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Emergence of collective dynamics in active biological systems

-- Swimming micro-organisms --

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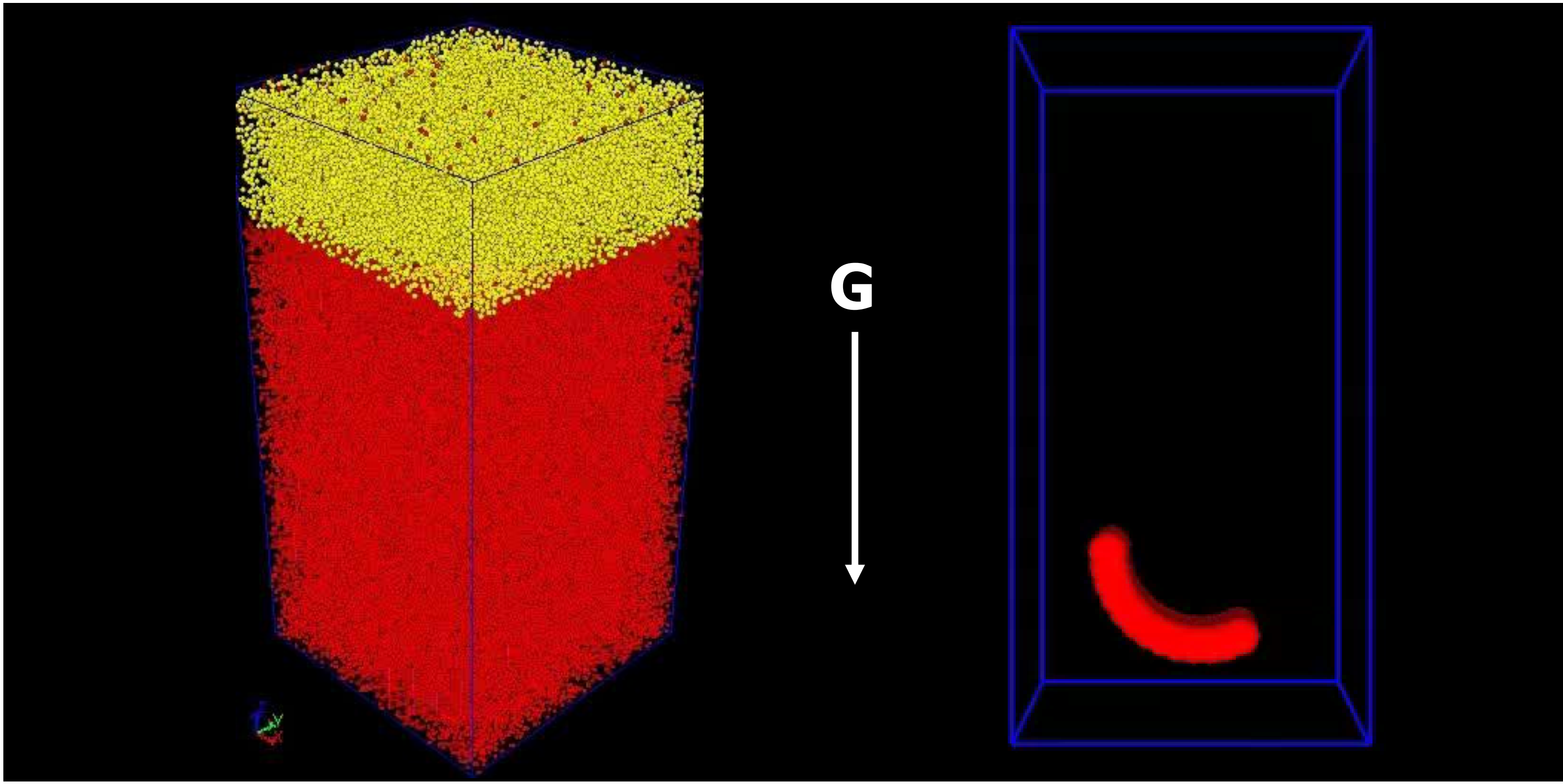
Outline

1. Introduction:
   - DNS for particles moving through Fluids

     Stokes friction, Oseen (RPY), … are not the end of the story -> Need DNS to go beyond

2. DNS of swimming (active) particles:
   - Self motions of swimming particles
   - Collective motions of swimming particles

Particles moving through fluids



Gravity:
Sedimentation
in colloidal disp.

Gravity:
A falling object
at high Re=10^3

Basic equations for DNS

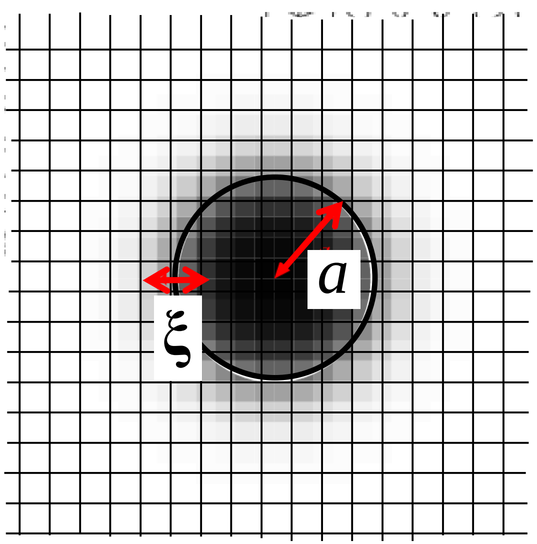
Navier-Stokes (Fluid)

$$\left(\frac{\partial}{\partial t}+\mathbf{u}\bullet\nabla\right)\mathbf{u}=-\frac{1}{\rho}\nabla p+\frac{\eta}{\rho}\nabla^2\mathbf{u}+\phi\mathbf{f}_p, \quad \nabla\bullet\mathbf{u}=0$$

exchange momentum

Newton-Euler (Particles)

$$\frac{d\mathbf{R}_i}{dt}=\mathbf{V}_i, \quad m_i\frac{d\mathbf{V}_i}{dt}=\mathbf{F}_i, \quad \mathbf{I}_i\bullet\frac{d\mathbf{\Omega}_i}{dt}=\mathbf{N}_i$$

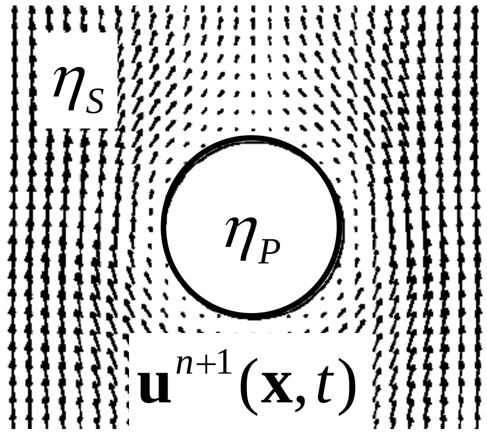


- **FEM**: sharp solid/fluid interface on irregular lattice
  → extremely slow…

- **FPD**/**SPM**: smeared out interface on fixed square lattice
  → much faster!!

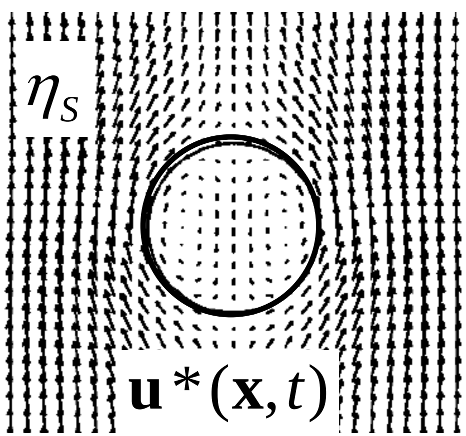
FPD and SPM

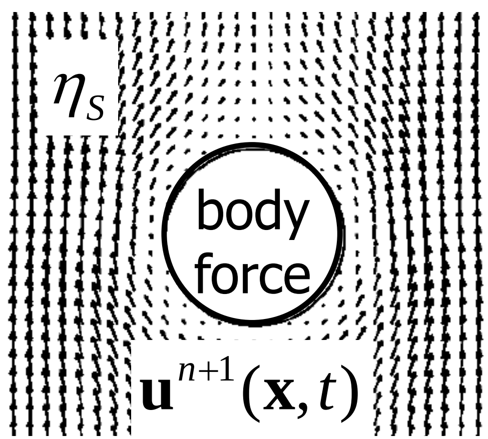
$\mathbf{u}^n(\mathbf{x}, t)$



FPD (2000)
Tanaka, Araki

$\eta_P \gg \eta_S$





SPM (2005)
Nakayama, RY

Define body force to enforce fluid/particle boundary conditions (colloid, swimmer, etc.)

Implementation of no-slip b.c.

$$\boldsymbol{R}_i^n, \boldsymbol{V}_i^n, \boldsymbol{\Omega}_i^n, \boldsymbol{u}^n(\boldsymbol{r})$$

Step 1

$$\boldsymbol{u}^* = \boldsymbol{u}^n + \int_{t_n}^{t_n+h} \mathrm{d}s\, \nabla \cdot \left[\frac{1}{\rho}(-p\mathbf{1} + \boldsymbol{\sigma}') - \boldsymbol{u}\boldsymbol{u}\right] \qquad \text{with } \nabla \cdot \boldsymbol{v}^* = 0$$

$$\underline{\boldsymbol{R}_i^{n+1}} = \boldsymbol{R}_i^n + \int_{t_n}^{t_n+h} \mathrm{d}s\, \boldsymbol{V}_i$$

Step 2

$$\underline{\boldsymbol{V}_i^{n+1}} = \boldsymbol{V}_i^n + M_p^{-1} \int \mathrm{d}\boldsymbol{x}\, \rho\phi_i^{n+1}(\boldsymbol{u}^* - \boldsymbol{u}_p^n)$$

where $\phi \boldsymbol{v}_p(\boldsymbol{x}, t) = \sum_{i=1}^{N_p} \phi_i(\boldsymbol{x}, t)[\boldsymbol{V}_i(t) + \boldsymbol{\Omega}_i(t) \times \boldsymbol{r}_i(t)]$

$$\underline{\boldsymbol{\Omega}_i^{n+1}} = \boldsymbol{\Omega}_i^n + \boldsymbol{I}_p^{-1} \cdot \int \mathrm{d}\boldsymbol{x}[\boldsymbol{r}_i^{n+1} \times \rho\phi_i^{n+1}(\boldsymbol{u}^* - \boldsymbol{u}_p^n)]$$

