Swimming Filaments in a Viscous Fluid with Resistance

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Swimming Filaments in a Viscous Fluid with Resistance

by

Nguyenho Ho

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Abstract

In this dissertation, we study the behavior of microscopic organisms utilizing lateral and spiral bending waves to swim in a fluid. More specifically, spermatozoa encounter different fluid environments filled with mucus, cells, hormones, and other large proteins. These networks of proteins and cells are assumed to be stationary and of low volume fraction. They act as friction, possibly preventing or enhancing forward progression of the swimmers. The flow in the medium is described as a viscous fluid with a resistance term known as a Brinkman fluid. It depends on the Darcy permeability parameter affecting the swimming patterns of the flagella. To further understand these effects we study the asymptotic swimming speeds of an infinite-length swimmer propagating planar or spiral bending waves in a Brinkman fluid. We find that, up to the second order expansion, the swimming speeds are enhanced as the resistance increases. The work to maintain the planar bending and the torque exerted on the fluid are also examined. The Stokes limits of the swimming speeds, the work and the torque are recovered as resistance goes to zero. The analytical solutions are compared with numerical results of finite-length swimmers obtained from the method of Regularized Brinkmanlets (MRB). The study gives insight on the effects of the permeability, the length and the radius of the cylinder on the performance of the swimmers.

In addition, we develop a grid-free numerical method to study the bend and twist of an elastic rod immersed in a Brinkman fluid. The rod is discretized using a Kirchhoff Rod (KR) model. The linear and angular velocity of the rod are derived using the MRB. The method is validated through a couple of benchmark examples including the dynamics of an elastic rod, and the planar bending of a flagellum in a Brinkman fluid. The studies
show how the permeability and stiffness coefficients affect the waveforms, the energy, and the swimming speeds of the swimmers.

Also, the beating pattern of the spermatozoa flagellum depends on the intracellular concentrations of calcium ([Ca$^{2+}$]). An increase of [Ca$^{2+}$] is linked to hyperactivated motility. This is characterized by highly asymmetrical beating, which allows spermatozoa to reach the oocyte (egg) or navigate along the female reproductive tract. Here, we couple the [Ca$^{2+}$] to the bending model of a swimmer in a Brinkman fluid. This computational framework is used to understand how internal flagellar [Ca$^{2+}$] and fluid resistance in a Brinkman fluid alter swimming trajectories and flagellar bending.
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Chapter 1

Introduction

The self-propulsion of microorganisms that utilize flagellar propulsion has been the topic of a vast number of analytical, experimental, and computational studies for many years (reviewed in [1]). Many species of spermatozoa and bacteria are able to swim by propagating lateral or spiral waves along their cylindrical flagella [2] [3] [4]. Similarly, larger organisms such as *C. elegans* (nematodes) are also able to make forward progression through soil via undulatory locomotion [5]. The native environment in which these organisms live varies greatly. For example, spermatozoa encounter different fluid environments in the female reproductive tract that include swimming through or around mucus, cells, hormones, and other large proteins [7] [6] [8]. Similarly, bacteria are able to swim in the mucus layer that coats the stomach and move in biofilms with extracellular polymeric substances [2] [9] [10]. Fig. 1.1 shows several sperm swimming in random directions in...

Figure 1.1: *The figure shows a snapshot of multiple bovine sperm swimming in vaginal fluid with a dense network of proteins.* The figure is taken from Rutllant et al. [6] with permission, reuse order license id is 3853640544521.
bovine vaginal fluid composed of a randomly oriented network of protein fibers [6].

The swimming speed or mode of swimming for microorganisms changes when encountering different environments. A study by Berg et al. [11] showed that Leptospira, a slender helical bacterium, swims faster in methylcellulose (MC), a gel with chains of long polymers. Another study showed that swimming speeds of seven different types of

![Images of human sperm cells in different fluid environments](image)

Figure 1.2: Images of human sperm cells in different fluid environments are captured where (a)–(b) show beat patterns of a sperm cell (for different time frames) in a salt solution, a liquid with low viscosity and (c)–(d) shows a cell rolling in high viscosity methylcellulose gel (for two time periods). The figures are taken from experiments by Smith et al. [4] and reproduced with permission, reuse order license id is 3853650445064.

bacteria were enhanced in higher viscosity solutions of MC and PVP (polyvinylpyrrolidone) [12]; beyond a certain viscosity or polymer concentration, this enhancement was no longer observed.

Experiments of sperm in MC and PA (polyacrylamide) gels showed that swimming speeds, beat frequency, and amplitude of undulation vary as the viscosity is changed from low to high [4, 13, 14]. Smith et al. [4] studied the flagellar movement of human sperm in low and high viscosity liquids using a salt solution and MC. In the medium with low viscosity, Figs. 1.2(a)–(b) are taken from two different time points and show that the flagellum has a high curvature waveform. This may be due to out-of-plane movement.
On the other hand, sperm cells may display rolling and exhibit planar bending at the end of the flagellum in a high viscosity solution such as MC as shown in Figs. 1.2(c)–(d) captured at two time points. In another study by Ho et al. [14], the bull sperm swims in a nearly straight trajectory with a symmetrical beat form with low intracellular or cytosolic calcium concentration as shown in Fig. 1.3(a). In the same experiment, the flagellum in Fig. 1.3(b) swims with a more asymmetrical pattern (deeper bends) with high intracellular calcium. The beat pattern changes significantly when the sperm is placed in a viscoelastic solution of long-chain polyacrylamide with high intracellular calcium. Here, we observe that the sperm flagellum in Fig. 1.3(c) beats vigorously at the end and shows no movement in the middle part of the flagellum.

![Figure 1.3: Images of bull sperm swimming in different fluid environments including (a) low intracellular calcium, (b) high intracellular calcium with the same viscosity of water and (c) high intracellular calcium in a viscoelastic solution with higher viscosity (polyacrylamide). Each image is from two photographs of the same sperm taken 1/60s apart and superimposed. The figure is reproduced from [14] with permission, reuse order license id is 3853650015322.](image)

The flagellum and cell body may also experience rolling. Previous experiments by [4] show that the viscosity not only changes the waveform of the flagellum but also alters the planarity of the swimmers. Recent developments show sperm trajectories that form chiral ribbons [16]. These have been observed and captured in experiments using horse sperm. Spermatozoa also display quasi-planar beating patterns [15]. Fig. 1.4 shows the 3D schematic of a planar bending flagellum (blue) and ‘quasi-planar’ patterns for sea urchin sperm (red) and human sperm (yellow). Some mammalian sperm also exhibit helical bending due to changes in viscosity [3]. In addition, to successfully reach the oocyte (egg) or navigate along the female reproductive tract, spermatozoa must alter their
bending pattern from symmetrical to highly asymmetrical, which is called hyperactivated motility [17, 18, 19]. The hyperactivity is linked to an increase of calcium concentration ([Ca^{2+}]) in the flagellum of the sperm.

The underlying idea is to understand the mechanisms that govern how the sperm flagellum propels itself in different fluid environments with different intracellular concentrations of calcium. Thus, it is important to study models of the flagellum and comprehend
its internal structure. Fig. 1.5(a) shows the cross-section of the sperm flagellum. There are 9 outer pairs of microtubules, surrounding a central microtubule pair making up the axoneme, the core of the flagellum [17]. The outer doublets, numbered clockwise from 1–9, are connected by nexin links and are tied with the central pair by radial spokes. The outer microtubules of the axoneme are also connected by the dynein arms, molecular motors [21, 17]. It is known that bending of the flagellum along its length is linked to forces induced by the dynein arms [17, 15]. In fact, when sliding occurs, doublets 1–4 generate bending in one side of the axoneme and doublets 6–9 cause the axoneme to bend in the opposite direction as shown in Fig. 1.5(b) [15, 17, 20]. These bends create different curvatures along the circumference of the sperm flagellum, which produce a propagating bending wave. Doublets 5 and 6 are permanently linked together and therefore can not slide past one another [22]. In the model we develop of sperm motility, we model the beating of the flagellum via a prescribed or preferred curvature. The curvature function is based on experimental results and parameters such as stiffness depend on measurements of microtubule flexural rigidity.

Since the length scale of these swimmers is small, they live in a viscosity dominated environment where inertia can be neglected. Many studies have focused on analyzing idealized swimmers in viscous fluids at zero Reynolds number. Formally, the Reynolds number is defined to be the nondimensional constant depending on the density \( \rho \) of the fluid, the characteristics velocity \( U \), the length scale \( L \), and the dynamic viscosity \( \mu \) as

\[
Re = \frac{\rho UL}{\mu}. \tag{1.1}
\]

In water, the viscosity is \( \mu = 10^{-3} \text{ kg m}^{-1} \text{ s}^{-1} \) and the density is \( \rho = 10^3 \text{ kg m}^{-3} \). The length of a human sperm is \( L = 50 \mu m \) and it swims with a velocity of \( U = 200 \mu m \text{ s}^{-1} \) [1]. Whereas, a swimming bacteria such as \textit{E.coli} has a typical length of \( L = 10 \mu m \) and swims at \( U = 10 \mu m \text{ s}^{-1} \) [1]. Thus, the resulting Reynolds number is on the order of \( 10^{-4} - 10^{-2} \) and can be approximated as zero. The incompressible Stokes equation, defined as

\[
\nabla p = \mu \Delta \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0, \tag{1.2}
\]
is often used to model fluid flow around microorganisms since it governs fluid motion at zero Reynolds number, for pressure $p \ (N \ \mu m^{-2})$, velocity $u \ (\mu m \ s^{-1})$, and viscosity $\mu \ (kg \ m^{-1} \ s^{-1} = N \ s \ m^{-2})$, where $N$ (Newton) is the unit of force. The Stokes equations model a homogeneous fluid with a given viscosity $\mu$. However, the fluid that these swimmers are moving through contains different amounts of proteins or other structures; thus, more complex fluid models than Stokes flow have been proposed and analyzed. For instance, viscoelastic fluid models at zero Reynolds number have been considered to describe the proteins or polymer chains in gels causing a fluid to exhibit a nonlinear strain response (frequency dependent) [23, 24].

Another approach is to think of the fluid with an embedded polymer network as a porous medium. Darcy’s law, written in the form

$$\nabla p = -\frac{\mu}{\gamma} u,$$

has been used to describe the fluid flow in porous media, where $\gamma \ (\mu m^2)$ is the permeability and average velocity $u \ (\mu m \ s^{-1})$ is proportional to the gradient in pressure. This law is not able to capture contributions of the viscous stress tensor and it is only valid on the macroscopic scale where the domain is large and boundary effects can be neglected [25, 26]. To overcome these disadvantages, the incompressible Brinkman flow equation has an additional diffusion term [25],

$$\nabla p = \mu \Delta u - \frac{\mu}{\gamma} u, \quad \nabla \cdot u = 0,$$

where $p \ (N \ \mu m^{-2})$ is the average fluid pressure, $u \ (\mu m \ s^{-1})$ is the average fluid velocity, $\gamma \ (\mu m^2)$ is the permeability of the porous medium, and the viscosity is $\mu \ (N \ s \ m^{-2})$. Thus, the pressure gradient has a unit of force per area per length (or force per volume).

This equation represents the effective flow through a network of stationary obstacles with small volume fraction [27, 25, 28, 29]. In Eq. (1.4), the term $\mu \Delta u$ is called the Brinkman term. The resistance due to the obstacles is characterized by $\mu/\gamma$; thus, $-\frac{\mu}{\gamma} u$ is called the resistance term. Fig. 1.6 shows the flow in a Brinkman fluid with randomly oriented...
spherical obstacles. Note that the incompressible Stokes equations as in Eq. (1.2) are recovered in the limit as $\gamma \to \infty$ where the resistance term vanishes. When $\gamma \to 0$, the Brinkman term becomes negligible and Eq. (1.4) behaves like Darcy’s law (Eq. (1.3)). Another characteristic of a Brinkman fluid is the Brinkman screening length, $\sqrt{\gamma}$, which marks the approximate length over which a disturbance to the velocity would decay. For comparison, in 3D, the flow due to a point force in Stokes flow decays as $1/r$ whereas the flow due to a point force in a Brinkman flow decays like $\gamma/r^3$ \cite{30, 31}. 

In order to consider a microorganism swimming in this environment, we assume that the obstacles are at a low enough volume fraction such that the distance between fibers is larger than the radius of the microorganism \cite{27}. Further, for randomly oriented fibers, Spielman and Goren \cite{29} have derived a relationship between the volume fraction $\phi$, the

Figure 1.6: *Flow in a Brinkman fluid with randomly oriented spherical obstacles.*
permeability $\gamma$, and the radius of the fiber $a_f$ as

$$\frac{a_f^2}{\gamma} = 4\varphi \left[ \frac{1}{3} \frac{a_f^2}{\gamma} + \frac{5}{6} \frac{a_f}{\sqrt{\gamma}} K_1\left(\frac{a_f}{\sqrt{\gamma}}\right) + \frac{5}{6} \frac{a_f}{\sqrt{\gamma}} K_0\left(\frac{a_f}{\sqrt{\gamma}}\right) \right].$$  \hspace{1cm} (1.5)

Here, $K_0(\cdot)$ and $K_1(\cdot)$ are the zero and first order modified Bessel functions of the second kind. We show in Fig. 1.7 the plot of the volume fraction $\varphi$ as a function of the ratio $a_f/\sqrt{\gamma}$. We also indicate the volume fraction of cervical mucus (red marker) and a collagen gel (green marker) where the values of $\varphi$ and $a_f$ are taken from [32]. The plot indicates the biological range of volume fractions or permeabilities we might want to work with. We note that the permeabilities for collagen gel and cervical mucus are estimated from Eq. (1.5) as $8.6 \mu m^2$ and $0.0085 \mu m^2$, respectively. Since the Brinkman model assumes that the fiber network is static, we must have that the distance between the fibers (or the interfiber spacing) is large enough for the swimmer to move through with little or no interaction with the fibers. To estimate the ratio of interfiber spacing and the fiber radius, we use the following equation [31]:

$$\frac{D}{a_f} \approx 2 \left( \frac{1}{2} \sqrt{\frac{3\pi}{\varphi}} - 1 \right),$$  \hspace{1cm} (1.6)

where $D$ is interfiber spacing.

To understand the propulsion of the flagellum bending in a viscous fluid, the swimming speeds of idealized swimmers have been studied. Seminal work by GI Taylor examined swimming speeds of an infinite sheet in two-dimensions (2D) and an infinite cylinder with circular cross section of small radius in three-dimensions (3D), propagating lateral displacement waves in the Stokes regime [33, 34]. This is the case where $\gamma \to \infty$ in Eq. (1.4) implying that there are no obstacles in the incompressible, viscous fluid. In these studies, it was shown that the second order swimming speed scales quadratically with amplitude and linearly with frequency for small amplitude bending. This analysis has been extended for several different cases including swimming speeds for cylinders with non-circular cross sections [35], as well as improvements to the perturbation series [36]. In addition, for the case of a swimming sheet, studies have looked at the asymptotic
swimming speeds in a gel represented as a two-phase fluid (elastic polymer network and viscous fluid) where enhancement in propulsion was observed for stiff and compressible networks [37].

In contrast, a two-fluid model (with intermixed fluids) exhibited a decreased swimming speed relative to the case of a fluid with a single viscosity in both asymptotics and numerical simulations [38]. In another model, Magariyama and Kudo [39] looked at a fluid governed by two viscosities using a modified resistive force theory and found that there is an enhancement in propulsion efficiency when the viscosity of the polymer solution increases and the other fluid viscosity is held constant. Swimming in a shear thinning fluid has also been studied; locomotion of finite-length swimmers is enhanced (2D numerical simulations) [40] and infinite undulating sheets exhibit a decrease in swimming speed relative to the Stokes case [41]. Through asymptotic analysis, it has been shown that the swimming speed of infinite sheets and cylinders in a viscoelastic fluid decreases relative to the speed in a purely viscous fluid [42, 43, 44]. Simulations of finite-length swimmers in a viscoelastic fluid at zero Reynolds number governed by the Oldroyd B equation revealed that enhancement in swimming speeds can be observed when asymmetrical beatforms and swimmer elasticity work together [23, 24]. Specifically, increases in swimming speeds were observed in a viscoelastic fluid when the beat frequency of the swimmer is on the same time scale as the polymer relaxation time [23]; when the polymer relaxation time is fast, other models may be more appropriate to understand swimming speeds.

