Simulation of individual cells in flow

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Simulation of individual cells in flow
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Abstract
In this thesis, simulations are performed to study the motion of individual cells in flow, focusing on the hydrodynamics of actively swimming cells like the self-propelling microorganisms, and of passively advected objects like the red blood cells. In particular, we develop numerical tools to address the locomotion of microswimmers in viscoelastic fluids and complex geometries, as well as the motion of deformable capsules in micro-fluidic flows.

For the active movement, the squirmer is used as our model microswimmer. The finite element method is employed to study the influence of the viscoelasticity of fluid on the performance of locomotion. A boundary element method is implemented to study swimming cells inside a tube. For the passive counterpart, the deformable capsule is chosen as the model cell. An accelerated boundary integral method code is developed to solve the fluid-structure interaction, and a global spectral method is incorporated to handle the evolving cell surface and its corresponding membrane dynamics.

We study the locomotion of a neutral squirmer with an emphasis on the change of swimming kinematics, energetics, and flow disturbance from Newtonian to viscoelastic fluid. We also examine the dynamics of different swimming gaits resulting in different patterns of polymer deformation, as well as their influence on the swimming performance. We correlate the change of swimming speed with the extensional viscosity and that of power consumption with the phase delay of viscoelastic fluids. Moreover, we utilise the boundary element method to simulate the swimming cells in a straight and torus-like bent tube, where the tube radius is a few times the cell radius. We investigate the effect of tube confinement to the swimming speed and power consumption. We analyse the motions of squirmers with different gaits, which significantly affect the stability of the motion. Helical trajectories are produced for a neutral squirmer swimming, in qualitative agreement with experimental observations, which can be explained by hydrodynamic interactions alone.

We perform simulations of a deformable capsule in micro-fluidic flows. We look at the trajectory and deformation of a capsule through a channel/duct with a corner. The velocity of capsule displays an overshoot as passing around the corner, indicating apparent viscoelasticity induced by the interaction between the deformable membrane and viscous flow. A curved corner is found to deform the capsule less than the straight one. In addition, we propose a new cell sorting device based on the deformability of cells. We introduce carefully-designed
geometric features into the flow to excite the hydrodynamic interactions between the cell and device. This interaction varies and closely depends on the cell deformability, the resultant difference scatters the cells onto different trajectories. Our high-fidelity computations show that the new strategy achieves a clear and robust separation of cells. We finally investigate the motion of capsule in a wall-bounded oscillating shear flow, to understand the effect of physiological pulsation to the deformation and lateral migration of cells. We observe the lateral migration velocity of a cell varies non-monotonically with its deformability.

Descriptors: Hydrodynamic interaction, swimming microorganisms, capsule, Stokes flow, finite element method, boundary integral method, general geometry Ewald method, spectral element method, viscoelastic fluid, cellular deformation, flow cytometry, cell sorting, microrheology
Simulering av enskilda celler i flödet
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Sammanfattning
I den här avhandlingen presenteras simuleringar utförda för att studera rörelsen hos individuella celler i strömmande medier. Detta görs med fokus på hydrodynamiken, dels hos aktivt simmande celler såsom självframdrivande mikroorganismer och dels hos passivt advekterade röda blodkroppar. I synnerhet har numeriska verktyg utvecklats för att behandla mikroskopiska simmande organismer och passiva röda blodkroppar. Numeriska verktyg har utvecklats för att behandla mikroskopiska störningar, samt tester deformerbara kapsylers rörelse i mikroskopiska störningar.


Rörelseformågan hos en neutral squirmer studeras med fokus på förändringen av simningens kinematik, energibalanse, and störningar från Newtonsk ill viskoelastisk fluid. Vi studerar även dynamiken vid olika simsätt som resulterar i olika deformationsmönster, samt deras inverkan på simningens prestation. För den neutral squirmer har vi analyserat rörelsen för en neutral squirmer i ett rör och för en deformerbar kapsel. Vi har sett att simningens kinematik och energibalanse bero på deformerbar kapsels form och dynamiken av fluiden. En global spectral metod har använts för att hantera dynamiken hos cell och membran.
geometriska egenskaper introduceras i flödet vilka existerar betydande hydro-
dynamiska interaktioner mellan cell och enhet. Nivån på detta samspel beror
på cellens deformbarhet och denna egenskap ger möjlighet att sprida cellerna
på olika rörelsebanor. Våra noggranna beräkningar visar att den nya strategin
uppnår en tydlig och robust separation. Slutligen studeras kapselns rörelsen i
ett väggbundet oscillerande skjuvflöde i syfte att förstå effekten av fysiologisk
pulsation på deformationen av celler och deras rörelse från väggen. För en fast
oscillationsfrekvens, upptäcker vi att det existerar ett icke-monotont beroende
hos cellens deformbarhet av migrationshastigheten.

**Nyckelord:** Hydrodynamisk växelverkan, simning mikroorganismer, kapsel,
Stokes flöde, finita elementmetoden, gräns integrerad metod, allmän geometri
Ewald metod, spektral elementmetoden, viskoelastisk vätska, cellulär deforma-
tion, flödescytometri, cell sortering, microrheology
Preface

This thesis investigates the active and passive motions of biological cells via numerical simulations. It mainly focuses on the microorganisms self-propelling in viscoelastic fluids and confined environments, as well as on the deformable micro-capsules transported in the micro-fluidic environments like a channel flow with a corner and cell-sorting devices. A brief introduction on the basic concepts and numerical methods is presented in the first part. The second part contains seven articles. The papers are adjusted to comply with the present thesis format for consistency, but their contents have not been altered as compared with their original counterparts.


**Paper 2.** L. Zhu, E. Lauga & L. Brandt, 2012


**Paper 4.** L. Zhu & L. Brandt, 2013
The motion of a deforming capsule through a corner. *Submitted to Journal of Fluid Mechanics.*

A microfluidic device to sort capsules by deformability. *Submitted to Lab on a Chip.*

**Paper 6.** OS. Pak, L. Zhu, L. Brandt & E. Lauga, 2012
The dynamics of a capsule in a wall-bounded oscillating shear flow. Internal report.
Related publications
Below is a list of the related work that has been partially performed by the author during the phd study, but not included in this thesis.

International Journals

Rotational propulsion from inertia. Submitted to the European Physical Journal E..

Peer-reviewed conference papers

Division of work among authors
The main supervisor for the project is Prof. Luca Brandt and the co-advisors are Dr. Minh Do-Quang and Prof. Gustav Amberg.

Paper 1
Lailai Zhu (LZ) built up the numerical model within the frame provided by Femlego (KTH Mechanics) with feedback from Minh Do-Quang (MDH) and Luca Brandt (LB). Simulations were performed by LZ. LZ and LB analysed the data in collaboration with Eric Lauga (EL). The paper was written by LB and LZ with the introduction by EL.

Paper 2
LZ built up the numerical implementation within the frame provided by COMSOL and performed the simulations. LZ analysed the data and wrote the paper with input from LB and EL.

Paper 3
The project was initiated by LZ, inspired by the experimental work of Jana et al. 2012. LZ developed the highly accurate boundary element method code from scratch and performed the simulations. LZ analysed the data and wrote the paper with input from LB and EL.

Paper 4
LZ developed the boundary integral flow solver accelerated by the general geometry Ewald method (Hernández-Ortíz et al. 2007), embedded with a global spectral method (Zhao et al. 2010) for the membrane dynamics. The numerical implementation is built on top of an open source Navier-Stokes solver NEK5000 (Fischer et al. 2008b) based on spectral element method. LZ developed the code from scratch except for NEK5000. LZ constructed the numerical setup, analysed the data and wrote the paper with feedback from LB.

Paper 5
LZ initiated the project of sorting cells by their deformability. LZ built up the numerical setup, based on the boundary integral implementation developed in the project of paper 4. Simulations are performed by LZ and Cecilia Rorai (CR). Data was analysed by LZ, Dhrubaditya Mitra (DM), CR and LB. CR, DM and LZ wrote the paper, with feedback from LB.

Paper 6
LZ built up the numerical model and performed the simulations. The paper was written by On Shun Pak and EL, with feedback from LZ and LB. LZ wrote
the numerical model description and provided the plots of flow field with the corresponding analysis.

**Paper 7**

LZ set up the numerical case based on the boundary integral implementation developed in the project of paper 4. LZ performed the simulations. LZ, Jean Rabault (JR) analysed the data. The paper was written by LZ, with feedback from JR and LB.
天下事有难易乎？为之，则难者亦易矣；不为，则易者亦难矣。

彭端淑《为学》
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Paper 2. Self-propulsion in viscoelastic fluids: pushers vs. pullers

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Part I

Overview
CHAPTER 1

Introduction

1.1. Dynamics of swimming microorganisms

The physics of animal locomotion has been studied for a long time. One particularly interesting topic is the hydrodynamics of swimming microorganisms. Due to its importance in a variety of biological and ecological processes, researchers have been addressing the problem from different perspectives, for instance, the mobility of spermatozoa crucial to mammalian fertilization, marine bacterial movement related to the biogeochemical transformation and cell swarming coupled to the biofilm formation (Verstraeten et al. 2008). More specific topics include the propulsion mechanisms of microorganisms (Evans et al. 2009; Hillinger et al. 2009; Spagnolie & Lauga 2010), directed bacterial responses to chemicals (chemotaxis) (Ahmed et al. 2010), gravitation (gyrotaxis) (Durham et al. 2011), temperature (thermotaxis) (Hamel et al. 2011) and flow shear (rheotaxis) (Marcos et al. 2012), swimming in complex fluids (Liu et al. 2011; Shen & Arratia 2011; Teran et al. 2010), nutrients uptake in the presence of external flow (Lambert et al. 2013; Magar et al. 2003), locomotion in confined environments (Felderhof 2010; Zhu et al. 2013) and collective swimming dynamics of bacteria suspensions (Ishikawa & Pedley 2008; Saintillan & Shelley 2008; Underhill et al. 2008).

Part of this thesis investigates two abovementioned topics: swimming in complex fluids and swimming within strongly confined environments.

1.1.1. Swimming in complex fluids

It is well known that microorganisms often have to swim through complex, non-Newtonian media. For instance, *spirochetes* burrows through the extracellular matrix in host tissues (Charon & Goldstein 2002; Goldenberg & Thompson 2003), mammalian spermatozoa progresses through the viscoelastic cervical mucus in the female reproductive tract (Fauci & Dillon 2006) and ulcer-causing bacterium *Helicobacter pylori* moves inside the mucus lining the stomach (Montecucco & Rappuoli 2001). From the practical point of view, potential manipulation of artificial microrobots through soft tissues, the digestive tract and the spinal canal will also benefit from the effective movement in complex media (Leshansky 2009). Therefore, a clear physical understanding of the microscale locomotion in these complex environments becomes important. Several
1. INTRODUCTION

Figure 1.1. The streamlines of flow around a swimming *Caenorhabditis elegans* in the Newtonian (left) and viscoelastic (right) fluid, the Reynolds number $Re < 1E - 3$. The red box zooms in the hyperbolic point owing to polymeric stretching. Reproduced from Shen & Arratia (2011).

groups have recently started to address the problem. Lauga (2007) investigated the kinematics and energetics of Taylor’s waving sheet in various model nonlinear polymeric fluids and found that, for a given waving stroke, viscoelasticity impeded the locomotion of swimming sheet. Similarly, Fu et al. (2009) derived analytically that the swimming speed of an infinite filament with a prescribed waveform will decrease in the Oldroyd-B fluid compared to the Newtonian case. Teran et al. (2010) numerically studied the influence of viscoelasticity on the dynamics of a finite-length Taylor’s waving sheet and showed that the swimming speed and efficiency can actually increase within a certain range of polymer relaxation time and sheet waveforms. Recently, Shen & Arratia (2011) experimentally demonstrated that fluid elasticity hindered the self-propulsion of the nematode *Caenorhabditis elegans*, primarily due to polymeric stretching near hyperbolic points in the viscoelastic flow (see figure 1.1). Liu et al. (2011) performed high-precision experiments to investigate the force-free locomotion of a rotating helix in a viscoelastic fluid, and showed that the swimming speed could be larger than that in a Newtonian fluid. The speed reaches the maximum when the polymeric relaxation time is close to the characteristic time scale of the flow. This polymer-induced increase of swimming speed is reproduced by the numerical simulations in Spagnolie et al. (2013) who attributed the velocity increase to the interplay between the helical motion and its viscoelastic wake.

All of the abovementioned investigations study the locomotion of cells propelled by undulatory motions, little knowledge is known about swimming by ciliary propulsion. Moreover, many of these previous numerical studies are limited to 2D cases. In this thesis, we perform 3D numerical simulations to investigate ciliated cells swimming in the viscoelastic fluids and we address these questions: how do the swimming speed and power consumption change due to
1.1. Dynamics of Swimming Microorganisms

Figure 1.2. Swimming *V. carteri*. (a) Top view. Superimposed images taken 4s apart. (b) Side, and (c) top views of a colony swimming near a solid boundary, with fluid streamlines. (d) A linear *Volvox* cluster viewed from above. Reproduced from Drescher et al. (2009).

the fluid viscoelasticity? How does the flow field interact with the surrounding polymer networks and thus influence the performance of locomotion?

1.1.2. Swimming in confined environments

Cell locomotion in confinements shows several interesting phenomena resulting from hydrodynamic effects. For example, the bull spermatozoa tend to accumulate near the solid walls (Rothschild 1963); *Escherichia coli* cells execute clockwise circular trajectories near the solid boundaries (Lauga et al. 2006) but swim in the anticlockwise circular direction beneath a liquid-air interface (Leonardo et al. 2011), owing to the counter-rotation of the cell body and flagella; two nearby *Volvox* colonies “waltz” or “minuet” around each other when swimming near a wall (Drescher et al. 2009) as a consequence of surface-mediated interactions (see figure 1.2). In this thesis, we study swimming microorganisms inside a tube, inspired by the experimental observation of *Paramecium* following helical trajectories. We develop an accurate and efficient code to simulate moving objects inside a tube in the Stokesian regime using the boundary element method (BEM) to explain such an interesting feature from the hydrodynamic point of view.
1. INTRODUCTION

1.2. Deformable cells, capsules and vesicles

Besides the previously mentioned self-propelling microorganisms, a large number of biological cells like red blood cells (RBCs), stem cells, ovums are not motile, instead carried by the external flow. These cells transported inside our body are responsible for distributing nutrients and oxygen, collecting waste, delivering genetic information, and more. Inspired by the delivery function of these natural particulates, synthetic micro and nano-particles have also been designed for targeted therapeutic delivery and more advanced purposes like microscopic imaging. Understanding the dynamics of these tiny objects in flow, object-object/object-flow interaction and how they together influence the surrounding environment becomes an interesting and important topic, indeed at the interface of biology, physics, mechanics, chemistry and computer science.

1.2.1. Biological phenomena

In the biological environment, circulating micro-particles are prevalent and red blood cells as the main ingredients of blood, are undoubtedly the best example. Millions of RBCs are simultaneously passing through our capillaries to transport nutrients and oxygen, remove CO2 and when necessary squeeze themselves significantly into the smallest veins. The deformability of RBCs plays such an important role, that any pathogenic variation of cells with abnormal deformability leads to serious and even deadly diseases, malaria-affected and sickle-cells being typical two (Freund 2014). Healthy RBCs deform to accelerate their journey and the flow around them: in a capillary of particular size, nicely-shaped RBCs achieve a higher volume flux higher than that of the overall suspension and reduce the total effective viscosity by inducing a blunted flow profile; a famous phenomenon called Fåhraeus effect (Fåhraeus & Lindqvist 1931). More surprisingly, our human body even develops delicate slit-shape structures (in the spleen) to remove aged RBCs (Freund 2013). There are many more applications of the mechanics of deformable cells, like the interaction between red and white blood cells, platelet transportation, activation and adhesion, shear-induced ATP release of RBCs (Wan et al. 2008), hematocrit reduction in bifurcating vessels due to plasma skimming (Jonsson et al. 1992) and so forth. These situations are characterized by complicated flow patterns transporting and deforming the suspended biological micro-particles. A proper understanding of these phenomena from the mechanical point view is important. The current thesis pays a special attention to the behaviours of deformable particles in micro-fluidic flows, more specifically to the interaction between fluid flow and cells.
1.2. Biomedical engineering

Flowing particles of micro and/or nano-scale is not only a fundamental natural phenomenon, but also prevalent in the biomedical engineering. A typical example is the micro-fluidic technology called flow cytometry designed to sort, count and analyse a large population of cells. Another application is the steered delivery of cell-inspired micro and nano-particles carrying drugs to the target region for the maximum therapeutic efficiency with minimum side-effects. Here, we shall just introduce flow cytometry.

1.2.2a. Flow cytometry. Flow cytometry is a routinely used biomedical device for manipulating microscopic particles, mostly biological cells, where these are suspended in a fluid and transported through an analysis apparatus. It is typically used to simultaneously measure and analyse the property of a large number of individual cells, like size, granularity, gene expressions and specific surface receptors; an alternative function is to separate cells with different properties or to capture those with specific properties (like rare or unhealthy cells).

Traditional devices utilize fluorescent-based and magnetic-based antibodies to label cells, subsequently performing the fractionation. Recently, new approaches without chemical labels have been developed to characterise cells based on the differences in the mechanical/physical (MP) properties like size, shape, deformability, magnetic susceptibility (Karimi et al. 2013), and so on. These devices have shown many advantages compared to their conventional counterparts, eliminating costly labelling and sample preparation, reducing the processing time and complexity (Mao & Huang 2012). Generally, label-free methods are classified into two groups, namely, active and passive methods. The active ones apply external fields (like optical, electric and magnetic) on the cells to achieve separation based on the disparity in the corresponding MP properties. The passive ones introduce carefully-designed geometric features, which excite cell-cell and/or cell-device interactions. The resultant hydrodynamic and non-hydrodynamic (like steric repulsion) forces can then be harnessed to reposition cells into desired locations for sorting or to stretch/deform cells determining their mechanical property. It is noteworthy that the cell deformability is relevant with the intracellular changes and hence a proper indicator of the cell states like the cycle stage and degree of differentiation. It can also be used to diagnose abnormal cells like the malaria-affected RBCs and tumour cells. In the current thesis, passive methods only employing hydrodynamic effects will be considered.

Micro-fluidic devices commonly have a characteristic length scale comparable with the size of biological cells, the length scale of flow is also of the same order. Therefore, the hydrodynamic force exerted on the cells varies considerably, closely depending on their size, shape and deformability: the force
differences lead these particles onto different trajectories. We report in figure 1.3 an illustration of two typical micro-fluidic devices for cell manipulation, the pinched flow fractionation (PFF) and deterministic lateral displacement (DLD). The PFF device in figure 1.3(a) consists of two inlets and a broadened funnel region connected by a pinched segment. By tuning the inlet flow rate, particles of different sizes injected from the top inlet are forced to be aligned with the top wall of pinched region. The particles are hence positioned at size-dependent vertical positions. The size-induced disparity, although small, is enlarged as the particles follow the diverging flow pattern in the funnel region. The DLD method employs the size-dependent response of particles to an asymmetric bifurcating flow around obstacles. As shown in figure 1.3(b), the flow between the top two obstacles is divided into three lanes. A particle smaller than the lane width is advected around the obstacle, hence, particles from different lanes display 'zigzag' motions however finally go into the same lane. The obstacles do not introduce any lateral displacement to the particle trajectory which then follows the mean flow direction. On the other hand, a particle whose diameter is larger than the lane width, does not fit into lane 1; it will be instead displaced horizontally every time it meets a post.

The PFF and DLD approaches are efficient and simple to sort cells based on their size; however in many situations, the cells have a similar size. In this case, the deformability of cells becomes a better biomarker. As illustrated in figure 1.4, Bow et al. (2011) achieved the separation of stiff malaria-affected cells out of the normal cells, by driving them through arrays of diverging or converging constrictions. The method exploits the fact that a stiff cell travels slower than a floppy one in the constriction, and the corresponding temporal difference even if small can be accumulated to accomplish a considerable net separation. An alternative deformability-based approach introduced by Beech et al. (2012) who drove RBCs around one cylindrical post. The shear around the post deforms the cells whose centroid positions hence are dependent on the deformability; a floppy cell is more flattened, hence its centre gets closer to the post. Since a cell tends to follow the streamlines crossing its centre, a floppy/stiff cell follows the streamline close/far away from the post.

A carefully designed flow pattern can also be used to measure the deformability of a population of cells, useful for the clinical diagnosis and cell characterisation (Gossett et al. 2012). Two recently developed devices are sketched in figure 1.6: Gossett et al. (2012) utilise the extensional flow to stretch a cell and captures its deformation; Zheng et al. (2013) fabricate a human-capillary-like channel supplemented by the hydrodynamic focusing to deform cells, where the deformation and relaxation time are measured in order to examine the quality and age of RBCs after banking/storage.
1.2. DEFORMABLE CELLS, CAPSULES AND VESICLES

Figure 1.3. Working principle of pinched flow fractionation (PFF) and deterministic lateral displacement (DLD). (a) Pinched flow fractionation of particles with two sizes. By controlling the flow rate of two inlets, particles are aligned with the upper wall in the pinched fragment regardless of size, but at size-dependent vertical positions. Entering the broadened funnel region, particles closely follow streamlines, hence, the differences in their positions are amplified. Reproduced with permission from Yamada et al. (2004), American Chemical Society. (b) Deterministic lateral displacement. Particles of different sizes are driven by the vertical flow, through an array of obstacles. Left: small particles follow the mean flow direction, without lateral displacement. Right: big particles are displaced horizontally as ‘bumping’ onto the obstacle and eventually separated. Reproduced from Huang et al. (2004).
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**Figure 1.4.** Schematic illustration of how to use constrictions to discriminate cells based on their deformability. Left: external flow is applied in the inlet to drive a dilute suspension of RBCs through periodic arrays of diverging or converging constrictions. Right: blue and red arrows indicate the positions of healthy and malaria-affected RBCs, respectively. Healthy cells are more floppy, hence pass through the constrictions faster. Reproduced from Bow et al. (2011).

**Figure 1.5.** Schematic illustration of using a cylindrical post to execute cell-sorting based on size and/or deformability. (A): size-based sorting, a smaller cell follows the streamline closer to the post. (B): sketch of the healthy and unhealthy RBCs. (C): increase in the flow rate (relatively enlarging the deformability of cells) flattens the cells as being aligned with the post and drive them to the streamline closer to the post. Reproduced from Beech et al. (2012).
Figure 1.6. Illustration of devices using hydrodynamic forces to measure the cell deformability. (a): Cells are deformed by the extensional flow. Reproduced from Gossett et al. (2012). (b): Cells are transported through a human-capillary-like channel, their deformation and relaxation time are measured. Reproduced from Zheng et al. (2013).
CHAPTER 2

Basic concepts of micro-scale locomotion

2.1. Governing equations

2.1.1. General flow equations

To study the locomotion or propulsion of a swimming microorganism in the viscous fluid, we need to solve the flow around the microorganism, including the velocity field \( u \) and pressure \( p \). Hence, the hydrodynamic force exerted on the cell body can be calculated. The flow of a Newtonian incompressible fluid with density \( \rho \) and viscosity \( \mu \) is governed by the continuity equation,

\[
\nabla \cdot \mathbf{u} = 0, \tag{2.1}
\]

and the momentum conservation equation,

\[
\rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u}. \tag{2.2}
\]

Boundary conditions are set on the surface \( S(t) \) of a cell and on solid boundaries, if considered. Knowing the solution \( \mathbf{u} \) and \( p \), one can calculate the stress tensor \( \mathbf{\sigma} = -p \mathbf{1} + \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \), the hydrodynamic force \( \mathbf{F}^h \) and the torque \( \mathbf{T}^h \) exerted on the cell:

\[
\mathbf{F}^h(t) = \int \int_{S(t)} \mathbf{\sigma} \cdot \mathbf{n} dS \tag{2.3}
\]

\[
\mathbf{T}^h(t) = \int \int_{S(t)} \mathbf{x} \times (\mathbf{\sigma} \cdot \mathbf{n}) dS. \tag{2.4}
\]

2.1.2. Swimming at low-Reynolds number

Reynolds number \( Re \) measures the importance of inertial force \( \rho \mathbf{u} \cdot \nabla \mathbf{u} \) compared to the viscous force \( \mu \nabla^2 \mathbf{u} \). For a cell of size \( L \) swimming at a characteristic speed of \( U \),

\[
Re = \frac{\rho (\mathbf{u}) \mathbf{u}}{\mu \nabla^2 \mathbf{u}} = \frac{UL}{\nu}, \tag{2.5}
\]

where \( \nu = \frac{\mu}{\rho} \) is the kinematic viscosity. For a typical swimming microorganism, \( Re \ll 1 \). For example, the size of \( E. \ coli \) is \( L \approx 1 - 10 \mu m \) and its swimming speed is about \( U \approx 10 \mu m/s \). If swimming in the water of density \( \rho \approx 10^3 kg/m^3 \) and viscosity \( \mu = 10^{-3} Pa \cdot s \), \( Re \approx 10^{-3} - 10^{-4} \) (Lauga & Powers...
A human sperm and *Paramecium* swim at $Re \approx 10^{-2}$ and $Re \approx 10^{-1}$ respectively. Therefore, it is reasonable to study the locomotion in the limit of zero Reynolds number. Navier-Stokes equations Eq. (3) and (2) are thus simplified to Stokes equations:

\[ \nabla \cdot \mathbf{u} = 0, \]
\[ -\nabla p + \mu \nabla^2 \mathbf{u} = 0. \]  

(2.6)

The swimming microorganism follows the Newton’s law of motion

\[ \frac{dI}{dt} = F^{\text{ext}}(t) + F^h(t), \]  

(2.7)

where $I$ is the momentum of the cell and $I \sim \rho_c L^3 U$ ($\rho_c$ is the density of the cell). $F^h(t)$ indicates the hydrodynamic force and $F^{\text{ext}}(t)$ stands for other external forces. $F^h(t) \sim \mu LU$, as the viscous force dominates the Stokes flow. Therefore, we have

\[ \frac{dI}{dt} / F^h(t) \sim \frac{\rho_c L^3 U}{L/U \mu LU} \sim \frac{\rho_c \rho}{Re}, \]  

(2.8)

showing that in the limit of very low Reynolds number, the momentum variation of cells is negligible. Moreover, $F^{\text{ext}}(t) = 0$ in most cases, thus we have

\[ F^h(t) = 0. \]  

(2.9)

In a similar fashion, $T^h(t) = 0$. Exceptional cases include the swimming of nose-heavy or bottom-heavy cells (Lauga & Powers 2009).

### 2.2. The scallop theorem

Purcell (1977) proved the so-called scallop theorem stating that a microorganism actuating via a reciprocal motion, like a scallop, cannot achieve any net motion in Stokes flow, whereas a scallop in the sea indeed moves by opening its mouth slowly and closing it fast to squirt water out (as this occurs at finite inertia, i.e., $Re > 0$). This peculiar phenomena results from two properties of the Stokes equation. The first one is the rate independence: if a cell body swims by the surface deformation, the distance it travels between two surface configurations does not depend on the rate at which the deformation occurs but only on the instantaneous geometry between the two configurations (Lauga & Powers 2009). The second property is the time-reversibility meaning that the fluid motion is reversible when reversing the driving force. The movement of the scallop shell is a reciprocal motion which remains identical after a reversal of time, hence in creeping flow, the scallop itself will also follow a reciprocal track, swimming forward and backward with a zero net displacement. In order to achieve an effective locomotion, microorganisms have to adopt other strategies, one of them is to use waves to break the time-reversal symmetry.
2.3. Propulsion mechanisms

Here we show two types of wavelike motion used by the microorganisms swimming at very low-Reynolds number. These tiny creatures actuate their lash-like appendages, the so-called flagella or cilia (see figure 2.1) to achieve locomotion. The first type of actuation is normally utilised by cells processing one or several slender flagella with their length comparable to the size of cell, e.g., *E. coli* or *Salmonella typhimurium*. These microorganisms rotate the screw-like flagella to generate helical waves while the sperm of many species whips its flexible flagellum to produce undulatory waves. Cells use such motions to obtain thrust purely from viscous drag and this so called drag-based thrust stems from the drag anisotropy of slender bodies. The second type of motion is used by cells with numerous short cilia covering their surface (right side of figure 2.1 shows one beating cilium). *Paramecium* beats its cilia collectively and each cilium undulates with a phase difference with respect to its neighbouring cilia. The resultant travelling wave along the cell surface is called the metachronal wave. Note that beating cilia in synchronisation is reciprocal and thus produces no net motion. In this thesis, we mainly investigate on the second motion, namely, the ciliary propulsion and we explain the mathematical model below.

2.4. Squirmer model

The squirmer model is a hydrodynamic model for the ciliated microorganisms achieving locomotion with metachronal waves. This model was firstly proposed by Lighthill (1952) and later on analysed by Blake (1971). The idea of the model is to utilize an ‘envelop’ representing the tips of all beating cilia, the dynamics of an individual cilium is thus neglected. The surface velocity is imposed on the envelop as the boundary condition to represent the travelling wave.

To derive the swimming dynamics analytically, the model cell is assumed to be a sphere with axisymmetric surface actuation, although we will extend it to the case of prolate swimmers. Spherical polar coordinates are now used. The metachronal wave is decomposed into an infinite number of modes, with the magnitude $A_n$ and $B_n$ for the $n$th mode of the normal and tangential surface actuation. We define the normal and tangential velocities with $u_r$ and $u_\theta$ in the frame of the squirmer, and express them as below (for detailed derivations we refer to Blake (1971); Lighthill (1952)),

\[ u_r |_{r=a} = \sum_{n=0}^\infty A_n(t)P_n(\cos \theta), \]

\[ u_\theta |_{r=a} = \sum_{n=1}^\infty B_n(t)V_n(\cos \theta), \]

where $a$ is the radius of the spherical cell, $P_n(\cos \theta)$ is the ordinary Legendre polynomial and $V_n = \frac{2}{n(n+1)}P'_n(\cos \theta)\sin \theta$. The swimming speed $U_s$ and power
2.4. SQUIRMER MODEL

Figure 2.1. Two types of bacterial propulsive organelle, a rotating helical flagellum (left) and a beating cilium (right), the cell body is not shown (Kohidai 2011).

The consumption $P_s$ of the squirmer are:

$$U_s = \frac{1}{3}(2B_1 - A_1)$$

$$P_s = 2\pi\mu a \left[ 8A_0^2 + \frac{8}{3}A_1^2 + \frac{8}{3}B_1^2 + \frac{16}{3}A_1B_1 \right] + \sum_{n=2}^{\infty} \left[ \frac{4n^2 + 6n + 8}{(2n + 1)(n + 1)} A_n^2 + \frac{8}{n(n + 1)} B_n^2 \right] + \frac{24}{(n + 1)(2n + 1)} A_nB_n \right]$$

In this thesis, we mainly study swimming by the tangential surface actuation, thus $A_n = 0 \ (n \geq 0)$, $B_n = 0 \ (n > 2)$ as used in many previous investigations.
CHAPTER 3

Basic concepts of deformable capsules

3.1. Models of cell: vesicle and capsule

A red blood cell is a droplet enclosed by an elastic membrane, with a negligible nucleus or other cellular appendages. The membrane is primarily a two dimensional fluid bilayer of phospholipids supported by an inner network of proteins. Simple models like vesicle and capsule have been developed to mimic the behaviours of cells like RBCs. A vesicle is made of a pure bilayer of phospholipid and a capsule of an extensible polymer shell (see figure 3.1).

Helfrich (1973) introduced a geometric model assuming that the energy of the cell membrane mostly appears in the form of bending. It can be formulated as a quadratic functional of the mean curvature $H$. The equilibrium shape of a cell is obtained by minimizing the overall bending energy with two invariants, the area of the membrane and its enclosed volume. The cell membrane can be regarded as a curved two dimensional incompressible fluid. The invariants represented as the two Lagrange multipliers $\lambda_1$ and $\lambda_2$ are imposed in the so called total ”free energy” $F_T$ for minimization,

$$F_T = \frac{\kappa}{2} \int H^2 dA + \lambda_1 \int dA + \lambda_2 \int dV,$$

where $\kappa$ is the bending modulus of the membrane. Note that the bending energy term is independent of the cell size but depends on how far away its shape is from a sphere (Misbah 2012). This is quantified by the so-called reduced volume, or swelling ratio, which is the ratio between the enclosed volume and that of a sphere with the same surface area. It is around 0.65 for human RBCs. The vesicle model has been used successfully to obtain the shape of RBCs at equilibrium and in the prediction of cellular dynamics in the external flow. In addition to its simple fabrication, it becomes a widely used model for the biological cells (Misbah 2012).

Capsule is another model for RBCs, as it accounts for the shear elasticity endowed by the spectrin network of RBCs. The elasticity is also important, having the same magnitude of the bending rigidity (Kaoui et al. 2009). In addition, synthetic cell-inspired carriers are commonly made from polymerized extensible membrane with considerable shear elasticity (Barthès-Biesel 2011), thus the capsule is a better model for them.
3.2. Mathematical and physical description

3.2.1. Fluid motion around cells

Having described the qualitative features of vesicles and capsules, it becomes natural to detail them mathematically. Although the dynamics of cells and their biomimetic counterparts span a broad range of scales in space, we limit our study to the very small scale where the characteristic length is of the order of the cell size. The phenomena typically correspond to the cellular/particulate flow in the microcirculation and micro-fluidic devices, where the viscous effect dominates. Therefore, Stokes equations can be adopted to solve the fluid motion inside/outside the model cells,

\[-\nabla p + \eta \nabla^2 \mathbf{u} = 0, \]
\[\nabla \cdot \mathbf{u} = 0,\]  

It is worth-noting that a RBC actually has both the property of the vesicle and capsule (Barthès-Biesel 2011), conserving the local area invariance (like a vesicle) and possessing the shear elasticity provided by the protein structure (like a capsule).
where \( u \) and \( p \) denote the velocity and pressure field outside. The quantities inside the cell will be indicated by an additional prime, for example, \( \eta' \) for the viscosity of the internal fluid. Boundary conditions have to be satisfied on the membrane:

- Continuity of the velocity field
  \[
  u = u' = u_m, \tag{3.4}
  \]
  where \( u_m \) denotes the velocity of the material points on the membrane. The continuity of the velocity inside and outside the cell is due to mass conservation and no-slip boundary condition on the interface. By assuming impermeable membrane, \( u_m \) attains the same value.

- Continuity of the stress
  \[
  \sigma \cdot n - \sigma' \cdot n + q = 0, \tag{3.5}
  \]
  where \( \sigma = -pI + \eta \left( \nabla u + \nabla u^T \right) \) is the stress tensor and \( n \) the outward unit normal vector. \( q \) denotes the force developed on the material point of the membrane owing to its local deformation.

3.2.2. Cell membrane dynamics

In this section, we describe the force developed on the membrane. As shown in Eq. (3.5), \( q \) represents the force density per unit area, but will be however denoted as the force for brevity. It consists of a bending part \( q_b \) and an elastic part \( q_e \).

3.2.2a. Geometrical setup and mathematical formulations. The membrane is modelled as a shell with zero thickness and curvilinear coordinates system will be used to describe the deformation of a capsule.

The coordinates \( x \) of a point on the surface can be written as a function of the curvilinear coordinates \( (\xi^1, \xi^2) \), such that \( x = x (\xi^1, \xi^2) \) can be expressed by the covariant base vector \((a_1, a_2, a_3)\) defined as:

\[
\begin{align*}
  a_1 &= \frac{\partial x}{\partial \xi^1},
  a_2 &= \frac{\partial x}{\partial \xi^2}, \\
  a_3 &= n = \frac{a_1 \times a_2}{|a_1 \times a_2|}. \tag{3.6}
\end{align*}
\]

The contravariant base vectors are introduced accordingly, \((a^1, a^2, a^3)\) satisfying \( a_\alpha \cdot a^\beta = \delta^\beta_\alpha = \delta^\alpha_\beta = a_\beta \cdot a^\alpha \), \( \delta \) is the Kronecker operator. Note that contravariant components are normally representing quantities ’contra’ vary with the change of base vectors, typically for positions or their time derivatives; covariant components co-vary, and are used for the spatial derivatives of positions. In addition, we introduce the metric tensors as below:

\[
\begin{align*}
  g_{\alpha\beta} = a_\alpha \cdot a_\beta, \quad g^{\alpha\beta} = a^\alpha \cdot a^\beta. \tag{3.7}
\end{align*}
\]
which defines the way of computing the distance between two points in a given space, \((ds)^2 = g_{\alpha\beta} d\xi^\alpha d\xi^\beta = g^{\alpha\beta} d\xi^\alpha d\xi^\beta\). Similarly, all quantities can be defined for the material points in the reference (undeformed) state and capital letters will be used accordingly.

A material point can be identified by its position in the undeformed and deformed state, with their coordinates being \(X(\xi^1, \xi^2)\) and \(x(\xi^1, \xi^2)\). We introduce the gradient of the transformation tensor \(\mathbf{F}^d = \mathbf{F} \cdot d\mathbf{X}\).

As \(d\mathbf{x} = \frac{\partial \mathbf{x}}{\partial \xi^\alpha} d\xi^\alpha = a_\alpha d\xi^\alpha\) and \(d\mathbf{X} = \frac{\partial \mathbf{X}}{\partial \xi^\beta} d\xi^\beta = A_\beta d\xi^\beta\), we obtain \(\mathbf{F} = a_\alpha \otimes A^\alpha\).

\(\mathbf{F}\) includes rigid body rotation and deformation, whereas the right Cauchy-Green dilation tensor \(\mathbf{C} = \mathbf{F}^T \cdot \mathbf{F}\) quantifies the pure local surface deformation. Moreover, the Green-Lagrange strain tensor is \(\mathbf{e} = \frac{1}{2} (\mathbf{C} - \mathbf{I})\), where \(\mathbf{I}\) is the identity tensor. Having defined \(\mathbf{C}\), we introduce its invariants, which are used to express the strain energy function per unit area \(W_S\). The variants \(I_1\) and \(I_2\),

\[ I_1 = A^{\alpha\beta} a_{\alpha\beta} - 2, \quad I_2 = |A^{\alpha\beta}||a_{\alpha\beta}| - 1, \quad (3.9) \]

which can also be determined from the principal dilations \(\lambda_1\) and \(\lambda_2\),

\[ I_1 = \lambda_1^2 + \lambda_2^2 - 2, \quad I_2 = \lambda_1^2 \lambda_2^2 - 1 = J_s^2 - 1. \quad (3.10) \]

The Jacobian, \(J_s = \lambda_1 \lambda_2\), shows the ratio of the deformed to the undeformed surface area.

### 3.2.2b. Shear elastic force

We firstly compute the in-plane Cauchy stress tensor \(\mathbf{T}\), from the strain energy function per unit area of the undeformed membrane, \(W_S(I_1, I_2)\),

\[ \mathbf{T} = \frac{1}{J_s} \mathbf{F} \cdot \frac{\partial W_S}{\partial \mathbf{e}} \cdot \mathbf{F}^T. \quad (3.11) \]

which can be further expressed by components as:

\[ T^{\alpha\beta} = \frac{2}{J_s} \frac{\partial W_S}{\partial I_1} A^{\alpha\beta} + 2 J_s \frac{\partial W_S}{\partial I_2} d^{\alpha\beta}. \quad (3.12) \]

We employ a widely-used model for \(W_S\) in our study, the Neo-Hookean law (NH) (Green & Adkins 1970) formulated as

\[ W_S = \frac{G_s}{2} \left( I_1 - 1 + \frac{1}{I_2 + 1} \right), \quad (3.13) \]

where \(G_s\) is the shear modulus. Local equilibrium connects \(\mathbf{T}\) with the external membrane load \(\mathbf{q}_e\), as

\[ \nabla_s \cdot \mathbf{T} + \mathbf{q}_e = 0, \quad (3.14) \]

where \(\nabla_s\) is the surface divergence operator in the deformed state. In curvilinear coordinates, the load vector is written as \(\mathbf{q}_e = q_e^\alpha a_\alpha + q_e^\alpha \mathbf{n}\). The local
balance in Eq. (17) is further decomposed into tangential and normal components,

\[
\frac{\partial T^{\alpha \beta}}{\partial \xi^\alpha} + \Gamma^\alpha_{\alpha \lambda} T^{\lambda \beta} + \Gamma^\beta_{\alpha \lambda} T^{\alpha \lambda} + q^\beta_e = 0, \quad \beta = 1, 2,
\]

\[
T^{\alpha \beta} b_{\alpha \beta} + q^n_e = 0,
\]

(3.15)

where \(\Gamma^\alpha_{\alpha \lambda}\) are the Christoffel symbols.

3.2.2c. Bending force. For a vesicle, only the bending force develops on the membrane. In contrast, bending is mostly not considered for capsules, which will affect the robustness of numerical simulations (see section 4.3.3a for the discussion). We take bending into account in our computation, following the work of Zhao et al. (2010). A linear isotropic model is used for moment \(M\),

\[
M^\alpha_{\beta} = -G_B (b^\alpha_{\beta} - B^\alpha_{\beta}),
\]

(3.16)

here \(G_B\) is the bending modulus, \(b^\alpha_{\beta} = a_{\alpha, \beta} \cdot n\) the second fundamental form of the surface of the deformed surface, and \(B^\alpha_{\beta}\) is corresponding quantity of the undeformed surface.

Torque balance is satisfied as

\[
M^\alpha_{[\beta} - q^\beta_{\alpha} = 0,
\]

(3.17)

\[
e^\alpha_{\beta} \left( T_{\alpha \beta} - b^\alpha_{\gamma} M^{\gamma \beta} \right) = 0,
\]

(3.18)

where \(\mid_\alpha\) is the covariant derivative. As \(b^\alpha_{\gamma} M^{\gamma \beta}\) is symmetric about \(\alpha\) and \(\gamma\), the antisymmetric part of the in-plane Cauchy stress tensor \(T\) is always zero (Zhao et al. 2010).
CHAPTER 4

Numerical methods

In this section, we briefly describe the numerical methods utilised in this thesis:

I ) Finite element method (FEM) to study the self-propulsion of microorganisms in the polymeric fluids, as well as the microrheology;
II ) Boundary element method (BEM) for simulating swimming cells in highly confined geometries;
III ) A hybrid integral mesh-based method (or a boundary integral method accelerated by the general geometry Ewald method proposed by Hernández-Ortiz et al. (2007)) for deformable model cells in micro-fluidic flows with arbitrary geometries. The membrane dynamics of model cells is solved by a spectral method based on spherical harmonics (Zhao et al. 2010).

The author is proud to comment that he built the BEM code (II) and the accelerated boundary integral code (III) from scratch during his PhD study. Code (II) is written in the framework of the parallel computational toolkit PETSC (Balay et al. 2013a,b) and Code (III) is built on top of the highly parallel and scalable general Navier-Stokes solver NEK5000 (Fischer et al. 2008). This uses spectral element method, as our algorithm needs a Stokes flow solution based on a mesh-based solver (see paper 4 or Hernández-Ortiz et al. (2007) for details).

4.1. Simulation of viscoelastic fluids with finite element method

4.1.1. Governing equations

For the steady incompressible inertialess flow of a viscoelastic fluid, the nondimensional momentum and continuity equation are written as

\[- \nabla p + \nabla \cdot \tau = 0, \quad (4.1)\]
\[\nabla \cdot u = 0, \quad (4.2)\]

where the velocity is scaled by the characteristic velocity $U$, length by the characteristic length $L$, time by $L/U$, pressure and stresses by $\mu U/D$, $\mu$ is the dynamic viscosity.
We follow the classical approaches (Bird 1976; Bird et al. 1987a, b) to split the deviatoric stress $\tau$ into two components, the viscous solvent stress ($\tau^s$) and polymeric stress ($\tau^p$),

$$\tau = \tau^s + \tau^p.$$ (4.3)

The solvent stress $\tau^s$ is governed by Newton’s law of viscosity, thus is formulated as

$$\tau^s = \beta (\nabla u + \nabla u^T),$$ (4.4)

where $\beta < 1$ represents the ratio of the solvent viscosity, $\mu_s$, to the total zero shear rate viscosity, $\mu$, of the solution. To close the model, a constitutive equation for the polymeric stress $\tau^p$ is necessary. Here we adopt the nonlinear Giesekus model (Giesekus 1982), which, in addition to displaying shear-thinning properties (viscosity and normal stress differences), provides two important features, namely the saturation of polymer elongation, and a non-negative entropy production during the time evolution of the polymers (see details in Beris & Edwards (1990); Dupret & Marchal (1986); Souvaliotis & Beris (1992)). Violation of these two properties may cause non-physical flow behaviours and numerical difficulties. The nondimensional constitutive equation for this model can be written as

$$\tau^p + We \tau^p + \frac{We \alpha_m}{1 - \beta} (\tau^p \cdot \tau^p) = (1 - \beta) (\nabla u + \nabla u^T),$$ (4.5)

where $\tilde{\nabla} A$ is the upper-convected time derivative, indicating the rate of a tensorial property $A$ of a fluid particle written in the coordinate system rotating and stretching with the fluid. $\tilde{\nabla}$ is defined as

$$\tilde{\nabla} A = \frac{\partial A}{\partial t} + u \cdot \nabla A - \nabla u^T \cdot A - A \cdot \nabla u.$$ (4.6)

In Eq. (4.5), $We$ denotes the Weissenberg number, defined as $We = \lambda U/L$. Here $\lambda$ is the relaxation time of viscoelastic fluid, indicating how long the internal molecules of fluid can sustain stress (Morrison 2001). $\lambda$ is equal to zero for a Newtonian fluid which deforms (and flows) subjected to stress but immediately stops deformation as the stress is removed. The coefficient $\alpha_m$ in the nonlinear term of Eq. (4.5) is called the mobility factor, representing an anisotropic hydrodynamic drag on the polymer molecules (Bird et al. 1987a) and thus limiting the extensional viscosity of the fluid. From thermodynamics considerations, $\alpha_m$ must vary in the range $[0, 0.5]$ (Bird et al. 1987a; Larson 1988). In this thesis we assume $\alpha_m = 0.2$.

4.1.2. Numerical challenges and solutions

Numerical instability has been a serious issue in computational rheology, as simulations fail when the nondimensional relaxation time $We$ becomes large
enough (Baaijens 1998; Walters & Webster 2003). The so-called high Weis-
sehenberg number problem (HWNP) appears in several cases (Walters & Webster 
2003): flow in a geometry with abrupt changes results in ‘corner singularities’; 
thin ‘stress boundary layer’ develops in the flow; a seemingly two-dimensional 
steady problem needs to be solved as a three dimensional and unsteady one. 
From the mathematical point of view, numerical instability arises from the de-
creased elliptic property of the momentum equations (Rajagopalan et al. 1990), 
as shown in the so-called ‘viscous formulation’ 

$$\beta \nabla^2 \mathbf{u} - \nabla p + \nabla \cdot \mathbf{\tau}_p = 0.$$  (4.7) 
The elliptic nature of the equation (weighted by $\beta$ in Eq. (4.7)) is important for 
numerical stability when applying the mixed finite element methods to solve 
the elliptic saddle point problem (Sun et al. 1999). Either a small solvent 
viscosity ($\beta$) or large polymer stress triggers the instability. For a better nu-
merical performance, reformulation of the momentum equation to ensure the 
ellipticity is thus proposed, yielding two successful schemes: Explicitly Elliptic 
Momentum Equation (EEME) and Elastic Viscous Split Stress (EVSS) (and 
its variation EVSS-G). We introduce EVSS here; it is derived by splitting $\mathbf{\tau}$ 
into a viscous part $\mathbf{\tau}_v$ and an elastic one $\mathbf{\tau}_e$ 

$$\mathbf{\tau} = \mathbf{\tau}_v + \mathbf{\tau}_e,$$  (4.8) 
where 

$$\mathbf{\tau}_v = \mu_a \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right)$$  (4.9) 
is a general viscous stress with viscosity $\mu_a$. The elastic stress $\mathbf{\tau}_e$ is defined 
from Eq. (4.3) and Eq. (4.8) as 

$$\mathbf{\tau}_e = \mathbf{\tau}_p + \mathbf{\sigma} - \mathbf{\tau}_v.$$  (4.10) 
Thus the momentum equations is rewritten as 

$$\nabla \cdot \left( \mu_a \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right) - \nabla p + \nabla \cdot \mathbf{\tau}_e = 0.$$  (4.11) 
A proper value of $\mu_a$ chosen to be 1 by the original version (Rajagopalan et al. 
1990) in Eq. (4.11) will certainly ensure the elliptic property of the momentum 
equation. However, the EEME and EVSS methods introduce terms into 
the constitutive equation that contain second-order spatial derivatives of the 
velocity, thus increasing complexity. The Discrete Elastic Viscous Split Stress 
(DEVSS) was proposed by Guénette & Fortin (1995) as a remedy by adding an 
additional elliptic term into the momentum equation and $\mathbf{\tau}_e$ is not required. 
The more generalized version proposed by Liu et al. (1998), DEVSS-G, in-
troduces an additional $\mathbf{G}^h$ as the finite element approximation of the velocity 
gradient $\nabla \mathbf{u}$ and $\mathbf{G}^h$ replaces $\nabla \mathbf{u}$ in the constitutive equation Eq. (4.5). 
Assume the approximate variables to be $(\mathbf{u}^h, p^h, \mathbf{\tau}_p^h, \mathbf{G}^h)$, we write the viscous 
formulation of Eq. (4.7) in a discretized form 

$$\beta \nabla \cdot \left( \mathbf{G}^h + (\mathbf{G}^h)^T \right) - \nabla p^h + \nabla \cdot \mathbf{\tau}_p^h = 0.$$  (4.12)
By adding the term
\[ \nabla \cdot \mu_a \left( \nabla u^h + \nabla (u^h)^T \right) - \nabla \cdot \mu_a \left( G^h + (G^h)^T \right) \] (4.13)
to the left side of Eq. (4.12), we get the DEVSS-G version of the momentum equation
\[ \nabla \cdot \mu_a \left( \nabla u^h + \nabla (u^h)^T \right) - \nabla p^h + \nabla \tau^h - \nabla \cdot (\mu_a - \beta) \left( G^h + (G^h)^T \right) = 0. \] (4.14)
As the grid size approaches zero, the added term cancels out and Eq. (4.14) recovers to the viscous formulation. In our paper 1, the viscous formulation is used while in paper 2 and 6, DEVSS-G is used.

