How hydrodynamics determines the (collective) motion of microswimmers

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Together with:

Davod Alizadherad, Igor Dudas, **Marc Hennes**, Max Schmitt, **Oliver Pohl**, **Katrin Wolff**, and **Andreas Zöttl**

Experiments on trypanosomes:

T.Pfohl, S. Uppaluri (Basel, Göttingen)

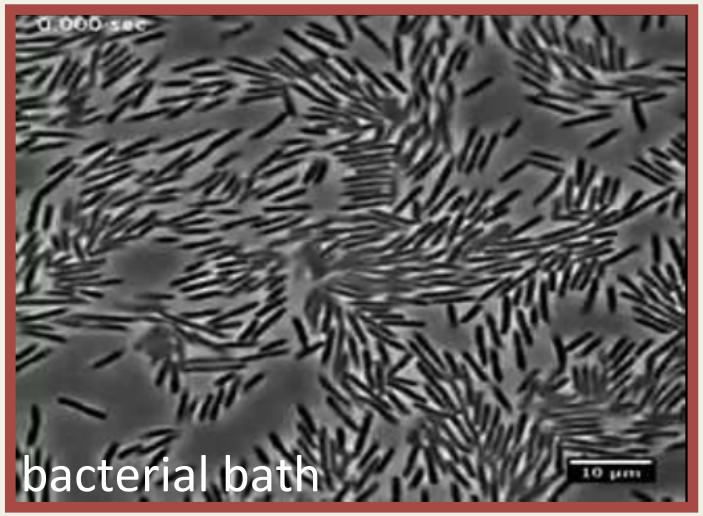
Deutsche Forschungsgemeinschaft DFG

GRK1558 research training group

SFB 910

VolkswagenStiftung

Active and collective motion in nature

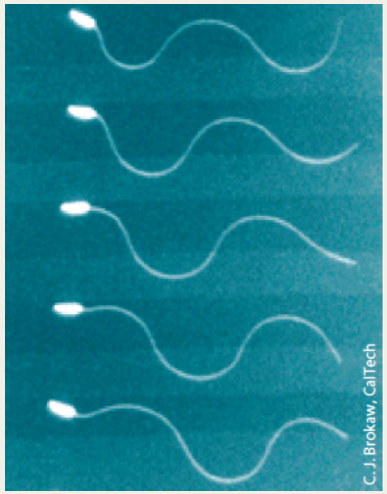


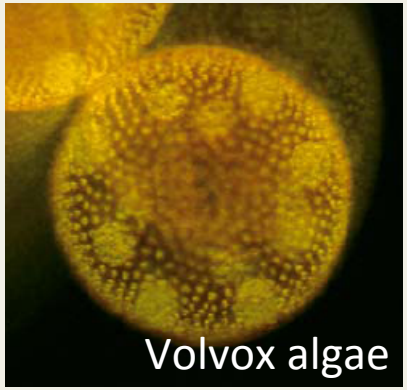
Weibel Lab (University of Wisconsin)

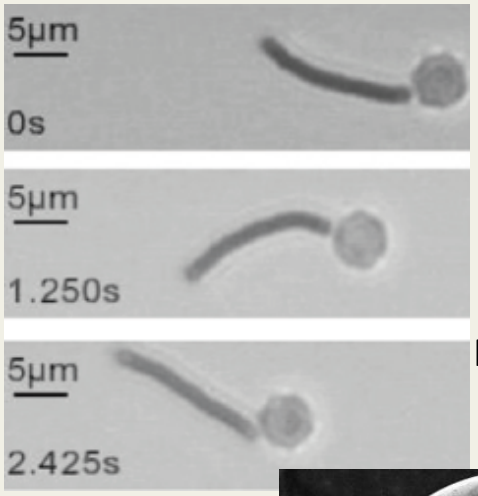
➔ aqueous environment
➔ microscopic world

Fascination: Active motion

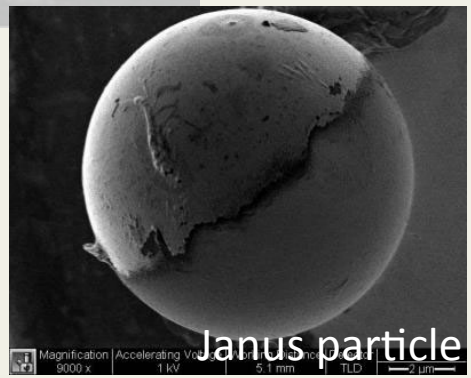
Nature versus artificial swimmers

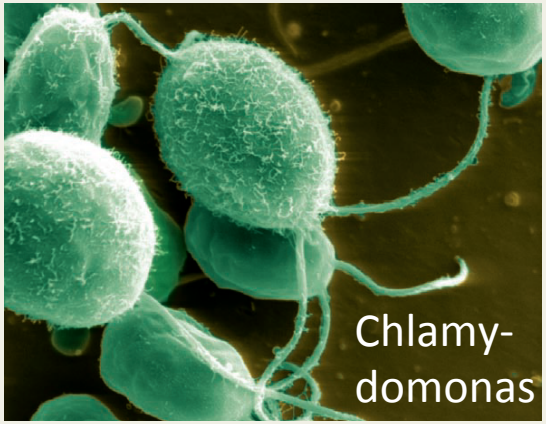


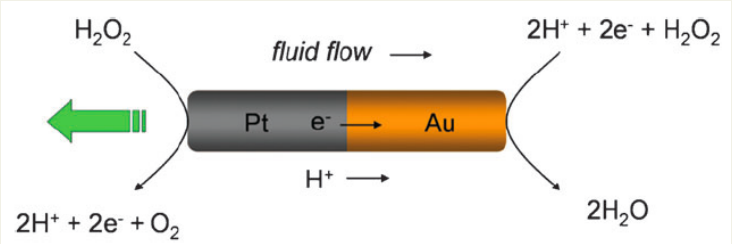




R. Dreyfus *et al.*
Nature (2005)



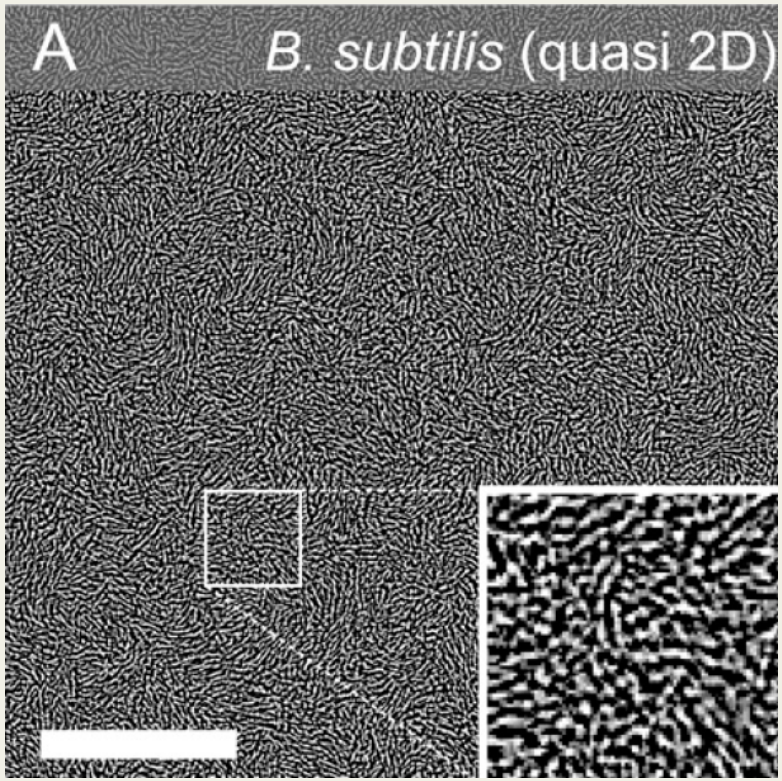




Fascination: Active motion

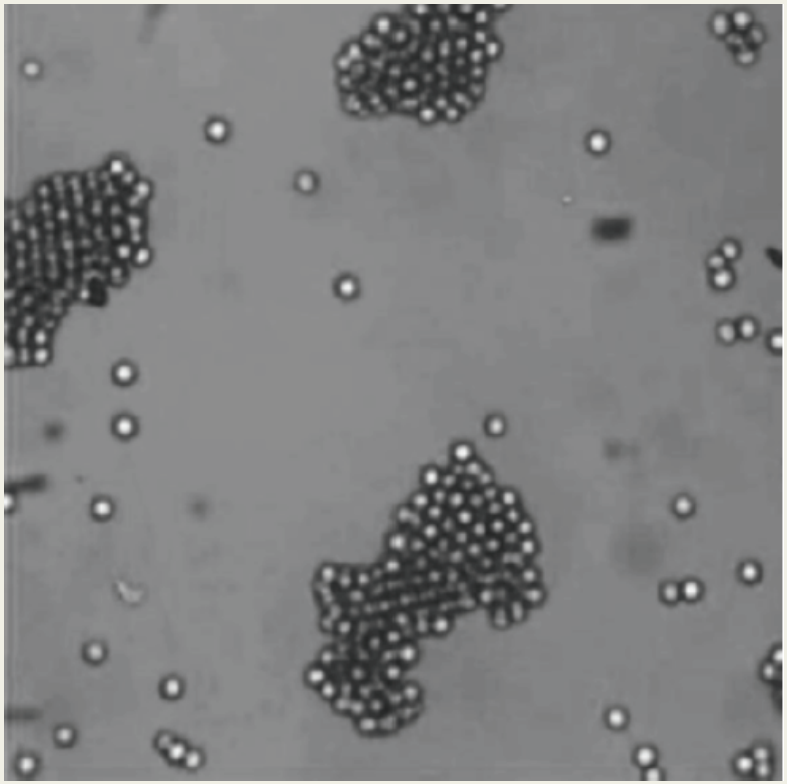
Collective dynamics

Bacterial turbulence



H.H. Wensink *et al.,* PNAS (2012)

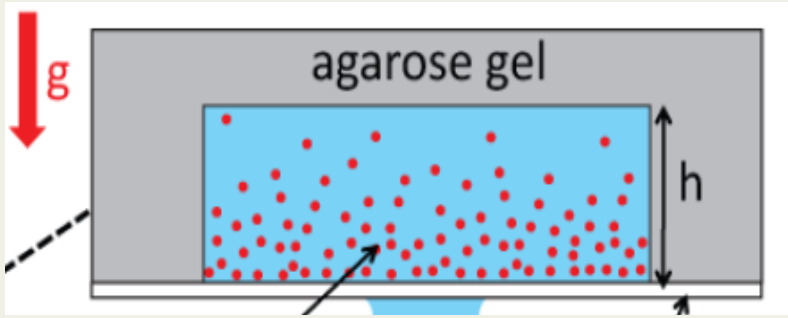
Novel dynamic states:
Clustering & phase separation



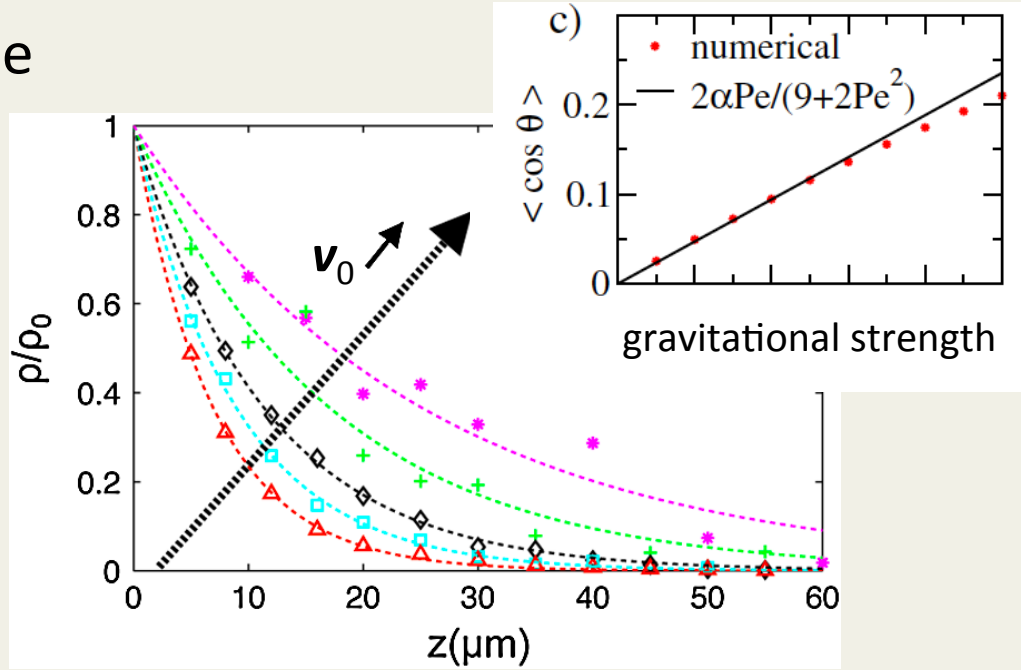
I. Buttinoni *et al.,* PRL (2013)

Generic features

Exponential sedimentation profile



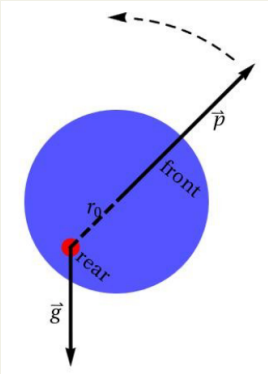
J. Palacci *et al.*, PRL (2010)



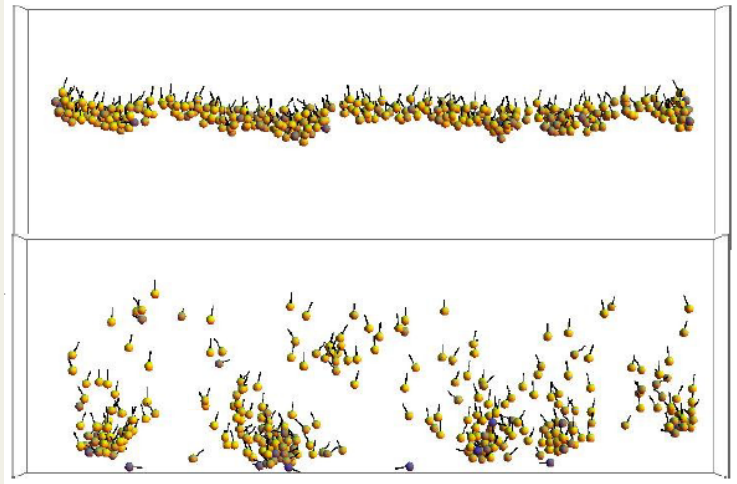
--> Polar order!

