Modelling bacteria in porous media

Kevin Vietz

July 16, 2021

1 Introduction

In contrast to passive Brownian particles, active particles can execute a systematic movement, because they can take in energy and dissipate the energy in the process of systematic movement [1]. Because motile bacteria perform such a systematic movement we can describe motile bacteria by assuming active Brownian particles. But due to their self-propulsion we cannot describe active particles within equilibrium and they are showing some interesting behaviours such as accumulation and transport properties.

To describe motile bacteria, section 2 firstly gives an introduction to active Brownian particles and how to describe the motion of them. Afterwards the mean square displacement will be discussed to find an effective temperature and describe the active particles within equilibrium. This assumption is indeed not correct for active particles and will therefore be disproved by discussing some non-equilibrium effects. In section 3 the fluid is described for the low Reynolds number regime where we look at the scallop theorem and comparing differences and properties of some flow fields. Section 4 will point out some biological details about the E. coli bacteria, in particular the run and tumble motion. Section 5 introduces a numerical simulation setup for simulating bacteria in a microporous channel and also discussing the results of this simulations.

2 Active Brownian particles

To describe the motion of active Brownian particles in a simple manner we can simply add a self propelling velocity to the motion of passive Brownian particles. This procedure will be explained in section 2.1. Afterwards section 2.2 shows the mean square displacement of free active Brownian particles, which will be used to define an effective temperature. The assumption of an effective temperature will then be disproved by some non-equilibrium effects in section 2.3.

2.1 Equations of motion

For Brownian particles the equations of motion are described by the Langevin equation [2]

$$m\dot{v} = -m\gamma v + F(t) \tag{1}$$

with the mass m, the velocity v, respectively the acceleration $\dot{v}$, the friction coefficient γ and a random force $F(t)$ acting on the particle. The friction coefficient provides a damping due to the collides with the fluid molecules. In the special case of an overdamped system $m\gamma v \gg m\dot{v}$ we can describe the

motion of a two dimensional passive Brownian particle with the coordinates x and y as well as the angular φ for the orientation of the motion. This leads to the equations

$$\begin{cases} \dot{x} &= \sqrt{2D_\mathrm{T}}W_\mathrm{x} \\ \dot{y} &= \sqrt{2D_\mathrm{T}}W_\mathrm{y} \\ \dot{\varphi} &= \sqrt{2D_\mathrm{R}}W_\varphi \end{cases} \tag{2}$$

where D_T is the translational, D_R is the rotational diffusion coefficient and the terms W_x, W_y and W_φ are presenting the white noise stochastic processes [3]. The diffusion coefficients are defined by the Stokes-Einstein relation as

$$D_\mathrm{T} = \frac{k_\mathrm{B}T}{6\pi\eta R}, \quad D_\mathrm{R} = \frac{k_\mathrm{B}T}{8\pi\eta R^3}, \tag{3}$$

with the radius R, the Boltzmann constant k_B, the temperature T and the viscosity of the fluid η. What we can recognize here is that the translational diffusion scales with the radius $\propto T/R$ whereas the rotational diffusion scales with the volume $\propto T/R^3$.

If we now assume to have active particles instead, the only thing we have to add to equation (2) is the self-propelled velocity of the active particle. We therefore get

$$\begin{cases} \dot{x} &= \sqrt{2D_\mathrm{T}}W_\mathrm{x} + v\cos\varphi(t) \\ \dot{y} &= \sqrt{2D_\mathrm{T}}W_\mathrm{y} + v\sin\varphi(t) \\ \dot{\varphi} &= \sqrt{2D_\mathrm{R}}W_\varphi, \end{cases} \tag{4}$$

for a two dimensional active Brownian particle in an overdamped system.

2.2 Mean square displacement

In contrast to passive particles, active particles are showing some behaviours we cannot describe by assuming equilibrium. To verify this statement, this section first take a look at the mean square displacement (MSD) for active particles and then assuming, that we can describe active particles within equilibrium states. This is indeed not valid and will be disproved in section 2.3 by pointing out some non-equilibrium effects.