In the case of a two-phase fluid composed of a polymer network and solvent, if the polymer is stationary, we obtain the Brinkman equation. In this limiting case of a two-phase fluid, an infinite-length sheet exhibits an enhancement in swimming speed [37]. Previously, Leshansky [31] derived the asymptotic swimming speed for an infinite sheet propagating waves of lateral bending in a fluid governed by the Brinkman equation. They observed that swimming speeds scaled similarly to those of Stokes, scaling quadratically with amplitude. In addition to the Stokesian swimming speed, there is an extra factor that depends on the permeability and is monotonically increasing for decreasing permeability (increasing the resistance in the fluid).
In this dissertation, we focus on calculating the asymptotic swimming speed for a waving cylindrical tail that exhibits lateral displacement waves in a Brinkman fluid. Since the waveform of the swimmer can be planar or nonplanar and the swimming occurs in 3D, studying the swimming speed of an infinite cylinder asymptotically gives us a better understanding on how a filament behaves in general. A second order asymptotic swimming speed is derived for planar bending and we find that swimming speeds are enhanced, similar to the 2D case for an infinite sheet. Swimming speeds are also calculated for cylindrical tails with spiral displacement waves, showing that fluid resistance enhances swimming speed. These results shed insight on how added fluid resistance changes propulsion of cylindrical tails when the kinematics are prescribed. In addition, as the resistance approaches zero, we recover the swimming speed, work, and torque for an infinite-length cylinder in a fluid governed by the Stokes equation. Through our analysis, we also find the range of enhancement in swimming speeds for the infinite cylinder in a Brinkman fluid and the relation to permeability, cylinder thickness, and wavenumber.

To validate our asymptotic results, we apply the method of Regularized Brinkmanlets to study finite-length filaments. This method was first developed by Cortez et al. [45] for a 3D Brinkman fluid and was later extended to 2D Brinkman flow [46]. It is an extension of the method of Regularized Stokeslets for the Stokes equation [47, 48]. Through validation, we find that the theoretical swimming speed of filaments with prescribed planar bending waves matches up well with the simulation data and that the asymptotics overestimate swimming speeds for shorter length cylindrical swimmers. In the helical bending wave case, we calculate the external torque exerted on the filament by the surrounding fluid. We observe that the numerical and the asymptotic findings may not consistently agree with one another; the asymptotics overestimate the torque of finite-length helical swimmers.

We also develop a grid-free numerical method to account for the bend and twist of an elastic rod propagating planar or spiral displacement waves in a Brinkman fluid using a Kirchhoff Rod (KR) model. This is an extension of the KR model for the Stokes equations [49, 50]. The rod is parameterized at the center line by the 3D space curve together with the associated orthonormal triads corresponding to the bend and twist of
the rod. In the fluid, an elastic rod is moved with the local fluid velocity and rotates with the local angular velocity. We derive the formulations for the linear and angular velocity of the rod in a Brinkman fluid using the method of Regularized Brinkmanlets. The evaluations of the velocity are done using two different approaches as detailed in Chapter 4. The solutions depend on the permeability, $\gamma$. We implement the method through a couple of benchmark examples including the dynamics of an elastic open rod and the planar bending sinusoidal swimmer in a Brinkman fluid. The test cases give us insight on the effect of stationary obstacles on the overall computed swimming speeds, energy as well as the bending and twisting of the rod. In addition, we study the effect of calcium concentration on the beating patterns of the flagellum in a Brinkman fluid. Here, the amplitude of the rod is no longer a constant but a function depending on the intracellular calcium along the length of the flagellum. The flagellum is parameterized as a sine wave using a KR model and the fluid is governed by the incompressible Brinkman equation. We observe that the emergent waveforms vary greatly as permeability $\gamma$ is varied. Specifically, for small permeability, the amplitude of bending achieved is much smaller and results in slower swimming speeds.
Chapter 2

Asymptotic Analysis

The emergent waveform of a swimmer is different in various environments. We observe that a sea urchin sperm (marine invertebrate), in artificial sea water (ASW) with viscosity of $4 \text{ Pa} \cdot \text{s}$, swims with planar bending as shown in Fig. 2.1(a). In Fig. 2.1(b), we also see that a sea urchin sperm in ASW with lower viscosity propagates a helical bending wave [3]. In addition, the swimming speed of the spermatozoa changes depending on amplitude and wavelength of the propagating wave [3]. These observations provide motivation to study the swimming speeds of swimmers with planar and spiral bending waves. To determine swimming speeds through asymptotic analysis, we study a cylinder or filament of infinite length. It is well known that asymptotic analysis has been used to study the swimming speeds of an infinite-length sheet in 2D (Fig. 2.2(a)) and an infinite-length cylinder in 3D (Fig. 2.2(b)) to provide insight into the propulsion of swimming microorganisms [33, 34]. The infinite swimmers are idealized assumptions since microorganisms...
are of finite length. The goal is to have the leading order (or second order) expansion of the swimming speed to further understand the effects of the properties of the fluid on the overall movements of the swimmers without carrying out lengthy calculations. Leshansky [31] derived the swimming speed of the 2D swimming sheet and the propulsion of a rotating helix in a Brinkman fluid.

In this chapter, we derive the asymptotic swimming speeds of a 3D infinite cylinder in the case of planar and spiral bending waves. We emphasize that the effective fluid environment is modeled as a viscous fluid moving through a porous, static network of low volume fraction fibers (obstacles) via the Brinkman equation. We proceed further by comparing the swimming speeds in the planar bending case with the one of the swimming sheet obtained by Leshansky for a Brinkman fluid [31] and the one in the Stokes regime by G. I. Taylor [34]. We also intend to derive the rate of work done to maintain the beating form of the flagellum in the planar bending case. The spiral bending velocity from our derivations is also used to compare with the propulsion of the rotating helix obtained through modified resistive force theory [31]. The torque exerted on the cylinder by the surrounding fluid is also considered. We end the chapter with an analysis on the range of parameters that enhance swimming speed and biological applications to validate our model.

Figure 2.2: Diagrams of (a) a finite swimming sheet and (b) swimming cylinder with amplitude b. The pictures are recreated from [51].
2.1 Swimming Speeds of a Cylinder with Planar Bending

2.1.1 Cylinder with Lateral Displacement Waves

Similar to previous work [43, 34], we consider a cylinder of constant cross section, bending with small amplitude in the $x$ direction, immersed in a fluid. The cylinder is bending in the $x - y$ direction with

$$x = b \sin(k(z + Ut)), \quad y = 0,$$

where $b$ is the amplitude, $U$ is the velocity of the propagating wave, and $k$ is the wavenumber, defined as $k = 2\pi/\lambda$ where $\lambda$ is the wavelength. With this, the velocity components of the cylinder have the form $u_x = bkU \cos(k(z + Ut))$ and $u_y = 0$. To simplify, we let

$$s = k(z + Ut)$$

and convert the above equations into cylindrical coordinates to obtain the boundary conditions on the surface of the cylinder,

$$u_r = bkU \cos \theta \cos s, \quad u_\theta = -bkU \sin \theta \cos s, \quad u_z = 0. \quad (2.1)$$

From this point, we regard the velocity components in cylindrical coordinates as $u_r = u, u_\theta = v$, and $u_z = w$. The time-dependent position of the cylinder at any given point
on the surface is given as

\[ r^2 = a^2 + b^2 \sin^2 s + 2ab \sin s \cos \theta', \quad (2.2) \]

as shown in Fig. 2.3 for \( \theta' = \theta + \xi \). We can rewrite Eq. (2.2) as

\[ r^2 = a^2 + b^2 \sin^2 s + 2ab \sin s \cos(\theta + \xi), \]

\[ = a^2 + b^2 \sin^2 s + 2ab \sin s (\cos \theta \cos \xi - \sin \theta \sin \xi), \]

where \( \sin \xi = \frac{b \sin s \sin \theta}{a} \). For small \( \xi \), we have:

\[ r^2 = a^2 + b^2 \sin^2 s + 2ab \sin s \cos \theta - 2b^2 \sin^2 s \sin^2 \theta, \]

\[ = (a + b \sin s \cos \theta)^2 - b^2 \sin^2 s \sin^2 \theta, \]

\[ = (a + b \sin s \cos \theta)^2 \left[ 1 - \frac{b^2 \sin^2 s \sin^2 \theta}{(a + b \sin s \cos \theta)^2} \right]. \]

Then \( r \) becomes

\[ r = (a + b \sin s \cos \theta) \sqrt{1 - \frac{b^2 \sin^2 s \sin^2 \theta}{(a + b \sin s \cos \theta)^2}}. \]

We can then arrive at the final equation of \( r \) in the first order of \( b/a \):

\[ r = a \left[ 1 + \frac{b}{a} \sin s \cos \theta + O \left( \frac{b}{a} \right)^2 \right], \quad (2.3) \]

or

\[ r = a + b \sin s \cos \theta. \quad (2.4) \]

**2.1.2 Fluid Model**

The 3D Brinkman equation in cylindrical coordinates is:

\[ \frac{1}{\mu} \frac{\partial p}{\partial r} = \frac{\partial}{\partial r} \left[ \frac{1}{r} \frac{\partial}{\partial r} (ru) \right] + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} - \frac{2}{r^2} \frac{\partial v}{\partial \theta} + \frac{\partial^2 u}{\partial z^2} - \frac{1}{\gamma} u, \quad (2.5) \]
\[
\frac{1}{\mu \theta} \frac{\partial p}{\partial \theta} = \frac{\partial}{\partial r} \left[ \frac{1}{r} \frac{\partial}{\partial r} (rv) \right] + \frac{1}{r^2} \frac{\partial^2 v}{\partial \theta^2} + \frac{2}{r^2} \frac{\partial u}{\partial \theta} + \frac{\partial^2 v}{\partial z^2} - \frac{1}{\gamma} v, \tag{2.6}
\]

\[
\frac{1}{\mu \theta} \frac{\partial p}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial w}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 w}{\partial \theta^2} + \frac{\partial^2 v}{\partial z^2} - \frac{1}{\gamma} w, \tag{2.7}
\]

where \( u, v, \) and \( w \) are the velocity components in the direction of \( r, \theta, \) and \( z, \) respectively. Again, we note that the Brinkman equation represents a heterogeneous viscous fluid with stationary polymer chains or fibers whose spacing is larger than the radius of the microorganism swimming through the fluid. The continuity equation for the incompressible flow is given by

\[
\frac{\partial u}{\partial r} + \frac{u}{r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{\partial w}{\partial z} = 0. \tag{2.8}
\]

Taking the divergence of Eq. (2.5) and using Eq. (2.8) to simplify, we find that the pressure satisfies \( \nabla^2 p = 0. \) Let \( \zeta = kr \) and recall \( s = k(z + Ut). \) The general solution for the pressure is thus

\[
p = \mu knA_{mn}K_m(n\zeta) \cos(m\theta) \cos(ns), \tag{2.9}
\]

where \( K_m \) is the \( m^{th} \) order modified Bessel function of the second kind and \( A_{mn} \) is a constant which is evaluated using the boundary conditions [52]. Based on the pressure in Eq. (2.9), we assume the velocity components can be described as

\[
u = \frac{u_{mn}}{m} \cos m\theta \cos ns, \quad v = \frac{v_{mn}}{m} \sin m\theta \cos ns, \quad \text{and} \quad w = \frac{w_{mn}}{m} \cos m\theta \sin ns. \tag{2.10}
\]

Note that \( u_{mn}, v_{mn}, \) and \( w_{mn} \) are functions with respect to \( \zeta \) only. Substituting \( u, v, w, \) and \( p \) from Eqs. (2.9)–(2.10) into Eqs. (2.5)–(2.6) and using the relations \( s = k(z + Ut) \) and \( \zeta = kr, \) we obtain the following system of equations:

\[
\begin{align*}
\left[ \frac{\partial^2}{\partial \zeta^2} + \frac{2}{\zeta} \frac{\partial}{\partial \zeta} \right] - \frac{(m+1)^2}{\zeta^2} - \left( \frac{n^2 + \alpha^2}{k^2} \right) \right] (u_{mn} + v_{mn}) &= -n^2 A_{mn} K_{m+1}(n\zeta), \tag{2.11} \\
\left[ \frac{\partial^2}{\partial \zeta^2} + \frac{2}{\zeta} \frac{\partial}{\partial \zeta} \right] - \frac{(m-1)^2}{\zeta^2} - \left( \frac{n^2 + \alpha^2}{k^2} \right) \right] (u_{mn} - v_{mn}) &= -n^2 A_{mn} K_{m-1}(n\zeta), \tag{2.12}
\end{align*}
\]

with \( \alpha^2 = 1/\gamma \) (where \( \gamma \) is the Darcy permeability). The parameter \( \alpha \) is known as the hydrodynamic resistance of the porous medium and has units of inverse length.
addition, $\alpha$ is proportional to the ratio of the diameter of the fiber over the spacing within the network. This ratio is usually characterized as the mesh spacing [30].

The homogeneous solutions for Eqs. (2.11)–(2.12) include the modified Bessel function of the first kind, which diverges as $\zeta \to \infty$. Thus, we eliminate this solution to maintain finite values for the velocities. The particular solutions are

$$(u_{mn} + v_{mn})_p = \frac{A_{mn}}{\beta^2} n^2 K_{m+1}(n\zeta) \quad \text{and} \quad (u_{mn} - v_{mn})_p = \frac{A_{mn}}{\beta^2} n^2 K_{m-1}(n\zeta), \quad (2.13)$$

where $\beta = \alpha/k$ is the scaled resistance. It is a nondimensional constant that characterizes the relationship between the resistance or average mesh size and the wavelength of the swimmer. After simplifying, the general solutions to Eqs. (2.11)–(2.12) are

$$u_{mn} + v_{mn} = B_{mn} K_{m+1}(\chi\zeta) + \frac{A_{mn}}{\beta^2} n^2 K_{m+1}(n\zeta), \quad (2.14)$$

$$u_{mn} - v_{mn} = C_{mn} K_{m-1}(\chi\zeta) + \frac{A_{mn}}{\beta^2} n^2 K_{m-1}(n\zeta), \quad (2.15)$$

for $\chi = \sqrt{n^2 + \beta^2}$. The constants $B_{mn}$ and $C_{mn}$ are determined by the boundary conditions of the cylindrical tail. The radial and tangential velocity components are found to satisfy the following equations:

$$2u_{mn} = B_{mn} K_{m+1}(\chi\zeta) + C_{mn} K_{m-1}(\chi\zeta) + \frac{A_{mn} n^2}{\beta^2} \left[ K_{m+1}(n\zeta) + K_{m-1}(n\zeta) \right], \quad (2.16)$$

$$2v_{mn} = B_{mn} K_{m+1}(\chi\zeta) - C_{mn} K_{m-1}(\chi\zeta) + \frac{2A_{mn}}{\beta^2 \zeta} mn K_m(n\zeta). \quad (2.17)$$

The axial component of the velocity is determined using the continuity condition given in Eq. (2.8) and is given by

$$nw_{mn} = -\left[ \frac{\partial u_{mn}}{\partial \zeta} + \frac{1}{\zeta} (u_{mn} + mv_{mn}) \right],$$

$$= \frac{A_{mn} n^3}{\beta^2} K_m(n\zeta) + \frac{1}{2} (B_{mn} + C_{mn}) \chi K_m(\chi\zeta). \quad (2.18)$$

Since our goal is to determine the swimming speed of the cylinder, we have to determine the first and second order solutions, using the condition that the disturbance caused by
the cylinder body should vanish at infinity \cite{34}. The expansions are detailed as follows.

The velocity components are expanded up to the second order about \( \zeta = \zeta_1 = ka \):

\[
\begin{align*}
  u &= (u)_{\zeta=\zeta_1} + bk \cos \theta \sin s(u')_{\zeta=\zeta_1} + \cdots, \\
  v &= (v)_{\zeta=\zeta_1} + bk \cos \theta \sin s(v')_{\zeta=\zeta_1} + \cdots, \\
  w &= (w)_{\zeta=\zeta_1} + bk \cos \theta \sin s(w')_{\zeta=\zeta_1} + \cdots, \\
\end{align*}
\] (2.19)

where Eq. (2.4) is used to rewrite \((\zeta - \zeta_1)\). Additionally, the velocity components \( u, v, \) and \( w \) are expanded in the powers of \( b/a \),

\[
\begin{align*}
  u &= u^{(1)} + u^{(2)} + \cdots, \\
  v &= v^{(1)} + v^{(2)} + \cdots, \\
  w &= w^{(1)} + w^{(2)} + \cdots. \\
\end{align*}
(2.20)

Substituting Eq. (2.20) into Eqs. (2.19) and (2.10):

\[
\begin{align*}
  u &= u_1 \cos \theta \cos s + u^{(2)}_{\zeta=\zeta_1} + bk \cos \theta \sin s \cos \theta \cos s(u')_{\zeta=\zeta_1}, \\
  v &= v_1 \sin \theta \cos s + v^{(2)}_{\zeta=\zeta_1} + bk \cos \theta \sin s \sin \theta \cos s(v')_{\zeta=\zeta_1}, \\
  w &= w_1 \cos \theta \sin s + w^{(2)}_{\zeta=\zeta_1} + bk \cos \theta \sin s \cos \theta \sin s(w')_{\zeta=\zeta_1}. \\
\end{align*}
\] (2.21-2.23)

By matching the above expansions with the boundary conditions in Eq. (2.1), we can determine the constant coefficients \( A_{mn}, B_{mn}, \) and \( C_{mn} \) for each order of the expansion.