M. Enculescu & H.S., PRL (2011)

Bottom-heavy particles



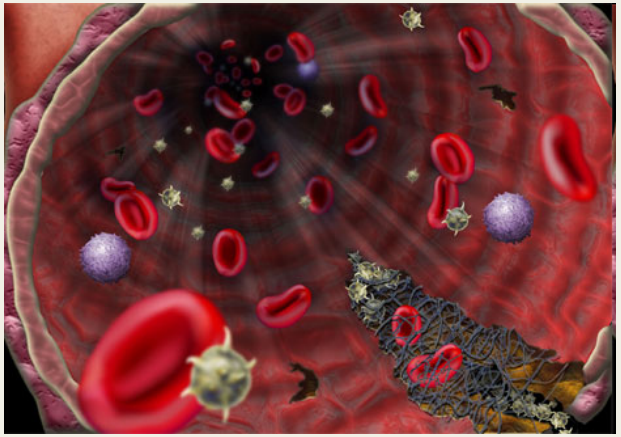
K. Wolff, A.M. Hahn & H.S., EPJE (2013)



M. Hennes, K. Wolff & H.S.

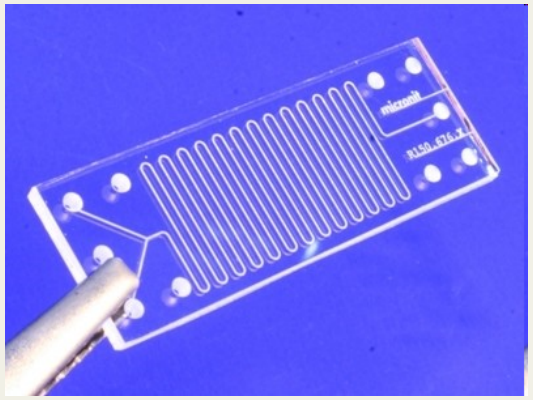
Swimming under confinement / in Poiseuille flow

parasites in bloodstream



Fallopian tube catheter →

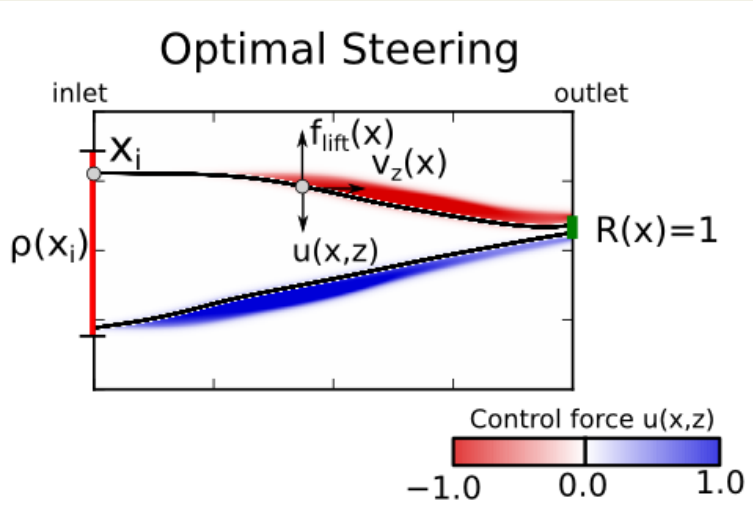
microfluidic channel

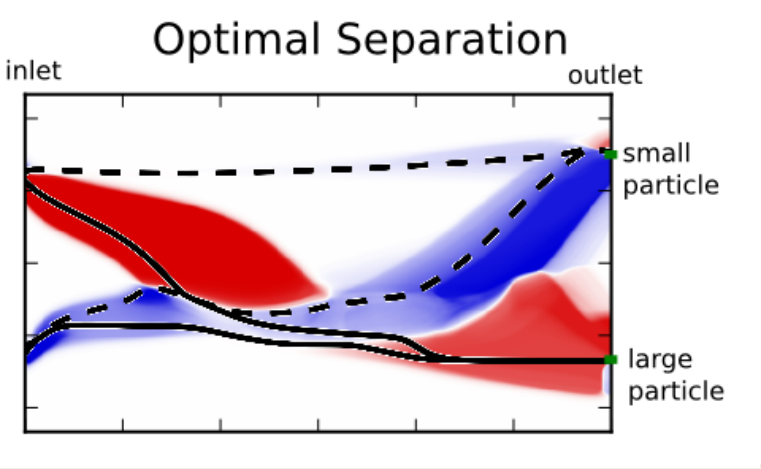


R. Rusconi, J.S. Guasto & R. Stocker, Nature Phys. (2014)

Inertial microfluidic

Design of optimal control forces





C. Prohm, F. Tröltzsch, & HS, EPJE (2013)

active motion:

non-equilibrium:
1. generic features & novel phenomena
2. external fields
3. collective dynamics

hydro- ⟷ dynamics

modeling of single microorganisms, active particles

I. A microswimmer in Poiseuille flow

→ from a Hamiltonian to a dissipative and chaotic system

II. Collective dynamics of spherical microswimmers („squirmers“)

→ hydrodynamics matters

III. Pump formation of active particles in a 3D harmonic trap

→ self-induced polar order: lessons from ferromagnetism

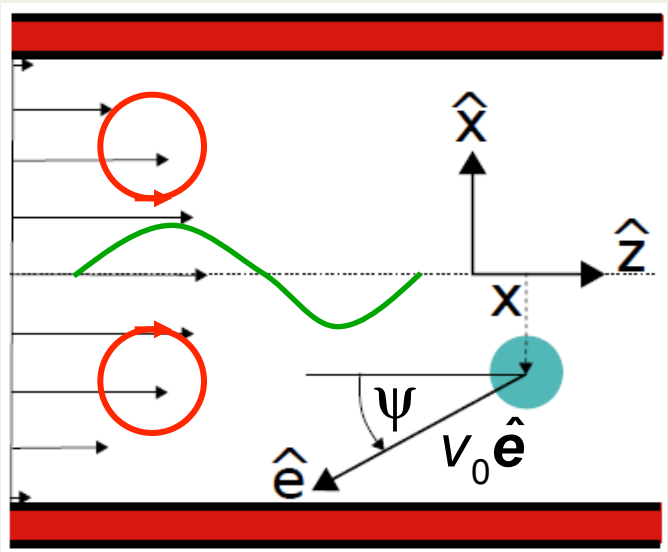
IV. „Chemotactic“ active colloids: Sensing the environment

→ dynamic clustering

I. SWIMMING IN POISEUILLE FLOW

Strong Poiseuille flow

(neglect wall effects)



swimmer performs nonlinear oscillations about centerline

$$\ddot{\psi} + \frac{v_F v_0}{R_{Ch}^2} \sin\psi = 0$$

v_F ... flow strength

v_0 ... swimming velocity

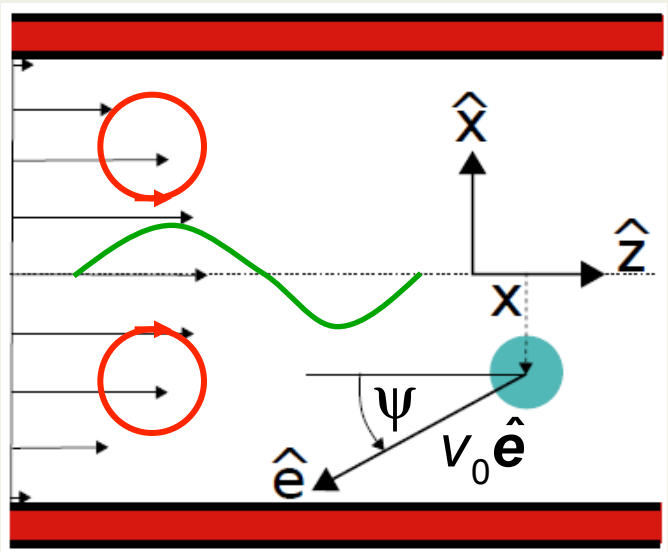
➔ Hamiltonian system in x and Ψ

(also in 3D)

A. Zöttl & H.S., PRL (2012), EPJE (2013); Zilman *et al.*, Mar. Biol. (2008)

Strong Poiseuille flow

(neglect wall effects)



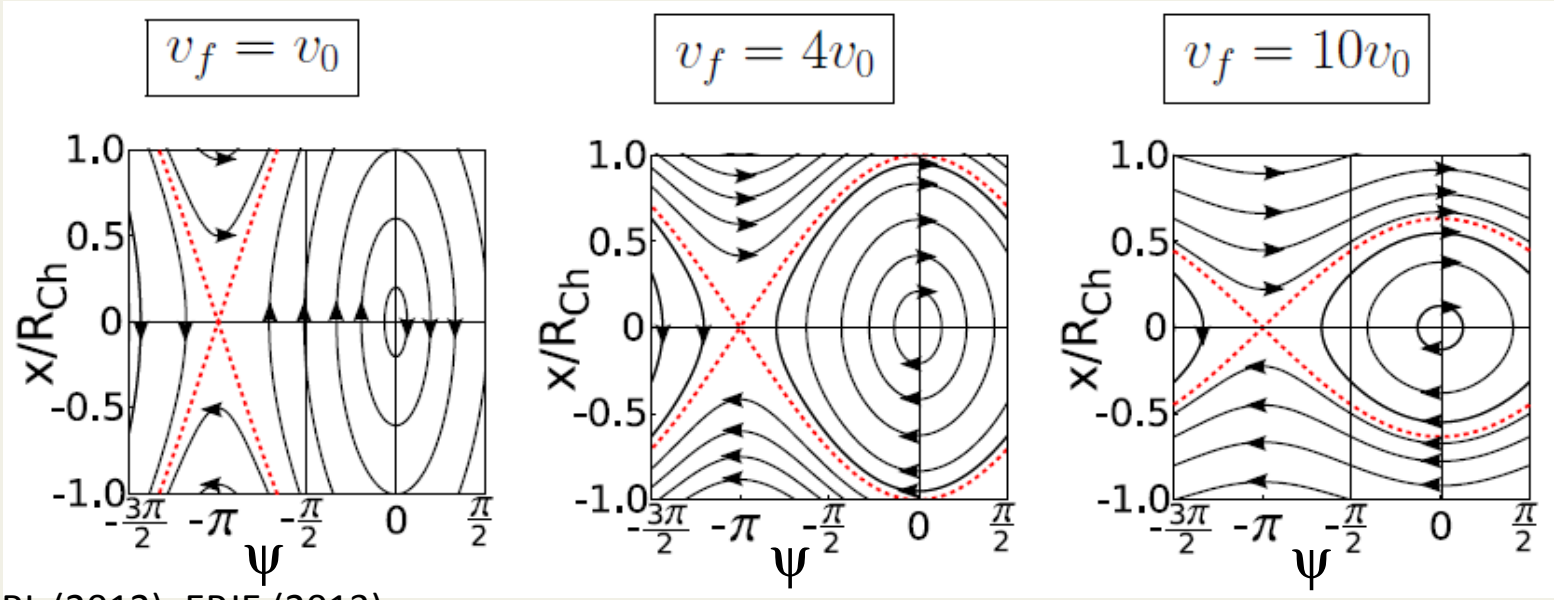
swimmer performs nonlinear oscillations about centerline

$$\ddot{\psi} + \frac{v_F v_0}{R_{Ch}^2}\sin\psi = 0$$

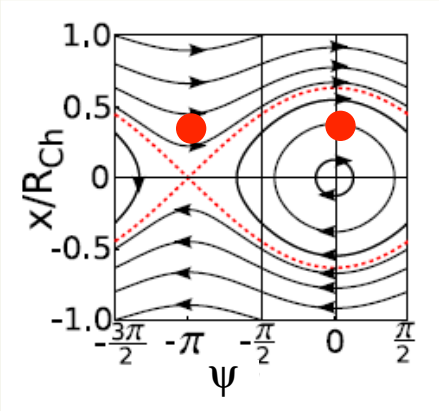
v_F ... flow strength

v_0 ... swimming velocity

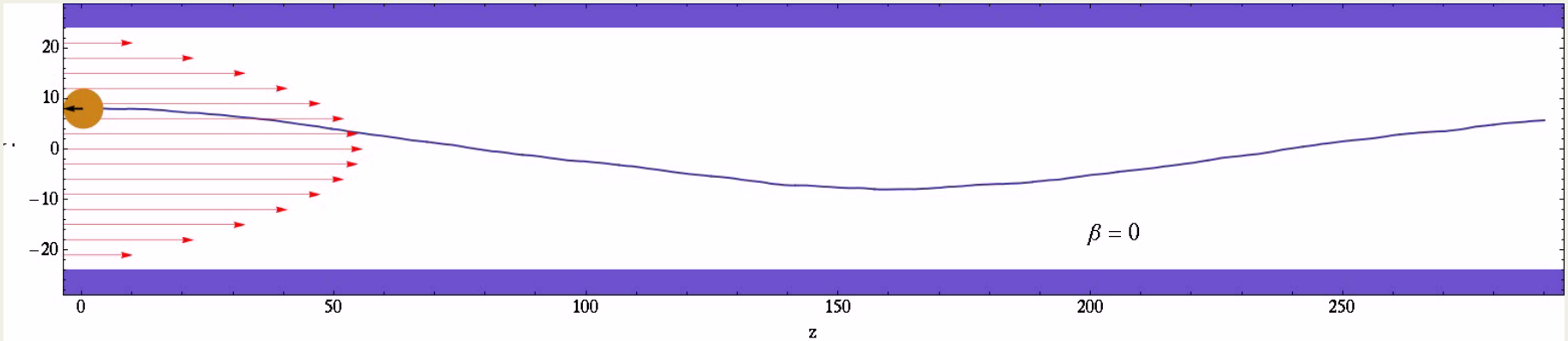
phase portrait

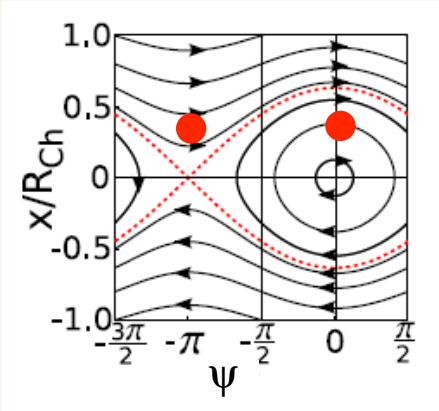


A. Zöttl & H.S., PRL (2012), EPJE (2013)

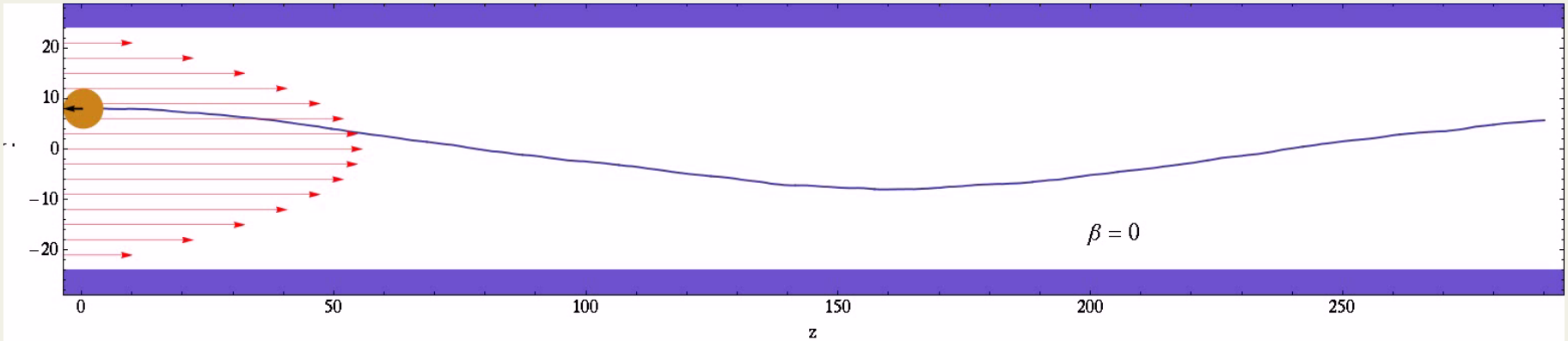

1.0
0.5
0
-0.5
-1.0
x/R_Ch
-3π/2
-π
-π/2
0
π/2
ψ

swinging

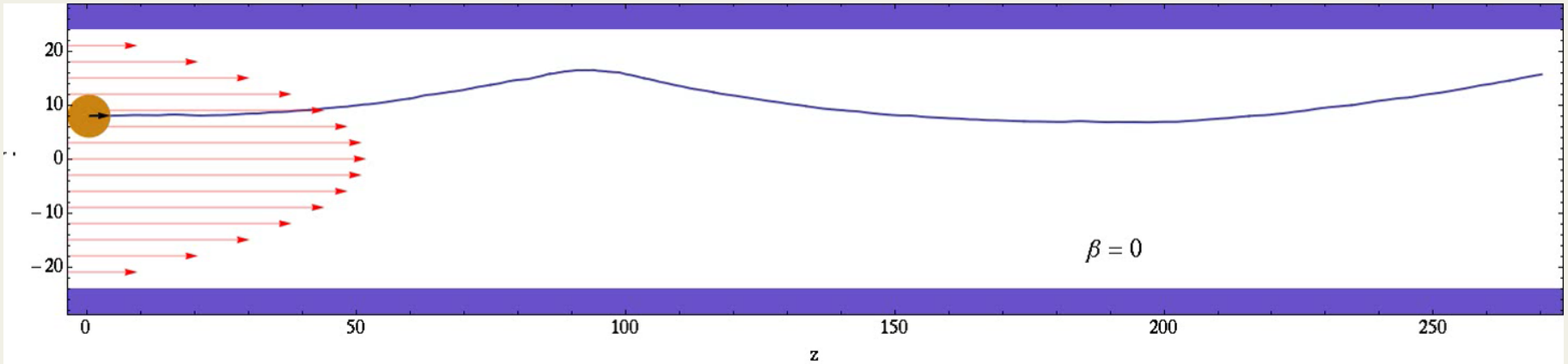

20
10
0
−10
−20
0
50
100
150
200
250
z
β = 0



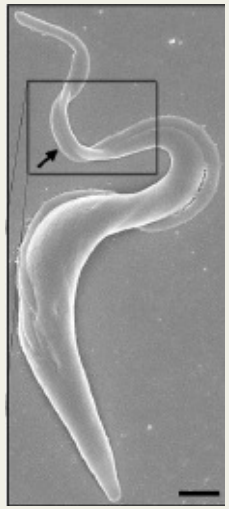
swinging

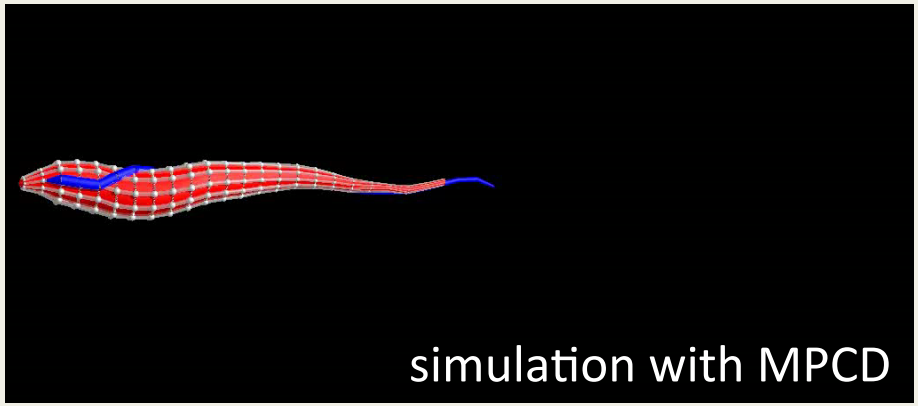


tumbling



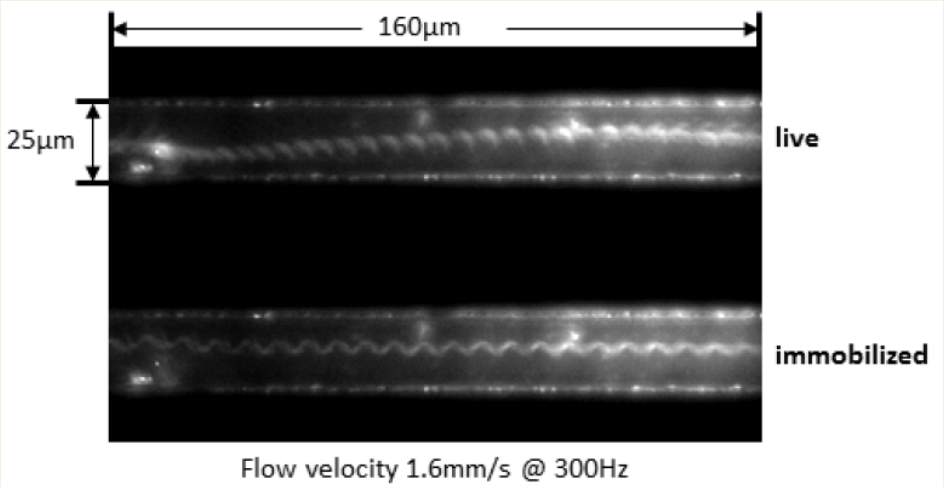
African trypanosome (sleeping sickness)