For passive particles in an overdamped system the MSD is given by

$$\mathrm{MSD}(\tau) = 4D_\mathrm{T}\tau \tag{5}$$

and for the MSD of an active Brownian particle we can assume [4]

$$\mathrm{MSD}(\tau) = \left[4D_\mathrm{T} + 2v^2\tau_\mathrm{R}\right]\tau + 2v^2\tau_\mathrm{R}^2\left[e^{-\tau/\tau_\mathrm{R}} - 1\right], \tag{6}$$

with a rotational diffusion time τ_R which corresponds to a persistence length

$$L = \frac{v}{D_\mathrm{R}} = v\tau_\mathrm{R}. \tag{7}$$

Considering different time regimes we get for equation (6)

$$\mathrm{MSD} = \begin{cases} 4D_\mathrm{T}\tau, & \tau \ll \tau_\mathrm{R} \\ 4D_\mathrm{T}\tau + 2v^2\tau_\mathrm{R}\tau, & \tau \approx \tau_\mathrm{R} \\ 4D_\mathrm{T}\tau + 2v^2\tau^2, & \tau \gg \tau_\mathrm{R} \end{cases} \tag{8}$$

This behaviour of the MSD is also shown in figure Figure 1 for self-propelled particles with different velocities v. The passive Brownian particle with $v = 0\,\mu\mathrm{m\,s^{-1}}$ shows a linear behaviour for the whole time scale. So the motion of the passive particle is always diffusive. But for increasing v one can recognizes a regime where the MSD scales quadratically with the time τ, which corresponds to the intermediate time scale in equation (8). In this ballistic regime, the particle is superdiffusive. For large time scales the active Brownian particles will again be proportional to τ and therefore diffusive. This is because the rotational diffusion no longer plays a role, better says it leads to a randomization of the orientation. Due to the particles velocities the MSD is enhanced for longer time scales.

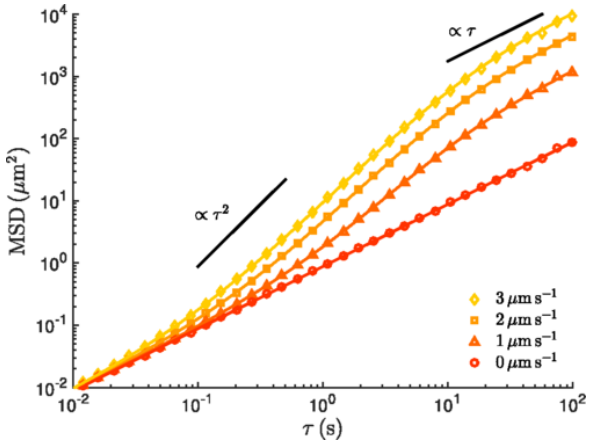


Figure 1: The mean square displacement (MSD) of free active Brownian particles for different velocities [3]. For short time scales the MSD is proportional to τ and the particles motions are diffusive. For intermediate time scales and velocities greater than $0\,\mathrm{m\,s^{-1}}$ the motion becomes superdiffusive and for large time scales again diffusive.

Due to the behaviour of the MSD we can define an effective diffusion coefficient

$$D_\mathrm{eff} = D_\mathrm{T} + \frac{1}{2}v^2\tau_\mathrm{R}. \tag{9}$$

By recalling the Stokes-Einstein relation, it would also be plausible to define a corresponding effective temperature for our effective diffusion like in equation (3). Therefore we would get

$$T_\mathrm{eff} \stackrel{?}{=} \frac{\gamma D_\mathrm{eff}}{k_\mathrm{B}} = T + \frac{\gamma v^2 \tau_\mathrm{R}}{2k_\mathrm{B}}. \tag{10}$$

and one could ask, if we can describe active particles within equilibrium and this effective temperature. But as experiments shows, this is not the case for interacting active particles.

2.3 Non-equilibrium effects

The assumption of an effective temperature would mean that active Brownian particles are in equilibrium which is indeed not the case. This section therefore shows some of non-equilibrium behaviours for active Brownian particles.

One example of breaking those quasi-equilibrium state theory is illustrated in Figure 2. This figure shows active Brownian particles of different velocities in a single pore with reflective boundaries. Also there is the position distribution shown for the different velocities underneath the trajectories. While the passive Brownian particles in figure 2a are distributed homogeneously over the entire pore, the probability increases towards the boundary if the velocity increases. This is because of the concave pore shape and the active particles persistence lengths. The active particles will hold their moving direction for a certain time and if they move against a boundary, they will move along it as long as the reorientation doesn't result a directed motion away from the boundary. Thus the position distribution is non-Boltzmann and therefore the system cannot be described by an effective temperature.

