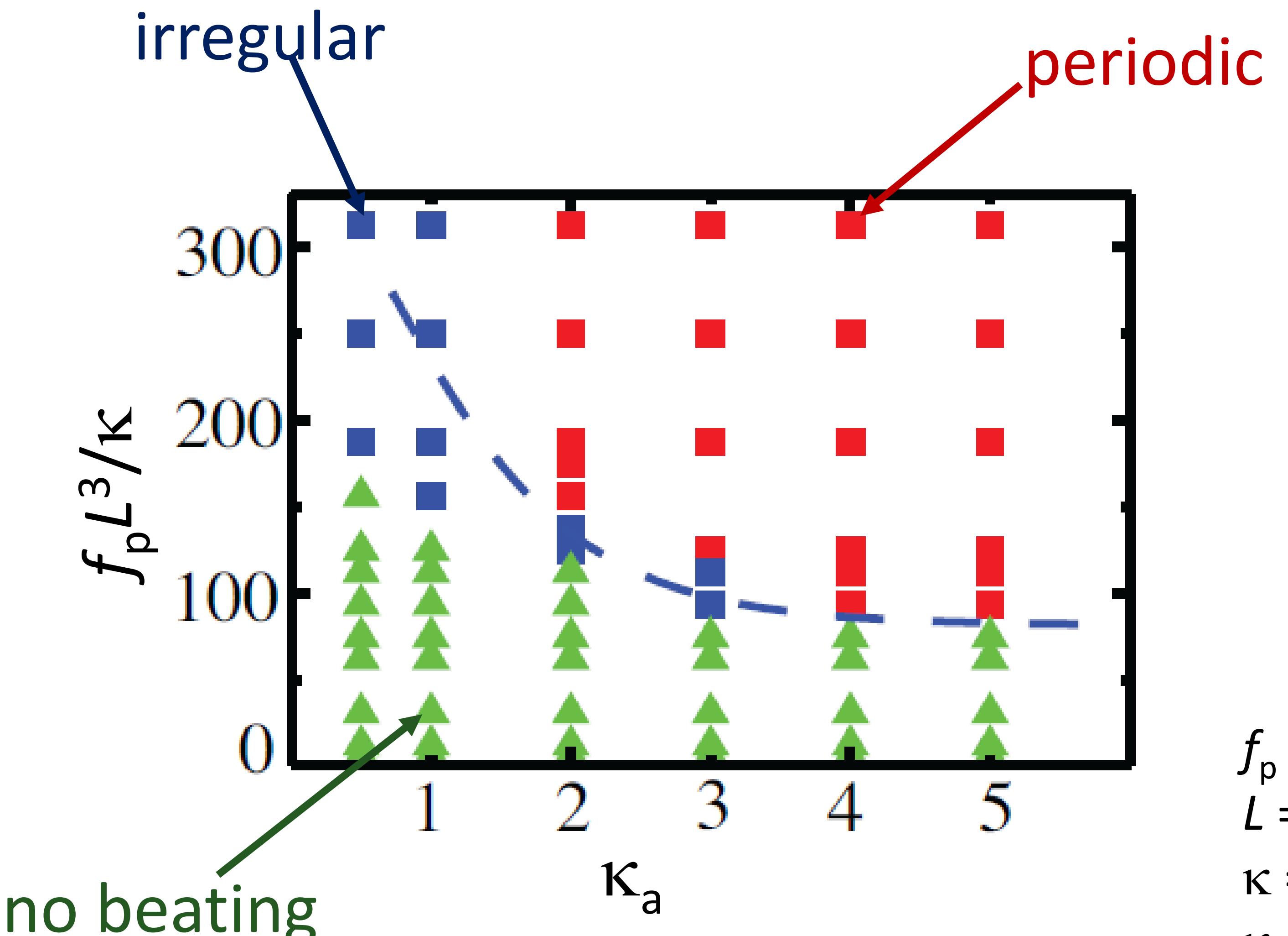
power spectrum for end-to-end length (L_{ee}) fluctuations

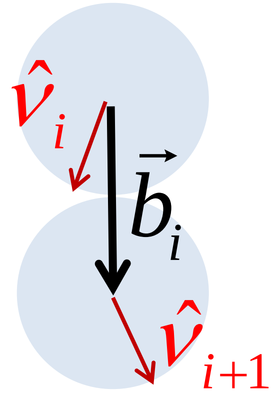




Pivoting Attachment

Phase Diagram





f_p = propulsion force
L = filament length
κ = bending rigidity
κ_a = propulsion orientational rigidity

Multiple Filaments

clamped anchor

pivoting anchor

no hydrodynamic interactions

Acknowledgements

$$: NIH: R01GM108021, R01GM100966
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