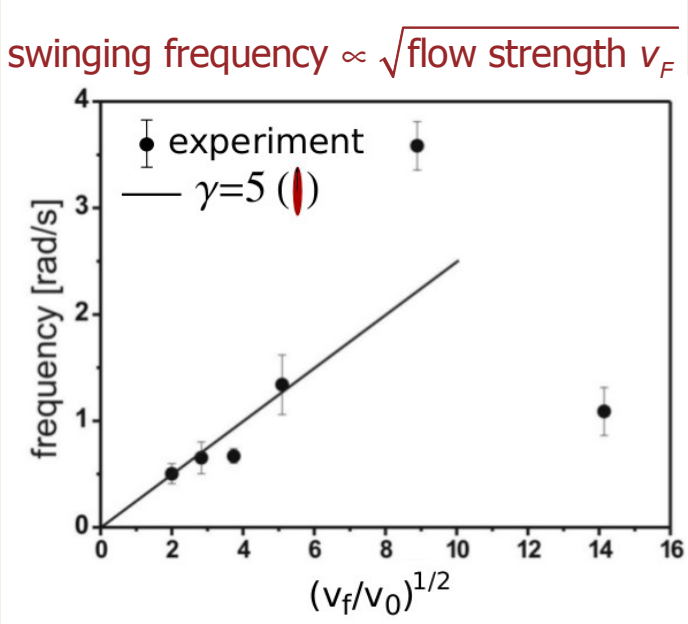


S. Babu & H.S., NJP (2012), D. Alizadherad

group of T. Pfohl (Basel, MPI Göttingen)



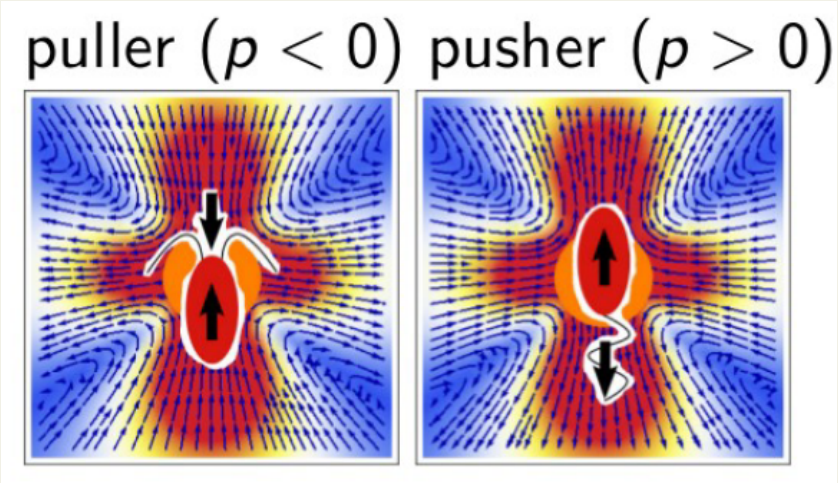
S. Uppaluri, ... Biophys. J. (2012)

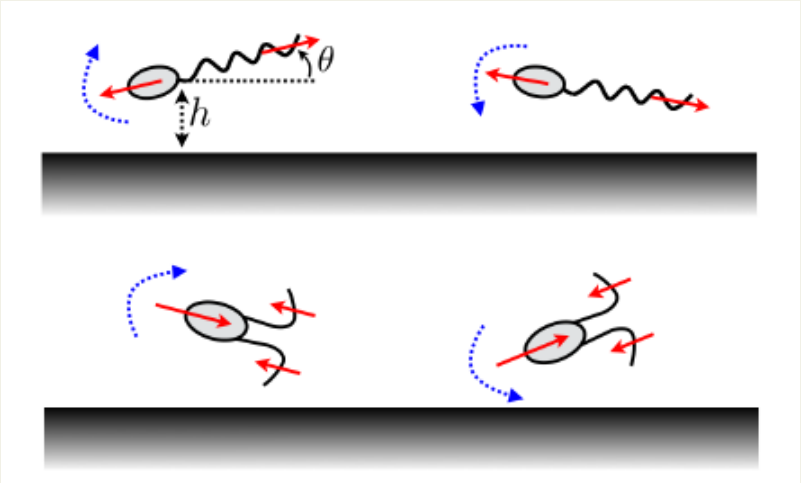


Hydrodynamic interactions with bounding walls

force-dipole swimmer:

$$\mathbf{v}(\mathbf{r}) = \frac{p}{8\pi\eta r^2}\left[3(\mathbf{e}\cdot\hat{\mathbf{r}})^2 - 1\right]\hat{\mathbf{r}}$$





→ wall induced velocity: $\boldsymbol{v}_W$

→ total swimming velocity: $\boldsymbol{v} = v_0\hat{\boldsymbol{e}} + \boldsymbol{v}_W$

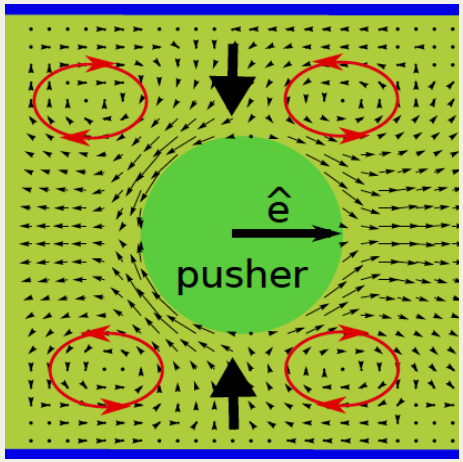
→ wall induced angular velocity: $\boldsymbol{\Omega}_W$

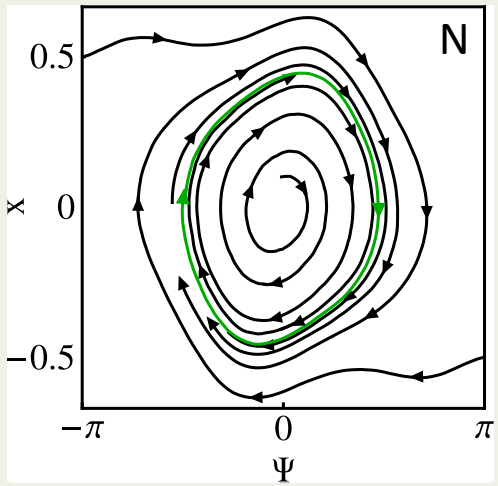
A.P. Berke, L. Turner, H.C. Berg and L. Lauga, PRL (2008)
L. Lauga, T. Powers, Rep. Prog. Phys. (2009)

2D motion in narrow channel ➔ „dissipation“

„analytic“ (A): 2-wall geometry numerics (N): cylindrical geometry

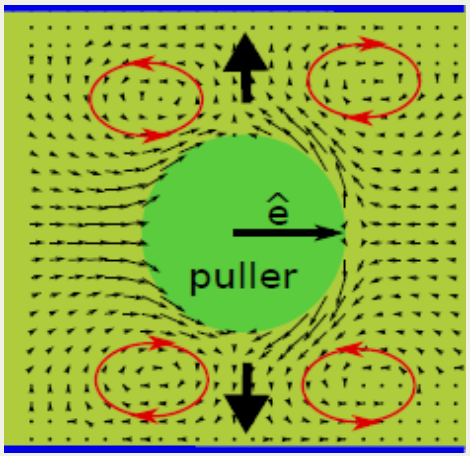
pusher:

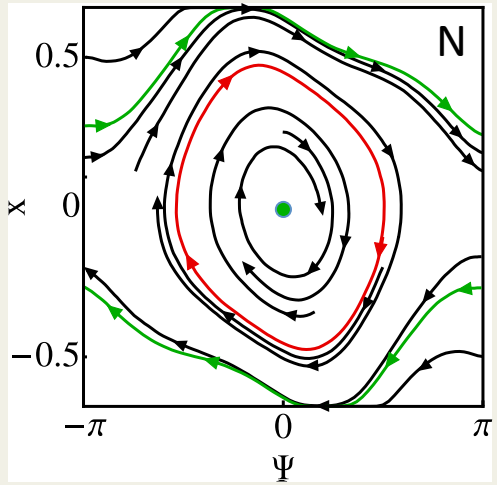




stable swinging motion around centerline

puller:





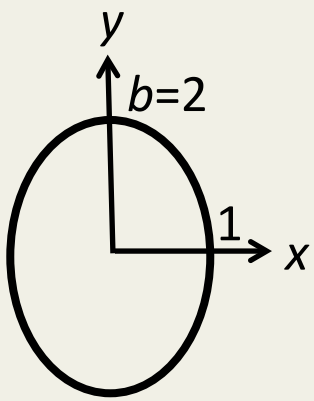
1. tumbling near wall
2. stable upstream swimming along centerline

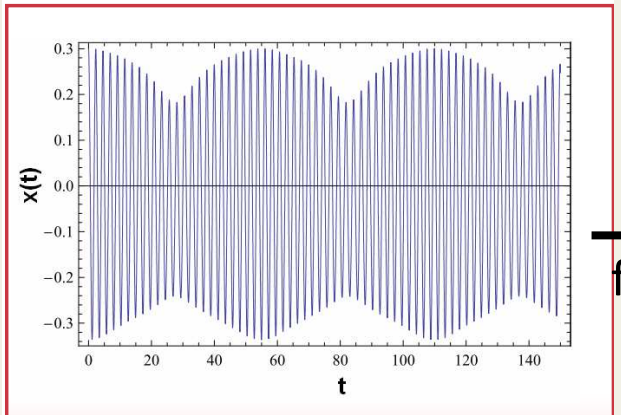
➔ hydrodynamic focussing

A. Zöttl & H.S., PRL (2012)

Chaotic motion

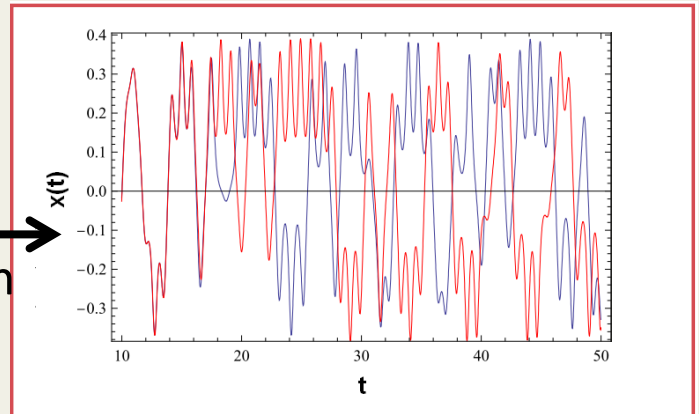
elliptical cross section:





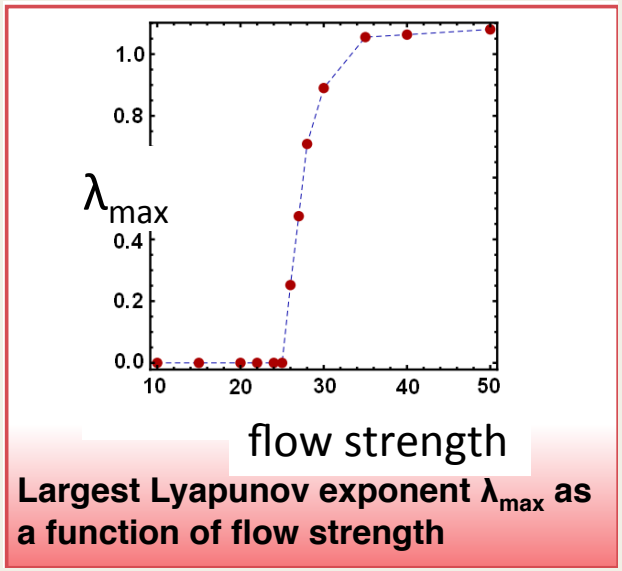
Time evolution of x(t) shows quasiperiodic behavior

increase of flow strength



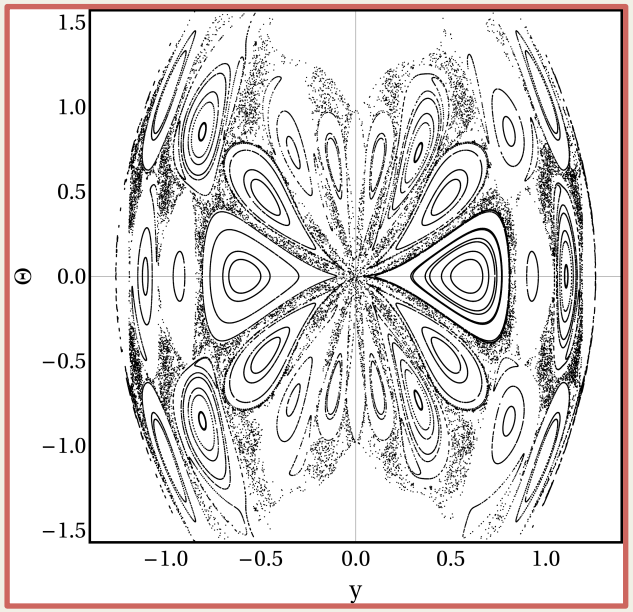
Time evolution of x(t) for two slightly different initial conditions

Lyapunov exponent:



Largest Lyapunov exponent λ_{max} as a function of flow strength

Poincaré section:

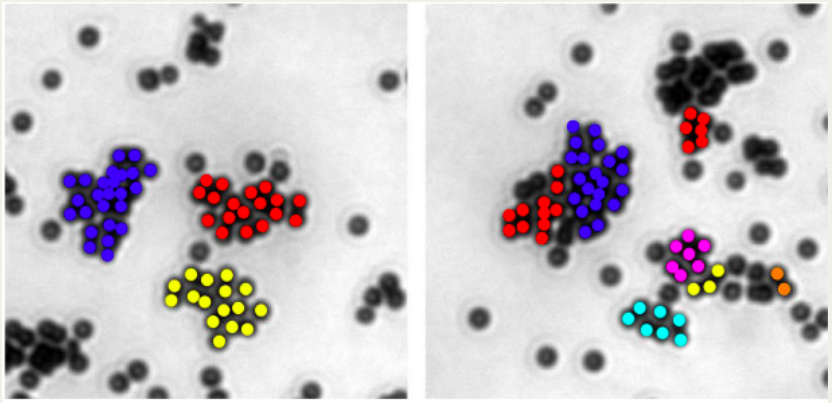


II. COLLECTIVE DYNAMICS OF SPHERICAL MICROSWIMMERS („SQUIRMERS“)

Experiment versus Theory in 2D

Active colloids: dynamic clustering

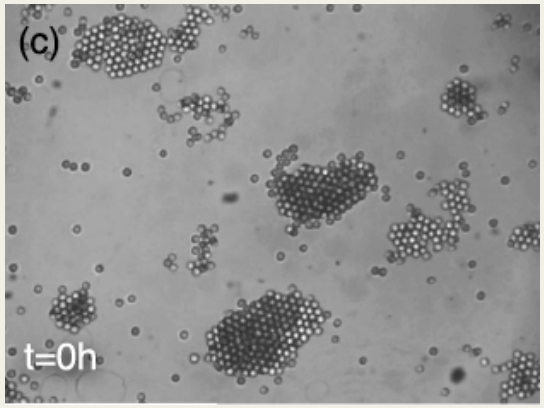
due to phoretic forces



I. Theurkauff, *et al.*, PRL (2012)

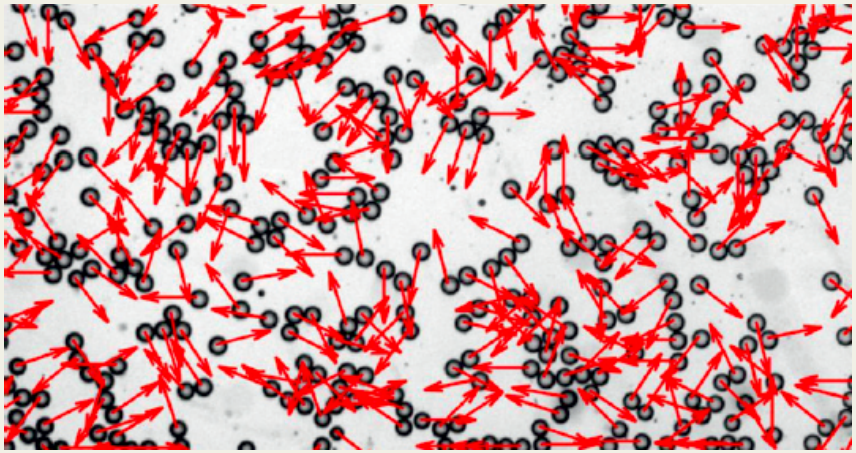
phase separation

pure hard core

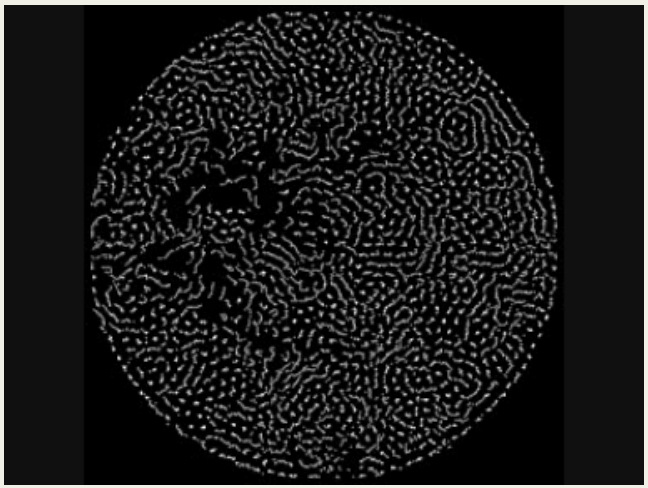


I. Buttinoni, *et al.*, PRL (2013)

Active droplets (squirmers): pure hydrodynamic interactions



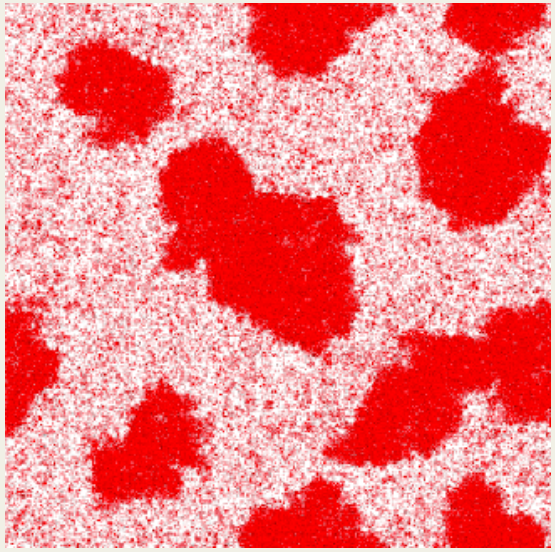
S. Thutupalli, R. Seemann & S. Herminghaus, NJP (2011)



Experiment versus Theory in 2D

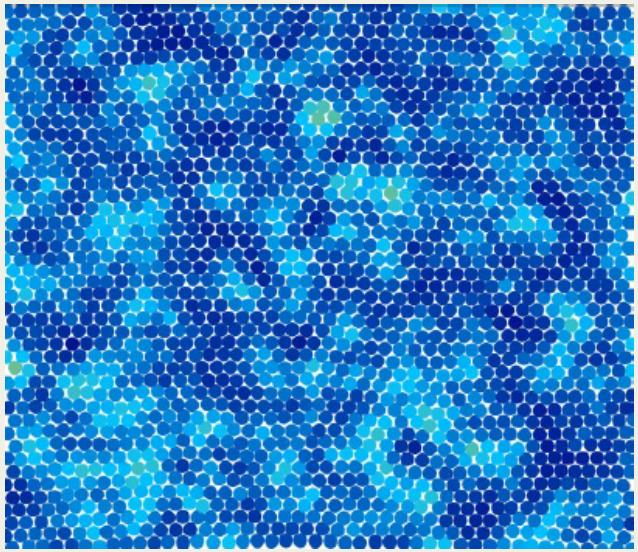
2D Brownian dynamics simulations

Phase separation



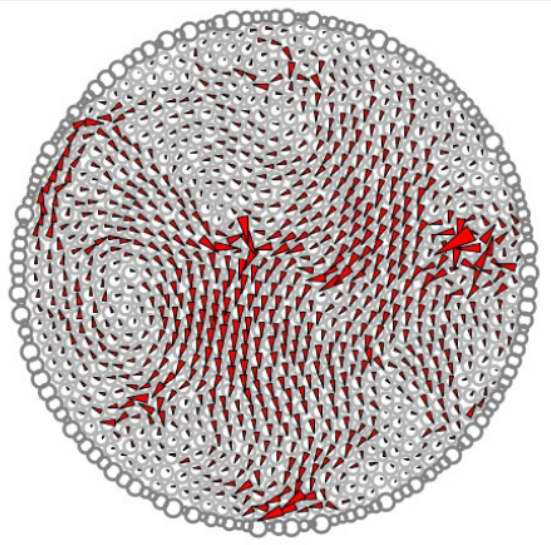
G.S. Redner, M.F. Hagan & A. Baskaran, PRL (2013)

Crystallization



J. Bialke, T. Speck & H. Löwen, PRL (2012)

Active jamming



S. Henkes, Y. Fily & M.C. Marchetti, PRE (2011)

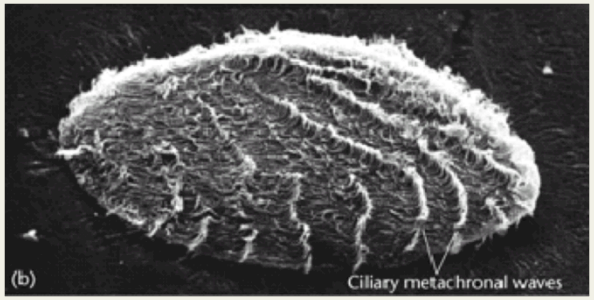
Motility-induced phase separation:

J. Tailleur & M.E. Cates, PRL (2008)
M.E. Cates & J. Tailleur, EPL (2013)

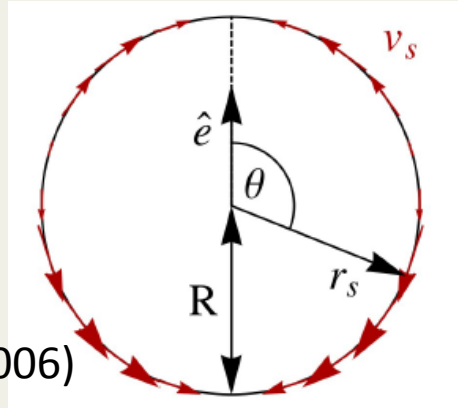
Influence of solvent/ hydrodynamic interactions ?

The squirmer

motivation:



Lighthill (1952)
Blake (1971)
Ishikawa &
Pedley, JFM (2006)



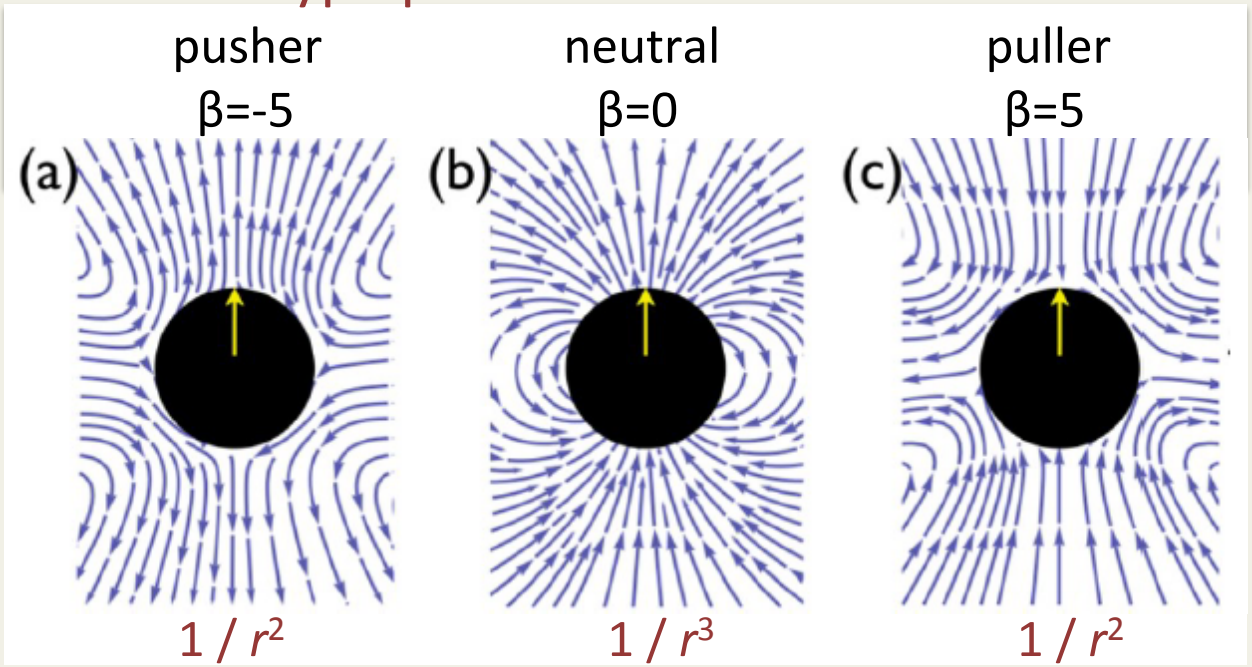
surface velocity

$$v_s = B_1(\sin\theta + \beta \sin 2\theta)$$

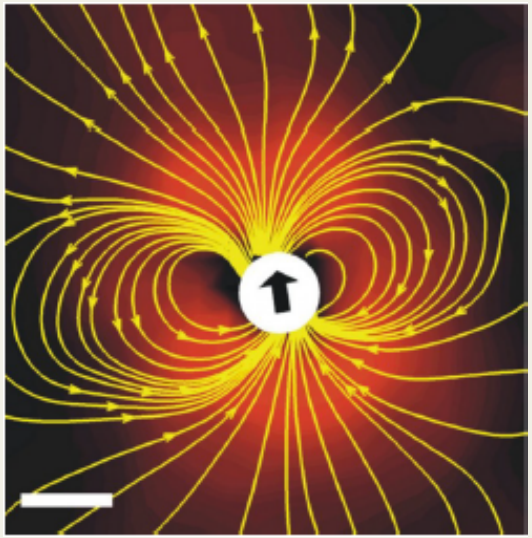
swimming velocity

$$v_0 = 2\,B_1 / 3$$

Swimmer type β



Evans *et al.*, Phys. Fluids (2011)



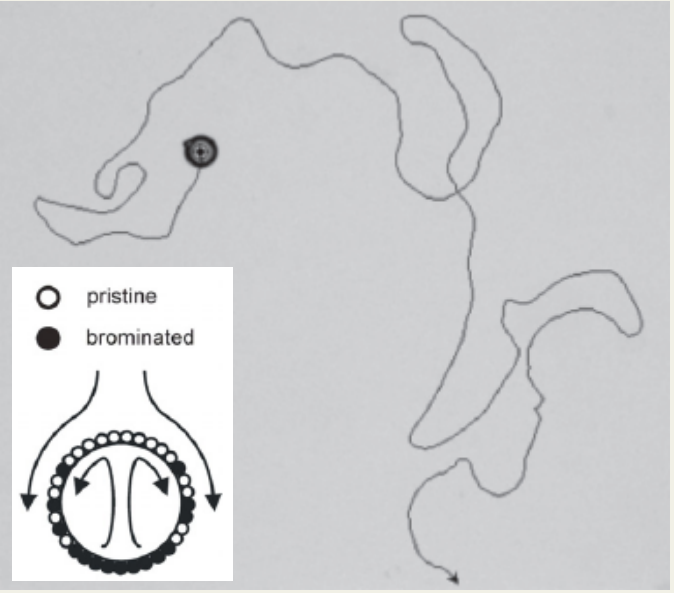
S. Thutupalli, R. Seemann &
S. Herminghaus, NJP (2011)

Experimental realization & modeling

- realization:

  surfactant-laden, bromide-water droplets in oil

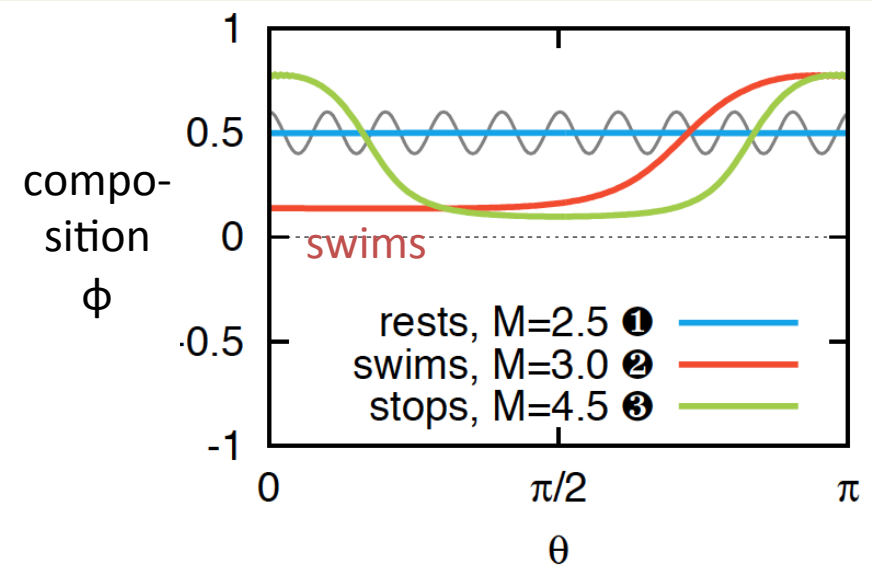
  ➔ surfactant mixture
  ➔ surface tension gradient
  ➔ Marangoni flow



S. Thutupalli, R. Seemann & S. Herminghaus, NJP (2011)

- modeling:

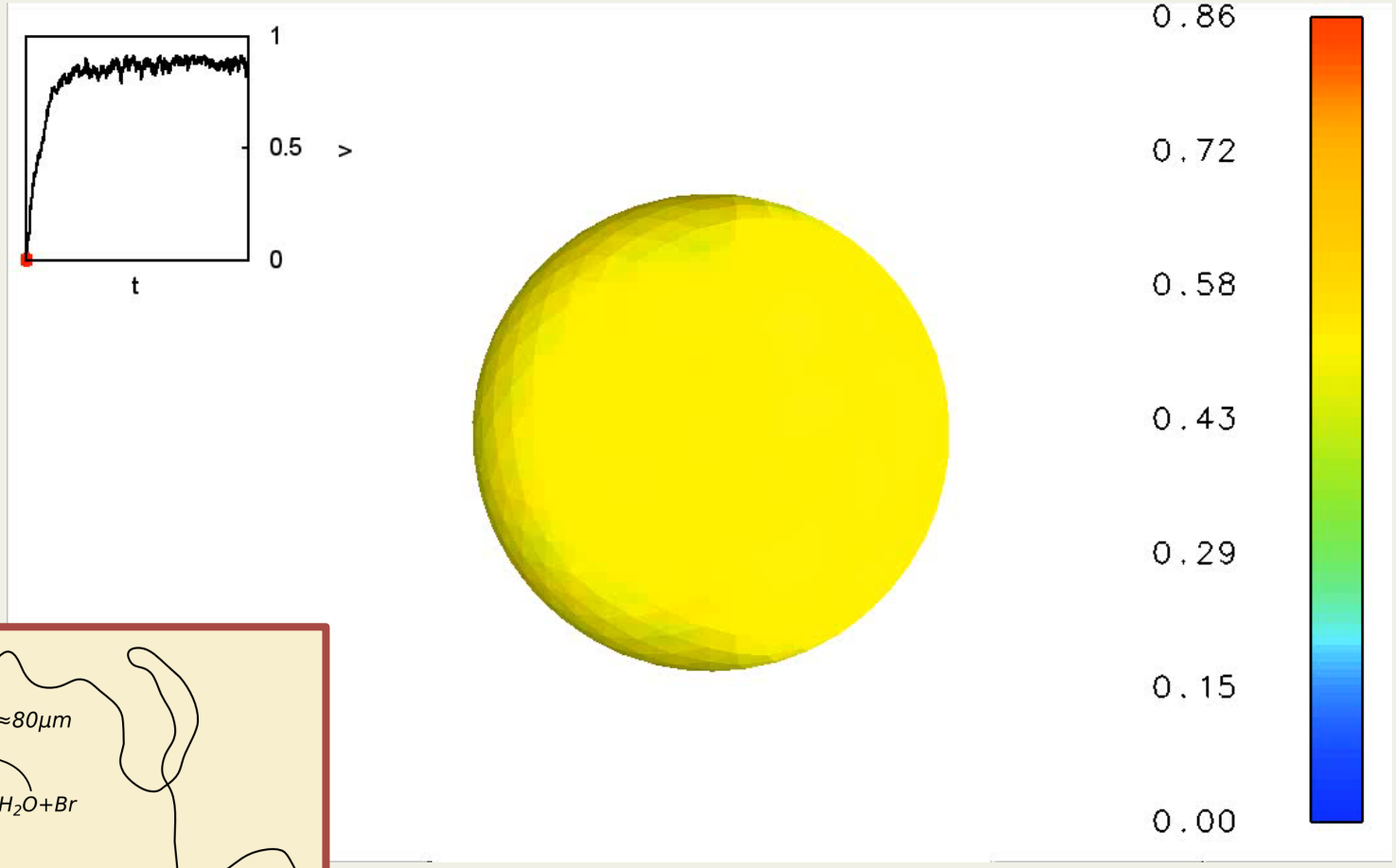
  free energy of mixture
  +
  diffusion-reaction-advection dynamics



M. Schmitt & H.S., EPL 2013

Full coarsening dynamics

(M. Schmitt)



compo-
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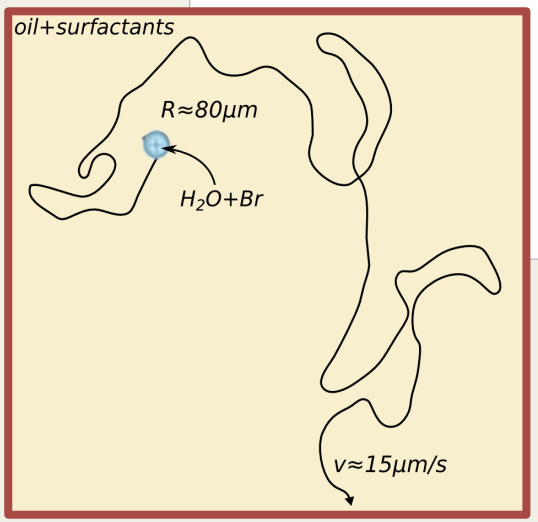
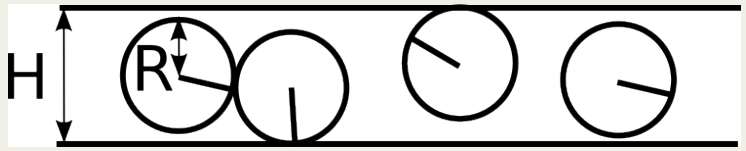


S. Thutupalli, R. Seemann &
S. Herminghaus, NJP (2011)

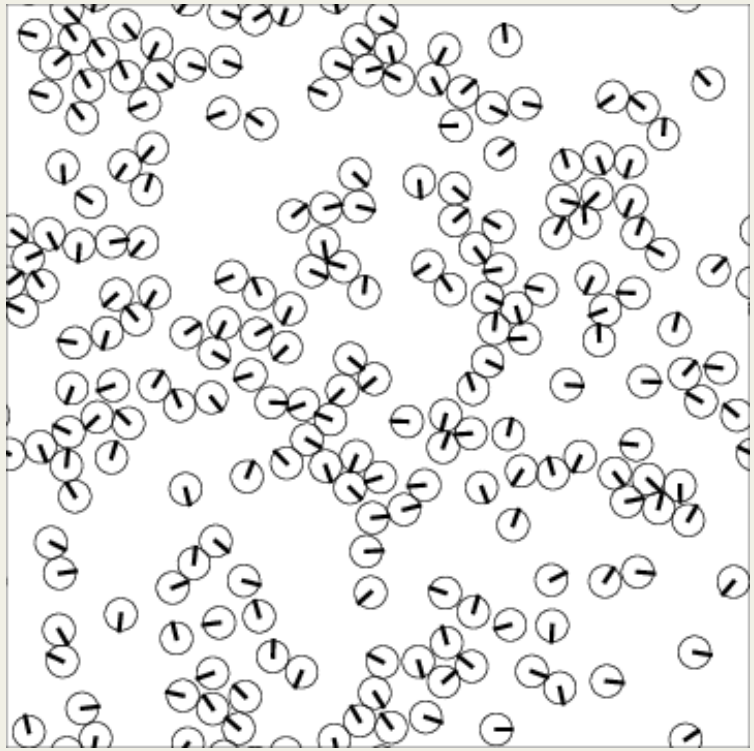
Squirmers in quasi-2D geometry

A. Zöttl & H.S.
to be published
in PRL

side view



top view



N = 208

squirmer parameter: β = -3 ... 3

areal density: Φ = 0.1 ... 0.83

Fluid:

simulation with

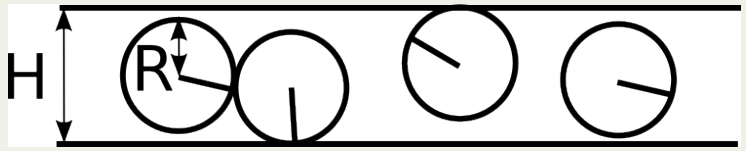
multi-particle collision dynamics

$N_{\text{fluid}} = 0.3 \ldots 4.4 * 10^6$

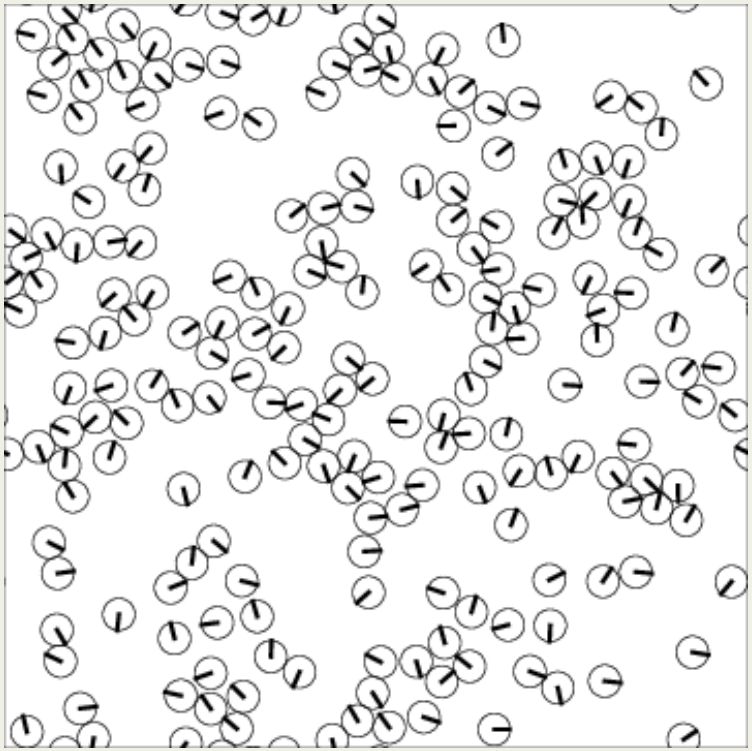
Squirmers in quasi-2D geometry

A. Zöttl & H.S.
submitted to PRL

side view



top view



N = 208

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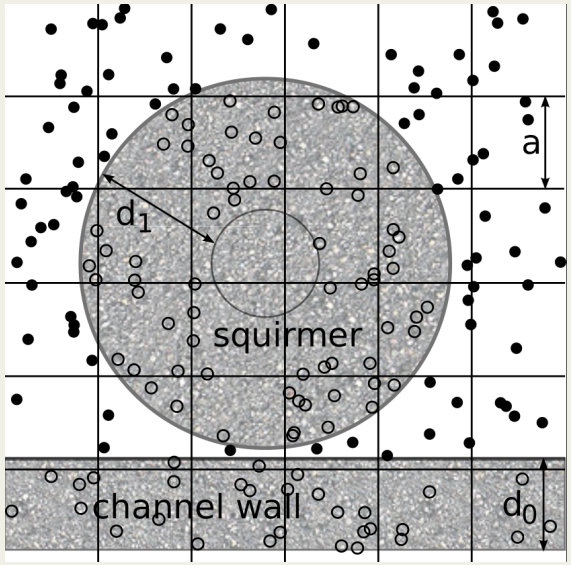
Fluid:

simulation with

multi-particle collision dynamics

$N_{\text{fluid}} = 0.3 \ldots 4.4 * 10^6$

Squirmers: coupled to fluid



M. Downton & H.S., JPCM (2009)
A. Zöttl & H.S. (2012)

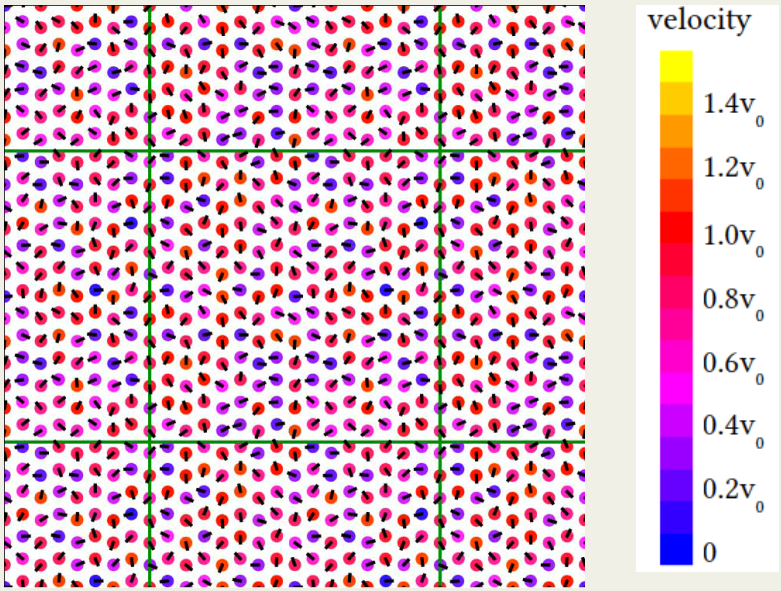
periodic boundary conditions

Collective dynamics

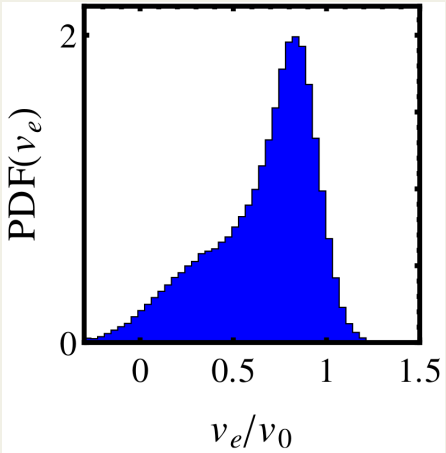
gas-like phase

$\Phi = 0.3$

$\beta = 0$



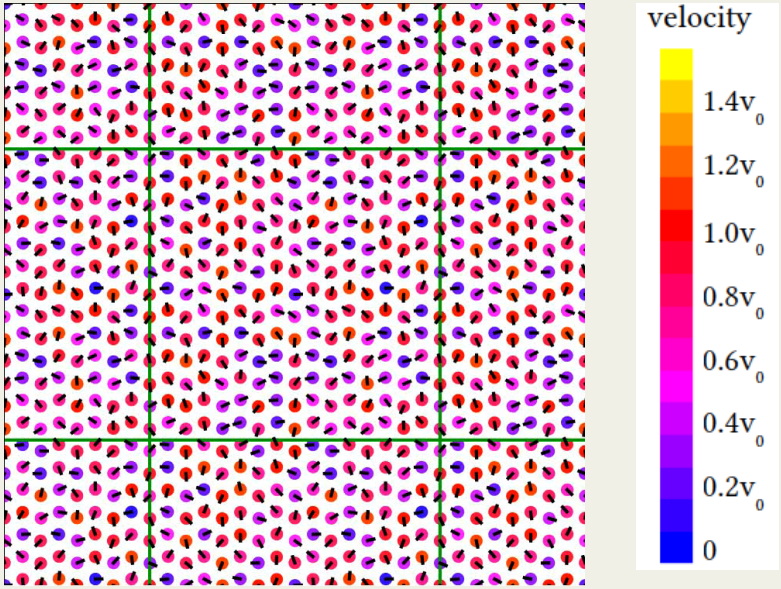
velocity distribution



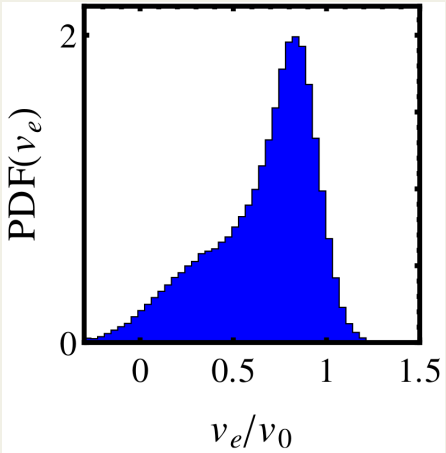
Collective dynamics

gas-like phase

$\Phi = 0.3$
$\beta = 0$

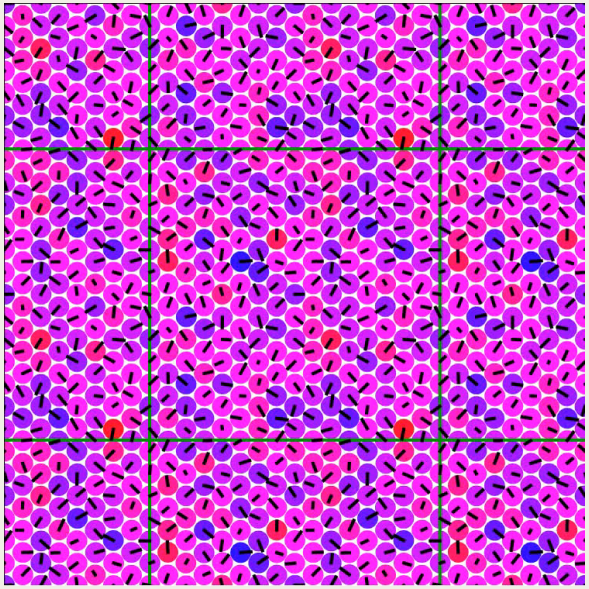


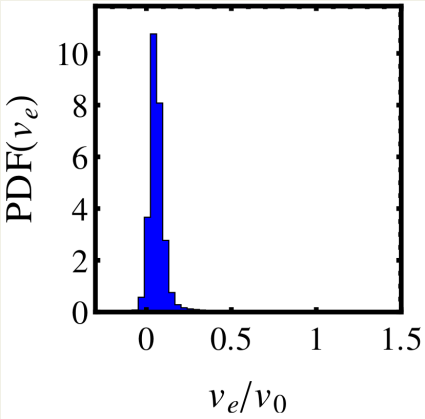
velocity distribution

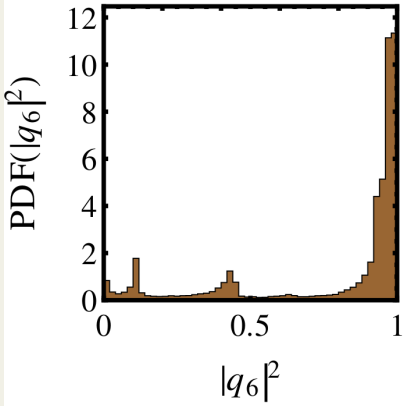


jammed crystalline phase

$\Phi = 0.83$
$\beta = 0$







local 6-fold bond orientation

$$|q_6^{(i)}|^2 \text{ with } q_6^{(i)} := \frac{1}{6} \sum_{j \in N_6^{(i)}} e^{i6\theta_{ij}}$$