2.1.3 First Order Solution

As outlined above, the velocity components are expanded about \( \zeta = \zeta_1 = ka \). To the first order, when \( m = 1 \) and \( n = 1 \), the boundary conditions are \( u_1 = bkU, v_1 = -bkU, \) and \( w_1 = 0 \). Plugging into Eqs. (2.14)-(2.15) and (2.18), we obtain:

\[
\begin{align*}
  u_1 + v_1 &= BK_2(\chi\zeta_1) + \frac{A}{\beta^2} K_2(\zeta_1) = 0, \\
  u_1 - v_1 &= CK_0(\chi\zeta_1) + \frac{A}{\beta^2} K_0(\zeta_1) = 2bkU, \\
  w_1 &= \frac{A}{\beta^2} K_1(\zeta_1) + \frac{1}{2}(B+C)\chi K_1(\chi\zeta_1) = 0, \\
\end{align*}
\] (2.24-2.26)
for $\chi = \sqrt{1 + \beta^2}$. From Eqs. (2.24)–(2.26), the constants are

\[
\begin{align*}
A &= \frac{1}{\beta^2} \frac{2bkU}{K_0(\chi \zeta_1)}\Phi(\zeta_1) K_0(\zeta_1) + \frac{1}{\Phi(\zeta_1)} K_0(\zeta_1) K_0(\chi \zeta_1), \\
B &= \frac{2bkU}{K_0(\chi \zeta_1)} \left[ 1 + \frac{1}{\Phi(\zeta_1)} K_0(\chi \zeta_1) \right],
\end{align*}
\]

(2.27)

\[
\begin{align*}
C &= \frac{2bkU}{K_0(\zeta_1)} \left[ 1 + \frac{1}{\Phi(\zeta_1)} K_0(\chi \zeta_1) \right].
\end{align*}
\]

(2.28)

where

\[
\Phi(\zeta_1) = \frac{2}{\chi} \frac{K_1(\zeta_1)}{K_1(\chi \zeta_1)} - \frac{K_0(\zeta_1)}{K_0(\chi \zeta_1)} - \frac{K_2(\zeta_1)}{K_2(\chi \zeta_1)}.
\]

(2.30)

To determine the velocity of the cylinder, we have that Eqs. (2.21)–(2.23) vanish at infinity [34]. Thus, there is no contribution to the swimming speed of the cylinder in the first order expansion and we have to evaluate the velocity using a higher order expansion.

### 2.1.4 Second Order Solution

The second order expansion gives:

\[
\begin{align*}
\mathbf{u}^{(2)} &= -bk \cos \theta \sin s \cos \theta \cos s(u')_{\zeta=\zeta_1} = -\frac{1}{4} bk(u'_1)_{\zeta=\zeta_1} (\sin 2s + \cos 2\theta \sin 2s), \\
\mathbf{v}^{(2)} &= -bk \cos \theta \sin s \sin \theta \cos s(v')_{\zeta=\zeta_1} = -\frac{1}{4} bk(v'_1)_{\zeta=\zeta_1} \sin 2\theta \sin 2s, \\
\mathbf{w}^{(2)} &= -bk \cos \theta \sin s \cos \theta \sin s(w')_{\zeta=\zeta_1} = -\frac{1}{4} bk(w'_1)_{\zeta=\zeta_1} (1 - \cos 2s + \cos 2\theta - \cos 2\theta \cos 2s).
\end{align*}
\]

(2.31)

(2.32)

(2.33)

The coefficients of the velocity in the second order expansion can be evaluated as:

\[
\begin{align*}
&u_{02} = -\frac{1}{4} bk(u'_1)_{\zeta=\zeta_1}, \quad u_{22} = -\frac{1}{4} bk(u'_1)_{\zeta=\zeta_1}, \\
&v_{22} = \frac{1}{4} bk(v'_1)_{\zeta=\zeta_1}, \\
&w_{02} = \frac{1}{4} bk(w'_1)_{\zeta=\zeta_1}, \quad w_{20} = -\frac{1}{4} bk(w'_1)_{\zeta=\zeta_1}, \quad w_{22} = \frac{1}{4} bk(w'_1)_{\zeta=\zeta_1}.
\end{align*}
\]
Using the same argument for the velocity of the filament at infinity, we arrive at

\[ U_\infty = \frac{1}{4} b k (w'_1)_{\zeta = \zeta_1 = ka}, \]

where \( w'_1 \) is the first derivative of the axial velocity component given in Eq. (2.18) with respect to \( \zeta \) (for \( m = 1, n = 1 \)). Using the first order solution, and evaluating \( w'_1 \) at the boundary, \( \zeta = \zeta_1 = ka \), we have

\[ w'_1 = \frac{2 bk U}{\Phi(\zeta_1)} \left[ \frac{K_0(\zeta_1)}{K_0(\chi \zeta_1)} - \chi \frac{K_1(\zeta_1)}{K_1(\chi \zeta_1)} \right]. \] (2.34)

The swimming speed \( U_\infty \) up to second order expansion is thus

\[ U_\infty = \frac{1}{2} b^2 k^2 U \frac{1}{\Phi(\zeta_1)} \left[ \frac{K_0(\zeta_1)}{K_0(\chi \zeta_1)} - \chi \frac{K_1(\zeta_1)}{K_1(\chi \zeta_1)} \right]. \] (2.35)

The asymptotic velocity for an infinite-length cylinder that is propagating planar bending waves in a Brinkman fluid is given above in Eq. (2.35) and depends on the scaled resistance \( \alpha/k \) through \( \chi \).

In the limiting case when \( \zeta_1 = ka \ll 1 \), the limit forms of the Bessel functions are [53]:

\[
K_1(\zeta_1) = \frac{1}{\zeta_1} + \mathcal{O}(\zeta_1), \quad K_1(\chi \zeta_1) = \frac{1}{\chi \zeta_1} + \mathcal{O}(\chi \zeta_1),
\]

\[
K_2(\zeta_1) = \frac{2}{\zeta_1^2} + \mathcal{O}(\zeta_1^2), \quad K_2(\chi \zeta_1) = \frac{2}{\chi^2 \zeta_1^2} + \mathcal{O}(\chi^2 \zeta_1^2),
\]

\[
K_0(\zeta_1) = -\log \zeta_1 + \log 2 - \gamma_e + \mathcal{O}(\zeta_1^2), \quad K_0(\chi \zeta_1) = -\log \zeta_1 + \log 2 - \gamma_e - \log \chi + \mathcal{O}(\chi^2 \zeta_1^2),
\]

where \( \gamma_e \) is the Euler-Mascheroni constant. Thus, for \( \zeta_1 = ka \ll 1 \) we can rewrite \( \Phi(\zeta_1) \) as

\[ \Phi(\zeta_1) = 2 - \chi^2 - \frac{K_0(\zeta_1)}{K_0(\zeta_1) - \log \chi}. \]

To second order, the nondimensional swimming speed, \( U_\infty/U \), in the case of a cylinder
propagating lateral bending waves is given as

$$\frac{U_\infty}{U} = \frac{1}{2} \beta^2 k^2 \left[ \frac{(1 - \chi^2)K_0(\zeta_1) + \chi^2 \log \chi}{(1 - \chi^2)K_0(\zeta_1) - (2 - \chi^2) \log \chi} \right], \quad (2.36)$$

for $ka \ll 1$. We note that this swimming speed scales quadratically with the amplitude of bending $b$ and depends on the resistance $\alpha$ through the parameter $\chi$. The swimming speeds are shown in Fig. 2.4(a) for several permeability values $\gamma$. For comparison, we also plot the swimming speed of the same infinite-length cylinder propagating planar bending in a fluid governed by the incompressible Stokes equation, as derived by Taylor [34]. We observe in Fig. 2.4(a) that as $\alpha \to 0$ (or $\gamma \to \infty$), we approach the Stokes swimming speed. In the next section, we study this case further.

2.1.5 Comparison of Swimming Speeds

The Brinkman equation is characterized by the Darcy permeability $\gamma$. In the case of $\gamma \to \infty$ (or resistance $\alpha \to 0$), we recover the Stokes equation. To understand what
happens to the swimming speed of the infinite-length cylinder (with \(ka \ll 1\)) as \(\alpha \to 0\), we work with Eq. (2.36) to obtain the following expression,

\[
\frac{U_\infty}{U} = \frac{1}{2} b^2 k^2 \left[ \frac{k^2}{K_0(\zeta_1)} - \frac{1}{2} \log \left(1 + \frac{\alpha^2}{k^2}\right) \frac{k^2}{\alpha^2 - \frac{1}{2} \log \left(1 + \frac{\alpha^2}{k^2}\right)} \right]. \tag{2.37}
\]

We note the following limits as \(\alpha \to 0\):

\[
\lim_{\alpha \to 0} \log \left(1 + \frac{\alpha^2}{k^2}\right) = 1, \quad \lim_{\alpha \to 0} \log \left(1 + \frac{\alpha^2}{k^2}\right) = 0. \tag{2.38}
\]

Thus, the second order asymptotic velocity of a cylinder with \(\zeta_1 = ka \ll 1\) in a Brinkman fluid becomes

\[
\frac{U_{\text{Stokes}}}{U} = \frac{1}{2} b^2 k^2 \left[ \frac{K_0(\zeta_1) - \frac{1}{2}}{K_0(\zeta_1) + \frac{1}{2}} \right].
\]

This is precisely the asymptotic velocity of the same cylinder immersed in a fluid governed by the Stokes equations as derived by Taylor [34]. The swimming speed of an infinite cylinder with planar bending in a Brinkman and Stokes fluid is compared using the following normalization, \(U_n = U_\infty/U_{\text{Stokes}}\). In Fig. 2.4(b), \(U_n\) is shown with the dashed line and is an increasing function, bounded below by 1 as \(\alpha/k \to 0\). We observe that as \(\alpha/k\) increases, the ratio is greater than 1, showing enhancement relative to the Stokes case.

Next, we study the swimming speed of the infinite-length 3D cylinder in comparison to the 2D sheet, where both are propagating planar bending waves. The propulsion of an undulating planar sheet was studied by Leshansky [31] and the swimming speed \(U_{\text{Les}}\) was found to be:

\[
\frac{U_{\text{Les}}}{U} = \frac{1}{2} b^2 k^2 \sqrt{1 + \frac{\alpha^2}{k^2}}, \tag{2.39}
\]
for $\alpha^2 = 1/\gamma$. The ratio of Eq. (2.37) and (2.39) is

$$U_{\text{ratio}} = \frac{U_{\infty}}{U_{\text{Les}}} = \frac{K_0(\zeta_1) - \frac{1}{2} \left( \frac{k^2}{\alpha^2} + 1 \right) \log \left( 1 + \frac{\alpha^2}{k^2} \right)}{K_0(\zeta_1) + \frac{1}{2} \left( \frac{k^2}{\alpha^2} - 1 \right) \log \left( 1 + \frac{\alpha^2}{k^2} \right)} \cdot \frac{1}{\sqrt{1 + \alpha^2 k^2}}. \quad (2.40)$$

We plot $U_{\text{ratio}}$ versus the scaled resistance $\alpha/k$ in Fig. 2.4(b). We observe that the ratio decreases as $\alpha$ increases. This implies that the 3D infinite-length cylinder swims slower than the 2D sheet in a fluid with the same Darcy permeability. When $\alpha/k \to 0$, we see that the ratio approaches

$$U_{\text{ratio}} = \frac{K_0(\zeta_1) - 1/2}{K_0(\zeta_1) + 1/2},$$

for a fixed $\zeta_1$. This is the ratio of the swimming speeds of the infinite-length 3D cylinder and 2D sheet in a fluid governed by the Stokes equation.

### 2.1.6 Energy to Maintain Planar Bending

The force on the surface is calculated as $\mathbf{F} = \sigma \cdot \mathbf{n}$ where $\sigma$ is the stress tensor and $\mathbf{n}$ is the normal vector. The velocity components of $\mathbf{u}$ at the boundary $r = a$ are given in Eq. (2.1). The stress tensor components are given by [25] as $\sigma_{rr} = -p + 2\mu \frac{\partial u}{\partial r}$ and $\sigma_{r\theta} = \mu \left( \frac{\partial v}{\partial r} - \frac{v}{r} + \frac{1}{r} \frac{\partial u}{\partial \theta} \right)$. Using the calculations from the preceding sections, the representations of $u, v,$ and $p$ are

$$p = \mu k A K_1(\zeta_1) \cos \theta \cos s,$$

$$u = \left\{ \frac{1}{2} BK_2(\chi \zeta) + \frac{1}{2} CK_0(\chi \zeta) + \frac{A}{2\beta^2} \left[ K_2(\zeta) + K_0(\zeta) \right] \right\} \cos \theta \cos s,$$

$$v = \left\{ \frac{1}{2} BK_2(\chi \zeta) - \frac{1}{2} CK_0(\chi \zeta) + \frac{A}{2\beta^2} K_1(\zeta) \right\} \sin \theta \cos s,$$

where $A, B,$ and $C$ are from (2.27)–(2.29). The derivatives of $u$ and $v$ are

$$\frac{\partial u}{\partial r} = \left\{ - \left[ \frac{A}{\beta^2 \zeta} K_2(\zeta) + \frac{B}{\zeta} K_2(\chi \zeta) \right] - \left[ \frac{A}{\beta^2} K_1(\zeta) + \frac{1}{2} \chi K_1(\chi \zeta)(B + C) \right] \right\} \cos \theta \cos s,$$

$$\frac{\partial u}{\partial \theta} = u_1 \sin \theta \cos s,$$
\[ \frac{\partial v}{\partial r} = \frac{\partial v_1}{\partial r} \sin \theta \cos s. \]

The calculation of \(\sigma_{rr}\) at the boundary \(\zeta = \zeta_1\) becomes

\[
(\sigma_{rr})_{\zeta=\zeta_1} = -\mu k A K_1(\zeta_1) \cos \theta \cos s \\
- 2\mu \left\{ \left[ \frac{A}{\beta^2} K_2(\zeta_1) + \frac{B}{\zeta_1} K_2(\chi \zeta_1) \right] + \left[ \frac{A}{\beta^2} K_1(\zeta_1) + \frac{1}{2} \chi K_1(\chi \zeta_1)(B + C) \right] \right\} \cos \theta \cos s.
\]

Using the relations in (2.24) and (2.26), the expressions in the curly brackets vanish and we are left with

\[
(\sigma_{rr})_{\zeta=\zeta_1} = -\mu k A K_1(\zeta_1) \cos \theta \cos s. \quad (2.41)
\]

Similarly, recalling that \(\zeta = kr\), the calculation for \(\sigma_{r\theta}\) is

\[
\sigma_{r\theta} = \mu k \left[ \frac{\partial v_1}{\partial \zeta} - \frac{v_1}{\zeta} - \frac{u_1}{\zeta} \right] \sin \theta \cos s.
\]

If we estimate \(\sigma_{r\theta}\) at the boundary \(\zeta = \zeta_1\) and use Eq. (2.24), we have

\[
(\sigma_{r\theta})_{\zeta=\zeta_1} = \mu \left( \frac{\partial v_1}{\partial \zeta} \right)_{\zeta=\zeta_1} \sin \theta \cos s. \quad (2.42)
\]

The stress tensor used to calculate the work done to maintain planar swimming becomes

\[
(\sigma_{rr})_{\zeta=\zeta_1} = \mu k [-AK_1(\zeta_1)] \cos \theta \cos s, \\
(\sigma_{r\theta})_{\zeta=\zeta_1} = \mu k \left( \frac{\partial v_1}{\partial \zeta} \right)_{\zeta=\zeta_1} \sin \theta \cos s,
\]

where \(r = \zeta/k\). Since we consider a fluid with a low volume fraction of stationary and randomly oriented fibers, the total stress applied to the filament is assumed to be entirely due to the fluid and not influenced by the fibers. This assumption is valid since the distance between the fibers is large compared to the radius of the filament. There is further discussion of this in Section 2.4.
The rate of work done to maintain planar bending is calculated as follows:

\[
dW = -\mathbf{F} \cdot \mathbf{u} = \mu b k^2 U \left[ A K_1(\zeta_1) \cos^2 \theta + \left( \frac{\partial v_1}{\partial \zeta} \right)_{\zeta=\zeta_1} \sin^2 \theta \right] \cos^2 s. \tag{2.43}
\]

Using Eq. (2.17), the derivative of \( v_1 \) is:

\[
\frac{\partial v_1}{\partial \zeta} = \frac{1}{2} (-B + C) \chi K_1(\chi \zeta) - \frac{1}{\zeta} \left[ \frac{A}{\beta^2} K_2(\zeta) + B K_2(\chi \zeta) \right], \tag{2.44}
\]

where \( \frac{A}{\beta^2}, B, C \) are from Eqs. (2.27)-(2.29). The mean value of the rate of work to maintain the filament motion is denoted by \( \overline{dW} \) and is given as

\[
\overline{dW} = \frac{1}{4} \mu b k^2 U \left\{ \frac{2b k U}{\zeta_1 \Phi(\zeta_1)} \left[ -\frac{\beta^2}{K_0(\chi \zeta_1)} - \frac{\chi^2}{2 K_0(\chi \zeta_1)} + \frac{1}{2} \Phi(\zeta_1) + \frac{1}{2} K_0(\zeta_1) \right] \right\}.
\]

For a cylinder immersed in a Brinkman fluid, the mean value of the total rate of work per unit length (\( \lambda \)) along the surface of the cylinder (\( r = a \)) is then calculated as

\[
\overline{W} = \frac{\mu \pi b^2 k^2 U^2}{K_0(\zeta_1) + \frac{1}{2} \left( \frac{k^2}{\alpha^2} - 1 \right) \log \left( 1 + \frac{\alpha^2}{k^2} \right)}, \tag{2.45}
\]

where \( \Phi(\zeta_1) = 2 - \chi^2 - \frac{K_0(\zeta_1)}{K_0(\chi \zeta_1)} \) when \( \zeta_1 \) is small, and \( \chi = \sqrt{1 + \beta^2} \). When the permeability approaches infinity, the Brinkman fluid behaves like Stokes flow. Thus, when \( \gamma \to \infty \) (or \( \alpha \to 0 \)) and using Eq. (2.38), we have

\[
\overline{W} = \frac{\mu \pi b^2 k^2 U^2}{K_0(\zeta_1) + 1/2}.
\]

This is exactly the same energy contribution to maintain the flagellum in motion in Stokes flow [34]. The nondimensional rate of work is shown in Fig. 2.5 for several different permeabilities \( \gamma \) and we observe that as \( \gamma \) gets large, it approaches the work done in a Stokesian fluid. In this analysis, as the permeability decreases, we observe that there are small changes in the swimming speed (shown in Fig. 2.4(a)), but the work done increases greatly (shown in Fig. 2.5). The mathematical analysis for this observation is detailed in
the next section. The physical meaning of this phenomenon can be explained as follows.