The constitutive equation Eq. (4.5) is a hyperbolic equation and the convective term also tends to cause numerical instability. To improve the numerical stability, we adopt the most widespread method (Baaijens 1998), Streamline Upwind Petrov Galerkin (SUPG). The weak form of Eq. (4.5) is thus written as
\[ \left\{ S + \frac{\mu}{U_C} \mathbf{u} \cdot \nabla S, \, \tau^p + \nabla \left( \mu (\nabla \mathbf{u} - \mathbf{u} \cdot \nabla) \mathbf{G}^h + (\mathbf{G}^h)^T \right) \mathbf{G} + \frac{\mu_0}{1-\beta} (\tau^p \cdot \tau^p) \right\} = 0, \] (4.15)
where \( S \) denotes the test function of \( \tau^p \), \( h \) is the characteristic length-scale of the element and \( U_C \) is the magnitude of the local characteristic velocity. In our case, we choose the norm of \( \mathbf{u} \) as \( U_C \).

4.2. Boundary element method

4.2.1. Governing equations

The boundary element method (BEM) has been successfully adopted to study the hydrodynamics of bacterial locomotion in the Stokesian regime (Ishikawa et al. 2006; Ramia et al. 1993; Shum et al. 2010). Our current work mainly follows the approach in Pozrikidis (2002), the important difference being that we use quadrilateral elements instead of triangle elements as typically used and originally proposed. The method is introduced briefly here. In the Stokesian realm, the flow is governed by the Stokes equation
\[ -\nabla p + \mu \nabla^2 \mathbf{u} = 0. \] (4.16)
Due to the linearity of the Stokes equation, the velocity field \( \mathbf{u}(\mathbf{x}) \) resulting from moving objects with smooth boundary \( S \) can be expressed as
\[ \mathbf{u}(\mathbf{x}) = \frac{1}{8\pi \mu} \int_S \mathbf{f}(\mathbf{x}') \cdot \mathbf{S}(\mathbf{x}, \mathbf{x}') \, dS_{\mathbf{x}'} \] (4.17)
where \( f(x') \) is the unknown force per unit area exerted by the object onto the fluid. \( S \) is the Stokeslet Green function

\[
S_{ij}(x, x') = \left( \frac{\delta_{ij}}{d} + \frac{d_i d_j}{d^3} \right),
\]

(4.18)

with \( d_i = x_i - x_i' \), \( d^2 = |x - x'|^2 = d_1^2 + d_2^2 + d_3^2 \), and \( \delta_{ij} \) denotes Kronecker delta tensor.

### 4.2.2. Discretization

We discretize the objects, the spherical squirmer and surrounding tube, into \( N \) zero-order elements with the centre locations \( \{x_q : q = 1, ..., N \} \) (\( x_q \) \( \in \) Squirmer : \( q = 1, ..., N_S \) and \( x_s \) \( \in \) Tube : \( q = N_S + 1, ..., N \). \( N_S \) is the number of elements on the squirmer). For the \( r \)th element, \( f(x') \) is assumed to be constant over the element and is thus approximated by the value \( f_r \). As a consequence, the discretized version of Eq. (4.17) is

\[
\mathbf{u}(x_q) = \frac{1}{8\pi\mu} \sum_{r=1}^{N} f_r \int_{S_r} S(x_q, x') dS_{x'} \quad \{q = 1, ..., N\}.
\]

(4.19)

To calculate the hydrodynamic force on a sphere with prescribed motions inside the tube, the left hand side of Eq. (6) is determined by our boundary condition. Thus we have \( 3N \) equations for \( 3N \) unknown force density components. Conversely, to solve for the instantaneous motion of the squirmer with surface deformation \( \mathbf{u}_S \), we need to introduce six more unknowns, namely its translational velocity \( \mathbf{U} \) and rotational velocity \( \Omega \). Thus, the left hand side of Eq. (6) becomes \( \mathbf{U} + \Omega \times \ddot{x}_q + \mathbf{u}_S(x_q) \) for \( q \) from 1 to \( N_S \) (here \( \ddot{x}_q = x - x^R \), where \( x^R \) is an arbitrary reference point, the centre of the spherical squirmer for convenience). By assuming zero external force and torque on the squirmer, we have the six additional equations necessary to close our linear system

\[
\int f(x) dS_x = 0 \quad x \in \text{Squirmer},
\]

\[
\int \ddot{x} \times f(x) dS_x = 0 \quad x \in \text{Squirmer}.
\]

(4.20)

### 4.3. Computational frameworks for deformable particles in flow

Flow of deformable particles is a typical fluid-structure problem, and different numerical techniques have been developed and used for a variety of problems (Hou et al. 2012; Mittal & Iaccarino 2005). Commonly, a computational framework to address them needs a flow solver to address the fluid-structure interactions (FSI), incorporating another solver for the structural dynamics of stiff and deformable particles, e.g., cells bounded by a soft membrane. A bunch
of methods are available for each solver, and in most cases, methods of different solvers can be conveniently integrated. Hence, we will introduce the two groups of methods separately.

4.3.1. A review of flow solvers

In the context of FSI simulations, opt-used flow solvers are categorized into three groups, depending on the discretization of the fluid: mesh-based solvers that mesh the whole fluid domain, including finite difference method (FDM), finite volume (FVM), finite element method (FEM) among others; mesh-free solvers that only discretize the surface of the immersed objects, like the boundary integral method (BIM); and stochastic particle-based methods which describe the motion of fluid by a large number of Lagrangian particles.

4.3.1a. Conformal mesh-based solver. The conformal mesh-based solver prescribes the exact physical boundary conditions on the fluid-solid interface and the mesh for the fluid and/or solid has to conform to the interface. Several techniques have been developed, and we only mention of them, namely the Arbitrary Lagrangian Eulerian (ALE) method (Donea et al. 1982; Hu et al. 2001) for brevity. The ALE method is commonly built on FEM, and uses the combined formulation of fluid and particle momentum equations with a moving unstructured mesh to account for the moving particles. ALE solves the fluid and membrane dynamics simultaneously, showing better numerical stability and accuracy than most other approaches that weakly couple the motion of fluid and solid. A typical work of using this technique for deformable model cells is that of Gao & Hu (2009). A similar method has also been implemented in the commercial FEM-based package FlexPDE which successfully simulated one and several two-dimensional RBCs in a channel flow (Secomb 2003), as well as flows with Y-shape and T-shape bifurcations (Barber et al. 2008). They provided results in qualitative agreement with the experimental observations. However, ALE with FEM requires frequent mesh generation and data-transferring between two successive meshes, imposing a non-trivial challenge to the robustness, simplicity and cost of a numerical implementation, especially for three-dimensional cases; hence it has only been opted by a limited number of research groups simulating deformable particles.

4.3.1b. Non conformal mesh-based solver. An alternative is the non conformal mesh-based solver which normally use a simple stationary Cartesian grid to solve the flow, whereas another set of mesh (Lagrangian grid points) discretizing the boundary of immersed objects cuts through the Cartesian grid. Imposing the boundary condition of immersed objects requires modifying the fluid equations near the boundaries (Mittal & Iaccarino 2005). In most cases, this technique can be readily embedded into an existing solver based on most
methods like FDD, FVM, FEM and so forth, thus is capable of taking advantage of the existing codes with few modifications. Owing to its simplicity and flexibility, the non conformal mesh-based approach has attracted a great amount of attention and has been used for many problems like particulate/bubbly flow, turbulence, swimming or flying animals and so on. For the deformable cells, the mostly used approach is the immersed boundary method (IBM) and its variations like the front tracking method (FTM). These methods have shown versatility in simulating cellular flows (Bagchi & Kalluri 2010; Doddi & Bagchi 2008; Huang et al. 2012). On the other hand, Lattice Boltzmann method (LBM) is also characterised by non conformal meshes for the FSI problems. Three-dimensional suspensions of RBCs (Ding & Aidun 2006) and deformable particles (Dupin et al. 2007) were simulated by LBM, which captured the key features of blood rheology (Freund 2014). Although IBM and LBM have achieved success for the cellular flow computation, several limitations do exist. For low Reynolds number flow typically in the microcirculation, both methods suffer from the temporal discretization. IBM usually utilises fractional-step methods which introduce significant errors into the momentum equations when \( Re \to 0; \) LBM loses efficiency as its computational time per time step scales with \( 1/Re. \) In addition, IBM smears the interfacial force and hence considerably spoils the numerical accuracy, particularly in resolving the strong cell-cell or cell-wall interactions. The accuracy of LBM based on the simple bounce-back algorithm degrades to first order near the interface. This can be improved by using complex boundary kinematics, which will however break the locality of LBM computations and their efficiency. A further challenge arises in the case of micro-fluidic devices that commonly have non-trivial and confined geometries. Although both methods are able to account for complex geometries by imposing proper boundary conditions, the scheme becomes inaccurate as the wall is very close to the cell surface that is represented also by a blurred interface. Hence, the boundaries of cell and wall interfere with each other, apparently deteriorating the estimation of the lubrication force playing an important role in the cellular dynamics.

4.3.1c. **Boundary integral method.** For flows in the microcirculation and micro-fluidic devices, the characteristic length is so small that the viscous effect dominates the inertia effect leading to a very small Reynolds number. When completely removing the inertia term from the momentum equations, we need to solve the Stokes equation. Due to its linearity, a very powerful numerical tool to for this problem is the boundary integral method (BIM) introduced by Youn- green & Acrivos (1975), which has been used successfully to simulate a great number of low-Reynolds-number problems (Pozrikidis 1992).

Here, we consider a fluid-filled cell enclosed by a infinitely-thin membrane \( S_m \), the fluid inside and outside the cell has a dynamic viscosity of \( \lambda \mu \) and \( \mu \). Given the force per unit area \( \Delta f(x_m) \) exerted by the fluid on the membrane
at \( \mathbf{x} = \mathbf{x}_m \), the flow field can be computed by solving the following equations:

\[
- \nabla p (\mathbf{x}) + \mu \nabla^2 \mathbf{u}(\mathbf{x}) = \int_{S_m} \Delta \mathbf{f}(\mathbf{x}_m) \delta(\mathbf{x} - \mathbf{x}_m) dS(\mathbf{x}_m),
\]

\[
\nabla \cdot \mathbf{u}(\mathbf{x}) = 0,
\]

where \( \delta(\cdot) \) is the Dirac delta function. Note that \( \Delta \mathbf{f} = (\mathbf{\sigma} - \mathbf{\sigma}') \cdot \mathbf{n} = -\mathbf{q} \) (see Eq. (3.5)) and its calculation will be discussed in Sec. 4.3.2. By exploiting the linearity of Eq. (2), the velocity of a material point on the membrane \( \mathbf{x} \) can be derived analytically as (Pozrikidis 1992):

\[
u_j (\mathbf{x}_m) = \frac{2}{1 + \lambda} \frac{1}{\mu} \frac{1}{2 \pi} \int_{S_m} \Delta f_i (\mathbf{y}) G_{ij}(\mathbf{y}, \mathbf{x}_m) dS(\mathbf{y}) + \frac{1 - \lambda}{1 + \lambda} \int_{S_m} u_i(\mathbf{y}) T_{ijk}(\mathbf{y}, \mathbf{x}_m)n_k(\mathbf{y}) dS(\mathbf{y}),
\]

where \( PV \) denotes the principal value of the double-layer potential, defined as the improper double-layer integral as the point \( \mathbf{y} \) is exactly located on \( S_m \). \( G(\cdot, \cdot) \) is the Green’s function, also called the Stokeslet, or the Oseen-Burgers tensor and \( T(\cdot, \cdot) \) is the stress tensor. For \( \mathbf{r} = \mathbf{y} - \mathbf{x} \) with a norm \( r = |\mathbf{r}| \), we have

\[
G_{ij}(\mathbf{y}, \mathbf{x}) = \frac{\delta_{ij}}{r} + \frac{r_ir_j}{r^3},
\]

\[
T_{ijk}(\mathbf{y}, \mathbf{x}) = -6 \frac{r_ir_jr_k}{r^5},
\]

here \( u_i = \frac{1}{8 \pi \mu} G_{ij} g_j \) and \( \sigma_{ij} = \frac{1}{8 \pi} T_{ijk} g_k \) respectively corresponds to the velocity field \( \mathbf{u}(\mathbf{x}) \) and stress field \( \mathbf{\sigma}(\mathbf{x}) \) of the Stokes flow driven by a point singular force \( \mathbf{g}(\mathbf{y}) \delta(\mathbf{x} - \mathbf{y}) \), respectively.

The simplicity of BIM stems from the reduction of the order of the problem by one, as shown by Eq. (4.22); only surfaces of the immersed objects are discretized, without meshing the fluid domain. This offers a special benefit for the accurate simulation of cellular flows: inter-cellular and cell-wall lubrication forces will be well resolved by increasing the surface mesh resolution, that is rather cumbersome and/or expensive for mesh-based methods. The second advantage of BIM is that the velocity of the cell surface comes directly with the solution, devoid of the interpolations errors that are common in the mesh-based methods. Nonetheless, the linearity is a double-sided sword. The velocity of one point has to take into account of all singular forces, due to the intrinsic long-range interactions of the Stokesian nature. For a system of \( N_p \) point forces, the number of operations scales with between \( O(N_p^2) \) (using an iterative solver whose iteration number is independent of \( N_p \)) and \( O(N_p^3) \) (using a direct solver) (Kumar & Graham 2012). This is the major difficulty of using BIM in many-body systems like suspensions. Acceleration techniques for BIM thus have been developed to turn the scaling down to the ideal \( O(N_p) \), based either on the particle-particle-particle-mesh method (PPPM) (Deserno & Holm 1998).
4.3. COMPUTATIONAL FRAMEWORKS FOR DEFORMABLE PARTICLES IN FLOW

(with its variants like particle mesh Ewald method (Darden et al. 1993) and the smoothed particle mesh Ewald method (Essmann et al. 1995)), or the fast multiple method (Greengard & Rokhlin 1987). The accelerated BIM enables the simulation of suspensions of different particles, including droplets (Zinchenko & Davis 2000), RBCs (Zhao et al. 2010), vesicles (Veerapaneni et al. 2011) and so forth.

It is noteworthy that BIM and its accelerated versions provide accurate simulations for low-Reynolds-number flow, however, strictly limited to configurations without inertia. To simulate multiphase flows with a finite inertia, one has to resort to the mesh-based methods or particle-based methods.

4.3.1d. Stochastic particle method. All the methods mentioned above solve the fluid motion based on continuous formations, another option is to discretize the fluid by a collection of stochastic mesoscopic particles. Each particle representing a number of molecules moves like a Lagrangian point and soft repulsive-only potential is activated between particles to coordinate their motion. This approach is also regarded as a coarse-grained molecular dynamics. Two variants, namely, the dissipative particle dynamics (DPD) method (Fedosov et al. 2010; Lei et al. 2013) and multiparticle collision dynamics (Noguchi & Gompper 2005) have been implemented to model the flow suspensions of cells. The main advantage of these particle-based methods is that the membrane viscosity and thermal fluctuation are intrinsically accounted for, which is not straightforward for most other methods.

4.3.2. Structural solver for the cell membrane

In this section, we present how to calculate the force $q$ developed on the membrane as introduced in Sec. 3.2.2. For one time step, $q$ is computed given the instantaneous shape of the cell. This procedure is in contrast to the traditional FEM-based approaches calculating nodal displacements with a known force distribution. Here, the displacements are derived following the fluid motion.

A number of strategies have been employed. The membrane loading was calculated as linear piece-wise functions on triangle meshes by Li & Sarkar (2008); Ramamurthy & Pozrikidis (1998). Numerous implementations have been developed based on the FEM (Charrier et al. 1989; Huang et al. 2012; Pranay et al. 2010; Walter et al. 2010) for its generality and versatility. Bi-cubic B-splines interpolation functions were adopted by Lac et al. (2007), producing very accurate results at a reasonable computational cost. Alternatively, a spectral boundary element algorithm was used by Dodson & Dimitrakopoulos (2008), thus coupling the numerical accuracy of the spectral method and the geometric flexibility of boundary element method. However, due to the discontinuity of geometric derivatives at the element boundaries, this method necessitates proper interfacial smoothing to avoid the numerical instability.
Global spectral method is devoid of this drawback, meanwhile attaining spectral accuracy, and it has therefore been suggested as a promising tool. Fourier spectral interpolation and spherical harmonics were used for 2D (Freund 2007) and 3D simulations (Kessler et al. 2008; Zhao et al. 2010) respectively.

4.3.3. Numerical framework of the current work

In the current work, we employ a boundary integral method accelerated by the general geometry Ewald method (GGEM) proposed by Hernández-Ortiz et al. (2007); Kumar & Graham (2012). GGEM is similar to PPPM, however, the Fourier-space part of PPPM is substituted by a general mesh-based Stokes flow solver in GGEM. Hence, compared to PPPM and other accelerating techniques, GGEM is characterised by its unique capacity to handle arbitrarily confined geometries, that are essential in micro-fluidic devices. GGEM decomposes the Stokes solution into two parts, one standing for the short-ranged interactions computed by traditional boundary integral techniques; and another for the long-ranged interactions solved by a mesh-based Stokes solver. In our implementation, we take the Stokes sub-solver of an open source code NEK5000 as the mesh-based solver. NEK5000 is a highly parallel and scalable general Navier-Stokes solver based on spectral element method, hence it contributes a double insurance of the generality and accuracy to our framework.

We use a global spectral method based on the spherical harmonics proposed by Zhao et al. (2010) to interpretate the surface of a deformable model cell and to solve its membrane dynamics. We emphasize its advantages here. Firstly, all grid points are used to fully capture the cell shape, hence the spatial derivatives are computed with high-fidelity. This special globality compared with the locality of other finite/spectral element approaches facilitates a superior accuracy for short-length-scale features (Freund 2014). Furthermore, the calculation of derivatives is straightforward, even for high order derivatives. Thus, we can easily take the bending moments into account, that is not trivial for other methods (like FEM) although important to maintain the numerical stability (see section 4.3.3a). Secondly, non-linearity arises from the differential geometry calculations (products, roots and inverse operations) on the membrane as well as from the complex constitutive law. So, the aliasing becomes another source of errors in addition to the truncation errors. This error spoils the numerical accuracy and stability. Luckily, the current spectral method offers a natural dealiasing procedure owing to its exact interpolation to a finer grid. As akin to the common treatment in direct numerical simulations of incompressible turbulence, filtering the aliased energy is expedite.

The detailed description of our implementation is described in paper 4.

4.3.3a. Calculation of the bending moments. As we have mentioned in section 3.2.2, the bending moments have been neglected often in the simulations of capsule dynamics. Neglecting the bending in capsule notably makes the
computation of the membrane dynamics less complex. Results in qualitative agreement with experiments have been obtained for a capsule being only stretched (Barthès-Biesel et al. 2010). The drawback arises with the compressive tensions on the membrane triggering the appearance of wrinkles on the surface; the physical buckling will deteriorate the numerical accuracy, causing numerical instabilities. Therefore, simulations of capsules without bending rigidity is limited to simple or weak flows. A remedy is pre-stressing the membrane (Hu et al. 2011; Lac et al. 2007) which introduces a new ad-hoc parameter. Alternatively, using a low-order finite element method with an artificial numerical bending stiffness alleviates the suffer to some extent (Pozrikidis 2010; Walter et al. 2010), although one loses full control of the results and unphysical effects can appear. For the strongly-confined cellular flow bending becomes so important for the robustness of physical model, hence has to be considered. This is clearly exemplified by the high-fidelity simulations of densely-packed RBCs recently appeared (Freund 2013; Freund & Orescanin 2011; Zhao et al. 2010). In our work, we employ the capsule model with bending stiffness closely following Zhao et al. (2010).
CHAPTER 5

Summary of papers

Paper 1
(Zhu et al. 2011)
Locomotion by tangential deformation in a polymeric fluid
In several biologically relevant situations, cell locomotion occurs in polymeric fluids with Weissenberg number larger than one. Here we present results of three-dimensional numerical simulations for the steady locomotion of a self-propelled body in a model polymeric (Giesekus) fluid at low Reynolds number. Locomotion is driven by steady tangential deformation at the surface of the body (so-called squirming motion). In the case of a spherical squirmer, we show that the swimming velocity is systematically less than that in a Newtonian fluid, with a minimum occurring for Weissenberg numbers of order one. The rate of work done by the swimmer always goes up compared to that occurring in the Newtonian solvent alone, but is always lower than the power necessary to swim in a Newtonian fluid with the same viscosity. The swimming efficiency, defined as the ratio between the rate of work necessary to pull the body at the swimming speed in the same fluid and the rate of work done by swimming, is found to always be increased in a polymeric fluid. Further analysis reveals that polymeric stresses break the Newtonian front-back symmetry in the flow profile around the body. In particular, a strong negative elastic wake is present behind the swimmer, which correlates with strong polymer stretching, and its intensity increases with Weissenberg number and viscosity contrasts. The velocity induced by the squirmer is found to decay in space faster than in a Newtonian flow, with a strong dependence on the polymer relaxation time and viscosity. Our computational results are also extended to prolate spheroidal swimmers and smaller polymer stretching are obtained for slender shapes compared to bluff swimmers. The swimmer with an aspect ratio of two is found to be the most hydrodynamically efficient.

Paper 2
(Zhu et al. 2012)
Self-propulsion in viscoelastic fluids: pushers vs. pullers
We use numerical simulations to address locomotion at zero Reynolds number in viscoelastic (Giesekus) fluids. The swimmers are assumed to be spherical,
Newtonian $\omega = 7$, $\beta = 0.1$

Figure 5.1. Flow streamlines and map of velocity magnitudes. Comparison between the Newtonian case (left) and polymeric case with $We = 7$ and $\beta = 0.1$ (right).

to self-propel using tangential surface deformation, and the computations are implemented using a finite element method. The emphasis of the study is on the change of the swimming kinematics, energetics, and flow disturbance from Newtonian to viscoelastic, and on the distinction between pusher and puller swimmers. In all cases, the viscoelastic swimming speed is below the Newtonian one, with a minimum obtained for intermediate values of the Weissenberg number, $We$. An analysis of the flow field places the origin of this swimming degradation in non-Newtonian elongational stresses. The power required for swimming is also systematically below the Newtonian power, and always a decreasing function of $We$. A detail energetic balance of the swimming problem points at the polymeric part of the stress as the primary $We$-decreasing energetic contribution, while the contributions of the work done by the swimmer from the solvent remain essentially $We$-independent. In addition, we observe negative values of the polymeric power density in some flow regions, indicating positive elastic work by the polymers on the fluid. The hydrodynamic efficiency, defined as the ratio of the useful to total rate of work, is always above the Newtonian case, with a maximum relative value obtained at intermediate Weissenberg numbers. Finally, the presence of polymeric stresses leads to an increase of the rate of decay of the flow velocity in the fluid, and a decrease of the magnitude of the stresslet governing the magnitude of the effective bulk stress in the fluid.

Paper 3
(Zhu et al. 2013)
Low-Reynolds number swimming in a capillary tube
We use the boundary element method to study the low-Reynolds number locomotion of a spherical model microorganism in a circular tube. The model
5. SUMMARY OF PAPERS

Figure 5.2. Vector plot of flow fields generated by pusher and puller squirmers in a Newtonian fluid. Left: co-moving frame. Right: laboratory frame. On each panel, the data for the pusher are displayed on the left, and those for the puller on the right. The large arrow (blue online) indicates the swimming direction and the background colour scheme indicates the velocity magnitudes.

cell propels itself by tangential and/or normal wavelike surface deformation in a tube whose radius is few times the cell size. It is found that confinement due to the capillary tube and the cell position significantly affect the average swimming speed and power consumption. Swimming speed of locomotion induced by tangential deformation decreases due to enhanced drag while it increases in the case of squirming with normal deformation when the fluid flow is directed against the surrounding walls. We show that the neutral squirmer follows helical trajectories inside the tube, in qualitative agreement with experimental observations and this can be solely explained by hydrodynamic interactions. Puller attains a stable motion inside the tube either on the axis or at a fixed distance depending on the magnitude of the actuation. Pusher and squirmer using normal deformation, instead, eventually descend onto the wall. The dynamic motion of a neutral and puller squirmer are therefore marginally and passively asymptotical stable, while other types of squirming are found to be unstable. Finally, we investigate squirming inside a torus-like bent tube and find that the main features of locomotion are as reported for the straight tube.
Figure 5.3. 3D helical trajectory executed by a neutral squirmer swimming in the tube.

Paper 4

The motion of a deforming capsule through a corner

A three-dimensional deformable capsule convected through a channel/duct with a corner is studied via numerical simulations using an accelerated boundary integral method adapted to general geometries. A global spectral method is adopted to resolve the dynamics of the capsule’s membrane developing elastic tensions and bending moments according to the Neo-Hookean constitutive law, while the flow obeys the Stokes equations. The simulations show that the trajectory of the capsule follows the underlying flow streamline with little deviation and the deformation of the capsule induces an anti-clockwise rotation of its material points with respect to the travelling direction. The surface area, principle tension and elastic energy of the capsule increase around the corner. Their temporal evolutions are characterised by a clear phase delay and the loss of the time-reversal symmetry of Stokes flow due to the elasticity of membrane. The capsule centroid velocity decreases near the corner as the mean flow does while a velocity overshoot is observed past the corner as a result of the interplay between the membrane elasticity and surrounding viscous flow. We show that the shear and bending moduli have a similar influence on the capsule behaviour where higher bending modulus inhibits the appearance of concavity during the deformation. Moreover, we examine how the wall confinement changes the dynamics: higher confinement generates higher deformation due to the sharper flow curvature whereas the spanwise confinement reduces the rotation of the membrane. Finally, we consider a round corner and show that it significantly reduces the mechanical stresses on the capsule.
Paper 5

**A microfluidic device to sort capsules by deformability** Guided by extensive numerical simulations, we propose a microfluidic device that can sort elastic capsules by their deformability. The device consists of a duct embedded with a semi-cylindrical obstacle, and a diffuser which further enhances the sorting capability. We demonstrate that the device can operate reasonably well under changes in the initial position of the capsule. The efficiency of the device remains essentially unaltered under small changes of the obstacle shape (from semi-circular to semi-elliptic cross-section). Confinement along the direction perpendicular to the plane of the device increases its efficiency. This work is the first numerical study of cell sorting by a realistic microfluidic device.

Paper 6

*(Pak et al. 2012)* **Micropropulsion and microrheology in complex fluids via symmetry breaking**

Many biological fluids have polymeric microstructures and display non-Newtonian rheology. We take advantage of such nonlinear fluid behaviour and combine it with geometrical symmetry-breaking to design a novel small-scale propeller able to move only in complex fluids. Its propulsion characteristics are explored numerically in an Oldroyd-B fluid for finite Deborah (De) numbers while the small Deborah number limit is investigated analytically using
Figure 5.5. Two-dimensional profiles of two capsules at different time instants, plotted on the $z = 0$ plane with flow streamlines. The plot in the dashed box displays the streamlines of the flow without capsules. The evolution of the stiff capsule $Ca = 0.05$ and the floppy one $Ca = 0.3$, is illustrated in the top and bottom row respectively. The centre of mass of the capsule is indicated by the cross, and its trajectory by the dashed line. Snapshots are taken for each capsule at three time instants when: (a)/(d), the capsule almost touches the obstacle; (b)/(e), it sits in the gap above the obstacle; (c)/(f), it is well past the obstacle.

a second-order fluid model. We then derive expressions relating the propulsion speed to the rheological properties of the complex fluid, allowing thus to infer the normal stress coefficients in the fluid from the locomotion of the propeller. Our simple mechanism can therefore be used either as a non-Newtonian micro-propeller or as a micro-rheometer.

Paper 7

The dynamics of a capsule in a wall-bounded oscillating shear flow
The motion of an initially spherical capsule in a wall-bounded oscillating shear flow
5. SUMMARY OF PAPERS

\[ v_r(\theta = 0)/R\Omega \]

**Figure 5.6.** Rotation of a single sphere in a second order fluid. Radial velocity along the rotation axis \((\theta = 0)\) as a function of \(r/R\) at \(De = 0.1\) and \(\zeta = 0.5\). Inset: streamline pattern and velocity (shaded/colour map) of the corresponding secondary flow.

Flow is studied via an accelerated boundary integral implementation. Neo-Hookean model is used as the constitutive law of the membrane of capsule. The lateral migration velocity of the capsule varies non-monotonically with its capillary number. It is negatively related with the initial height of the capsule above the wall. A positive correlation between the lateral migration velocity and normal stress difference is identified. The correlation becomes strongest for the capsule with the highest lateral migration velocity. For a fixed capillary number, the lateral migration velocity decreases linearly with the frequency of oscillating shear, and approaches an asymptotic value of zero for high frequency. The deformation of capsule displays a wave-like variation in time and its frequency is twice that of the underlying shear. A phase delay is observed between the variation of capsule deformation with that of the oscillatory flow, more pronounced for a more deformable capsule.
Figure 5.7. Lateral migration velocity $U_{\text{lat}}$ denoted by the solid curve and nondimensional normal stress difference $(N_1 - N_2) / \mu \phi \dot{\gamma}_{\text{max}}$ by the dashed curve versus the nondimensional time $t \omega / 2 \pi$, for three capillary numbers $Ca = 0.0375$ ((a)), 0.12 ((b)) and 0.6 ((c)). The initial offset $h_{\text{ini}} = 2$ and the frequency of shear $\omega = 5/3$. The left scale is for $U_{\text{lat}}$ and the right for $(N_1 - N_2) / \mu \phi \dot{\gamma}_{\text{max}}$. Their local maximums are marked by the circles and squares respectively.
CHAPTER 6

Conclusions and Outlook

Hydrodynamics of swimming microorganisms in viscoelastic fluids

We present numerical investigations using the finite element methods on the hydrodynamics of swimming microorganisms in viscoelastic fluids. The steady squirmer model is used to represent the swimming microorganisms with ciliary propulsion. We investigate the flow field and polymer distribution around a swimming cell. We observe and pinpoint regions with high polymeric stress, attributed to a unique property of complex fluids, increasing extensional viscosity. This property hinders the locomotion of swimming ciliates in the polymeric fluids. We also show that the power consumption decreases monotonically with the fluid elasticity. By analytically decomposing the power consumption into several contributions, we show that the energy-saving stems from spatial decorrelation between flow shear and induced polymer deformation. Such a phase delay is indeed another typical feature of the complex fluids.

As shown by recent experimental studies (Drescher et al. 2010; Guasto et al. 2010), the flow field generated by swimming microorganisms is usually time-periodic. A natural extension of the current work is to simulate swimming squirmers with unsteady surface deformations, focusing on the polymeric dynamics coupled with oscillating flow field and its consequent influence on the performance. Moreover, the effect of fluidic viscoelasticity on the microscale locomotion is still controversial and the physics is not fully understood. For instance, the experiments of a rotating model helix (Liu et al. 2011) and simulations of a undulatory flagella (Teran et al. 2010) showed that the swimming speed of these model cells increases within certain range of fluid elasticity (indicated by polymer relaxation time), whereas the experiments performed by Shen & Arratia (2011) observed that the locomotion of undulating nematode Caenorhabditis elegans is hindered by viscoelasticity. Such a discrepancy might be due to the difference between the way we describe the cell actuation in model studies and that in real cases, model studies fix the magnitude of actuation while bacteria itself might change the magnitude as a response to the surrounding environment. A possible extension might be to describe the cell actuation in another way, e.g., computing the motion of an actuated flagella with a fixed power consumption.
Hydrodynamic of swimming microorganisms in confined geometries

We have developed a boundary element method implementation to study locomotion of a spherical model cell inside a straight and bent tube. The radius of the tube is a few times the radius of the cell. It is found that the confinement due to the capillary tube and the cell position significantly affect the average swimming speed and power consumption. We show that the neutral squirmer follows helical trajectories inside the tube, in qualitative agreement with experimental observations and this can be solely explained by hydrodynamic interactions. The dynamic motions of a neutral and puller squirmer are marginally and passively asymptotical stable, respectively. The motions of others types of squirming are found to be unstable (the cell moves into the wall).

As in many cases, the bacteria do not swim in a quiescent environment but indeed in the presence of flow shear, possibly resulting in swimming in a preferred direction. From the practical perspective, artificial microswimmers either for in-vivo applications or lab-on-a-chip devices also need to go through background flow. Therefore, a possible extension of the current work is to take the background flow into account, e.g., examining the self-propulsion in a corner flow (Rusconi et al. 2010).

Deformable cells in the micro-fluidic flow

We develop a boundary integral implementation accelerated by a general geometry Ewald summation, to simulate the motion of deformable cells in micro-fluidic flow. A global spectral method based on spherical harmonics is embedded for the membrane dynamics of model cells. Our numerical framework combines the elegance of boundary integral and mesh-based methods. Boundary integrals are computed to accurately account for the singular and fast-varying interactions while the smooth part of solution is handled by a highly-parallel general Stokes solver based on the spectral element method. Our hybrid scheme therefore couples the high accuracy of boundary integrals for short-ranged interactions, to the geometrical flexibility of mesh-based methods for the long-ranged interactions.

In the thesis, we use the capsule with neo-Hookean membrane as the model cell. We firstly study its motion through, a channel/duct with a corner that is common in the microcirculation or micro-fluidic devices. We examine the temporal variation of the area, velocity, elastic stress and energy of the capsule around the corner. We observe the broken symmetry of the capsule motion stemming from the interplay between the elastic membrane and viscous flow. The shape of corner is also studied, which shows that a curved corner deforms less the cell than a straight corner. Secondly, we propose a flow-based cell sorting device based on the deformability of cells. Our high-fidelity simulations
indicate that carefully-designed geometrical features can be used to excite considerable hydrodynamic interaction between the cell and device. This effect is exploited to scatter passing-by cells to different positions according to their deformability and hence accomplishes an efficient label-free cell sorting.

In the microcirculation, cells move in the form of suspensions and the role of the interactions between cells is not fully understood even when they are loosely bounded. Cellular flow computations mimicking the real psychological configurations have been pioneered by Freund & Orescanin (2011); Lei et al. (2013) investigating the suspension of RBCs in the tubular flow, the extensions to more complicated geometries (with branches and junctions) will give more insight to the understanding of microcirculation. It is also interesting to examine the interaction between RBCs and the endothelial cells as well as cilia, between healthy and diseased cells like malaria-affected and tumour cells. In the thesis, the capsule is a suitable model pure fluid-filled cells (like RBCs) without any organelle, nevertheless, most cells do have complicated internal structures like nucleus and vacuoles which are themselves membrane-bounded compartments. Numerical techniques need to be developed to cope with these complex cellular configurations, as in the work of Kaoui et al. (2011) for example. This might also pave the way for simulating cellular hydrodynamics at smaller scales. Our current work proposes a deformability-based cell sorting device; likewise, it is also possible to numerically investigate other cell sorting approaches employing the response of cells to magnetic and/or electric fields. Finally, we comment that our numerical platform can be extended for the above-mentioned cases. We also plan to make it a unified framework for the simulation of an individual droplet, solid particle and vesicle as well as their suspensions.
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Part II

Papers
Paper 1
Locomotion by tangential deformation in a polymeric fluid

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In several biologically relevant situations, cell locomotion occurs in polymeric fluids with Weissenberg number larger than one. Here we present results of three-dimensional numerical simulations for the steady locomotion of a self-propelled body in a model polymeric (Giesekus) fluid at low Reynolds number. Locomotion is driven by steady tangential deformation at the surface of the body (so-called squirming motion). In the case of a spherical squirmer, we show that the swimming velocity is systematically less than that in a Newtonian fluid, with a minimum occurring for Weissenberg numbers of order one. The rate of work done by the swimmer always goes up compared to that occurring in the Newtonian solvent alone, but is always lower than the power necessary to swim in a Newtonian fluid with the same viscosity. The swimming efficiency, defined as the ratio between the rate of work necessary to pull the body at the swimming speed in the same fluid and the rate of work done by swimming, is found to always be increased in a polymeric fluid. Further analysis reveals that polymeric stresses break the Newtonian front-back symmetry in the flow profile around the body. In particular, a strong negative elastic wake is present behind the swimmer, which correlates with strong polymer stretching, and its intensity increases with Weissenberg number and viscosity contrasts.
The velocity induced by the squirmer is found to decay in space faster than in a Newtonian flow, with a strong dependence on the polymer relaxation time and viscosity. Our computational results are also extended to prolate spheroidal swimmers and smaller polymer stretching are obtained for slender shapes compared to bluff swimmers. The swimmer with an aspect ratio of two is found to be the most hydrodynamically efficient.

1. Introduction

Small organisms displaying the ability to move usually do so in the presence of a viscous fluid (Vogel 1996). This is the case, in particular, for swimming cells such as bacteria, protozoa, or spermatozoa, which exploit the viscous forces induced by the movement of appendages such as flagella or cilia in order to propel themselves in a fluid environment (Berg 2004; Bray 2000).

The peculiar fluid mechanics properties at low Reynolds numbers, which is the regime in which motile cells live, dictate the manner in which they are able to swim (Purcell 1977). Classical work emphasized the relationship between the time-varying deformation of the cell bodies and appendages, and their swimming and transport kinematics, for a variety of cell families (Childress 1981; Brennen & Winet 1977; Lighthill 1976). More recent work has focused on nonlinear aspects such as cell-cell interactions, and the coupling between external mechanical forces and internal biophysical activity (Lauga & Powers 2009). For example, the role of hydrodynamic interactions in collective modes of locomotion has been the focus of much work (Dombrowski et al. 2004; Simha & Ramaswamy 2002; Sokolov et al. 2007; Cisneros et al. 2007; Saintillan & Shelley 2008). In addition to their relevance to biology, the physical principles of cell locomotion has allowed for the design of synthetic swimming devices on small scales (Behkam & Sitti 2006, 2007; Dreyfus et al. 2005; Ishiyama et al. 2001a,b).

One topic of renewed interest concerns the locomotion of biological cells in complex (non-Newtonian) fluids. As a counterpart to large organisms known to deal with non-Newtonian fluids, most notably gastropods crawling on pedal mucus (Denny 1980a,b; Trueman 1975), in many instances eukaryotic or prokaryotic cells move in fluids displaying time-dependent and nonlinear rheological properties (Doi & Edwards 1988; Larson 1999; Tanner 1988; Bird 1976; Bird et al. 1987a,b). Examples include the progression of spermatozoa through the cervical mucus of mammals and along the mucus-covered fallopian tubes (Fauci & Dillon 2006; Katz & Berger 1980; Katz et al. 1981, 1978; Suarez & Dai 1992; Suarez & Pacey 2006), or the locomotion of bacteria through host mucus and
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tissues (Montecucco & Rappuoli 2001; Wolgemuth et al. 2006). Bacteria in biofilms are also embedded in a viscoelastic matrix (Donlan & Costerton 2002; O’Toole et al. 2000; Costerton et al. 1987, 1995).

In these instances where locomotion occurs in a non-Newtonian fluid, one can define a dimensionless Weissenberg number for the flow, $\text{We}$, defined as the product of the fluid relaxation time scale with the typical shear rate in the flow (Tanner 1988; Bird et al. 1987, a, b). In many cases, $\text{We} \gtrsim 1$ (Fu et al. 2008, 2009; Lauga 2009; Teran et al. 2010; Lauga 2007; Fu et al. 2008), indicating that elastic effects should play an important role in the distribution of forces acting on cells.

A number of theoretical models have been proposed in the past to study small-scale locomotion in complex fluids. Linearized approach have used integral (Chaudhury 1979) or differential constitutive relationships (Fulford et al. 1998). Since cells relies on geometrical nonlinearities to swim — a waving flagellum leads to locomotion at a speed scaling with the square of the wave amplitude (Lauga & Powers 2009) — nonlinearities in the constitutive modelling are essential, a result which has prompted renewed modelling interest. Small-amplitude theories for swimming sheets (Lauga 2007), filaments (Fu et al. 2008, 2009, 2008), and arbitrary surface deformations (Lauga 2009) were recently obtained. Similarly, force generation arising from simple one-degree-of-freedom actuation modes were characterized (Normand & Lauga 2008; Pak et al. 2010).

In practice, finite-size cells swim with large-amplitude motion, and in three dimensions. There is therefore fundamental interest in characterizing locomotion kinematics and energetics in cases for which analytical treatment is not possible. A recent numerical study in two dimensions addressed the locomotion of waving sheets of large-amplitude, showing in particular that swimmers with non-constant wave amplitude could be more efficient and swim faster than their Newtonian counterparts (Teran et al. 2010).

In this paper we take a further step in this direction. We present results of numerical simulations for a steady squirmer free-swimming in a model (Giesekus) polymeric fluid. Locomotion is achieved by steady tangential surface deformation of the cell, which displays no shape change. It is thus a model for locomotion by cells which swim using the propulsion generated by large arrays of short cilia (Blake & Sleigh 1974), and is akin to the spherical envelope approach first proposed by Blake (1971). To the best of our knowledge, the results we present below are the first three-dimensional simulations for self-propelled motion in a complex fluid.

This paper is organized as follows. In Sec. 2 we present the modelling approach chosen in this paper, both for the swimmer and the complex fluid dynamics. In Sec. 3 we detail the numerical method used in our work, and the validation of the code. The main results are then presented in Sec. 4, where we
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consider the case of a spherical squirmer, and present both integral properties of the locomotion (swimming speed, energetics, efficiency) as well as detailed flow characteristics (polymeric wake, flow streamlines, and polymer stretching). A generalization to prolate swimmers is also offered in Sec. 5. Our results are finally discussed in Sec. 6.

2. Problem formulation

2.1. Swimmer model

In order to focus on the fundamental physics of locomotion in polymeric fluids, a model microorganism is used in this paper with several simplifying assumptions. First, we mostly assume the microorganism to be spherical in shape, as is the case for some unicellular ciliates such as *Opalina*, or multicellular algae such as *Voleanx* (Larson *et al.* 1992; Brennen & Winet 1977). Other organisms, such as *Paramecium* or *Cyanobacteria* (Waterbury *et al.* 1985) have elongated shapes, and thus we also consider prolate ellipsoidal swimmers of varying aspect ratios in Sec. V. Second, swimmers are considered to be neutrally buoyant as their sedimentation velocity is much smaller than their swimming speed (Ishikawa *et al.* 2006). Third, the small swimming speed and cell size make it reasonable to neglect inertial effects in the flow, as commonly done in investigations of small-scale biological locomotion (Teran *et al.* 2010; Lauga 2007; Ishikawa *et al.* 2006; Lauga & Powers 2009). Finally, Brownian effects are neglected, an assumption which is valid for all but the smallest bacteria.

In this paper, the swimmers self-propel by generating tangential surface motion, as a model for the time-averaged ciliary propulsion by means of synchronized beating arrays of cilia (Blake & Sleigh 1974). This forms the basis of the so-called envelope model, as first introduced by Blake (1971), where the dynamics of the ciliary tips are replaced by that of their continuous envelope. In this approximation, an effective non-homogeneous boundary condition is imposed at a fixed outer surface, which is impermeable to the fluid. For the simulations presented in this paper, the surface velocity is assumed to be axi-symmetric and time independent. That second assumption is justified if we are interested in the mean motion of a cell averaged over a fast beating period (Ishikawa *et al.* 2006). This model microorganism is also referred to as “squirmer” in the literature.

The surface velocity of a squirmer $u_S$, the co-moving frame, is that considered by Blake (1971) with a concise formulation introduced in Ishikawa & Pedley (2008) as

$$u_S(R) = \sum_{n \geq 1} \frac{2}{n(n+1)} B_n P_n' \left( \frac{e \cdot R}{R} \right) \left( \frac{e \cdot R}{R} - e \right). \tag{1}$$
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Figure 1. Sketch of the prolate swimmer and the coordinate system used; \((r, z)\) denote cylindrical coordinates and \((R, \theta)\) the spherical coordinates with \(\phi\) the azimuthal angle. The results presented below assume axisymmetric flow.

Here, \(e\) is the orientation vector of the squirmer, \(B_n\) is the \(n\)th mode of the surface squirming velocity (Blake 1971), \(P_n\) is the \(n\)th Legendre polynomial, \(\mathbf{R}\) is the position vector, and \(R = |\mathbf{R}|\). (See figure 1 for a sketch of the notations)

In a Newtonian fluid, the swimming speed of the squirmer is \(2B_1/3\) (Blake 1971) and thus only dictated by the first mode. In previous studies, it is commonly assumed \(B_n = 0\) for \(n > 2\) (Downton & Stark 2009; Ishikawa & Pedley 2008).

Consequently, the tangential velocity on the sphere in the co-moving frame is expressed as \(u_\theta(\theta) = B_1 \sin \theta + (B_2/2) \sin 2\theta\), where \(\theta = \arccos(e \cdot r/r)\) and an additional parameter, representing the ratio of the second to the first squirming mode, is introduced \(\beta_{SW}\), i.e., \(\beta_{SW} = B_2/B_1\). A squirmer with positive \(\beta_{SW}\) is a “puller”, and has its propeller located ahead of the cell body, while a squirmer with negative \(\beta_{SW}\) is a “pusher”, and has its propeller located behind the cell body in the swimming direction (Ishikawa & Pedley 2008; Lauga & Powers 2009). In this paper we limited ourselves to the simple case \(\beta_{SW} = 0\), which gives the most energy-saving swimming gait in a Newtonian fluid (Downton & Stark 2009). This convenient mathematical assumption allows us to numerically explore a large range of values of polymeric elasticity and viscosity. Thus, the surface velocity on our squirmer is \(u_\theta(\theta) = B_1 \sin \theta\), and has its maximum surface velocity located at the equator. For the simulations of the prolate organisms we assume the same boundary condition for the velocity component tangential to the surface of the ellipsoid.

...
2.2. Polymeric fluid dynamics

For incompressible low-Reynolds number flow in a viscoelastic fluid, the momentum and continuity equation are written as

\[-\nabla p + \nabla \cdot \tau = 0, \quad (2)\]
\[\nabla \cdot u = 0, \quad (3)\]

upon nondimensionalizing velocity with \(B_1\), length with the diameter of the squirmer \(D\), time with \(D/B_1\), and pressure and stresses with \(\mu B_1/D\), where \(\mu\) is the solution viscosity. Note that for numerical convenience we actually retain the partial time derivative in the momentum equation and present the final steady state results (E. O. A. Carew & Webster 1993; Baaijens 1998).