Step 3

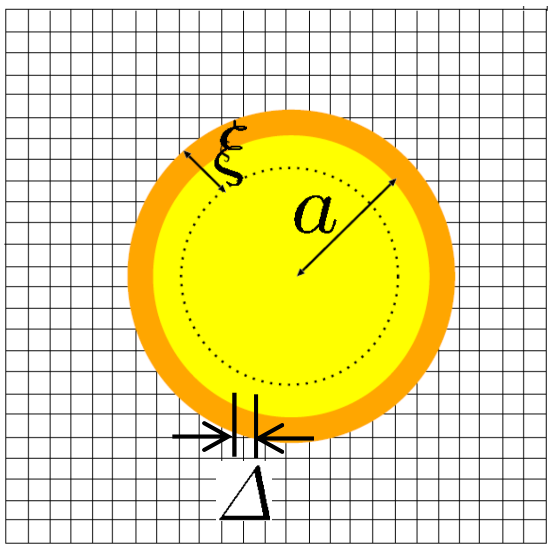
$$\underline{\boldsymbol{u}^{n+1}} = \boldsymbol{u}^* + \phi^{n+1}(\boldsymbol{v}_p^{n+1} - \boldsymbol{u}^*) \qquad \text{with } \nabla \cdot \boldsymbol{u}^{n+1} = 0$$

$$n+1 \rightarrow n$$

- - - - - - Momentum conservation

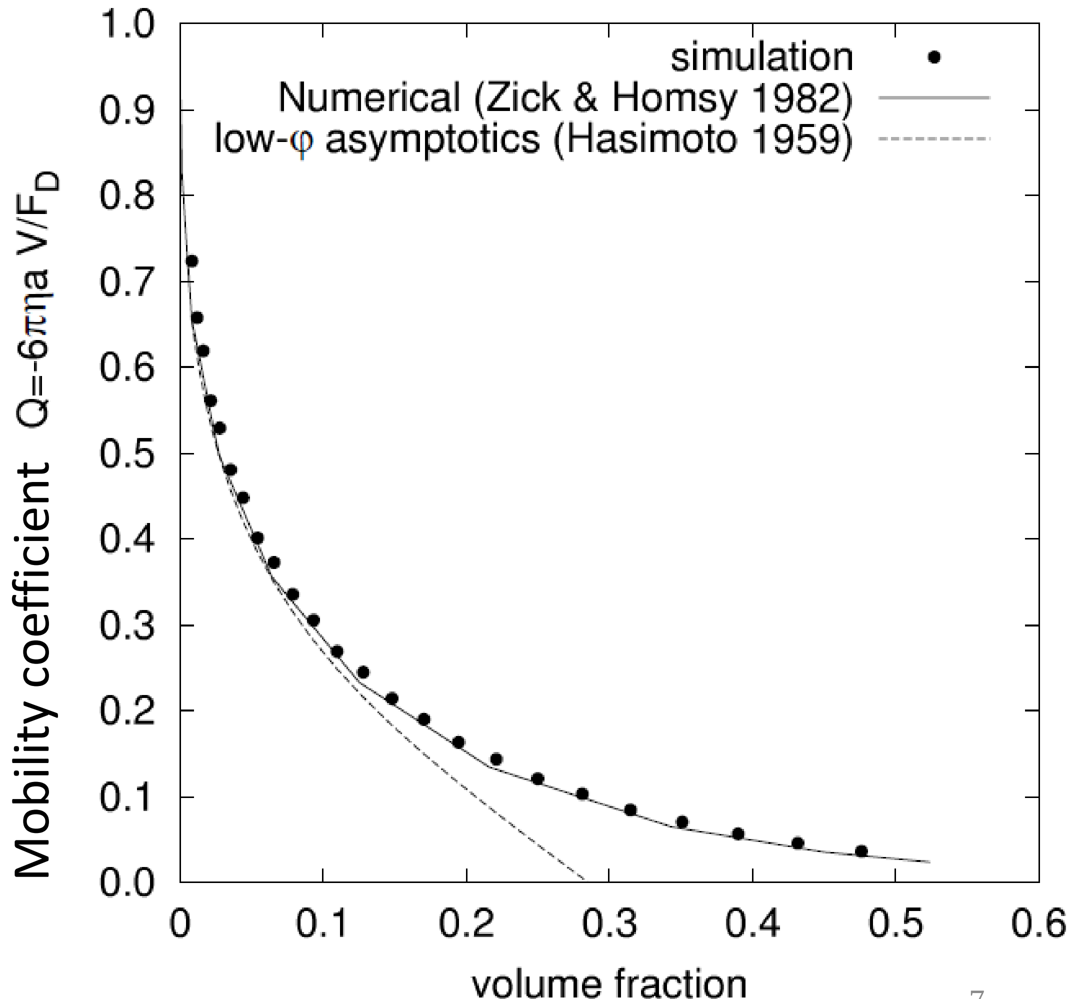
Numerical test: Drag force (1)

Mobility coefficient of spheres at Re=1



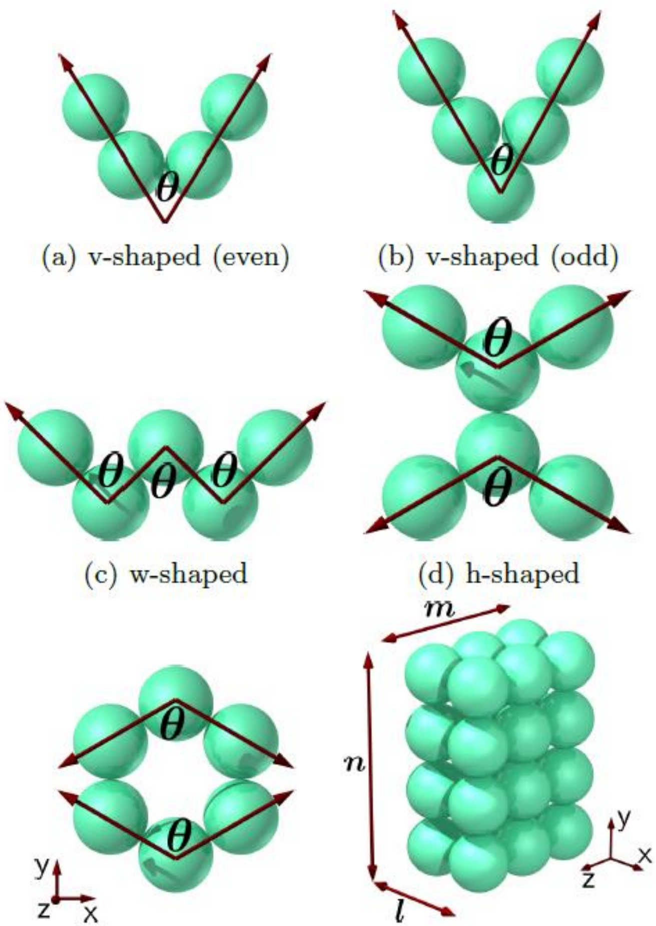
$a = 4 \sim 12,\ \xi = 1$

This choice can reproduce the collect Stokes drag force within 5% error.



Numerical test: Drag force (2)

Drag coefficient of non-spherical rigid bodies at Re=1



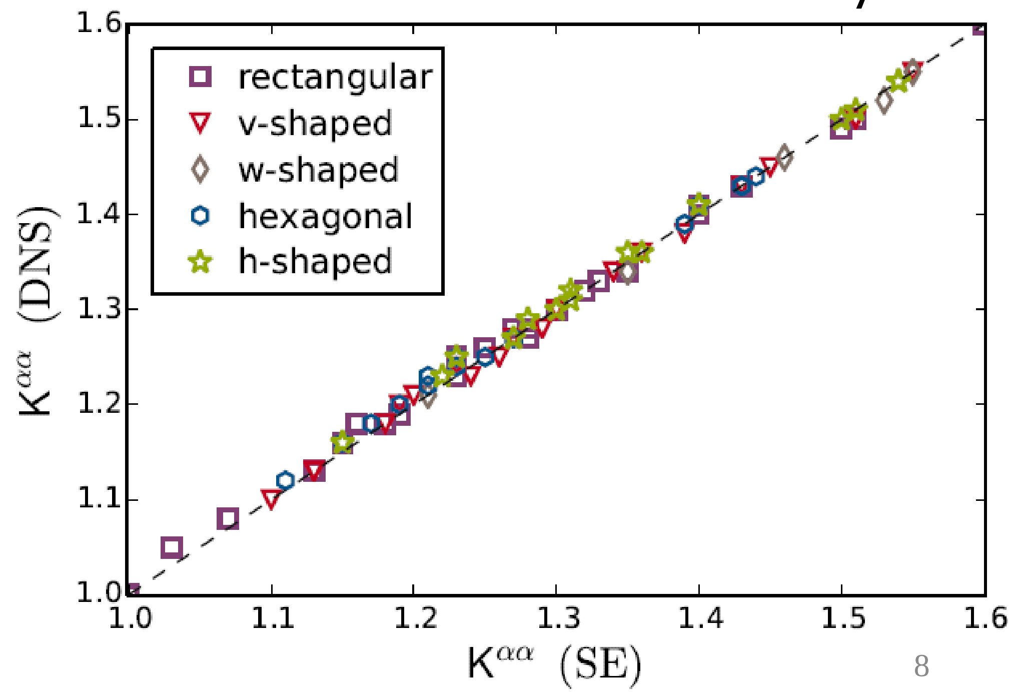
(a) v-shaped (even) (b) v-shaped (odd)