For a small permeability, there is a large added resistance present in the fluid, preventing
the swimmer from propelling itself forward. Therefore, it requires more work to move
with the same prescribed kinematics. We note that the rate of work of the swimming
sheet has been previously calculated and is also an increasing function of resistance $\alpha$ [31].

Figure 2.5: The nondimensional rate of mean work done to maintain planar bending along
the infinite-length cylinder, calculated from Eq. (2.45) for several permeabilities $\gamma$ where
$\lambda = 24$ and $a = 0.05$. The Stokes case is also plotted for comparison.

2.1.7 Analysis of the Asymptotic Functions

We look more closely at the behavior of the velocity in Eq. (2.37) and the work done in
Eq. (2.45). Rewriting in terms of the scaled resistance $\beta = \alpha/k$,

$$f(\beta) = \frac{U\infty}{(1/2)b^2k^2U} = \frac{K_0(\zeta_1) - \frac{1}{2} \left( \frac{1}{\beta^2} + 1 \right) \log (1 + \beta^2)}{K_0(\zeta_1) + \frac{1}{2} \left( \frac{1}{\beta^2} - 1 \right) \log (1 + \beta^2)}, \quad (2.46)$$

$$g(\beta) = \frac{\bar{W}}{\mu \pi b^2 k^2 U^2} = \frac{1}{K_0(\zeta_1) + \frac{1}{2} \left( \frac{1}{\beta^2} - 1 \right) \log (1 + \beta^2)}. \quad (2.47)$$

The two functions are plotted in Fig. 2.6. Using the condition in (2.65), $f(\beta)$ and $g(\beta)$
are positive functions and $f(\beta)$ is bounded by 1. The first derivatives of $f(\beta)$ and $g(\beta)$
with respect to $\beta$ are

$$f'(\beta) = \frac{2\beta^2 \left\{ K_0(\zeta_1) \left[ -1 + \log(1 + \beta^2) + \frac{1}{\beta^2} \log(1 + \beta^2) \right] - \frac{1}{2} \left( 1 + \frac{1}{\beta^2} \right) \log^2(1 + \beta^2) \right\}}{(1 + \beta^2) \left[ K_0(\zeta_1) + \frac{1}{2} \left( \frac{1}{\beta^2} - 1 \right) \log(1 + \beta^2) \right]^2},$$

(2.48)

$$g'(\beta) = \frac{(1 + \beta^2) \log(1 + \beta^2) + \beta^4(1 + \beta^2)}{(1 + \beta^2) \left[ K_0(\zeta_1) + \frac{1}{2} \left( \frac{1}{\beta^2} - 1 \right) \log(1 + \beta^2) \right]^2}. \quad (2.49)$$

We observe that all terms in the denominator and the numerator of $g'(\beta)$ are always positive for all $\beta$ which implies $g(\beta)$ is an increasing function. On the other hand, the function inside the curly bracket of $f'(\beta)$ is positive when

$$K_0(\zeta_1) > \frac{(1 + 1/\beta^2) \log^2(1 + \beta^2)}{2[-1 + \log(1 + \beta^2) + (1/\beta^2) \log(1 + \beta^2)]}. \quad (2.50)$$

In other words, $f(\beta)$ is an increasing function when it satisfies the condition in (2.50). We note that the expression $-1 + \log(1 + \beta^2) + (1/\beta^2) \log(1 + \beta^2)$ is always positive. The

![Figure 2.6](image)

**Figure 2.6:** The plot of the functions $f$ in Eq. (2.46) and $g$ in Eq. (2.47).

Taylor expansions of $f(\beta)$ and $g(\beta)$ about $\beta \ll 1$ are as follows:

$$f(\beta) \approx \frac{K_0(\zeta_1) - 1/2}{K_0(\zeta_1) + 1/2} + O(\beta^2), \quad g(\beta) \approx \frac{1}{K_0(\zeta_1) + 1/2} + O(\beta^2). \quad (2.51)$$
This shows that when $\beta$ is small, $f(\beta) > g(\beta)$ as in Fig. 2.6. When $\beta$ is large, we can expand the two functions in terms of the Puiseux series [51] as:

\[
f(\beta) \approx 1 + \frac{2\log(1/\beta)}{\beta^2 [K_0(\zeta_1) + \log(1/\beta)]} + O\left(\frac{1}{\beta^4}\right), \tag{2.52}
\]

\[
g(\beta) \approx \frac{1}{K_0(\zeta_1) + \log(1/\beta)} + O\left(\frac{1}{\beta^2}\right). \tag{2.53}
\]

Clearly, $f(\beta)$ is bounded by 1 when $\beta$ is large while $g(\beta)$ is unbounded. The two formulations above give insight as to why a decrease in permeability $\gamma$ causes a small increase in swimming speed and a large increase on the rate of work done.

### 2.2 Cylinder with Spiral Bending

#### 2.2.1 Asymptotic Swimming Speeds

Next, we consider an infinite-length cylinder propagating spiral waves, motivated by experiments where sperm flagella are able to exhibit helical bending [3]. Thus, it is compelling to consider the rotational movements of a cylinder propagating spiral bending waves (helical bending waves with constant radius). One can verify from Fig. 2.7 that

\[
a^2 = r^2 + b^2 - 2br \cos(\theta - s),
\]

\[
= [r - b \cos(\theta - s)]^2 + b^2 \sin^2(\theta - s),
\]

or equivalently,

\[
r = b \cos(\theta - s) + \sqrt{a^2 - b^2 \sin^2(\theta - s)}.
\]

Similar to the planar case, to the first order of $b/a$,

\[
r = a + b \cos(\theta - s), \tag{2.54}
\]

where $s = k(z + Ut)$. Eq. (2.54) corresponds to a cylinder that achieves the form of a right-handed helix about its axis with angular velocity $kU$ in the direction of increasing
The formulation for the cylinder is

\[ x = b \cos s, \quad y = b \sin s, \quad z = bs, \]

and the velocity components become

\[ u_x = -bkU \sin s, \quad u_y = bkU \cos s, \quad u_z = 0. \]

Converting the above equations to cylindrical coordinates, we have

\[ u = bkU \sin(\theta - s), \quad v = bkU \cos(\theta - s), \quad w = 0. \] (2.55)

Figure 2.7: Model geometry for a cylinder propagating spiral bending waves. The circle is the cross section of the deformed cylinder (current configuration) which is centered at \( O' \). The undeformed cylinder is centered at \( O \).

The motion of the helix includes the contributions of two orthogonal planar motions that are perpendicular to the \( z \)-axis, namely the \( xz \)-plane and \( yz \)-plane. The analysis for each plane proceeds in a similar fashion to that of the planar case, satisfying the boundary conditions in Eq. (2.55). As previous analysis has shown, the second-order solution can only be determined through first-order expansions (see [35, 34]). The second-order velocity components at the boundary are

\[ u_{22} = -\frac{1}{2} bk(u'_{1})_{\zeta = \zeta_1}, \quad v_{22} = -\frac{1}{2} bk(v'_{1})_{\zeta = \zeta_1}, \quad w_{22} = -\frac{1}{2} bk(w'_{1})_{\zeta = \zeta_1}. \] (2.56)
Let $V_s$ be the propulsion velocity of the helix in the opposite direction of the propagating spiral bending waves. With this, similar to \[34\], we have

$$V_s = \frac{1}{2} b k \omega_1'(\zeta = \zeta_1),$$

where $\omega_1'$ is the same as in Eq. (2.34). By a simple calculation, we observe

$$\frac{V_s}{U} = b^2 k^2 \cdot \frac{K_0(\zeta_1) - \chi^2 K_0(\chi \zeta_1)}{(2 - \chi^2) K_0(\chi \zeta_1) - K_0(\zeta_1)}. \tag{2.57}$$

Similar to the results obtained in the planar case, when $\alpha \to 0$, we recover the speed $V_s$ in the incompressible Stokes equations,

$$\frac{V_s}{U} = b^2 k^2 \cdot \frac{K_0(\zeta_1) - 1/2}{K_0(\zeta_1) + 1/2}.$$

Thus, the swimming speed of a spiral bending wave is double that of a planar bending wave with the same kinematics. We note that modified resistive force theory calculations have also been used to determine expressions for the swimming speed of a spiral bending wave in a Brinkman fluid \[31\].

### 2.2.2 Torque Exerted on the Cylinder

In addition to determining the asymptotic swimming speed from spiral bending, we can find the expression for the torque exerted on the cylinder by the surrounding fluid. Since the fluid in this case flows in a circular motion, the radial and axial velocity components are zero and only tangential velocity plays a role in this calculation. That is,

$$u = 0, \quad v = \frac{\Omega}{r} = \frac{\Omega k}{\zeta}, \quad w = 0,$$

where $\Omega$ is the angular velocity of the helix. With this, we simplify the expression for mean torque per unit length applied on the filament by the fluid, $T_\infty = 2\pi r^2 \sigma_{r\theta}$, to

$$T_\infty = -4\pi \mu \Omega. \tag{2.58}$$
To solve for $\Omega$, we use the boundary condition for $v_{22}$ in Eq. (2.56) to obtain

$$\frac{\Omega k}{\zeta_1} = -\frac{1}{2} b k (v'_1)_{\zeta=\zeta_1}. \quad (2.59)$$

Substituting Eq. (2.59) into Eq. (2.58) and using Eq. (2.44) for $v'_1$ and Eqs. (2.27)-(2.29) to simplify, we have

$$T_\infty = \frac{4\pi \mu b^2 k U}{K_0(\zeta_1) + \frac{1}{2} \left( \frac{k^2}{\alpha^2} - 1 \right) \log \left( 1 + \frac{\alpha^2}{k^2} \right)}. \quad (2.60)$$

In the limit as $\alpha \to 0$, the torque exerted on the cylinder reduces to

$$T_\infty = \frac{4\pi \mu b^2 k U}{K_0(\zeta_1) + 1/2},$$

which is the same torque calculated for the Stokes regime by Drummond [55]. Note that this derivation differs from the work of Taylor [34] (where $w'_1$ was used instead of $v'_1$).

### 2.2.3 Asymptotic Solutions versus Resistive Force Theory Results

Next, we compare our spiral asymptotic swimming velocity with Leshansky’s propulsion speed for a rotating helical filament in a Brinkman fluid derived using a modified resistive force theory (RFT). RFT is a local drag model that describes swimming of a slender and finite-length flagellum with small amplitude immersed in a viscous fluid [1, 56]. The local velocity, $u$, relative to the fluid is decomposed into tangential ($u_\|)$ and normal ($u_\perp$) components. This leads to drag force components per unit length as $f_\| = -\xi_\| u_\|$ and $f_\perp = -\xi_\perp u_\perp$, where $\xi_\|$ and $\xi_\perp$ are the corresponding drag coefficients [1, 56]. The self-propulsion of the slender flagellum is possible when $\xi_\| \neq \xi_\perp$. The difference between the drag coefficients allows the drag force and local velocity to be in different directions, inducing net propulsion [1, 57].

Leshansky [31] developed a modified RFT to calculate the propulsion velocity for a
rigid rotating helix. The configuration of the helix is

\[ \mathbf{r}(s, t) = \{ b \cos(ks + \omega t), b \sin(ks + \omega t), ds + Ut \}, \]

for \( kb = \sin \theta \) and \( d = \cos \theta \) where \( \theta \) is the pitch angle of the helix. The propulsion speed \( U \) was previously determined to be \[31\]

\[ \frac{U}{b \omega} = \frac{(\xi - 1) \sin 2\theta}{2[1 + (\xi - 1) \sin^2 \theta]}, \quad (2.61) \]

where \( \xi \) is defined as the drag coefficient and is given as

\[ \xi = 2 + \frac{\alpha a K_0(\alpha a)}{2 K_1(\alpha a)}. \]

In a purely viscous fluid, \( \xi = 2 \) \[31, 1\]. We recall that \( \alpha = 1/\sqrt{\gamma} \), and \( 2a \) is the thickness of the filament. We want to rewrite the propulsion velocity in Eq. (2.61) in terms of the wavenumber \( k \), the amplitude \( b \), \( \alpha \), and \( a \) only. That is,

\[ \frac{U}{b \omega} = \frac{(\xi - 1) \sin 2\theta}{2[1 + (\xi - 1) \sin^2 \theta]} = \frac{kb}{1 + \frac{\alpha a K_0(\alpha a)}{2 K_1(\alpha a)}} \frac{\sqrt{1 - (kb)^2}}{1 + \frac{\alpha a K_0(\alpha a)}{2 K_1(\alpha a)}}. \quad (2.62) \]

Eq. (2.62) is compared with the asymptotic swimming velocity of the spiral bending wave. Recall that \( \zeta_1 = ka \) or \( \zeta_1 = \frac{ka}{\alpha a} \). Then we can rewrite Eq. (2.57) in terms of \( b, k, \alpha \) and \( a \) as

\[ \frac{V_s}{b \omega} = \frac{K_0(\alpha a) - \frac{1}{2} \left( \frac{(ka)^2}{(\alpha a)^2} + 1 \right) \log \left[ 1 + \frac{(\alpha a)^2}{(ka)^2} \right] - \log \frac{ka}{\alpha a}}{K_0(\alpha a) + \frac{1}{2} \left( \frac{(ka)^2}{(\alpha a)^2} - 1 \right) \log \left[ 1 + \frac{(\alpha a)^2}{(ka)^2} \right] - \log \frac{ka}{\alpha a}}. \quad (2.63) \]

We note the solution from RFT is for a rigid rotating helix which is different from our model of a spiral bending filament. Another difference between the two approaches is that RFT works for a finite-length swimmer while our model is valid only for an infinite-length cylinder. The ratio between the spiral bending swimming speed with the propulsion
velocity obtained using RFT is plotted in Fig. 2.8. We observe that our results compare well with the RFT calculations for small resistance and are less than that predicted by RFT for moderate to larger values of resistance.

2.3 Range of Parameters That Lead To Swimming Speed Enhancement

To identify the range of parameter values that lead to enhancement in swimming speeds of the infinite-length cylinder with planar waves, we rearrange Eq. (2.37) as follows:

\[
\frac{U_{\infty}}{U} = \frac{1}{2} b^2 k^2 \frac{K_0(\zeta_1) - \frac{1}{2}}{K_0(\zeta_1) + \frac{1}{2}} \left\{ 1 + \frac{K_0(\zeta_1) - \frac{1}{2}}{K_0(\zeta_1) - \frac{1}{2}} \frac{K_0(\zeta_1) k^2}{\alpha^2} \log \left( \frac{1 + \alpha^2}{k^2} \right) \right\}.
\]

Note that Eq. (2.64) illustrates the velocity behavior in the spiral bending wave case when the constant 1/2 is removed. For any fixed permeability, the swimming speed is enhanced relative to the Stokes case when the following inequalities hold:

\[
K_0(\zeta_1) > \frac{\frac{1}{2} \alpha^2}{k^2} \log \left( \frac{1 + \alpha^2}{k^2} \right),
\]

\[
\frac{\alpha^2}{k^2} - \log \left( \frac{1 + \alpha^2}{k^2} \right).
\]

Figure 2.8: The ratio between the asymptotic swimming speed of a spiral bending wave and the speed obtained by Leshansky [31] using RFT for a rigid rotation of a helix.
\[ \zeta_1 = ka < \frac{2}{e^{\gamma_e}} \exp \left\{ -\frac{1}{2} \frac{\alpha^2}{k^2} \log \left( 1 + \frac{\alpha^2}{k^2} \right) \right\} = h\left(\frac{\alpha}{k}\right). \]  

(2.66)

Figure 2.9: The plot of the right hand side of Eq. (2.66) as a function of \( \alpha/k \).