Following classical modelling approaches (Bird 1976; Bird et al. 1987a, b), the deviatoric stress \(\tau\) can be split into two components, the viscous solvent stress \((\tau^s)\) and the polymeric stress \((\tau^p)\); \(\tau^s\) is thus given by

\[\tau^s = \beta (\nabla u + \nabla u^T), \quad (4)\]

where \(\beta < 1\) represents the ratio of the solvent viscosity, \(\mu_s\), to the total zero shear rate viscosity, \(\mu\). To complete the model, a transport equation for the polymeric stress \(\tau^p\) is required. Here we adopt the nonlinear Giesekus model (Giesekus 1982), which, in addition to shear-thinning material properties, provides two important features, namely saturation of polymer elongation, and a non-negative entropy production during the time evolution of the polymers (see details in Beris & Edwards (1990); Dupret & Marchal (1986); Souvaliotis & Beris (1992)). Violation of these two properties may cause numerical difficulties and non-physical flow behaviour. The nondimensionalized constitutive equation can be written as

\[\frac{\tau^p}{W e} + \frac{\nu}{W e} + \frac{\alpha}{1 - \beta} (\tau^p \cdot \tau^p) = \frac{1 - \beta}{W e} (\nabla u + \nabla u^T), \quad (5)\]

where upper-convected derivative, \(\nabla^C\), defined for a tensor \(A\), is given by

\[\nabla^C A = \frac{\partial A}{\partial t} + u \cdot \nabla A - \nabla u^T \cdot A - A \cdot \nabla u. \quad (6)\]

In the expression above, \(We\) is the Weissenberg number, defined as \(We = \lambda B_1/D\) where \(\lambda\) is the polymer relaxation time. The so-called mobility factor \(\alpha\) is introduced in the nonlinear stress term representing an anisotropic hydrodynamic drag on the polymer molecules (Bird et al. 1987a), and it limits the extensional viscosity of the fluid. From thermodynamics considerations, the mobility factor \(\alpha\) must be in the \(0 - 0.5\) range (Bird et al. 1987a; Larson 1988). We fix it to be 0.2 in all our simulations.
2.3. Swimming power and efficiency

In the realm of low Reynolds number locomotion, where inertia can be neglected, the swimming speed is determined at each instant as the speed at which the total force on the microorganism is zero. Given that swimming speed, it is of interest to compute the power required to move, and the efficiency of the motion. The power $P$ consumed by a swimming microorganism is defined as Stone & Samuel (1996)

$$ P = - \int_S n \cdot \sigma \cdot u \, dS, $$

where $n$ is the unit normal outward the swimmer surface $S$, $\sigma$ is the stress tensor, $\sigma = -pI + \tau^s + \tau^p$, and $u$ is the velocity of the fluid in the laboratory reference frame. The swimming efficiency

$$ \eta = \frac{F_p U}{P} $$

is then defined as the ratio between the work rate $F_p U$ necessary to pull the swimmer body at the swimming speed in the same fluid (same We and $\beta$) without active boundary motion and the swimming power $P$ defined above (Lauga & Powers 2009). The force acting on the pulled object is given by

$$ F_p = - \int_S n \cdot \sigma \, dS. $$

3. Numerical method

The finite-element code Femlego, developed at the Royal Institute of Technology (KTH), Stockholm (Amberg et al. 1999) is used in our simulations. Femlego has provided a variety of successful simulations in the area of microfluids (Carlson et al. 2009) and multiphase flow (Do-Quang & Amberg 2009). For the incompressible isothermal Navier-Stokes equations, a projection method introduced by Guermond & Quartapelle (1997) is used to solve the conservation equation for mass and momentum, Eqs. (2) and (3), with a Galerkin discretization. However, Galerkin discretization is not the optimal choice for the constitutive equation, Eq. (5), owing to the increasing importance of the convective term with increasing Weissenberg number (King et al. 1988). Serving as a remedy, we follow Baaijens (1998) and Marchal & Crochet (1987) and adopt the streamline-upwind/Petrov-Galerkin (SUPG) method for the convective term in the constitutive equation. The weak form of the constitutive equation is therefore written as

$$ \left\{ S + \frac{h}{U} u \cdot \nabla S, \tau^p + \lambda \nabla \cdot \tau^p + \frac{\alpha}{\mu_p} (\tau^p \cdot \tau^p) - \mu_p (\nabla u + \nabla u^T) \right\} = 0 $$
where $S$ denotes the weighting function for $\tau_p$, $h$ is a characteristic length-scale of the element and $U$ is the magnitude of the local characteristic velocity. In our case, we choose the norm of $u$ as the value of $U$.

The fact that the flow is axisymmetric is exploited in our simulations, degenerating the computational domain to a half circle representing the squirmer bounded by a rectangular box. Inflow boundary is placed 10 diameters away from the object with prescribed velocity and zero polymeric stress (equilibrium status). The outflow boundary is 30 diameters downstream of the object, with zero pressure specified as the flow is fully developed. The centreline is treated as an axisymmetric boundary condition. Tangential velocity is imposed on the surface of the squirmer to realize the prescribed swimming gait, as discussed above. Neumann boundary conditions are set for the remaining variables.

Spatial discretization is performed with piecewise linear functions for the whole set of equations. Use of triangular elements in our simulations enabled sufficient grid refinement to better capture the unique flow structure in the polymeric flow, such as elastic boundary layers (King et al. 1988) and elastic wake (McKinley et al. 1993). The number of elements typically used in our simulations is of about 90,000 with necessary grid refinement up to 150,000 elements to avoid numerical instabilities at higher Weissenberg number. Mesh independence of the results has been tested for the most difficult cases, and a relative error below 1% has been observed for both swimming speed and power.

The computation of the swimming speed is based on the fact there is no net force or torque on self-propelled swimming microorganisms. Therefore, we performed simulations of the same squirmer with three different free-stream conditions (the simulations are performed in the comoving reference frame) and computed the hydrodynamic forces for the three cases. By interpolation, we are thus able to estimate the swimming speed as the free-stream velocity for which the total force on the body is zero. For all the cases, simulations are then performed at the estimated swimming speed in order to verify that the force were below a given tolerance and to provide a more accurate evaluation of the swimming power.

4. Locomotion of a spherical squirmer

4.1. Integral quantities

We first present our results on integral quantities of the swimming motion, namely the swimming speed, work done, and the swimmer efficiency. In the following the different quantities will be made non dimensional with the diameter of the spherical squirmer and its swimming velocity and power in the Newtonian fluid. Simulations are performed with different values of the Weissenberg number, $\text{We}$, and for three values of the viscosity ratio, $\beta$ (0.1, 0.3, and 0.6). The swimming speed in the polymeric fluid divided by that of the
Newtonian swimmer is displayed in figure 2 as a function of $We$. We see that the swimming speed of the squirmer decreases for low Weissenberg numbers, reaches its minimum value near $We = 1$, and then slowly recovers with increasing polymeric elasticity (or $We$). The largest decrease in swimming speed is observed for the lowest value of $\beta$ considered, i.e., for the largest polymer viscosity under investigation. It is interesting to note that the minimum speed is always obtained when the polymer relaxation time is approximately equal to the time it takes for the swimmer to swim its own length.

Newtonian swimmer is displayed in figure 2 as a function of $We$. We see that the swimming speed of the squirmer decreases for low Weissenberg numbers, reaches its minimum value near $We = 1$, and then slowly recovers with increasing polymeric elasticity (or $We$). The largest decrease in swimming speed is observed for the lowest value of $\beta$ considered, i.e., for the largest polymer viscosity under investigation. It is interesting to note that the minimum speed is always obtained when the polymer relaxation time is approximately equal to the time it takes for the swimmer to swim its own length.
The rate of work done by the swimmer divided by that in the Newtonian fluid with identical total viscosity is displayed in figure 3 as a function of $We$. The power needed to swim decreases for all cases considered and seems to approach a constant asymptotic value at large Weissenberg number. It is important to note that, if scaled with the solvent viscosity, the actual value of the work performed by the microorganism is increasing when decreasing $\beta$. However, the work done is significantly less than that of a swimmer in a Newtonian fluids with the same viscosity, similarly to what was observed for the swimming sheet (Lauga 2007). This relative power saving in a polymeric fluid increases with Weissenberg numbers in all cases. Note that the fact that the swimming speed and power approach the Newtonian values as $We \to 0$ contributes to an a posteriori validation of our code.

The power expended by the squirmers is approaching a final value in the high-$We$ limit independent of the fluid elasticity and increasing with the total viscosity. As will be discussed below, for long relaxation times, the stretching/relaxation of polymers in the wake of the body takes place further away from the organism. This may explain why the results become independent of the Weissenberg number: the elastic wake moves far enough not to affect the stress distribution close to the surface. At the same time, the work performed against the fluid is larger for larger viscosity and therefore the value of the power needed to swim when $We \to \infty$ increases when $\beta$ decreases. The swimming power is seen numerically to scale with $\beta$ approximately as $P \sim \beta^{-0.8}$.

Figure 4. Swimming efficiency, $\eta$, in a polymeric fluid: ratio between the power needed to pull the spherical body at the velocity equal to its swimming speed and the power required to swim in the same fluid. Efficiency is displayed as a function of $We$ for three values of $\beta$. Inset: Value of the efficiency at large $We$ as a function of $\beta$ (log-log plot); the line is a guide for the eye showing a 1/3 power law.
The swimming efficiency, $\eta$, is shown in figure 12 as a function of $We$. The efficiency is defined here as the ratio between the power needed to pull the spherical body at the swimming velocity of the squirmer and the power required to swim in the same fluid. The efficiency is seen to always be larger in the viscoelastic fluid than in a Newtonian fluid, which is one of the main results of our work. This is in agreement with the findings of Teran et al. (2010) who simulated a two-dimensional swimming sheet finite length in an Oldroyd B-fluid, as well as the results by Leshansky (2009) who considered the locomotion of a squirmer in a suspension of rigid spheres. The efficiency is seen to remain essentially constant beyond $We \gtrsim 3$. By considering the averaged values of the efficiency in the large-$We$ limit, the relation between the viscosity ratio and the asymptotic efficiency is examined. As shown by the inset in figure 12, there seems to be a power-law relationship with exponent close to $1/3$, $\eta \sim \beta^{-1/3}$. Using the definition of efficiency given in Eq.(8) and $P \sim \beta^{-0.8}$, we conclude that the relative decrease in power with viscosity ratio observed at large $We$ is faster for swimming micro-organisms than for pulled bodies.

4.2. Flow visualization

![](image)

**Figure 5.** Flow streamlines and map of velocity magnitudes.

Comparison between the Newtonian case (left) and polymeric case with $We = 7$ and $\beta = 0.1$ (right).

4.2a. Comparison with Newtonian swimming: Elastic wake. In this section we consider the detailed flow (solvent plus polymer) around the swimming microorganism. We start by showing in figure 5 the difference in velocity field between a Newtonian and a non-Newtonian squirmer. The figure depicts the Newtonian case (left-hand side) and the polymeric flow with $We = 7$ and $\beta = 0.1$ (right-hand side), both in the co-moving frame. The streamlines are shown close to the body and the background map indicates the velocity magnitude.
We first note the similarity in the shape of the streamlines. The only noticeable difference is a slight upstream shift upstream with increasing $We$ of the streamlines behind the cylinder. In the case of translation of a sphere, a similar observation has been attributed to the shear-thinning characteristics of the viscosity, see among others Harlen (2002).

The first important difference between Newtonian and polymeric swimming is the magnitude of the fluid velocity. The flow approaching the swimmer is hardly changed by the presence of polymers, while important quantitative differences exist on the side and the front of the body. The velocity induced by the swimming gait, maximum in the equatorial plane $z = 0$, decays faster in the viscoelastic fluid where a thinner boundary layer is observed. This fast decay was identified by Leshansky (2009) as a possible cause of larger efficiency for locomotion in a non-Newtonian media.

The second notable difference is the presence of a so-called negative elastic wake downstream of the object. This is clearly visible about one diameter behind the sphere, and it extends to about six diameters downstream for the longer polymer relaxation times. The front-back flow symmetry of a Newtonian swimmer is thus broken in a viscoelastic fluid.

![Figure 6. Flow streamlines and map of velocity magnitudes. Comparison between two polymeric fluids with same viscosity ($\beta = 0.3$) with $We = 1$ (left) and $We = 9$ (right).](image)

The negative wake was studied for spheres sedimenting in polymeric flows (Bisgaard 1983; Hassager 1979). It appears as a velocity overshoot behind the body in the co-moving reference frame and as a negative velocity in the laboratory frame, and is related to the relative magnitude of the normal and shear stress and their spatial gradients. Stresses generated in the extensional flow at the rear of the squirmer drive the flow towards the body and produce a region of slower decay, the so-called extended wake. In contrast, the force induced by the downstream relaxation of shear stresses generated near the side
of the body gives rise to flow directed away from the swimmer, and causes a negative wake (Harlen 2002). Away from the axis of symmetry, the principal direction of extension is no longer aligned with the axis, which produces stresses directed away from the body. The polymers away from the axis have memory of the shear flow experienced near the side of the sphere and for large relaxation times the stresses built up in this region are still relevant as fluid particles are advected downstream.

Figure 7. Axial flow in front and behind the swimmer nondimensionalized by the swimming speed of the organism for different values of the Weissenberg number and $\beta = 0.3$.

Figure 8. Asymmetry measure (see text) as a function of the Weissenberg number for swimming motion (red circles, solid line) and forced motion at same speed with $\beta = 0.3$ (black squares, solid line).

A wake number is defined in Harlen (2002) to show that both limited polymer extension and large relaxation times contribute to the formation of a negative wake. The extensional viscosity plays an important role in the generation of the elastic wake, and a shear-thinning first normal stress coefficient enhances
the velocity overshoot. Negative wakes are not expected in dilute solutions, such as those modelled e.g. by the Oldroyd-B constitutive equation at moderate Weissenberg numbers. Fitting of experimental data of semi-concentrated solutions using Giesekus and Phan-Thien-Tanner models allow one to reproduce negative wakes in numerical simulations (Arigo & Mckinley 1998). Our results are thus relevant to locomotion in concentrated polymer solutions, and to relatively high values of the polymer relaxation times.

In figure 6 we further show a comparison of the flow field for two different values of the Weissenberg number, \( We = 1 \) and 9, at fixed viscosity ratio \( \beta \). The elastic wake is evident for the largest \( We \) considered while it appears not yet formed for \( We = 1 \), as expected since \( We \) is the ratio between the characteristic time scales for polymer relaxation and advection.

![Figure 9. Influence of polymer viscosity on flow streamlines and velocity magnitudes for \( We = 7 \). Left: \( \beta = 0.6 \). Right: \( \beta = 0.1 \).](image)

To further investigate the occurrence of an elastic wake, we show the axial profile of the axial velocity along the symmetry axis \( r = 0 \) in figure 7 divided by the swimming speed. The symmetric Newtonian case is also reported for comparison. For a sedimenting sphere, the extent of the negative velocity just downstream of the wake increases with \( We \) (see Harlen (2002) and references therein). In the polymeric fluid the largest negative value is found at \( We \approx 5 \). This seems to result from two competing effects: When the Weissenberg number increases, the extent of the region of negative velocity increases as for the pulled object. However, the negative peak velocity decreases since the shear stress responsible for its formation is acting further downstream in the region of larger fluid velocity (seen in the co-moving frame).
To quantify this effect, we consider as measure of the fore-aft asymmetry the difference in the axial velocity upstream and downstream of the object

\[ A_s = \int_{D/2}^{\infty} [u_z(r) - u_z(-r)] \, dz. \]  

(11)
The variation of the asymmetry, \( A_s \), with the Weissenberg number is shown in figure 8 at \( \beta = 0.3 \) for both the swimmer and the forced motion of the spherical body in the same polymeric solution. For the swimmer, the asymmetry, which is zero in the Newtonian limit, always increases and reaches a constant value when \( We \gtrsim 5 \). As shown in figure 7, this is due to a compensation between the elongation of the wake and the negative peak just behind the swimmer. In the case of the forced motion of a sphere, \( A_s \) is first negative for lower values of \( We \) and then increases monotonically. This is explained by the fact that the decrease of the velocity in front of the object is faster for forced motion, and is observed already for the lowest Weissenberg number considered while the negative wake, leading to positive values of \( A_s \), is formed in this case only when \( We \gtrsim 3 \).

Finally, the influence of polymer viscosity on flow streamlines and velocity magnitudes is illustrated in figure 9 for \( We = 7 \). For increased flow viscosity, the effect of swimming actuation on the side of the object is felt over shorter distances. Similarly, the negative elastic wake is found about one diameter downstream of the swimmer at \( \beta = 0.1 \), while it is further downstream, at \( r/D \approx 2.5 \), for \( \beta = 0.6 \).

**Figure 10.** Power law exponent \( \gamma \) for decay of the axial velocity along the \( z = 0 \) plane \( (u \sim r^{-\gamma}, \text{see text}) \), as a function of the Weissenberg number.

4.2b. Spatial decay. In order to quantify the spatial signature of the velocity perturbation introduced by the swimmer in directions other than that of the wake, we now consider the decay of the axial velocity in the radial direction along the equatorial plane, i.e. \( u_z(r, z = 0) \). For a Newtonian squirmer with
\(\beta_{SW} = 0\) the velocity decays as \(\sim 1/r^3\), whereas the decay is only \(\sim 1/r^2\) for pusher and puller-type cells \((\beta_{SW} \neq 0)\). We numerically estimate the radial decay of the velocity for locomotion in a polymeric fluid by fitting a power law from about \(r \approx D\) to the end of the computational domain. The values of the exponent \(\gamma\) obtained with this procedure are reported in figure 13 as a function of the Weissenberg number. The flow, which decays as \(\sim 1/r^3\) in the Newtonian case, always decays faster in the polymeric case. We observe that the variation of the decay rate with \(We\) is not monotonic, and that for the two largest values of the viscosity ratio \((\beta = 0.6, 0.3)\) a maximum is reached near \(We = 1\), which coincides with the occurrence of the minimum swimming speed. Finally, the decay rate increases with increased viscosity contrast between the polymer and the solvent (decrease of \(\beta\)). In agreement with Leshansky (2009) we find therefore that a more rapid decay leads to larger efficiency.

![Figure 11. Polymeric stretching field: trace of the polymer conformation tensor, Tr(\(C\)). Comparison between forced motion (left) and free-swimming at the same speed (right), with \(We = 7\) and \(\beta = 0.3\).](image)

4.2c. Polymer stretching. The trace of the polymer conformation tensor, \(C\), defined as

\[
C = \frac{We}{1 - \beta} (\tau^p + I),
\]

indicates the elongation of the polymers in the fluid. We plot \(Tr(C)\) in figure 11 and 12 for the forced motion of the sphere and for swimming with different polymer relaxation times. In figure 11 we compare polymer stretching for forced motion and free swimming at the same speed in the case where \(We = 7\) and \(\beta = 0.3\). The region around the body where stretching is evident is much larger in the case of forced motion. The spatial decay of stretching is more rapid.
on the side of the swimmer while the largest elongation is observed in the wake right behind the organism. In figure 12 we show the variation of stretching at different values of $We$. As expected a larger Weissenberg number leads to a larger region of elongated polymers, and correlates with a more pronounced elastic wake.

![Figure 12. Polymeric stretching field: trace of the polymer conformation tensor, $Tr(C)$. Comparison of polymer stretching between $We = 1$ and $We = 9$ for $\beta = 0.3$.](image)

**Figure 12.** Polymeric stretching field: trace of the polymer conformation tensor, $Tr(C)$. Comparison of polymer stretching between $We = 1$ and $We = 9$ for $\beta = 0.3$.

![Figure 13. Dependence of the maximum polymer stretching, $Max(Tr(C))$, on the Weissenberg number, $We$. In the range of Weissenberg numbers considered, the relationship is approximately linear, with a slope $s$. Inset: dependence of the slope, $s$, on the viscosity ratio $\beta$ (log-log plot); the solid line is a guide to the eye showing a power law of 1/4.](image)

**Figure 13.** Dependence of the maximum polymer stretching, $Max(Tr(C))$, on the Weissenberg number, $We$. In the range of Weissenberg numbers considered, the relationship is approximately linear, with a slope $s$. Inset: dependence of the slope, $s$, on the viscosity ratio $\beta$ (log-log plot); the solid line is a guide to the eye showing a power law of 1/4.
The increase of the magnitude of the polymer elongation is further quantified in figure 13 where the maximum of $\text{Tr}(\mathbf{C})$ inside our computational domain is displayed as a function of $We$ for the different values of $\beta$ considered. The relationship between elongation and relaxation time is found to be approximately linear, with a slope $s$ dependent on the viscosity ratio. The dependence of the slope with $\beta$ is shown in the inset in figure 13, and a power law $s \approx \beta^{-1/4}$ provides an appropriate fit to our numerical results.

<table>
<thead>
<tr>
<th></th>
<th>$C_{rr}$</th>
<th>$C_{zz}$</th>
<th>$C_{rz}$</th>
<th>$C_{\phi\phi}$</th>
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<td>$39.3$</td>
<td>$-9.4$</td>
<td>$16.3$</td>
</tr>
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<tr>
<td>$We = 5$</td>
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<td>$223.6$</td>
<td>$-38.3$</td>
<td>$84.2$</td>
</tr>
<tr>
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<td>$0.529$</td>
<td>$0.5$</td>
<td>$0.5$</td>
</tr>
<tr>
<td>$\theta$ (°)</td>
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<td>$171$</td>
<td>$7$</td>
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<td>$426.6$</td>
<td>$-89.7$</td>
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<tr>
<td>$\theta$ (°)</td>
<td>$4$</td>
<td>$178.3$</td>
<td>$171.7$</td>
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Table 7.1. Maxima of individual components of polymer stretching (bold numbers) and corresponding location where these maxima are attained for different values of $We$, and in the case $\beta = 0.3$. The position is reported in spherical polar coordinate, with $\theta$ in degrees and $R$ nondimensionalized by the sphere diameter, while the polymeric stresses are in cylindrical coordinate (see figure 1).
Finally, we report in Table 7.1 the maxima of the different components of the conformation tensor \((C_{rr}, C_{zz}, C_{rz}, C_{\phi\phi})\) together with the location where these maxima are attained (spherical coordinates with \(R\) the distance from the centre of the swimmer and \(\theta\) in degrees measured from the front of the swimmer). Three values of the Weissenberg number are considered with \(\beta = 0.3\). The maximum elongation is in axial stretching, \(C_{zz}\), and occurs just behind the body (see also figure 12). The maximum of radial stretching \(C_{rr}\) is observed on the swimmer, just off the symmetry line at the front stagnation, while the peak of the shear \(C_{rz}\) is characterized by negative values and is observed on the back of the body with values of \(\theta\) slightly increasing with polymer elasticity; this component will be responsible for the negative wake further downstream (Harlen 2002). In addition, and as expected, the component \(C_{\phi\phi}\) is also nonzero. Its amplitude is in fact comparable to that of the radial stretching \(C_{rr}\) and it attains its maximum value in front of the cylinder.

5. Prolate swimmers

After considering spherical bodies, we extend in this section our results to the case of prolate swimmers of different aspect ratios. We assume the body to be an axisymmetric prolate spheroid with an aspect ratio, \(AR > 1\), defined as the ratio between its major (symmetry) axis, and its minor axis. In order to present a proper comparison between organisms of different shapes, we keep their volume fixed. As a consequence, we adopt as reference length for our dimensionless numbers \(2\tilde{R}\), with \(\tilde{R} = (3V/4\pi)^{1/3}\); \(\tilde{R}\) is thus the radius of a sphere having same volume \(V\) as the prolate ellipsoid. As an example, for a swimmer with aspect ratio \(AR = 4\), the semi-major axis is \(0.315D\), the semi-minor axis is \(1.26D\), and simulations are performed for the same values of \(We\) and \(\beta\) as for the sphere of diameter \(D\).

Computational results for swimming speed, power and efficiency as a function of the Weissenberg number and the viscosity ratio show similar trends as those discussed earlier for spherical squirming, and will not be repeated. As example of flow, we show in figure 14 the flow streamlines and polymer elongation for a prolate swimmer of aspect ratio \(AR = 4\). Large values of \(Tr(C)\) are observed in a thin region around the body and in the wake, similarly to the spherical swimmer. The thickness of this stretching boundary layer, as well as the length of the wake, is found to decrease for an elongated swimmer.

Comparing the polymer stretching reported in figure 11 and in figure 14, we note also that the maximum of \(Tr(C)\) is more than twice as big in the case of a spherical swimmer. In addition, for the prolate swimmer the velocity displays a weak overshoot just behind the body and, more interestingly, the streamlines are seen to converge toward the centre of the body \((z = 0)\), and then depart further downstream. This is explained by the formation of a region of negative (resp. positive) pressure near the surface on the front (resp. rear)
Figure 14. Locomotion of a prolate swimmer of aspect ratio $\mathcal{AR} = 4$ in a viscoelastic fluid with $We = 7$ and $\beta = 0.3$.

Left: Trace of the conformation tensor, $Tr(C)$. Right: Velocity magnitude, $|u|$. Streamlines are reported on both sides.

of the body. Such an antisymmetric pressure distribution with respect to the plan $z = 0$ is not observed for spherical squirmers.

Figure 15. Swimming speed in the polymeric fluid with $We = 7$ and $\beta = 0.3$ divided by that of the spherical Newtonian swimmer for the prolate microorganism sharing the same volume but with different aspect ratio $\mathcal{AR}$.

In figure 15 we show the variation of the swimming speed with the prolate aspect ratio. We plot the results in the Newtonian case (black squares) as well as the polymeric case with $We = 7$ and $\beta = 0.3$ (red circles). The swimming speed is normalized with the swimming velocity of the spherical Newtonian.
squirmer, and is seen to decrease with the aspect ratio. To explain this finding we consider the pressure distribution around the organism. For the spherical squirmer, the two regions of minimum and maximum pressure are close to each other and on the rear of the body, whereas for the elongated squirmer we find high pressure on the front and low pressure on the rear. This implies that the pressure forces act in the direction opposite to that of swimming for prolate organisms.

The swimming power, normalized by that of the sphere in the Newtonian fluid with the same total viscosity, is shown in figure 16, and also decreases with the aspect ratio of the body. The relative reduction in consumed power is increasing with decreasing aspect ratio.

The swimming efficiency is displayed in figure 17. We find that the swimmer of aspect ratio $AR \approx 2$ is the most efficient, a result which is valid both in the Newtonian and non-Newtonian limit. In addition, a robust increase in efficiency in the viscoelastic fluid is also evident.

6. Conclusion

Although significant progress has been made in the analysis of low-Reynolds number locomotion in Newtonian fluids, many biological cells encounter viscous environments with suspended microstructures or macromolecules. It is thus of fundamental importance to develop modelling tools addressing the effect of non-Newtonian stresses on propulsion. In our study, we presented the results of numerical simulations for a steady squirmer free-swimming in a model (Giesekus) polymeric fluid. Locomotion is achieved by a prescribed steady tangential surface deformation of the body, which thus displays no shape change. To the best of our knowledge, the results discussed in our paper are the first
three-dimensional simulations for self-propelled motion in a complex fluid. In addition, as stresses in the Giesekus model saturate for large elongation, our results are relevant to cell locomotion in concentrated polymeric solutions, and long polymer relaxation times, as demonstrated by the appearance of negative wakes behind the swimmer.

Our main results are as follows. We first showed that the swimming speed is lower than in a Newtonian fluid, with a minimum near $We \approx 1$. Swimming power also decreases with polymer relaxation time and increased viscosity contrast between the polymer and the solvent. Rescaling the data, it is possible to show when keeping constant the consumed power, the velocity at the boundary increases and the swimming speed increases. Swimming at constant power gives therefore larger speeds in viscoelastic fluids. The swimming efficiency, defined as the ratio between the power required to pull the swimmer in the same fluid at the same speed, and the power consumed by the swimmer, is found to systematically increase in viscoelastic fluids. The gain in efficiency is larger for the longest relaxation times and higher polymer viscosity contrast, and approaches a constant asymptotic value at high Weissenberg number. The increase in efficiency is consistent with the analysis in Leshansky (2009) for a squirmer in a suspension of rigid spheres and with the numerical results of Teran et al. (2010) for a two-dimensional sheet of finite length. Flow visualizations further reveal that the fore-aft symmetry of a Newtonian swimmer is broken in a viscoelastic fluid. The appearance of a negative elastic wake, i.e. one with velocity directed towards the object, is numerically demonstrated. The analysis of the main flow features indicates that the swimming speed of a viscoelastic squirmer increases for $We \gtrsim 1$ when the elastic wake moves further downstream, and the polymer molecules experience larger elongations. The minimum speed is observed at $We \approx 1$ when the distance travelled by the polymer during their relaxation
time is of the order of the body length. In this case, a region of strong normal stress $\tau_{zz}$ is forming on the back of the swimmer, pulling it backward. This region is weaker for lower $We$ and located further downstream for larger $We$. The spatial decay rate of the flow induced by the swimmer is found to be larger in a viscoelastic flow, suggesting different collective behaviour of active suspensions of self-propelled bodies in Newtonian vs. non-Newtonian fluids. Finally, we extended our results to the case of prolate swimmers of different aspect ratios, and found that bodies with an aspect ratio of two have the largest swimming efficiency. The gain in efficiency provided by the fluid viscoelasticity is more pronounced for the spherical swimmer. This suggests that bluff bodies have larger possibilities to exploits the advantages of such an environment.

The work presented in this paper could be extended in a number of non-trivial and interesting ways. First, we have focused here on a single squirming mode, but most swimming cells have a dipolar nature in the far field, and thus the case $\beta_{SW} \neq 0$ should be investigated next. In particular, the distinction between pushers and pullers should be addressed. Second, real cells do not deform the surrounding fluid in a steady fashion, but usually apply time-dependent kinematics, and these unsteady effects, when they occur for Deborah numbers of order unity or above, can in general not be neglected. Third, more realistic cell geometries should be considered, in particular for flagellated bacteria. Fourth, the breakdown of the front-back flow symmetry and the appearance of wakes will surely have interesting consequences on hydrodynamic interactions between swimmers. Finally, most cells do not swim with prescribed kinematics, but instead their deformation kinematics are obtained as a physical balance between an internal (or boundary) actuation and the outside fluid, and this coupled fluid-solid problem should be further investigated.

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References


Locomotion by tangential deformation in a polymeric fluid


Paper 2
Self-propulsion in viscoelastic fluids: pushers vs. pullers

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We use numerical simulations to address locomotion at zero Reynolds number in viscoelastic (Giesekus) fluids. The swimmers are assumed to be spherical, to self-propel using tangential surface deformation, and the computations are implemented using a finite element method. The emphasis of the study is on the change of the swimming kinematics, energetics, and flow disturbance from Newtonian to viscoelastic, and on the distinction between pusher and puller swimmers. In all cases, the viscoelastic swimming speed is below the Newtonian one, with a minimum obtained for intermediate values of the Weissenberg number, $We$. An analysis of the flow field places the origin of this swimming degradation in non-Newtonian elongational stresses. The power required for swimming is also systematically below the Newtonian power, and always a decreasing function of $We$. A detail energetic balance of the swimming problem points at the polymeric part of the stress as the primary $We$-decreasing energetic contribution, while the contributions of the work done by the swimmer from the solvent remain essentially $We$-independent. In addition, we observe negative values of the polymeric power density in some flow regions, indicating positive elastic work by the polymers on the fluid. The hydrodynamic efficiency, defined as the ratio of the useful to total rate of work, is always above
the Newtonian case, with a maximum relative value obtained at intermediate Weissenberg numbers. Finally, the presence of polymeric stresses leads to an increase of the rate of decay of the flow velocity in the fluid, and a decrease of the magnitude of the stresslet governing the magnitude of the effective bulk stress in the fluid.

1. Introduction

The physical mechanisms of microorganism locomotion accompany a variety of natural phenomena, including human spermatozoa approaching the ovum in the mammalian female reproductive tract (Fauci & Dillon 2006), algal blooms moving to nutrient rich environment in maritime regions (Hill & Pedley 2005; Pedley & Kessler 1992), biofilm formation (Costerton et al. 1987), and paramecia cells escaping from their predators (Hamel et al. 2011). Much work has been done to shed light on the different physical mechanisms at play in the locomotion of microorganisms, including classical kinematics studies (Blake 1971a; Stone & Samuel 1996; Brennen & Winet 1977; Lauga & Powers 2009), nutrients uptake (Magar & Pedley 2005; S.Michelin & Lauga 2011), collective behaviour (Cisneros et al. 2007; Hernandez-Ortiz et al. 2005; Moore et al. 2002; Saintillan & Shelley 2008; Ishikawa & Pedley 2008) and hydrodynamic interactions (Giacché & Ishikawa 2010; Ishikawa & Hota 2006; Ishikawa et al. 2006).

Most past work has however been limited to the study of locomotion in Newtonian fluids, whereas in many biological instances microorganisms swim in complex polymeric fluids. Several groups have recently started to address the effect of viscoelasticity on the locomotory features and hydrodynamic performance of swimming microorganisms. Lauga (2007) investigated the kinematics and energetics of Taylor’s waving sheet in various model nonlinear polymeric fluids and found that, for a given waving stroke, viscoelasticity impeded the locomotion of the swimming sheet. Similarly, Fu et al. (2009) derived analytically that the swimming speed of an infinite filament with a prescribed waveform will decrease in Oldroyd-B fluid compared to the Newtonian case. Teran et al. (2010) numerically studied the influence of viscoelasticity on the dynamics of a finite-length Taylor’s waving sheet and showed that the swimming speed and efficiency can actually increase within a certain range of polymer relaxation time and sheet waveforms. Recently, Shen & Arratia (2011) experimentally demonstrated that fluid elasticity hindered the self-propulsion of the nematode Caenorhabditis elegans, primarily due to polymeric stretching near hyperbolic points in the viscoelastic flow.
In our previous work (Zhu et al. 2011), we carried out three-dimensional axisymmetric simulations to study the effect of viscoelasticity on the locomotion speed and energy consumption of a spherical squirmer swimming by tangential surface deformations, as a model of ciliated protozoa. A non-linear viscoelastic model (Giesekus) was used to describe the polymer dynamics. We showed the dependency of swimming speed, power consumption, and swimming efficiency on the fluid elasticity. This work was however restricted to the most energetically efficient swimming gait, one associated with no vortices generated around the cell in the Newtonian case (a potential flow squirmer in the Newtonian limit).

In the current paper we numerically investigate the hydrodynamic performance of a squirmer utilizing other swimming gaits in a viscoelastic fluid. The gaits correspond to pusher and puller swimmers, a natural distinction for biological organisms. We assume the gait to be steady and thus ignore, as a first model, the oscillatory flow field around a swimming cell. As recently shown by Guasto et al. (2010) and Drescher et al. (2010), the flow field generated by some microorganisms such as Chlamydomonas reinhardtii cannot be accurately described by a steady analysis, and in fact, the flow generated by many swimmers is usually time-periodic, with large fluctuations around the mean. However, the simple steady model we utilize here has been used to understand several fundamental processes related to the physics of swimming microorganisms, such as nutrient uptake (Magar et al. 2003), locomotion in stratified fluid (Doostmohammadi et al. 2012), biomixing (Lin et al. 2011) and the collective behaviour of microorganisms (Evans et al. 2011; Ishikawa & Pedley 2008). Note that in the case of viscoelastic fluids like those studied here, the presence of an additional time scale (stroke frequency) leads to the definition of a Deborah number, different from the Weissenberg number defined below based on shear rates, and possibly leading to a rich dynamical behaviour. Therefore, we assume as in Ref. (Ishikawa et al. 2006) that the stroke frequency is higher than the inverse of the polymer relaxation times and we study the mean motion of a cell averaged over a fast beating period.

The paper is organized as follows. We first investigate in detail how fluid elasticity affects the swimming speed of the spherical model cells applying different locomotive gaits and the resulting polymeric dynamics in the flow field. We then analytically derive a decomposition of the power associated to cell locomotion by surface deformation in the viscoelastic fluid, extending the analysis presented for the Newtonian fluid in Stone & Samuel (1996). We further compute the change in the swimming speed of the squirmer in the viscoelastic fluid under constant-power conditions, as well as the hydrodynamic efficiency. Finally, in order to quantify the influence of the squirmer motion on nearby swimmers as well as on the bulk stress of the surrounding fluid, we analyse the velocity decay around the model swimming cells and calculate their effective stresslets.
2. Mathematical Model

2.1. Squirmer Model

In this so-called envelope approach, first proposed by Blake (1971), one assumes the squirmer imposes a non-zero tangential velocity on its surface, \( u_S \), in the co-moving frame. Here we adopt the concise formulation introduced in Ishikawa & Pedley (2008)

\[
    u_S(r) = \sum_{n \geq 1} \frac{2}{n(n+1)} B_n P_n'(e \cdot r) \left( \frac{e \cdot r r - e}{r} \right),
\]

(1)

where \( e \) is the orientation vector of the squirmer, \( B_n \) is the \( n \)th mode of the surface squirming velocity (Blake 1971), \( P_n \) is the \( n \)th Legendre polynomial, \( r \) is the position vector, and \( r = |r| \). In a Newtonian fluid, the swimming speed of the squirmer is \( U_{\text{New}} = 2B_1/3 \) (Blake 1971) and thus only dictated by the first mode. As in many previous studies (Magar & Pedley 2005; Ishikawa & Hota 2006; Ishikawa & Pedley 2008; Ishikawa et al. 2006), we assume \( B_n = 0 \) for \( n \geq 3 \). The tangential velocity on the sphere in the co-moving frame is therefore expressed as \( u_\theta(\theta) = B_1 \sin \theta + (B_2/2) \sin 2\theta \), where \( \theta = \arccos(e \cdot r/r) \). We introduce an additional parameter \( \alpha \), representing the ratio of the second to the first squirming mode, thus \( \alpha = B_2/B_1 \). When \( \alpha \) is positive, the swimmer get impetus from its front part, and is termed a puller (swimmers in this category include the alga genus Chlamydomonas). As a difference, when \( \alpha \) is negative, the thrust comes from the rear part of the body and the swimmer is a pusher (swimmers in this category include all peritrichous bacteria such as Escherichia coli). If not otherwise stated, here we will present results obtained with \( \alpha = -5 \) (simply denoted as pusher), \( \alpha = 5 \) (puller) and \( \alpha = 0 \) (neutral squirmer inducing a potential velocity field in the Newtonian case).

2.2. Polymeric Dynamics

For steady incompressible low-Reynolds number flow in a viscoelastic fluid, the momentum and continuity equation are written as

\[
    -\nabla p + \nabla \cdot \tau = 0, \quad (2)
\]

\[
    \nabla \cdot u = 0. \quad (3)
\]

The velocity is scaled by \( B_1 \)—related by the expressions above to the magnitude of the velocity of the boundary and to the swimming speed—while lengths are scaled by the diameter of the spherical swimmer \( D \), time is scaled by \( D/B_1 \), and pressure and stresses are scaled by \( \mu B_1/D \), where \( \mu \) is the coefficient of viscosity.

Following classical modelling approaches (Bird 1976; Bird et al. 1987a,b), the deviatoric stress \( \tau \) is split into two components, the viscous solvent stress \( (\tau^s) \) and the polymeric stress \( (\tau^p) \), so \( \tau = \tau^s + \tau^p \). The stress \( \tau^s \) is governed
by Newton’s law of viscosity, thus is formulated as
\[ \tau^s = \beta (\nabla u + \nabla u^T), \]
where \( \beta < 1 \) represents the ratio of the solvent viscosity, \( \mu_s \), to the total zero shear rate viscosity, \( \mu \), of the solution. To close the model, a transport equation for the polymeric stress \( \tau^p \) is required. Here we adopt the nonlinear Giesekus model (Giesekus 1982), which, in addition to displaying shear-thinning material properties (viscosity and normal stress differences), provides two important features, namely saturation of polymer elongation, and a non-negative entropy production during the time evolution of the polymers (see details in Beris & Edwards (1990); Dupret & Marchal (1986); Souvaliotis & Beris (1992)). Violation of these two properties may cause non-physical flow behaviour as well as numerical difficulties. The nondimensional constitutive equation for this model can be written as
\[ \tau^p + \text{We} \tau^p + \frac{\text{We} \alpha_m}{1 - \beta} (\tau^p \cdot \tau^p) = (1 - \beta)(\nabla u + \nabla u^T), \]
where \( \text{We} = \frac{\lambda B_1}{D} \) is the Weissenberg number, defined as \( \text{We} = \frac{\lambda B_1}{D} \), where \( \lambda \) is the polymer relaxation time. The so-called mobility factor \( \alpha_m \) is introduced in the nonlinear stress term to represent an anisotropic hydrodynamic drag on the polymer molecules (Bird et al. 1987a) and limits the extensional viscosity of the fluid. From thermodynamics considerations, the mobility factor \( \alpha_m \) must be in the 0 to 1/2 range (Bird et al. 1987a; Larson 1988), and in this paper we assume \( \alpha_m = 0.2 \).

3. Numerical method
A numerically stable and accurate finite element model is built, based on the formulation denoted Discrete Elastic-Viscous Split Stress (DEVSS-G) (Guénette & Fortin 1995; Liu et al. 1998). The governing equations are rewritten as
\[ \nabla \cdot \mu_a (\nabla u + \nabla u^T) - \nabla p + \nabla \cdot \tau^p - \nabla \cdot (\mu_a - \beta)(G + G^T) = 0, \]
where an additional tensor \( G = \nabla u \) is introduced as an independent interpolation of the velocity gradient tensor \( \nabla u \) and an additional elliptic term \( \nabla \cdot \mu_a (\nabla u + \nabla u^T) - \nabla \cdot G + G^T \) is added into the momentum equation (Sun et al. 1999). In our computations, \( \mu_a \) is chosen to be 1 as in Liu et al. (1998), and the velocity gradient term in equation for the polymeric stress, Eq. (5), is approximated by \( G \).
A Galerkin method is used to discretize the momentum equations, continuity equation, and the equation for the additional unknown $G$. We use quadratic elements for $u$ and linear elements for both $p$ and $G$. To improve the numerical stability, the streamline-upwind/Petrov-Galerkin (SUPG) (Marchal & Crochet 1987) method is used to discretize the constitutive equation, Eq. (5). Finally, the weak form for the constitutive equations is written as

\[
\left\{ \mathbf{S} + \frac{h}{U_C} u \cdot \nabla \mathbf{S}, \quad \tau^p + W e (u \cdot \nabla \tau^p - G^T \cdot \tau^p - \tau^p \cdot G + \frac{\alpha_m}{1-\beta} (\tau^p \cdot \tau^p)) - (1-\beta)(G + G^T) \right\} = 0,
\]

where $\mathbf{S}$ denotes the test function for $\tau^p$, $h$ is the characteristic length-scale of the element and $U_C$ is the magnitude of the local characteristic velocity. In our case, we choose the norm of $u$ as the value of $U_C$. The finite-element framework for our implementation is provided by the commercial software COMSOL.

We perform three-dimensional axisymmetric simulations on a two-dimensional mesh. Triangle elements are used for all the simulations and the number of elements are dependent on the swimming gait. We generate sufficiently refined mesh in regions with high magnitude of polymeric stress to overcome numerical instabilities (Baaijens 1998; Walters & Webster 2003). In all cases, high resolution near the cell body is required in order to resolve the thin stress boundary layers. Fine meshes are also necessary to capture the high polymer elongation rates. Typical mesh size at the cell boundary is $5E10^{-4}$ of the reference (swimmer) length. The total number of elements used for the results reported here ranges from 150,000 to 250,000.

The numerical implementation is first validated against the theoretical results for the swimming speed and power of squirmers of different gaits in Newtonian fluids (Blake 1971). For viscoelastic fluids, we validate the present numerical approach against the simulations in Lunsmann et al. (1993) of a sphere sedimenting in a tube filled with an Oldroyd-B fluid (the mobility factor $\alpha_m$ equals to zero) and against the results in G. & Harlen (2002) where the authors numerically study the negative wake of a sphere sedimenting in a tube filled with a Giesekus fluid.

4. Swimming speed in viscoelastic fluids

To illustrate the difference between the swimming modes considered, the flow fields generated by a pusher and a puller in a Newtonian fluid are shown in figure 1, where data for the pusher are displayed on the left of each panel, and those for the puller on the right. Vectors display the in-plane velocity magnitude and direction while the background colour indicates velocity magnitudes. We see an axisymmetric vortex ring generated in the front of the pusher and behind the puller; as a difference the neutral swimmer generates a symmetric velocity field with no vorticity (Zhu et al. 2011).
To address the dynamics in a viscoelastic fluid, we first examine the dependency of the squirmer swimming speed, $U$, on the Weissenberg number, $We$. The swimming speed is computed as in Zhu et al. (2011). Simulations are performed in the co-moving frame with different values of the inflow velocity, and the total force on the body is computed. The swimming speed is then estimated by interpolating to the inflow velocity yielding zero net force on the swimmer. A new simulation is then performed to ensure that the value of the predicted swimming speed used as free-stream velocity indeed gives values of the total force below a given tolerance. The numerical results are shown in figure 2, for three different swimming gaits, where the swimming speed is scaled with the speed of the Newtonian squirmer, $U_{\text{New}} = 2B_1/3$.

Considering the data in figure 2, we first observe that viscoelasticity clearly distinguishes between the three swimming gaits in terms of $U$, while they produce the same swimming speed in the Newtonian fluid. The neutral gait, $\alpha = 0$, generally gives the highest value of $U$ for most $We$ numbers while pushers generally have the lowest velocity. Second, for all the gaits and $We$ numbers considered here, the swimming speed of swimmers in the viscoelastic fluid is lower than that of swimmers in the Newtonian fluid. Finally, for all three gaits, $U$ systematically displays a minimum in the range of $We$ considered. The swimming speed initially decreases as $We$ increases from 0, while it eventually always increase for the largest values of $We$. The value of the
Figure 2. Nondimensional swimming speed, $U$, of the swimmer as a function of the Weissenberg number, $We$, for pusher $\alpha = -5$ (squares, green), puller $\alpha = 5$ (triangles, blue) and neutral squirmer $\alpha = 0$ (circles, red). The swimming speed is scaled by its corresponding value in the Newtonian fluid, $U_{New}$.

Weissenberg number corresponding to the minimum swimming speed varies with the gait: it increases from 0.5 to 4 when moving from puller to neutral to pusher.

Different swimming gaits generate different polymer dynamics around the swimmer and this, in turn, influences the swimming speed as shown above. To gain insight into the numerical results, we start by showing in figure 3 the distribution of axial polymeric stress, $\tau_{zz}$, for the neutral swimmer ($\alpha = 0$) in the cases $We = 0.1$ and $We = 2$. The value $We = 0.1$ is chosen since it is close to the Newtonian case ($U = 0.987$), while $U$ is close to the minimum swimming speed when $We = 2$. As seen in the figure, there exists a significant difference in the $\tau_{zz}$ distribution behind the swimmer. In the case $We = 2$, the magnitude of $\tau_{zz}$ is much higher, indicating a higher extent of polymer stretching in this region. As suggested in figure 1, an elongational flow (Bird et al. 1987a) is generated aft the cell body. In the viscoelastic fluid such flow would be responsible for polymer stretching which in return increases the local elongational viscosity (Dealy 1984, 1994), yielding a strong elastic resistance against locomotion. We further see in figure 3 that, upon increasing the polymer relaxation time to $We = 6$, the region of largest elongation becomes narrower and closer to the pole, leading to a reduced elastic resistance and consistent with the results of figure 2.
Figure 3. Distribution of the $\tau_{zz}^p$ component of the polymeric stress for the neutral squirmer and three values of the Weissenberg number, $We = 0.1, 2$, and $6$. (Left: $We = 0.1$ and $2$. Right: $We = 6$ and $2$.)

Figure 4. Distribution of the $\tau_{zz}^p$ component of the polymeric stress for the pusher (left) and puller (right) swimming in the viscoelastic fluid. For both gaits, $We = 0.1$ and $We = 2$ are chosen for comparison. The inset plots show regions with high value of $\tau_{zz}^p$.

The polymer contribution for the pusher swimmer is displayed in figure 4 (left). In this case, the kinematics of surface deformation draws fluid from the side and pushes it towards the two poles, resulting in strong elongational flows at the poles (see figure 1). Such flow aligns the polymer chains near the poles.
Figure 5. Distribution of the $\tau_{zz}$ component of the polymeric stress along the symmetry axis. Shaded circles and arrows indicate the squirmer and its swimming direction. Data for the pusher are shown in the top whereas the neutral squirmer and the puller are reported at the bottom. The solid and short-dashed lines correspond to $\text{We} = 0.1$, the long-dashed and dot-dashed lines to $\text{We} = 2$.

in the swimming direction, leading to high elongational viscosities in the front of and behind the squirmer. Comparing figure 3 and figure 4, we see that the magnitude of $\tau_{zz}$ on the back is much larger in the case of pushers. This is further illustrated in figure 5 where we display the value of the normal polymeric stress along the symmetry axis. It is noteworthy that for the pusher squirmer, significant $\tau_{zz}$ is evident also in the region ahead of the body. In this case, the stretched polymers might contribute an elastic driving force on the swimmer. However, the magnitude of $\tau_{zz}$ at the front is lower than that behind, and thus the net effect is that of an additional drag. Note that for the neutral squirmer, the region of polymer elongation becomes narrower at large $\text{We}$ and we observe a recovery of the swimming speed.