(c) w-shaped (d) h-shaped

(e) hexagonal (f) rectangular

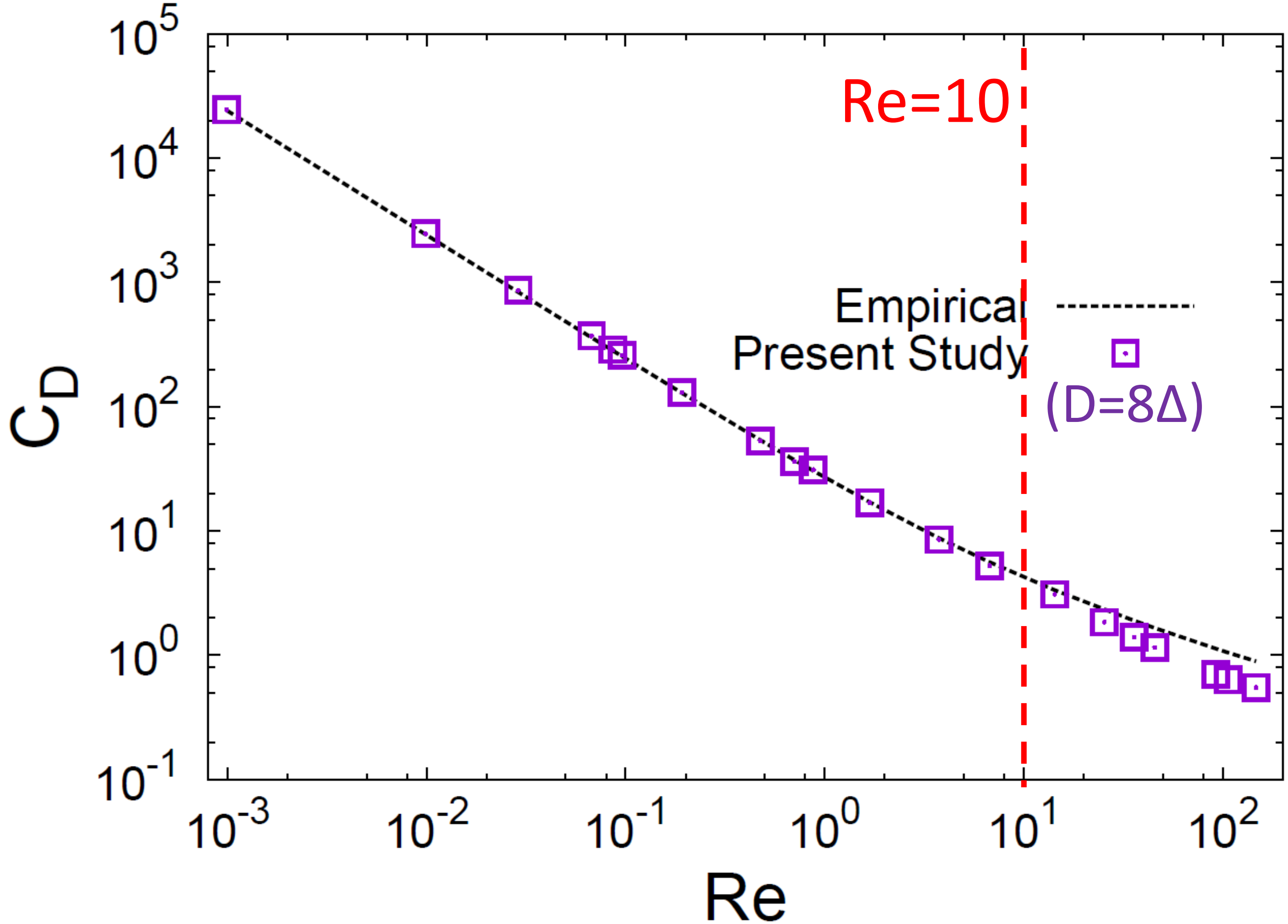
Any shaped rigid bodies can be formed by assembling spheres

Simulation vs. Stokes theory



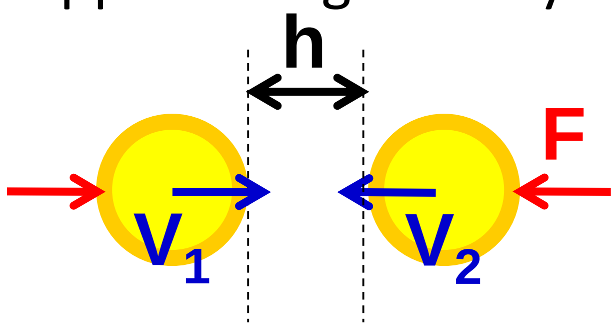
Numerical test: Drag force (3)

Drag coefficient of a sphere C_D at Re<200



Numerical test: Lubrication force

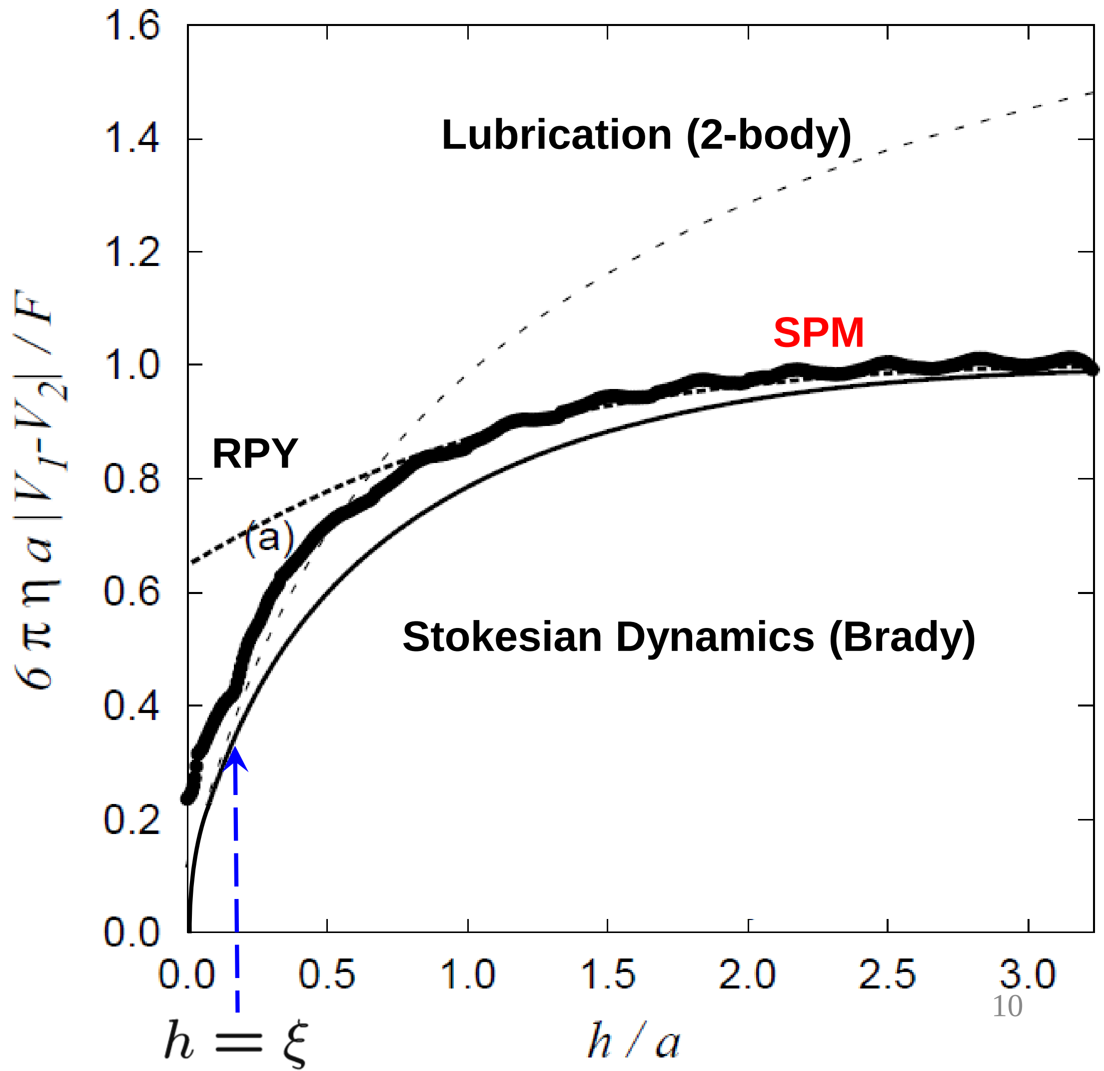
Approaching velocity of a pair of spheres at Re=0 under a constant F



Two particles are approaching with velocity V under a constant force F. V tends to decrease with decreasing the separation h due to the lubrication force.

$$a = 5,\ \xi = 1$$

SPM can reproduce lubrication force very correctly until the particle separation becomes comparable to ξ (= grid size)



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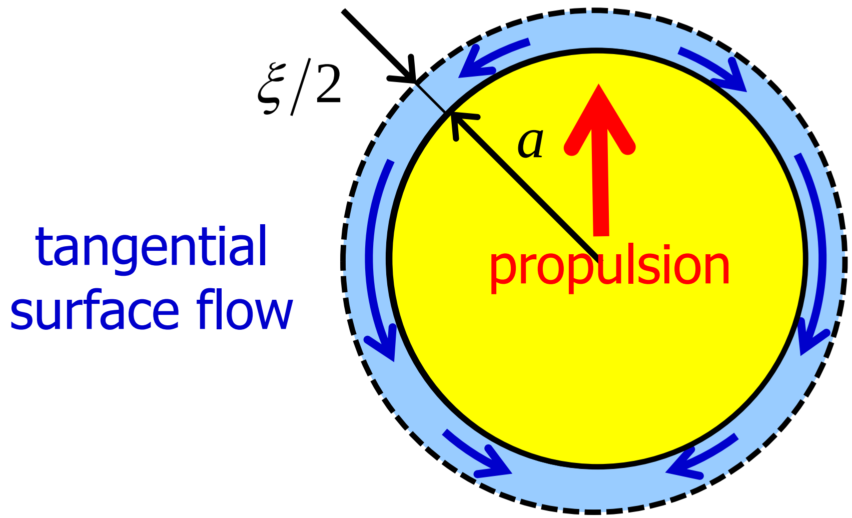
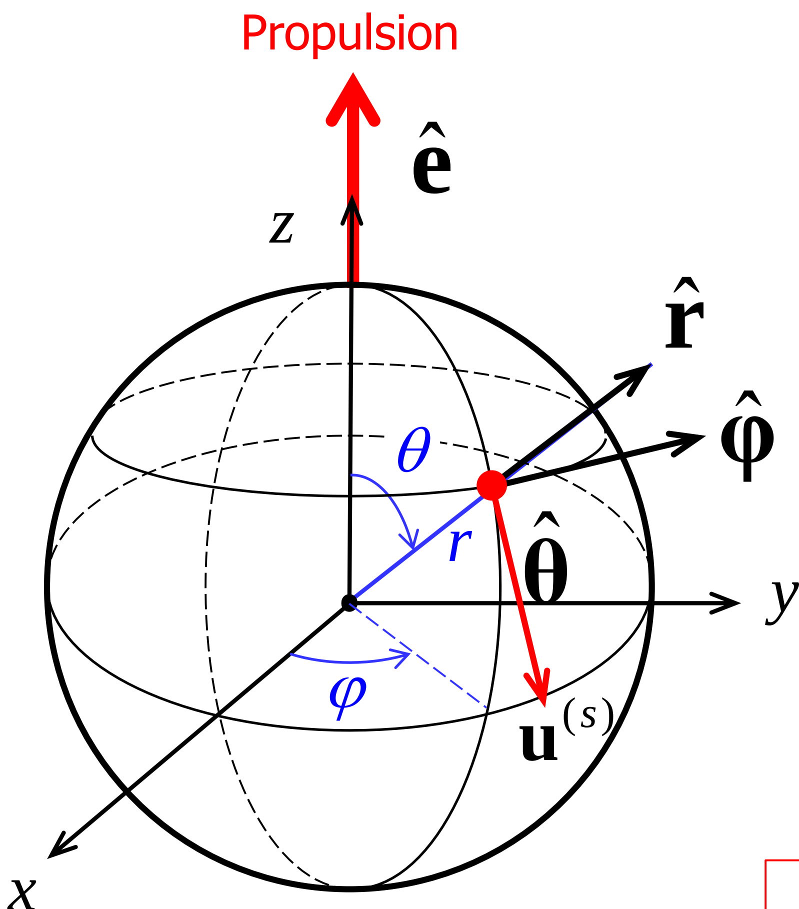
Implementation of surface flow