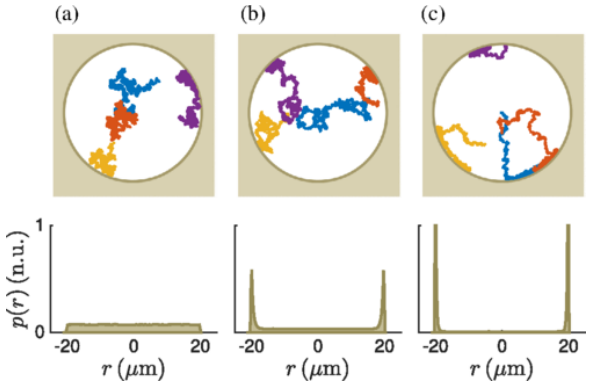
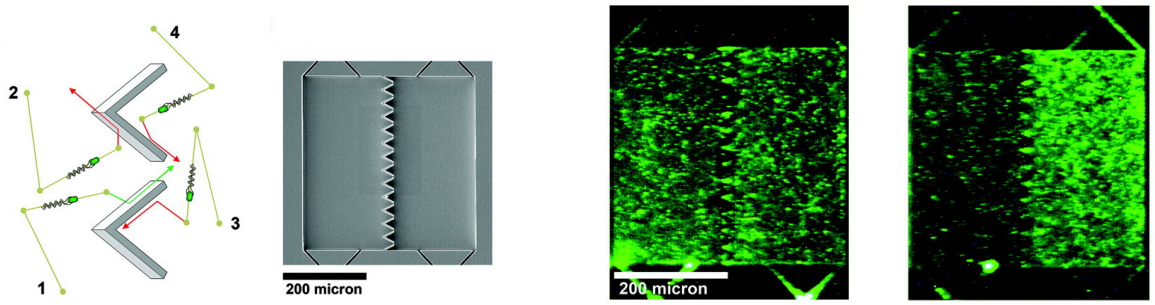


Figure 2: Simulated trajectories and associated position distributions for active Brownian particles of different velocities in a pore [5].

A similar kind of non-equilibrium effect is shown in Figure 3. The schematic setup in Figure 3a consists of obstacles in a funnel shape with a gap between the obstacles. This setup will lead to an increased position distribution on the ride half of the system for active Brownian particles. Passive Brownian particles instead will be homogeneously distributed due to the equipartition theorem. But because the self-propelling velocities and the shape of the obstacles, the active particles are more inclined to trace the gap from the left side, whereas the possibility to trace the gap from the right side is restricted.

This kind of setup has also been used in an experiment and the results are shown in Figure 3b. The left side shows the initial setup, where all the active particles are distributed homogeneously over the whole system. The right side shows the system after a certain time and therefore the density on the right half is enhanced. This is only caused by the self-propelling of the particles, it didn't need any kind of additional force to move the particles there.



(a) Schematic setup

(b) Experimental results

Figure 3: A setup to concentrate active particles. (a) show the schematic setup. The micro-structure uses funnel walls with a gap which active particles can trace more likely from the left side. (b) shows the experimental results for this kind of setup. The initial uniform distribution on the left side becomes a steady-state distribution after 80 min, which is shown on the right [6].

3 Hydrodynamics

The motion of fluids can be described by the Navier–Stokes equations. To describe bacteria in a fluid we consider afterwards the dimensionless Navier-Stokes equations and transfer them into the Stokes equations by assuming a vanishing Reynolds number.

To describe bacteria in a fluid it is kind of practical to make the Navier–Stokes equations dimensionless. Thereby we get

$$\mathrm{Re}\left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\boldsymbol{u}\right) = \boldsymbol{\nabla}^2\boldsymbol{u} - \boldsymbol{\nabla}p + \boldsymbol{f} \tag{11}$$

with the Reynolds number Re and the fluid velocity $\boldsymbol{u}$, as well as the dimensionless pressure p and outer forces $\boldsymbol{f}$. The Reynolds number is coming from the non-dimensionalisation of the Navier-Stokes equations and is defined as the ratio between inertial forces and viscous forces as follows:

$$\mathrm{Re} = \frac{\text{inertial forces}}{\text{viscous forces}} = \frac{\rho L v}{\eta}. \tag{12}$$