We then consider the puller swimmer, which is about 20% faster than the pusher (as seen in figure 2). The polymeric stresses in this case are shown in Figs. 4 (right), 5 and 6. The results in figure 6 are displayed for $\text{We} = 0.5$, corresponding to the minimal swimming speed for the viscoelastic puller (and thus the maximum influence of viscoelastic stresses). In the case of pullers, the inward velocity imposed by the surface deformation on the front and back of the body takes fluid away from the back of the swimmer, and thus stretched fluid is removed from the region behind the body. As shown in figure 5, $\tau_{zz}$ is
Figure 6. Distribution of the $\tau_{zz}^p$ and $\tau_{rz}^p$ components of the polymeric stress for pullers in the viscoelastic fluid with $We = 0.5$. Both the $\tau_{zz}^p$ and $\tau_{rz}^p$ components lead to a net polymeric (elastic) force indicated by the gray arrows, hindering locomotion. The location of this elastic forces is right above the vortex ring, implying that they are generated by the elongational flow.

smaller for the puller than for the neutral squirmer in the region immediately behind the body. One may thus expect the puller may swim faster than the neutral squirmer. However, large magnitude of $\tau_{zz}$ and $\tau_{rz}$ are observed in conjunction to the vortex ring, with maximum values attained near the swimmer surface. Both components contribute to a polymeric (elastic) force applied on the swimmer as indicated by the grey arrows in figure 6. We observe an elongational flow generated on top of the vortex ring, and polymer chains stretched by such flow result in a strong force opposing the swimmer motion, possibly explaining why the puller swimmer is not faster than the neutral squirmer despite displaying a significant reduction in polymer stretching behind its body.

To summarize, we observe elongational flows generated by all three swimmers around their bodies (neutral squirmer, pusher, and puller). The strength, orientation and position of the elongational flow is dependent on the swimming gaits. Such flows yield increasing elongational viscosities which serve as an additional elastic force, possibly positive or negative, to the locomotion. For the three gaits considered here, the force is predominantly resistive, thus impeding locomotion. These computational results are in agreement with a recent experimental study of swimming Caenorhabditis elegans in polymeric
fluids where the authors suggest that elongational viscosities can explain the measured decrease in swimming speeds (Shen & Arratia 2011).

5. Swimming power in viscoelastic fluids

![Swimming Power Diagram](image)

Figure 7. Swimming power, $P$, for pusher (squares, green), puller (triangles, blue) and neutral (circles, red) squirmers, nondimensionalized by the swimming power in the Newtonian case, $P_{\text{New}}$. The power consumption of swimming in the Newtonian fluid are equal to $P_{\text{New}} = 8/3\pi$ (neutral squirmer) and $P_{\text{New}} = 36\pi$ (both pusher and puller).

The mechanical power, $P$, expended by the spherical squirmer is reported as a function of the Weissenberg number, $We$, for the three different gaits under investigation in figure 7. When considering dimensional quantities, we observe that both the puller and pusher require significantly more power than the neutral squirmer due to the strong vortex rings (see figure 1). Indeed, as reported in Blake (1971), $P$ grows quadratically with the dipole magnitude $\alpha$. In order to factor out the influence of the swimming gait on the power expenditure, thereby isolating the effect of elasticity on the energy budget, we normalize the power with its corresponding value in the Newtonian fluid, termed $P_{\text{New}}$. In figure 7, we observe a significant reduction in power in the viscoelastic fluid for all gaits; $P$ decreases first rapidly in the range $We \in [0,2]$, and tends to an asymptotic value when further increasing the polymer relaxation time. The limiting value of $P$ for $We \gg 1$ is close to half the value of the Newtonian case ($We = 0$), namely, $P|_{We\gg1}/P_{\text{New}} \approx 0.5$. The result is in agreement with the asymptotic analysis of Lauga (2007) which predicts $P|_{We\gg1}/P_{\text{New}} = \beta$ ($\beta = 0.5$ for the computations presented here).
As we will show below, the component of the power consumption associated with the Newtonian solvent is almost constant with variations in \( W_e \), while the contribution of the polymeric stresses decreases significantly (up to one order of magnitude decrease at large \( W_e \)). Since, for \( \beta = 0.5 \), the Newtonian and polymeric contribution are the same for \( W_e = 0 \), the power at large Weissenberg numbers is about half that of a Newtonian fluid.

To probe the power saving for microswimmers in viscoelastic fluids, we decompose the power into three parts. First, we use the divergence theorem to transform the total power, \( P \), which is the integral of the stress at the surface times the swimming speed, into a volume integral as done in Stone & Samuel (1996)

\[
P = -\int_S \mathbf{u} \cdot \mathbf{\tau} \cdot \mathbf{n} dS = \int_V \nabla \cdot (\mathbf{u} \cdot \mathbf{\tau}) dV,
\]

where \( \mathbf{n} \) is the unit normal outward the swimmer surface \( S \), \( \mathbf{u} \) is the velocity in the laboratory frame and \( \mathbf{\sigma} \) is the stress tensor introduced above. Rearranging the integrand, one can write

\[
\nabla \cdot (\mathbf{u} \cdot \mathbf{\tau}) = \beta \mu \omega^2 + 2\beta \mu (\nabla \mathbf{u} : \nabla \mathbf{u}) + \mathbf{E} : \mathbf{\tau}_p.
\]

Consequently, \( P \) is found to be the sum of three contributions, \( P = P_\Omega + P_{DV} + P_P \); a component related to the flow vorticity, \( P_\Omega = \int_V \beta \mu \omega^2 dV \), a component related to the velocity gradient, \( P_{DV} = \int_V 2\beta \mu (\nabla \mathbf{u} : \nabla \mathbf{u}) dV \), and a polymeric component, \( P_P = \int_V \mathbf{E} : \mathbf{\tau}_p dV \), where \( \mathbf{E} \) is the rate-of-strain tensor. The component related to the velocity derivative, \( P_{DV} \), is only dependent on the tangential velocity distribution we impose on the surface and thus is only a function of \( \alpha \). This can be seen by re-writing

\[
P_{DV} = 2\beta \mu \int_V (\nabla \mathbf{u}) : (\nabla \mathbf{u}) dV = -2\beta \mu \int_S \mathbf{n} \cdot (\mathbf{u} \cdot \nabla \mathbf{u}) dS.
\]

The three different contributions to the total consumed power are displayed in figure 8 as a function of the Weissenberg number, \( W_e \), for two swimming gaits, neutral swimmer (left panel) and puller (right panel). Energetic results for pushers are qualitatively similar to those for pullers. First note that for \( W_e = 0 \) and our choice \( \beta = 0.5 \), the power component due to the polymeric stress is \( P_P = P_\Omega + P_{DV} \). As seen from the definition of the polymeric model, \( \mathbf{\tau}_p \) reduces to Newtonian stress \( (1 - \beta)(\nabla \mathbf{u} + \nabla \mathbf{u}^T) \) when \( W_e = 0 \) in Eq. (5).

For a fixed mode of surface motion, \( P_{DV} \), is strictly constant with \( W_e \) since it depends only on the values of the velocity at the surface (see Eq.11). For both gaits, we observe computationally that the vorticity contribution, \( P_\Omega \), shows little variations with \( W_e \). The major contribution to the reduction in swimming power stems thus from the significant reduction of the polymeric part, \( P_P \), with increasing values of the Weissenberg number.

The contribution of polymeric stresses to the consumed power is the double dot product of two tensors, the rate-of-strain tensor, \( \mathbf{E} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \), and
Figure 8. Contributions to the total power expended by swimming, $P$, versus Weissenberg number $We$, $\beta = 0.5$, for neutral squirmer (left) and puller (right). The three contributions are defined as: $P_\Omega = \int_V \beta \mu \omega^2 dV$, $P_{DV} = \int_V 2\beta \mu (\nabla u : \nabla u) dV$ and $P_P = \int_V E : \tau_p dV$.

the polymeric stress tensor, $\tau_p$. Polymer chains get stretched by the rate-of-strain. In fluids with low relaxation times, polymeric stretching occurs immediately, resulting in high spatial correlation between the polymeric stress tensor and the rate-of-strain tensor. Thus, the product of the two tensors takes large values. In contrast, for fluids with large relaxation times, polymer chains get fully stretched at a position far away from where they get excited, and the spatial correlation of the two tensors decreases. Polymeric deformation and rate-of-strain become therefore separated in space as $We$ increases, which gives a systematically smaller power consumption, as observed computationally.

In figure 9, we plot the power density, $D_P = 2\pi |r| E : \tau_p$, for the spherical pusher for two different values of $We$. When $We = 0.1$ (left half of the figure), large values of $D_P$ are observed in the region very close to the swimmer, especially in the equatorial region. This is the region where most of the energy is expended to elongate the polymers. A region of positive $D_P$ also exists near the equatorial $z = 0$ plane for the case with $We = 2$ shown on the right, although of reduced size. In addition, negative density can be seen on the planes $z \approx \pm 0.4$ (indicated by elliptical circles in the figure), which can also be clearly identified in figure 10 where we display the value of $D_P$ evaluated along the surface of the pusher. These areas of negative power density produce further decrease of the total expended power by providing energy to the system. This energy analysis allows us to understand the reduction in swimming power observed in viscoelastic fluids for any type of surface deformation considered.
Self-propulsion in viscoelastic fluids: pushers vs. pullers

Figure 9. Polymeric power density, $D_P$, for pushers in fluids with $We = 0.1$ (left) and $We = 2$ (right). Dotted elliptical circles mark areas with negative values of $D_P$. The values of $D_P$ along the swimmer surface are displayed in figure 10.

Figure 10. Spatial distribution of polymeric power density, $D_P$, along the surface of pushers in viscoelastic fluids with $We = 0.1$ (solid line, red) and 2 (dashed line, blue); $\theta$ is defined in Sec. 2, as the angle between the swimming direction and the position vector of each point.

We finally consider the situation of locomotion at constant power. Some bacteria have been observed to swim with kinematics consistent with constant-power conditions (Schneider & Doetsch 1974), and it is thus interesting to
consider the swimming speed which would be attained by squirmers if they were under the constraints of expending the same power as in a Newtonian fluid (the results in figure 2 were obtained at constant intensity of the velocity at the boundary). The swimming speed obtained rescaling the previous data to obtain constant-power locomotion is displayed in figure 11. To calculate the velocity at constant power, we need to increase the value of the surface velocity $B_1$ to account for the power-saving in polymeric fluid discussed above. If we use $B'_1$ to denote the new value of $B_1$, constant power requirement is written as $(B'_1)^2 P|_{We(B'_1)} = B_1^2 P_{New}$, where $We(B'_1) = \frac{\lambda B'_1}{D} = \frac{B'_1}{B_1} We$; we use a simple interpolation from our computational results in order to obtain $P|_{We(B'_1)}$. Thus, the swimming speed with constant power is computed as $\tilde{U} = \frac{B'_1}{B_1} U|_{We(B'_1)}$. As can be seen in figure 11, $\tilde{U}$ is found to be systematically larger than that in the Newtonian conditions for all the cases considered, and the swimming speed systematically increases with the Weissenberg number. The puller and the neutral squirmers are about 20% faster than the pusher.
6. Swimming Efficiency in viscoelastic fluids

The hydrodynamic efficiency of squirmers in viscoelastic fluid is displayed in figure 12. The efficiency is defined as the ratio between the rate work needed to pull a sphere of same size in the same fluid at the swimming speed $U$ and the swimming power $P$ of a self-propelled swimmer (S. Michelin & Lauga 2010; Lauga & Powers 2009)

$$\eta = \frac{F U}{P},$$

where $F$ is the force required to drag the spherical squirmer body at the speed $U$. Similarly to what we did for the power consumption, the efficiency is normalized in figure 12 by its Newtonian value. We observe that all swimmers have a higher swimming efficiency than in a Newtonian fluid. For all three gaits, as $We$ increases from 0, the scaled efficiency firstly increases rapidly with $We$, then decreases asymptotically. We can thus identify an optimal $We$ number corresponding to the maximum efficiency; this is around 2 for the neutral and puller swimmer and around 0.5 for the pusher.

![Figure 12. Swimming efficiency, $\eta$, normalized by the corresponding value for Newtonian swimming, $\eta_{\text{New}}$, versus Weissenberg number, $We$. The efficiencies of swimming in the Newtonian fluid are equal to $\eta_{\text{New}} = 0.5$ (neutral squirmer) and $\eta_{\text{New}} = 0.037$ (both pusher and puller).](image)

7. Velocity decay in viscoelastic fluids

Because of its implications to collective cell behaviour (Shen & Arratia 2011; Lauga & Powers 2009), it is of interest to investigate the effect of the fluid elasticity on the spatial decay of the flow perturbation induced by the swimming motion. We compute the axial velocity along the symmetry axis of the
domain for the pusher and puller (similar analysis was carried out for the neutral swimmer in our previous paper (Zhu et al. 2011)). The velocity decays with a power-law behaviour, $|u| \sim 1/r^\gamma$, with $\gamma = 2$ in the Newtonian case for both pushers and pullers, as sufficiently far away from the cell the higher order terms ($1/r^3$ and $1/r^4$) give negligible contribution to the flow field ($\gamma = 3$ in the neutral potential-flow case). In the non-Newtonian case, we estimate the value of $\gamma$ by fitting a power law to the numerical results in a measurement region extending from about $r \approx 5D$ to the end of the computational domain. The estimated values of $\gamma$ are displayed in figure 13 as a function of the Weissenberg number, $We$. We see clearly that the velocity always decays faster in viscoelastic fluids than in the Newtonian fluid. For both pusher and puller, $\gamma$ is not monotonically increasing when with $We$, but instead reaches a maximum value at intermediate Weissenberg numbers. The maximum value of $\gamma$ is seen to take place as $We$ is around 5 for the pusher and around 1 for the puller, which approximately corresponds with the values of the Weissenberg numbers at which the swimming speed, $U$, is minimum for both gaits (although slightly above). We thus observe a negative correlation between the swimming speed and the velocity decay rate. We further note that the velocity decay rate is larger for the pusher than for the puller, which is consistent with our observation of the negative correlation as the swimming speed of a pusher is smaller than that of a puller.

![Figure 13](image-url)

**Figure 13.** Power law exponent, $\gamma$, for spatial decay of the axial velocity along the axis of the domain ($r = 0$) ($|u| \sim r^{-\gamma}$, see text), as a function of the Weissenberg number, $We$. The inset plot highlights the difference between pusher and puller.
8. Stresslet in viscoelastic fluids

In this final section we address how the viscoelastic modification of the squirming motion would affect the rheology of an active suspension of squirmers. When the size of the microorganisms is much smaller than the scale of the flow field under consideration, it is convenient to use a continuum model of the active suspension. The first order correction to the bulk viscosity in terms of the volume fraction of swimmers is then given by the stresslet associated with an individual swimmer. Batchelor (1970) derived a relation between the bulk stress and the conditions at the surfaces of individual particles embedded in a Newtonian solvent (his original formulation is given in dimensional form and we present the nondimensional version here using the scaling we introduced in Sec. 2). The bulk stress \( \hat{\sigma} \) is given by

\[
\hat{\sigma} = I \cdot T + 2 \bar{E} + \sigma',
\]

where \( I \cdot T \) is an isotropic tensor, i.e. \( I \cdot T = \hat{\sigma}_{kk} I \), \( \bar{E} \) is the volume-averaged rate-of-strain tensor \( \bar{E}_{ij} = \frac{1}{2V} \int_V \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \, dV \), where \( V \) is the volume occupied by the fluid and the particles) and \( \sigma' \) represents the disturbance stress due to the presence of squirmers; see also Ishikawa et al. (2007) for the application to active suspensions in Newtonian fluids. The particle bulk stress \( \sigma' \) induced by force- and torque-free particles (such as swimmers) in the volume \( V \) can be expressed as

\[
\sigma' = \frac{1}{V} \sum S,
\]

where \( S = \int_{A_S} \left[ \frac{1}{2} \left( (\sigma \cdot n) x + x (\sigma \cdot n) \right) - \frac{1}{3} x \cdot \sigma \cdot n I - (u n + n u) \right] \, dA. \quad (15)
\]

The stress is thus given by the volume average of the so-called stresslet \( S \), where the sum is taken over all the swimmers. The stresslet \( S \) is defined Eq. (15) where \( \sigma \) is the stress tensor, \( A_S \) is the surface of one of the squirmers, \( n \) is the unit outward normal vector, \( x \) is the position vector and \( I \) is the unit tensor.

Ishikawa et al. (2006) exploited the formulation above to study the stresslet \( S \) of a single squirmer and a pair of squirmers in the Newtonian fluid both analytically and numerically. They showed that for single squirmers

\[
S = \frac{1}{3\pi} (3ee - I) B_2,
\]

where \( e \) is the swimming direction and \( B_2 \) the second squirming mode defined in Sec. 2. The assumption of axisymmetric bodies makes the off-diagonal part of \( S \) zero. In a Newtonian fluid, the first mode \( B_1 \) determines the swimming speed while \( B_2 \) the stresslet magnitude; the stresslet of a neutral squirmer \( (B_2 = 0) \) is therefore zero.

In order to derive a similar formalism for a squirmer in a non-Newtonian flow, we consider the additional polymeric contribution, \( \tau^p \), to the Newtonian
stress, $\sigma = -pI + \beta (\nabla u + \nabla u^T) + \tau_p$. The same derivation as in Batchelor (1970); Batchelor & Green (1972) can be performed for non-Newtonian fluids, see for example Ref. Patankar & Hu (2001). In our case, we seek an expression for $\sigma' = I.T. + 2\beta \bar{E} + \bar{\tau}_p + \sigma'$. The total bulk stress can be written as (Batchelor 1970)

$$\bar{\sigma} = \frac{1}{V} \int_{V - V_S} \{ -pI + \beta (\nabla u + \nabla u^T) + \tau_p \} dV + \frac{1}{V} \int_{V_S} \sigma dV,$$

(18)

where $V_S$ is the volume occupied by the squirmer. Combining Eq. (17) and Eq. (18), we have

$$\sigma' = \frac{1}{V} \int_{V_S} \beta (\nabla u + \nabla u^T) dV - \frac{1}{V} \int_{V_S} \tau_p dV + \frac{1}{V} \int_{V_S} \sigma dV.$$

(19)

The volume integral of the Newtonian contribution to the total stress inside the squirmer is re-written as a surface integral by applying the divergence theorem: the first term on the right hand side of Eq. (19) becomes $\frac{1}{V} \int_{A_S} \beta (\mathbf{un} + \mathbf{nu}) dA$, whereas the total stress inside the particles contributes to the stresslet

$$\int_{V_S} \sigma dV = \int_{A_S} (\mathbf{\sigma} \cdot \mathbf{n}) x dA - \int_{V_S} (\nabla \cdot \mathbf{\sigma}) x dV,$$

(20)

where we have assumed $\nabla \cdot \mathbf{\sigma} = 0$ inside the solid body. For a swimming squirmer which is force-free and torque-free, $(\mathbf{\sigma} \cdot \mathbf{n}) x = \frac{1}{2} \{ (\mathbf{\sigma} \cdot \mathbf{n}) x + x (\mathbf{\sigma} \cdot \mathbf{n}) \} - \frac{1}{3} x \cdot \mathbf{\sigma} \cdot \mathbf{n} I$ as in Ishikawa et al. (2006). Finally we obtain the new definition of the stresslet

$$\mathbf{S} = \int_{A_S} \left[ \frac{1}{2} \{ (\mathbf{\sigma} \cdot \mathbf{n}) x + x (\mathbf{\sigma} \cdot \mathbf{n}) \} - \frac{1}{3} x \cdot \mathbf{\sigma} \cdot \mathbf{n} I - \beta (\mathbf{un} + \mathbf{nu}) \right] dA - \int_{V_S} \tau_p dV.$$

(21)

The stresslets $\mathbf{S}$ computed from Eq. (21) for the pusher ($\alpha = -5$), puller ($\alpha = 5$) and neutral squirmer ($\alpha = 0$) are displayed in figure 14. Because of axisymmetry, there are only two non-zero components of $\mathbf{S}$, namely, the $rr$ component in the direction normal to the swimming direction and the $zz$ component in the swimming direction.

First, we see that for the pusher and puller the magnitude of both the $rr$ and $zz$ components decreases monotonically with increasing $We$, and reaches an asymptotic value (while keeping the same sign). This corresponds to a maximum decrease of approximately 20% with respect to the Newtonian value at $We = 10$. This implies that a dilute suspension of swimming cells will have a weaker rheological effect in a viscoelastic fluid.

The decrease in the stresslet can tentatively be explained by the fact that the polymeric stress always opposes the flow which generates it. Let us consider
Self-propulsion in viscoelastic fluids: pushers vs. pullers

Figure 14. Stresslets induced by swimmers in viscoelastic fluids: \( rr \) and \( zz \) components of the tensor \( S \), Eq. (21), for different swimming gaits. Left: pusher (\( \alpha = -5 \)) and puller (\( \alpha = 5 \)). Right: neutral squirmer (\( \alpha = 0 \)).

Interestingly, we also observe in figure 14 that for the neutral squirmer, which has zero stresslet in the Newtonian limit, viscoelastic stresses induce a non-zero stresslet. The value of the \( rr \) component is lower than that of the \( zz \) component and of same sign. Considering two squirmers swimming in the same direction side by side, at leading order in their separation distance they have no influence on each other in a Newtonian fluid, but will repel each other due to the negative value of the \( rr \) component of the stresslet. Similarly, two neutral squirmers swimming in line along the same swimming direction will tend to increase their relative distance owing to the negative value of the \( zz \) component of the stresslet. The peak value of the \( rr \) and \( zz \) components occur at \( We \approx 1 \), at which the minimum swimming speed of the neutral squirmer appears, as well as the fastest velocity decay. Interestingly, this viscoelastic repulsion between swimming squirmers has the sign opposite to the viscoelastic attraction observed between sedimenting spheres in polymeric fluids.
9. Conclusion

In the current paper, we numerically compute the swimming speed, power, and hydrodynamic efficiencies of model ciliated cells swimming in a viscoelastic Giesekus fluid. We use the squirmer model where the self-propulsion is driven by tangential surface deformation and consider three types of boundary conditions to mimic swimming gaits typical of cell locomotion (potential squirmer, pusher, and puller) all having the same swimming speed in a Newtonian fluid. The characteristics of the flow and of the polymeric stress are examined to help understand our computational results.

For constant magnitude of the surface deformation velocity, we show that the swimming speed decreases in the viscoelastic fluid compared its the Newtonian value for all cases considered, with a minimum obtained at intermediate values of the Weissenberg number. Neutral swimmer and puller have the highest velocity, whereas the pusher is about 15% slower. For the potential squirmer and the pusher, the reduced self-propulsion is explained by the accumulation of highly stretched polymers behind the body. For low values of the polymer relaxation times, \( We \ll 1 \), the stretching of the polymers increases hence the initial decrease in the swimming speed. For the largest values of the Weissenberg number, however, the region of stretched polymers behind the swimmer becomes thinner and the induced elastic resistance decreases, thus explaining the slow recovery of the swimming speed. In the case of pullers, a different velocity field is created and stretched polymers are advected away from the cell on the sides. This induces a force with a component both in the radial and axial direction, the latter explaining the reduced swimming speed. Similar kinematic analysis could be used to provide detailed guidelines for the design of efficient swimmers in viscoelastic fluids - the basic design principle consisting in reducing the accumulation of stretched polymers at the cell surface in the direction of motion.

Along with the decrease in swimming speed, we observe a significant reduction of swimming power in all cases. To understand this observation, we analytically decompose the expression for the power expended by cells swimming in viscoelastic fluids into three contributions (integrals over the flow domain): one associated to the vorticity induced in the flow, one only set by the surface deformation, and one related to the polymeric stresses. In this way, we are able to clearly identify the reduction in consumed power with a reduction in the polymeric contribution and interpret the observed reduction in power as due to an increasing spatial de-correlation between the flow shear and the induced polymer deformation. In addition, we observe regions of negative power density indicating that the polymers in the fluid have the capacity to first transform the mechanical energy into potential energy (polymer deformation), and then feed it back to the fluid thus reducing the consumed power. We also consider
the hydrodynamic efficiencies and show that self-propulsion is always more efficient in a viscoelastic fluid, with a maximum relative efficiency obtained for intermediate values of the Weissenberg number.

We further investigate the influence of the fluid elasticity on the decay rate of the perturbation velocity induced by the squirmer. We find that the decay rate is faster in viscoelastic fluid and is larger for the pusher than for the puller. Finally, to address the influence of viscoelasticity on the rheology of an active suspension of swimmers, we extract from the computational results the stresslet associated with an isolated swimmer. Notably, viscoelasticity induces a non-zero stresslet for the potential squirmer (rigorously equal to zero in the Newtonian case). As a difference, the magnitude of the stresslet for both pushers and pullers decrease by about 20%. These results presents a first quantitative step toward an understanding of the dynamics and rheology of active suspensions in viscoelastic fluids.

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Self-propulsion in viscoelastic fluids: pushers vs. pullers


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Low-Reynolds number swimming in a capillary tube

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We use the boundary element method to study the low-Reynolds number locomotion of a spherical model microorganism in a circular tube. The swimmer propels itself by tangential or normal surface motion in a tube whose radius is of the order of the swimmer size. Hydrodynamic interactions with the tube walls significantly affect the average swimming speed and power consumption of the model microorganism. In the case of swimming parallel to the tube axis, the locomotion speed is always reduced (resp. increased) for swimmers with tangential (resp. normal) deformation. In all cases, the rate of work necessary for swimming is increased by confinement. Swimmers with no force-dipoles in the far field generally follow helical trajectories, solely induced by hydrodynamic interactions with the tube walls, and in qualitative agreement with recent experimental observations for \textit{Paramecium}. Swimmers of the puller type always display stable locomotion at a location which depends on the strength of their force dipoles: swimmers with weak dipoles (small $\alpha$) swim in the centre of the tube while those with strong dipoles (large $\alpha$) swim near the walls. In contrast, pusher swimmers and those employing normal deformation are unstable and end up crashing into the walls of the tube. Similar dynamics is observed for
swimming into a curved tube. These results could be relevant for the future design of artificial microswimmers in confined geometries.

1. Introduction

The locomotion of self-propelled microorganisms have recently attracted sizeable attention in both the applied mathematics and biophysics communities (Berg 2000; Brennen & Winet 1977; Fauci & Dillon 2006; Lauga & Powers 2009; Lighthill 1975, 1976; Yates 1986; Purcell 1977). A number of novel phenomena have been discovered, including the dancing behaviour of pair Volvox algae (Drescher et al. 2009), the collective motion of motile Bacillus subtilis bacteria (Dombrowski et al. 2004), and tumbling dynamics of flagellated Chlamydomonas (Polin et al. 2009; Stocker & Durham 2009). One area of particularly active research addresses the variation in cell mobility as a response to complex environments, including the dependence on the rheological properties of the medium where cells swim (Elfring et al. 2010; Fu et al. 2008; Lauga 2007; Shen & Arratia 2011; Zhu et al. 2011, 2012; Liu et al. 2011), the presence of an external shear flow (Hill et al. 2007; Kaya & Koser 2012), gravity (Durham et al. 2009), or a sudden aggression (Hamel et al. 2011).

Many microorganisms swim close to boundaries, and as a result the effect of boundaries on fluid-based locomotion has been extensively studied. E. coli bacteria display circular trajectories near boundaries, clockwise when the wall is rigid (Lauga et al. 2006) and anti-clockwise near a free surface (Leonardo et al. 2011). Experiments, simulations, and theoretical analysis are employed to investigate locomotion near a plane wall (Berke et al. 2008; Fauci & Mcdonald 1995; Goto et al. 2005; Katz 1974, 1975; Ramia et al. 1993; Shum et al. 2010; Smith et al. 2009; Spagnolie & Lauga 2012) explaining in particular the accumulation of cells by boundaries (Berke et al. 2008; Drescher et al. 2011; Fauci & Mcdonald 1995; Ramia et al. 1993; Shum et al. 2010; Smith et al. 2009). Most of these past studies consider the role of hydrodynamic interaction in the kinematics and energetics of micro-scale locomotion, developing fundamental understanding of how microorganisms swim in confined geometries.

Although most past studies consider interactions with a single planar, infinite surface, microorganisms in nature are faced with more complex geometries. For example, mammalian spermatozoa are required to swim through narrow channel-like passages (Katz 1974; Winet 1973), Trypanosoma protozoa move in narrow blood vessels (Winet 1973), and bacteria often have to navigate microporous environments such as soil-covered beaches and river-bed sediments (Biondi et al. 1998).

Locomotion of microorganisms in strongly confined geometries is therefore biologically relevant, and a few studies have been devoted to its study. An
Low-Reynolds number swimming in a capillary tube

Experimental investigation was conducted by Winet (1973) to measure the wall drag on ciliates freely swimming in a tube. Perturbation theory was employed to analyse the swimming speed and efficiency of an infinitely long model cell swimming along the axis of a tube (Felderhof 2010). Numerical simulations using multiple-particle collision dynamics were carried out to study the motion of model microswimmers in a cylindrical Poiseuille flow (Zöttl & Stark 2012). Recent experiments (Jana et al. 2012), which originally inspired the present paper, showed that Paramecium cells tend to follow helical trajectories when self-propelling inside a capillary tube.

In this article, we model the locomotion of ciliated microorganisms inside a capillary tube. Specifically, we develop a boundary element method (BEM) implementation of the locomotion of the squirmer model (Blake 1971; Lighthill 1952) inside straight and curved capillary tubes. The boundary element method has been successfully used in the past to simulate self-propelled cell locomotion at low Reynolds numbers (Ishikawa et al. 2006; Nguyen et al. 2011; Ramia et al. 1993; Shum et al. 2010). Our specific computational approach is tuned to deal with strong geometrical confinement whereas traditional BEM show inaccuracy when the tube becomes too narrow (Pozrikidis 2005).

After introducing the mathematical model, its computational implementation and validation, we calculate the swimming speed and power consumption of spherical squirmers with different swimming gaits inside a straight or curved capillary tube. The effect of tube confinement, swimming gait, and cell position is investigated. By studying trajectories of squirmers with varying initial cell positions and orientations, we show that cells end up either swimming parallel to the tube axis or performing wavelike motions with increasing/decreasing wave magnitudes. The dynamic stability of the cell motion is also analysed revealing the importance of the swimming gaits. In particular, squirmers employing the gait leading to minimum work against the surrounding fluid are seen to generically execute helical trajectories, in agreement with the experimental observation of swimming Paramecia inside a capillary tube (Jana et al. 2012).

2. Mathematical Model

2.1. Squirmer model

In this work we use steady squirming as a model for the locomotion of ciliated cells such as Paramecium – more specifically, as a model for the envelope of the deforming cilia tips at the surface of the cells. This steady model has been employed in the past to address fundamental processes in the physics of swimming microorganisms, such as nutrient uptake (Magar et al. 2003), locomotion in stratified and viscoelastic fluids (Doostmohammadi et al. 2012; Zhu et al. 2012).
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2012), biomixing (Lin et al. 2011), and the collective behaviour of microorganisms (Evans et al. 2011; Ishikawa & Pedley 2008; Underhill et al. 2008). Furthermore, simulations of two interacting Paramecium using the squirmer model showed good agreement with corresponding experiments (Ishikawa & Hota 2006).

In the model, a non-zero velocity, $u_{ST}$, is imposed at the surface of the spherical swimmer as first proposed by Blake (1971); Lighthill (1952). In this work, we consider for the most part pure tangential surface deformation (normal surface deformation will be covered in §4.6 only) and adopt the concise formulation introduced in Ishikawa & Pedley (2008) where the imposed velocity on the surface of a squirmer centred at the origin is explicitly given as

$$u_{ST}(r) = \sum_{n\geq 1} \frac{2}{n(n+1)} B_n P'_n \left( \frac{\hat{e} \cdot r}{r} \right) \left( \frac{\hat{e} \cdot r}{r} r - \hat{e} \right),$$

(1)

where $\hat{e}$ is the orientation vector of the squirmer, $B_n$ is the $n$th mode of the tangential surface squirming velocity (Blake 1971), $P_n$ and $P'_n$ are the $n$th Legendre polynomial and its derivative with respect to the argument, $r$ is the position vector, and $r = |r|$. In a Newtonian fluid, the swimming speed of the squirmer in free space is $U_{ST}^F = 2B_1/3$ (Blake 1971) and thus dictated by the first mode only. The second mode, $B_2$, governs the signature of the flow field in the far field (stresslet). As in many previous studies (Ishikawa & Pedley 2008; Ishikawa et al. 2006), we assume $B_n = 0$ for $n > 2$. In that case, the power consumption by the swimmer is $P_{ST}^F = 8\pi \mu a (2B_1^2 + B_2^2) / 3$, where $\mu$ is the dynamic viscosity of the fluid and $a$ the radius of the sphere.

The tangential velocity on the sphere in the co-moving frame is therefore simply expressed, in spherical coordinates, as $u_\theta(\theta) = B_1 \sin \theta + (B_2/2) \sin 2\theta$, where $\theta = \arccos(\hat{e} \cdot r / r)$ is the polar angle between the position vector $r$ and the swimming direction $\hat{e}$. We introduce an additional dimensionless parameter, $\alpha$, representing the ratio of the second to the first squirming mode, $\alpha = B_2 / B_1$.

When $\alpha$ is positive, the swimmer is called a puller and obtain the impetus from its front part. As $\alpha$ is negative, the cell is called a pusher and thrust is generated from the rear of the body. A puller (resp. pusher) generates jet-like flow away from (resp. towards) its sides, as shown in Ishikawa (2009) and references therein. A squirmer with $\alpha = 0$ is termed a neutral squirmer, and it is associated with a potential velocity field.

We note that the current model does not capture flow unsteadiness (Drescher et al. 2010; Guasto et al. 2010) arising from the periodic cilia-beating of micro-organisms like Paramecium or Volvox. Here we assume that the steady time-averaged velocity beyond the cilia tips dominates the overall dynamics. Including the underlying unsteadiness is of great interest, and may be the object of future work.
2.2. Swimming in a tube

The spherical squirmer (radius, $a$) is swimming in a cylindrical tube of radius $R$, as illustrated in figure 1. The centre of the squirmer is located at a distance $b$ from the tube axis. We use Cartesian coordinates with an origin at the centre of the tube and the $x$-direction along the tube axis. As in Higdon & Muldowney (1995) we introduce the nondimensional position $\beta$ as

$$\beta = b/(R - a),$$

so that $\beta = 0$ indicates that the squirmer is at the centre of the tube while for $\beta = 1$ the squirmer is in perfect contact with the tube wall.
3. Numerical method

3.1. Formulation

The boundary element method (BEM) has already been successfully adopted to study the hydrodynamics of swimming micro-organisms in the Stokesian regime (Ishikawa et al. 2006; Ramia et al. 1993; Shum et al. 2010). Our current work mainly follows the approach in Pozrikidis (2002), the important difference being that we use quadrilateral elements instead of triangle elements as typically used and originally proposed. The method is introduced briefly here.

In the Stokesian realm, fluid motion is governed by the Stokes equation

\[-\nabla p + \mu \nabla^2 \mathbf{u} = 0,\]

(3)

where \(p\) is the dynamic pressure and \(\mathbf{u}\) the fluid velocity. Due to the linearity of the Stokes equation, the velocity field, \(\mathbf{u}(\mathbf{x})\), resulting from moving bodies with smooth boundary \(S\) can be expressed as

\[\mathbf{u}(\mathbf{x}) = \frac{1}{8\pi \mu} \int_S \mathbf{f}(\mathbf{x}') \cdot \mathbf{S}(\mathbf{x}, \mathbf{x}') \, dS_{\mathbf{x}'},\]

(4)

where \(\mathbf{f}(\mathbf{x}')\) is the unknown force per unit area exerted by the body onto the fluid. The tensor \(\mathbf{S}\) is the Stokeslet Green’s function

\[\mathbf{S}_{ij}(\mathbf{x}, \mathbf{x}') = \left( \frac{\delta_{ij}}{d} + \frac{d_i d_j}{d^3} \right),\]

(5)

with \(d_i = x_i - x_i', \ d^2 = |\mathbf{x} - \mathbf{x}'|^2 = d_1^2 + d_2^2 + d_3^2\), and \(\delta_{ij}\) denoting the Kronecker delta tensor.

We discretize the two bodies in the problem, namely the spherical squirmer and the surrounding tube, into \(N\) zero-order elements with centres at the locations \(\{\mathbf{x}_q, q = 1 \rightarrow N\}\), with \(q = 1 \rightarrow N_S\) denoting the elements on the squirmer surface and \(q = N_S + 1 \rightarrow N\) the elements on the surface of the tube. For the \(r^{th}\) element, \(\mathbf{f}(\mathbf{x}')\) is assumed to be constant over the element and is thus approximated by the value \(\mathbf{f}_r\). As a consequence, the discretized version of (4) is, when evaluated on one of the elements,

\[\mathbf{u}(\mathbf{x}_q) = \frac{1}{8\pi \mu} \sum_{r=1}^N \mathbf{f}_r \cdot \int_{S_r} \mathbf{S}(\mathbf{x}_q, \mathbf{x}') \, dS_{\mathbf{x}'}, \ q = 1 \rightarrow N.\]

(6)

In its discrete form, equation (6) represents a total of \(3N\) equations for the \(3N\) unknown force density components.

3.2. Swimming and squirmer boundary conditions

On the squirmer surface, the left-hand side of (6) is not fully known. The swimmer has an instantaneous surface deformation, \(\mathbf{u}_S\), plus 6 unknown components, namely its instantaneous translational velocity vector, \(\mathbf{U}\), and its instantaneous rotational velocity vector, \(\Omega\). Thus, the left hand side of (6), when
evaluated on the surface of the squirmer, becomes \( \mathbf{u}(\mathbf{x}_q) = \mathbf{U} + \mathbf{\Omega} \times \tilde{\mathbf{x}}_q + \mathbf{u}_S(\mathbf{x}_q) \) for \( q \) from 1 to \( N_S \) (here \( \tilde{\mathbf{x}}_q = \mathbf{x} - \mathbf{x}^R \), where \( \mathbf{x}^R \) is an arbitrary reference point, the centre of the spherical squirmer for convenience). The 6 additional equations necessary to close the linear system are the force- and torque-free swimming conditions, namely
\[
\int \mathbf{f}(\mathbf{x}) \, dS_x = 0, \quad \int \tilde{\mathbf{x}} \times \mathbf{f}(\mathbf{x}) \, dS_x = 0,
\]
for \( \mathbf{x} \in \text{squirmer} \).

3.3. Other boundary conditions

The situation addressed in our paper is that of a squirmer swimming inside an infinitely long tube filled with a quiescent fluid. Numerically, we close both ends of the tube with appropriate boundary conditions. If the tube caps are sufficiently far away from the squirmer, the velocity near the caps is almost zero, so we have \( \mathbf{u}_B = \mathbf{u}_T = \mathbf{0} \), and the pressure over the bottom and top cap is \( p_B \) and \( p_T \) respectively (Pozrikidis 2005). The force density \( \mathbf{f}_T \) over the top cap can be approximated by \( \mathbf{f}_T = p_T \mathbf{n} \) (Pozrikidis 2005), where \( \mathbf{n} \) is the unit normal vector pointing from the top cap into the fluid domain. Since pressure is defined up to an arbitrary constant, without loss of generality, we set \( p_T = 0 \), \( \mathbf{f}_T = \mathbf{0} \) and the top cap does not requires discretization. However, unlike (Pozrikidis 2005), we do perform discretization on the bottom cap, solving for the normal and tangential components of the force density \( \mathbf{f}_B \) there. For the conduit part of the tube, we use no-slip boundary condition, thus write \( \mathbf{u}_C = \mathbf{0} \).

Since we set the velocity on both caps of the tube to be zero, the error due to domain truncation need to be carefully considered. A truncated tube length \( L \) of \( \pi R \) or \( 2\pi R \) was chosen in Pozrikidis (2005) and \( L = 3R \) in Higdon & Muldowney (1995). In our computation of hydrodynamic force on a moving sphere inside, we tested different values \( L \) and examined the truncation error. We find the length, \( L = 2\pi R \), to be long enough for required accuracy (see figure 3 and details below). In the case of swimming squirmers, we set \( L = 3\pi R \), and larger values of \( L \) were shown to have negligible differences in the results.

3.4. Discretization and integration

Zero-order constant quadrilateral elements are used to discretize all the surfaces. We use six-patch structured grid to discretize the sphere (Cortez et al. 2005; Higdon & Muldowney 1995; Smith 2009), mapping six faces of a cube onto the surfaces of a sphere with each face latticed into a square mesh. The conduit part of the tube is divided into cylindrical quadrilateral elements obtained from the intersections of evenly spaced planes normal to tube axis and evenly spaced azimuthal planes (Higdon & Muldowney 1995; Pozrikidis 2005; Wen et al. 2007). Moreover, orange-like quadrilateral elements are used for the
Figure 2. Local mesh refinement of the cylinder (red) and the sphere (green). The geometrical parameters are $a/R = 0.3$ and $\beta = 0.95$. For a better visualisation, the mesh on the squirmer surface is reproduced on the displaced sphere as indicated by the black arrow.

bottom cap of the tube (Higdon & Muldowney 1995; Wen et al. 2007). For the sphere we adopt the six-patch quadrilateral grid with parameterized coordinates instead of triangle elements (Pozrikidis 2002, 2005). Such discretization with its natural parametrisation facilitates Gauss-Legendre quadrature when performing numerical integration. Template points used in the quadrature lie exactly on the sphere surface since their coordinates are derived from the parametrisation. The resulting improved quadrature gives superior accuracy (see Table 9.1). The integration for singular elements are performed by using plane polar coordinates with Gauss-Legendre quadrature (Pozrikidis 2002).

In many instances, the squirmer is so close to the cylindrical wall that near-singular integration has to be performed, a key point to achieve the required accuracy and efficiency (Huang & Cruse 1993). We perform local mesh refinement in the near-contact regions between the squirmer and the tube (Ishikawa & Hota 2006; Ishikawa et al. 2006) as illustrated in figure 2. The agreement between numerical results with our method and existing results from high-order spectral boundary element method (Higdon & Muldowney 1995) improves significantly when applying such local mesh refinement as shown in the next section where we compute the resistance of a translating sphere inside a cylindrical tube.

3.5. Validation and accuracy

We first compute the drag force, $F$, on a translating sphere in an unbounded domain and compare it with the analytical expression, $F = 6\pi \mu a U$, where $\mu$ is the dynamic viscosity of the fluid and $U$ is the translational speed of the sphere.
As shown in Table 9.1, the current method is very accurate when compared to the three similar approaches (Cortez et al. 2005; Pozrikidis 2002; Smith 2009). We then compute the drag force and torque on a sphere translating parallel to an infinite, flat, no-slip surface. The surface is modelled by a discretized plate of size $40a \times 40a$. Our simulation agree well with analytical results (Goldman et al. 1967), as shown in Table 9.2. Finally, we compute the drag force acting on a sphere translating inside the tube with confinement $a/R = 0.4$, up to a maximum value of $\beta = 0.99$, and compare our results with published data obtained with high-order spectral boundary element method (Higdon & Muldowney 1995). As illustrated in figure 3, the maximum relative error is less than 1.2%. In all simulations, we keep the confinement $\beta \leq 0.99$ to obtain sufficient accuracy; the cell is considered to be too close to the wall when $\beta > 0.99$.

### 4. Swimming inside a tube: results

We now have the tools necessary to characterise the locomotion of squirmers inside a tube. Our computational results, presented in this section, are organised as follows. We first compute the swimming kinematics and power consumption

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<td>Relative error (%)</td>
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<td>0.431</td>
<td>$9.6 \times 10^{-3}$</td>
<td>$1.4 \times 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 9.1. Relative error, in percentage, in the drag force on a translating sphere in an unbounded domain between the method in this paper and three other methods. The parameter $\epsilon$ is the regularization parameter first introduced in Cortez et al. (2005).
Table 9.2. Relative error in the drag force, $F_{err}$, and torque, $T_{err}$, in percentage, on a sphere translating parallel to an infinite wall between our computations and the analytical results (Goldman et al. 1967). Here $a$ is the radius of the sphere and $h$ the distance between the centre of the sphere and the wall.

<table>
<thead>
<tr>
<th>$h/a$</th>
<th>$F_{err}$ (%)</th>
<th>$T_{err}$ (%)</th>
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<tbody>
<tr>
<td>3.7622</td>
<td>0.00426</td>
<td>0.09488</td>
</tr>
<tr>
<td>2.3523</td>
<td>0.01911</td>
<td>0.37879</td>
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<tr>
<td>1.5431</td>
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<tr>
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<td>1.0453</td>
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<td>0.74217</td>
</tr>
<tr>
<td>1.0050</td>
<td>0.17669</td>
<td>1.13493</td>
</tr>
<tr>
<td>1.0032</td>
<td>0.27472</td>
<td>1.74313</td>
</tr>
</tbody>
</table>

Figure 3. Relative error in the three components of the drag force, $R_x$, $R_y$, and $R_z$, on a sphere translating inside a tube ($a/R = 0.4$) between the present paper and Higdon & Muldoney (1995). Note that the three largest values of $\beta$ chosen are 0.95, 0.975 and 0.99.
of a squirmer instantaneously located at various positions inside the tube while its orientation is kept parallel to the tube axis. These results then enable us to understand the origin of the two-dimensional wave-like trajectory for a neutral squirmer inside the tube. We also analyse the asymptotic stability of trajectories close to solid walls (Crowdy & Yizhar 2010; Or & Murray 2009). We then move on to examine the general three-dimensional helical trajectory of a neutral squirmer and also consider the kinematics of pusher and puller swimmers. Finally, we study locomotion induced by normal surface deformation and consider locomotion inside a curved tube.

4.1. Static kinematics and energetics

To start our investigation, we first numerically calculate the swimming speed and power consumption for a squirmer exploiting pure tangential surface deformation (for completeness, results on squirmers with normal surface deformations are shown in Sec. 4.6). We fix $B_1 = 1$ and vary the value of $\alpha$, while
different values of $a/R$ and $\beta$ are chosen to address the effect of confinement and eccentricity on the instantaneous swimming kinematics.

In figure 4, we plot the instantaneous swimming speed of a squirmer with orientation parallel to the tube axis (positive $x$ direction) and location $(x, y, z) = (0, 0, -\beta (R - a))$. The swimming velocity parallel to the tube axis ($U_x$) is displayed in figure 4 (left) while the velocity perpendicular to it ($U_z$) is shown in figure 4 (right). Interestingly, both pushers and pullers have the same swimming speed, $U_x$, as the neutral squirmer. This is due to the fact that the second squirming mode, $\sim B_2 \sin 2\theta$, is front back symmetric, and thus produces zero wall-induced velocity (Berke et al. 2008), as confirmed by our simulation. We observe numerically that when $\alpha = 0$, there is only one non-zero velocity component, namely $U_x$. In contrast, for pushers and pullers ($\alpha \neq 0$) a non-zero transverse velocity component, $U_z$, is induced. The value of $U_z$ is seen to decrease with confinement, $a/R$, and eccentricity, $\beta$, as shown in figure 4 (left). The sharp decrease when $\beta$ is beyond $\approx 0.8$ is due to the strong drag force experienced closer to the wall which overcomes the propulsive advantage from near-wall locomotion.

The transverse velocity, $U_z$, shown in figure 4 (right), is plotted against the swimmer position, $\beta$, for different values of $\alpha$ while the confinement is fixed at $a/R = 0.3$. In the case of a puller ($\alpha > 0$), the swimmer will move away from the nearest wall ($U_z > 0$) while a pusher ($\alpha < 0$) will move towards the nearest boundary ($U_z < 0$), as expected considering the dipolar velocity field generated by squirmers (see also Sec. 4.4). The absolute value of $U_z$ increases with $\alpha$ and is of the same magnitude for pushers and pullers of equal and opposite strength. A similar effect was explained in Berke et al. (2008) for a plane wall, although in that case, the cell was approximated by a point stresslet and the cell-wall distance was considerably larger than the cell size. By probing hydrodynamics very close to the wall, we observe that the magnitude of $U_z$ does actually not vary monotonically with $\beta$, instead reaching a maximum value as $\beta \approx 0.9$. Moving away from the tube centre, the transverse velocity increases due to stronger hydrodynamic interactions with the tube walls before decreasing owing to a significantly larger hydrodynamic resistance very close to the tube boundaries.