$$\boldsymbol{u}^{**} = \boldsymbol{u}^{*} + \sum_i \varphi_i \cdot \left(\boldsymbol{V}_i' + \boldsymbol{\Omega}_i' \times \boldsymbol{r}_i + \boldsymbol{u}_i^{(s)} - \boldsymbol{u}^{*} \right) + \sum_i \phi_i \left(\delta \boldsymbol{V}_i + \delta \boldsymbol{\Omega}_i \times \boldsymbol{r}_i \right)$$



Total momentum is conserved

A model micro-swimmer: Squirmer



J. R. Blake (1971)

Polynomial expansion of surface slip velocity. Only $\hat{\boldsymbol{\theta}}$ component is treated here.

$$\boldsymbol{u}^{(s)} = \sum_{n=1}^{n=\infty} \frac{2}{n(n+1)} B_n \left(\hat{e}\cdot\hat{\boldsymbol{r}}\hat{\boldsymbol{r}} - \hat{e}\right) P_n'(\hat{e}\cdot\hat{\boldsymbol{r}})$$
$$= \sum_{n=1}^{\infty} \frac{2}{n(n+1)} B_n P_n'(\cos\theta)\sin\theta\hat{\boldsymbol{\theta}}$$

neglecting n>2

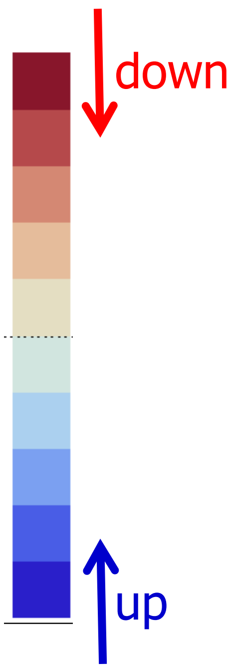
$$\boxed{\mathbf{u}^{(s)} = \left(B_1 \sin\theta + B_2 \sin 2\theta\right)\hat{\boldsymbol{\theta}}}$$

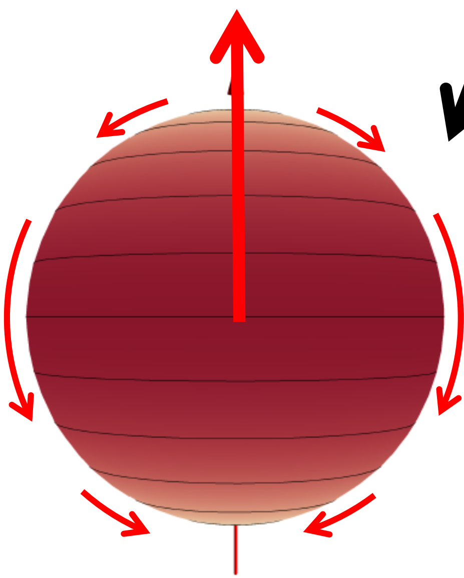
A spherical model: Squirmer

J. R. Blake (1971) Ishikawa & Pedley (2006-)

$$\boxed{\mathbf{u}^{(s)} = B_1\left(\sin\theta + {\color{red}\alpha}\sin 2\theta\right)\hat{\boldsymbol{\theta}}}$$

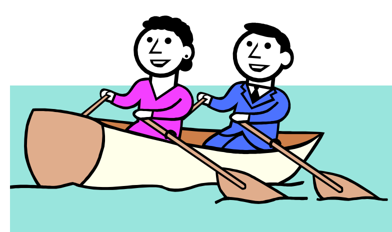
Surface flow velocity

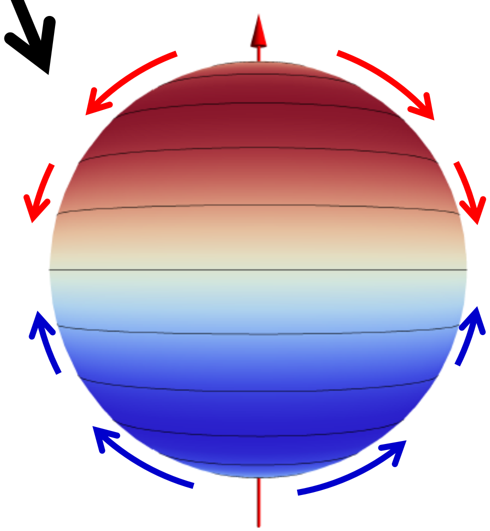




$$\boldsymbol{U} = \frac{2}{3}B_1\hat{\boldsymbol{e}}$$

propelling velocity

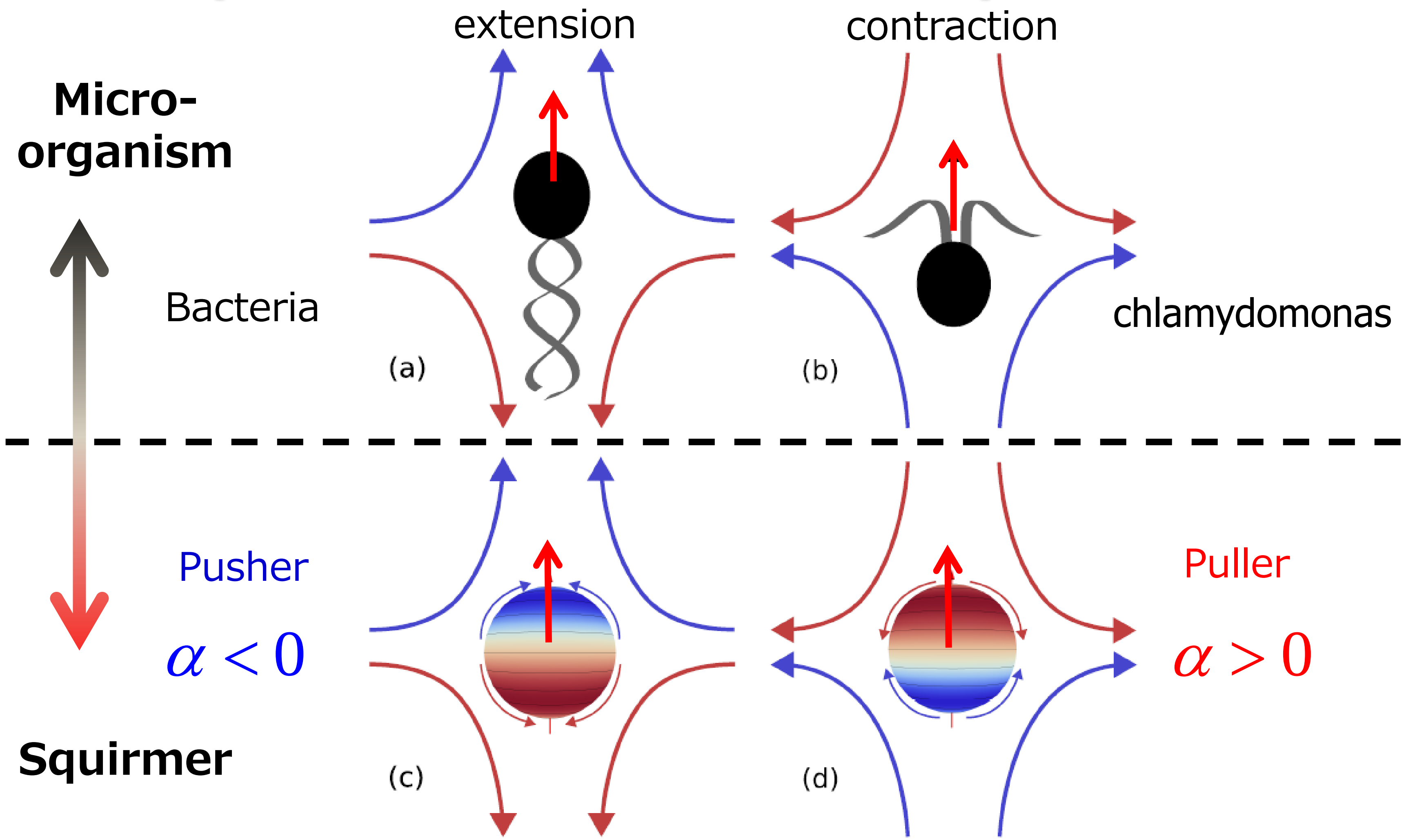




$$\boldsymbol{S} = \frac{4}{3}\pi\eta a^2(3\hat{\boldsymbol{e}}\hat{\boldsymbol{e}} - \boldsymbol{I})B_2$$

stress against shear flow

A spherical model: Squirmer



Sim. methods for squirmers

SD

Ishikawa, Pedley, … (2006-)
Swan, Brady, … (2011-)

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DNS

LBM:
Llopis, Pagonabarraga, … (2006-)

MPC / SRD:
Dowton, Stark (2009-)
Götze, Gompper (2010-)

Navier-Stokes:
Molina, Yamamoto, … (2013-)