In Fig. 2.9 we plot the right hand side of Eq. (2.66), \( h(\alpha/k) \), to show that it is, in fact, decreasing in a manner that is dependent on the scaled resistance. This means that if the permeability is reduced, then \( ka \) must also be reduced to observe swimming enhancement in a Brinkman fluid. Hence, the cylinder radius and/or wavenumber must decrease in order to observe an increase in swimming speed. This finding makes sense since the mesh size decreases as the permeability decreases, thus there is less room for the swimmer to move. We note that in addition to an enhancement in swimming speed, an increase in torque and rate of work is also observed when Eq. (2.66) is satisfied.

2.4 Biological Application and Swimming Enhancement

As mentioned in Chapter 1, the model assumes that the proteins and fibers are arranged randomly in the fluid. The distance between the fibers, the radius of the fibers and the permeability are related through the equations given in Eq. (1.5) and Eq. (1.6). We note that in the case where this ratio of \( D/a_f \) is large, there are little or no interactions
between a stationary network of fibers and the swimmers. Thus, it is assumed that the fibers do not impart any additional stress onto the filament.

In Table 2.1 we report a few parameter ranges in which we see enhancement of swimming speed. In particular, we report ranges of the cylinder radius $a$, with a fixed wavelength of $\lambda = 25 \, \mu m$. To find these ranges, we use fiber volume fractions and radii from the literature [32], together with our own computed values of permeability from Eq. (1.5) and average separation from Eq. (1.6).

<table>
<thead>
<tr>
<th>Media</th>
<th>$\varphi$</th>
<th>$a_f$ (nm)</th>
<th>$D$ (nm)</th>
<th>$\gamma$ ($\mu m^2$)</th>
<th>Eq. (2.66)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Collagen gels, [32]</td>
<td>0.00074</td>
<td>75</td>
<td>8314</td>
<td>8.6</td>
<td>$a &lt; 1.337 , (\mu m)$</td>
</tr>
<tr>
<td>Cervical mucus, [32]</td>
<td>0.015</td>
<td>15</td>
<td>346</td>
<td>0.0085</td>
<td>$a &lt; 0.102 , (\mu m)$</td>
</tr>
</tbody>
</table>

Table 2.1: The calculated permeability $\gamma$ using the given volume fractions $\varphi$ and fiber radii $a_f$. The range of cylinder thickness $a$ where an enhancement in swimming speed is observed for $\lambda = 25 \, \mu m$ is reported.

The radii of the principal piece of human, bull, and ram sperm are 0.5 $\mu m$, 0.29 $\mu m$ and 0.15 $\mu m$, respectively [58, 59, 60]. We note that that flagellar radius decreases along the length of the flagellum from the principal piece (closer to cell body) to the endpiece. Thus, swimmers experience enhancement when placed in a collagen gel. However, there is no enhancement for the three swimmers when they are put in cervical mucus at a volume fraction of $\varphi = 0.015$. Further, it is well known that the composition of the cervical and vaginal fluid varies greatly through the menstrual or oestrous cycle [61, 6], and this experimental value of $\varphi = 0.015$ is taken at one time point in the cycle [32]. For instance, around the time of ovulation, the interfiber spacing $D$ may reach up to 25 $\mu m$ [6]. Using this interfiber spacing and a given fiber radius $a_f = 15$ nm, we can further estimate the volume fraction $\varphi = 0.00033$ from Eq. (1.6) and the permeability $\gamma = 0.868 \, \mu m^2$ from Eq. (1.5). Then, the cylinder radii for which enhancement is seen is $a < 0.765 \, \mu m$ when the wavelength $\lambda$ is 25 $\mu m$. At this volume fraction, all three spermatozoa species experience an enhancement in swimming speed in cervical fluid.
Chapter 3

The Method of Regularized Brinkmanlets

In this chapter, we study a Lagrangian numerical algorithm to solve for the 3D Brinkman flow when a swimmer is immersed in the fluid. The method is used to validate the asymptotic solutions from the preceding Chapter and to understand the swimming speed or emergent waveform of a swimmer numerically. We want to focus on rederiving solutions for the velocity of an infinite fluid in the 3D case. We first introduce the background of the numerical method and present some of the known derivations in the literature. We then extend this method for the case of a Kirchhoff Rod in Chapter 4.

3.1 Background

Suppose there is an elastic structure immersed in a Brinkman fluid. The Brinkman equation should include an external force term $f = f_0 \delta(x - x_0)$ for a point force $f_0$ at $x_0$ to account for the disturbance of the structure to the motion of the fluid. Then, the incompressible Brinkman equation becomes

\[
\nabla p = \mu \Delta u - \frac{\mu}{\gamma} u + f_0 \delta(x - x_0), \quad \nabla \cdot u = 0, \quad (3.1)
\]
where \( \mathbf{x} \) is any point in the fluid, \( \mathbf{x}_0 \) is the point where the force is applied, and \( \delta(\cdot) \) is the delta distribution. Recall that the unit of the pressure gradient is force per volume; thus, \( \mathbf{f} \) should have a unit of force per volume as well. The fundamental solutions to Eq. (3.1) in 3D are called the Brinkmanlets which are written as [45]:

\[
\mu \mathbf{u} = \mathbf{f}_0 \cdot \nabla \nabla B(\mathbf{x} - \mathbf{x}_0) - \mathbf{f}_0 \Delta B(\mathbf{x} - \mathbf{x}_0),
\]

(3.2)

and the corresponding pressure is

\[
p = \mathbf{f}_0 \cdot \nabla G(\mathbf{x} - \mathbf{x}_0),
\]

(3.3)

where \( G(r) \) is the Green’s function and \( B(r) \) is related to \( G(r) \) by the non-homogeneous Helmholtz differential equation \((\Delta - \alpha^2)B(r) = G(r)\) for \( r = \|\mathbf{x} - \mathbf{x}_0\| \) and \( \alpha^2 = 1/\gamma \).

The solutions of \( G(r) \) and \( B(r) \) are well known [62, 45]:

\[
G(r) = -\frac{1}{4\pi r}, \quad B(r) = \frac{1 - e^{-\alpha r}}{4\pi \alpha^2 r}.
\]

(3.4)

Thus, the Brinkmanlets velocity in (3.2) becomes

\[
\mu \mathbf{u} = \mathbf{f}_0 H_1(r) + (\mathbf{f}_0 \cdot (\mathbf{x} - \mathbf{x}_0))(\mathbf{x} - \mathbf{x}_0)H_2(r),
\]

(3.5)

where \( H_1(r) \) and \( H_2(r) \) are functions of \( G(r), B(r), \) and their derivatives

\[
H_1(r) = -\frac{1}{4\pi \alpha^2 r^3} + \frac{e^{-\alpha r}}{4\pi r} \left( \frac{1}{\alpha^2 r^2} + \frac{1}{\alpha r} + 1 \right),
\]

(3.6)

\[
H_2(r) = \frac{3}{4\pi \alpha^2 r^5} - \frac{e^{-\alpha r}}{4\pi r^3} \left( \frac{3}{\alpha^3 r^3} + \frac{3}{\alpha r} + 1 \right).
\]

(3.7)

However, Eq. (3.4), (3.6), and (3.7) present singularities where the force is applied. To eliminate these singular solutions we apply the technique called the Method of Regularized Brinkmanlets (MRB) developed by Cortez et al. [45]. The MRB is an extension of the Method of Regularized Stokeslets also developed by Cortez [47, 48] for use with the Stokes equations. The general idea is to compute regularized fundamental solutions
by replacing singular point forces with a smooth approximation. With this, the resulting equations can be solved exactly to obtain non-singular fundamental solutions. The smooth approximations to a delta distribution, often called ‘blob’ functions, $\phi_\varepsilon(r)$, are characterized by a small parameter $\varepsilon$ that controls their width.

We note the similarities of a blob function to a mollifier used in distribution theory \[63\]. For simplicity, we define a mollifier in $\mathbb{R}^3$. By definition, a radially symmetric smooth function $\phi(x) \in \mathbb{R}^3$ is called a mollifier if $\phi$ satisfies the following conditions \[63\]. One, $\phi$ is compactly supported. Two, $\phi$ satisfies $\int_{\mathbb{R}^3} \phi(x) dx = 1$. Three, for $\varepsilon > 0$, a regularization function (also a mollifier) $\phi_\varepsilon(x)$ of $\phi(x)$ is scaled by volume as $\phi_\varepsilon(x) = \frac{1}{\varepsilon^3} \phi\left(\frac{x}{\varepsilon}\right)$ and $\lim_{\varepsilon \to 0} \phi_\varepsilon(x) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^3} \phi\left(\frac{x}{\varepsilon}\right) = \delta(x)$, where $\delta(x)$ is the Dirac delta function. The function $\phi$ is a non-negative mollifier if $\phi(x) \geq 0$. For any $\varepsilon > 0$, a smooth function $g_\varepsilon(x)$ can be calculated in terms of the convolution as \[63\]

$$
g_\varepsilon(x) := (g \star \phi_\varepsilon)(x) = \int_{\mathbb{R}^3} \phi_\varepsilon(x-y) g(y) dy = \int_{\mathbb{R}^3} \phi_\varepsilon(y) g(x-y) dy,$$

where $x, y \in \mathbb{R}^3$ and ‘$\star$’ denotes the convolution of two functions. The convolution can be estimated by approximating the integral using the trapezoidal rule. The convolution of a force against a blob function can be done in the same way \[64\]. We note that a mollifier requires compact support while a blob function can have infinite support or compact support. An infinite support blob function allows for easier numerical evaluation since a single formula can be used. A compactly supported blob would result in a fluid calculation that differs inside and outside of the compactly supported region \[65, 66\].

We also assume that the blob is a radially symmetric function that satisfies the condition $4\pi \int_0^\infty r^2 \phi_\varepsilon(r) dr = 1$ in 3D. One example of such a function is given in \[47\] as

$$
\phi_\varepsilon(r) = \frac{15\varepsilon^4}{8\pi(r^2 + \varepsilon^2)^{7/2}}.
$$

(3.8)

This blob function is widely used in the literature \[47, 48, 50\]. The function $\phi_\varepsilon(r)$ is plotted in Fig. \[3.1\] with three different values of the regularization parameter $\varepsilon = 1, 3/2$ and $\varepsilon = 2$. We note that for illustration in Fig. \[3.1\] we set the regularization parameter.
to be $\varepsilon \geq 1$. In our simulations, $\varepsilon$ is chosen in the interval between 0 and 1. As $\varepsilon$ decreases, the base of the blob function gets narrower. When $\varepsilon \to 0$, the blob function approaches the Dirac delta function. The singular solutions can also be recovered by letting $\varepsilon \to 0$. The force is now written as $f = f_0 \phi_\varepsilon(r)$. Then the regularized Brinkman equation becomes

$$\nabla p = \mu \Delta u - \frac{\mu}{\gamma} u + f_0 \phi_\varepsilon(r).$$

(3.9)

To define units of $f_0 \phi_\varepsilon(r)$, we consider the blob function in Eq. (3.8). We see that $r$ has a unit of length, as does the regularization parameter $\varepsilon$. Then, $\phi_\varepsilon(r)$ has a unit of inverse length cubed or inverse volume. Thus, $f_0 \phi_\varepsilon(r)$ carries a unit of force per volume.

Next, the regularized fundamental solutions can be derived by first taking the divergence of Eq. (3.9) and applying the incompressibility condition. Next, utilizing some vector calculus identities in Appendix A.1 we arrive at the regularized pressure and regularized velocity as

$$p = f_0 \cdot \nabla G_\varepsilon,$$

(3.10)

$$\mu u = (f \cdot \nabla) \nabla B_\varepsilon(x - x_0) - f_0 G_\varepsilon(x - x_0).$$

(3.11)

Figure 3.1: Plot of the blob function $\phi_\varepsilon(r)$ from Eq. (3.8) for different $\varepsilon$ values.
In this case, $G_\varepsilon(r)$ and $B_\varepsilon(r)$ relate to the blob function $\phi_\varepsilon(r)$ as follows

\[ G_\varepsilon(r) = \phi_\varepsilon(r), \quad (\Delta - \alpha^2)B_\varepsilon(r) = G_\varepsilon(r). \]  

(3.12)

Since we require that $\phi_\varepsilon(r)$ is radially symmetric, we can also assume $G_\varepsilon(r)$ and $B_\varepsilon(r)$ are as well. Then, Eq. (3.11) can be written as \[ \mu \mathbf{u}(\mathbf{x}) = f_0 H_1^\varepsilon(r) + (f_0 \cdot (\mathbf{x} - \mathbf{x}_0))(\mathbf{x} - \mathbf{x}_0) H_2^\varepsilon(r), \]  

(3.13)

where $H_1^\varepsilon(r)$ and $H_2^\varepsilon(r)$ are functions of $G_\varepsilon(r)$, $B_\varepsilon(r)$, and their derivatives. There are two ways to regularize the fundamental solutions. The first one is to rewrite the singular solutions of $H_1$ and $H_2$ in terms of the regularized solutions and derive the associated blob function, $\phi_\varepsilon(r)$. The second way is to choose a suitable blob function and calculate the corresponding $G_\varepsilon(r)$ and $B_\varepsilon(r)$ functions. We give the derivations for the 3D forms of $G_\varepsilon(r)$, $B_\varepsilon(r)$, and their associated derivatives.

### 3.2 Finding $G_\varepsilon(r)$, $B_\varepsilon(r)$ by Regularizing $G(r)$ and $B(r)$

The 3D regularized fundamental solutions for the Brinkman equation have been completed previously \[45\]. Here, we want to give a brief summary to the solutions given in \[45\]. These results are necessary since they are reconsidered in Chapter 4 for the derivation of the 3D Kirchhoff Rod model. To regularize the fundamental solution, the expression for $B(r)$ is rewritten as

\[ B_\varepsilon(r) = \frac{1 - \varepsilon R}{4\pi \alpha^2 R}, \]  

(3.14)

where $R^2 = r^2 + \varepsilon^2$ so that the singularity is removed. In 3D, $H_1^\varepsilon(r)$ and $H_2^\varepsilon(r)$ can be written in terms of derivatives of $B_\varepsilon(r)$ as

\[ H_1^\varepsilon(r) = -\frac{rB_\varepsilon''(r) + B_\varepsilon'(r)}{r}, \quad H_2^\varepsilon(r) = \frac{rB_\varepsilon''(r) - B_\varepsilon'(r)}{r^3}. \]
Taking the derivative of $B_\varepsilon(r)$ we have \[45\] (the details can be found in Appendix A.2)

\[
H_2^\varepsilon(r) = \frac{3}{4\pi\alpha^2 R^5} - e^{-\alpha R} \left( \frac{3}{\alpha^3 R^3} + \frac{3}{\alpha R} + 1 \right), \tag{3.15}
\]

\[
H_1^\varepsilon(r) = -\frac{1}{4\pi\alpha^2 R^3} + e^{-\alpha R} \left( \frac{1}{\alpha^2 R^2} + \frac{1}{\alpha R} + 1 \right) + \varepsilon^2 H_2^\varepsilon(r). \tag{3.16}
\]

The corresponding $G_\varepsilon(r)$ and $\phi_\varepsilon(r)$ are also given in \[45\]

\[
G_\varepsilon(r) = -\frac{1}{4\pi R} - \varepsilon^2 \Delta H_2^\varepsilon(r), \tag{3.17}
\]

\[
\psi_\varepsilon(r) = \frac{3\varepsilon^2}{4\pi R^5} - \varepsilon^2 \Delta H_2^\varepsilon(r). \tag{3.18}
\]

The blob in Eq. (3.18) depends on the choice of $\alpha$ through $H_2^\varepsilon(r)$. The limits of the blob function when $\alpha \to 0$ and $\alpha \to \infty$ are \[45\]

\[
\lim_{\alpha \to 0} \psi_\varepsilon_1(r) = \frac{15\varepsilon_1^4}{8\pi(r^2 + \varepsilon_1^2)^{3/2}}, \quad \lim_{\alpha \to \infty} \psi_\varepsilon_1(r) = \frac{3\varepsilon_1^4}{4\pi(r^2 + \varepsilon_1^2)^{5/2}}. \tag{3.19}
\]

Unless stated differently, $\varepsilon_1$ denotes the regularization parameter of the blob function in Eq. (3.19). Also, we let $\psi_\varepsilon_1(r)$ be the notation of the blob function determined from the regularized fundamental solutions of $G_\varepsilon(r)$ and $B_\varepsilon(r)$ in Section 3.2. The notation $\phi_\varepsilon(r)$ is used for the blob function in Section 3.3.