Beyond the translational velocities, the squirmers also rotate due to hydrodynamic interactions with the tube boundaries. Numerical results show that the magnitude of the rotational velocity, $\Omega_y$, is independent on the dipole strength, $\alpha$, and that all squirmers rotate away from the closest wall. This is also attributed to the front-back symmetric distribution of the second squirming mode. Using our notation, we therefore obtain that squirmers rotate in the $-y$ direction. The value of $\Omega_y$ is displayed in figure 5 (left). Its magnitude increases with eccentricity, $\beta$, and confinement, $a/R$, as a result of stronger hydrodynamic interactions. To explain the sign of the rotational velocity, we look in detail at a neutral squirmer in figure 5 (right), in the case where the
Figure 5. Left: Rotational velocity of the squirmer in the direction normal to the plane of locomotion, $\Omega_y$. The squirmer is located at $(0, 0, -\beta (R - a))$ with its orientation parallel to the tube axis. Different values of $a/R$ are plotted with maximum value of $\beta = 0.99$. Right: Physical picture of cell rotation near the walls. The circle indicates the spherical squirmer and the green arrows denote the tangential surface velocity imposed by the squirmer. Blue straight arrow and curved arrow denote the cell orientation and rotational velocity respectively; 1 indicates the closest point on the cell to the top wall and 2 the closest point to the bottom wall while $F^P_1$ and $F^P_2$ are the wall-induced shear forces generated near point 1 and 2.
et al. (2006), the unknown \( f \) is the sum of the force density from outer (\( f_{\text{out}} \)) and inner (\( f_{\text{in}} \)) surface. We therefore rewrite the power as \( P = \int_S f \cdot u_S dS - \int_S f_{\text{in}} \cdot u_S dS \), where \( \int_S f_{\text{in}} \cdot u_S dS \) denotes the viscous dissipation of the flow inside the squirmer. We thus need to subtract the internal viscous dissipation in the fluid given by the numerics where \( f_{\text{in}} \) can be derived analytically based on the squirming velocity. In figure 6, we depict \( P \), scaled by the corresponding value in free space for different values of \( \alpha \). For each gait, \( P \) increases slowly until \( \beta \approx 0.8 \) followed by a rapid increase for cells closer to the wall. Such a drastic power increase is in agreement with the sharp decrease in swimming speed close to the tube, and consequently, a significant decrease in swimming efficiency is expected. In addition, as the confinement is getting stronger, the eccentricity of the swimmer’s position becomes more important. For example, as \( \beta \) changes from 0 to 0.99, power consumption of a neutral squirmer \( P \) increases only by around 45% for \( a/R = 0.2 \) but by 85% for \( a/R = 0.5 \).

\[ \alpha = 0 \quad \alpha = 5 \]

Figure 6. Power consumption \( P \) of the neutral squirmer (\( \alpha = 0 \), left) and puller (\( \alpha = 5 \), right), scaled by their corresponding values in free space. Insets display \( P \) as a function of \( a/R \) in the case \( \beta = 0 \). The orientation of the squirmer is parallel to the tube axis with the maximum value of \( \beta = 0.99 \).

4.2. Two-dimensional wavelike motion of the neutral squirmer

We next study in detail the trajectory of a squirmer inside a tube with fixed confinement; unless otherwise stated, all results in this section use the same value, \( a/R = 0.3 \). The cell is neither a pusher nor a puller, but a neutral squirmer generating potential flow field (\( \alpha = 0 \)). The initial position and
orientation of the cell are defined as in figure 7. The cell is initially placed at $(0,0,-b_I)$, with $b_I = \beta_I (R - a)$, and oriented parallel to the axis ($\xi_I = 0$); the motion of the cell will also be restricted to the $x-z$ plane ($\chi_I = 0$).

We calculate the translational and rotational velocity of the cell at each time step and update its position using fourth-order Adams-Bashforth scheme as in Giacché & Ishikawa (2010). Note that in the simulations the cell always remains in the centre of the computational domain (while its axial velocity is stored for post-processing), which allows to minimise the error introduced by domain truncation.

Our computations show that the squirmer always displays a periodic wave-like trajectory in the tube, with amplitude $A$ and wavelength $\lambda$. This is illustrated in figure 8 for $\beta_I = 0.9$ (top) and $\beta_I = 0.7$ (bottom). The wave amplitude does not change over time and is twice the initial off-axis distance, namely, $A = 2b_I$. The presence of a nonzero rotational velocity, $\Omega_y$, discussed above and shown in figure 5, is the key parameter leading to the periodic trajectory.

By considering cases where the initial orientation of the cell is not parallel to the axis (thus for which the orientation vector has non-zero $x$ and $z$ components) and we find that as long as the squirmer does not immediately descend into the wall, a wave-like trajectory is also obtained. To present all results in a concise manner, we consider the motion of the neutral squirmer as a dynamical system similarly to recent work on two-dimensional swimming (Crowdy &
Figure 8. Two-dimensional trajectories of a neutral squirmer inside a capillary tube with confinement $a/R=0.3$. All positions are measured in the units of cell radius $a$, same for figures hereinafter unless otherwise specified. Blue circles and red arrows indicate, respectively, the instantaneous position and orientation of the squirmer. The cell is released from $(0, 0, -\beta I(R-a))$ with $\beta I = 0.9$ (up) and $\beta I = 0.7$ (bottom), while the initial orientation is parallel to the axis. We denote $\lambda$ the wavelength of the periodic trajectory and $A$ its amplitude.

Samson 2011; Or & Murray 2009). The trajectory is defined by two parameters, the off-axis distance ($z$) and the angle between the swimmer orientation and the tube axis ($\xi$). We report the phase portrait of the neutral squirmer in the ($z, \xi$) plane in figure 9, where the solid curves show the trajectories. The marginally stable point $(0, 0)$ corresponds to locomotion along the axis of the tube. For any initial conditions ($z, \xi$), the neutral squirmer swims along wave-like trajectories corresponding to the periodic orbits in figure 9 (the largest periodic orbit in the figure has a maximum $\beta$ of 0.95).

The main characteristics of the squirmers’ trajectories are shown in figure 10 for different initial positions, $\beta I$. We display the trajectory wavelength, $\lambda$, and the wavelength-to-amplitude ratio, $\lambda^* = \lambda/(A/2)$. It is clear that $\lambda$ and $\lambda^*$ both decrease with $\beta I$. Indeed, when the swimmer is at the crest or trough of the periodic trajectory, stronger rotation occurs for larger $\beta I$. Therefore, the swimmer will escape from the nearest wall more rapidly, resulting in a decrease
of the wavelength. We also show in figure 10 that the time-averaged axial speed, $\bar{U}_x$, and the time-averaged swimming speed along the trajectory, $\bar{U}$, decrease with $\beta$ whereas the time-averaged power consumption, $\bar{P}$, increases when the squirmers move closer to the wall.

4.3. Three-dimensional helical trajectory of the neutral squirmer

By tilting the initial cell orientation, $\hat{e}$, off the $x-z$ plane, the squirmer trajectories become three dimensional and take the shape of a helix, a feature we address in this section. As in the two-dimensional case, these three-dimensional trajectories are a consequence of hydrodynamics interactions only. Recent experiments in Jana et al. (2012) showed that Paramecium cells display helical trajectories when swimming inside capillary tubes, a feature our simulations are thus able to reproduce. It is noteworthy that Paramecium cells follow occasionally helical trajectories also in free space due to the asymmetry of the body shape and of its beating; however, we do not study these effects in the current work, to focus purely on hydrodynamics within confinement.

We introduce $\chi_I$ as the yaw angle between the initial cell orientation and the $x-z$ plane (see figure 7), so that the initial orientation becomes $(\cos(\chi_I), \sin(\chi_I), 0)$. In our simulations, $\beta_I$ ranges from 0.3 to 0.9 and $\chi_I$ from 20° to 40°. Within these parameters, squirmers always display helical trajectories. One such helix is plotted in figure 11, for an initial position $\beta_I = 0.8$ and a yaw angle $\chi_I = 40°$. The helical trajectory is a combination of wavelike motions developed in the azimuthal $y-z$ plane and in the axial direction, see figure 11b and c. In figure 11b, we show the projected circular trajectory of
Figure 10. Dynamics and kinematics of the neutral squirmer in a tube as a function of the initial dimensionless off-axis position, $\beta_I$. Top left: wavelength, $\lambda$, of the periodic trajectory. Top right: wavelength-to-amplitude ratio, $\lambda^* = \lambda/(A/2)$. Bottom left: time-averaged swimming speed in the axial direction, $\bar{U}_x$, and along the trajectory, $\bar{U}$, both rescaled by the free-space swimming velocity. Bottom right: time-averaged power consumption $\bar{P}$, rescaled by value in free space.

the swimmer in the $y-z$ plane. In figure 11c, we show that the curves $y(x)$ and $z(x)$ share the same wavelength and time period. We then plot the values of $z$ and $h$ (cell off-axis distance) as a function of the axial position, $x$, during one period in figure 11d to show that the wave frequency of $h(x)$ is three times that of $z(x)$. Indeed, the trajectory projected in the plane perpendicular to the tube axis resembles a regular triangle ($\Delta_1\Delta_2\Delta_3$), with vertices corresponding to locations of maximum off-axis distance where the cell bounces back inside the tube. In this particular case, the cell bounces off the wall three times during one orbit with an angle $\psi = 60^\circ$. A variety of other wave patterns can be
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Figure 11. Three-dimensional trajectory of the neutral squirmer in the tube. The initial position and orientation are given by $\beta_0 = 0.8$, $\chi_0 = 30^\circ$, $\xi_0 = 0^\circ$. (a): trajectory in perspective view; the empty circle and solid triangle stand for the start and end of one periodic orbit; (b): trajectory in the $y-z$ plane (axes shown in figure 11a); (c): trajectories in the $x-y$ (dashed) and $x-z$ (dot dashed) planes; (d): relation between the wavelike motion developed in the axial and azimuthal direction.

observed for different initial cell positions and yaw angels $(\beta_I, \chi_I)$. We display two of them in figure 12 in the $y-z$ plane, with $(\beta_I, \chi_I) = (60, 30^\circ)$ (figure 12, left) and $(60, 20^\circ)$ (figure 12, right). The swimmer on the left approaches the wall 21 times during one periodic orbit with $\psi = 42.86^\circ$, whereas the example on the right displays a 5 fold helix with $\psi = 36^\circ$.

Finally in figure 13 we show the variation of the averaged swimming speed (left) and power consumption (right) with the initial cell position $(\beta_I)$ and orientation $(\chi_I)$; where both the speed and power are nondimensionalized by
Figure 12. Periodic orbits of the neutral squirmer in the transverse plane for two different initial positions and orientations. Left: \((\beta_I, \chi_I) = (0.6, 30^\circ)\). Right: \((\beta_I, \chi_I) = (0.6, 20^\circ)\).

their corresponding values in free space. The time-averaged swimming speed along the axial direction, \(\bar{U}_x\), and along the trajectory, \(\bar{U}\), decrease clearly with \(\chi_I\) but slowly with \(\beta_I\). Larger values of \(\chi_I\) and \(\beta_I\) result in larger maximum off-axis distance, leading to higher hydrodynamic resistance from the boundaries and thus hindering locomotion. We also observe that \(\bar{U}_x\) decreases with \(\chi_I\) more rapidly than \(\bar{U}\). As \(\chi_I\) increases, the swimmer trajectory becomes more coiled, which significantly decreases the swimming velocity in the axial direction. We also note that the power consumption, \(\bar{P}\), increases with the the initial orientation, \(\chi_I\), but does not change significantly with \(\beta_I\).

4.4. The trajectory of a puller inside the tube

In this section, we study the trajectories of a puller swimmer \((\alpha > 0)\) in the tube. We first consider the case where the motion is restricted to the \(x-z\) plane, as in Sec. 4.2. In figure 14 we show the two-dimensional trajectories of pullers having force dipole parameters of \(\alpha = 3\) (left) and \(\alpha = 5\) (right), for different initial positions, \(\beta_I\), and orientations, \(\xi_I\). In both cases, the swimmers initially follow wavelike trajectories with decreasing magnitude, and eventually settle along straight trajectories, displaying thus passive asymptotic stability (Or & Murray 2009). The puller with \(\alpha = 3\) ends up swimming along the tube axis, with \((r_{CYL}, \xi_{CYL}) = (0, 0)\) as its equilibrium point (cylindrical coordinates are used here, and \(r_{CYL}\) and \(\xi_{CYL}\) denote the off-axis distance and orientation of the cell respectively). In contrast, the puller with \(\alpha = 5\) swims parallel to the axis near the top or bottom wall depending on its initial position and
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Figure 13. Nondimensional time-averaged swimming speed and power consumption of squirmers with different initial position ($\beta_I$) and orientation ($\chi_I$) with three-dimensional kinematics.

Figure 14. Two-dimensional trajectories, $z(x)$, of pullers in a tube (left: $\alpha = 3$; right: $\alpha = 5$). Different combinations of the initial position ($\beta_I$) and pitching angle ($\xi_I$) are chosen. The inset plots display the trajectories near the starting positions.
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Figure 15. Equilibrium points, \{r_{CYL}, \xi_{CYL}\}, of the puller in the tube as a function of the force dipole parameter, \(\alpha\), and for a confinement \(a/R = 0.3\). Blue dashed lines (\(\alpha < 3.86\)) show the equilibrium point at (0, 0), corresponding to swimming in the centre of the tube and along its axis. For \(\alpha > 3.86\), the combination \(\{r_{CYL}, \xi_{CYL}\}\) characterises the equilibrium state for swimming along a straight line with off-axis distance \(r_{CYL}\) and orientation towards the wall \(\xi_{CYL}\).

We further examine the coordinates of equilibrium points (\(r_{CYL}, \xi_{CYL}\)) as a function of the force dipole strength, \(\alpha\), in figure 15. For \(\alpha\) below a critical value, \(\alpha_c \approx 3.86\) for the confinement chosen here (\(a/R = 0.3\)), the equilibrium point is \(\{r_{CYL}, \xi_{CYL}\} = (0, 0)\) denoted by the dashed blue line. For \(\alpha > 3.86\), the equilibrium point corresponds to swimming stably along a straight line with off-axis distance \(r_{CYL}\) and orientation \(\xi_{CYL}\), both of which grow with increasing \(\alpha\). The relationship between confinement, \(a/R\), and the critical value \(\alpha_c\) is examined in figure 16. Determining precisely the value of \(\alpha_c\) is not possible due to the large computational cost so we report approximate values, with an upper (resp. lower) limit of the error bar corresponding to the asymptotically-stable swimming motion near the wall (resp. along the tube axis). The critical
Figure 16. Critical value of the dipole parameter, $\alpha_c$, for stable swimming of the puller in the tube centre as a function of the confinement, $a/R$. The approximate values of $\alpha_c$ are denoted by the square symbols and the upper (resp. lower) limit of the error bar corresponds to the asymptotically-stable swimming motion away from the centre (resp. along the tube axis).

dipolar strength first increases with the confinement, reaching its maximum as $a/R \approx 0.3$, before decreasing.

By starting with different combinations of $\alpha$, $\beta_I$ and $\chi_I$, we obtain different three-dimensional trajectories for the puller. Some of these trajectories are illustrated in figure 17. Results similar to the two-dimensional simulations are obtained. For $\alpha$ below a critical value, pullers eventually swim along the tube axis indicating the equilibrium point $(r_{CYL}, \xi_{CYL}) = (0,0)$. For larger values of $\alpha$, the equilibrium point corresponds to swimming motion with constant off-axis distance and orientation. Hydrodynamic interactions between the swimmer and the tube alone are responsible for such a passive stability, which could be of importance to guarantee, for example, robust steering of artificial micro-swimmers in capillary tubes without on-board sensing and control (Or & Murray 2009).
Figure 17. Three-dimensional trajectories of pullers in the tube with confinement $a/R = 0.3$. The red dashed line indicates the tube axis. Different combinations of the force dipole parameter, $\alpha$, initial position, $\beta_I$, and initial orientation, $\chi_I$, are chosen. Light green trajectories correspond to pullers with one equilibrium point in the tube centre whereas blue ones are for pullers with equilibrium near the wall.

We conclude this section by investigating in figure 18 the swimming speed of the puller along the stable trajectory and the dependency of its magnitude on the force dipole parameter, $\alpha$. In the case of confinement $a/R = 0.3$, the swimming speed $U_x$ is larger than that in free space as $\alpha$ is above a critical value (around 4 here) and it increases by about 16% as $\alpha = 5$. This is an example of swimming microorganisms taking propulsive advantage from near-wall hydrodynamics, as discussed in previous analytical studies (Felderhof 2009, 2010; Katz 1974). In our case, as the squirmer is oriented into the wall, the direction of the wall-induced hydrodynamic force, $F_R$, resulting from flow being ejected on the side of the puller, is not normal to the wall but possesses a component in the swimming direction, as shown in figure 19. This force contributes thus to an additional propulsion and increases the swimming speed.
Figure 18. Swimming speed, $U_x$ (blue lower triangles), and power consumption, $\mathcal{P}$ (light green upper triangles), of the puller as a function of the force dipole parameter, $\alpha$, both quantities being scaled by their corresponding values in free space (with $a/R = 0.3$). The critical value $\alpha_c = 3.86$, shown by the cross, is the transition between stable swimming at the tube centre vs. stable swimming near the tube walls. The blue dashed line indicates the swimming speed in free space.

4.5. *The trajectory of a pusher inside the tube*

We next address the spherical pusher squirmer, with a negative value of force dipole parameter, $\alpha$. We find that the motion of the pushers inside the tube is unstable. The trajectories of pushers confined in the $x-z$ plane ($\chi_I = 0$) are plotted in figure 20 for different combinations of force dipole, initial position, and initial orientation. The pushers always execute wavelike motions
Figure 19. The orientation, $\hat{e}$, of a puller swimming (red arrow) on the stable trajectory near the tube wall. Curved green arrows stand for the flow imposed at the surface of the swimmer, black ($F_N^P$) and grey ($F_F^P$) dashed arrows for the hydrodynamic force while $F_R$ is the repulsive force.

with decreasing wavelengths and increasing amplitude, eventually crashing into the walls. Pushers and pullers display therefore very different swimming behaviours, a difference which stems from the opposite front-back asymmetry of the force dipole.

4.6. Squirmers with normal surface velocity

For the sake of completeness, we investigate in this section the dynamics of squirmers in the tube in the case where the squirming motion is induced by normal (instead of tangential) surface velocity, modelled as

$$u_{SN}(r) = \sum_{n=0}^{2} \frac{2}{n(n+1)} A_n P_n \left( \frac{\hat{e} \cdot r}{r} \right),$$

where $A_n$ is the $n$th mode of the normal squirming velocity (Blake 1971). In free space, the swimming velocity is $U_{SN}^F = -A_1/3$ (Blake 1971). For simplicity, we only consider the instantaneous kinematics of a squirmer with $A_1 = -1$
and $A_{n\neq 1} = 0$, corresponding thus to $U_{SN}^F = 1/3$. The swimmer is located at $(0, 0, -\beta (R - a))$, and is oriented in the positive $x$ direction. We plot the axial velocity component, $U_x$, (scaled by $U_{SN}^F$) together with the rotational velocity, $\Omega_y$, in figure 21. Both $U_x$ and $\Omega_y$ are seen to increase monotonically with the confinement and eccentricity. This is in agreement with past mathematical analysis stating that microorganisms utilising transverse surface displacement speed up when swimming near walls (Katz 1974), between two walls (Felderhof 2009), or inside a tube (Felderhof 2010).

This increase (resp. decrease) of swimming speed in the tube of a squirmer with normal (resp. tangential) surface deformation can be related to the problem of micro-scale locomotion in polymer solutions. It is well known that actuated biological flagella generate drag-based thrust due to larger resistance to normal than to tangential motion (Lauga & Powers 2009). When swimming in polymer solutions, flagella undergoing motion normal to its shape push directly onto the neighbouring polymer network, whereas tangential motion barely perturb these micro obstacles (Berg & Turner 1979; Leshansky 2009; Magariyama & Kudo 2002; Nakamura et al. 2006). In this case, the drag force increases more in the normal direction than in the tangential, resulting in larger swimming speeds (Berg & Turner 1979; Leshansky 2009; Magariyama & Kudo 2002;
Figure 21. Swimming velocity in the axial direction, $U_x$, and rotational velocity, $\Omega_y$, of the squirmer with normal surface deformation with modes $A_n = -\delta_{n1}$; $U_x$ is scaled by the swimming speed in free space, $U_{SN}^F$. The squirmer is located at $(0, 0, -\beta (R - a))$ and oriented parallel to the axis. Different values of $a/R$ are reported with maximum value of $\beta = 0.99$.

Nakamura et al. 2006; Liu et al. 2011). Likewise, it was shown for a spherical squirmer that polymeric structures in the fluid always decrease the swimming speed in case of tangential surface deformation (Leshansky 2009; Zhu et al. 2011, 2012) but increase for normal deformation (Leshansky 2009). The increase of swimming speed observed here in the case of a squirmer with normal surface deformation can similarly be attributed to the flow directly onto the tube wall.

The value of rotational velocity, $\Omega_y$, shown in figure 21 shows however that the squirmer rotates into the nearest wall, thus getting eventually trapped there. In order to avoid being trapped while at the same time taking advantage of the wall-induced enhanced propulsion, ideally swimmers should thus use a combination of tangential and normal deformation.

Interestingly, a superposition of the neutral squirming mode ($B_n = \delta_{n1}$, see §2) with the first normal squirming mode ($A_n = -\delta_{n1}$) results in a special swimmer able to move without creating any disturbance in the surrounding fluid, characterised by a uniform squirming velocity of $-1$ everywhere on the body (in the co-moving frame), no body rotation, and a swimming speed equal to 1. This remains true regardless of the degree of confinement as confirmed by our numerical simulations.
5. Swimming inside a curved tube

In this final section, we investigate the squirmer motion inside a curved tube that is a part of a torus. The axis of the torus is a circle on the plane \( y = 0 \) with its radius \( R_B = 20a \). Trajectories of a neutral squirmer and a puller with the force dipole parameter \( \alpha = 1 \) are shown in Figs. 22 and 23 respectively. In both cases, the trajectory is displayed in both the \( x - z \) and \( y - z \) planes. The motion in the radial direction, represented by \( R(\sigma) - R_B \), is plotted as a function of the azimuthal position of the swimmer, \( \sigma \), where \( R(\sigma) \) is the distance between the cell and the centre of the circle. In both cases, the dynamics of swimmers initially starting aligned with the tube axis is wavelike. For the neutral squirmer, the wavelength and wave magnitude approach a constant value \( \sigma > \pi \) (figure 22, right), indicating marginal stability of the motion. In contrast, for the puller, decaying waves are observed (figure 23, right), indicating passive asymptotic stability. As in the straight-tube case, pushers are unstable and crash into walls in finite time.

6. Conclusion and outlook

In this paper, a Boundary Element Method code was developed, validated, and used to present computations for the locomotion of model ciliates inside
straight and curved capillary tubes. We used the spherical squirmer as our model microorganism and studied the effect of confinement on the kinematics, energetics, and trajectories of the cell. We also investigated the stability of the swimming motion of squirmers with different gaits (neutral, pusher, puller).

We found that tube confinement and near-wall swimming always decrease the swimming speed of a squirmer with tangential surface deformation for swimming parallel to the tube axis. In contrast, a swimmer with normal surface deformation improves its swimming speed by directly pushing against the surrounding tube wall. In both cases however, tube confinement and near-wall swimming always lead to additional viscous dissipation, thus increasing the power consumption.

Focusing on swimming with tangential forcing, we then studied in detail the dynamics of neutral, puller, and pusher squirmers inside a straight tube. For a neutral squirmer, swimming motion on the tube axis is marginally stable and generically displays three-dimensional helical trajectories as previously observed experimentally for *Paramecium* cells. Importantly, these helical trajectories arise purely from hydrodynamic interactions with the boundaries of the tube.

In the case of puller swimmers, their trajectories are wavelike with decreasing amplitude and increasing wavelength, eventually leading to stable swimming parallel with the tube axis with their bodies slightly oriented toward the nearest wall. The locations for these stable trajectories depend on the strength of the force dipole, \( \alpha \). Swimmers with weak dipoles (small \( \alpha \)) swim in the centre of the tube while those with strong dipoles (large \( \alpha \)) swim near the walls. The stable orientation of the swimmers makes an non-zero contribution of the wall-induced hydrodynamic forces in the direction of locomotion, thus leading to an increase of the swimming speed (although accompanied by an increase of
the rate of viscous dissipation). In contrast, pushers are always unstable and crash into the walls of the tube in finite time. Similar results are observed for locomotion inside a curved tube.

We envision that our study and general methodology could be useful in two specific cases. First, our results could help shed light on and guide the future design and maneuverability of artificial small-scale swimmers inside small tubes and conduits. Second, the computational method could be extended to more complex, and biologically-relevant, geometries, to study for example the locomotion of flagellated bacteria or algae into confined geometries, as well as their hydrodynamic interactions with relevant background flows. It would be also interesting to relax some of our assumptions in future work, and address the role of swimmer geometry on their stability (we only considered the case of spherical swimmers in our paper) and quantify the role of noise and fluctuations on the asymptotic dynamics obtained here.

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Paper 4
The motion of a deforming capsule through a corner

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A three-dimensional deformable capsule convected through a channel/duct with a corner is studied via numerical simulations using an accelerated boundary integral method adapted to general geometries. A global spectral method is adopted to resolve the dynamics of the capsule’s membrane developing elastic tensions and bending moments according to the Neo-Hookean constitutive law, while the flow obeys the Stokes equations. The simulations show that the trajectory of the capsule follows the underlying flow streamline with little deviation and the deformation of the capsule induces an anti-clockwise rotation of its material points with respect to the travelling direction. The surface area, principle tension and elastic energy of the capsule increase around the corner. Their temporal evolutions are characterised by a clear phase delay and the loss of the time-reversal symmetry of Stokes flow due to the elasticity of membrane. The capsule centroid velocity decreases near the corner as the mean flow does while a velocity overshoot is observed past the corner as a result of the interplay between the membrane elasticity and surrounding viscous flow. We show that the shear and bending moduli have a similar influence on the capsule behaviour where higher bending modulus inhibits the appearance of concavity during the deformation. Moreover, we examine how the wall confinement changes the dynamics: higher confinement generates higher deformation due to the sharper flow curvature whereas the spanwise confinement reduces the rotation of the
membrane. Finally, we consider a round corner and show that it significantly reduces the mechanical stresses on the capsule.

1. Introduction

Elastic micro-capsules are ubiquitous in nature, appearing in the form of seeds, eggs, cells and similar. The elasticity of the cells plays an important role for their proper biological functioning. For example, red blood cells (RBC) deform significantly in micro vessels to ease oxygen transportation; leukocytes squeeze through small gaps into the endothelial cell wall during inflammation (Springer 1994) so as tumour cells do in tumour metastasis (Hanahan & Weinberg 2000). On the other hand, artificial micro-capsules are commonly used in the food and cosmetic industry for a controlled release of effective ingredients (Barthés-Biesel 2011) and synthetic nano-capsules promise a potentially powerful medical therapy for a precise and targeted drug delivery. The ability of biological and artificial capsules to dynamically adapt, restructure their shapes on time and withstand stresses from the surrounding medium has thus attracted remarkable attention from research groups in different fields.

In micro-fluidic applications, one of the most fundamental issues is the behaviour of these tiny deformable structures when interacting with an external applied flow. Early experimental studies discovered several interesting features of RBCs: the well-known tank-treading and tumbling motion in shear flow (Goldsmith & Marlow 1972; Fischer & Schmid-Schönbein 1978), ‘parachute’ shaped deformation (Skalak & Branemark 1969) and the ‘zipper’ flow pattern (Gaëtgens et al. 1980) in the micro-capillaries. These observations show that the capsule shape is not given a priori but determined by the dynamic balance of interfacial forces with fluid stresses (Finken et al. 2011), which poses a challenge to theoretical approaches. Several analytical studies deal with unbounded domains for the modelling of tank-treading and tumbling motions of an initially spherical capsule by asymptotic analysis (Barthès-Biesel 1980, 1981); the proof of the existence of ‘slipper’ shaped cells in the capillary flow (Secomb & Skalak 1982); the prediction of the vacillating-breathing behaviour (Misbah 2006) and swinging-tumbling transition (Vlahovska et al. 2011).

Numerical simulations have also been successfully carried out to solve the nonlinear fluid-structure problem; examples are the deformation of a spherical (Foessel et al. 2011; Pozrikidis 2001, 1995), elliptical (Ramanujan & Pozrikidis 1998; Walter et al. 2011) or RBC-shaped (Sui et al. 2008; Tsubota & Wada 2010) capsule in an unbounded shear flow. However, in a realistic situation, biological cells and artificial capsules are convected in bounded flows
such as the Poiseuille flow. Motivated by early experiments showing the centre-
ward migration of RBCs (Goldsmith 1971), Zarda et al. (1977) and Ozkaya
(1987) simulated the axisymmetric cellular flow in a cylindrical tube using the
finite element method (FEM). Simulations based on boundary integral method
(BIM) for the inertia-less fluid motion combined with FEM for the membrane
dynamics were performed to study axisymmetric capsules (Leyrat-Maurin &
Barthès-Biesel 1994) and RBCs (Pozrikidis 2005a) in strongly confined tubes
with or without constrictions. Later simulations have addressed complex phe-
nomena like the migration and slipper-shaped deformation of cells (Pozrikidis
2005b), suspension of RBCs in a capillary tube (Lei et al. 2013), and the shape
transition between nonaxisymmetric and axisymmetric RBCs (Danker et al.
(2011) examined the effect of strong confinement on the capsule motion in a
square and circular duct of size comparable to the cell radius. Inertial effects
on the cell migration have also been investigated (Doddi & Bagchi 2008; Shi
et al. 2012).

These previous computational studies focus on the capsule motion in
straight geometries. Nevertheless, capsules are seldom transported in such sim-
ples configurations, but rather in highly complicated capillary networks in the
in-vivo micro-recirculation for RBCs or through micro-fluidic devices, where
corrugations, bifurcations and corners are common. Less is known about
the dynamics of capsules in these complex geometries, although these are at-
tracting growing interest. Experiments (Braunmüller et al. 2011) and simula-
tions (Noguchi et al. 2010) have shown rich behaviours of RBCs and vesicles
going through sawtooth-shaped channels; a transition from shape oscillations
to orientational oscillations was identified for such deformable micro-objects,
depending on the flow rate and the confinement. 2D FEM computations have
been carried out by Barber et al. (2008) to examine the cell partitioning in
small vessel bifurcations, showing that the cells preferentially enter the branch
with higher flow rate; such an effect is intensified by the cell migration towards
the centre, however hindered by the cell obstruction near the bifurcations. Re-
cently, Woolfenden & Blyth (2011) reported 2D simulations of a capsule in a
pressure-driven channel with a side branch. They found that the capsule de-
formation strongly depends on the branch angle and the cells selected different
paths at the branch junction according to their deformability.

The flow past a sharp corner is one of the most basic flow configurations;
despite its universality in biological systems and micro-fluidic devices, its in-
fluence on deformable micro-objects is not fully understood. Steps in this direction
have been taken only recently: the experiments by Rusconi et al. (2010) have
revealed the rapid formation of bacterial streamers near the corners of a curved
microchannel at low Reynolds number due to the nearby vortical flow struc-
ture. This secondary flow appears as long as the curvature of the boundary
varies, even in the Stokes flow (Lauga et al. 2004). Simulations of an elastic
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filament in a 2D corner flow (Autrusson et al. 2011) display a crossing over the curved streamlines in the corner, instead of alignment with the flow as seen in a rectilinear flow.

In this work, we numerically study the motion and deformation of an individual capsule transported in a channel/duct with a straight and/or curved corner. A three-dimensional code is developed to compute the motion of deformable capsules in arbitrary configurations. A boundary integral method with Ewald acceleration (Hernández-Ortiz et al. 2007) is implemented, sharing the elegance of both boundary integral and mesh-based methods. Boundary integrals are computed to accurately account for the singular and fast-varying interactions while the smooth part of solution is handled by a highly-parallel general Stokes solver based on the spectral element method. The boundary integration is performed with a global spectral surface interpolation based on spherical harmonics (Zhao et al. 2010). Our hybrid scheme therefore couples the high accuracy of boundary integrals for short-ranged interactions, to the geometrical (and boundary-condition) flexibility of mesh-based methods (Freund 2014) for long-ranged interactions. The spherical harmonics are utilised to resolve the membrane dynamics with spectral accuracy.

The paper is organised as follows. In section 2, we present the geometrical setup and describe the numerical method. Results of the simulations are presented in section 3, together with a detailed discussion. A summary of the main conclusions is provided in section 4.

2. Problem setup and numerical method

2.1. Flow geometry and numerical procedure

We investigate the motion of an elastic capsule transported through a micro-channel of width $H$. Figure 1 displays the flow configuration and the coordinate system, where half of the domain is removed to better visualise the deforming capsule. Streamlines and colour contours, coded by the velocity magnitude, are shown on the $z = 0$ mid-plane. The channel is characterised by a 90 degree sharp corner for most of the results presented here. We initially assume spanwise periodicity, and neglect wall confinement in the $z$ direction; the capsule motion in a square duct is examined in section 3.2.

We consider an initially spherical capsule of radius $a$, enclosed by an infinitely thin hyperelastic membrane with surface shear module $G_s$. The fluid inside and outside the capsule has the same density $\rho_F$, buoyancy forces and sedimentation effects are thus neglected. The viscosity of the two fluids is $\mu$ and $\lambda\mu$, with $\lambda = 1$ without loss of generality.

As capsules are usually small, the Reynolds number $Re$ defined with the capsule radius $a$ is $Re = \rho_F U a / \mu \ll 1$. Viscous forces are dominant over inertial forces, and consequently, the flow inside and outside the capsule is
Figure 1. (Colour online) Schematic of the flow configuration. (a) A deformable capsule transported in a duct with a straight sharp corner, only half of the domain displayed. Poiseuille flow is imposed at the inlet with a maximum centre-line velocity of 1.5. Flow periodicity is assumed in the spanwise $z$ direction, with no-slip at the walls. The flow field without capsules is depicted by the streamline and grey-scale colour indicating the velocity magnitude. (b) The discretized fluid domain and the capsule at four positions on the $x-y$ plane. The red box represents one spectral element with $5 \times 5 \times 5$ GLL points. Inset: the dashed line denotes the trajectory of the centre of capsule, the red solid line the axis of geometrical symmetry and the cross the instant $t = 0$ when the centre of the capsule reaches the corner axis.

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governed by the linear Stokes equations and determined instantaneously by the boundary conditions. A proper tool for the problem is therefore the boundary integral method (BIM) and we adopt an accelerated variant of the BIM here.

The fluid-structure interaction problem is solved as follows: the flow conveys and distorts the capsule while its reacting elastic forces give feedback to the fluid motion (Walter et al. 2010). We start with an undeformed capsule near the inflow and compute, at each time step, the force on the membrane from the deformed (and out-of-equilibrium) shape of the capsule. Neglecting inertia
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and Brownian fluctuations, the force density exerted onto fluid is equal to the membrane load. With this feedback forcing, the velocities in the channel and at the membrane nodes are computed explicitly with the BIM (see the following section). The integration is then repeated for the new membrane displacement and deformation.

2.2. Numerical method

2.2a. Accelerated boundary integral method. We develop a boundary integral implementation accelerated by the General Geometry Ewald like method (GGEM), proposed by Hernández-Ortiz et al. (2007) and later on used in a variety of micro-multiphase simulations (Kumar & Graham 2011; Pranay et al. 2010). An introduction is given here, the readers are referred to the above-mentioned articles for more details. We consider the Stokesian flow with \( M \) point forces

\[
-\nabla p(x) + \mu \nabla^2 u(x) = -\rho(x), \nabla \cdot u(x) = 0 \tag{1}
\]

where the force density \( \rho(x) = \sum_{i=1}^{M} f_i \delta(x - x_i) \) and \( f_i \) denotes the force exerted onto the fluid at point \( x_i \). Owing to the linearity of the Stokes problem, the flow field is a superposition of the flow induced by the localized forces \( f_i (i = 1, ..., M) \), where the velocity contribution from \( f_i \) is analytically known

\[
u_i(x) = G(x - x_i) \cdot f_i. \tag{2}
\]

Here \( G(x) \) is the Green’s function of the Stokes problem

\[
G(x) = \frac{1}{8\pi \mu \alpha^3} \left( \delta + \frac{\hat{x} \hat{x}}{r^2} \right),
\]

where \( r = |\hat{x}| \).

The GGEM method decomposes the force density \( \rho(x) \) into a local part \( \rho^l(x) \) and a global part \( \rho^g(x) \), with \( \rho(x) = \rho^l(x) + \rho^g(x) \), and

\[
\rho^l(x) = \sum_{i=1}^{M} f_i [\delta(x - x_i) - g(x - x_i)], \tag{3}
\]

\[
\rho^g(x) = \sum_{i=1}^{M} f_i [g(x - x_i)]. \tag{4}
\]

These two forcing are responsible for the local velocity \( u^l(x) \) and global velocity \( u^g(x) \) respectively, with \( u(x) = u^l(x) + u^g(x) \). After this decomposition, we address a local and a global problem separately. The quasi-Gaussian function \( g(\hat{x}) = (\alpha^3/\pi^{3/2}) \exp(-\alpha^2 r^2)[5/2 - \alpha^2 r^2] \), smears the delta-function \( \delta(\hat{x}) \) (Eq. 3) over a length scale \( \alpha^{-1} \). The resulting modified Green’s function \( G^l(x) \) can be found to be

\[
G^l(\hat{x}) = \frac{1}{8\pi \mu} \left( \delta + \frac{\hat{x} \hat{x}}{r^2} \right) \frac{\text{erfc}(\alpha r)}{r} - \frac{1}{8\pi \mu} \left( \delta - \frac{\hat{x} \hat{x}}{r^2} \right) \frac{2\alpha}{\pi^{1/2}} e^{-\alpha^2 r^2}, \tag{5}
\]

(5)
and the local solution written as

$$ u_l^i(x) = \sum_{i=1}^{M} G^i_l(x - x_i) \cdot f_i. $$

(6)

If the summation only considers point forces within a spherical domain of radius $R_{\text{cut}}$ centred at $x$, the local velocity $u_l^i(x)$ becomes then

$$ u_l^i(x) = \sum_{\nu=1}^{M_{\text{cut}}} G^i_l(x - x_{\nu}) \cdot f_{\nu}, $$

(7)

where $M_{\text{cut}}$ is the reduced number of point forces actually used. Such a domain truncation, stemming from the Ewald summation decreases the number of operations from $O(M^2)$ to $O(M)$. The corresponding error decreases for a larger cut-off radius $R_{\text{cut}}$. Carefully balancing computational cost and accuracy, we choose $R_{\text{cut}} = 4/\alpha$ as in the work of Pranay et al. (2010). The local velocity, see Eq. (7), accounts for the singular but short-ranged interactions, and is computed with classical boundary integral implementations. Regularised Stokeslet is therefore an expedient for the calculation, as applied among others in Pranay et al. (2010); Hernández-Ortiz et al. (2007). Nonetheless, BIM with regularisation suffers a degradation of the numerical accuracy and robustness for cases involving strong confinement or closely packed objects owing to the increasingly important hydrodynamic interactions. Descent singular and nearly-singular integration is a key point to achieve the required accuracy (Huang & Cruse 1993; Zhu et al. 2013), which is performed here in the framework of a spectral surface representation for the capsule, following Zhao et al. (2010) (detailed in the following section). As the local velocity is computed from the modified Green’s function for free space (Eq. 5), errors come in for arbitrary domains, to be rectified in the global solution.

The global problem solves the steady Stokes flow driven by the smooth forcing $\rho^g(x)$ in Eq. (4), with specified boundary conditions $u^g(x_\Omega)$ ($\Omega$ denoting the boundary). This is solved numerically in GGEM, requiring the total velocity $u(x_\Omega) = u_l^i(x_\Omega) + u^g(x_\Omega)$ to satisfy the correct boundary conditions. For Dirichlet boundary conditions, $u^g(x_\Omega)$ is imposed to be $u(x_\Omega) - u_l^i(x_\Omega)$, a special case being $u^g(x_\Omega) = -u_l^i(x_\Omega)$ for static no-slip wall. For periodic boundary conditions, applying the minimum image convention (Deserno & Holm 1998) in the local problem guarantees periodicity. In our simulation, we keep a large distance ($> R_{\text{cut}}$) between periodic boundaries and capsule to avoid this additional complexity.

We compute the global solution with the open-source Navier-Stokes solver NEK5000 (Fischer et al. 2008) based on the spectral element method. NEK5000 has been extensively used for stability analysis (Schrader et al. 2010) and turbulent flow (Fischer et al. 2008a) in complex domains. As akin to FEM, the physical domain is decomposed into elements with each element subdivided into arrays of Gauss-Lobatto-Legendre (GLL) nodes for the velocity and
Gauss-Legendre (GL) nodes for the pressure field. The Galerkin approximation is employed for the spatial discretization with different velocity and pressure spaces, following the so-called $P_N - P_{N-2}$ approach (Maday & Patera 1989). Accordingly, the velocity (respectively pressure) space consists of $N$th (respectively $(N-2)$th) order Lagrange polynomial interpolants, defined on the GLL (respectively GL) quadrature points in one element. We note that any Stokes solvers based on any other method can be readily used for the global problem. NEK5000 is chosen here for its spectral accuracy, high parallel performance and most importantly its geometric flexibility fully exploiting the general-geometry merit of GGEM.

Since point forces $x_i (i = 1, ..., M)$ do not necessarily coincide with the Eulerian mesh points, interpolation is needed for the global velocity $u^g (x_i)$, in order to get the total velocity $u^g (x_i) + u^p (x_i)$. The interpolation error is minimised thanks to the spectral accuracy of NEK5000.

2.2b. Spectral method for the membrane dynamics. The membrane loading was calculated as linear piece-wise functions on triangle meshes by Li & Sarkar (2008); Ramanujan & Pozrikidis (1998); Pozrikidis (1995). Numerous implementations have been developed based on the FEM (Charrier et al. 1989; Huang et al. 2012; Pranay et al. 2010; Walter et al. 2010) for its generality and versatility. Bi-cubic B-splines interpolation functions were adopted by Lac et al. (2007), producing very accurate results at a reasonable computational cost. Alternatively, a spectral boundary element algorithm was used by Dodson & Dimitrakopoulos (2008), thus coupling the numerical accuracy of the spectral method and the geometric flexibility of the boundary element method. However, due to the discontinuity of the geometric derivatives at the element boundaries, this method necessitates proper interfacial smoothing to avoid numerical instability. Global spectral method is devoid of this drawback, meanwhile attaining spectral accuracy, and it has therefore been suggested as a promising tool. Fourier spectral interpolation and spherical harmonics were used for 2D (Freund 2007) and 3D simulations (Kessler et al. 2008; Zhao et al. 2010) respectively. Here, we follow the approach of Zhao et al. (2010) as outlined below.

We map the capsule surface onto a unit reference sphere, using its spherical angles $(\theta, \phi)$ for the parametrisation. The parameter space $\{ (\theta, \phi) | 0 \leq \theta \leq \pi, 0 \leq \phi \leq 2\pi \}$ is discretized by a quadrilateral grid consisting of Gauss-Legendre quadrature points in $\theta$ and uniform spacing in $\phi$. All other surface quantities are defined on the same mesh. The surface coordinates $x^c (\theta, \phi)$ are expressed by a truncated series of spherical harmonic functions,

$$x^c (\theta, \phi) = \sum_{n=0}^{N_{SH}} \sum_{m=0}^{n} \hat{P}_n^m (\cos \theta) \left( a_{nm} \cos m\phi + b_{nm} \sin m\phi \right), \quad (8)$$
yielding $N_{SH}^2$ spherical harmonic modes. The normalised associated Legendre polynomials are

$$P_n^m(x) = \frac{1}{2^n n!} \sqrt{\frac{(2n+1)(n-m)!}{2(n+m)!}} \left(1 - x^2\right)^{\frac{m}{2}} \frac{d^{n+m}}{dx^{n+m}} \left(x^2 - 1\right)^n. \quad (9)$$

Both forward and backward transformations are calculated with the SPHEREPACK library (Adams & Swarztrauber 1997; Swarztrauber & Spotz 2000). Aliasing errors arise due to the intricate nonlinearity from both the membrane model and the complicated geometry. We implement an approximate dealiasing by performing the nonlinear operations on $M_{SH} > N_{SH}$ points and filtering the result back to $N_{SH}$ points, to significantly reduce the aliasing errors and improve the numerical stability.

A point on the surface is expressed by the curvilinear coordinates, $(\theta, \phi)$, defined on the covariant base, $(a_1, a_2, a_3)$, following the local deformation. The base vectors are

$$a_1 = \frac{\partial x}{\partial \theta} \cdot a_3 = n = \frac{a_1 \times a_2}{|a_1 \times a_2|}, \quad (10)$$

and the covariant and contravariant metric tensors

$$a_{\alpha \beta} = a_\alpha \cdot a_\beta, a^{\alpha \beta} = a^\alpha \cdot a^\beta. \quad (11)$$

The base vectors and metric tensors are also defined for the undeformed state and denoted here by capital letters $(A^\alpha, A^{\alpha \beta})$.

The second fundamental form of the surface is $b_{\alpha \beta} = n \cdot a_{\alpha \beta}$ and the two invariants of the transformation $I_1$ and $I_2$ are defined as

$$I_1 = A^{\alpha \beta} a_{\alpha \beta} - 2, I_2 = |A^{\alpha \beta}| |a_{\alpha \beta}| - 1. \quad (12)$$

$I_1$ and $I_2$ can also be determined from the principal dilations $\lambda_1$ and $\lambda_2$,

$$I_1 = \lambda_1^2 + \lambda_2^2 - 2, I_2 = \lambda_1^2 \lambda_2^2 - 1 = J_2^2 - 1. \quad (13)$$

The Jacobian, $J_s = \lambda_1 \lambda_2$, shows the ratio of the deformed to the undeformed surface areas. We compute the in-plane Cauchy stress tensor $T$, from the strain energy function per unit area of the undeformed membrane, $W_S(I_1, I_2)$,

$$T = \frac{1}{J_s} F \cdot \frac{\partial W_S}{\partial \varepsilon} \cdot F^T. \quad (14)$$

where $F$ is $a_\alpha \otimes A^\alpha$. Eq. (14) can be further expressed by components as

$$T^{\alpha \beta} = \frac{2}{J_s} \frac{\partial W_S}{\partial I_1} A^{\alpha \beta} + 2J_s \frac{\partial W_S}{\partial I_2} a^{\alpha \beta}. \quad (15)$$

We employ a widely-used model of the strain energy function $W_S$ in our study, the Neo-Hookean law (NH) (Green & Adkins 1970) formulated as

$$W_S^{NH} = \frac{G_s}{2} \left(I_1 - 1 + \frac{1}{I_2 + 1}\right), \quad (16)$$
where $G_s$ is the shear modulus. The local equilibrium connects $T$ with the external membrane load $q$, as
\[
\nabla_s \cdot T + q = 0, \tag{17}
\]
where $\nabla_s \cdot$ is the surface divergence operator in the deformed state. In curvilinear coordinates, the load vector is written as $q = q^\beta a_\beta + q^n n$. The local balance in Eq. 17 is further decomposed into tangential and normal components,
\[
\frac{\partial T^{\alpha \beta}}{\partial \xi^\alpha} + \Gamma^{\beta}_{\alpha \lambda} T^{\lambda \beta} + \Gamma^{\alpha}_{\alpha \lambda} T^{\alpha \lambda} + q^\beta = 0, \beta = 1, 2, \tag{18}
\]
where $\Gamma^{\alpha \beta}_{\alpha \lambda}$ are the Christoffel symbols and $(\xi^1, \xi^2) = (\theta, \phi)$.

We incorporate bending stiffness into our model using the linear isotropic model for the bending moment $M$:
\[
M^{\alpha \beta} = -G_B \left( b^{\beta}_{\alpha} - B^{\beta}_{\alpha} \right), \tag{20}
\]
where $G_B$ is the bending modulus, and $B^{\beta}_{\alpha}$ is the second fundamental form of the reference surface. We obtain the surface transverse tensor $Q$ from the bending moment. Local equilibrium of the stress including bending gives
\[
\frac{\partial T^{\alpha \beta}}{\partial \xi^\alpha} + \Gamma^{\beta}_{\alpha \lambda} T^{\lambda \beta} + \Gamma^{\alpha}_{\alpha \lambda} T^{\alpha \lambda} - b^{\beta}_{\alpha} Q^{\alpha} + q^\beta = 0, \beta = 1, 2,
\]
\[
T^{\alpha \beta} b_{\alpha \beta} + Q^{\alpha}_{\alpha} + q^n = 0. \tag{19}
\]

2.3. Nondimensionalization

Here, we study the property of a membrane characterised by its resistance to shearing and bending. The capillary number $Ca$, the ratio of viscous over elastic forces, is defined based on the shear modulus $G_s$,
\[
Ca = \frac{\mu V_C}{G_s}, \tag{20}
\]
where $V_C$ is the characteristic flow velocity, here the mean velocity. The reduced bending modulus, $Cb$, is the ratio of bending and shearing, $Cb = G_B/a^2 G_s$. All the length scales are nondimensionalized by the radius of the capsule $a$.