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.
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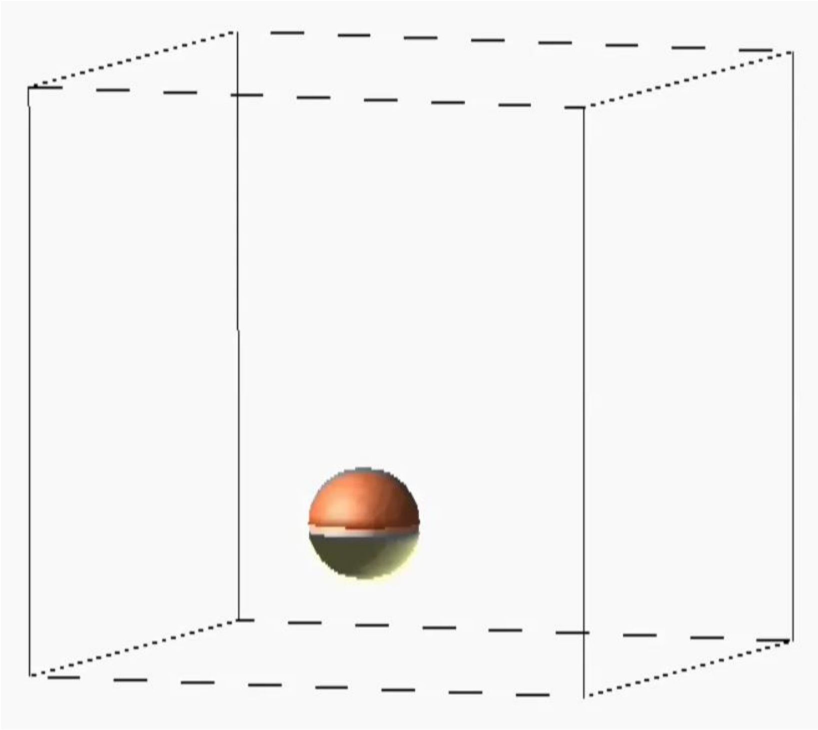
A single swimmer

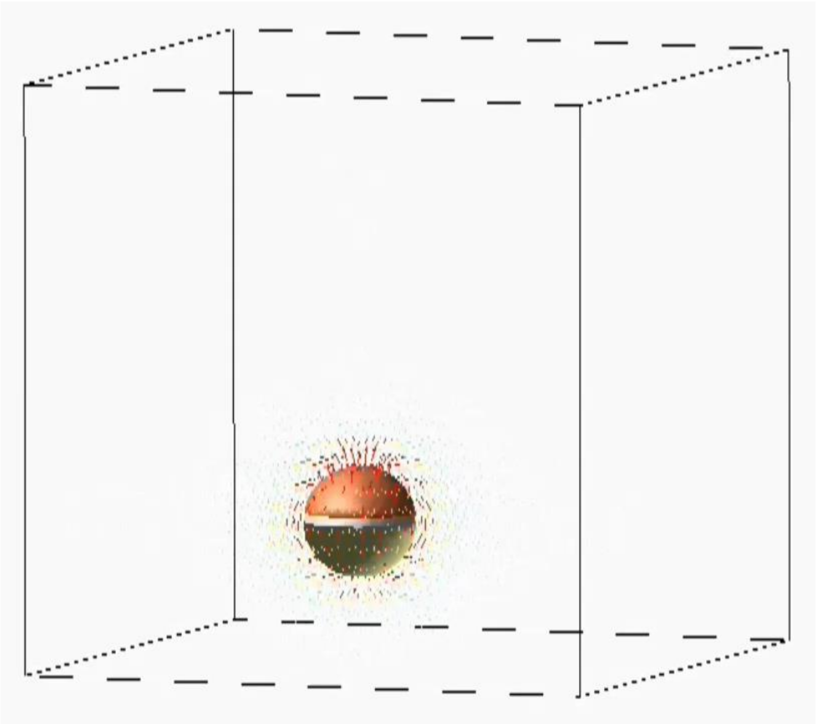
Externally driven colloid
(gravity, tweezers, etc…)



$\mathbf{u}(\mathbf{r}) \sim |\mathbf{r}|^{-1}$

Neutral swimmer

$\alpha = 0$



$\mathbf{u}(\mathbf{r}) \sim |\mathbf{r}|^{-3}$

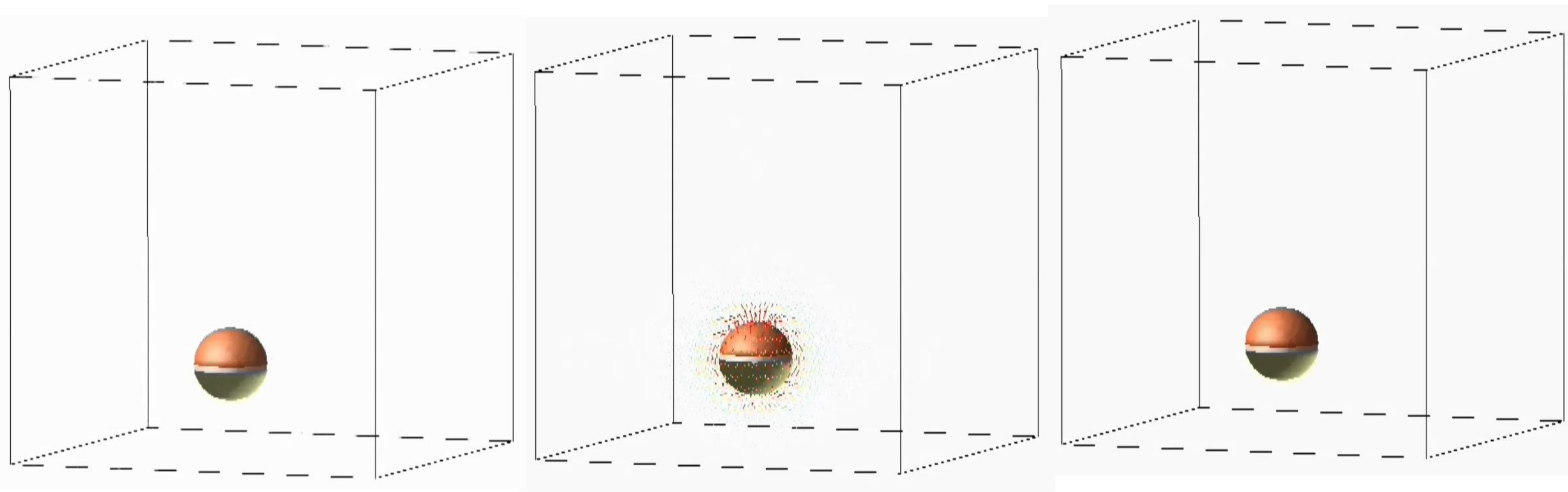
Box: 64 x 64 x 64 with PBC, Particle radius: a=6, φ=0.002
Re=0.01, Pe=∞, Ma=0

A single swimmer

Pusher $\alpha = -2$

Neutral $\alpha = 0$

Puller $\alpha = 2$



$\mathbf{u}(\mathbf{r}) \sim |\mathbf{r}|^{-2}$

$\mathbf{u}(\mathbf{r}) \sim |\mathbf{r}|^{-3}$

$\mathbf{u}(\mathbf{r}) \sim |\mathbf{r}|^{-2}$

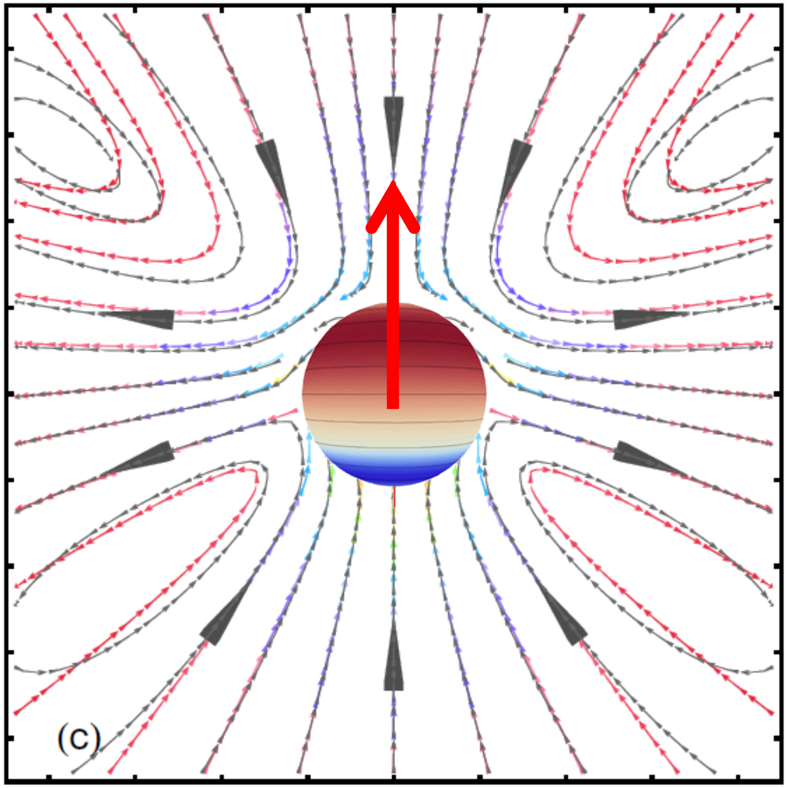
Box: 64 x 64 x 64 with PBC, Particle radius: a=6, φ=0.002
Re=0.01, Pe=∞, Ma=0