If we now assuming to describe bacteria, we can neglect the left term of equation (11), due to the fact that the Reynolds number is very small. For a bacteria in water we can use for example $\rho = 1000\,\mathrm{kg\,m^{-3}}$, $L \approx 1\,\mu\mathrm{m}$, $v = 30\,\mu\mathrm{m\,s^{-1}}$ and $\eta = 1\times10^{-3}\,\mathrm{Pa\,s}$ and get a Reynolds number about $\mathrm{Re} \approx 3\times10^{-5} \ll 1$ [3]. We can therefore use the simpler Stokes equations

$$\begin{cases} \boldsymbol{\nabla}^2\boldsymbol{u} - \boldsymbol{\nabla}p + \boldsymbol{f} &= 0 \\ \boldsymbol{\nabla}\cdot\boldsymbol{u} &= 0 \end{cases} \tag{13}$$

and also recognize, that we lost the time evolution we had in the Navier-Stokes equations. This independence in time makes the motion fully reversible and we can illustrate this by the scallop theorem. In Figure 4 are shown two states for the scallop movement. At state A the scallop is open and by performing a quick closing of the shells the scallop is pushed forward and gets into state B. By

open the two shells very slowly one would assume that the movement backwards is not as much as the movement forwards. But this is indeed not the fact in the low Reynolds number regime and thus the scallop cannot generate propulsion by this kind of motion.

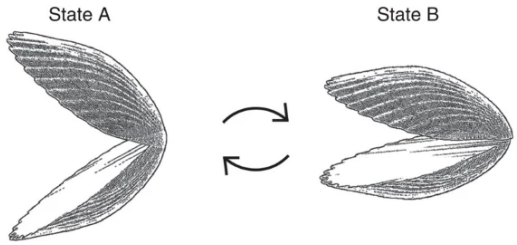


Figure 4: The two states of a scallop movement by opening and closing the two shells. In the low Reynolds number regime the scallop cannot generate propulsion by this kind of motion [7].

By considering the scallop theorem one can wonder how motile bacteria actually are moving, because we know they do move. One simple example for moving in an low Reynolds number regime consists of a body and a rotating paddle at the tail. This kind of schematic arrangement is also used by E. coli and will be discussed in section 4 in more detail.

To analyze the flow field created by a freely swimming bacterium of this type we are looking at Figure 5. This figure shows the measured average flow field for a freely swimming bacterium and the streamlines indicates the direction of the fluid flow. The bacterium in the center is swimming to the right. What we can recognize is, that this flow field is close to stokes dipole in Figure 6 for a pusher. So in a simple manner we can describe the flow field for a freely swimming pusher bacterium by a force dipole.

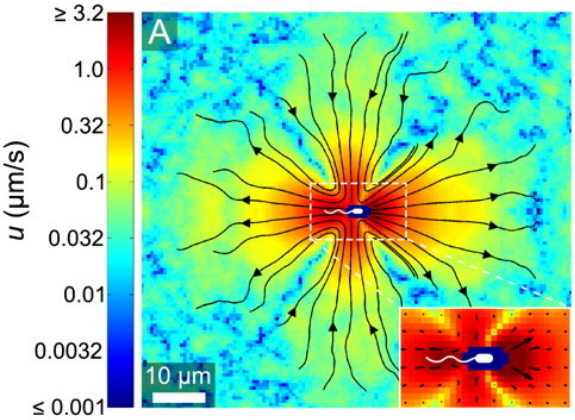


Figure 5: Experimental average flow field for a freely swimming bacterium, the streamlines indicate the flow direction [8].

In contrast to the Navier-Stokes equations the Stokes equations are linear. We can therefore describe the flow field by the superposition of singular solutions. If we assume the particles are driven by external forces, the dominant singularity is the Stokes flow which is generated by a point force and

showed in Figure 6 left [3]. Figure 6 also shows the dipole singularities. Here the far-field flow for the Stokes dipoles are represented by two nearby forces pointing in the opposite direction. Figure 6 middle shows the Stokes dipole for two point forces pointing apart from each other. Therefore it is called pusher. The point forces for the Stokes dipole on the right pointing against each other, therefore this dipole is a puller. Both Stokes dipoles moving horizontally.