### 3.3 Finding $G_\varepsilon(r), B_\varepsilon(r)$ by Selecting a Blob Function

The detailed procedure to determine $G_\varepsilon, B_\varepsilon$ from choosing a blob function has been previously completed \[45\]. Here, we want to give a detailed derivation of these functions since we utilize them in later chapters. The regularized Green’s function satisfies $[rG_\varepsilon(r)]'' = r\phi_\varepsilon(r)$. Integrating both sides twice we have

\[
[rG_\varepsilon(r)]' = \int_0^r t\phi_\varepsilon(t)dt, \]

\[
rG_\varepsilon(r) = \int_0^r \int_0^t x\phi_\varepsilon(x)dxdt.
\]
Let \( u = \int_0^t x \phi_\varepsilon(x)dx \) and \( dv = dt \), then \( du = x \phi_\varepsilon(x)dx \) and \( v = t \), we obtain

\[
\begin{align*}
 rG_\varepsilon(r) &= t \int_0^t x \phi_\varepsilon(x)dx \Bigg|_0^r - \int_0^r tx \phi_\varepsilon(x)dx.
\end{align*}
\]

Since \( t \) and \( x \) are dummy variables, we can replace \( x \) with \( t \). In addition, we impose an extra constant that is later determined. Then,

\[
\begin{align*}
 rG_\varepsilon(r) &= rG_\varepsilon(0) + r \int_0^r t \phi_\varepsilon(t)dt - \int_0^r t^2 \phi_\varepsilon(t)dt. \\
(3.20)
\end{align*}
\]

Since the total integral of the blob is \( 4\pi \int_0^\infty t^2 \phi_\varepsilon(t)dt = 1 \), we can enforce the condition on \( r \) such that \( rG_\varepsilon(r) \to \frac{1}{4\pi} \) as \( r \to \infty \) Thus, as \( r \to \infty \), we obtain

\[
\begin{align*}
 -\frac{1}{4\pi} = \lim_{r \to \infty} \left( rG_\varepsilon(0) + r \int_0^r t \phi_\varepsilon(t)dt \right) - \frac{1}{4\pi}, \\
0 = \lim_{r \to \infty} \left( rG_\varepsilon(0) + r \int_0^r t \phi_\varepsilon(t)dt \right).
\end{align*}
\]

We now can choose \( G_\varepsilon(0) \) such that \( G_\varepsilon(0) = -\int_0^\infty t \phi_\varepsilon(t)dt \). Dividing both sides of (3.20) by \( r \) and using \( G_\varepsilon(0) \), we have

\[
\begin{align*}
 G_\varepsilon(r) &= -\int_0^\infty t \phi_\varepsilon(t)dt + \int_0^r t \phi_\varepsilon(t)dt - \frac{1}{r} \int_0^r t^2 \phi_\varepsilon(t)dt, \\
 &= -\int_0^\infty t \phi_\varepsilon(t)dt + \int_0^r \left( 1 - \frac{t}{r} \right) t \phi_\varepsilon(t)dt, \\
 G_\varepsilon(r) &= -\int_0^\infty t \phi_\varepsilon(t)dt + \frac{1}{r} \int_0^r (r - t) t \phi_\varepsilon(t)dt. \\
(3.21)
\end{align*}
\]

From the last equation we can see that as \( r \to \infty \), we can obtain \( G_\varepsilon(r) \to -\frac{1}{4\pi r} \). In 3D, the relation between \( B_\varepsilon(r) \) and \( G_\varepsilon(r) \) can be expressed as

\[
[rB_\varepsilon(r)]'' - \alpha^2 [rB_\varepsilon(r)] = rG_\varepsilon(r). \\
(3.22)
\]

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We solve this second order non-homogeneous differential equation using the Laplace transform. Assume that \( Z = rB_\varepsilon(r) \), then equation (3.22) is written as

\[
Z'' - \alpha^2 Z = rG_\varepsilon(r). \tag{3.23}
\]

Recall that \( \mathcal{L}(Z'') = s^2\mathcal{L}(Z) - Z'(0) - sZ(0) \). Also, we need to know the Laplace transform of the right hand side of (3.23) that is \( \mathcal{L}[rG_\varepsilon(r)] \). From (3.21), if we let \( C_1 = \int_0^\infty t\phi_\varepsilon(t)dt \), we have

\[
rG_\varepsilon(r) = -rC_1 + \int_0^r (r - t) t\phi_\varepsilon(t)dt
\]

so that if we take Laplace transform of (3.21) we have

\[
\mathcal{L}[rG_\varepsilon(r)] = -C_1 \mathcal{L}\{r\} + \mathcal{L}\left\{ \int_0^r (r - t) t\phi_\varepsilon(t)dt \right\}.
\]

The second Laplace transform from the last equation is the convolution of two functions which can be broken down as follows,

\[
\mathcal{L}\left\{ \int_0^r (r - t) t\phi_\varepsilon(t)dt \right\} = \mathcal{L}\{(f * g)(r)\} = \mathcal{L}\{\mathcal{L}^{-1}(F(s)G(s))\} = F(s)G(s),
\]

for \( f(r) = r, g(r) = r\phi_\varepsilon(r) \) and \( F(s) = \mathcal{L}\{r\} = \frac{1}{s^2}, G(s) = \mathcal{L}\{r\phi_\varepsilon(r)\}(s) \). Then

\[
\mathcal{L}[rG_\varepsilon(r)] = -\frac{C_1}{s^2} + \frac{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)}{s^2}.
\]

Now, take Laplace transform of (3.23), and assume that \( Z(0) = 0 \) and \( Z'(0) = B_\varepsilon(0) \).

Since \( B_\varepsilon(r) \) is a smooth function, we obtain

\[
\mathcal{L}\{Z''\} - \alpha^2 \mathcal{L}\{Z\} = \mathcal{L}\{rG_\varepsilon(r)\},
\]

\[
s^2\mathcal{L}(Z) - Z'(0) - sZ(0) - \alpha^2 \mathcal{L}\{Z\} = -\frac{C_1}{s^2} + \frac{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)}{s^2},
\]

\[
(s^2 - \alpha^2) \tilde{Z} - B_\varepsilon(0) = -\frac{C_1}{s^2} + \frac{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)}{s^2}. \tag{3.24}
\]
Next, to solve for $\hat{Z}$ we first divide both sides of (3.24) by $(s^2 - \alpha^2)$ then take the inverse Laplace transform. That is,

$$\hat{Z} - \frac{B_z(0)}{s^2 - \alpha^2} = -\frac{C_1}{s^2 (s^2 - \alpha^2)} + \frac{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)}{s^2 (s^2 - \alpha^2)},$$

$$Z = \mathcal{L}^{-1}\left\{\frac{B_z(0)}{s^2 - \alpha^2}\right\} - \mathcal{L}^{-1}\left\{\frac{C_1}{s^2 (s^2 - \alpha^2)}\right\} + \mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)}{s^2 (s^2 - \alpha^2)}\right\}.$$

We can obtain the result for each inverse Laplace transform as follows,

$$\mathcal{L}^{-1}\left\{\frac{B_z(0)}{s^2 - \alpha^2}\right\} = \frac{B_z(0)}{\alpha} \sinh(\alpha r),$$

$$\mathcal{L}^{-1}\left\{\frac{C_1}{s^2 (s^2 - \alpha^2)}\right\} = \frac{C_1}{\alpha^3} \sinh(\alpha r) - \frac{C_1}{\alpha^2} r,$$

$$\mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)}{s^2 (s^2 - \alpha^2)}\right\} = -\mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)}{\alpha^2 s^2}\right\} + \mathcal{L}^{-1}\left\{\frac{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)}{\alpha^2 (s^2 - \alpha^2)}\right\},$$

$$= -\frac{1}{\alpha^2} \mathcal{L}^{-1}\left\{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)\mathcal{L}\{r\varepsilon\}\right\} + \frac{1}{\alpha^3} \mathcal{L}^{-1}\left\{\mathcal{L}\{r\phi_\varepsilon(r)\}(s)\mathcal{L}\{\sinh(\alpha r)\}\right\},$$

$$= \frac{1}{\alpha^3} \left\{\int_0^r \left[\sinh(\alpha(r - t)) - \alpha(r - t)\right] t\phi_\varepsilon(t) dt\right\}.$$
The final form of $B_\varepsilon(r)$ is

$$B_\varepsilon(r) = \frac{1}{\alpha^2} \int_0^\infty \left[ 1 - e^{-\alpha t} \sinh(\alpha r) \right] t \phi_\varepsilon(t) dt + \frac{1}{\alpha^3 r} \int_0^r \left[ \sinh(\alpha(r - t)) - \alpha(r - t) \right] t \phi_\varepsilon(t) dt. \quad (3.25)$$

The expressions for $G_\varepsilon(r)$ and $B_\varepsilon(r)$ depend on the choice of a blob function $\phi_\varepsilon(r)$. We consider a blob function of the form

$$\phi_\varepsilon(r) = (a_0 + a_1 r^2)e^{-r^2/\varepsilon^2}, \quad (3.26)$$

where $a_0$ and $a_1$ can be determined given that $\phi_\varepsilon(r)$ satisfies certain conditions previously derived [67]. The blob function needs to satisfy the property $4\pi \int_0^\infty r^2 \phi_\varepsilon(r) dr = 1$. This means that the total volume integrates to 1 and the smooth approximation decays sufficiently fast as $r \to \infty$ [45]. Together with the first property, the condition $\lim_{\varepsilon \to 0} \phi_\varepsilon(r) = 0$ guarantees the blob approaches the Dirac delta function as $\varepsilon \to 0$. We also impose the property $\frac{1}{\alpha} \int_0^\infty r \phi_\varepsilon(r) \sinh(\alpha r) dr = \frac{1}{4\pi}$ [67]. This property plays a similar role as the second-moment condition, $\int_0^\infty r^4 \phi_\varepsilon(r) dr = 0$, used in the method of regularized Stokeslets. Using these conditions, $a_0$ and $a_1$ are [67]

$$a_0 = \frac{1}{\alpha^2 \varepsilon^2 \pi^{3/2}} \left( \alpha^2 \varepsilon^2 + 6 - 6e^{-\alpha^2 \varepsilon^2/4} \right), \quad a_1 = -\frac{4}{\alpha^2 \varepsilon^7 \pi^{3/2}} \left( 1 - e^{-\alpha^2 \varepsilon^2/4} \right).$$

The limits of the blob function in Eq. (3.26) when $\alpha \to 0$ and $\alpha \to \infty$ are [67]

$$\lim_{\alpha \to 0} \phi_{\varepsilon_2}(r) = \frac{1}{\pi^{3/2} \varepsilon_2^3} \left( \frac{5}{2} - \frac{r^2}{\varepsilon_2^2} \right) e^{-r^2/\varepsilon_2^2}, \quad \lim_{\alpha \to \infty} \phi_{\varepsilon_2}(r) = \frac{1}{\pi^{3/2} \varepsilon_2^3} e^{-r^2/\varepsilon_2^2}. \quad (3.27)$$

Unless stated otherwise, we denote $\varepsilon_2$ to be the regularization parameter of the blob function (3.26) in Section. 3.3. We plot the blob function in Eq. (3.26) for five different $\alpha$’s ($\alpha = 0.1, 1/\sqrt{10}, 1, \sqrt{10}, 10$) and its limits in Eq. (3.27) ($\alpha \to 0$ and $\alpha \to \infty$). We see in Fig. 3.2 that the smaller $\alpha$ becomes, the narrower the base of the blob function gets.
Figure 3.2: The blob function in Eq. (3.26) is plotted for $\alpha$ ranging from 0.1 to 10 (in dashed lines). The limit functions of $\alpha \to 0$ and $\alpha \to \infty$ in Eq. (3.27) are also plotted (in solid lines) for comparison. The regularization parameter is chosen to be $\varepsilon_2 = 0.909$.

### 3.4 Comparing Blob Functions

We notice that as $r \to \infty$ the function in Eq. (3.18) decays in the range between $r^{-7}$ and $r^{-5}$ while the function in Eq. (3.26) decays exponentially with $e^{-r^2/\varepsilon_2^2}$ independent of the choice of $\alpha$. To compare the two functions fairly, we match their limits and obtain the relation $\varepsilon_2 = 0.909 \varepsilon_1$. This is the scale between the two blob functions so that they agree at $r = 0$. We plot the functions in Eq. (3.19) and Eq. (3.27) for the case when $\alpha \to 0$ with $\varepsilon_1 = 1$ and $\varepsilon_2 = 0.909$. Fig. 3.3 shows the agreement between the two functions at $r = 0$.

Figure 3.3: Blob functions in Eq. (3.19) and Eq. (3.27) are plotted for the case of $\alpha \to 0$. The regularization parameter $\varepsilon_1 = 1$ and $\varepsilon_2 = 0.909$. 
Chapter 4

Kirchhoff Rod Model

The movement of microorganisms, including spermatozoa, can be both planar and non-planar depending on the conditions of the fluid. In this Chapter, we extend a grid-free numerical method to capture the bend and twist of the filament immersed in a Brinkman fluid using a Kirchhoff Rod (KR) model. An immersed boundary formulation of the KR model was first developed by Lim et al. [68] to study supercoiling instabilities of a circular rod in a viscous fluid. The method was later extended by Lim to study the dynamics of an open elastic rod and E. coli flagellar bundling [49, 69]. Recently, this method was extended to study sperm motility using a grid-free numerical algorithm based on the method of regularized Stokeslets [50, 70]. Here, we extend the regularized method to now study spermatozoa in a fluid governed by the Brinkman equation. This provides insight on how stationary obstacles of low volume fraction in the Brinkman fluid model affect waveform, energy, and the swimming speed of the swimmer.

4.1 Background

Using the KR model, a flagellum is described as a 3D space curve $X(s)$ where $0 < s < L$ is the Lagrangian parameter initialized as the arclength and $L$ is the length of the unstressed rod with associated orthonormal triads $\{D^1(s), D^2(s), D^3(s)\}$. The triads can be thought of as the normal, binormal, and tangent vectors and follow the right-handed rule $(D^1(s) \times D^2(s)) = D^3(s)$, $D^2(s) \times D^3(s) = D^1(s)$, or $D^3(s) \times D^1(s) = D^2(s)$,
where ‘×’ denotes the cross product of two vectors). These triads are subjected to the constraint \( \mathbf{D}^i \cdot \mathbf{D}^j = \mathbf{I} \), where \( \mathbf{I} \) is the identity matrix for \( i, j = 1, 2, 3 \). Fig. 4.1 shows a rod discretized as a helix using the centerline approximation with the associated orthonormal triads plotted at one point on the space curve. In the standard model, \( \mathbf{D}^3(s) \) is enforced to be the tangent vector, that is \( \partial \mathbf{X}/\partial s = \mathbf{D}^3(s) \). The rod is also inextensible, \( \| \partial \mathbf{X}/\partial s \| = 1 \).

For our model, we employ an unconstrained version of the Kirchhoff rod model developed by Lim et al. \[68, 49\], where we do not exactly enforce the two conditions above. Instead, an elastic energy penalty, (which is described later in this section) is used such that it can numerically maintain the inextensibility of the rod and keep \( \mathbf{D}^3(s) \) as a unit tangent vector along the rod \[49, 50\].

The balance of force and balance of torque and their associated orthonormal triads have been described in detail by \[68, 50\]. Here, we summarize the main equations of the KR model which are utilized later. The balance of force and torque are given as

\[
0 = \mathbf{f} + \frac{\partial \mathbf{F}}{\partial s}, \tag{4.1}
\]

\[
0 = \mathbf{m} + \frac{\partial \mathbf{M}}{\partial s} + \left( \frac{\partial \mathbf{X}}{\partial s} \times \mathbf{F} \right), \tag{4.2}
\]
where \( f \, (N \ m^{-1}) \), \( m \, (N) \) are external force and external torque densities applied on the rod, where \( N \) (Newton) is the unit of force and \( m \) (meter) is a unit of length. Whereas, \( F \, (N) \), \( M \, (N \ m) \) are internal force and internal torque transmitted across each section of the rod in terms of \( X(s) \) and its triads. Each of the force and torque components can be expanded in the basis of the triads

\[
\begin{align*}
F &= \sum_{i=1}^{3} F^i D^i, & M &= \sum_{i=1}^{3} M^i D^i, \\
f &= \sum_{i=1}^{3} f^i D^i, & m &= \sum_{i=1}^{3} m^i D^i,
\end{align*}
\]

for \( i = 1, 2, 3 \). The constitutive relations for the unconstrained version of the Kirchhoff rod are given as [50, 68]

\[
\begin{align*}
M^1 &= a_1 \left( \frac{\partial D^2}{\partial s} \cdot D^3 - \Omega_1 \right), & M^2 &= a_2 \left( \frac{\partial D^3}{\partial s} \cdot D^1 - \Omega_2 \right), & M^3 &= a_3 \left( \frac{\partial D^1}{\partial s} \cdot D^2 - \Omega_3 \right), \\
F^1 &= b_1 \frac{\partial X}{\partial s} \cdot D^1, & F^2 &= b_2 \frac{\partial X}{\partial s} \cdot D^2, & F^3 &= b_3 \left( \frac{\partial X}{\partial s} \cdot D^3 - 1 \right),
\end{align*}
\]

where \( a_1, a_2 \) are the bending moduli, and \( a_3 \) is the twisting modulus while \( b_1, b_2 \) are the shear moduli, and \( b_3 \) is the extension modulus. In addition, \( \{\Omega_1, \Omega_2, \Omega_3\} \) is defined to be the strain-twist vector where \( \Omega_1, \Omega_2 \) are associated with the intrinsic curvature through the equation \( \kappa = \sqrt{\Omega_1^2 + \Omega_2^2} \) and \( \Omega_3 \) is the intrinsic twist. This vector determines the preferred configuration of the rod. When all three values are non-zero and the rod is open, it has a helical shape. As we discuss in Chapter 5, we can have a preferred curvature corresponding to a planar or spiral bending wave (a function of time and arclength) that is representative of sperm flagellar beatforms observed in experiments [41].