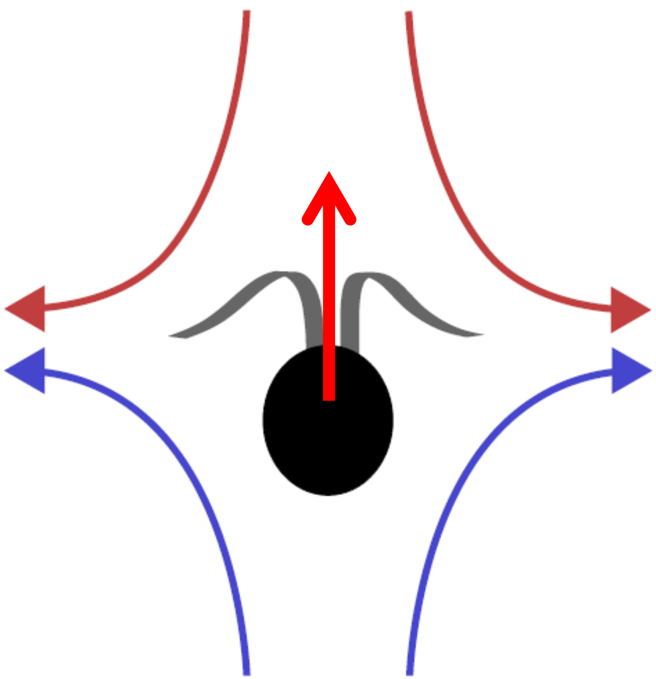
A single swimmer

Stream lines

Puller $\alpha = 2$

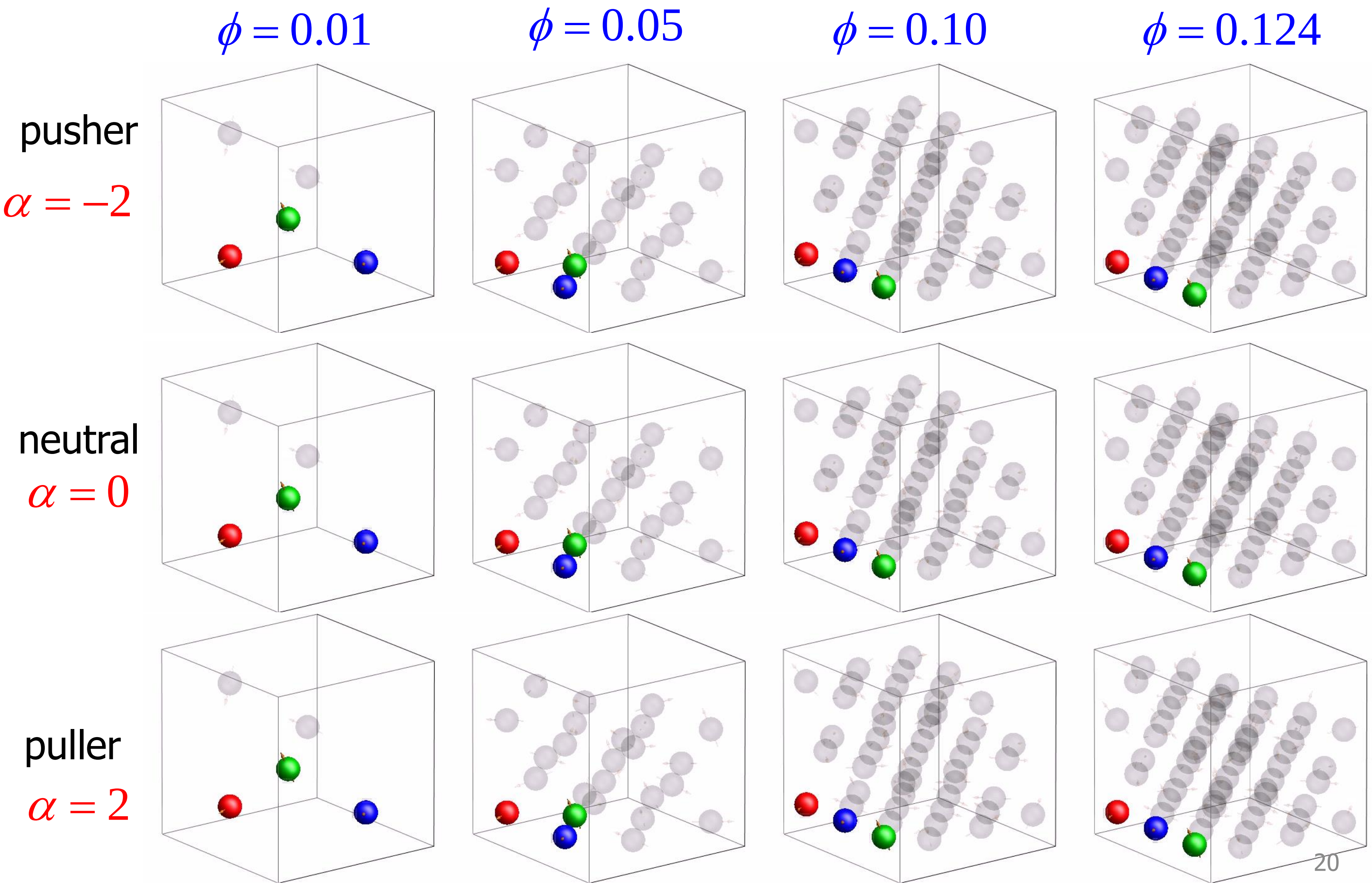
$\mathbf{u}(\mathbf{r})$





SM 2013

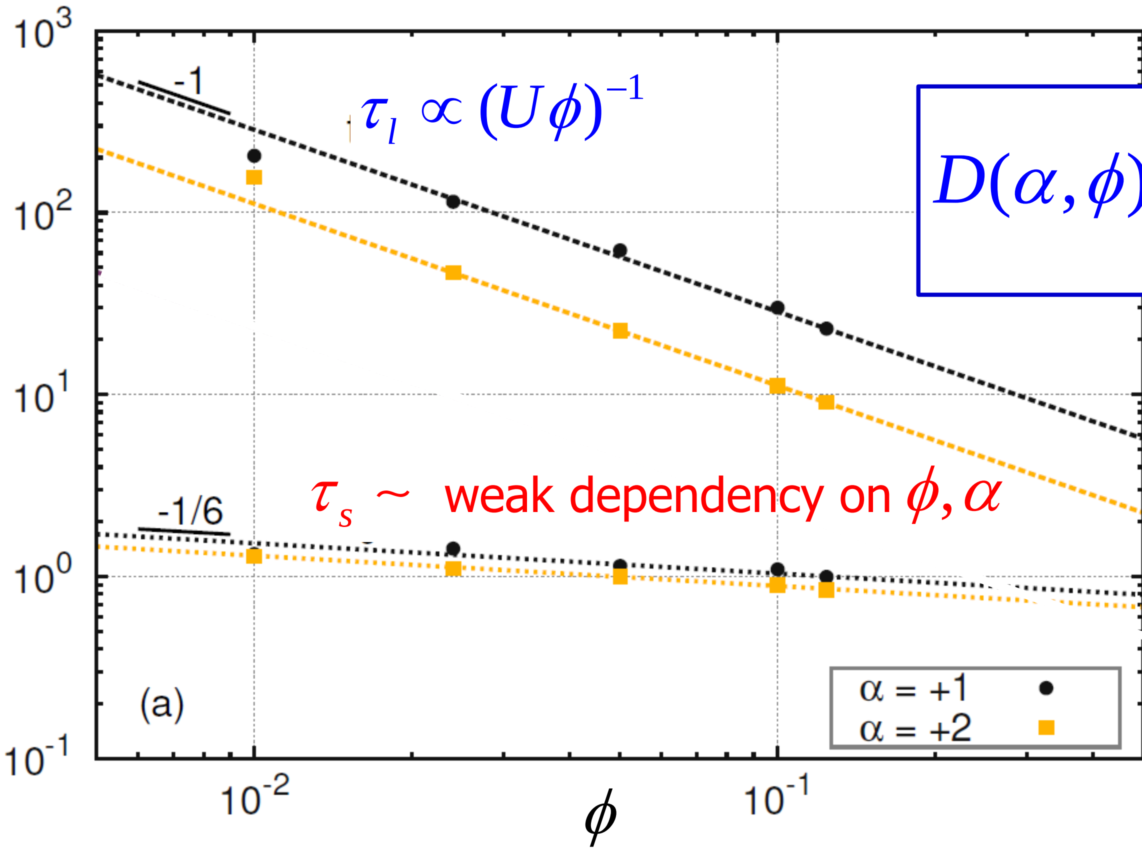
Swimmer dispersion (α, ϕ)



Velocity auto correlation

$$C(t) = U\phi \exp\left(-\frac{t}{\tau_s(\phi,\alpha)}\right) + U^2 \exp\left(-\frac{t}{\tau_l(\phi,\alpha)}\right)$$

Short-time   Long-time



$$\boxed{D(\alpha,\phi) \sim U^2\tau_l \sim \frac{U}{\phi\, r_c^2(\alpha)}}$$

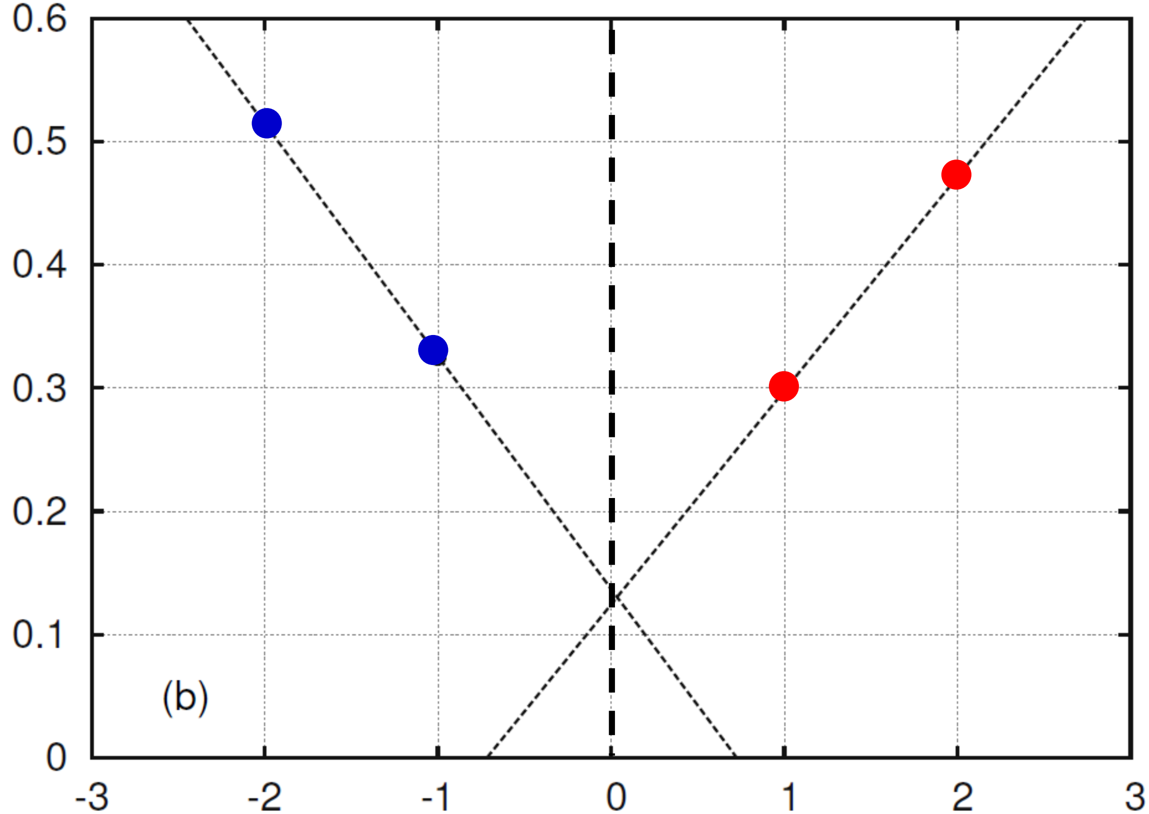
↑ collision radius

Analogous to
low density gas
(mean-free-path)