2.4. Validation

We firstly introduce the parameters used in the discretization. For the fluid solver, $\alpha = 1$ is adopted following Pranay et al. (2010), indicating that the local solution is negligible beyond a length scale of 1. Cubic spectral elements of size $1 \times 5 \times 5$ GLL points are used to discretize the fluid domain, and the mean grid spacing $h_{\text{mean}} = 1/4$ well satisfies the relation $\alpha h_{\text{mean}} \leq 0.5$ suggested in Kumar & Graham (2012). Rigorous tests are carried out to ascertain mesh independence, supporting the current choice. For the membrane dynamics, $N_{SH} = 25$ modes with a dealiasing factor $M_{SH}/N_{SH} = 2$ are chosen for most
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The tank-treading motion of an initially spherical capsule in shear flow is selected as the first validation case of our implementation. The capsule will evolve into a prolate and reach a steady deformed shape where the membrane continuously rotates in a tank-treading fashion. The time-dependent capsule deformation is measured by the Taylor parameter

\[ D = \frac{L_{\text{max}} - L_{\text{min}}}{L_{\text{max}} + L_{\text{min}}} \]  

where \( L_{\text{max}} \) and \( L_{\text{min}} \) are the maximum and minimum dimensions of the capsule in the shear plane. We plot \( D \) as a function of time for Neo-Hookean capsules with a varying \( Ca \) and no bending stiffness. Good agreement is observed between our simulations and those of Pranay et al. (2010). We next compare cases involving bending modulus, with the results of Huang et al. (2012) and Le (2010). Figure 10.2(b) shows that our results are in between theirs. To verify the nearly-singular integration, we simulate a capsule compressed in a confined square duct, and again report excellent agreement with the data by Hu et al. (2011), see figure 3.

**Figure 2.** (Colour online) (a) Variation of the deformation parameter \( D \) versus time, for an initially spherical Neo-Hookean capsule in shear flow. Different \( Ca \) are chosen. The profile of capsule in the shear plane is an ellipse with a long axis \( L_{\text{max}} \) and short axis \( L_{\text{main}} \); the Taylor parameter quantifying the capsule deformation is \( D = \frac{L_{\text{max}} - L_{\text{min}}}{L_{\text{max}} + L_{\text{min}}} \). (b) Same as figure (a), \( Ca \) is fixed to be 0.15, and we vary the reduced bending modulus \( Cb \).
3. Results

We consider the capsule in the centre of the channel, as deformable objects tend to move towards the centreline due to the Fåhraeus effect. We anchor the centre of the capsule at $(0, -5, 0)$, 5 units away from both the computational inlet and the corner, and release it after it has reached the equilibrium shape. This distance is large enough for the interaction between the capsule and the inlet/corner to be negligible during the initial phase.

3.1. Channel flow with a 90° sharp corner and no spanwise confinement

We begin by investigating the motion of a capsule transported in a moderately confined channel of width $H_x = 3$ where we assume periodicity in the spanwise direction. This configuration is denoted as the channel flow hereinafter; the duct flow including spanwise confinement is studied later (see section 3.2).

The background flow without capsules is referred to as the single-phase flow and its flow field in the $z = 0$ plane is illustrated in figure 4. We show five trajectories ($S_1, S_2, S_3, S_4, S_5$) starting from equally-spaced points on the line $y = -9, \ x \in [-1.2,1.2]$; they are ordered from the outer to the inner corner where $S_3$ goes through the centre of the domain. The velocity magnitude $V_S(t)$ is symmetric about $t = 0$, when the minimum is reached for $S_1, S_2$ and $S_3$, but a maximum for $S_5$. $S_4$ displays a wavy variation around $t = 0$, intermediate between the two extremes.
3.1a. *Capsule behaviour varying the shear modulus.* We investigate the effect of the shear modulus $G_s$, proportional to the inverse of the capillary number, on the capsule dynamics focusing on the temporal evolution of the surface area, the centroid velocity, the principle tension and the elastic energy of the capsule. Its trajectory and deformation are also analysed.
As expected, a 'floppy' capsule with capillary number \( Ca = 0.45 \) deforms more, as shown by the time evolution of the capsule surface area \( A \) in figure 10.5(a). As we let the capsule move only after it has reached equilibrium, the value of the capsule surface area when the capsule is released is the equilibrium value \( A_{\text{equ}} \neq A_{\text{ini}} \) with \( A_{\text{ini}} \) the reference undistorted area. The surface area varies slowly far away from the corner, starts increasing shortly before \( t = 0 \), reaches the maximum \( A_{\text{max}} \) and finally relaxes to the equilibrium value. The relation between the nondimensional area variations \( A_{\text{max}}/A_{\text{ini}} - 1 \), \( A_{\text{equ}}/A_{\text{ini}} - 1 \) and \( Ca \), are shown in figure 10.5(b). Here we identify a power-law scaling,

\[
\left( \frac{A_{\text{max}}}{A_{\text{ini}}} - 1 \right) \sim (Ca)^{1.5}, \\
\left( \frac{A_{\text{equ}}}{A_{\text{ini}}} - 1 \right) \sim (Ca)^2.
\]

(22)

We suggest that this relationship could be used to infer the membrane mechanical properties from measurements of the area variation of capsules through a corner flow, in addition or in alternative to methods based on the measurement of capsule deformation and velocity (Lefebvre et al. 2008).

The velocity of the capsule centre, \( V_{\text{cap}} \), is displayed in figure 10.6(a) versus time for different values of \( Ca \). The velocity scaled by that at equilibrium \( V_{\text{equ}} \) is depicted in figure 10.6(b), together with the velocity on the streakline \( S3 \) of the single-phase flow (cf. figure 4). We observe that all capsules move faster than the average flow velocity, as expected because of the Fåhræus effect. The velocity of the capsule decreases when approaching the corner and increases as leaving, influenced by the background flow; the profile is characterised by a minimum located at \( t = 0 \), when the particle centre is on the corner bisetrix. Soft capsules move faster, both at the equilibrium and around the corner. In contrast to the underlying flow, the capsule velocity profile breaks the time-reversal symmetry about \( t = 0 \), revealing an overshoot during the recovery stage; this symmetry breaking becomes more evident for softer membranes. Only the stiffest case \( Ca = 0.0375 \) maintains the symmetry to the eye’s accuracy (see figure 10.6(b)). The loss of symmetry is indeed related to the viscoelasticity induced by the fluid-capsule interplay, in analogy with the dynamics of Stokesian polymeric flows over a sphere. In that case, the fore-aft flow asymmetry is induced by the fluid elasticity, and characterised by a ‘negative wake’ in the rear of the body or velocity overshoot (Bisgaard 1983; Hassager 1979; Zhu et al. 2011). The ‘negative wake’ grows with the polymer relaxation time (Arigo & McKinley 1998), exactly as the velocity overshoot increases with the capillary number here, which can be as seen as the nondimensional membrane relaxation time. It is noteworthy that the dependence of the capsule velocity on its shear modulus could be used to deduce the cell membrane property, similar to the monitoring of the capsule velocity in a pore flow (Hu et al. 2011; Lefebvre et al. 2008) or the passage time of cells traversing constrictions (Adamo et al. 2012; Qi et al. 2012). A potential application is the
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Figure 5. (Colour online) (a) Time evolution of the surface area $A$ of capsules of different Capillary number, scaled by the initial value $A_{\text{ini}}$. Green squares and blue circles denote the maximum area over time $A_{\text{max}}/A_{\text{ini}}$ and area at equilibrium $A_{\text{equ}}/A_{\text{ini}}$, respectively; the inset shows their dependence on $Ca$; (b) Log-log plot of the nondimensional area variation $A_{\text{max}}/A_{\text{ini}} - 1$ and $A_{\text{equ}}/A_{\text{ini}} - 1$ as function of $Ca$.

precise temporal control of drug delivery, where the chemicals are encapsulated in soft nano-capsules or nano-vesicles (Chen et al. 2010; Singh et al. 2007).

The membrane tension developing on the capsule is of great importance, since it influences the release of molecules (Goldsmith et al. 1995) and ATP (Wan et al. 2008) by RBCs and also causes haemolysis. We analyse the principal tension $\tau_i^P$ ($i = 1, 2$), to better understand the potential mechanical damage of capsules passing through a corner. For any definition of strain energy function $W_S(I_1, I_2)$, $\tau_i^P$ are derived as (Skalak et al. 1973):

$$\tau_1^P = 2\frac{\lambda_1}{\lambda_2}\left(\frac{\partial W_S}{\partial I_1} + \lambda_2^2 \frac{\partial W_S}{\partial I_2}\right),$$

$$\tau_2^P = 2\frac{\lambda_2}{\lambda_1}\left(\frac{\partial W_S}{\partial I_1} + \lambda_1^2 \frac{\partial W_S}{\partial I_2}\right).$$

(23)
Figure 6. (Colour online) Time evolution of the velocity of the capsule centre, $V_{\text{cap}}$, scaled by the bulk channel velocity $V_C$ in (a), and by the cell velocity at equilibrium in the straight channel $V_{\text{equ}}$ in (b). The solid line corresponds to the velocity of a tracer particle passing through the centre in the single-phase flow. Time $t = 0$ denotes the instant when the capsule centre cuts the corner.

We consider the major principal tension: \( \max(\tau^P_1(x, t), \tau^P_2(x, t)) \) and the isotropic principal tension \( \left( \tau^P_1(x, t) + \tau^P_2(x, t) \right)/2 \); their spatial maximum $\tau^P_{\text{max}}(t)$ and $\tau^{P,\text{ISO}}_{\text{max}}(t)$ are,

\[
\tau^P_{\text{max}}(t) = \max_{x,i=1,2} \left( \tau^P_i(x, t) \right),
\]

\[
\tau^{P,\text{ISO}}_{\text{max}}(t) = \max_x \left( \left( \tau^P_1(x, t) + \tau^P_2(x, t) \right)/2 \right),
\]

where \((t)\) will be omitted hereinafter for the sake of clarity. Figure 10.7(a) shows that for all capillary numbers, $\tau^P_{\text{max}}$ increases sharply as the capsule is passing through the corner, and then relaxes back to the equilibrium value. Much less variation in the isotropic counterpart $\tau^{P,\text{ISO}}_{\text{max}}$ is observed as the velocity gradient in the spanwise direction is very weak. We mark the temporal peak of $\tau^P_{\text{max}}$ in figure 10.7(a) by green squares and find that it scales with \((Ca)^{0.8}\) (see figure 10.7(b)). We measure the elapsed time $t^P_{\text{max}}$, taken by the capsule to reach the peak tension, from $t = 0$. As shown in figure 10.7(b), $t^P_{\text{max}}$ grows with
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Figure 7. (Colour online) (a) The spatial maximum of the nondimensional major and isotropic principal tension, $\tau P_{\text{max}}$ and $\tau P_{\text{ISO,max}}$, versus time. $\tau P_{\text{max}}|\text{peak}$ denotes the temporal peak of $\tau P_{\text{max}}$. (b) $\tau P_{\text{max}}|\text{peak}$, and the elapsed time to reach that peak $t_{\text{max}}|\text{peak}$ versus the capillary number $Ca$ (the former in log-log).

$Ca$, linearly as $Ca \leq 0.15$, much slowly as $Ca \in [0.15, 0.3]$, finally reaching a plateau as $Ca \geq 0.35$. Clearly, a stiff capsule gets mostly distorted immediately after the corner, while a compliant one takes longer time. This variation with the capillary number is also observed for the time needed to reach the peak surface area and the velocity overshoot (see figure 10.5(a) and figure 10.6(a)). This clearly indicates a phase delay, a typical feature of viscoelastic media, which results from the interaction of the elastic membrane and the surrounding flow. Such a delay occurs for two interacting spherical (Lac et al. 2007) or RBC-shape capsules (Omori et al. 2013) in shear flow; in those cases, a more deformable pair needs longer time to reach the maximum vertical separation during the collision. Another case worth-noting is that of RBCs in a channel of oscillating width (Braunmüller et al. 2011), whose deformation follows the geometric oscillations with a phase delay.

We next analyse the evolution of the elastic energy stored in the capsule membrane. Following the work of Walter et al. (2011), we split the elastic energy into two parts, shear strain energy $E_S$ and bending energy $E_B$. $E_S$ is the integral of the Lagrangian strain energy function $W_S$ on the capsule surface $S_0$, $E_S = \int_{S_0} W_S (x,t) \, dS_0$ and $E_B = \int_{S_0} G_B H^2 \, dS_0$, where $H$ is the mean
curvature, expressed as $H = \frac{1}{2} a^{\alpha \beta} b_{\alpha \beta}$. The temporal evolution of their nondimensional form $E_S/G_s a^2$ and $E_B/G_B$ is depicted in figure 8 for the different values of $Ca$ under investigation. Both forms increase significantly with capsule elasticity. The shear strain energy reaches its peak value around $t = 1$, similarly to what is observed for the surface area and the maximum major principle tension. The similarity implies that the extension of the membrane is the main ingredient of the capsule deformation, induced by the accelerating flow right after the corner. We recall that the capsule velocity (see figure 6) decreases before the corner and goes up after. The peak velocity appears when the shear strain energy $E_S$ drops down sharply and the observed velocity overshoot can therefore be related to the release of the elastic energy accumulated during the extensional deformation.

The temporal variation of the nondimensional bending energy $E_B/G_B$ displays a more complicated dependence on the membrane elasticity. Stiff capsules
develop an energy peak when severely extended by the accelerating flow after corner but show negligible response to the upstream decelerating flow. Conversely, the softer capsule $Ca = 0.45$, displays a wavy variation in $E_B/G_B$, which decreases before $t = 0$, showing its sensitivity to the deceleration. To better clarify this point, four instants $T_A$, $T_B$, $T_C$ and $T_D$ are marked in figure 8 and the corresponding distribution of the bending energy density $H^2$ is visualised in figure 10.9(b), where the viewpoint is chosen to focus on the trailing tips. At $t = T_A$, the capsule is not far from the equilibrium shape in Poiseuille flow, thus the density distribution is almost left-right symmetric. The symmetry breaks as $E_B/G_B$ reaches the local minimum at $t = T_B$, and the energy density peak on the right tip shrinks in size and magnitude. This is mirrored in the $x - y$ plane (see figure 8), the right tip is slightly less sharper from $t = T_A$ to $t = T_B$; at $t = T_B$, the capsule experiences the underlying flow deceleration and hence its deformation is relaxed. Right after the corner, the flow acceleration drives the energy to the next peak at $t = T_C$ by elongating
the capsule that develops high curvature on its left trailing tip. At $t = T_D$, the capsule relaxes as leaving the corner and the energy goes down.

![Graphs and diagrams showing capsule profiles and tension distribution](image)

**Figure 10.** (Colour online) Profiles and principal tension distribution of capsules with capillary number $Ca = 0.15$ and $Ca = 0.45$, bending modulus $Cb = 0.01$ and confinement $H_x = 3$. (a) Profiles on the $x - y$ plane, where the yellow shading denotes the initial equilibrium shape. The black curve with circles represents the centroid path. The grey dash-dotted curve is the streamline of the single-phase flow. Dash-dotted green curves with filled and hollow diamonds show trajectories of front and rear apexes, respectively; dashed red curves with squares stand for that of left and right apexes. (b) Contours of the scaled major principal tension $\tau^P/G_s$. Five snapshots denoted by $t_1, t_2, t_3, t_4$ and $t_5$ for each case correspond to the profiles marked in (a); $t_i = t_{\text{start}} + \frac{(t_{\text{end}} - t_{\text{start}})(i+1)}{14}$, $i = 1$ to 5, where $t_{\text{start}}, t_{\text{end}}$ corresponds to the beginning and end of the capsule trajectory; this definition of $t_i$ will be used in the following.
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The trajectories of capsules with $Ca = 0.15$ and $Ca = 0.45$ are illustrated in figure 10.10(a). The centroid trajectory (black curves with circles) closely match the centre streakline $S3$ (dash-dotted grey curve) and is insensitive to the membrane elasticity. We also mark and trace the four apexes of the capsule from the equilibrium shape. The front and rear apexes initially on $S3$, follow trajectories (indicated by filled and hollow diamonds respectively) deviating from $S3$ significantly; the front/rear apex drifts towards the outer/inner corner, eventually staying above/below the centroid trajectory. The left/right apex starts from the same vertical position and approximately moves along the streakline $S1/S5$, characterised by a decreasing/increasing velocity around the corner (see figure 4); as a result, the right apex travels beyond the left, as shown in figure 10.10(a). The vertical and horizontal displacements of the tips suggest that the material points of the capsule have rotated anti-clockwise with respect to its moving direction. This rotation is induced by the flow near the corner: as discussed above, this is spatially nonuniform across the channel and the material points near the inner/outer corner are advected by the accelerating/decelerating flow, which result in a net anticlockwise membrane rotation.

Unlike the trajectory, the deformation of capsules displays strong dependence on the elasticity, see figure 10.10(a). The softer capsule ($Ca = 0.45$) exhibits a stronger deformation than its stiff counterpart, especially in the $x-y$ plane. It has a parachute shape at the instant $t_1$, preserving the left-right symmetry far away from the corner. Right before the corner, at time $t = t_2$, the parachute shape is distorted and develops a double concavity. At $t_3$, the acceleration of the flow on the centre streakline $S3$ (see figure 4) stretches the capsule horizontally; meanwhile, the material points close to the outer corner lag behind because of the underlying flow deceleration, and hence form a sharp tail. Leaving the corner, the capsule recovers the equilibrium shape at $t_5$. Due to the absence of any spanwise confinement, the deformation is less evident in the $x-z$ plane than in the $x-y$ plane.

We investigate the distribution of the scaled major principal tension, $\tau_P(x, t)/G$, in figure 10.10(b). The soft capsule, $Ca = 0.45$, experiences a significantly higher tension than the stiffer one, $Ca = 0.15$, as shown in figure 10.7(a). For both cases, the tension grows and reaches the peak at the time denoted by $t_3$. The maximum tension is located in proximity of the outer part of the corner. Interestingly, at $t_3$, the maximum tension appears on the lateral sides of the capsule, even if no confinement is imposed in the spanwise direction.

3.1b. Effect of the bending modulus. By modulating the reduced bending modulus $Cb$, we study the effect of the bending resistance of the membrane. The capillary number is fixed to $Ca = 0.3$ and the results presented in figure 11.
The data reveal that decreasing $C_b$, the surface area $A/4\pi a^2$, maximum principal tensions $\tau_{\text{max}}^P/G_s$ and $\tau_{\text{max}}^\text{ISO}/G_s$ and elastic energies $E_S/G_s a^2$, $E_B/G_B$ increase (cf. figure 11). Indeed, the bending modulus has an influence similar to that of the shear modulus, both modelling the resistance of the membrane to deformation. Figure 10.11(b) shows that the capsule velocity $V_{\text{cap}}$...
The motion of a deforming capsule through a corner

\[ \tau^P / G_s \]

\[ CB = 0.01 \]
\[ CB = 0.04 \]
\[ CB = 0.1 \]

\[ x-y \]  \[ x-z \]  \[ x-y \]  \[ x-z \]  \[ x-y \]  \[ x-z \]

Figure 12. (Colour online). Distribution of the scaled major principle tension \( \tau^P / G_s \) in the \( x-y \) and \( x-z \) plane, for capsules with \( Ca = 0.3 \), and varying bending modulus \( CB = 0.01 \), \( CB = 0.04 \) and \( CB = 0.1 \). The five snapshots indicate different instants during the flow past the corner.

increases noticeably for weaker bending stiffness as long as \( CB > 0.01 \), thanks to the enhanced capsule deformation towards the centre of the channel. This effect is nonetheless limited when \( CB \) is further decreased since the deformation is mainly determined by the shear modulus for very low \( CB \).

In figure 12, we examine the dependence of the capsule deformation and the distribution of the major principle stress on the modulus \( CB \). In the \( x-y \) plane, the shape of the capsule with \( CB = 0.01 \) is similar to a skewed parachute at \( t_2 \) and to a flipper at \( t_3 \); the stiffer body, \( CB = 0.1 \), deforms instead into almost symmetric prolatas; the bending stiffness suppresses both the convexity and concavity, smoothing the surface. In the \( x-z \) plane, the capsule shrinks as \( CB \) increases, since it is squeezed less in the wall-normal direction and hence
expands more in the spanwise direction at fixed volume. Note also that the peak of the principle tension is found at $t_3$ for $Cb = 0.01$ and $Cb = 0.04$, and at $t_2$ for $Cb = 0.1$. The stiffer capsule, characterised by a shorter relaxation time, reaches the maximum deformation earlier.

3.1c. Effect of the wall confinement: varying the channel width $L$. Micro-fluidic devices are designed to be small and compact. Owing to the wall confinement, the size of the device influences its performance and the motion of the objects transported inside. We therefore investigate the effect of the channel width $L$; in addition to the value $L = 3$ used for the simulations reported so far, the two configurations with $L = 2.7$ and $3.3$ are studied, with the membrane elasticity defined by $Cu = (0.075, 0.3)$ and $Cb = 0.01$. As clearly illustrated in figure 10.13(a), the capsule deforms more in the smaller channel, being more elongated and with sharper trailing tips. Surprisingly, figure 10.13(b) shows that stronger confinement enlarges the capsule around the corner, especially in the $x - y$ plane; the effect is also mirrored by the increase of the membrane area for the case with smaller $H_x$ (see figure 14). This is not intuitive: for a fixed flow rate, reducing the channel width indeed increases the wall-normal velocity gradient and consequently stretches the capsule more.

![Figure 13](image-url)

**Figure 13.** (Colour online) Profiles and principal tension of capsules transported in channels of width $H_x = 2.7$ and $H_x = 3.3$. $(Ca,Cb) = (0.3,0.01)$. Same plot as in figure 10.
Figure 14. (Colour online) The effect of the channel width $L$ on the dynamics of capsules with $Ca = (0.075, 0.3)$ and $Cb = 0.01$. Three values of $L$ are chosen: 2.7, 3.0 and 3.3. (a) The capsule surface area $A$; (b) The velocity of the capsule centre $V_{\text{cap}}$; (c) The spatial maximum of the scaled major and isotropic principal tension, $r_{\text{max}}^P/G_s$ and $r_{\text{max}}^{P_{\text{ISO}}}/G_s$; (d) The scaled shearing and bending elastic energies, $E_S/G_s a^2$ and $E_B/G_B$.

Figure 14 shows that stronger wall confinement increases the area, elastic energy and maximum principle tension of the capsule. While the increment is small for the stiff capsule $Ca = 0.075$, it becomes important for softer bodies. The area, elastic energy and principle tensions measure the deformation of the
membrane and quantify its elastic response. At the low \(Ca\), the capsule is relatively stiff compared to viscous forces and the flow variation induced by the confinement has a weak effect on the capsule. A significant decrease in the velocity \(V_{\text{cap}}\) as a result of the wall effects is however observed for both stiff and soft capsules. While the behaviour of the membrane is mainly determined by the capsule elasticity, the velocity of the capsule centre is related to the speed of the fluid inside and around the membrane, and therefore it reflects more the behaviour of the flow. This explains the sensitivity of the capsule velocity to wall confinement.

We conclude this section by examining the overshoot of the capsule velocity observed just behind the corner. To quantify the increased speed behind the corner, we introduce the parameter \(\chi = \left( \max_t (V_{\text{cap}}(t)) - V_{\text{equ}} \right) / V_{\text{equ}}\), and display it versus the capillary number and for the three values of \(L\) considered in figure 15. The overshoot \(\chi\) increases with \(Ca\), as discussed in section 3.1a, and with the confinement. Indeed, reducing the channel width increases the curvature of the channel flow profile, generating relatively stronger flow. In other words, the effective capillary number, accounting for the flow curvature, increases with confinement, thus promoting a higher overshoot.

### 3.2. Duct flow (spanwise confined) with a 90° sharp corner

Micro-fluidic devices and biological vessels commonly consist of ducts and pipes, confining objects in all transverse directions. 3D surface-vortices and shear layers of non-negligible velocity are formed on vesicles in a duct flow (Coupier
et al. 2012), unlike 2D cases with the confinement in one direction only. In this section, we present results for a square duct of dimensions $H_x = H_z = 3$.

![Figure 16](image)

**Figure 16.** (Colour online) Nondimensional properties of a capsule convected through a corner flow with and without spanwise confinement. For the case with confinement, a square duct is studied, $H_x = H_z = 3$. The capsule membrane is defined by $Cb = 0.04$, while $Ca = (0.15, 0.3)$. (a) Surface area of capsule $A/4\pi a^2$; (b) Velocity of the capsule centre $V_{\text{cap}}/V_C$; (c) Spatial maximum of the major principal tension $\tau^P_{\text{max}}/G_s$; (d) Shear strain energy $E_S/G_s a^2$.

In the duct flow, the ratio between the maximum and the mean velocity is higher than that of a channel flow because the additional spanwise confinement intensifies the velocity gradients. As a result, the capsule is more distorted, as
seen by the different quantities displayed in figure 16. Interestingly, the anti-clockwise rotation of the membrane in the $x-y$ plane is reduced, as indicated by the orientation of the line connecting the lateral apexes (see figure 10.17(a)). Such a phenomenon might have useful implications on the alignment of soft particles, as discussed in the work of Omori et al. (2012). These authors observed that the orientation of a non-spherical capsule displays a transition depending on its elasticity; in our configuration, the capsule orientation is influenced by the spanwise confinement. As the additional confinement introduces velocity gradients in the spanwise direction $z$, the capsule shape is significantly altered in the $x-z$ plane. This effect is depicted in figure 10.17(b) where results for the channel and duct are compared.

![Figure 17](image_url)

**Figure 17.** (Colour online) Profiles and principal tension of capsules transported in a channel and in a square duct with $H_x = 3$. $(Ca, Cb) = (0.3, 0.01)$. Same plot as in figure 10. The double-sided arrows connect the lateral apexes of the capsule, indicating its initial and eventual orientation.

### 3.3. Channel flow with a round corner

Corners are typically curved and smoother in real micro capillaries (Woolfenden & Blyth 2011); its biological relevance is however still unclear. As a first step, we study a channel with a round 90-degree corner, as sketched in figure 18. The
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Figure 18. (Colour online) Profiles and principal tension distribution of capsules transported in channels with round and 90 degree sharp corner, $H_x = 3$. $(Ca, Cb) = (0.3, 0.01)$.

(a) Profiles on the $x - y$ plane, where the yellow shading denotes the equilibrium shape of the released capsule. The black curve with filled circles represent the centroid path. (b) Distribution of principal tension $\tau_{\text{P max}}$ scaled by $G_s$. The five snapshots correspond to the profiles marked in figure 10.18(a).

radius of curvature of the inner and outer arc are $R_c$ and $R_c + H_x$, respectively, with $R_c = 1$ (see figure. 10.18(a)). This setup, characterised by a constant channel width, minimises the streamwise flow variation. As a result, the area, principle tension and elastic energy of the capsule vary more smoothly when compared to those of a cell convected through a sharp corner, see figure 19; the maximum values of the different quantities decrease significantly and the variation of the capsule shape seems less noticeable, see figure 10.18(a).

To quantify the relative reduction in the temporal maximum of the capsule surface area, we introduce the ratio between the values in the round and sharp corner $\mathcal{R}[A_{\text{max}}^\text{peak}] = \frac{A_{\text{max}}^\text{peak}(\text{sharp}) - A_{\text{max}}^\text{peak}(\text{round})}{A_{\text{max}}^\text{peak}(\text{sharp})}$, and similarly for the other quantities characterising the cell motion and deformation, $\mathcal{R}[\tau_{\text{max}}^\text{P max}]$, $\mathcal{R}[\tau_{\text{max}}^\text{ISO}]$, and $\mathcal{R}[\frac{E_G}{\sigma_s}]$. 

Figure 19. (Colour online) Nondimensional properties of a capsule convected in a channel flow with a straight and round corner. $R_c = 1, L = 3$. For the capsule, $C_b = 0.01$, while $Ca = (0.15, 0.45)$. (a) Surface area of capsule $A/4\pi a^2$; (b) velocity of the capsule centre $V_{cap}/V_C$; (c) Spatial maximum of the major principal tension $\tau_{max}/G_s$; (d) Shear strain energy $E_S/G_s a^2$ and bending energy $E_B/G_B$.

As shown in figure 20, the reduction is most evident for the principle tension and elastic energy, approaching about 20% for $\tau_{max}^P$ (also reflected by the distribution of $\tau^P/G_s$ in figure 10.18(b)) and 40% for $E_S/G_s a^2$. In general, stiffer capsules display the larger reduction. The round corner reduces the mechanical stresses on the membrane, showing an advantage over the sharp corner. This is thus potentially relevant in complex micro-fluidic devices where
multiple branches and corners are utilised for the precise control and manipulation of micro-particles, a typical example being the novel cell-sorting setup proposed by Cartas-Ayala et al. (2012). Finally, we note that no velocity shoot is observed for the \( Ca = 0.15 \) capsule when flowing past the round corner. From this, we can conclude that the viscoelastic effects induced by the membrane deformability are more relevant when due to the velocity gradients along the flow direction rather than by the curvature of the streamlines.

![Figure 20](image_url)

Figure 20. (Colour online) Relative reduction of the temporal peak of the surface area \( A \), maximum major principle tension \( \tau^{P\max} \), maximum isotropic principle tension \( \tau^{P\text{ISO}\max} \) and scaled shear strain energy \( \frac{E_S}{G_S a^2} \) of a capsule convected in the channel with a round corner with respect to the case of a sharp corner. The relative reduction is defined as \( R[A|\text{peak}] = \frac{A[\text{peak}\text{ (sharp)}] - A[\text{peak}\text{ (round)}]}{A[\text{peak}\text{ (sharp)}]} \), \( R[\tau^{P\max}|\text{peak}] \), \( R[\tau^{P\text{ISO}\max}|\text{peak}] \) and \( R[\frac{E_S}{G_S a^2}|\text{peak}] \) are defined correspondingly.

4. Conclusion and outlook

We present an implementation of the general geometry accelerated boundary integral method (Hernández-Ortiz et al. 2007) to simulate fluid-structure interactions in arbitrary geometries at low Reynolds number, coupled with a spectral method for the membrane dynamics. The boundary integral is accelerated by an Ewald method adapted to cope with general geometries and boundary conditions. We use this validated tool to investigate the motion of a 3D deformable Neo-Hookean capsule flowing in a micro-channel/duct with a corner. In particular, we examine the evolution of its surface area, centroid
velocity, principle tension and elastic energy. We analyse the influence of the shear modulus, bending modulus and wall confinement on the deformation and trajectory of the capsules; the effect of the corner shape is also investigated.

The temporal evolution of the surface area, centroid velocity, principle tension and elastic energy of the capsule display a clear loss of the time-reversal symmetry of the Stokes flow; this is induced by the nonlinear effects stemming from the strong interplay between the viscous flow and the deforming structure. A clear phase delay, function of the capsule elasticity, is also documented, another signature of the two-way complex interaction. The surface area, principle tension and elastic energy reach a maximum soon after the capsule passes the corner, owing to the membrane's extensional deformation induced by the flow acceleration after the corner. Before reaching the corner the velocity of the centre of the capsule follows that of the underlying streamline closely, whereas it displays a distinct overshoot right after.

The shear and bending modulus of the membrane have a similar effect on the capsule dynamics; a lower modulus results in larger deformability and stronger deformations inducing more significant viscoelastic features. The trajectory of a capsule is however insensitive to either moduli and mostly follows the underlying streamline, with only little deviation: viscosity turns out to be more important for the particle motion for the configurations considered in this work.

We also show that a stronger confinement produces a larger capsule deformation and higher viscoelasticity, owing to the sharper velocity profile (stronger velocity gradients), able to deform more the immersed objects. We finally simulated a channel with a round corner and demonstrate that the hydrodynamic stresses exerted on the capsule are significantly reduced with respect to the case of flow past a straight sharp corner.

We believe that this implementation will enable us to continue this work in several interesting directions. First, as the variation of the surface area and of the capsule centroid velocity is highly dependent on its stiffness, flow in a corner may provide new way to measure the membrane properties. Second, these results on the corner shape could help designing micro-fluidic devices with multiple branches and corners. Finally, the numerical framework presented here can be readily extended to perform high-fidelity simulations of vesicles, droplets, solid particle as well as their suspensions in arbitrary geometries, thus showing great potential for the study of micro-multiphase flow in complex lab-on-a-chip devices.

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Paper 5
A microfluidic device to sort capsules by deformability

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Submitted to Lab on a Chip

1. Introduction

One vitally important challenge in the field of biotechnology is to design devices to sort cells by chemical and physical properties. These devices can be used for rapid medical diagnoses at the cellular level, and screening to guard against deliberate contamination (Prasad 2003). To quote a few specific examples, such devices would be effective tools to (a) measure the altered deformability of Red Blood Cells (RBCs) e.g., due to malaria (Suresh 2006), (b) sort bacteria or yeast cells by their length, or (c) extract circulating tumour cells from blood of a cancer patient (Lim & Hoon 2014). An oft-used device in this category is a flow cytometer that can sort cells based on their optical responses (Prasad 2003).

It is clear from the examples quoted above that the physical properties of a cell, e.g., size, shape, or deformability are important bio-markers; it is hence crucial to try to develop cell-sorting devices based on them. Furthermore, these markers may even be preferable to biochemical markers used in traditional medical diagnostics because they are label-free. A device to sort cells by biophysical markers can be low cost, convenient to maintain, and characterized by shorter assay times and good throughput (Mao & Huang 2012).

As a further motivation, we note a remarkable use of biophysical markers in natural biological systems: the spleen separates old and damaged RBCs from healthy ones by passing them through slits between endothelial cells. Only RBCs deformable enough are recirculated back to the venous system, while ageing RBCs are phagocytosed in the cord of the spleen red pulp (Mebius & Kraal 2005).

In recent times, several microfluidic devices have been fabricated to detect biophysical markers and to sort cells accordingly (Beech et al. 2012; Bow
et al. 2011; Gossett et al. 2012; Holm et al. 2011; Hou et al. 2010; Hur et al. 2011; Mao & Huang 2012). The challenge in this field lies in designing clever geometries that allow for an efficient sorting. Microfluidic devices possess the unique ability to sort cells by deformability because they operate by balancing the elastic stresses of the cell against the fluid stresses. It then behoves us to try to understand and model flows carrying suspended cells; let us elaborate on this point. Given a geometric configuration of a microfluidic device it is computationally straightforward to find out the flow in the absence of cells. This is because the small size of microfluidic devices implies that the viscous effects dominate over inertia and hence the solution to the flow problem can be obtained by solving the linear Stokes equations. But as soon as a deformable object, e.g., a cell, is introduced, the mutual interaction between the elastic stresses at the cell surface and the viscous fluid stresses turns the problem into a formidable, nonlinear one.

Over the last decade, numerical techniques and computational capabilities have developed hand-in-hand such that it is now possible to solve such microscale complex flows in a computer (Freund 2014). The time is now ripe to use simulations to complement and speed up the usual experimental trial-and-error process required to perfect a microfluidic device. As an example of such an exercise, in this paper we use extensive numerical simulations to propose the design of a microfluidic device, sketched in figure 1, that can potentially sort cells by their deformability.

2. Models
The simplest model of a cell is a fluid-filled closed membrane, i.e., a capsule. Given the molecular complexity and the active nature of a living cell, it would be unrealistic to assume that any single constitutive model can capture the diverse behaviour of cells in flows; see, e.g., the illuminating discussion in Section 3 of Freund (2014) to appreciate the difficulties in choosing a constitutive model for RBCs. As recommended by Freund (2014), the best option is to choose a model with parameters tuned for a particular circumstance. Without much ado, we assume that the membrane of the cell is two-dimensional and isotropic. This implies that the local strain energy function \( W(I_1, I_2) \) is a function of only \( I_1 = \lambda_1^2 + \lambda_2^2 - 2 \) and \( I_2 = \lambda_1^2 \lambda_2^2 - 1 \), which are the two invariants constructed from the two principal components of the strain, \( \lambda_1 \) and \( \lambda_2 \). Among several possibilities we choose the oft-used neo-Hookean model (Barthès-Biesel et al. 2010) for which

\[
W = \frac{G_s}{2} \left[ I_1 - 1 + \frac{1}{I_2 + 1} \right],
\]

where \( G_s \) is the isotropic shear modulus. Another commonly used alternative is the Skalak model, used e.g., in Freund (2013); Freund & Orescanin (2011) for RBCs; see also Barthes-Biesel et al. (2002) for a comparison between several
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constitutive models. We also employ a linear isotropic model for the bending moment (Zhao et al. 2010), with a bending modulus $G_b = C_b a_c^2 G_s$, where $a_c$ is the radius of the capsule and $C_b = 0.01$ is held constant in our simulations. The choice of $C_b$ is consistent with the available experimental data for RBCs (Freund 2014). Finally we also assume that the fluid inside and outside the cell has exactly the same density and viscosity; and the equilibrium shape of the cell is a sphere of radius $a_c$. To summarize, we solve for capsules with neo-Hookean membrane in flows. Even stripped of all its biological context, this problem is

Figure 1. A two-dimensional ($x$-$y$ plane) sketch of our computational domain with the paths of two capsules, a stiff one ($Ca = 0.05$, solid blue line) and a floppy one ($Ca = 0.3$, broken red line), starting from the same initial position, at an offset $h_{ini} = 0.015a_c$ above the mid-plane ($y = 0$). The flow is driven from left to right. The diffuser (the diverging duct) make an angle of 45° with the $x$ axis. All length scales are normalized by the equilibrium radius, $a_c$, of the capsule. The extent of the device in the $z$ direction (perpendicular to the plane shown) is $H_z = 4a_c$. 
interesting in its own right for its potential applications to the fields of chemical engineering, bioengineering, and food processing among others.

There are two dimensionless numbers in this problem, the capillary number, \( Ca \equiv \frac{\mu U}{G_s} \), and the Reynolds number, \( Re \equiv \frac{\rho U a_c}{\mu} \), where \( U \) is the characteristic velocity, and \( \mu \) the dynamic viscosity and \( \rho \) the density. The Reynolds number is typically below 0.01 in microfluidic devices by virtue of the small length scales involved. Hence we use the linear Stokes equations (\( Re = 0 \)) to solve the flow.

For the sake of completeness, we provide a short description of the numerical algorithm (Freund 2014; Zhu & Brandt 2013) we use. The surface of the capsule is discretized into \( N \) points; the \( j \)-th point has the coordinate \( x_j \). In the spirit of immersed boundary methods (Mittal & Iaccarino 2005); at the \( j \)-th point, a force \( f_j \) is exerted on the flow. These forces are determined by the deformation of the capsule with respect to its equilibrium shape through an appropriate constitutive law; in this case the neo-Hookean model. We use a spectral method (Zhao et al. 2010) to calculate \( f_j \) given the positions \( x_j \). The flow field can then be obtained by solving the Stokes problem, with the forces \( f_j \) added to the right hand side, i.e.,

\[
-\nabla p + \mu \nabla^2 u = -\sum_{j=1}^{N} f_j \delta (x - x_j), \quad (2)
\]
\[
\nabla \cdot u = 0. \quad (3)
\]

Here \( p \) is the pressure, \( u \) is the velocity, and \( \delta \) denotes the Dirac delta function.

Equations 2 and 3 are solved by a hybrid Integral-Mesh method (Kumar & Graham 2012; Hernández-Ortiz et al. 2007). In our implementation, the mesh-based part (responsible for the long-range part of the Green’s function) is calculated by the spectral-element solver NEK5000 (Fischer et al. 2008) which allows us to cope with non-trivial boundaries. The short-range part is handled by standard boundary integral techniques. Once the Stokes problem is solved we know the velocity of the flow at every point including each point on the surface of the capsule, \( x_j ; u(x_j) \). The values of \( x_j \) at the next time step are obtained by solving,

\[
\frac{dx_j}{dt} = u(x_j). \quad (4)
\]

This implies that the \( j \)-th point on the surface of the cell moves with the velocity, \( u(x_j) \), i.e., a no-slip, non-penetrating boundary condition is satisfied on the cell surface. With this algorithm, we are able to perform high-fidelity simulations of deformable capsules suspended in microfluidic flows with complex domains.
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3. Results

The device we propose is a rectangular duct attached to a diverging one (a diffuser), as shown in figure 1. An obstacle which encompasses the entire depth of the device (z direction), is positioned at the junction of the duct and the diffuser symmetrically about the mid-plane (y = 0). A capsule, whose equilibrium shape is a sphere of radius $a_c$, is placed at the inlet. Initially, the centre of the capsule is not on the mid-plane but is displaced (along the y-direction) by an amount $h_{ini}$. The analytical flow profile (Spiga & Morino 1994) of a rectangular duct is maintained at the inlet, extreme left in figure 1,
and the zero-stress boundary condition is imposed at the outlet, extreme right in figure 1. The width and thickness of the duct (the extent of the y and z direction) is $8\alpha_c$ and $4\alpha_c$, respectively; non-penetrating, no-slip boundary conditions are imposed on the wall of the device.

The functioning of the device is demonstrated by a series of images in figure 2 (see also the supplementary videos). The flow field in the absence of the capsule is plotted in Fig. 2(a). When the capsule is at the inlet, the flow is very similar to that without the capsule. As the capsule approaches the obstacle, it slows down, deforms significantly (the deformation depends on Ca) and substantially modifies the flow as shown in Fig. 2(a)-(f). Due to the interaction between the elastic membrane and the viscous flow, the capsules follow different paths depending on their deformability. Two extreme cases are sketched in figure 1 which demonstrate that at the outlet of the device two capsules with $Ca = 0.05$ (stiff) and 0.3 (floppy) are clearly separated. This completes our primary objective, i.e., to demonstrate that our device can sort capsules by deformability.

The deformed shapes of the capsules for $Ca = 0.05$ (stiff) and $Ca = 0.3$ (floppy) at different positions along their trajectories are shown in figure 3. When the capsule passes around the obstacle, it blocks the flow and enhances the flow velocity on the opposite side of the obstacle; clearly, a stiffer (smaller Ca) capsule produces a stronger blockage. The deformation of the capsules are accompanied by large changes in their surface area as shown in the inset of figure 4. Note that, the fractional change of the area of the capsules is roughly proportional to their capillary number as can be seen from the collapsed curves shown in figure 4.

The elastic stresses on the surface of the capsule are given by the two principal tensions, $\tau_1^P$ and $\tau_2^P$, defined by (Skalak et al. 1973):

$$\tau_1^P = 2\lambda_1 \left( \frac{\partial W}{\partial \xi_1} + \lambda_1 \frac{\partial W}{\partial \xi_2} \right),$$

$$\tau_2^P = 2\lambda_2 \left( \frac{\partial W}{\partial \xi_1} + \lambda_2 \frac{\partial W}{\partial \xi_2} \right).$$

(5)

The time evolution of the maximum stress, $\tau_{\text{max}}^P$, which is the maximum value of $\tau_1^P$ and $\tau_2^P$ calculated over the surface of the cell, is shown in figure 5 for three capillary numbers, $Ca = 0.05, 0.2, \text{ and } 0.3$. The stress is maximum when the capsules pass through the gap and increases with Ca; for $Ca = 0.3$ it can be as large as 3.5 times $G_\alpha$. Clearly, too strong mechanical stresses can rupture capsules although rupturing depends not only on the maximum value of the stress but also on how long it is applied. For example, RBCs at room temperature can even survive stresses up to 5000 Pascals for a very short time (Musielak 2009). The time evolution of the maximum stress in figure 5 determines the type of cells that can be sorted in this device.
Figure 3. Shapes of the capsule, with the computational grid sketched on the surface, at different instances during its passage through the device. Top row: $Ca = 0.05$. Bottom row: $Ca = 0.3$. At a time when (A) the capsule almost touches the obstacle, (B) the capsule sits in the gap between the obstacle and the duct-walls, (C) the capsule has gone well past the obstacle. The pseudocolors show the variation of the local strain energy function non-dimensionalized by $G_s a_c^2; \mathcal{E} \equiv W/(G_s a_c^2)$. Each plot is normalized by the maximum value of $\mathcal{E}, \mathcal{E}_{\text{max}}$. In the top row, $Ca = 0.05$, $\mathcal{E}_{\text{max}} = 0.04(A), 1(B), 0.004(C)$. In the bottom row, $Ca = 0.3$, $\mathcal{E}_{\text{max}} = 0.47(A), 3(B), 0.07(C)$. 

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The basic working principle of this device is the following. To distinguish capsules by deformability we apply an external flow that forces the capsules to pass through a narrow gap. The path of each capsule is then determined by the interaction between the viscous stresses and the elastic stresses; a relative measure of these two is the capillary number, $Ca$. For capsules with large $Ca$ the viscous stresses dominate over the elastic ones, hence the trajectories of their centre-of-mass are close to the flow streamlines; these capsules deform far from their equilibrium shape. As an illustration, consider the limit $Gs \rightarrow \infty$, $Ca = 0$. In this limit, the membrane of the capsule does not resist deformation and its material points ($x_j$s) are advected by the flow as Lagrangian points. Consequently their centre of mass follows the streamline of the underlying flow.
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Figure 5. The maximum value of the principal tension (Equation (5)), nondimensionalized by $G_s$, $\tau_{p_{\text{max}}}/G_s$ as a function of time for $Ca = 0.05$ (black filled circles), 0.2 (red squares), and 0.3 (blue triangles).

In contrast, capsules with smaller $Ca$ deform less and can alter the flow more, hence their paths deviate further from the underlying flow; i.e., their centres are deflected further from the obstacle. This is also the basic principle that acts in the Deterministic Lateral Displacement (DLD) devices (Beech et al. 2012). This variation in the trajectories after passing around a single obstacle is much smaller than the radius of the capsule, $a_c$. Hence, by merely driving the capsules through a narrow gap (between the obstacle and the duct-walls) it is not possible to generate large enough differences between their trajectories to separate them. The DLD device (Beech et al. 2012) overcomes this limitation by using an array of obstacles to generate an accumulative outcome. We solve this problem by adding the diffuser where small displacements are magnified. The Pinched Flow Fractionation devices (Yamada et al. 2004), which sort particles by their size, also use a diffuser. So far they have not been used to sort capsules by their deformability.
Let us now discuss the typical length scales involved in designing this device. In the sketch shown in figure 1 all the length scales have been normalized by $a_c$. The radius of the obstacle is $2a_c$. The gaps through which the capsules pass have a width of $2a_c$ too. Although the exact values of these sizes are not crucial, they must be of the same order of the size of the cells.

Symmetry dictates that, if initially the capsule is placed exactly on the mid-plane it would get stuck in front of the obstacle, in the absence of thermal fluctuations. Estimates show that thermal fluctuations can be ignored in this problem. Even without Brownian fluctuations, in an experimental realization, it would certainly be impossible that all the capsules are placed near the inlet with a precise initial offset, $h_{ini}$, from the mid-plane. How do small changes in $h_{ini}$ affect the sorting capability of our device? To answer this question, we run simulations, for a range of values of Ca, each with several different values of $h_{ini}$. Let us concentrate on the stiffest capsule, $Ca = 0.05$, and the most floppy one, $Ca = 0.3$. If they are released from the same initial offset ($h_{ini}$) then at the outlet the vertical displacement between their centres is larger than their diameter ($2a_c$), i.e., they are clearly separated, as shown in figure 1. Such a clear separation is not achieved if the capsules are released from different $h_{ini}$s. For example, the trajectories for the two cases, $h_{ini} = 0.3$, $Ca = 0.3$ and $h_{ini} = 0.15$, $Ca = 0.05$, are such that at the outlet the exit regions for the two cases overlap, see figure 6(a). To estimate this overlap, we plot, in figure 6(b), the displacements of the centre of the capsules from the mid-plane (at the outlet), $\Delta y$, as a function of $Ca$, for $h_{ini} = 0.15$ and 0.3. The overlap between the capsules in figure 6(a) corresponds to the shaded region in figure 6(b). Figure 6(b) can be similarly used to calculate the overlap between any two points in the figure. Figure 6(b) clearly shows that the paths of floppy capsules

To estimate the strength of the thermal fluctuations in this problem, we note that while in contact with a fluid at temperature $T$ and viscosity $\mu$, a rigid sphere of radius $a_c$ performs a random walk (in the absence of any other external forces) where its displacement $\langle r^2 \rangle \approx 4D_T t$, with the diffusion coefficient $D_T = k_B T / (6 \pi \mu a_c)$ where $k_B$ is the Boltzmann constant (Saffman & Delbrück 1975). Using $T = 300K$, $a_c \approx 10\mu m$ and using the viscosity of water $\mu = 0.01$ (in cgs units), we obtain $D_T \approx 7 \times 10^{-7} \text{cm}^2 \text{s}^{-1}$; hence over the time of transit of the capsule through the microfluidic device the root-mean-square displacement of the capsule due to thermal fluctuations will be about $\langle r^2 \rangle \approx 7 \times 10^{-7} \times 20a_c/U$ as we take a device which is about twenty cell-lengths long. Typical velocities in microfluidic devices are of the order of $\mu$litre per minute. The cross-section of our device is about $10\mu m \times 10\mu m$ which gives typical velocities of the order of $U \approx 0.1 \text{cms}^{-1}$. Hence the total displacement due to the Brownian motion during the passage of the cell through this device is about $10^{-5}$ times the typical cell-length. Hence the Brownian fluctuations can be ignored in this problem.
(larger Ca) are more affected by the change in \( h_{\text{ini}} \). Note that, the overlap is quite small compared to \( a_c \) and can be reduced by using a longer diffuser.