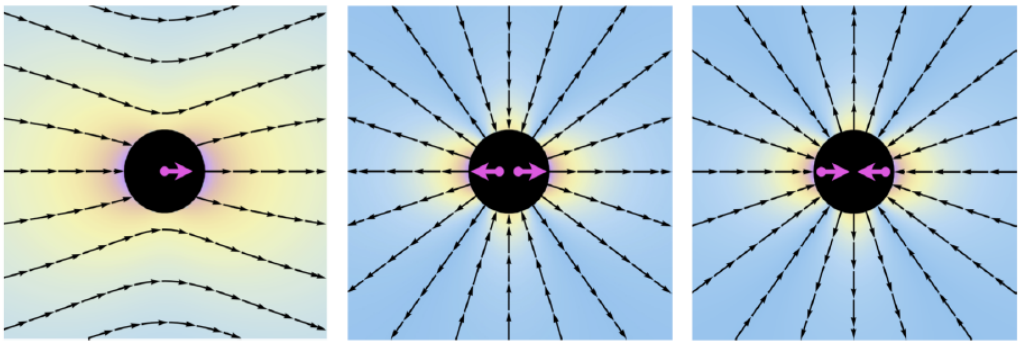


Figure 6: The flow singularities for the the far field on the left. In the middle the Stokes dipole for a pusher and on the right the Stokes dipoles for a puller. The Stokes dipoles are representing active particles driven by an internal force and moving horizontally [3].

4 Biological details

The prime example of a motile bacteria is the E. coli, which is one of the most intensively studied organism on the planet. As already mentioned in section 3, we can describe them as pushers because they are moving by rotating the so called flagella at their backside. Normally bacteria could have up to a few of those flagella. They rotating with rates around 100 Hz and they have a helical shape [9]. The motion of the cells basically consists of runs and tumbles. Together they build the so called run and tumble motion. This motion is described afterwards in more detail.

If the flagella are all bundled together at the tail of the bacterium this leads to a run motion and the bacterium is moving steadily forwards for a specific time. This type of motion is illustrated by the schematic drawing in Figure 7 on the left side. The bacterium in this figure would swim to the left.

The other part of the motion is the so called tumble. If one ore more of the flagella are not in the bundle anymore this will lead to a reorientation of the bacterium. This kind of motion is illustrated in Figure 7 where all flagella are spread out.

Both parts are alternating to find nutrient in the fluid. Whereas the average tumble times are relatively short about 0.1 s, the runs are relatively long about 1 s [9]. By alternating those motion parts, the bacterium can perform a systematical movement. So if the bacterium detects a higher density of nutrient in the fluid, the probability to re-orientate by performing the tumble motion decreases and therefore the systematical movement will be more directed to the nutrient. In contrast to this, the probability for the tumble motion increases if the nutrient density decreases.

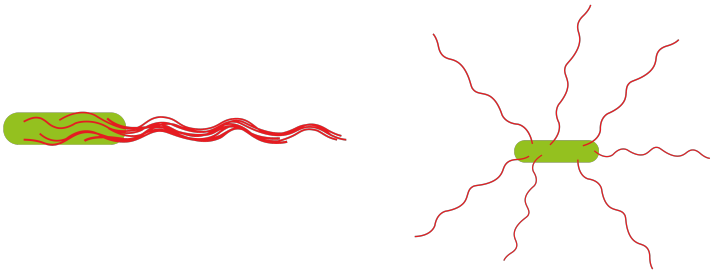


Figure 7: The schematic drawing of the run and tumble motion. Left the run motion, where all flagella are bundled at the tail of the bacterium and rotating together. On the right side the schematic drawing of the tumble motion where the flagella are not bundled together and the bacterium can therefore reorientate itself.

5 Numerical application

This section shows an example to simulate bacteria in porous media. First the simulation setup will be described and afterwards the results are discussed in section 5.2.

5.1 Setup

Figure 8 shows the an example setup for modelling bacteria in porous media. The setup consists of a channel with a microfluide flow and a cylindrical obstacle inside the channel. Due to this setup a basic porous media is given, because there are solid boundaries and we have also different velocities in the fluid stream because of the obstacle inside the channel. For the bacteria this model uses a set of five rigid collected particles. The reason for using multiple particles aligned to each other, is to put torque on it. This wouldn't be able with a single point like particle [10].

The flow direction of the fluid is in the positive x direction. In this direction periodic boundary conditions are applied such that the swimmer will come in from the left, if it reaches the right boundary and vice versa. In the other two directions no-slip boundaries are used.

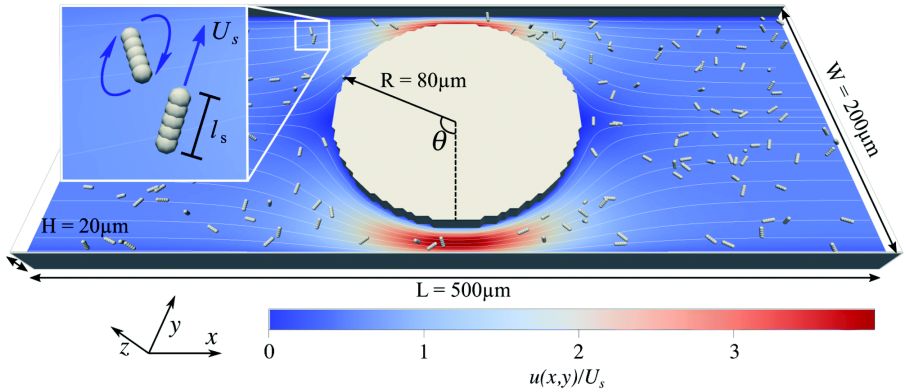


Figure 8: A simulation setup for a fluid-filled channel with an cylindrical obstacle in the center of the channel and 159 swimmers [11].