Collision radius of swimmers

$$r_c(\alpha) = \left(2\sqrt{2} U \tau_l \phi\right)^{-1/2}$$

$r_c(\alpha)$



Pusher ⟵ α ⟶ Puller

$r_c \ll a\,(=5)$

r_c increases with increasing $|\alpha|$

Nearly symmetric for puller ($\alpha>0$) and pusher ($\alpha<0$)

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Collective motion: flock of birds

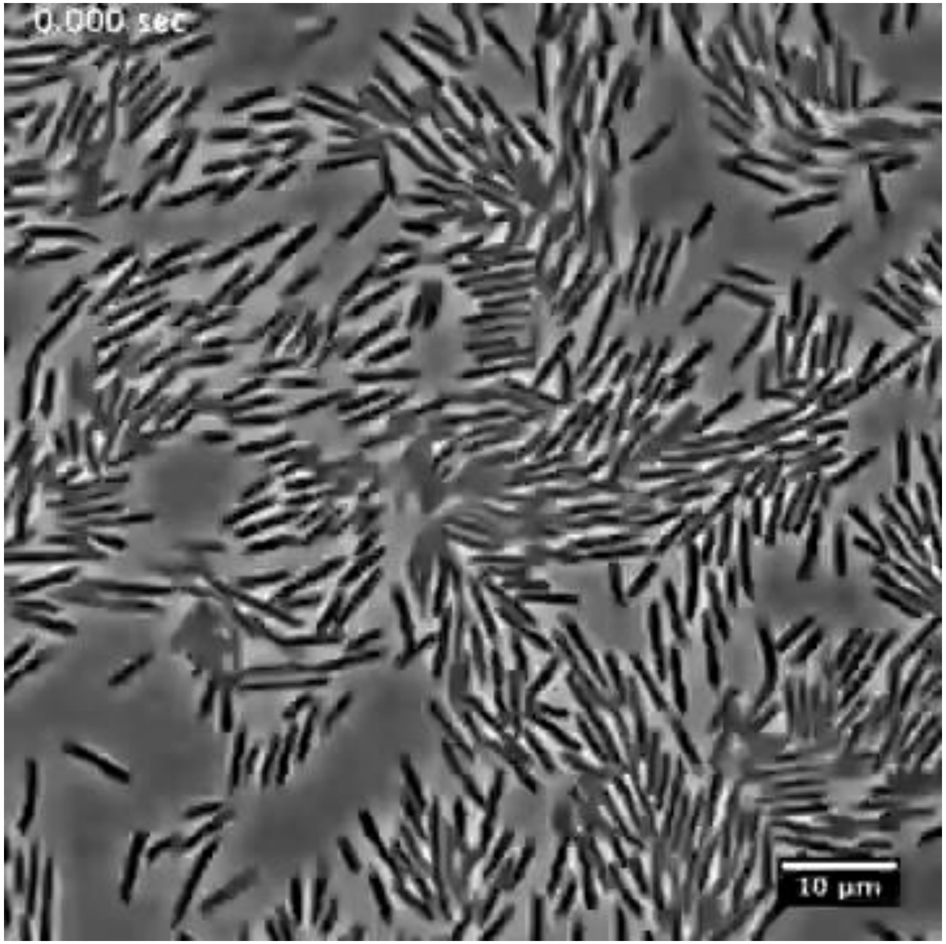
Interactions:

- Hydrodynamic
- Communication

$Re \sim 10^{3\sim5}$

Ex. Vicsek model

Collective motion: E-coli bacteria



Interactions:

- Hydrodynamic
- Steric (rod-rod)

$\mathrm{Re} \sim 10^{-3\sim-5}$

Ex. Active LC model

Question

Can any non-trivial collective motions take place in a system composed of spherical swimming particles which only hydrodynamically interacting to each other?

↓

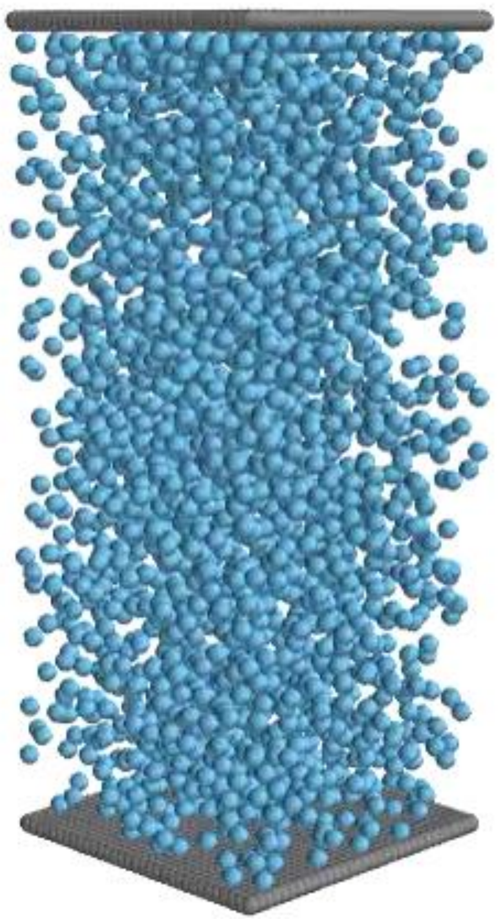
DNS is an ideal tool to answer this question.

unpublished

Collective motion of squirmers

confined between hard walls (at a volume fraction = 0.13)

puller with α = +0.5



pusher with α = -0.5

Dynamic structure factor

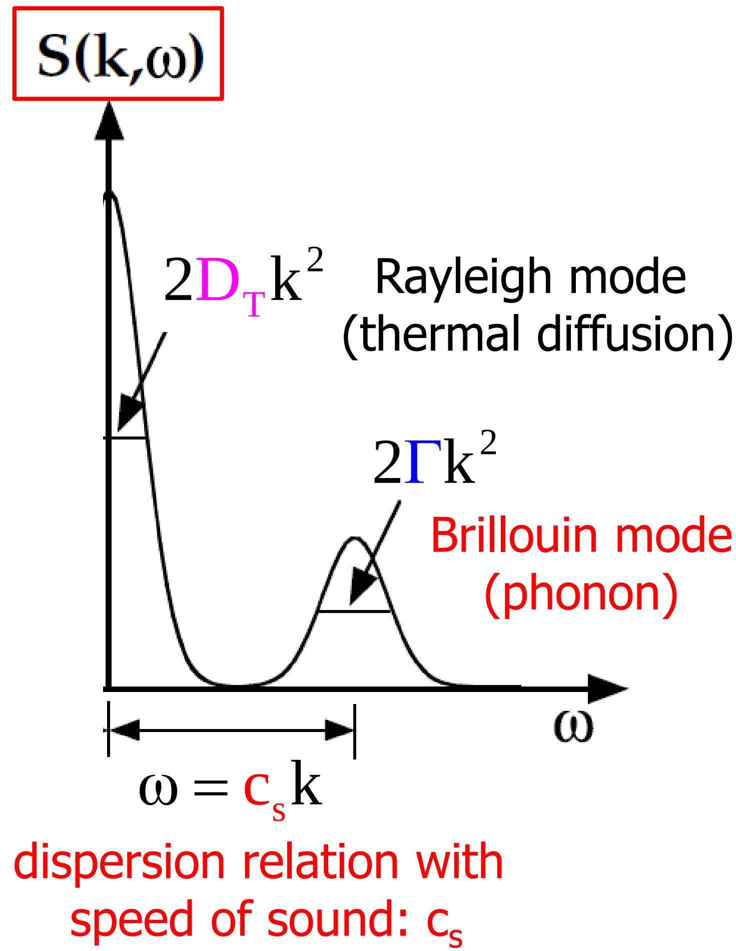
Summary for bulk liquids

$$F(\mathbf{k},t) = \frac{1}{N}\langle \rho_{\mathbf{k}}(t)\rho_{-\mathbf{k}} \rangle$$

$$\boxed{S(\mathbf{k},\omega)} = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\mathbf{k},t)\exp(i\omega t)\,\mathrm{d}t$$

$$c_s \propto \frac{1}{\sqrt{\rho\chi_T}}$$

$$\Gamma \propto aD_T + b\nu$$



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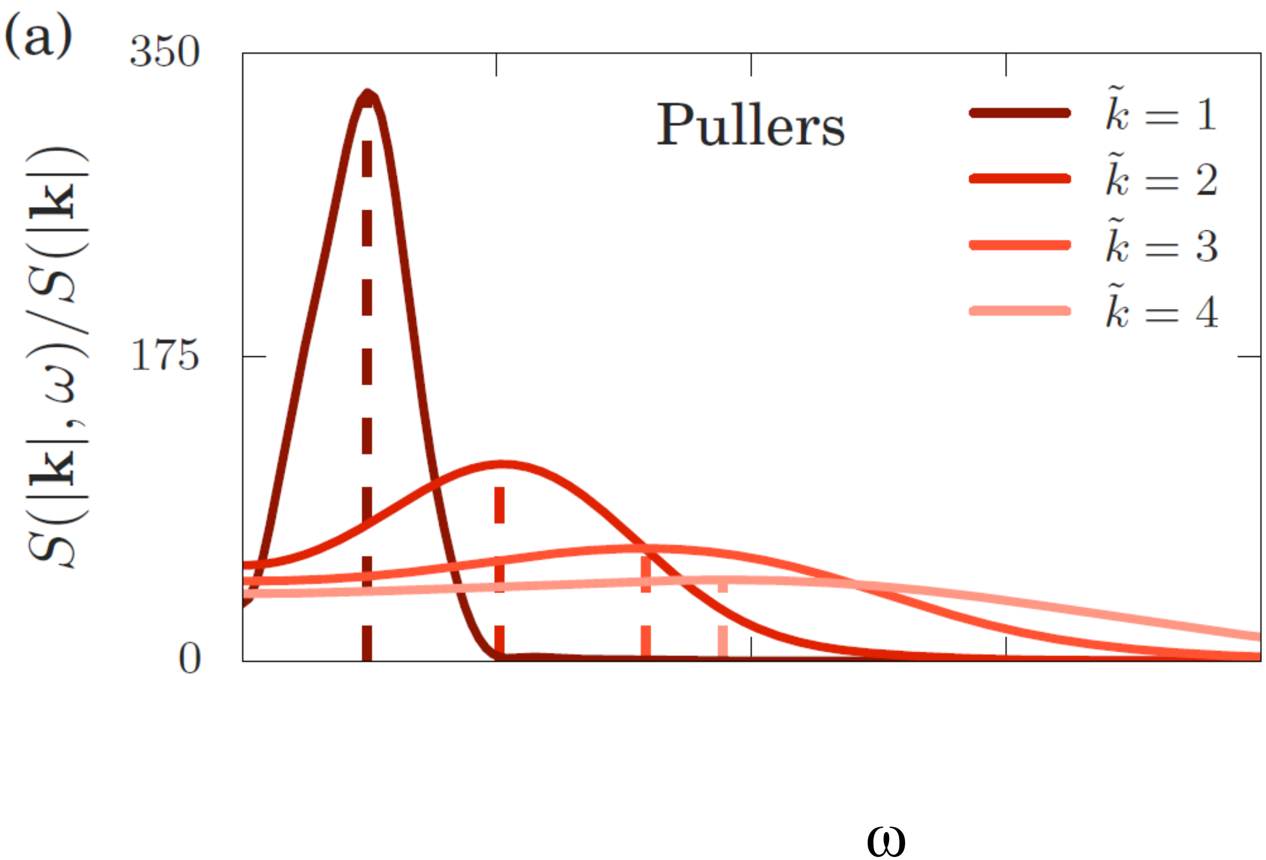
Dynamic structure factor

of bulk squirmers (puller with $\alpha = +0.5$)



Brillouin mode
(phonon-like?)