To further understand how crucially the performance of this device depends on its design, we remove its spanwise confinement and impose periodic boundary conditions along the \( z \) direction; the results are plotted in figure 6 with the label “unconfined”. As expected, the absence of the spanwise confinement implies that for the same value of Ca, the vertical displacement decreases, in other words, the sorting capability of the device becomes weaker. Note that this comparison is made with the mean velocity of the underlying flow being held fixed. Next, instead of a perfect semi-cylindrical post, we test two more obstacles with semi-elliptic cross sections, made by stretching the semi-cylinder in the \( x \) direction by a factor of \( \xi = 2 \) and \( \xi = 2/3 \). Their cross sections are then two semi-ellipses with a major axis along the \( x \) and \( y \) direction, respectively. We find that the displacements between capsules with different deformability are essentially not altered by this geometric change, there is however a minor improvement in the sorting capability when the major axis is oriented along the \( x \) direction (\( \xi = 2 \)).

4. Conclusions

We model cells as fluid-filled capsules enclosed by neo-Hookean membranes characterized by two elastic moduli, the shear modulus \( G_s \) and the bending modulus \( G_b \); the ratio between the two is held constant. Depending on the type of targeted cells, this model needs to be calibrated with the elastic measurements performed on the particular cells. For human RBCs, different methods, e.g., the measurements by micro-pipette (Liu et al. 2007) or that by optical tweezers (Heinon et al. 1999; Lenormand et al. 2001) give slightly different values of \( G_s \). Diseases, e.g., sickle cell anaemia, can change this elastic coefficient by a factor of two to three (Lei & Karniadakis 2012), which is consistent with the range of variation of the capillary number studied here. If we take a representative value of \( G_s \approx 2.5 \mu N/m \), and use water as our fluid, then a typical flow rate of 0.1 \( \mu \)litre-per-minute gives \( \text{Ca} \approx 0.06 \) which is well within the operating range of our device. Furthermore, as the sorting behaviour depends on \( \text{Ca} \) and not on \( G_s \) alone, the same device can be used in a different range of \( G_s \) values by merely changing the flow rate.

To compare against other cell-sorting devices, the throughput of this device will be of the same order as that of the optical flow cytometers (Prasad 2003) because we can only allow one cell at a time to pass through the device. Margination devices (Hou et al. 2010) have a higher throughput as they operate on very many cells simultaneously, but the accuracy of the device we propose is expected to be significantly higher. We further note that optical flow cytometers can be modified to sort by deformability too by adding obstacles in the path of the cells and by optical recognition of their deformation. Due
to the relatively simple model of the cell membrane used, and the fact that possible surface interactions between the cells and the walls of the device have been ignored, we do believe that further refinements of the suggested devices are possible. This work is the first numerical study of cell sorting in a realistic microfluidic device and shows how accurate simulations may guide the initial stages of the design of new devices. We hope that our work will inspire the experimental realization of devices based on the mechanism presented.

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Figure 6. (a) Trajectories for \( Ca = 0.05 \) (stiff, red) and \( Ca = 0.3 \) (floppy, blue) for two initial offsets \( h_{init} = 0.15 \) (solid) and 0.3 (dashed). The profiles of the capsules, at the outlet, clearly show an overlap. (b) The displacements of the centre of the capsules (\( \Delta y \)), above the mid-plane, measured at the outlet as a function of \( Ca \) for \( h_{init} = 0.15 \) (solid) and \( h_{init} = 0.3 \) (dashed). The vertical axis is normalized by the equilibrium radius of the capsule, \( a_c \). To calculate the overlap (the shaded region), for the pair of points \( Ca = 0.05, h_{init} = 0.3 \) (red filled circle) and \( Ca = 0.3, h_{init} = 0.15 \) (blue filled square), we draw circles of unit radius with the position of the centre of the capsule as their respective origins. The overlap for any pair of points can be calculated in a similar manner. The dashed-dotted line with the symbol asterisk (\( * \)) corresponds to the "unconfined" case where we use periodic boundary conditions along the \( z \) direction.
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Micropropulsion and microrheology in complex fluids via symmetry breaking

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Many biological fluids have polymeric microstructures and display non-Newtonian rheology. We take advantage of such nonlinear fluid behaviour and combine it with geometrical symmetry-breaking to design a novel small-scale propeller able to move only in complex fluids. Its propulsion characteristics are explored numerically in an Oldroyd-B fluid for finite Deborah numbers while the small Deborah number limit is investigated analytically using a second-order fluid model. We then derive expressions relating the propulsion speed to the rheological properties of the complex fluid, allowing thus to infer the normal stress coefficients in the fluid from the locomotion of the propeller. Our simple mechanism can therefore be used either as a non-Newtonian micro-propeller or as a micro-rheometer.

1. Introduction

Life at low Reynolds numbers has attracted considerable attention in the past few decades (Brennen & Winet 1977; Fauci & Dillon 2006; Lauga & Powers 2009; Purcell 1977). The absence of inertia plays a remarkable role in the swimming of microorganisms. In a Newtonian flow, the scallop theorem (Purcell 1977) constrains the types of locomotion strategies which are effective
in the microscopic world and reciprocal motion – as are called those with a time-reversal symmetry – cannot lead to any net propulsion (or fluid transport). Microorganisms evolved different propulsion strategies to achieve micropropulsion, including the active propagation of flagellar waves for eukaryotic cells and the passive rotation of rigid helical flagella for bacteria (Brennen & Winet 1977).

The physics of low Reynolds number locomotion is relatively well explored in the Newtonian limit (see reviews in Brennen & Winet (1977); Fauci & Dillon (2006); Lauga & Powers (2009); Purcell (1977) and references therein). Beyond improving our understanding of biological processes, applications of these physical principles led to progress in the design of synthetic micro-swimmers for potential future biomedical applications (Dreyfus et al. 2005; Ebbens & Howse 2010; Lauga 2011; Lauga & Powers 2009; Wang 2009). In contrast, fundamental properties of life in complex, non-Newtonian, flows remain surprisingly unaddressed. Non-Newtonian flow behaviours can be appreciated through well-known manifestations from daily life, for example the climbing of dough up kitchen mixing blades (termed rod-climbing, or Weissenberg, effect) or the remarkable behaviour of Silly Putty, a popular toy which bounces like a solid rubber ball when thrown to the floor but melts like a fluid when left on a surface for some time (Bird et al. 1987a; Larson 1999; Morrison 2001).

Many situations exist wherein microorganisms encounter biological fluids which have polymeric microstructures and non-Newtonian rheological properties. For example, spermatozoa swim through the viscoelastic cervical mucus and along the mucus-covered fallopian tubes (Fauci & Dillon 2006; Katz & Berger 1980; Katz et al. 1981, 1978; Suarez & Dai 1992; Suarez & Pacey 2006); cilia lie in a layer of mucus along the human respiratory tract (Sleigh et al. 1988); Helicobacter pylori, a bacterium causing ulcer, locomotes through mucus lining of the stomach (Montecucco & Rappuoli 2001); spirochetes moves through host tissue during infection (Wolgemuth et al. 2006); in biofilms, bacteria are embedded in cross-linked polymer gels (Costerton et al. 1987, 1995; Donlan & Costerton 2002; O’Toole et al. 2000; Wilking et al. 2011).

Physically and mathematically, the presence of polymeric stresses in a complex fluid means that the usual properties associated with the absence of inertia in the Newtonian limit cease to be valid, in particular kinematic reversibility and the linearity of the flow equations. In return, non-Newtonian effects such as stress relaxation, normal stress differences, and shear-rate dependent viscosity manifest themselves (Bird et al. 1987a,b; Larson 1999; Morrison 2001).

discussion in the biomechanics community has recently focused on the simple question: does fluid elasticity enhance or deteriorate propulsion at the microscopic scale? Theoretical studies on infinite models (Fu et al. 2007, 2009; Lauga 2007) showed that, for fixed body-frame kinematics, the propulsion speed decreases in a viscoelastic fluid. Numerical studies on a finite swimmer (Teran et al. 2010) demonstrated that the propulsion speed could be enhanced by the presence of polymeric stress for some prescribed kinematics. Experimental investigations suggested evidences for both (Liu et al. 2011; Shen & Arratia 2011). It was also shown that reciprocal actuation on a fluid, unable to provide net locomotion or flow transport in the Newtonian case, can be rendered effective by viscoelasticity (Lauga 2009; Normand & Lauga 2008; Pak et al. 2010).

The presence of polymeric stress has also interesting consequences on the rate of flagellar synchronization (Elfring et al. 2010).

Normal stress differences in a complex fluid are responsible for a number of important non-Newtonian effects (Bird et al. 1987a; Larson 1999; Morrison 2001) including the rob-climbing effect mentioned above impacting many applications such as mixing, and the swelling of polymer melts when extruded from dies in manufacturing processes posing constraints on the rate of extrusion. In a pure shear flow with an arbitrary Reynolds number and a shear rate \( \dot{\gamma} \), assuming that the flow is in the \( x \)-direction and the velocity varies in the \( y \)-direction, the \( z \)-direction being called the neutral direction (Bird et al. 1987a), the first and second normal stress coefficients are defined as \( \Psi_1 = (\tau_{xx} - \tau_{yy})/\dot{\gamma}^2 \) and \( \Psi_2 = (\tau_{yy} - \tau_{zz})/\dot{\gamma}^2 \) respectively, where \( \tau_{ij} \) are the components of the deviatoric stress tensor. In a Newtonian flow, there are no normal stress differences (\( \Psi_1 = \Psi_2 = 0 \)), whereas for polymeric fluids typically \( \Psi_1 > 0 \) and \( \Psi_2 < 0 \). The magnitude of the second normal stress coefficient is usually much smaller than that of the first normal stress coefficient (\( |\Psi_2| \ll \Psi_1 \)). In the rob-climbing phenomenon, both first and second normal stress coefficients contribute to the effect (Bird et al. 1987a). However, due to its small magnitude, the effect of the second normal stress coefficient is shadowed by that of the first normal stress difference (Bird et al. 1987a). The existence of the second normal stress difference can be demonstrated in a free-surface flow driven by gravity through a tilted trough: a Newtonian fluid has a flat free surface (with negligible meniscus effect), while the free surface of a non-Newtonian fluid becomes convex due to second normal stresses (Couturier et al. 2011; Tanner 1970; Wineman & Pipkin 1966).

In this work, we propose a simple mechanism able to take advantage of the presence of normal stress differences to propel in a complex fluid. Our geometry, shown in figure 1, consists of two linked small spheres propelling under the action of an external torque, a setup we will refer to as a “snowman”. Locomotion is enabled solely by the presence of normal stress differences, and no motion exists in a Newtonian environment, a fact that can in turn be used to infer the normal stress coefficients of a complex fluid. In essence, as complex
fluids lead to new modes of small-scale propulsion, symmetrically the presence of propulsion in an environment can be used to locally probe the rheological properties of the fluid.

The first normal stress coefficient of a fluid can be measured directly from a conventional cone-and-plate rheometer (Bird et al. 1987a; Larson 1999; Morrison 2001); the measurement of the second normal stress coefficient however has been a longstanding challenge (Baek & Magda 2003; Brown et al. 1995; Kulkarni et al. 2006; Schweizer 2002). A number of methods were proposed (see a review in Schweizer (2002)), including a modified cone-and-plate rheometry with pressure transducers (Baek & Magda 2003; Bird et al. 1987a), a subtle evaluation of a combination of cone-and-plate and parallel-plate experiments (Brown et al. 1995), rheo-optical measurements (Brown et al. 1995; Kulkarni et al. 2006), and the use of a cone-and-partitioned plate tool (Schweizer 2002). Recently, a microrheological technique was proposed to measure the first and second normal stress coefficients (Khair & Squires 2010). In microrheology, colloidal probes are either actively driven, or passively diffusing, and their dynamics allows to infer local rheological information. Microrheology enjoys many advantages over conventional macroscopic rheological measurements (Squires & Mason 2010; Waigh 2005), including the reduction in sample size, the ability to probe spatially-inhomogeneous environments, and the possibility of performing measurements in living cells (Squires & Mason 2010; Waigh 2005; Weihs et al. 2006; Wirtz 2009). The mechanism we propose in this paper would be classified as “active” microrheology, a situation where colloidal probes are actively manipulated to drive the material out of equilibrium and probe its nonlinear mechanical properties (Squires 2008; Squires & Mason 2010). We offer in this paper an alternative microrheological technique capable of probing both first and second stress coefficients by using only kinematic measurements.

This paper is organized as follows. In Sec. 2, we introduce the geometric and kinematic setup of our proposed mechanism and the polymeric fluid models adopted in our study. We first investigate in Sec. 3 the propulsion characteristics of the snowman in a complex fluid, followed in Sec. 4 by the method of inferring the normal stress coefficients from its locomotion. We then provide a qualitative, and intuitive, explanation of the locomotion enabled by normal stresses in Sec. 5 before concluding the paper in Sec. 6.

2. Setup

2.1. Kinematics

By symmetry, the rotation of a single sphere in any homogeneous fluid produces no net locomotion. Inserting a second sphere, of different size, breaks the geometrical symmetry and can potentially allow locomotion. We first consider the rotation of two unequal spheres touching each other as a single rigid body
Figure 1. Geometrical setup of two spheres (“snowman”) rotating with angular velocity $\Omega$ along their separation axis. The radii of the upper and lower spheres are denoted by $R_U$ and $R_L$ respectively. The centers of the spheres are separated by a distance, $h$ (for touching spheres, $h = R_U + R_L$).

(see the geometry and notations in figure 1), the “snowman” geometry. We label the line of centers of the spheres as the $z$-axis. Without loss of generality, we assume the radius of the upper sphere ($R_U$) is smaller than that of the lower sphere ($R_L \geq R_U$). The distance between the centers of the spheres is denoted by $h$. For the case of touching spheres, we thus have $h = R_U + R_L$.

From a kinematic standpoint we assume that the rigid body rotates with a steady angular velocity about the $z$-axis, $\Omega = (0, 0, \Omega > 0)$, but is otherwise free to move. Given that the snowman is axisymmetric, the only direction it could potentially move is the $z$-direction. We assume the net hydrodynamic force acting on the snowman is zero for all times (free-swimming condition), and aim at computing the rigid body (swimming) velocity necessary to maintain force-free motion.

In a Newtonian fluid without inertia, it is straightforward to show using kinematic reversibility and reflection symmetry that a rotating snowman cannot swim – a result true for any degree of geometrical asymmetry. The central question at the heart of this paper is: Can elasticity of the fluid enable propulsion of the snowman? We answer this question in the following sections by studying the locomotion of a rotating snowman in polymeric fluids described by the two constitutive relations.

2.2. Polymeric fluid dynamics

We consider an incompressible low-Reynolds-number flow in a complex fluid. Denoting the velocity field as $\mathbf{u}$ and the fluid stress as $\sigma = -pI + \tau$, where $p$ is the pressure, and $\tau$ is the deviatoric stress tensor, the conservation of mass
and momentum are given by the continuity equation and Cauchy’s equation of motion respectively

$$\nabla \cdot u = 0,$$

$$\nabla \cdot \sigma = 0.$$  

For closure, we require a constitutive equation relating the deviatoric stresses \( \tau \) to the kinematics of the flow. Obviously a large number of models have been proposed in the past to describe polymeric fluids. In this work two constitutive equations are used to study the viscoelastic locomotion of a snowman.

2.2a. Oldroyd-B fluid. The classical Oldroyd-B constitutive equation is arguably the most famous constitutive model for polymeric fluids (Bird et al. 1987a,b; Larson 1999; Morrison 2001). It has a sound physical origin and can be derived from a kinetic theory of polymers in the dilute limit by modeling polymeric molecules as linearly elastic dumbbells. The predictions also agree well with experimental measurements up to order one Weissenberg numbers, although it is known to suffer deficiencies for larger values (Bird et al. 1987a,b; Larson 1999; Morrison 2001). In an Oldroyd-B fluid, the deviatoric stress is the sum of two components, \( \tau = \tau^s + \tau^p \), where \( \tau^s \) and \( \tau^p \) denote, respectively, the Newtonian solvent contribution and polymeric contribution to the stress. The constitutive relation for the Newtonian contribution is given by

$$\tau^s = \eta_s \dot{\gamma},$$

where \( \dot{\gamma} = \nabla u + (\nabla u)^T \) is the rate of strain tensor and \( \eta_s \) is the solvent contribution to the viscosity. The momentum equation can thus be written as

$$-\nabla p + \eta_s \nabla \cdot \dot{\gamma} + \nabla \cdot \tau^p = 0,$$  

The polymeric stress \( \tau^p \) is then assumed to be governed by the upper-convected Maxwell equation

$$\tau^p + \lambda \frac{\partial}{\partial t} \tau^p = \eta_p \dot{\gamma},$$

where \( \lambda \) is the polymeric relaxation time and \( \eta_p \) is the polymer contribution to the viscosity (Bird et al. 1987a; Larson 1999; Morrison 2001). The upper-convected derivative for a tensor \( A \) is defined as

$$\nabla A = \frac{\partial A}{\partial t} + u \cdot \nabla A - (\nabla u^T \cdot A + A \cdot \nabla u),$$

which calculates the rate of change of \( A \) while translating and deforming with the fluid.

Combining the Newtonian and polymeric constitutive relations, we obtain the Oldroyd-B constitutive equation for the total stress, \( \tau \), as

$$\tau + \lambda \frac{\partial}{\partial t} \tau = \eta(\dot{\gamma} + \lambda_2 \dot{\gamma}),$$

where the total viscosity is given by \( \eta = \eta_s + \eta_p \), and \( \lambda_2 = \lambda \zeta \) denote the retardation times (we define the relative viscosity \( \zeta = \eta_s/\eta < 1 \)). For steady
shear of an Oldroyd-B fluid, both the viscosity and the first normal stress coefficient are constant, and the second normal stress coefficient is zero (Bird et al. 1987a). The Oldroyd-B fluid is the model we will use for our numerical approach.

2.2b. Second-order fluid. For slow and slowly varying flows, the second-order fluid model applies. It is the first non-Newtonian term in a systematic asymptotic expansion of the relationship between the stress and the rate of strain tensors called the retarded-motion expansion. It describes small departures from Newtonian fluid behaviour, and the instantaneous constitutive equation is given in this model by

\[ \tau = \eta \dot{\gamma} - \frac{1}{2} \Psi_1 \dot{\gamma}^T + \Psi_2 (\dot{\gamma} \cdot \dot{\gamma}), \]

where \( \Psi_1 \) and \( \Psi_2 \) are the first and second normal stress coefficients respectively. Note that if \( \lambda = 0 \) while \( \lambda_2 \neq 0 \) in the Oldroyd-B model, Eq. (6), it reduces to a second-order fluid with a vanishing second normal stress coefficient (\( \Psi_2 = 0 \)) (Bird et al. 1987a). The second-order fluid model will enable us to derive theoretically the behaviour of the snowman for small deformations.

2.3. Non-dimensionalization

We non-dimensionalize lengths by the radius of the lower sphere \( R_L \), times by \( 1/\Omega \), and use the total fluid viscosity, \( \eta \), to provide the third fundamental unit. Hence, velocities, shear rates, and stresses are scaled by \( R_L \Omega \), \( \Omega \), and \( \eta \Omega \) respectively. The dimensionless radius of the upper sphere becomes then \( r^* = R_U/R_L \) while the lower sphere has now radius 1. We have \( h^* = h/R_L \) denoting the dimensionless distance between the centers of the sphere (\( h^* = 1 + r^* \) for two touching spheres). Both spheres rotate at the same dimensionless unit speed, \( \Omega^* = 1 \). The starred variables represent dimensionless variables in this paper. The Deborah number (Bird et al. 1987a; Larson 1999; Morrison 2001), \( \text{De} = \lambda \Omega \), is a dimensionless number defined as the ratio of a characteristic time scale of the fluid (the polymeric relaxation time, \( \lambda \)) to a characteristic time scale of the flow system (1/\( \Omega \)), and appears in the dimensionless momentum equation and upper-convected Maxwell equation

\[ -\nabla p^* + \zeta \nabla \cdot \dot{\gamma}^* + \nabla \cdot \tau^{ps} = 0, \]

\[ \tau^{ps} + \text{De} \tau^{ps} = (1 - \zeta) \dot{\gamma}^*. \]

The limit \( \text{De} = 0 \) corresponds to a Newtonian fluid.

Alternatively, the upper-convected Maxwell equation of the polymeric stress, Eq. (9), can be combined with the constitutive relation of the Newtonian contribution to obtain the dimensionless Oldroyd-B constitutive equation for
the total stress $\tau^*$ as

$$\tau^* + \text{De} \frac{\nabla}{\nabla} \tau^* = \dot{\gamma}^* + \text{De}_2 \dot{\gamma}^*, \tag{10}$$

where we have defined another Deborah number, $\text{De}_2$, in terms of the retardation time, $\text{De}_2 = \lambda_2 \Omega = \text{De} \zeta$.

The dimensionless constitutive relation for a second-order fluid is now given by

$$\tau^* = \dot{\gamma}^* - \text{De}_{\text{so}} \left( \nabla \dot{\gamma}^* + B \dot{\gamma}^* \cdot \dot{\gamma}^* \right), \tag{11}$$

where we have defined another Deborah number for the second-order fluid, namely $\text{De}_{\text{so}} = \Psi_1 \Omega / 2 \eta$, and $B = -2 \Psi_2 / \Psi_1 \geq 0$.

Importantly, we note that the definition of the Deborah number of an Oldroyd-B fluid is different from that of a second-order fluid, because the relaxation time of an Oldroyd-B fluid is defined only by the polymer, whereas the relaxation time of a second-order is defined by both the polymer and the solvent (Lee et al. 2010). The two Deborah numbers are related by the relation $\text{De}_{\text{so}} = \text{De}(1 - \zeta)$. We shall mostly use the Deborah number defined for an Oldroyd-B fluid ($\text{De}$) for the presentation of our final results, since we feel it is the one with the most intuitive definition. The Oldroyd-B equation is valid up to moderate $\text{De}$, and the second order fluid is valid for small $\text{De}$ (or $\text{De}_{\text{so}}$), and we thus expect the results from both models to match when $\text{De}$ (or $\text{De}_{\text{so}}$) is sufficiently small.

3. Propulsion of snowman in a complex fluid

As argued in Sec. 2.1, asymmetry alone does not lead to net locomotion upon rotating a snowman in a Newtonian fluid. We now explore the effects of fluid elasticity on the propulsion of a snowman: Does it even move? Which direction does it go? And how fast? Using the Oldroyd-B fluid model, we first explore numerically the propulsion characteristics of the snowman from small to moderate Deborah numbers. Next, the small $\text{De}$ limit is studied analytically via the second-order fluid model.

3.1. Moderate Deborah number

We employed a finite element model to compute the polymeric flow as described by Eqs. (8) and (9). A formulation called the Discrete Elastic-Viscous Split Stress (DEVSS-G) (Guénette & Fortin 1995; Liu et al. 1998) is implemented here to improve numerical stability. The momentum equation, Eq. (8), is rewritten as

$$\nabla \cdot \mu_a (\nabla u^* + \nabla u^{*T}) - \nabla p^* + \nabla \cdot \tau^{*p} - \nabla \cdot (\mu_u - \zeta)(\nabla \Delta + \nabla^T) = 0, \tag{12}$$
where the tensor \( G \equiv \nabla \mathbf{u}^* \) is introduced as a finite element approximation of the velocity gradient tensor \( \nabla \mathbf{u}^* \). An additional elliptic term, 
\[
\nabla \cdot \mu_a (\nabla \mathbf{u}^* + \nabla \mathbf{u}^{*T}) - \nabla \cdot \mu_a (G + GT),
\]
is added into the momentum equation for stabilization (Sun et al. 1999). In the limit that the mesh size in the finite element approximation tends to zero, \( G \) approaches \( \nabla \mathbf{u}^* \) and the elliptic term vanishes, reducing Eq. (12) to Eq. (8). \( G \) is also used to approximate the velocity gradient term \( \nabla \mathbf{u}^* \) in the constitutive equation, Eq. (9). For simulations in this work, we choose \( \mu_a = 1 \) as in Liu et al. (Liu et al. 1998).

A Galerkin method is used to discretize the momentum equations, continuity equation, and the equation for the additional unknown \( G \). Quadratic elements are used for \( \mathbf{u}^* \) and linear elements for both \( p^* \) and \( G \). The streamline-upwind/Petrov-Galerkin (SUPG) (Marchal & Crochet 1987) method is adopted to discretize the constitutive equation, Eq. (9), to improve numerical stability. The resulting weak form of the model is formulated as
\[
\{ S + \frac{h_c}{U_c} \mathbf{u}^* \cdot \nabla S, \ \tau^{p*} + \text{De}(\mathbf{u}^* \cdot \nabla \tau^{p*} - GT \cdot \tau^{p*} - \tau^{p*} \cdot G) - (1 - \zeta)(G + GT) \} = 0,
\]
where \( S \) denotes the test function for \( \tau^{p*} \), \( h_c \) is a characteristic mesh size, and \( U_c \) is the magnitude of a local characteristic velocity (we choose the norm of \( \mathbf{u}^* \) as \( U_c \)). The framework for the implementation is provided by the commercial software COMSOL, which was successfully used for simulating the locomotion of squirmers in a viscoelastic fluid at low Reynolds numbers (Zhu et al. 2012).

We perform three-dimensional axisymmetric simulations on a two-dimensional mesh constructed with triangle elements. Sufficiently refined mesh is generated near rotating objects to resolve the thin stress boundary layers, necessary to overcome numerical instabilities (Baaijens 1998; Walters & Webster 2003) and improve accuracy. We validate our implementation by comparing numerical and analytical values of the hydrodynamic torque on a rotating sphere in the Newtonian fluid. For the viscoelastic model, we validate our approach against the simulations in Lunsmann et al. (Lunsmann et al. 1993) of a sedimenting sphere in a tube filled with Oldroyd-B fluid and the analytical results in Bird et al. (Bird et al. 1987a) of a rotating sphere in a second-order fluid.

Equipped with our computational model, we are able to show that fluid elasticity does indeed enable the propulsion of the snowman provided the two spheres have unequal sizes \( (r^* < 1) \). The snowman always swim in the positive \( z \)-direction (see figure 1), i.e. from the larger to the smaller sphere. For illustration, we compute the dimensionless propulsion speed, \( U^* = U/RL\Omega \), of a typical snowman \( (r^* = RU/RL = 0.5) \) as a function of the Deborah number, \( \text{De} \) (dot-dashed line - red online, figure 2), for a fixed relative viscosity \( \zeta = 0.5 \). When \( \text{De} = 0 \), the fluid reduces to the Newtonian limit and we recover that no propulsion is possible in this case. For small values of \( \text{De} \), the propulsion speed

\[
\text{Eq. (13)}
\]
Figure 2. Demonstration of snowman locomotion. In the case $r^* = R_U/R_L = 0.5$ and $\zeta = 0.5$, we plot: (a) Dimensionless propulsion speed, $U/R_L \Omega$, as a function of the Deborah number, De. Dot-dashed line (red online): numerical simulations in an Oldroyd-B fluid; solid line (blue online): theoretical calculation using the reciprocal theorem in a second-order fluid, Eq. 36; (b) The streamline pattern and speed (shaded/color map) of the secondary flow for De = 0.1 (streamline patterns at higher De are qualitatively similar).

appears to grow linearly with De, a result confirmed analytically in the next section. A maximum swimming speed is reached at De $\approx 1.75$, before decaying as De continues to increase.

In addition to the primary flow (the Newtonian component, De = 0), elastic stresses around the snowman generate a secondary flow, understood simply as the difference between the total flow and the Newtonian component. A typical secondary flow pattern is shown in the frame of the snowman in figure 2b (De = 0.1 and $\zeta = 0.5$). We depict the velocity vectors and streamlines with the shaded/color map representing the flow speed. Fluid is drawn towards the snowman parallel to the equatorial plane and then expelled along the axis, while a ring vortex is detected in the front. The maximum speed of the secondary flow is observed at the rear of the snowman, only about 0.7% of the characteristic speed of the primary flow $R_L \Omega$. 
Micropropulsion and microrheology in complex fluids via symmetry breaking

3.2. Small Deborah number

To provide a theoretical approach to the snowman locomotion and to quantify the connection between locomotion and rheology in the following sections we now consider the second-order fluid, which we remind is valid in the small-$De$ limit only (Eq. 11). All variables are expanded in powers of the Deborah number, $De_{so}$, as

\[
\sigma = \sigma_0 + De_{so}\sigma_1 + O(De_{so}^2),
\]
\[
u = \nu_0 + De_{so}\nu_1 + O(De_{so}^2),
\]
\[
\dot{\gamma} = \dot{\gamma}_0 + De_{so}\dot{\gamma}_1 + O(De_{so}^2),
\]
\[
U = U_0 + De_{so}U_1 + O(De_{so}^2),
\]

where $U$ denotes the propulsion velocity, $U = (0, 0, U)$. Other variables are expanded similarly. We drop the stars hereafter for simplicity, and all variables in this section are dimensionless unless otherwise stated. The locomotion problem is then solved order by order.

3.2a. Zeroth-order solution. The zeroth order solution, \( \{\sigma_0 = -p_0I + \dot{\gamma}_0, u_0\} \), satisfies the Stokes equations,

\[
\nabla \cdot \sigma_0 = 0,
\]
\[
\nabla \cdot u_0 = 0,
\]

where $\sigma_0 = -p_0I + \dot{\gamma}_0$. This is the Newtonian flow for two touching spheres rotating (at a rate of $\Omega$) about the line of their centers ($z$-axis). The exact solution in terms of analytical functions was given by Takagi (Takagi 1974) in tangent-sphere coordinates. No propulsion occurs in the Newtonian limit, $U_0 = 0$, as expected.

3.2b. First-order solution. The first order solution $(\sigma_1, u_1)$ of the main problem satisfies

\[
\nabla \cdot \sigma_1 = 0,
\]
\[
\nabla \cdot u_1 = 0,
\]

where

\[
\sigma_1 = -p_1I + \dot{\gamma}_1 - \frac{\dot{\gamma}_0}{\Omega} - B\dot{\gamma}_0 \cdot \dot{\gamma}_0.
\]

To compute the value of the first order propulsion velocity, $U_1$, we will use a version of the reciprocal theorem for Stokes flows adapted to self-propulsion in viscoelastic fluids (Brunn 1976a, b; Chan et al. 2005; Ho & Leal 2010; Khair & Squires 2010; Lauga 2009; Leal 1975, 1980; Phillips 1996).
Consider an auxiliary problem with identical geometry, \( \{ \sigma_{aux}, u_{aux} \} \), satisfying
\[
\nabla \cdot \sigma_{aux} = 0, \tag{23}
\]
\[
\nabla \cdot u_{aux} = 0. \tag{24}
\]

Taking the inner product of Eq. (20) with \( u_{aux} \), minus the inner product of Eq. (23) with \( u_1 \), and integrating over the entire fluid volume, we have trivially
\[
\int_{V_f} u_{aux} \cdot (\nabla \cdot \sigma_1) - u_1 \cdot (\nabla \cdot \sigma_{aux}) dV = 0. \tag{25}
\]

Using vector calculus we can rewrite the integral in the following form (Leal 2007)
\[
\int_{V_f} \nabla \cdot (u_{aux} \cdot \sigma_1 - u_1 \cdot \sigma_{aux}) dV = \int_{V_f} (\nabla u_{aux} : \sigma_1 - \nabla u_1 : \sigma_{aux}) dV. \tag{26}
\]

The left-hand side of Eq. (26) can be converted to a sum of surface integrals by the divergence theorem while the right-hand side can be simplified using the first-order constitutive equation, Eq. (22), leading to
\[
\sum_{\alpha} \int_{S_{\alpha}} n \cdot (u_{aux} \cdot \sigma_1 - u_1 \cdot \sigma_{aux}) dS = \int_{V_f} \left[ \left( \gamma + B \gamma_0 \cdot \dot{\gamma}_0 \right) \cdot \nabla u_{aux} \right] dV, \tag{27}
\]
where \( S_{\alpha} \) denotes the surface of different spheres \((\alpha = 1, 2)\) and \( n \) represents the outward normal vector on the surface. The important simplification which took place in the right hand-side of Eq. (26) is that all Newtonian terms included in \( \sigma_{aux} \) and \( \sigma_1 \) have canceled each other out by symmetry, and thus the only piece remaining in the right-hand side of Eq. (27) is the non-Newtonian contribution (Chan et al. 2005; Phillips 1996).

Now, let \( U_1 \) and \( \Omega_1 \) be the (unknown) first order translational and rotational velocities of the spheres in our main problem, while the translational and rotational velocities of the spheres in the auxiliary problem (known) are given by \( U_{aux} \) and \( \Omega_{aux} \). On the surface \( S_{\alpha} \) of one sphere, the no-slip and no-penetration boundary conditions lead to
\[
\begin{align*}
\quad u_{aux} &= U_{aux} + \Omega_{aux} \times r, \tag{28} \\
\quad u_1 &= U_1 + \Omega_1 \times r, \tag{29}
\end{align*}
\]
where $r$ is the position vector describing the surface. The integral relation, Eq. (27), becomes

\[
\sum_{\alpha} U_{\alpha}^0 \cdot \int_{S_{\alpha}} n \cdot \sigma_{1} dS + \Omega_{\alpha}^0 \cdot \int_{S_{\alpha}} r \times (n \cdot \sigma_{1}) dS
\]

\[
- U_{1}^0 \cdot \int_{S_{\alpha}} n \cdot \sigma_{aux} dS - \Omega_{1}^0 \cdot \int_{S_{\alpha}} r \times (n \cdot \sigma_{aux}) dS
\]

\[
= \int_{V_f} \left[ \frac{\gamma}{\gamma} \frac{\gamma}{\gamma} \frac{B \gamma \gamma + \gamma \gamma}{\gamma} : \nabla u_{aux} \right] dV.
\]

(30)

In Eq. (30), the integrals $\int_{S_{\alpha}} n \cdot \sigma_{1} dS$ and $\int_{S_{\alpha}} r \times (n \cdot \sigma_{1}) dS$ represent the net hydrodynamic force and torque acting on the sphere $\alpha$ by the first order flow field. Let us denote $F_{1}^{aux} = - \int_{S_{\alpha}} n \cdot \sigma_{1} dS$ and $T_{1}^{aux} = - \int_{S_{\alpha}} r \times (n \cdot \sigma_{1}) dS$ the net external force ($F_{1}^{aux}$) and external torque ($T_{1}^{aux}$) acting on each sphere; the appearance of a minus sign comes from the fact that the total force and torque (external + fluid) acting on a body have to sum to zero in the absence of inertia. In the free-swimming case there is an additional stronger constraint, namely the total external force (or equivalently, the total fluid force) has to remain zero at all instant (we will enforce this constraint shortly). Defining also $F_{aux}^\alpha$ and $T_{aux}^\alpha$ as the external force and torque required to balance the fluid drag and torque on each sphere in the auxiliary problem we see that Eq. (30) is transformed into

\[
\sum_{\alpha} - U_{aux}^\alpha \cdot F_{1}^{\alpha} - \Omega_{aux}^\alpha \cdot T_{1}^{\alpha} + U_{1}^\alpha \cdot F_{aux}^\alpha + \Omega_{1}^\alpha \cdot T_{aux}^\alpha = \int_{V_f} \left[ \frac{\gamma}{\gamma} \frac{\gamma}{\gamma} \frac{B \gamma \gamma + \gamma \gamma}{\gamma} : \nabla u_{aux} \right] dV.
\]

(31)

The above relation remains actually true for any number of spheres and kinematics. In the case of a snowman, we have two spheres connected as a rigid body in both the main and auxiliary problems, hence $U_1^1 = U_1^2 = U_1$, $\Omega^1 = \Omega^2 = \Omega_1$, $U_{aux}^1 = U_{aux}^2 = U_{aux}$, and $\Omega_{aux}^1 = \Omega_{aux}^2 = \Omega_{aux}$. In the main problem we impose a rotational rate $\Omega$ on the snowman, which has been accounted for in the zeroth order (Newtonian) solution, hence $\Omega_{aux}^\alpha = 0$ for all $n \geq 1$. In addition, we define in the main problem the total external force and torque acting on the rigid body as $F_1 = F_1^1 + F_1^2$, $T_1 = T_1^1 + T_1^2$, and in the auxiliary problem $F_{aux} = F_{aux}^1 + F_{aux}^2$, and $T_{aux} = T_{aux}^1 + T_{aux}^2$. Using these simplifications the general relation, Eq. (31), simplifies to

\[
- (U_{aux} \cdot F_1 + \Omega_{aux} \cdot T_1) + U_1 \cdot F_{aux} = \int_{V_f} \left[ \frac{\gamma}{\gamma} \frac{\gamma}{\gamma} \frac{B \gamma \gamma + \gamma \gamma}{\gamma} : \nabla u_{aux} \right] dV.
\]

(32)

We now need to find an auxiliary problem that facilitates the determination of the first order propulsion velocity, $U_1$, in the main problem. An appropriate candidate is the translation of two touching spheres along the line of their
centers without rotation, $\mathbf{\Omega}_{\text{aux}} = 0$. The exact analytical solution was given by Cooley and O’Neill (Cooley & O’Neill 1969). By choosing this auxiliary problem, the relation further simplifies to

$$-\mathbf{U}_{\text{aux}} \cdot \mathbf{F}_1 + \mathbf{U}_1 \cdot \mathbf{F}_{\text{aux}} = \int_{V_f} \left[ \left( \mathbf{\nabla} \cdot \mathbf{\gamma}_0 + B \mathbf{\gamma}_0 \cdot \mathbf{\gamma}_0 \right) : \mathbf{u}_{\text{aux}} \right] dV. \quad (33)$$

If we do not allow the spheres to translate along the $z$-axis, $\mathbf{U}_1 = 0$, an external force, $\mathbf{F}_1$, is required to hold the snowman in place given by

$$-\mathbf{U}_{\text{aux}} \cdot \mathbf{F}_1 = \int_{V_f} \left[ \left( \mathbf{\nabla} \cdot \mathbf{\gamma}_0 + B \mathbf{\gamma}_0 \cdot \mathbf{\gamma}_0 \right) : \mathbf{u}_{\text{aux}} \right] dV. \quad (34)$$

On the other hand, if we allow the snowman to translate freely without imposing any external forces, $\mathbf{F}_1 = 0$, then the first order propulsion velocity, $\mathbf{U}_1$, can be determined from

$$\mathbf{U}_1 \cdot \mathbf{F}_{\text{aux}} = \int_{V_f} \left[ \left( \mathbf{\nabla} \cdot \mathbf{\gamma}_0 + B \mathbf{\gamma}_0 \cdot \mathbf{\gamma}_0 \right) : \mathbf{u}_{\text{aux}} \right] dV, \quad (35)$$

where both $\mathbf{F}_{\text{aux}}$ and the integral are expressed in terms of known Newtonian solutions of the main and auxiliary problems. Since the propulsion velocity $\mathbf{U}_1$ (with magnitude $U_1$) and the force in the auxiliary problem $\mathbf{F}_{\text{aux}}$ (with magnitude $F_{\text{aux}}$) act both vertically, the first order propulsion speed is finally given by

$$U_1 = \frac{1}{F_{\text{aux}}} \int_{V_f} \left[ \left( \mathbf{\nabla} \cdot \mathbf{\gamma}_0 + B \mathbf{\gamma}_0 \cdot \mathbf{\gamma}_0 \right) : \mathbf{u}_{\text{aux}} \right] dV, \quad (36)$$

where a positive value represents upward propulsion.

Using Eq. (36) with the zeroth-order solution (Takagi 1974) and the auxiliary Newtonian solution (Cooley & O’Neill 1969) we are able to determine theoretically the leading order propulsion speed of the snowman, $U = \text{De}_{\text{so}} U_1 + O(\text{De}_{\text{so}}^2) = \text{De}(1 - \zeta) U_1 + O(\text{De}^2)$. The quadrature is performed in the tangent-sphere coordinates, with somewhat lengthy differential operations in evaluating the integrand. Our asymptotic results are shown in figure 2 as a solid line (blue online). We see that our results predict very well the propulsion speed of the snowman for small $\text{De}$ when compared with numerical computations of the Oldroyd-B fluid (dot-dashed line - red online, in figure 2), and the agreement is excellent up to $\text{De} \sim 1$.

Note that in order to compare the results between the second-order fluid calculation and the Oldroyd-B numerics, the dimensionless parameter $B = -2\Psi_2/\Psi_1$ in the second-order fluid has to be taken to be zero because the second normals stress coefficient is zero in the Oldroyd-B model. Experimentally, indeed we have $B \ll 1$. Mathematically, the propulsion velocity varies linearly with $B$, and a transition of propulsion direction occurs at $B = 1$. Such a transition also occurs in the direction of radial flow for a single rotating sphere in a second-order fluid (see Sec. 5 for a related discussion).
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3.3. Propulsion characteristics

Anticipating the section where we make the link between rheology and locomotion, we now investigate the impact of the snowman geometry on its propulsion performance in the low-De regime where our asymptotic results via reciprocal theorem are quantitatively accurate.

3.3a. Touching spheres. In the case of two touching sphere \( h^* = 1 + r^* \), the only free dimensionless geometric parameter is the ratio of the radius of the upper to that of the lower spheres \( r^* = R_U / R_L \in [0, 1] \). In the limit \( r^* = 0 \), the snowman reduces to a single sphere, while the limit \( r^* = 1 \) corresponds to two equal touching spheres; in both cases, there is no propulsion by symmetry. We therefore expect an optimal ratio \( r^* \) for a maximum propulsion speed. Using the reciprocal theorem, Eq. (36), we calculate the propulsion speed as a function of \( r^* \) (Fig 3, solid line - blue online) and compare with the numerical results in an Oldroyd-B fluid (figure 3, dots - red online) at \( De = 0.1 \) and a typical relative viscosity \( \zeta = 0.5 \). The asymptotic results agree very well with the Oldroyd-B computations. The optimal sphere size ratio occurs at \( r^*_opt \approx 0.58 \). In addition to our computations and theoretical calculations, and based on physical understanding of the behaviour of a single rotating sphere in a second-order fluid, a simplified analytical model can be constructed to predict the snowman dynamics with results shown as a dotted line (black online) in figure 3; the details of this simple model are given in Sec. 5.

3.3b. Separated spheres. Next, we let the two spheres be separated at a distance \( h^* > 1 + r^* \) (no longer touching). The two spheres still rotate at the same speed as a rigid body and the separation distance is kept fixed by connecting the spheres with a drag-less slender rigid rod (a mathematically phantom rod) with negligible hydrodynamic contribution. Experimentally, this may be realized using, for example, using nanowires \( \dagger \). To compute the propulsion speed by the method described in Sec. 3.2b and therefore Eq. (36), we need two new Newtonian solutions, namely the zeroth-order solution and the auxiliary problem. The zeroth order solution considers two separated unequal spheres rotating at the same rate in a Newtonian fluid, the exact solution of which was given by Jeffery (Jeffery 1915) in bi-spherical coordinates. The appropriate auxiliary problem is the translation in a Newtonian fluid of the same two-sphere geometry along their axis of symmetry. Stimson and Jeffery (Stimson & Jeffery 1926) calculated that exact solution also in bi-spherical coordinates.

For very separated spheres \( h^* \gg 1 \), the propulsion is expected to decay with the separation distance. Hydrodynamic interactions between the two spheres is weak in this limit and each sphere behaves approximately as a single rotating sphere which does not propel. In figure 4a, the variation of the propulsion speed as a function of the separated distance is calculated for different fixed values of \( r^* \). The propulsion speed decays as expected for large \( h^* \). Interestingly, a
non-monotonic variation occurs when the spheres are close to each other (small $h^*$). The swimming speed first increases with $h^*$, reaching a maximum around $h^* \approx 2.5$, before decaying to zero with further increase in $h^*$. In Sec. 5, a simple physical explanation to this non-monotonicity is discussed; the dotted line (black online) in figure 4a corresponds to the predictions by a simplified analytical model based on this explanation.

For separated spheres, we can again vary the radii ratio, $r^*$, at different fixed separated distance $h^*$ (figure 4b) and results similar to the case of touching spheres is observed: for any value of $h^*$ there exists an optimal value of $r^*$ at which the dimensionless propulsion speed reaches a maximum. The simplified model (Sec. 5) again captures this trend qualitatively (dotted line - black online, figure 4b).

Finally, by plotting the isovalues of the propulsion speed as a function of both $r^*$ and $h^*$ (figure 5), we are able to optimize the snowman geometry for the overall maximum propulsion speed. The optimal geometry occurs at $(r^*, h^*) = (0.46, 2.5)$, and a schematic diagram of the optimal snowman is drawn to-scale in figure 5.
Figure 4. Propulsion speed of a separated snowman as a function of (a) the separation distance, and (b) ratio of the radii, at $\text{De} = 0.1$ and $\zeta = 0.5$. Dots (red online): numerical results in an Odroyd-B fluid. Solid line (blue online): second-order fluid analytical calculation. Dotted line (black online): simplified model (Eq. 50).

4. Microrheology via snowman

4.1. Scaling

In the sections above we have derived an analytical expression, valid in the small De regime, relating the propulsion speed to the intrinsic properties of the complex fluid, namely the normal stress coefficients (Eq. 36). Turning all dimensionless variables back in dimensional form, this relationship reads formally

$$U = \left( C_S^1 \Psi_1 + C_S^2 \Psi_2 \right) \frac{R_L \Omega^2}{\eta},$$

where $C_S^1$ and $C_S^2$ are dimensionless coefficients depending solely on the snowman geometry ($h^*$ and $r^*$) and defined as

$$C_S^1 = \frac{\int_{V_t} \nabla \cdot \gamma_0^* \mathbf{u}_{aux}^* dV^*}{2 F_{aux}^*},$$

$$C_S^2 = -\frac{\int_{V_t} (\gamma_0^* \cdot \gamma_0^*) : \nabla \mathbf{u}_{aux}^* dV^*}{F_{aux}^*}.$$
Figure 5. Optimization snowman propulsion. Iso-values of the dimensionless propulsion speed with dimensionless separation distance, $h^*$, and ratio of sphere radii, $r^*$. The optimal geometry for maximum propulsion speed is given by $(r^*, h^*)_{opt} = (0.46, 2.5)$. A schematic diagram showing the optimal geometry is drawn to scale above.

Since the second normal stress coefficient $\Psi_2$ is usually much smaller than the first normal stress coefficients $\Psi_1$, we might ignore $\Psi_2$ and obtain an estimation of $\Psi_1$ by measuring the propulsion speed of a snowman $U$, i.e.

$$\Psi_1 \approx \frac{U}{C_{S1} \frac{\eta}{R_L \Omega^2}}, \quad (40)$$

where $C_{S1}^S$ depends only on geometry and can be computed using Eq. (38). This expression demonstrates the use of locomotion ($U$) to probe the local non-Newtonian properties of the fluid ($\Psi_1$).

4.2. Second Experiment: Repulsion of two equal spheres

In scenarios where both values of $\Psi_1$ and $\Psi_2$ are desired, a second experiment is necessary to obtain a second, independent, measurement of a combination of the normal stress coefficients. We propose to measure in the second experiment the relative speed (repulsion) of two rotating equal spheres of radius $R_E$, with their centers separated by a distance $h$ (see figure 6 inset for notations and geometry). Should the two equal spheres be connected as a rigid body, no propulsion would occur by symmetry. However, if the equal spheres are not connected but allowed to freely translate along their separation axis, upon imposing rotation they will translate with velocities of equal magnitude but opposite directions provided the fluid is non-Newtonian.
We adopt the same non-dimensionalizations as previous sections (all lengths are now scaled by $R_E$) and drop the stars for simplicity; all variables in this section are dimensionless unless otherwise stated. Denoting the dimensionless velocity of the lower sphere as $V$, we again expand the repulsion velocity in powers of $D_{so}$, $V = D_{so} V_1 + O(D_{so}^2)$, and determine the first order velocity $V_1$ using our use of the reciprocal theorem as described in Sec. 3.2b. By symmetry, the upper sphere translates with velocity $-V$ (equal speed but opposite direction as the lower sphere).