5.2 Results

Some results of the simulations are shown in Figure 9. Here the swimmers distribution is shown for various external flow inputs. Also the dashed lines are showing regions where the magnitude of the averaged flow velocity u_{avg} is greater than the magnitude of the swimmer velocity U_{S}. In the first case (upper left figure) there is no flow velocity applied to the fluid. The distribution shows, that there is a high position probability for the swimmers at the walls of the channel and also around the obstacle. What one can also observe is that more swimmers are accumulated on the lateral walls than around the obstacle, which can be explained by the convex shape of the obstacle [11].

By introducing an external flow, the ratio between averaged flow velocity and the swimmer velocity becomes greater than 0. What we can also see in Figure 9 is that the accumulation for the bacteria enhances at the downstream side of the obstacle, whereas the accumulation at the upstream side around the obstacle is reduced.

Another result can be obtained by also looking at the extension of the accumulation regions. With stronger flow velocities the extension for accumulation mainly at the downstream side of the obstacle is reduced. This extension reduces with increasing flow strengths and can also be obtained by looking at the dashed regions where the local flow velocity is higher than the swimmer velocity.

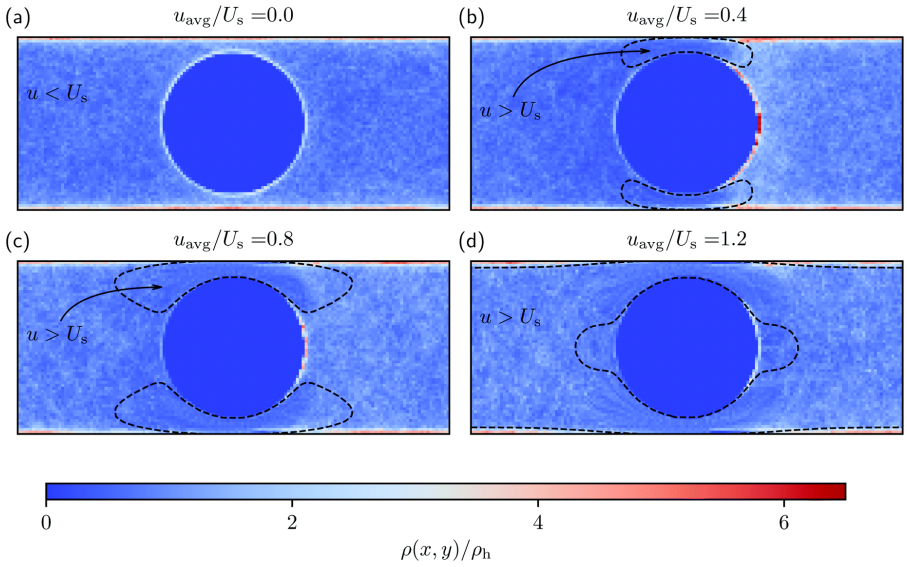


Figure 9: Distribution of the swimmers $\rho(x, y)$, normalized by the homogeneous swimmer distribution ρ_{h} for various external flow inputs [11].

6 Conclusion

To describe the motion of active Brownian particles we can simply add a velocity to the overdamped Langevin equation. Also we have seen that we can define an effective temperature for the active Brownian particles, but indeed this assumption is incorrect due to the fact that they are not in equilibrium.

Because bacteria live in low Reynolds number regimes we can use the Stokes equations and due to their linearity use superposition to find solutions and describe the flow fields. By looking at some flow singularities and comparing them to experimental results we have seen, that the flow field created by the bacterium in the experiment could be approximated with a Stokes pusher dipole.

In the end we discussed a simulation example which consists of a microporous channel and a cylinder inside the channel. This setup has solid boundaries and generates different flow zones of different flow velocities, therefore this setup describes a simple porous media. As a result the distribution shows that the swimmers prefer to accumulate in regions with lower flow velocities.

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