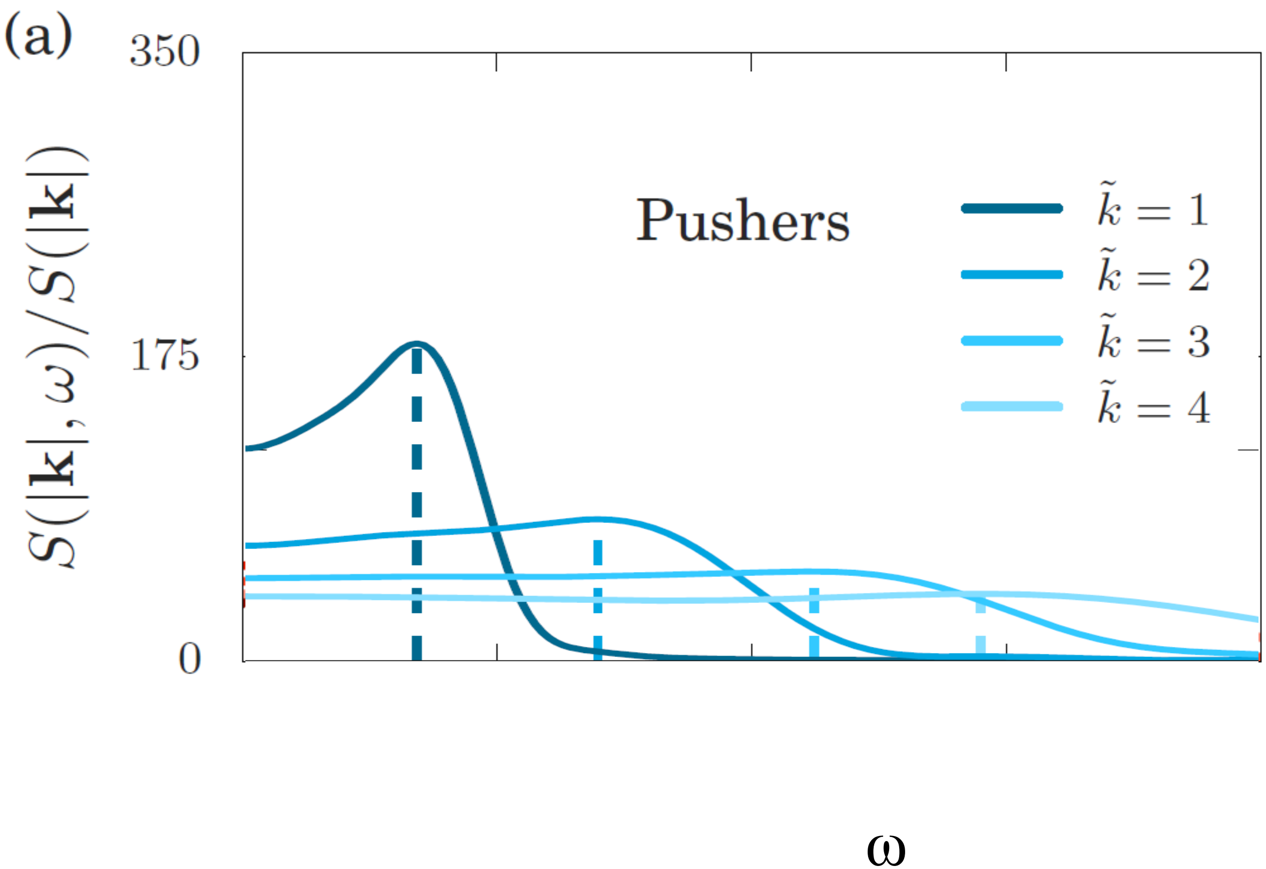
$$\omega = c_s k$$

dispersion relation with
speed of wave: c_s

unpublished

Dynamic structure factor

of bulk squirmers (pusher with α=-0.5)



Similar to the previous puller case (α = +0.5), but the intensity of the wave is much suppressed.

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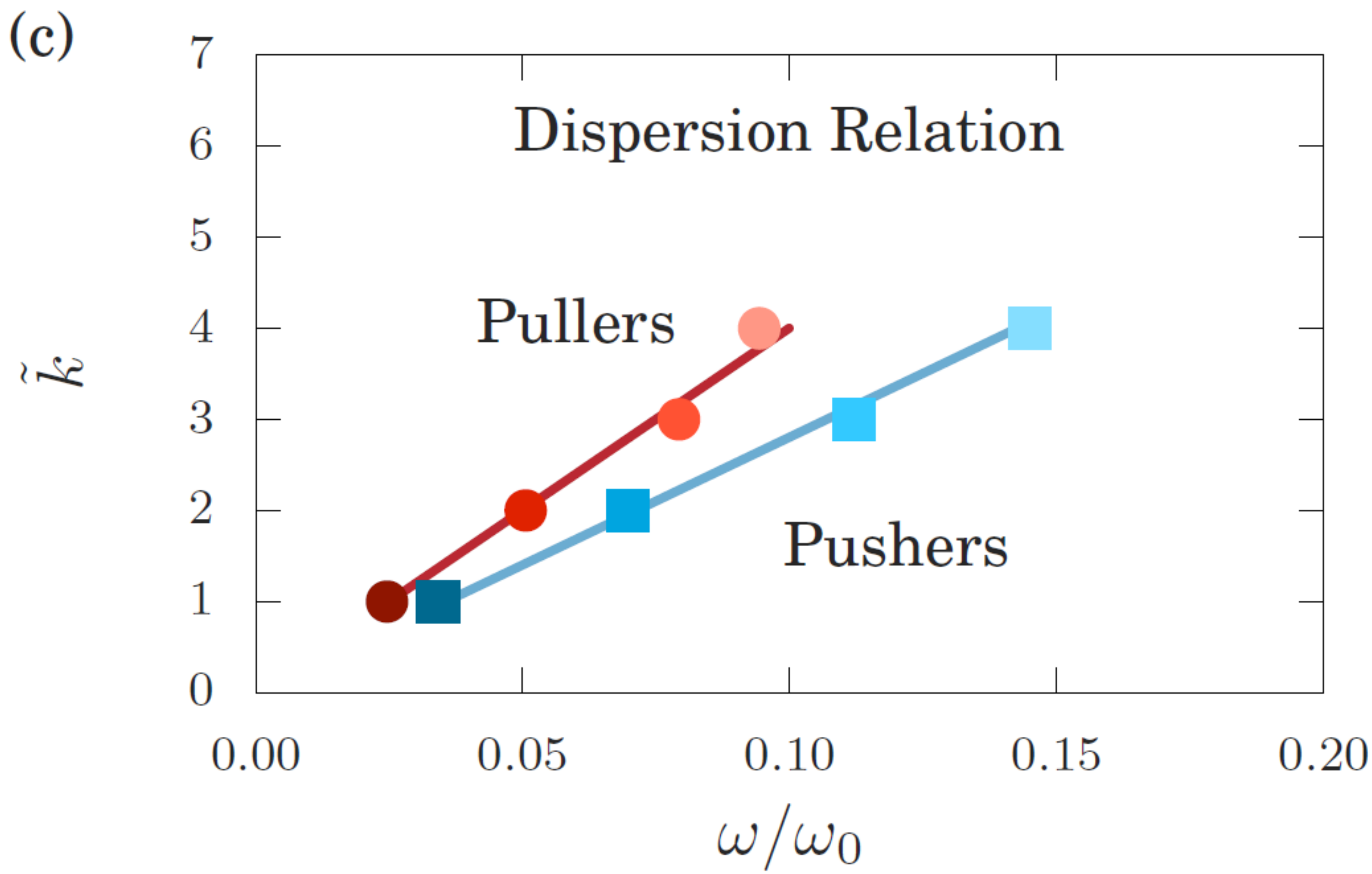
Dynamic structure factor

Dispersion relation



$\omega = c_s k$

unpublished

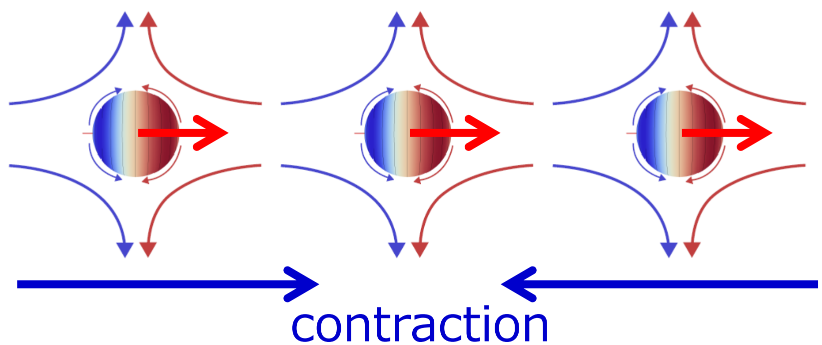
Open questions

- Dependencies of the phenomena on (α, ϕ, L)

- Mechanism of density wave

naive guess …

for pullers



- Corresponding experiments