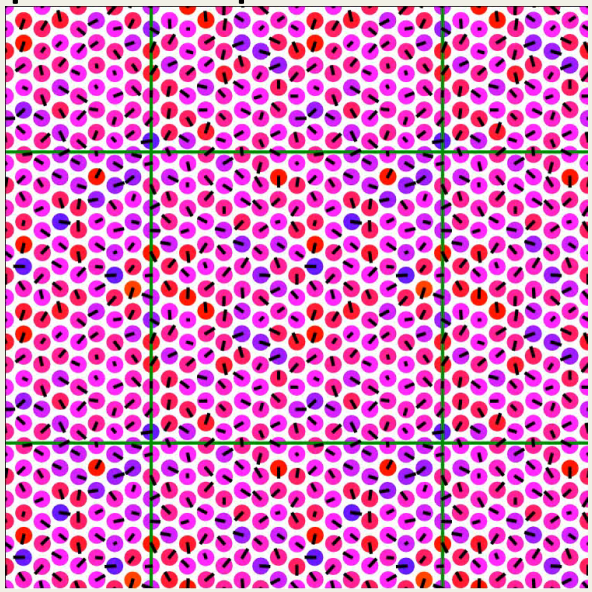
J. Bialke *et al.*, PRL (2012)

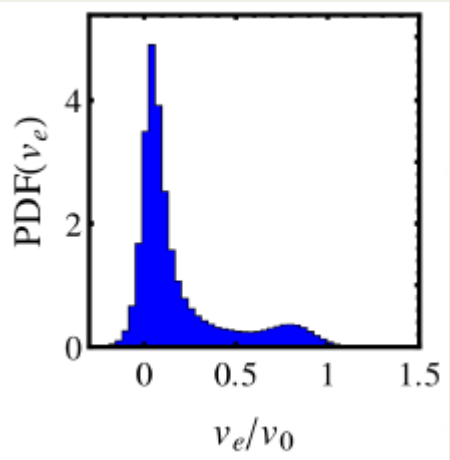
Collective dynamics

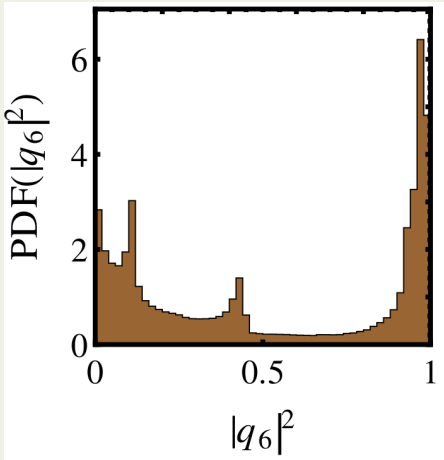
phase separation

$\Phi = 0.57$

$\beta = 0$



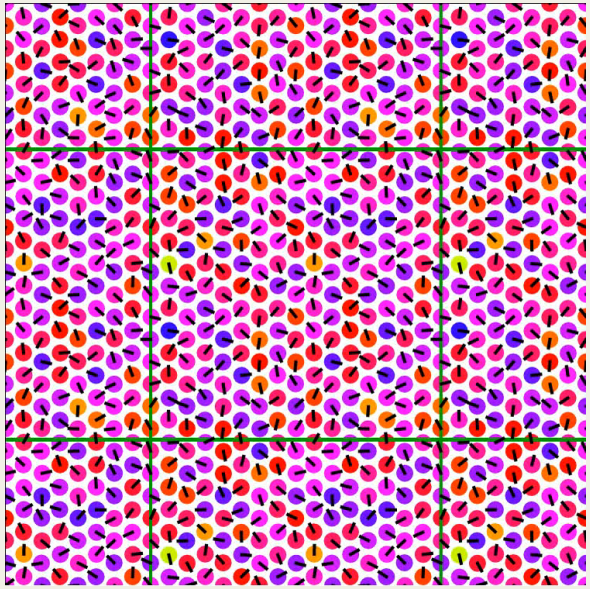


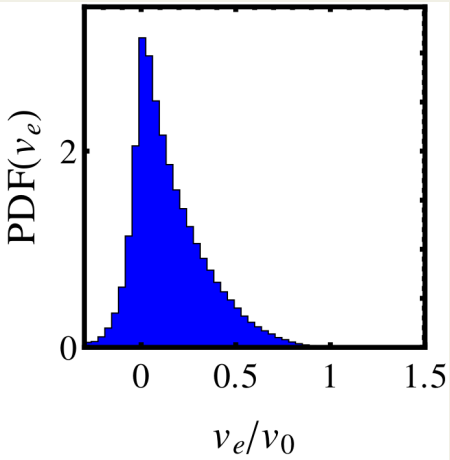


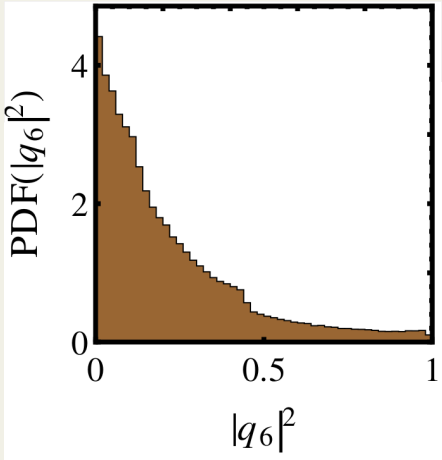
no phase separation

$\Phi = 0.57$

$\beta = -3$



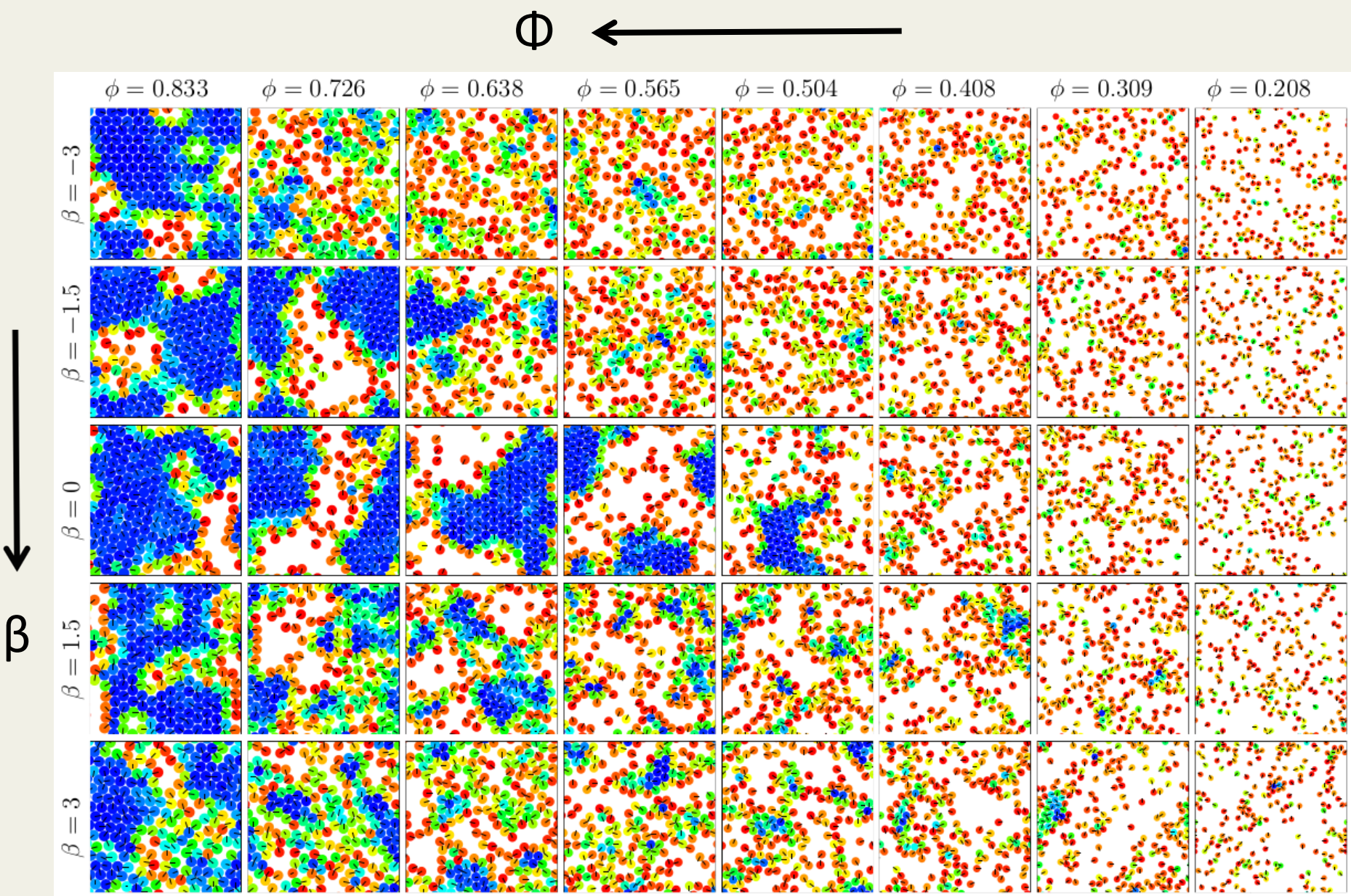




suppression of phase separation!

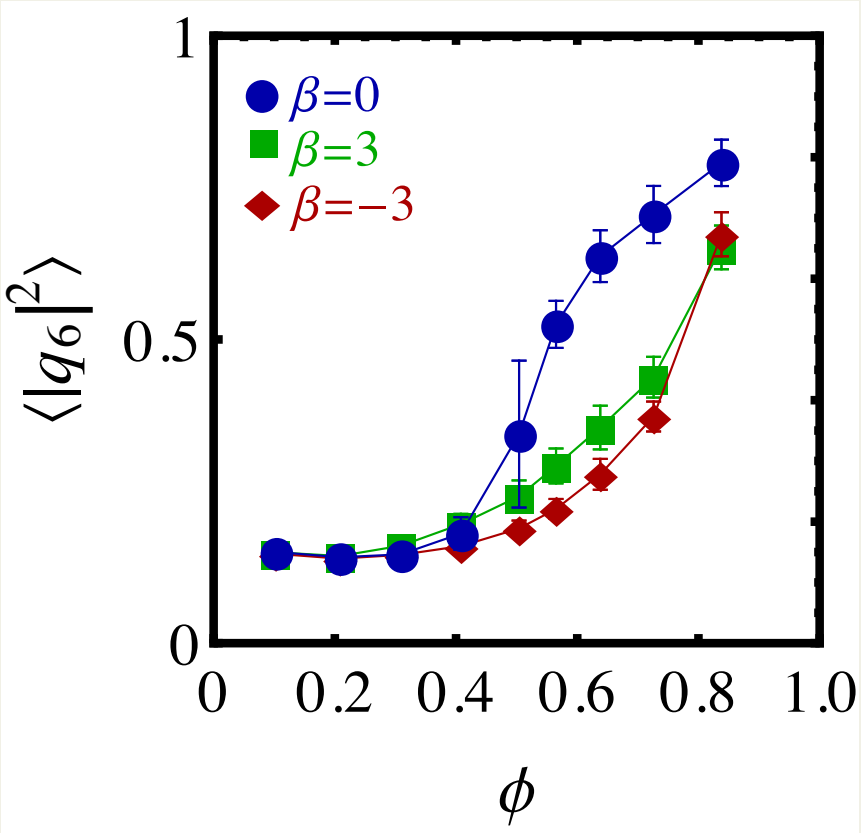
local flow fields are important!