In this scenario we have to again define two setups, one for the main problem and one for the auxiliary problem. For the main problem, we consider the rotational motion of two free equal spheres about their line of centers (Jeffery 1915). Since the motion is force-free ($F_1 = 0$ at each instant), Eq. (36) simplifies to

$$-\Omega_{aux}^1 \cdot T^1 - \Omega_{aux}^2 \cdot T^2 + U_1^1 \cdot F_{aux}^1 + U_2^1 \cdot F_{aux}^2 = \int_{V_f} \left[ \left( \tilde{\gamma}_0 + B\dot{\gamma}_0 \cdot \dot{\gamma}_0 \right) : \nabla u_{aux} \right] dV,$$

(41)

where $\Omega_{aux}^1 = 0$ for the same reason as explained in Sec. 3.2b.

For the auxiliary problem, we consider the Newtonian translational motion ($\Omega_{aux}^1 = 0$) of two equal spheres moving towards each other at the same speed and hence force, $F_{aux}^1 = -F_{aux}^2 = F_E^{aux}$. The exact solution to this problem was found by Brenner (Brenner 1961) in bi-spherical coordinates. We therefore have

$$(U_1^1 - U_1^2) \cdot F_{aux}^E = \int_{V_f} \left[ \left( \tilde{\gamma}_0 + B\dot{\gamma}_0 \cdot \dot{\gamma}_0 \right) : \nabla u_{aux} \right] dV.$$  

(42)

Note that the main problem here is a special case of that considered in Sec. 3.2b, but the auxiliary problem is completely different. We however still use the same symbols as in Sec. 3.2b for simplicity.

By symmetry, the two equal spheres propel with equal speed in opposite directions $U_1^2 = -U_1^1 = V_1$, hence

$$-2V_1 \cdot F_{aux}^E = \int_{V_f} \left[ \left( \tilde{\gamma}_0 + B\dot{\gamma}_0 \cdot \dot{\gamma}_0 \right) : \nabla u_{aux} \right] dV.$$  

(43)

Since the repulsion velocity $V_1$ (with magnitude $V_1$) and the force in the auxiliary problem $F_{aux}^E$ (with magnitude $F_{aux}^E$) both act vertically, the equation above can be rewritten as

$$V_1 = -\frac{1}{2F_{aux}^E} \int_{V_f} \left[ \left( \tilde{\gamma}_0 + B\dot{\gamma}_0 \cdot \dot{\gamma}_0 \right) : \nabla u_{aux} \right] dV,$$

(44)

where a positive value of $V_1$ represents repulsion.

The only dimensionless parameter in this second experiment is the ratio of the separation distance to the radius of the spheres, which we write as $h^* = h/R_L$. Using Eq. (44) we calculate the repulsion speed ($V_1 > 0$) as a
Figure 6. Dimensionless repulsion speed, $V/R_E\Omega$, of two equal co-rotating spheres as a function of their dimensionless separation distance, $h^*$, at $De = 0.1$ and $\zeta = 0.5$. Dots (red online): numerical results in an Odroyd-B fluid. Solid line (blue online): theoretical calculation for a second-order fluid.

function of the dimensionless separation $h^*$ (solid line - blue online, figure 6, for $De = 0.1$ and $\zeta = 0.5$), and the results are found to be in excellent agreement with the Oldroyd-B calculations (dots - red online, figure 6).

Back to dimensional variables, the leading order repulsion speed is formally given by

$$V = (C_1^E\Psi_1 + C_2^E\Psi_2) \frac{R_E\Omega^2}{\eta},$$

(45)

where $C_1^E$ and $C_2^E$ are dimensionless coefficients evaluated with the solution to the main and auxiliary problems described above

$$C_1^E = -\frac{\int_{V^*} \gamma_0^* \cdot \nabla^* \mathbf{u}_{aux}^* dV^*}{4F_{aux}^*},$$

(46)

$$C_2^E = \frac{\int_{V^*} (\dot{\gamma}_0^* \cdot \dot{\gamma}_0^*) \cdot \nabla^* \mathbf{u}_{aux}^* dV^*}{2F_{aux}^*}.$$  

(47)

4.3. Determination of normal stress coefficients

From measuring both the propulsion speed $U$ of a snowman (given by Eq. 37) and repulsion speed $V$ of the equal spheres (given by Eq. 45), we now have enough information to deduce both the first and second normal stress coefficients ($\Psi_1, \Psi_2$). If we choose the same radius for the lower sphere in both
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experiments $R_E = R_L$ (we use $R_L$ hereafter), we can write Eqs. (37) and (45) in a matrix form as

$$\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} C^S_1 & C^E_1 \\ C^S_2 & C^E_2 \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \frac{R_L \Omega^2}{\eta},$$

(48)

where we denote by $C$ the matrix containing the dimensionless coefficients $(C^S_1, C^S_2, C^E_1, C^E_2)$ in Eq. (48). The matrix $C$ depends only on three geometric parameters, namely the ratio of the radii of the spheres in the snowman ($r^* = R_U/R_L$), the dimensionless separation distance in the snowman ($h^*_S = h/R_L$) and that for the equal spheres in the second experiment ($h^*_E = h/R_E$). The coefficients of the matrix can be readily computed via Eqs. (38)–(39) and Eqs. (46)–(47), and thus the matrix in Eq. (48) can be inverted to obtain the values of $\Psi_1$ and $\Psi_2$.

For practical implementation of this microrheological technique, measurement errors in the velocity of the snowman are inevitable and depend on the specific equipment employed for tracking the motion of the probe. However, the geometry of the snowman can be designed so that $\Psi_1$ and $\Psi_2$ are insensitive to measurement errors in the velocities $U$ and $V$. The condition number (CN) of the matrix $C$ to be inverted represents the maximum amplification factor of the relative measurement errors. The maximum relative errors in the normal stress coefficients would be equal to the condition number multiplied by the maximum relative measurement error. A small condition number is therefore desired. Similarly to the study by Khair and Squires (Khair & Squires 2010), we now investigate the value of condition number as a function of the geometry.

To simplify the parametric studies, we first adopt the same separation distance in the first and second experiments ($h^*_S = h^*_E = h^*/R_L$), and explore the dependence of the condition number on $r^*$ and $h^*$, with results shown in figure 7a. The condition number does not vary monotonically with the parameters, which implies that optimization is possible. Under this requirement and within the ranges of values considered ($r^* \in [0.2, 0.98]$ and $h^* \in [2.1, 4]$), the geometry yielding the lowest condition number is $r^* = 0.46$ and $h^* = 2.1$ (the corresponding condition number for $C$ is $\approx 27.6$). When the requirement of $h^*_S = h^*_E$ is removed, by examining all combinations of the parametric values within the ranges ($r^* \in [0.2, 0.98]$, $h^*_S \in [2.1, 4]$, and $h^*_E \in [2.1, 4]$), the minimum CN obtainable appears to be $\approx 25.7$ with $r^* = 0.46$, $h^*_S = 2.6$, and $h^*_E = 2.1$.

The condition number can be further fine-tuned if we allow $R_L \neq R_E$, in which case we have the new matrix relation

$$\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} C^S_1 & C^S_2 \\ C^E_1 R_E/R_L & C^E_2 R_E/R_L \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \frac{R_L \Omega^2}{\eta},$$

(49)

The modified dimensionless matrix $C$ in Eq. (49) now depends on one more parameter $R_L/R_E$, which is the ratio of the lower sphere radius in the snowman, $R_L$, to that of the equal sphere, $R_E$. In figure 7b, we investigate the dependence of the condition number of $C$ with this new parameter, and adopt for
all other parameters the optimal geometric parameters we determined before ($r^* = 0.46$, $h^*_S = 2.6$, and $h^*_E = 2.1$). The variation turns out to be also non-monotonic, and a minimum is achieved when $R_L/R_E = 3.5$ with $CN \approx 13.4$.

A schematic diagram showing the corresponding geometrical setup of the two sets of experiment is given to scale in the inset of figure 7. The condition number could be brought further down with a full four-dimensional parametric study and expanding the domains of the parametric studies. However, geometries yielding a lower CN may correspond to a negligible speeds undesirable for measurement. The current geometry ($r^* = 0.46$, $h^*_S = 2.6$, $h^*_E = 2.1$, and $R_L/R_E = 3.5$) has both a relatively low CN and a high propulsion speed, making it ideal for experimental implementation. It is interesting to note that the optimal geometry for a small condition number we find here is close to the optimal geometry producing the maximum propulsion speed for the snowman ($r^* = 0.46$, $h^*_S = 2.5$) determined in Sec. 3.3b.

5. Qualitative physical explanation

In this section, we turn to an explanation of the physical origin of the non-Newtonian propulsion of a snowman. Based on physical intuition we present a simple model which successfully captures all the qualitative features of this mode of propulsion.

We first look into the simplest related problem, that of a single sphere rotating in a complex fluid (a textbook problem discussed, for example in Bird et al. (1987a)). Non-Newtonian stresses lead to the creation of a secondary flow in which the fluid moves towards the sphere in the equatorial plane and
away from the sphere near the axis of rotation (see the inset of figure 8 for an illustration of the secondary flow field) (Bird et al. 1987a).

This secondary flow can be understood physically as a consequence of the hoop stresses along the curved streamlines. Polymer molecules in the fluid get stretched by the flow, leading to an extra tension along streamlines. The presence of that extra tension along the closed circular streamlines leads to an inward radial contraction (like a stretched rubber band) pushing the fluid to thus go up vertically in both directions (by continuity) to produce the secondary flow. Notably, this secondary flow is independent of the direction of rotation of the sphere.

The argument for locomotion of the snowman is then the following. Based on the one-sphere result, we see that when the two spheres in a snowman are aligned vertically and subject to a rotation they generate secondary flows and push against each other. For a single sphere, the strength of the secondary flow increases with the size of the sphere (Bird et al. 1987a). Consequently the smaller sphere is being pushed harder by the larger sphere than it is able to push against, and hence the two-sphere system is subject to a force imbalance, leading to propulsion. This physical understanding agrees with our results: propulsion always occurs in the direction of the smaller sphere, independently of the direction of rotation. Should the two spheres not be connected as a rigid body but free to translate vertically, they would repel each other, explaining physically our results in Sec. 4.2.

Based on this intuitive argument, we can now construct a simple mathematical model. Using the same notations as above, for a sphere of radius $R$ rotating with an angular velocity $\Omega$ in a second-order fluid, the leading order solution $v(\phi, r, \theta)$ in spherical coordinates (Bird et al. 1987a) is

$$v^\ast = v/R\Omega = (1/r^2)^2 \sin \theta \hat{e}_\phi + D_{\text{eso}}(1-B)/(1/2r^4 - 3/2r^6 + 1/r^8)\left(3 \cos^2 \theta - 1\right) \hat{e}_r - 3(1/r^4 - 1/r^6) \sin \theta \cos \theta \hat{e}_\theta + O(D_{\text{eso}}^2).$$

The Newtonian component of the flow field ($D_{\text{eso}} = 0$) is the primary flow field, and it has only a azimuthal ($\phi$) component. The secondary flow field, proportional to $D_{\text{eso}}$, is due to fluid elasticity and has only radial ($r$) and polar ($\theta$) components. As expected, the dimensional secondary flow $v$ is quadratic in $\Omega$, confirming our physical intuition that it should be independent of the direction of rotation of the sphere. In the case where $B < 1$ (recall that $B = -2\Psi_2/\Psi_1$), the relevant limit for polymeric fluids, the secondary flow occurs in the direction intuited above and shown in the inset of figure 8. Note that the secondary flow field of a rotating single sphere would switch its direction when $B$ went above one, explaining the switch in the propulsion direction of a snowman reported in Sec. 3.2b in that limit.

The dimensionless fluid velocity along the vertical axis ($\theta = 0$) is given by $v^\ast(r, \theta = 0) = D_{\text{eso}}(1/r^2 - 3/r^4 + 2/r^6) \hat{e}_r(\theta = 0)$, where we have set $B = 0$ to allow comparison with the numerical results. The velocity along the
vertical axis, shown in figure 8, is expected to display non-monotonic variation with the distance from the sphere since the velocity decreases to zero both in the far field and on the solid surface. This is at the origin of the non-monotonic dependence of the snowman propulsion speed with the separation distance between the spheres shown in figure 4a.

The forces experienced by the upper and lower spheres can be approximately estimated by considering the individual flow fields generated by their own rotation without the presence of the other sphere. We place an upper sphere at a distance $h^* = h/R_L$ from the center of the lower sphere. Using the same notations as in the previous sections, the dimensionless velocity generated by the lower sphere, and evaluated at the location of the upper sphere, is given by $v_L^*(h^*) = \text{De}_{\text{so}} \left( \frac{1}{h^*} - \frac{3}{h^*^4} + 2 \frac{h^*}{h^*} \right) \hat{e}_L^r(\theta^L = 0)$, where $\hat{e}_L^r(\theta^L = 0)$ is the unit radial vector in the polar direction $\theta^L = 0$, with respect to the coordinates system at the center of the lower sphere. Similarly, the dimensionless velocity generated by the upper sphere at the same distance, $h^*$, but measured from the center of the upper sphere is given by $v_U^*(h^*) = r^* \text{De}_{\text{so}} \left( \frac{(r^*)^2}{h^*} - 3 \frac{(r^*)^4}{h^*^4} + 2 \frac{(r^*)^5}{h^*} \right) \hat{e}_U^r(\theta^U = \pi)$, where $\hat{e}_U^r(\theta^U = \pi)$ is the unit radial vector in the polar direction $\theta^U = \pi$, with respect to the coordinates system at the center of the upper sphere. Note
that $\hat{e}^U_\theta(\theta_U = \pi) = -\hat{e}^L_\theta(\theta_L = 0)$. As a simple approximation, we estimate the viscous drag force experienced by the upper and lower spheres to be $\mathbf{F}_U^\ast \sim 6\pi r^\ast \mathbf{v}_L^\ast(h^\ast)$ and $\mathbf{F}_L^\ast \sim 6\pi \mathbf{v}_U^\ast(h^\ast)$ respectively. The difference between these two forces results in a net propulsive thrust. When dividing by an approximation of the translational resistance of the snowman at zero Deborah number with no hydrodynamic interactions, $6\pi(1 + r^\ast)$, we obtain a simple estimate of the dimensionless propulsion speed as $U^\ast \approx |\mathbf{F}_U^\ast + \mathbf{F}_L^\ast|/6\pi(1 + r^\ast)$. This leads to

$$U^\ast \approx \frac{|r^\ast \mathbf{v}_L^\ast(h^\ast) + \mathbf{v}_U^\ast(h^\ast)|}{(1 + r^\ast)} = \text{De}_{\text{so}} \frac{r^\ast \left[3h^\ast(r^{\ast 4} - 1) - h^{\ast 3}(r^{\ast 2} - 1) - 2r^{\ast 5} + 2\right]}{h^{\ast 5}(1 + r^\ast)}.$$  

(50)

In Eq. (50), we verify that $U^\ast$ vanishes when $r^\ast = 0$ (single sphere) and $r^\ast = 1$ (equal spheres). For the case of touching spheres ($h^\ast = 1 + r^\ast$), Eq. (50) simplifies to

$$U^\ast_{\text{touch}} \approx \text{De}_{\text{so}} \frac{2r^{\ast 3}(1 - r^\ast)}{(1 + r^\ast)^{\ast 6}}.$$  

(51)

Does this simple model capture the essential propulsion characteristics? In figure 3, we plot the dimensionless propulsion speed of a touching snowman estimated by this simple model (Eq. 51) as a function of $r^\ast$ (dotted line - black online) and compare with the theoretical results from the reciprocal theorem approach (solid line - blue online) and the numerical computations (symbols - red online). The simple model correctly predicts the order of magnitude and captures qualitatively the variation with $r^\ast$. For non-touching snowman, the qualitative model (Eq. 50) also captures qualitatively the variation of the dimensionless propulsion speed with $h^\ast$ (dotted line - black online - for $r^\ast = 0.6$, figure 4a), also predicting an optimal separation distance and therefore supporting our understanding of a non-monotonic dependence with $h^\ast$ as arising from the non-monotonicity of the single-sphere velocity (figure 8). As expected, Eq. (50) also captures the non-monotonic variation with respect to $r^\ast$ for separated snowman (dotted line - black online - for $h^\ast = 8$, figure 4b).

6. Discussion and Conclusions

In this work, we present the design and mathematical modeling for a new non-Newtonian swimmer – the snowman – which propels only in complex fluids by exploiting asymmetry and the presence of normal stress differences under rotational actuation. The simple shape of our swimmer makes it ideally suited for experimental measurements. Note that if kept in place, the snowman would then act as a micro-pump for complex fluids.

The propulsion characteristics of the snowman are investigated by a combination of numerical computations (moderate values of De in an Odroyd-B
fluid) and analytical treatment (small De in a second-order fluid). The underlying physics of propulsion, relying on elastic hoop stresses and geometrical asymmetry, is explained and based on this physical understanding a simple analytical model capturing all qualitative features is successfully constructed. Note that since, as a rule of thumb, inertial and elastic effects tend to produce secondary flows in opposite directions (Bird et al. 1987a), we expect that an inertial (instead of viscoelastic) snowman should swim in the opposite direction (from small to large sphere).

The two-sphere setup proposed in this work is arguably the simplest geometry able to swim in a complex fluid under uniform rotation. It of course simplifies the analysis since the required Newtonian solutions to be used in our integral approach are all available. Any axisymmetric but top-down asymmetric geometry should also work, for example a cone, and clearly there remains room for shape optimization in that regard. Additionally, studying the snowman dynamics under a time-varying rotation could lead to a rich dynamics with potentially non-trivial stress relaxation effects.

One of the main ideas put forward in this work is the use of locomotion as a proxy to probe the local non-Newtonian properties of the fluid. The snowman can be used as a micro-rheometer to estimate the first normal stress coefficient on its own, or to measure both the first and second normal stress coefficients with the help of another complementary experiment. Khair and Squires (Khair & Squires 2010) recently proposed to measure normal stress coefficients by pulling microrheological probes and measuring the relative forces on the probes. In our work, we propose alternatively to perform only kinematic measurements of the sphere speeds instead of forces, which could present an interesting alternative from an experimental standpoint.

We finally comment on a potential experimental implementation of the snowman technique. We are aware of a number of rotational micro-manipulation techniques (see a short review in Bishop et al. 2004)). For example, spinning micro-particles may be achieved by the use of optical tweezers and birefringent objects (Friese et al. 1998). Birefringence allows the transfer of angular momentum from the circularly polarized laser to the particle, producing controlled rotation. By rotating spherical birefringent crystals (vaterite), this technology has been implemented as a micro-viscometer to probe fluid viscosity (Bishop et al. 2004; Knöner et al. 2005; Parkin et al. 2007). A similar mechanism may be useful for the two-sphere setup in this work although simultaneous rotation of two spheres may introduce experimental challenges. Our dual-purpose snowman, both a micro-propeller and a micro-rheometer, invites experimental implementation and verification.
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† If the drag on the slender rod is taken into account in modeling, the overall force balance should include the small contribution from the drag on the rod, which will slightly decrease the propulsion speed of the snowman.


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Paper 7
The dynamics of a capsule in a wall-bounded oscillating shear flow

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Internal report

The motion of an initially spherical capsule in a wall-bounded oscillating shear flow is studied via an accelerated boundary integral implementation. Neo-Hookean model is used as the constitutive law of the membrane of capsule. The lateral migration velocity of the capsule varies non-monotonically with its capillary number. It is negatively related with the initial height of the capsule above the wall. A positive correlation between the lateral migration velocity and normal stress difference is identified. The correlation becomes strongest for the capsule with the highest lateral migration velocity. For a fixed capillary number, the lateral migration velocity decreases linearly with the frequency of oscillating shear, and approaches an asymptotic value of zero for high frequency. The deformation of capsule displays a wave-like variation in time and its frequency is twice that of the underlying shear. A phase delay is observed between the variation of capsule deformation with that of the oscillatory flow, more pronounced for a more deformable capsule.

1. Introduction

The dynamics of a capsule in external flows have attracted enormous interest due to their physiological and biological significance, leading to the discovery of a variety of interesting and complex phenomena. Since the observation
of the tank-treading (TT) motion of a human red blood cell in the viscometer (Fischer & Schmid-Schönbein 1978; Fischer et al. 1978), shear flow, one of the simplest flows, has been applied onto cells and their models experimentally, theoretically and numerically to understand the motions of biological cells for decades (Barthès-Biesel 1980; Cordasco & Bagchi 2013; Eggleton & Popel 1998; Ha & Yang 2000; Koleva & Rehage 2012; Kraus et al. 1996; Lac et al. 2004; Le 2010; Lebedev et al. 2007; Ma et al. 2009; Omori et al. 2012; Peng & Zhu 2013; Sui et al. 2008; Zhao et al. 2012). The starting focus was on an initially spherical capsule that performed a shear-induced TT motion and reached a steady ellipsoidal shape (Barthès-Biesel 1981; Pozrikidis 1995). The membrane elements of the capsule rotated along the stationary configuration, like the caterpillar driving of a tank. The undeformed shape of biological cells is seldom a sphere but geometrically anisotropic, for example, the shape of undeformed red blood cells (RBCs) is bi-concave. The non-spherical capsule has a shape memory, tending to orient in a preferential direction (Finken et al. 2011). As a consequence, the capsule tank-treads and oscillates around a preferred direction as the shear rate is above a certain value (Keller & Skalak 1982; Skotheim & Secomb 2007); this oscillatory behaviour is termed as the swinging mode (Abkarian et al. 2007). Furthermore, the oscillating shear flow has been used to account for the physiological pulsation, more complex and diverse motions of the capsules have been explored. Experiments (Nakajima et al. 1990) showed that the RBCs deform more in the retarding phase than in the accelerating phase. The harmonically modulated shear was examined by theoretical approaches (Kessler et al. 2009), exhibiting a resonance behaviour; a particular combination of the oscillation frequency and phase could induce the tumbling motion of a capsule which would otherwise swing under steady shear flow. Dupire et al. (2010) theoretically produced the disordered motions of model RBCs in sinusoidally varying flows with physiologically relevant parameters, that was also attested by their experiments. A similar chaotic behaviour was also realized analytically by Noguchi (2010) who found multiple limit-cycle solutions of the model RBCs subject to an oscillating shear flow with a high frequency; their TB-based or TT-based swinging motions were found at a high or low shear amplitude. Recent numerical simulations by Zhao & Bagchi (2011) reproduced the two swinging modes of an initially oblate-shaped by varying the frequency of the shear; they also displayed the high sensitivity of the motion of capsule to its initial orientation, indirectly confirming the chaotic manner reported in Dupire et al. (2010).

The previous work mainly focused on the dynamics of capsules in an unbounded oscillatory shear flow. While in the micro-recirculation, cells like the RBCs also move in strongly confined oscillating flows, an example being the physiological process called vasomotion. This corresponds to the spontaneous and rhythmic oscillations performed by large arteries as well as microvessels (Haddock & Hill 2005; Nilsson & Aalkjær 2003; Shimamura et al.
A capsule in a wall-bounded oscillating shear flow

1999). Vasomotion is independent of the common physiological pulsations like the heart beat, innervation or respiration (Alkjaer & Nilsson 2005), but induced by the smooth muscle constriction and dilation. Its possible benefits include reducing the time-averaged hydraulic resistance to the blood flow (Meyer et al. 2002) and the enhancement of oxygen transport (D. Goldman & Popel 2001; Secomb et al. 1989). Hence, it is important to understand the dynamics of deformable particles like the biological cells in a confined oscillating flow. Despite the complexity introduced by the oscillation, the influence of wall confinement on cells itself is crucial and has been mostly investigated in steady flows. Fähræus & Lindqvist (1931) started to unravel the biological importance of confinement. He discovered that the RBCs tend to deform significantly and migrate towards the centre of a microvessel, owing to the hydrodynamic lift resulting from the interaction between the cellular deformation and wall confinement; the towards-centre cellular migration facilitates a lower flow resistance and a more effective mass transport. A numerical study (Pranay et al. 2012) was carried out to quantitatively investigate the cross-streamline migration of a spherical capsule in the wall-bounded shear flow, showing that a more deformable capsule tends to migrate more rapidly. Simulations (Zhao & Bagchi 2011) of a vesicle in a similar flow exhibited that the wall confinement delayed its transition from the tank-treading motion to trembling and tumbling. Regarding the importance of wall confinement, in this paper, we study the motion of a capsule in a wall-bounded oscillatory shear flow. We therefore take into account of both the wall confinement and flow unsteadiness, aiming to understand and elucidate their interplay and its influence on the dynamics of deformable cells.

2. Problem setup and numerical methods

2.1. Problem setup

We compute the motion and deformation of a capsule subject to a wall-bounded shear flow, see the sketch in figure 1. The undeformed shape of the capsule is a sphere with radius $a$ and its centre of mass is initially above the wall by a distance of $h_{\text{ini}}$. A sinusoidally varying shear flow $\dot{\gamma}(t) = \dot{\gamma}_{\text{max}} \cos(\omega t)$ is applied. $\dot{\gamma}_{\text{max}}$ denotes the maximum value of the shear, and $\omega$ is the frequency of the shear. In this paper, we focus on the model cell, the capsule, in the flow at a small scale, in order to mimic its dynamics in the micro-circulation or in micro-fluidic devices. Therefore, we assume that the capsule is advected by the creeping flow and the Reynolds number $Re$ indicating the ratio of the viscosity over inertia is zero.

We model the capsule as a fluid-filled droplet enclosed by an infinitely thin elastic membrane. The fluid inside and outside the capsule has the same density $\rho$ and dynamic viscosity $\mu$. The capsule is deformed by the fluid stress exerted
\[ \dot{\gamma}(t) = c \dot{\gamma}_{\text{max}} \cos(\omega t) \]

Figure 1. Sketch of the setup. We consider a capsule whose undeformed shape is a sphere of radius \( a \), subject to an oscillating wall-bounded shear flow \( \dot{\gamma}(t) = c \dot{\gamma}_{\text{max}} \cos(\omega t) \). The centre of the capsule is initially above the wall by \( h_{\text{ini}} \) and its lateral migration measured from the initial position is denoted \( h_{\text{lat}} \).

on its membrane and the membrane dynamics is calculated based on the neo-Hookean constitutive law (Barthès-Biesel et al. 2010). The membrane has a shear modulus of \( G_s \) and zero bending stiffness. Elastic stress will develop on the surface of the capsule due to its deformation, this stress will modify the surrounding flow in return. In this fluid-structure interaction problem, the viscous stress of the flow and elastic stress of the deformable membrane compete with each other. Hence, we introduce the ratio of them, the capillary number \( \text{Ca} \) defined as \( \text{Ca} = \mu \dot{\gamma}_{\text{max}} / G_s \).

2.2. Numerical methods

The membrane of the capsule is discretized into \( N \) Lagrangian points. Neglecting the inertia of capsule, the elastic force balances the flow viscous force on its surface,

\[ \rho^e + (\sigma_{\text{out}} - \sigma_{\text{in}}) \cdot n_{\text{out}} = 0, \]

where \( \rho^e \) is the elastic force per unit area exerted by the surrounding membrane, \( \sigma_{\text{out}} \), \( \sigma_{\text{in}} \) are the stress tensor of the flow outside and inside the capsule, and \( n_{\text{out}} \) is the unit out normal vector. At a time instant, given the distribution of \( \rho^e \) on the membrane, the solution of the flow can be obtained by solving the
Stokes flow with $N$ point forces exerted to the fluid:

$$
-\nabla p + \mu \nabla^2 u = -\sum_{i=1}^{N} f_i \delta(x - x_i),
$$

$$
\nabla \cdot u(x) = 0,
$$

(2)

where $p$ and $u$ is the pressure and velocity field of the flow respectively. $f_i$ denotes the force exerted onto the fluid at the position $x_i$ and can be derived as

$$
f_i = \int_{S_i} \rho_e dS_i,
$$

(3)

where $S_i$ represents the elemental patch around the $i$th Lagrangian point. We solve the flow by a boundary integral method accelerated by the general geometry Ewald method (GGEM) proposed by Hernández-Ortiz et al. (2007). GGEM decomposes the Stokes solution into two parts, one standing for the short-ranged interactions computed by traditional boundary integral techniques; and the other for the long-ranged interactions handled by a mesh-based Stokes solver. In our implementation, we take the Stokes sub-solver of an open source software NEK5000 (Fischer et al. 2008) as the mesh-based solver. We further mention that we perform the singular integration following Zhao et al. (2010), a proper treatment guarantees the numerical accuracy of the solution (Huang & Cruse 1993; Zhu et al. 2013).

After getting the flow solution, the velocity in the domain is known including that on each Lagrangian point, $u(x_i)$ for the $i$th point at $x_i$. Due to the no-slip, non-penetrating boundary condition on the membrane of capsule, we can update the position of the $i$th point, following

$$
\frac{dx_i}{dt} = u(x_i).
$$

(4)

Given the new coordinates of the $N$ Lagrangian points, we are able to calculate the elastic force per unit area developed on each point. The computation is based on their displacements with respect to the undeformed shape of the capsule, through the constitutive law of membrane, the neo-Hookean model here. We use a global spectral method based on the spherical harmonics (Zhao et al. 2010) to interpretate the surface of capsule and to solve the elastic force $\rho^e$. This accuracy provided by the approach is twofold: the high order spatial derivatives on the material points are computed with high accuracy, which is crucial for the calculation of the elastic force; the same spectral discretization can be used for the boundary integration performed when solving the short-ranged hydrodynamic interactions. For a detail of our implementation, the readers are refer to Zhu & Brandt (2013).
3. Results

3.1. Trajectories

We firstly look at the trajectories of capsules. The centre of mass of the capsule is plotted in figure 13.2(a) for three cases, \((Ca, \omega) = (0.15, 1)\), \((Ca, \omega) = (0.3, 1)\) and \((Ca, \omega) = (0.3, 2)\). The motion of capsule is a combination of the reciprocal motion in the streamwise \((x)\) direction due to the oscillating background flow and the wall-normal lateral migration due to the hydrodynamic lift. Although, the applied shear is time-reversal symmetric, the nonlinear interplay between the membrane and fluid breaks the symmetry. Indeed, the starting direction of the flow will be remembered by the capsule and reflected in its motion; its trajectory shows a clear left-right asymmetry that will be absent for a solid particle. This is also illustrated in figure 13.2(b) showing the lateral migration \(h_{\text{lat}}\) of capsules versus the nondimensional time \(\omega t/2\pi\). For all cases, \(h_{\text{lat}}\) increases periodically and its profile is irregular compared to the sinusoidal wave pattern of the applied shear. However, \(h_{\text{lat}}\) varies at a same frequency with that of the applied shear. It is noteworthy that a solid spherical particle will not move at all in the wall-normal direction at any instant, while its ellipsoidal counterpart will exhibit a oscillatory vertical drift but with a zero mean. The physical picture is in analogy with a microswimmer employing nonlinearity for a net locomotion by performing reciprocal motions, an interesting case in the low-Reynolds-number swimming dynamics (Lauga & Powers 2009). In detail, in the Stokes regime, a reciprocal swimming pattern is able to render a net displacement in the viscoelastic fluid (Keim et al. 2012; Pak et al. 2010), which will otherwise be zero as in a Newtonian fluid (Lauga & Powers 2009; Purcell 1977)!

We further notice that for the same frequency of shear \(\omega = 1\), the motion of two capsules \(Ca = 0.15\) and \(Ca = 0.3\) with different deformability is similar. While, for the same capsule \(Ca = 0.3\), its trajectory varies significantly under the shear with two frequencies, \(\omega = 1\) and \(\omega = 2\). Clearly, the range of the capsule spans in the \(x\) direction reduces to its half as doubling \(\omega\) from 1 to 2, which is expected. Its lateral migration also diminishes considerably as shown in figure 13.2(b).

3.2. Velocity of the lateral migration

In this section, we analyse the velocity of the lateral migration \(U_{\text{lat}}\) defined as \(U_{\text{lat}} = dh_{\text{lat}}/dt\). Its temporal evolution is plotted in figure 13.3(a) for three capsules with the same initial offset \(h_{\text{ini}} = 2\) and frequency \(\omega = 5/3\). The migration velocity varies periodically with time, as can be inferred from the periodic growing of \(h_{\text{lat}}\) seen in figure 13.2(b). We plot the time-averaged values \(\bar{U}_{\text{lat}}\) for the three cases and observe that the capsule with an intermediate capillary number \(Ca = 0.15\) has a greater velocity \(\bar{U}_{\text{lat}}\) than its floppy \((Ca =\)
A capsule in a wall-bounded oscillating shear flow

Figure 2. The centre of mass of three capsules \((Ca, \omega) = (0.15, 1)\) (solid curve), \((Ca, \omega) = (0.3, 1)\) (dashed) and \((Ca, \omega) = (0.3, 2)\) (dot-dashed) released from the initial offset \(h_{\text{ini}} = 2\). Left: trajectories of the centre of mass in the shear plane \((x - y)\) plane. Right: lateral migration \(h_{\text{lat}}\) as a function of the nondimensional time \(t^* = \omega t/(2\pi)\). The dotted curve stands for the applied oscillating shear \(\dot{\gamma}_{\text{max}} \cos (\omega t)\), arbitrarily scaled for visualization.

0.0375) and stiff \((Ca = 0.6)\) counterpart. Conversely, in the case of a steady wall-bounded shear flow, the lateral migration velocity of a capsule increases monotonically with \(Ca\) (Graham 2005; Pranay et al. 2012).

In the steady flow, the lateral migration velocity is linearly dependent with the normal stress differences \(\Delta N = N_1 - N_2\) as proved in Ref. Graham (2005); Pranay et al. (2012). Hence, we investigates the relation between \(U_{\text{lat}}\) and \(\Delta N\). The normal stresses \(N_1\) and \(N_2\) are defined as,

\[
N_1 = \sigma_{xx} - \sigma_{yy}, \\
N_2 = \sigma_{yy} - \sigma_{zz},
\]

where \(\sigma\) denotes the extra stress due to the presence of the capsule:

\[
\sigma_{ij} = -\frac{1}{V} \int_S \rho^e x_j dS,
\]

where \(V\) is the volume of the domain. For a better illustration, we nondimensionalize \((N_1 - N_2)\) by \(\mu \phi \dot{\gamma}_{\text{max}}\), \(\phi\) is the local volume fraction; thus, the nondimensional value \((N_1 - N_2) / (\mu \phi \dot{\gamma}_{\text{max}})\) represents the stress induced by the
Figure 3. Lateral migration velocity $U_{\text{lat}}$ as a function of the dimensional time $\omega t/2\pi$ and the capillary number $Ca$, $\omega = 5/3$ is fixed. figure (a): $U_{\text{lat}}$ versus time, for the capsule $Ca = 0.0375$ (solid curve), $Ca = 0.15$ (dashed) and $Ca = 0.6$ (dot-dashed), the initial offset $h_{\text{ini}} = 2$. The time-averaged migration velocities $\bar{U}_{\text{lat}}$ are denoted by horizontal lines with circles ($Ca = 0.0375$), squares ($Ca = 0.15$) and diamonds ($Ca = 0.6$). figure (b): $\bar{U}_{\text{lat}}$ as a function of the capillary number $Ca$, for three initial offsets, $h_{\text{ini}} = 1.5$, $h_{\text{ini}} = 2$ and $h_{\text{ini}} = 3$ indicated by the triangles, circles and squares respectively.

capsule scaled with the viscous stress. We plot the migration velocity $U_{\text{lat}}$ together with the nondimensional normal stress difference in figure 4 for capsules $Ca = 0.0375$, $Ca = 0.12$ and $Ca = 0.6$. Both quantities vary periodically and reach their local maximum values with negligible phase differences. This implies a considerable correlation between the two, even in the oscillating shear flow. We next examine their local maximums, marked by the circles for the migration velocity $U_{\text{lat}}$ and squares for the nondimensional normal stress difference $(N_1 - N_2)/\mu\dot{\gamma}_{\text{max}}$. We do not count the first peak appearing in the initial stage when the capsule starts its movement. As displayed in figure 13.4(a), for the stiff capsule $Ca = 0.0375$, the maximum values of the two quantities reach the same magnitude approximately with respect to their own scales, at the time $\omega t \approx 1$ and $\omega t \approx 2$. At other instants when the peaks are reached, like $\omega t \approx 0.75$ and $\omega t \approx 1.75$, their magnitude vary with each other apparently.
The same trend is observed for the floppy capsule \( Ca = 0.6 \). In contrast, for the one \( Ca = 0.12 \) that is featured with the largest mean migration velocity, its two quantities, namely, \( U_{\text{lat}} \) and \( (N_1 - N_2) / \mu \dot{\gamma}_{\text{max}} \) have roughly the same magnitude every time they reach the local maximums (see figure 13.4(b)); in other words, the local maximums of the lateral migration velocity and the normal stress difference co-appear and the ratio of the maximum values keeps almost constant with time. This implies the correlation between the two quantities of the capsule \( Ca = 0.12 \) is stronger than that of the other two \( Ca = 0.0375 \) and 0.6. A high correlation may indicates that migration velocity and the normal stress difference is well synchronised, possibly contributing to a more pronounced lateral migration. For a deeper understanding of the relation, in figure 5, we plot the time-averaged migration velocity \( \bar{U}_{\text{lat}} \) together with the time-averaged nondimensional normal stress difference \( \bar{\Delta}N \), versus the capillary number \( Ca \). It is clearly detected that the two follow closely a same trend, initially increase sharply with \( Ca \), reach the peak when \( Ca \in (0.1, 0.2) \) and then decrease with \( Ca \). The agreement between their variations in \( Ca \) is especially clear before they approach the peaks. We note that the capillary number \( Ca \) can also be regarded as a ratio between the relaxation time of the capsule and the characteristic flow time. The non-monotonic dependence of the lateral migration velocity on this ratio \( Ca \) is analogous to the relation of the swimming speed of a model microswimmer, a rotating helix, propelling in the viscoelastic fluid with the Deborah number. Deborah number is the ratio of the relaxation time of the elastic fluid over the characteristic flow time. Both experiments (Liu et al. 2011) and simulations (Spagnolie et al. 2013) have shown that the helical model swimmer moves fastest when \( De \approx 1 \), i.e., the two time scales are close and the elastic and viscous effect balances.

We also examine the dependence of the lateral migration velocity on the frequency of the oscillatory shear, \( \omega \). Figure 3.2 displays the time-averaged migration velocity \( \bar{U}_{\text{lat}} \) versus \( \omega \) for the capsule \( Ca = 0.3 \) released from the wall by an initial offset \( h_{\text{ini}} = 1.5, 2 \) and 3. As \( \omega < 2 \), \( \bar{U}_{\text{lat}} \) decreases with \( \omega \) sharply and their relation is almost linear; as \( \omega > 2 \), the migration velocity declines with \( \omega \) much slower, approaching zero asymptotically for large \( \omega \). Indeed, \( \omega = 0 \) corresponds to the case of a capsule subject to a steady wall-bounded shear flow, it will move away from the wall with a certain velocity. As \( \omega \rightarrow \infty \), the characteristic flow time is too small compared to the relaxation time of the capsule; it fails to sense the shear with almost no deformation or lateral migration. In figure 3.2, We plot \( U_{\text{lat}}^{PK} \), the first peak value of the \( U_{\text{lat}} \) in time, as a function of \( \omega \), for the same capsule \( Ca = 0.3 \) released from different initial offsets. Surprisingly, \( U_{\text{lat}}^{PK} \) is not altered significantly as changing the initial offset of the capsule \( h_{\text{ini}} \). For the three \( h_{\text{ini}} \)s examined, \( U_{\text{lat}}^{PK} \) decreases with monotonically with \( \omega \).
Figure 4. Lateral migration velocity $U_{\text{lat}}$ denoted by the solid curve and nondimensional normal stress difference $(N_1 - N_2)/\mu \dot{\gamma}_{\text{max}}$ by the dashed curve versus the nondimensional time $t \omega / 2\pi$, for three capillary numbers $Ca = 0.0375$ ((a)), 0.12 ((b)) and 0.6 ((c)). The initial offset $h_{\text{ini}} = 2$ and the frequency of shear $\omega = 5/3$. The left scale is for $U_{\text{lat}}$ and the right for $(N_1 - N_2)/\mu \dot{\gamma}_{\text{max}}$. Their local maximums are marked by the circles and squares respectively.

Figure 5. $\bar{U}_{\text{lat}}$ is the time-averaged value of the lateral migration velocity $U_{\text{lat}}$, and $\bar{\Delta N}$ is that of the nondimensional normal stress differences $(N_1 - N_2)/\mu \dot{\gamma}_{\text{max}}$. $\bar{U}_{\text{lat}}$ (resp. $\bar{\Delta N}$) versus the capillary number $Ca$ is indicated by the solid (resp. dashed) curve with circles (resp. diamonds), measured by the left (resp. right) scale. The results are shown for three initial offsets, (a) $h_{\text{ini}} = 1.5$, (b) $h_{\text{ini}} = 2$ and (c) $h_{\text{ini}} = 3$. 
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Figure 6. Time-averaged migration velocity $\bar{U}_{\text{lat}}$, as a function of the frequency of the oscillating shear $\omega$. The capillary number $Ca$ of the capsule is 0.3 and three initial positions of the capsules are chosen, $h_{\text{ini}} = 3$ denoted by squares, $h_{\text{ini}} = 2$ by circles and $h_{\text{ini}} = 1.5$ by triangles.

Figure 7. The first peak value of the migration velocity $U_{\text{lat}}$, $U_{\text{PK}}^{\text{lat}}$, as a function of the frequency of the oscillating shear $\omega$. The capillary number $Ca$ of the capsule is 0.3 and three initial positions of the capsules are chosen, $h_{\text{ini}} = 3$ denoted by squares, $h_{\text{ini}} = 2$ by circles and $h_{\text{ini}} = 1.5$ by triangles.

3.3. Deformation of the capsule

The capsule commonly evolves into a prolate as subject to the unbounded shear flow. Hence, its deformation can be easily quantified by the so-called Taylor parameter $D = (L_{\text{max}} - L_{\text{min}})/(L_{\text{max}} + L_{\text{min}})$ (Barthès-Biesel et al. 2010), where $L_{\text{max}}$ and $L_{\text{min}}$ are the length of the major and minor axis of the elliptical profile.
The deformation index $\hat{D}$ of the capsules versus the nondimensional time $\omega/2\pi$, the initial offset is $h_{\text{ini}} = 10$ and the frequency of the shear is $\omega = 5/3$. $\hat{D}$ of the capsule $\text{Ca} = 0.03$, $\text{Ca} = 0.15$ and $\text{Ca} = 0.6$ is indicated by the solid, dot-dashed and dashed curve respectively. The dotted curve denotes the oscillating shear $\dot{\gamma}_{\text{max}} \cos(\omega t)$, arbitrarily scaled for visualization. (b), the temporal peak of $\hat{D}$, versus the capillary number $\text{Ca}$. $\omega = 5/3$, the results for $h_{\text{ini}} = 1.5$, 2 and 3 are represented by the curves with triangles, circles and squares respectively. Note we take the peak value after the capsule has undergone the initial period when the peak values are not varying.

in the shear plane. In our case, the profile of the capsule on the shear plane is not a ellipse, as the symmetry is broken by the presence of wall. We thus introduce the deformation index, $\hat{D} = (L'_{\text{max}} - L'_{\text{min}})/(L'_{\text{max}} + L'_{\text{min}})$, where $L'_{\text{max}}$ is the maximum distance measured from the capsule to the its centre of mass and $L'_{\text{min}}$ is the minimum distance accordingly. The deformation index $\hat{D}$ tells how far away the capsule is from its initial shape, a sphere in the current case.

The deformation index $\hat{D}$ versus the nondimensional time is illustrated in figure 8(a) for three capsules $\text{Ca} = 0.03$, 0.15 and 0.6 starting from the same initial offset $h_{\text{ini}} = 2$. The frequency of the oscillating shear is $\omega = 5/3$. The index $\hat{D}$ displays wake-like variations in time. The wave magnitude increases
A capsule in a wall-bounded oscillating shear flow during the initially stage, which then keeps more or less constant. The initial increase is especially apparent for the relatively soft capsules, $Ca = 0.15$ and 0.6; indeed, a higher capillary number implies a longer relaxation time, hence the capsule needs more time to adapt itself to the unsteady flow. Moreover, the frequency of the periodically varying deformation index $\hat{D}$ is roughly twice that of the background shear. The stiffest capsule $Ca = 0.03$, displays the maximum deformation roughly after the local extremum points of the shear, and the minimum deformation as the shear flow reverses its direction. The stiff capsule senses and responds to the variation of flow so fast that it immediately changes its shape according to the strength of the flow. The capsule deforms closely following the flow with a negligible phase delay. In contrast the floppy capsule $Ca = 0.6$ deforms most, roughly when the flow reverses, exhibiting a phase delay of about $\pi/4$. Regardless of the difference in the phase delay between different capsules, the sinusoidally varying shear either reaches the extremum points or changes its sign at a frequency exactly twice its own wave frequency $\omega$. Consequently, the deformation index $\hat{D}$ of both capsules changes with time twice as fast as the flow oscillation.

We plot the temporal peak value of deformation index $\hat{D}$, as a function of the capillary number $Ca$ in figure 13.8(b). Three initial heights $h_{ini} = 1.5$, 2 and 3 are chosen. We see that the maximum deformation of the capsule does not vary significantly with the initial offset $h_{ini}$, in contrast with the strong dependence of its lateral migration velocity on $h_{ini}$. The deformation $\hat{D}$ increases almost linearly with the capillary number $Ca$ as it is small, $Ca < 0.1$ in this case. This resembles the linear relation between the deformation of a capsule and its capillary number in an unbounded steady shear flow. $\hat{D}$ increases very slowly as $Ca > 0.2$ and reaches an asymptotic value close to 0.3 as $Ca > 0.6$. This is different with that happens in the unbounded steady shear. In that case, $\hat{D}$ increases slowly but keep growing with $Ca$ when $Ca$ is large. Here, the deformation not only depends on $Ca$ but also on the frequency of the shear flow $\omega$. For a capsule with a large $Ca$ whose relaxation time is much larger than the characteristic flow time $2\pi/\omega$, it fails to reach its maximum deformation before the flow changes its direction. In other words, the maximum deformation of the capsule is limited by the period of time the flow applies in one direction, instead of its own deformability.

4. Conclusions
We study the motion and deformation of an initially spherical capsule in a wall-bounded oscillating shear flow, with an accelerated boundary integral method. The lateral migration velocity of the capsule varies non-monotonically with its capillary number $Ca$; the velocity reaches the peak value when $Ca \approx 0.15$. The migration velocity decreases as the initial distance between the capsule and the
wall becomes larger. We investigate the correlation between the lateral migration velocity and the normal stress difference due to the presence of capsule. The maximum of the two quantities co-appear in time, however the ratio between the corresponding maximum values can vary depending on the capillary number. The capsule either stiff (Ca = 0.0375) or floppy (Ca = 0.6) has a low migration velocity and accordingly the ratio varies considerably with time. The capsule with a medium deformability Ca = 0.12 has the highest migration velocity and the ratio keeps constant with time. This indeed implies a stronger correlation between the lateral migration velocity and normal stress difference for the fastest capsule Ca = 0.12 than the other two. We also examine the time-averaged value of the normal stress difference as a function of Ca, their relation is highly similar with that between the mean lateral migration velocity and Ca. This confirms the positive correlation between the lateral migration velocity and normal stress difference. For a fixed capsule Ca = 0.3, the migration velocity decreases linearly with the frequency of shear $\omega$ and approaches a asymptotic value of zero for large $\omega$.

The deformation of capsule varies periodically with time, following the change of shear in time with a phase delay. The phase delay increases with the capillary number, up to around $\pi/4$ for Ca = 0.6. For all capsules with different Ca, the variation of capsule deformation is roughly twice as fast as that of the underlying oscillatory shear. The peak deformation of the capsule increases linearly with Ca when Ca < 0.1 and much more slowly as Ca > 0.2, approaching an unchanged value as Ca > 0.6. The deformation of capsule is limited here by the period of time it is exerted by the flow before reversing its direction, instead of the deformability of capsule.

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