As mentioned earlier, equations (4.5)–(4.6) are derived from a variational argument of the elastic energy penalty

\[
E = \frac{1}{2} \int_0^L \left[ \sum_{i=0}^{3} a_i \left( \frac{\partial D^i}{\partial s} \cdot D^k - \Omega_i \right)^2 + \sum_{i=0}^{3} b_i \left( \frac{\partial X}{\partial s} \cdot D^i - \delta_{3i} \right)^2 \right] ds,
\]

where \( \delta_{ij} \) is the Kronecker delta function. We note that \( (i, j, k) \) is any cyclic permutation of (1, 2, 3). Based on a variational argument, as \( b_i \to \infty \) the unconstrained algorithm reduces to a standard KR model [68, 49, 50].
4.2 Regularized Solutions for a Kirchhoff Rod Model in a Brinkman Fluid

Similar to the MRB, the equation of motion for Brinkman flow is modified to have an extra external effect $f^b$ as

$$\nabla p = \mu \Delta \mathbf{u} - \frac{\mu}{\gamma} \mathbf{u} + f^b,$$  \hspace{1cm} (4.8)

subject to the no-slip boundary conditions for the positions and the orthonormal triads of the rod

$$\frac{\partial \mathbf{X}(s,t)}{\partial t} = \mathbf{u}(\mathbf{X}(s,t)),$$  \hspace{1cm} (4.9)

$$\frac{\partial \mathbf{D}(s,t)}{\partial t} = \omega(\mathbf{X}(s,t)) \times \mathbf{D}(s,t),$$  \hspace{1cm} (4.10)

where ‘×’ is the cross product between two vectors and $\omega(\mathbf{X}(s,t))$ is the angular velocity of the rod. Since we want to capture both the bending and twisting motions of the rod in a 3D infinite fluid, the expression of $f^b$ is a contribution of point forces and torques. To simplify the derivation, we focus on a single point force $f_0$ and a single point torque $m_0$ applied at the point $X_0$ as

$$f^b = f_0 \phi_\varepsilon(r) + \frac{1}{2} \nabla \times m_0 \phi_\varepsilon(r),$$  \hspace{1cm} (4.11)

for $r = ||\mathbf{x} - X_0||$ where $\mathbf{x}$ is any point in the fluid domain including the points where the force and torque are applied. The force $f_0$ ($N$) and the torque $m_0$ ($N \cdot m$) are assumed to be constant but can also depend on time and on the spatial parameter $s$ \[50]. We note again that $\phi_\varepsilon(r)$ is the blob function whose width depends on the parameter $\varepsilon \ll 1$. When $\varepsilon \to 0$, $\phi_\varepsilon(r)$ approaches the Dirac delta function \[47]. From Section 3.1, we show that $f_0 \phi_\varepsilon(r)$ has a unit of force per volume. Since $\phi_\varepsilon(r)$ has units of inverse length cubed and $m_0$ has units of force times length, the term $\nabla \times m_0 \phi_\varepsilon(r)$ has units of force per volume. This means that $f^b$ also has units of force per volume.

Next we find the solutions of the pressure with the contributions of a point force $f_0$ and a point torque $m_0$. We take the divergence of both sides of Eq. (4.8) where the force is given by Eq. (4.11)

$$\Delta p = \mu \Delta (\nabla \cdot \mathbf{u}) + \frac{\mu}{\gamma} \nabla \cdot \mathbf{u} + \nabla \cdot (f_0 \phi_\varepsilon) + \frac{1}{2} \nabla \cdot (\nabla \times m_0 \phi_\varepsilon).$$  \hspace{1cm} (4.12)
Applying the incompressibility condition and using several vector identities that are detailed in Appendix A.1, all the terms on the right hand side of Eq. (4.12) vanish except
\[ \nabla \cdot (f_0 \phi_\varepsilon) = f_0 \cdot \nabla \phi_\varepsilon. \]

We consider the following relations
\[ \Delta G_\varepsilon = \phi_\varepsilon \quad \text{and} \quad (\Delta - \alpha^2) B_\varepsilon = G_\varepsilon, \]
for \( \alpha = 1/\sqrt{\gamma} \), the pressure becomes \( p = f_0 \cdot \nabla G_\varepsilon \). To find the solution of the linear velocity, we simply substitute the expression for the pressure back into Eq. (4.8) and use \( \Delta B_\varepsilon = \alpha^2 B_\varepsilon + G_\varepsilon \), then
\[ \mu u = (f_0 \cdot \nabla) \nabla B_\varepsilon - f_0 \Delta B_\varepsilon - \frac{1}{2} \alpha^2 \nabla B_\varepsilon \times m_0 - \frac{1}{2} \nabla G_\varepsilon \times m_0. \quad (4.13) \]

Next, we show the derivation for the angular velocity. The angular velocity \( \omega \) is given by definition as \( \omega = \frac{1}{2} \nabla \times u \), or \( \mu \omega = \frac{1}{2} \nabla \times (\mu u) \). Then we can write the angular velocity as
\[
\mu \omega = \frac{1}{2} \nabla \times \left[ (f_0 \cdot \nabla) \nabla B_\varepsilon - f_0 \Delta B_\varepsilon - \frac{1}{2} \alpha^2 \nabla B_\varepsilon \times m_0 - \frac{1}{2} \nabla G_\varepsilon \times m_0 \right],
\]
\[ = \frac{1}{2} \nabla \times \left[ (f_0 \cdot \nabla) \nabla B_\varepsilon \right] - \frac{1}{2} \nabla \times (f_0 \Delta B_\varepsilon) - \frac{1}{4} \alpha^2 \nabla \times (\nabla B_\varepsilon \times m_0) - \frac{1}{4} \nabla \times (\nabla G_\varepsilon \times m_0). \]

Using the identities in Appendix A.1, the angular velocity becomes
\[ \mu \omega = \frac{1}{2} \alpha^2 f_0 \times \nabla B_\varepsilon + \frac{1}{2} f_0 \times \nabla G_\varepsilon - \frac{1}{4} \alpha^2 (m_0 \cdot \nabla) \nabla B_\varepsilon \]
\[ + \frac{1}{4} \alpha^2 \Delta B_\varepsilon m_0 - \frac{1}{4} (m_0 \cdot \nabla) \nabla G_\varepsilon + \frac{1}{4} \Delta G_\varepsilon m_0. \quad (4.14) \]

As we can see, both the linear and angular velocity depend on the parameter \( \alpha \) which is inversely proportional to the square root of the Darcy permeability coefficient, \( \gamma \). If \( \gamma \) is large or \( \alpha \) is small (close to zero), then all the terms associated with \( \alpha \) vanish. The equations for linear and angular velocities approach those previously derived for the Stokes regime as \( \alpha \to 0 \) [50].

These limits are detailed in Appendix A.4.1–A.4.2. For convenience in evaluating the solutions of (4.13) and (4.14) numerically, we write the local linear and angular velocity obtained from Appendix A.3 as
\[
\mu u = f_0 H_1^\varepsilon (r) + (f_0 \cdot \hat{x}) \hat{x} H_2^\varepsilon (r) + \frac{1}{2} (m_0 \times \hat{x}) \left[ Q_1^\varepsilon (r) + \alpha^2 Q_2^\varepsilon (r) \right],
\]
\[
\mu \omega = \frac{1}{2} (f_0 \times \hat{x}) \left[ Q_1^\varepsilon (r) + \alpha^2 Q_2^\varepsilon (r) \right] - \frac{1}{4} \alpha^2 [m_0 H_1^\varepsilon (r) + (m_0 \cdot \hat{x}) \hat{x} H_2^\varepsilon (r)]
\]
\[ + \frac{1}{4} [m_0 D_1^\varepsilon (r) + (m_0 \cdot \hat{x}) \hat{x} D_2^\varepsilon (r)]. \]
where the coefficient functions are

\[
H_1^\varepsilon(r) = -\frac{rB''_\varepsilon(r) + B'_\varepsilon(r)}{r}, \quad H_2^\varepsilon(r) = \frac{rB''_\varepsilon(r) - B'_\varepsilon(r)}{r^3},
\]

\[
Q_1^\varepsilon(r) = \frac{G'_\varepsilon(r)}{r}, \quad Q_2^\varepsilon(r) = \frac{B'_\varepsilon(r)}{r},
\]

\[
D_1^\varepsilon(r) = \phi_\varepsilon(r) - \frac{G'_\varepsilon(r)}{r} = \phi_\varepsilon(r) - Q_1^\varepsilon(r), \quad D_2^\varepsilon(r) = -\frac{rG''_\varepsilon(r) - G'_\varepsilon(r)}{r^3}.
\]

The expressions for the Green’s function \(G_\varepsilon(r)\) and \(B_\varepsilon(r)\) are determined after the choice of an appropriate blob function or can be regularized from the singular solutions, which are presented in Chapter 3. In the next section, we present the explicit forms of these functions and their associated derivatives using two different approaches.

### 4.3 Evaluating the Coefficient Functions

#### 4.3.1 Regularizing Fundamental Solutions Approach

The first approach is to solve the pressure, linear, and angular velocity in Eq. (4.13)–(4.14) by regularizing the fundamental solutions as developed by Cortez [45] and detailed in the preceding Chapter. That is, the functions \(G_\varepsilon(r)\) and \(B_\varepsilon(r)\) are written as

\[
G_\varepsilon(r) = -\frac{1}{4\pi R}, \quad B_\varepsilon(r) = \frac{1 - e^{-\alpha R}}{4\pi\alpha^2 R}, \quad (4.15)
\]

for \(R = \sqrt{r^2 + \varepsilon^2}\). When \(\varepsilon \to 0\), we recover the singular solutions. Using \(G_\varepsilon(r)\) and \(B_\varepsilon(r)\) we can derive in Mathematica the corresponding regularized solutions of \(H_i^\varepsilon(r)\), \(Q_i^\varepsilon(r)\), and \(D_i^\varepsilon(r)\) where \(i = 1, 2:\)

\[
H_1^\varepsilon(r) = \frac{e^{-\alpha R}}{4\pi R} \left( \frac{1}{\alpha^2 R^2} + \frac{1}{\alpha R} + 1 \right) - \frac{1}{4\pi\alpha^2 R^3}, \quad (4.16)
\]

\[
H_2^\varepsilon(r) = \frac{e^{-\alpha R}}{4\pi\alpha^2 R^3} \left( \frac{1}{\alpha^2 R^2} + \frac{1}{\alpha R} + 1 \right) + \frac{3}{4\pi\alpha^2 R^5}, \quad (4.17)
\]

\[
Q_2^\varepsilon(r) = \frac{e^{-\alpha R}}{4\pi\alpha^2 R^3} (1 + \alpha R) - \frac{1}{4\pi\alpha^2 R^5}, \quad (4.18)
\]

\[
Q_1^\varepsilon(r) = \frac{5\varepsilon^2}{R^2} H_2^\varepsilon(r) - \frac{\alpha^2 \varepsilon^2}{R^2} Q_2^\varepsilon(r) + \frac{1}{4\pi R^3} \left( 1 - \frac{\varepsilon^2}{R^2} \right), \quad (4.19)
\]

\[
D_2^\varepsilon(r) = \frac{35\varepsilon^2}{R^4} H_2^\varepsilon(r) - \frac{10\alpha^2 \varepsilon^2}{R^4} Q_2^\varepsilon(r) - \frac{1}{4\pi R^6} \left( \frac{10\varepsilon^2}{R^2} + \alpha^2 \varepsilon^2 e^{\alpha R} - 3 \right). \quad (4.20)
\]
The corresponding blob function is

\[
\psi_\varepsilon(r) = \frac{\varepsilon^2}{4\pi\alpha^2 R^2} \left\{ 3\alpha^2 R^2 + e^{-\alpha R} \left[ \alpha^2 \varepsilon^4 \left( -18 + \alpha^2 r^2 - 3\alpha R \right) + \varepsilon^2 \left( -45 + 45e^{\alpha R} + \alpha (45R + \alpha r^2 + 4\alpha R) \right) \right] + r^2 \left( 60 - 60e^{\alpha R} + \alpha(60R + \alpha r^2(27 + \alpha^2 r^2 + 7\alpha R)) \right) \right\}.
\]

(4.21)

### 4.3.2 Choosing a Blob Function Approach

The second approach is to choose a suitable blob function to substitute into Eq. (3.21) and Eq. (3.25) as shown in Chapter 3,

\[
G_\varepsilon(r) = -\int_0^\infty t\phi_\varepsilon(t)dt + \frac{1}{r}\int_0^r (r-t)t\phi_\varepsilon(t)dt,
\]

\[
B_\varepsilon(r) = \frac{1}{2\alpha^2}\int_0^\infty \left( 1 - \frac{\sinh(\alpha r)}{\alpha r} e^{-\alpha t} \right) t\phi_\varepsilon(t)dt + \frac{1}{\alpha^3 r}\int_0^r \left[ \sinh(\alpha r - t) - \alpha(r-t) \right] t\phi_\varepsilon(t)dt.
\]

The corresponding functions \(H_i^\varepsilon(r), Q_i^\varepsilon(r),\) and \(D_i(r)\) where \(i = 1, 2\) in terms of \(\phi_\varepsilon(r)\) are

\[
H_1^\varepsilon(r) = -\frac{1}{\alpha^2 r^3}\int_0^r t^2\phi_\varepsilon(t)dt + \frac{e^{-\alpha r}}{\alpha r} \left( 1 + \frac{1}{\alpha r} + \frac{1}{\alpha^2 r^2} \right) \int_0^\infty t\phi_\varepsilon(t) \sinh(\alpha t)dt
\]

(4.22)

\[
-\frac{e^{-\alpha r}}{2\alpha r} \left( 1 + \frac{1}{\alpha r} + \frac{1}{\alpha^2 r^2} \right) \int_0^\infty t\phi_\varepsilon(t)e^{\alpha t}dt + \frac{e^{\alpha r}}{2\alpha r} \left( 1 - \frac{1}{\alpha r} + \frac{1}{\alpha^2 r^2} \right) \int_0^\infty t\phi_\varepsilon(t)e^{-\alpha t}dt,
\]

\[
H_2^\varepsilon(r) = -\frac{3}{\alpha^2 r^3}\int_0^r t^2\phi_\varepsilon(t)dt + \frac{e^{-\alpha r}}{\alpha r} \left( 1 + \frac{3}{\alpha r} + \frac{3}{\alpha^2 r^2} \right) \int_0^\infty t\phi_\varepsilon(t) \sinh(\alpha t)dt
\]

(4.23)

\[
-\frac{e^{-\alpha r}}{2\alpha r^3} \left( 1 + \frac{3}{\alpha r} + \frac{3}{\alpha^2 r^2} \right) \int_0^\infty t\phi_\varepsilon(t)e^{\alpha t}dt + \frac{e^{\alpha r}}{2\alpha r^3} \left( 1 - \frac{3}{\alpha r} + \frac{3}{\alpha^2 r^2} \right) \int_0^\infty t\phi_\varepsilon(t)e^{-\alpha t}dt,
\]

\[
Q_1^\varepsilon(r) = \frac{1}{r}G_1^\varepsilon(r) = \frac{1}{r^3}\int_0^r t^2\phi_\varepsilon(t)dt,
\]

(4.24)

\[
Q_2^\varepsilon(r) = \frac{1}{r}B_1^\varepsilon(r) = -\frac{1}{r^3}\int_0^r \left[ \sinh(\alpha r - t) - \alpha(r-t) \right] t\phi_\varepsilon(t)dt,
\]

(4.25)

\[
D_1^\varepsilon(r) = \phi_\varepsilon(r) - Q_1^\varepsilon(r),
\]

(4.26)

\[
D_2^\varepsilon(r) = -\frac{rG_\varepsilon''(r) - G_\varepsilon'(r)}{r^3} = -\frac{3}{r^3}\int_0^r t^2\phi_\varepsilon(t)dt.
\]

(4.27)

We recall that the 3D blob function derived in Chapter 3 has the form

\[
\phi_\varepsilon(r) = (a_0 + a_1 r^2)e^{-r^2/\varepsilon^2}
\]

(4.28)
where \( a_0 \) and \( a_1 \) are \[ 67 \]

\[
a_0 = \frac{1}{\alpha^2 \varepsilon^3 \pi^{3/2}} \left( \alpha^2 \varepsilon^2 + 6 - 6e^{-\alpha^2 \varepsilon^2/4} \right), \quad a_1 = -\frac{4}{\alpha^2 \varepsilon^3 \pi^{3/2}} \left( 1 - e^{-\alpha^2 \varepsilon^2/4} \right).
\]