Color-coded local bond order

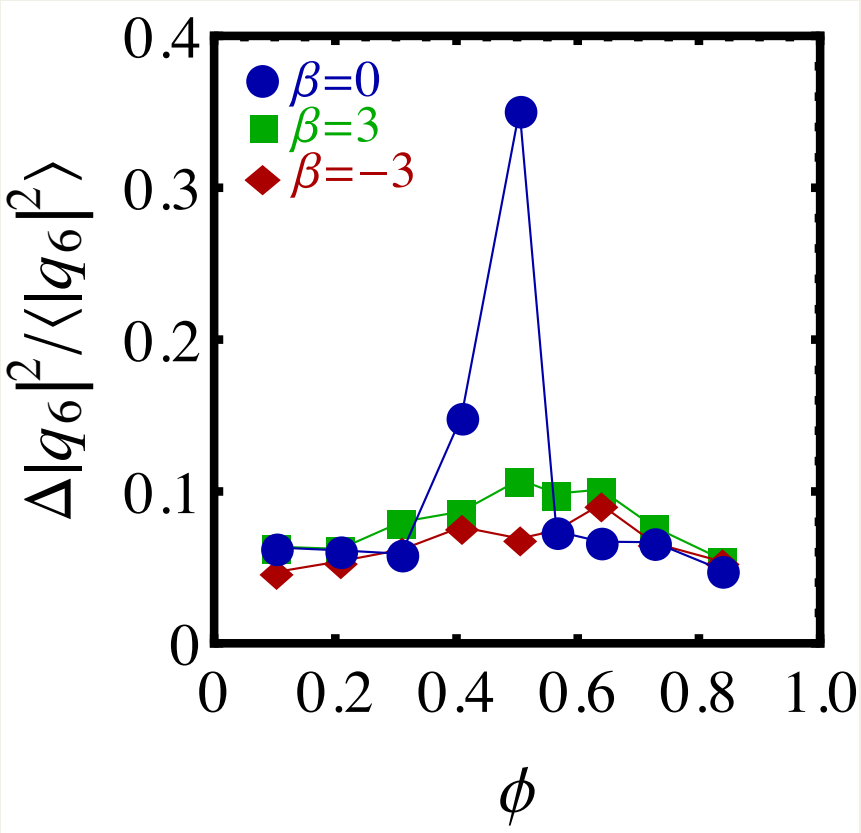


Mean local bond-orientational order

order parameter

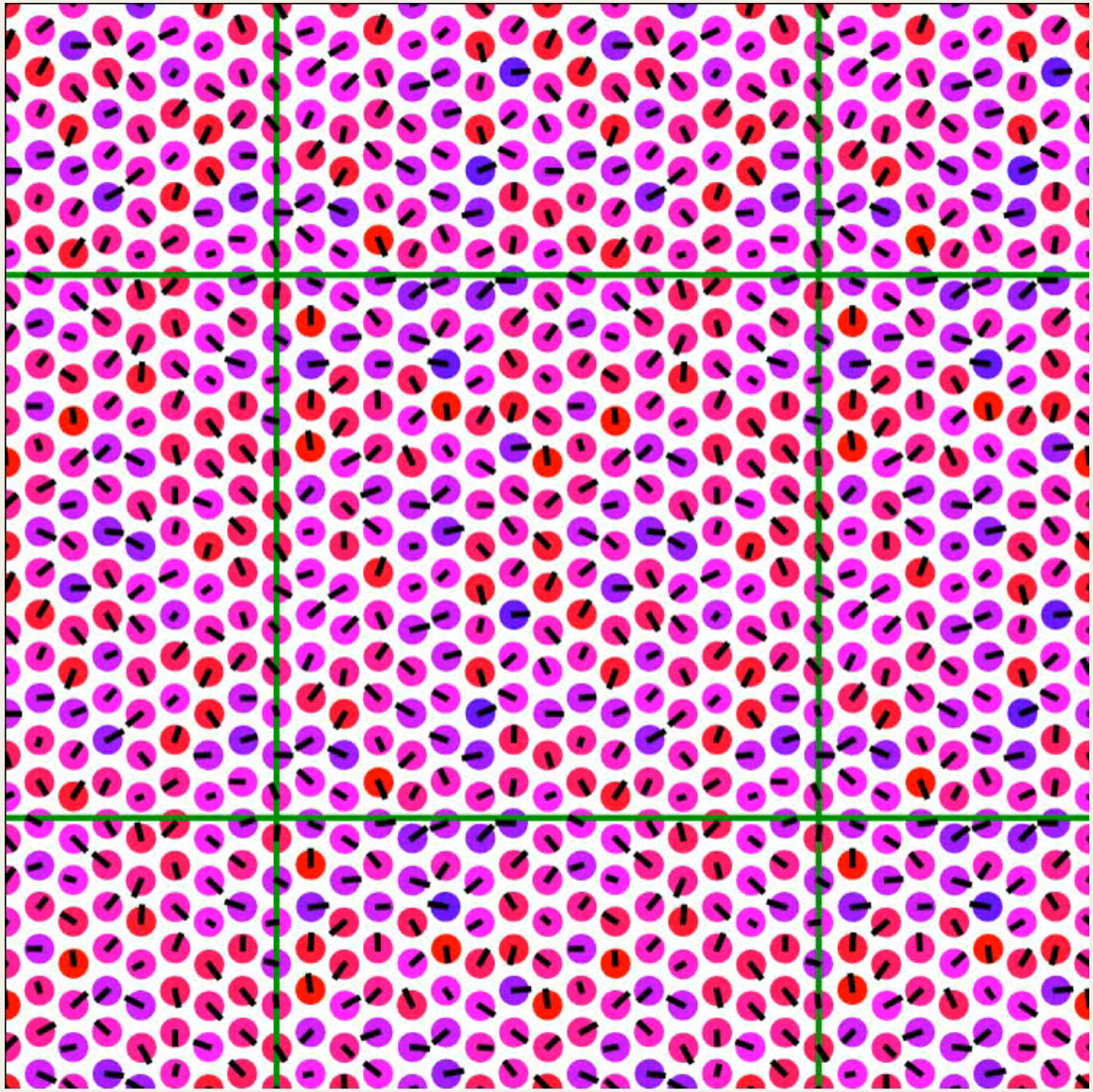


fluctuations



„Critical density“ – onset of phase separation

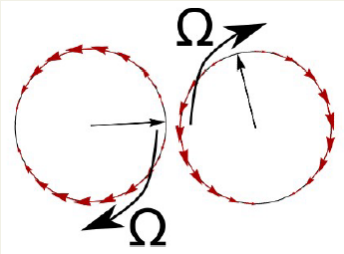
$\beta = 0$
$\Phi = 0.5$

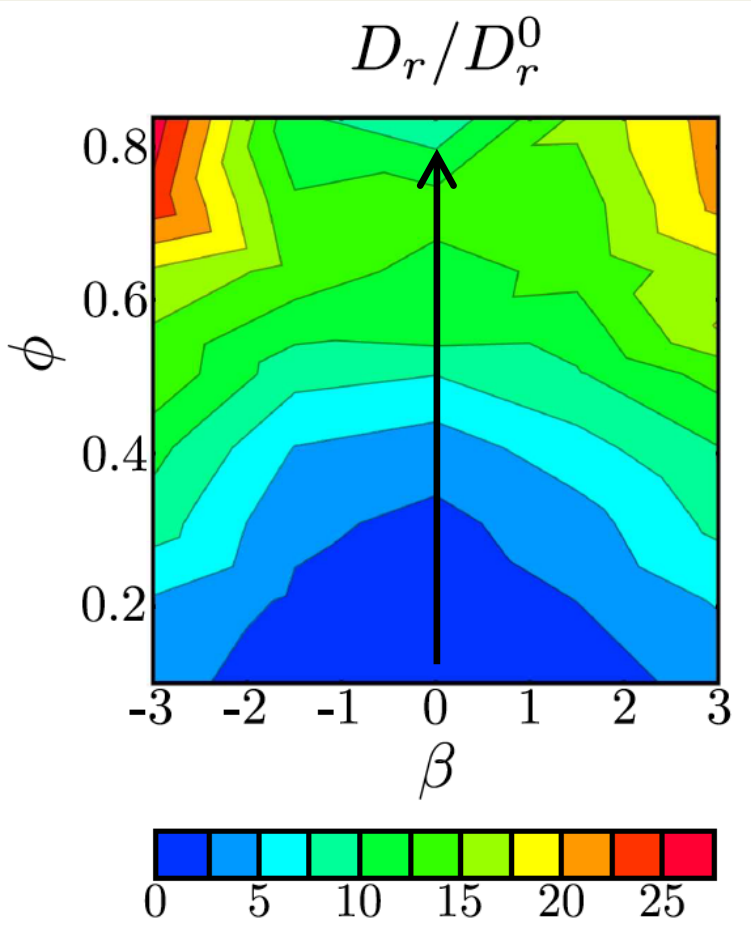


Swimmer flow field strongly influences:

1. rotational diffusion

D_r^0 ... thermal value





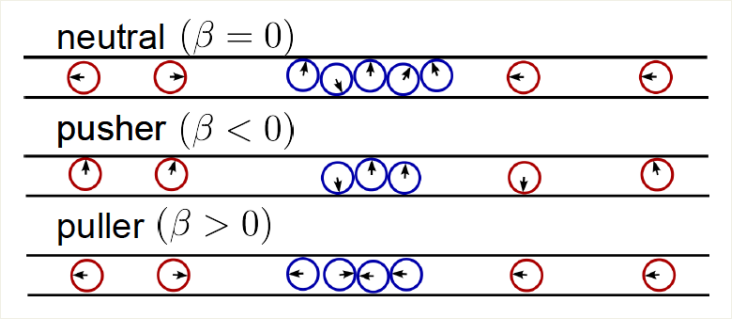
- strong increase with area fraction Φ
- near-field hydrodynamics matters:

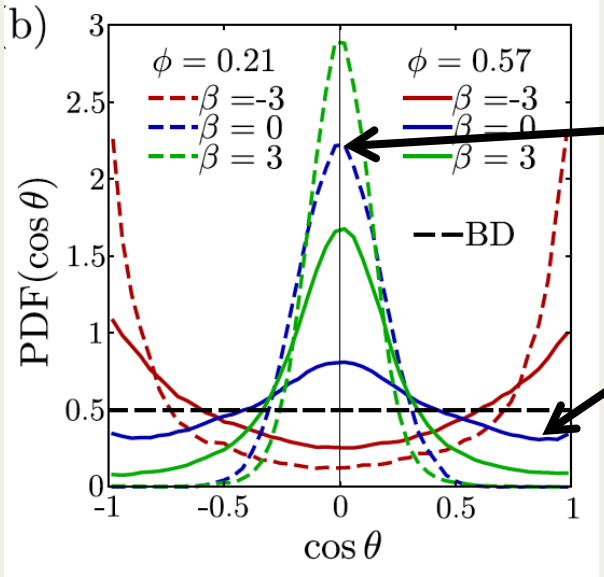
  increase with |β|

Swimmer flow field strongly influences:

2. orientation:

orientational distribution





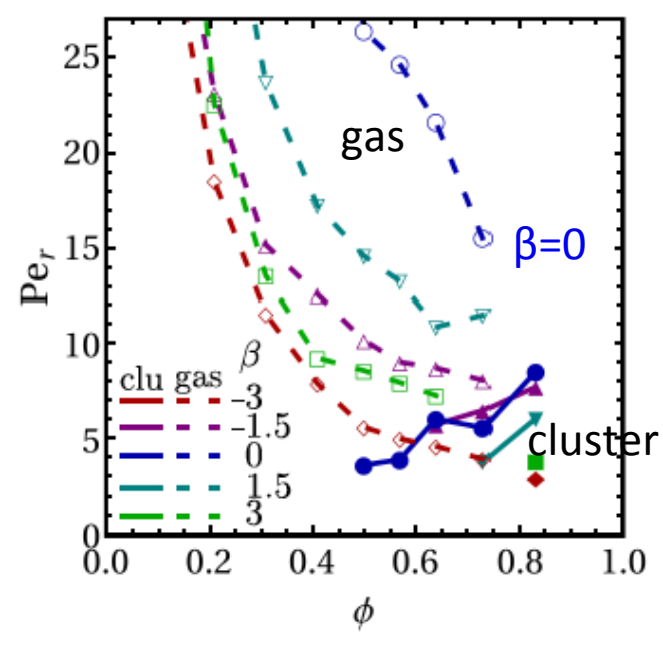
„in plane“

perpendicular to bounding walls

--> self-trapping!

➔ effective persistence number:

$$\mathrm{Pe}_r = \frac{\text{persistent drift length}}{\text{particle radius}} = \frac{v_0 \langle \sin\theta \rangle}{2RD_r}$$



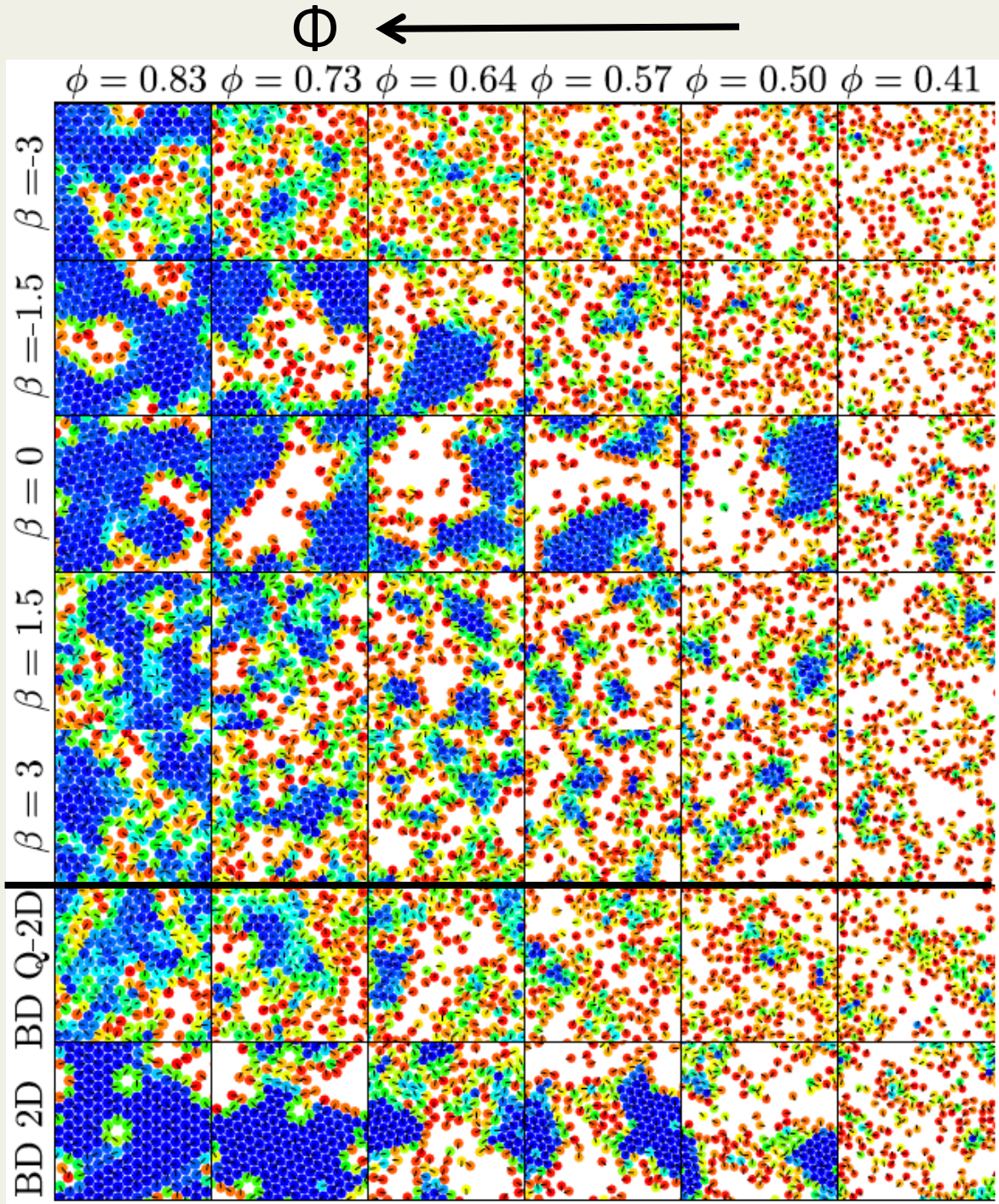
Color-coded local bond order

MPCD for squirmers: quasi-2D

Brownian dynamics & no HI

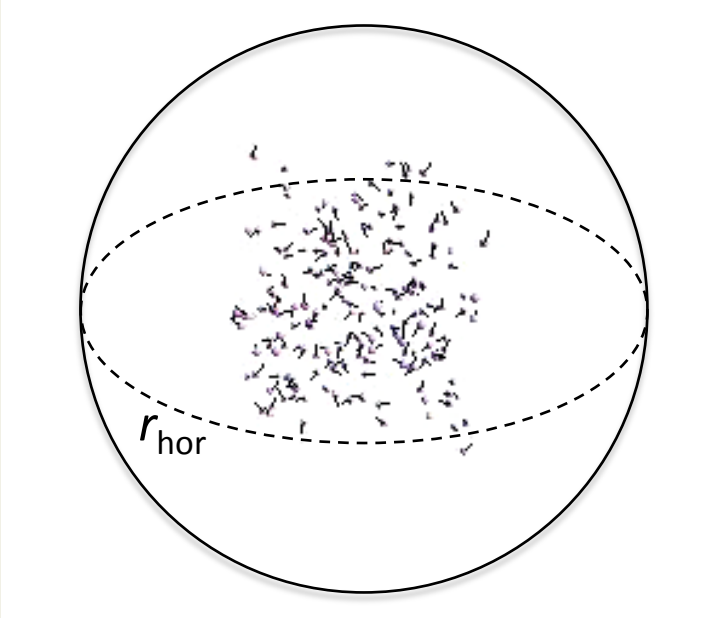
--> quasi-2D = same geometry

--> active circular disks in 2D



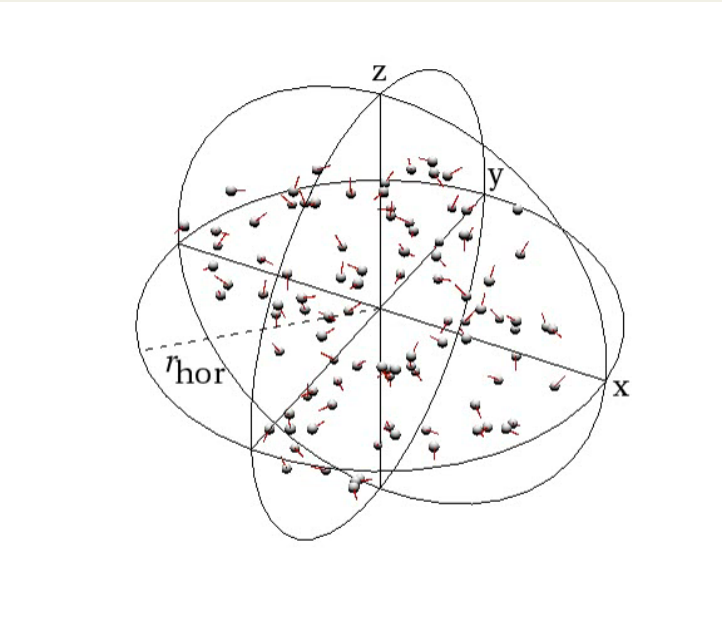
III. PUMP FORMATION OF ACTIVE PARTICLES IN A 3D HARMONIC TRAP

active particle pump



no HI

with HI



- active particle i:
  swimming velocity $v_0 \boldsymbol{p}_i$
  radius: a
- harmonic trap force: $\boldsymbol{F}_i = -k_{trap} \boldsymbol{r}_i$

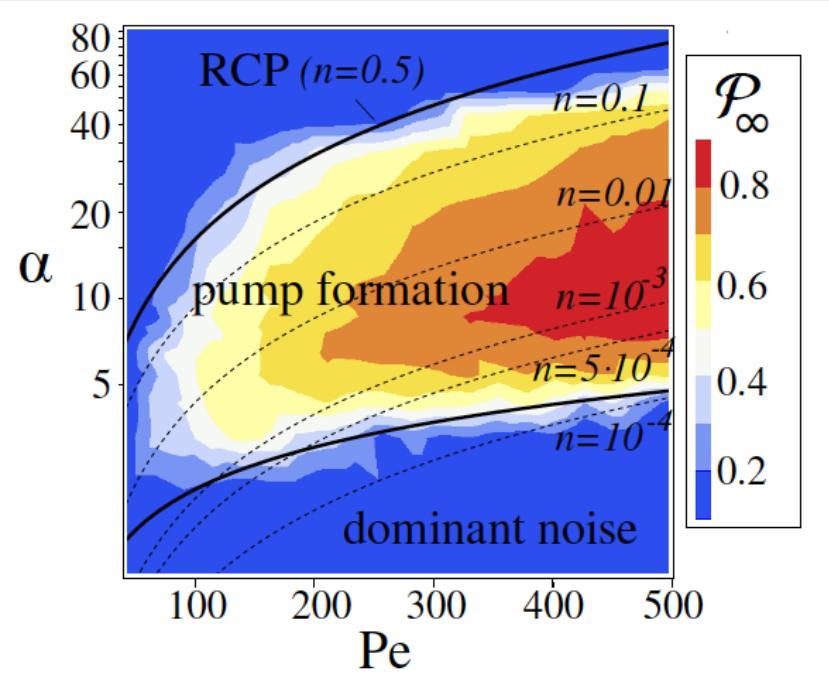
- BD simulations for $\boldsymbol{r}_i$, $\boldsymbol{p}_i$
- Stokeslet of particle i

$$\boldsymbol{u}(\boldsymbol{r}) = \frac{1}{8\pi r}\left(\mathbf{1} + \frac{\boldsymbol{r} \otimes \boldsymbol{r}}{r^2}\right)\boldsymbol{F}_i$$

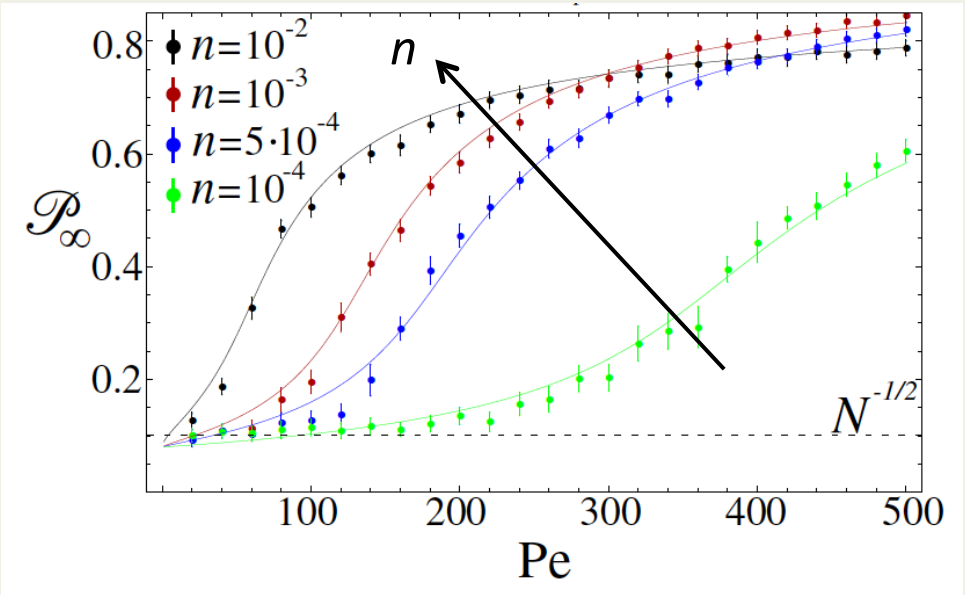
R.W. Nash, R. Adhikari, J. Tailleur & M. E. Cates, PRL (2010).

pump formation

state diagram



constant density *n*



- trapping strength: $\alpha = k_{\text{trap}} a^2 / k_B T$
- Peclet number: $\text{Pe} = v_0 a / D$
- polar order parameter:

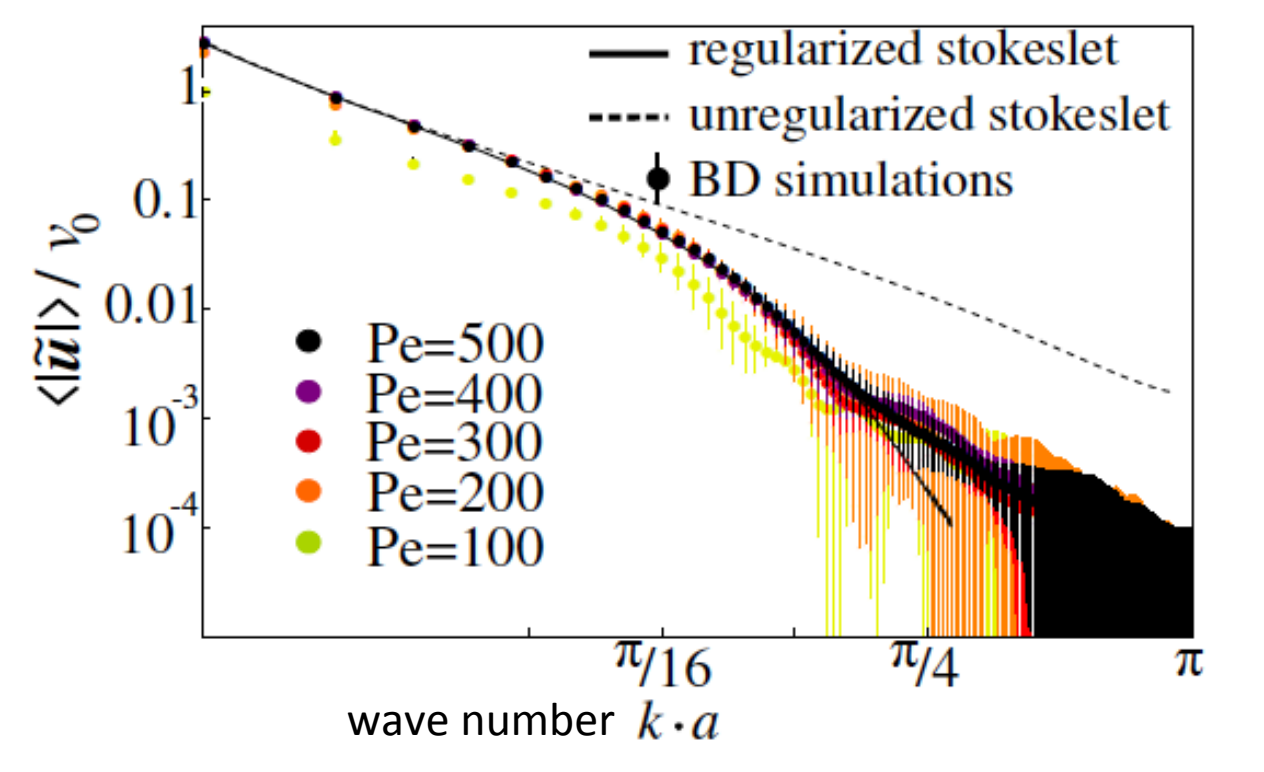
$$\mathcal{P}_\infty = \frac{1}{N} \left| \sum_{i=1}^{N} \boldsymbol{p}_i(t) \right|$$

alignment in self-induced (mean) flow field

M. Hennes, K. Wolff & H.S.
arXiv:1402.1397

mean flow field

angular-averaged Fourier transform



regularized stokeslet:

$$\boldsymbol{u}_{\text{reg}}(\boldsymbol{r}) = \frac{v_0 \varepsilon}{2\left(r^2 + \varepsilon^2\right)^{3/2}} \left[\left(r^2 + 2\varepsilon^2\right)\mathbf{1} + \boldsymbol{r} \otimes \boldsymbol{r} \right]$$

M. Hennes, K. Wolff & H.S.
arXiv:1402.1397

mean-field theory for self-induced order

- Smoluchowski equation:

$$\partial_t \psi(\boldsymbol{r},\boldsymbol{p}) = -\nabla \cdot \boldsymbol{J}_T - \mathcal{R} \cdot \boldsymbol{J}_R \quad \text{with} \quad \mathcal{R} = \boldsymbol{p} \times \nabla_{\boldsymbol{p}}$$

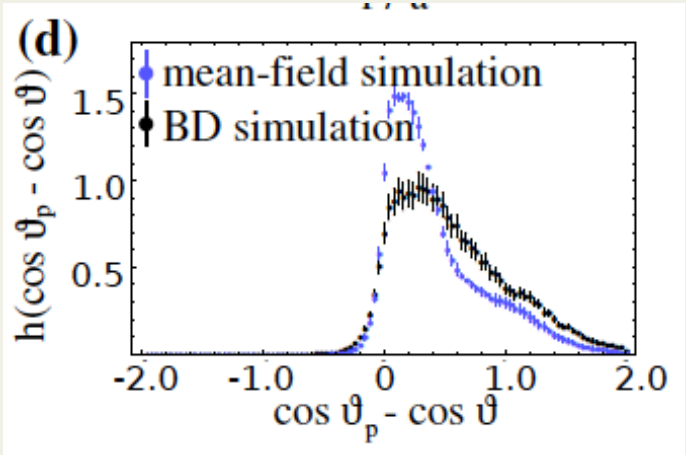
translational flux: $\boldsymbol{J}_T = [\ \underbrace{v_0 \boldsymbol{p}}_{\text{swimming}} + \underbrace{\mu_t \boldsymbol{F}_{\text{trap}}(\boldsymbol{r})}_{\text{trap force}} + \underbrace{\boldsymbol{u}_{\text{reg}}(\boldsymbol{r})}_{\text{mean flow field}}\ ]\ \psi(\boldsymbol{r},\boldsymbol{p})$

rotational flux: $\boldsymbol{J}_R = [\ \underbrace{\left(\nabla \times \boldsymbol{u}_{\text{reg}}(\boldsymbol{r})\right)/2}_{\text{vorticity}} - \underbrace{D_R \mathcal{R}}_{\text{diffusion}}\ ]\ \psi(\boldsymbol{r},\boldsymbol{p})$

- ansatz for $\psi(\boldsymbol{r},\boldsymbol{p})$:

in pump: $\boldsymbol{p}$ || radial direction

$$\rightarrow \psi(\boldsymbol{r},\boldsymbol{p}) = \phi(\boldsymbol{p})\, f(r) \times \delta(\cos\theta - \cos\theta_p)\, \delta(\varphi - \varphi_p)$$



Orientational distribution

$$\rightarrow \quad \partial_t \phi(\boldsymbol{p}) = -\mathcal{R} \cdot \left[\langle \boldsymbol{\omega} \rangle(\boldsymbol{p}) - D_R \mathcal{R} \right] \phi(\boldsymbol{p})$$

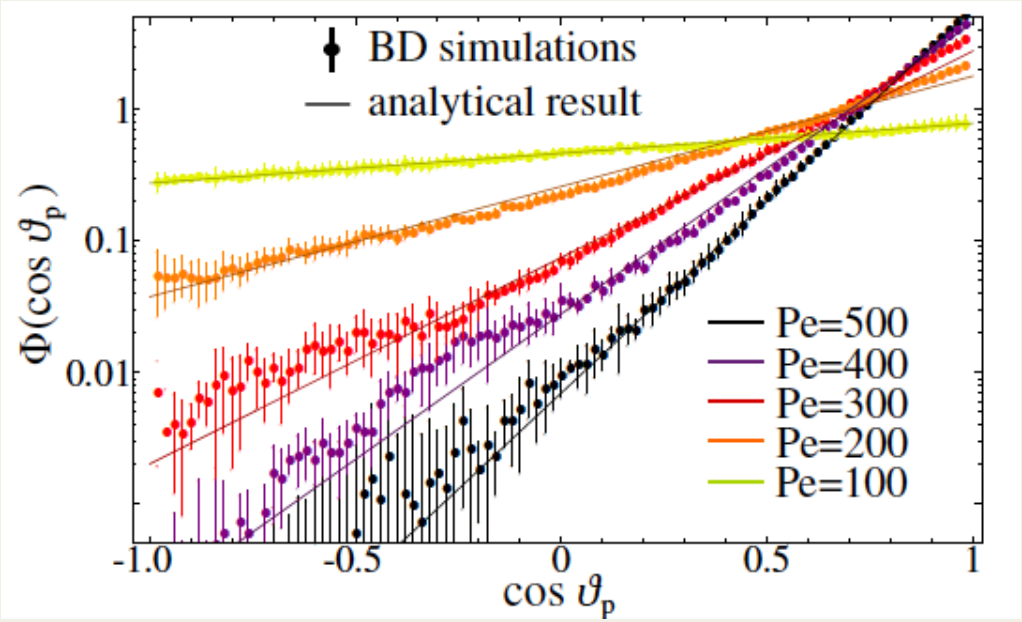
with mean vorticity ~ torque:

$$\langle \boldsymbol{\omega} \rangle(\boldsymbol{p}) = \left\langle \left(\nabla \times \boldsymbol{u}_{\text{reg}}(\boldsymbol{r}) \right) / 2 \right\rangle$$

$$\propto A \sin\theta_p \boldsymbol{e}_\varphi$$

$\rightarrow$ A ... mean field strength

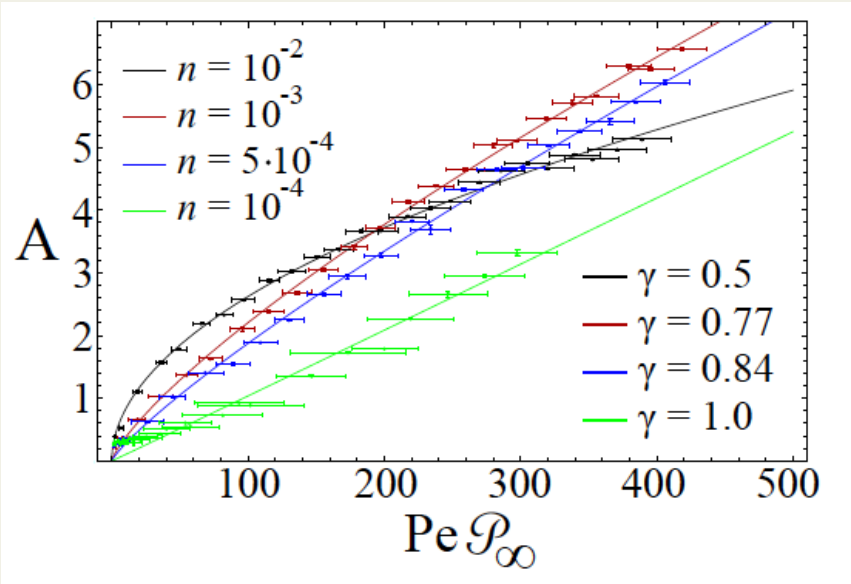
steady state: $\phi(\boldsymbol{p}) \propto e^{A \cos\theta_p}$

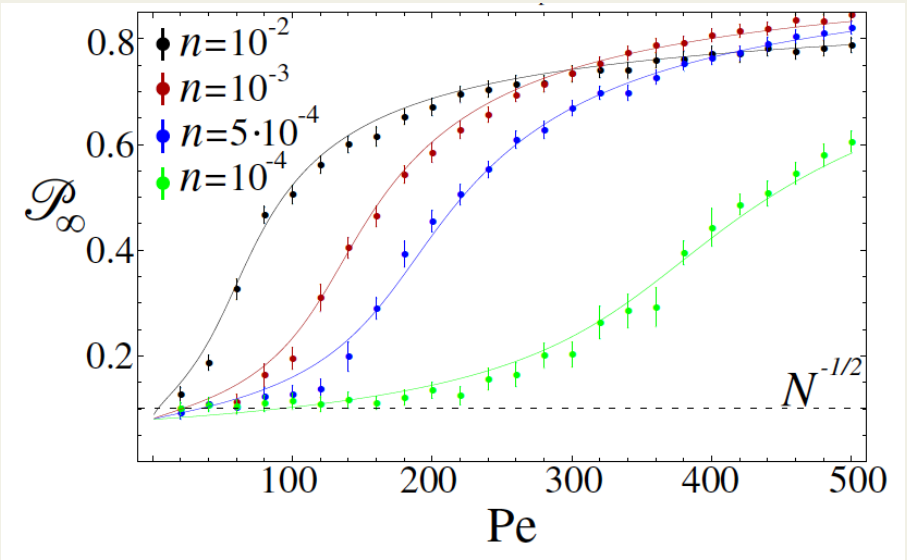


M. Hennes, K. Wolff & H.S.
arXiv:1402.1397

Mean polar order

$$\mathcal{P}_\infty = \int_{-1}^{1} \boldsymbol{p}\cdot\boldsymbol{e}_z\, \phi(\boldsymbol{p})\, d\cos\theta_p = \mathcal{L}(A) = \coth A - 1/A$$





$$A[\psi(\boldsymbol{r},\boldsymbol{p})] \propto (\mathrm{Pe}\,\mathcal{P}_\infty)^\gamma$$

$$\frac{\mathcal{P}_\infty - N^{-1/2}}{\mathcal{P}_\infty^{\max}} = \mathcal{L}[3(\mathrm{Pe}\,\mathcal{P}_\infty / \mathrm{Pe}_c)^\gamma]$$

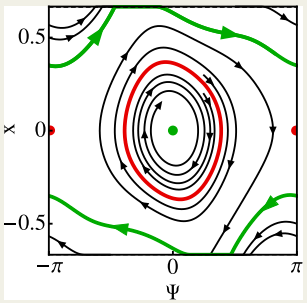
generalized Weiss molecular field!

M. Hennes, K. Wolff & H.S.
arXiv:1402.1397

Summary

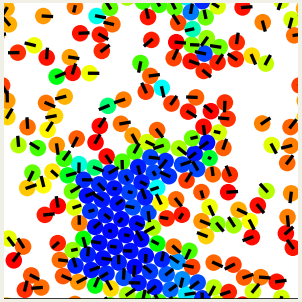
I. A microswimmer in Poiseuille flow

→ from a Hamiltonian to a dissipative system & chaos



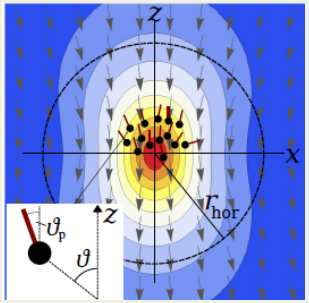
II. Collective dynamics of spherical microswimmers („squirmers“)

→ hydrodynamics matters



III. Pump formation of active particles in a 3D harmonic trap

→ self-induced polar order: lessons from ferromagnetism



IV. Chemotactic active colloids: Sensing the environment

→ dynamic clustering