The functions \( G_{\varepsilon}(r) \) and \( B_{\varepsilon}(r) \) are

\[
G_{\varepsilon}(r) = -\frac{1}{\pi^{3/2} \alpha^2 \varepsilon^3} \left( e^{\alpha^2 \varepsilon^2/4} - 1 \right) e^{-\alpha^2 \varepsilon^2/4 - r^2/\varepsilon^2} - \frac{1}{4\pi r} \text{erf}\left( \frac{r}{\varepsilon} \right),
\]

\[
B_{\varepsilon}(r) = \frac{1}{8\pi \alpha^2 r} \left[ 2 - 2\text{erf}\left( \frac{r}{\varepsilon} \right) - e^{-\alpha r} \text{erfc}\left( \frac{\alpha \varepsilon}{2} - \frac{r}{\varepsilon} \right) + e^{\alpha r} \text{erfc}\left( \frac{\alpha \varepsilon}{2} + \frac{r}{\varepsilon} \right) \right],
\]

where the functions \( \text{erf}(z) \) and \( \text{erfc}(z) \) for an arbitrary \( z \) are given as

\[
\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt, \quad \text{erfc}(z) = 1 - \text{erf}(z).
\]

The solutions of \( H_{1i}^\varepsilon \), \( Q_{1i}^\varepsilon \), \( D_{1i}^\varepsilon \) for \( i = 1, 2 \) using Eq. (4.28) can be derived from Eqs. (4.22)–(4.27). We note that at \( r = 0 \) these expressions can not be computed exactly. Instead, these functions are evaluated in the limit of \( r \to 0 \). The formulations of \( H_{1i}^\varepsilon \), \( Q_{1i}^\varepsilon \), \( D_{1i}^\varepsilon \) are as follows

\[
H_{1i}^\varepsilon(r) = \begin{cases} 
\frac{(e^2 + 2r^2)e^{-r^2/\varepsilon^2}}{2\pi^{3/2} \alpha^2 \varepsilon^3 r^2} \left( 1 - e^{-\alpha^2 \varepsilon^2/4} \right) + \frac{1 + \alpha r + \alpha^2 r^2}{8\pi \alpha^2 \varepsilon^3} \text{erfc}\left( \frac{\alpha \varepsilon}{2} - \frac{r}{\varepsilon} \right) e^{-\alpha r} \\
\frac{1}{4\pi \alpha^2 \varepsilon^3} \left[ 1 - \text{erf}\left( \frac{r}{\varepsilon} \right) \right] - \frac{1}{8\pi \alpha^2 \varepsilon^3} \text{erfc}\left( \frac{r}{\varepsilon} + \frac{\alpha \varepsilon}{2} \right) e^{\alpha r}, & r > 0 \\
\frac{2}{3\pi^{3/2} \alpha^2 \varepsilon^3} \left( 1 - e^{-\alpha^2 \varepsilon^2/4} \right) - \frac{\alpha}{6\pi} \left[ 1 - \text{erf}\left( \frac{\alpha \varepsilon}{2} \right) \right] + \frac{1}{3\pi^{3/2} \varepsilon} e^{-\alpha^2 \varepsilon^2/4}, & r = 0
\end{cases}
\]

(4.29)

\[
H_{2i}^\varepsilon(r) = \begin{cases} 
\frac{-3e^2 + 2r^2}{2\pi^{3/2} \alpha^2 \varepsilon^3 r^4} \left( 1 - e^{-\alpha^2 \varepsilon^2/4} \right) - \frac{3 + 3\alpha r + \alpha^2 r^2}{8\pi \alpha^2 \varepsilon^5} \text{erfc}\left( \frac{\alpha \varepsilon}{2} - \frac{r}{\varepsilon} \right) e^{-\alpha r} \\
\frac{3}{4\pi \alpha^2 \varepsilon^5} \text{erf}\left( \frac{r}{\varepsilon} \right) + \frac{3 - 3\alpha r + \alpha^2 r^2}{8\pi \alpha^2 \varepsilon^5} \text{erfc}\left( \frac{\alpha \varepsilon}{2} + \frac{r}{\varepsilon} \right) e^{\alpha r}, & r > 0 \\
\frac{e^{-\alpha^2 \varepsilon^2/4}}{30\pi^{3/2} \alpha^2 \varepsilon^3} \left( 2 - \alpha^2 \varepsilon^2 \right) + \frac{2}{5\pi^{3/2} \alpha^2 \varepsilon^5} \left( 1 - e^{-\alpha^2 \varepsilon^2/4} \right) + \frac{\alpha^3}{60\pi} \left[ 1 - \text{erf}\left( \frac{\alpha \varepsilon}{2} \right) \right], & r = 0
\end{cases}
\]

(4.30)
\[ Q_1^e(r) = \begin{cases} 
\frac{2 e^{-r^2/\varepsilon^2}}{\pi^{3/2} \alpha^2 \varepsilon^5} \left( 1 - e^{-\alpha^2 \varepsilon^2/4} \right) - \frac{1}{2 \pi^{3/2} \varepsilon^2} e^{-r^2/\varepsilon^2} + \frac{1}{4 \pi r^3} \text{erf} \left( \frac{r}{\varepsilon} \right), & r > 0 \\
\frac{1}{3 \pi^{3/2} \alpha^2 \varepsilon^5} \left( 6 + \alpha^2 \varepsilon^2 - 6 e^{-\alpha^2 \varepsilon^2/4} \right), & r = 0 
\end{cases} \]  

\[ Q_2^e(r) = \begin{cases} 
\frac{1}{2} H_1^e(r) - \frac{r^2}{2} H_2^e(r), & r > 0 \\
\frac{e^{-\alpha^2 \varepsilon^2/4}}{6 \pi^{3/2} \varepsilon} + \frac{1}{3 \pi^{3/2} \alpha^2 \varepsilon^5} \left( -1 + e^{-\alpha^2 \varepsilon^2/4} \right) + \frac{\alpha}{12 \pi} \left[ 1 - \text{erf} \left( \frac{\alpha \varepsilon}{2} \right) \right], & r = 0 
\end{cases} \]  

\[ D_1^e(r) = \begin{cases} 
\phi(r) - Q_1^e(r), & r > 0 \\
-\frac{4}{\pi^{3/2} \alpha^2 \varepsilon^5} e^{-\alpha^2 \varepsilon^2/4} + \frac{2(6 + \alpha^2 \varepsilon^2)}{3 \pi^{3/2} \alpha^2 \varepsilon^5}, & r = 0 
\end{cases} \]  

\[ D_2^e(r) = \begin{cases} 
\frac{4}{\pi^{3/2} \alpha^2 \varepsilon^5} e^{-r^2/\varepsilon^2} \left( 1 - e^{-\alpha^2 \varepsilon^2/4} \right) - \frac{3 \varepsilon^2 + 2 r^2}{2 \pi^{3/2} \varepsilon^3} e^{-r^2/\varepsilon^2} + \frac{3}{4 \pi r^3} \text{erf} \left( \frac{r}{\varepsilon} \right), & r > 0 \\
\frac{2}{5 \pi^{3/2} \alpha^2 \varepsilon^7} \left( 10 + \alpha^2 \varepsilon^2 - 10 e^{-\alpha^2 \varepsilon^2/4} \right), & r = 0. 
\end{cases} \]  

### 4.4 Numerical Algorithm

In this section, we describe the detailed numerical algorithm solving Eq. (4.13) and Eq. (4.14) as well as updating the configuration of the rod through the no-slip boundary conditions in Eqs. (4.9)–(4.10). The algorithm is similar to previous derivations [68, 49, 50], except that we are now solving the Brinkman equation and have additional terms as described in the previous sections. Let \( N \) be the number of immersed boundary points discretizing the centerline of the rod. We denote the superscript \( n \) to be the time-step index and time \( t = n \Delta t \) where \( \Delta t \) is the time step. Also, let \( s_k = k \Delta s \), for \( k = 1, \ldots, N \) and \( \Delta s \) be a fixed uniform interval of the Lagrangian parameter \( s \). For simplification, we use the notations \( X_k = X(k \Delta s) \) and \( u^n = u(n \Delta t) \) to be the velocity at time-step \( n \).

1. Evaluate the orthonormal triads at half grid points \( s_{k+1/2} \) between \( s_k \) and \( s_{k+1} \). That means we need to find a rotation matrix (an orthogonal matrix) that maps the orthonormal triads \( \mathbf{D}_k^i \) to \( \mathbf{D}_{k+1/2}^i \), where \( i = 1, 2, 3 \). This matrix can be determined as follows. We
observe that \((D_i^k)^T D_i^k = I\). Then,

\[
D_{i+1}^k = D_{i+1}^k \cdot I,
\]

\[
= D_{i+1}^k \left[ (D_i^k)^T D_i^k \right],
\]

\[
= \left[ D_{i+1}^k (D_i^k)^T \right] D_i^k,
\]

where \(I\) is the identity matrix and \(T\) is the transpose of a matrix. If we let \(A\) be a rotation matrix that maps \(D_i^k\) to \(D_i^{k+1}\), then \(A\) can be uniquely defined as \(A = D_{i+1}^k (D_i^k)^T\). The interpolation from \(D_i^k\) to \(D_i^{k+1/2}\) can be done by applying the principal square root of \(A\), namely \(\sqrt{A}\), on \(D_i^k\) as

\[
D_{i+\frac{1}{2}}^k = \sqrt{A} D_i^k.
\]

(4.35)

Here, \(\sqrt{A}\) is a rotation about the same axis as \(A\) but by half the angle.

2. Using the updated triad at the half point, the internal force and internal moment transmitted across the cross section of the rod can be evaluated at \(s_{k+1/2}\) using the following equations

\[
M_{i+\frac{1}{2}}^k = a_i \left( \frac{D_{i+1}^k - D_i^k}{\Delta s} \cdot D_{i+\frac{1}{2}}^k - \Omega_i \right),
\]

(4.36)

\[
F_{i+\frac{1}{2}}^k = b_i \left( \frac{X_{k+1} - X_k}{\Delta s} \cdot D_{i+\frac{1}{2}}^k - \delta_{3i} \right).
\]

(4.37)

The force \(F_{k+1/2}\) and moment \(M_{k+1/2}\) vectors are assembled as

\[
F_{k+\frac{1}{2}} = \sum_{i=1}^{3} F_{i+\frac{1}{2}}^k D_i^{k+\frac{1}{2}}, \quad M_{k+\frac{1}{2}} = \sum_{i=1}^{3} M_{i+\frac{1}{2}}^k D_i^{k+\frac{1}{2}}.
\]

(4.38)

The force and torque exerted on the fluid by the rod from Eqs. (4.1) – (4.2) are discretized as

\[
-f_k = \frac{F_{k+\frac{1}{2}} - F_{k-\frac{1}{2}}}{\Delta s},
\]

(4.39)

\[
-m_k = \frac{M_{k+\frac{1}{2}} - M_{k-\frac{1}{2}}}{\Delta s} + \frac{1}{2} \left( \frac{X_{k+1} - X_k}{\Delta s} \times F_{k+1}^k + \frac{X_k - X_{k-1}}{\Delta s} \times F_{k-\frac{1}{2}}^k \right).
\]

(4.40)

3. Since we now have \(N\) point forces and torques applied on the fluid and since the Brinkman equation is linear, we can take a superposition of fundamental solutions to determine the
resulting flow at each point in space. Thus, the linear and angular velocities of the fluid at any point \( \mathbf{x} \) are calculated as

\[
\mu \mathbf{u}(\mathbf{x}) = \sum_{k=1}^{N} \left[ (\mathbf{f}_k \cdot \nabla) \nabla B_{\epsilon}(r) - \frac{1}{2} \alpha^2 \nabla B_{\epsilon}(r) \times \mathbf{m}_k - \frac{1}{2} \nabla G_{\epsilon}(r) \times \mathbf{m}_k \right], \tag{4.41}
\]

\[
\mu \mathbf{\omega}(\mathbf{x}) = \sum_{k=1}^{N} \left[ \frac{1}{2} \alpha^2 \mathbf{f}_k \times \nabla B_{\epsilon}(r) + \frac{1}{2} \mathbf{f}_k \times \nabla G_{\epsilon}(r) - \frac{1}{4} \alpha^2 (\mathbf{m}_k \cdot \nabla) \nabla B_{\epsilon}(r)
+ \frac{1}{4} \alpha^2 \Delta B_{\epsilon}(r) \mathbf{m}_k - \frac{1}{4} (\mathbf{m}_k \cdot \nabla) \nabla G_{\epsilon}(r) + \frac{1}{4} \Delta G_{\epsilon}(r) \mathbf{m}_k \right], \tag{4.42}
\]

where \( r = ||\mathbf{x} - \mathbf{X}_k|| \).

4. Next, to update the position, we use the no-slip boundary condition in (4.9) written in terms of the Euler method as

\[
\mathbf{X}_k^{n+1} = \mathbf{X}_k^n + \mathbf{u}(\mathbf{X}_k^n) \Delta t. \tag{4.43}
\]

The orthonormal triads are updated through Eq. (4.10)

\[
(D_i^k)^{n+1} = \mathcal{R} \left( \frac{\mathbf{\omega}(\mathbf{X}_k^n)}{||\mathbf{\omega}(\mathbf{X}_k^n)||}, ||\mathbf{\omega}(\mathbf{X}_k^n)|| \Delta t \right)(D_i^k)^n, \tag{4.44}
\]

where \( \mathcal{R}(\mathbf{e}, \theta) \) is an orthogonal matrix rotating around an angle \( \theta \) about the axis of the unit vector \( \mathbf{e} \) and is defined as

\[
\mathcal{R}(\mathbf{e}, \theta) = (\cos \theta) \mathbf{I} + (1 - \cos \theta) \mathbf{e} \mathbf{e}^T + \sin \theta (\mathbf{e} \times),
\]

where \( \mathbf{I} \) is the \( 3 \times 3 \) identity matrix. The matrix \( \mathcal{R}(\mathbf{e}, \theta) \) is often called the Rodrigues rotation matrix [71]. We rederive \( \mathcal{R}(\mathbf{e}, \theta) \) in Appendix A.5 We note that one can also use higher order methods to update \( \mathbf{X}_k^{n+1} \), e.g. second order or fourth order Runge-Kutta methods.
Chapter 5

Numerical Studies

In this chapter, we study different test cases for our numerical methods presented in the previous chapters. We first want to use the Method of Regularized Brinkmanlets (MRB) to explore swimming speeds and torque, comparing to the asymptotic analysis as well as understanding the more important cases of finite-length swimmers. We discretize the filament using a centerline approximation or the entire cylinder. Next, in terms of the Kirchhoff Rod model, we study the dynamics of an open elastic rod with different permeabilities in a Brinkman fluid as we vary the permeability. The numerical results are also used to compare with the asymptotic solutions. A cylinder with a preferred curvature corresponding to a planar bending wave is also studied.

5.1 The Method of Regularized Brinkmanlets Test Cases

We note that in the case where the fluid flow is generated due to $N$ point forces, the linearity of the Brinkman equation allows the resulting flow to be written as

$$
\mu \mathbf{u}(\mathbf{x}) = \sum_{k=1}^{N} M_{\epsilon}(\mathbf{x} - \mathbf{x}_k) \mathbf{f}_k, \quad (5.1)
$$

where $k = 1, \cdots, N$ and $M_{\epsilon}(\hat{\mathbf{x}}_k) = H_1 I + \hat{\mathbf{x}}_k \hat{\mathbf{x}}_k H_2$ for $\hat{\mathbf{x}}_k = \mathbf{x} - \mathbf{x}_k$ and identity matrix $I$. Note that $\mathbf{x} = (x, y, z)$ is a point in the fluid and force $\mathbf{f}_k$ is located at $\mathbf{x}_k$. Eq. (5.1) is compactly written from Eq. (3.13) and determines the velocity field on the fluid domain at any given point $\mathbf{x}$. Explicitly, $\mathbf{f}_k = (f_k^x, f_k^y, f_k^z)$ where the force components are the forces in the $x, y$ and $z$
directions, respectively.

For all test cases, the number of discretization points \( N \) depends on the length \( L \) of the swimmer. Additionally, for a cylinder of larger thickness \( a \), each cross-section along the length is discretized with \( m_b \) points at a distance of \( \Delta s = 2a \sin(\pi/m_b) \) apart. The distance between each cross-section along the length is also imposed to be \( \Delta s \). For a cylinder of small thickness \( a \ll 1 \), a centerline approximation to the cylinder is used where there are only \( N = 1 + L/\Delta s \) points along the length. Unless otherwise stated, the regularization parameter \( \varepsilon \) is 0.01.

### 5.1.1 Planar Bending

We first compare the numerical data obtained from the MRB with the asymptotic swimming speed for the case of planar bending. Consider an undulating cylinder parametrized by the following space curve equation as

\[
x(s,t) = s, \quad y(s,t) = b \sin(ks - \omega t) + a \cos(\theta), \quad z(s,t) = a \sin(\theta),
\]

(5.2)

for \( 0 \leq \theta \leq 2\pi \) and \( 0 < s < L \) where \( s \) is a parameter initialized as arclength. The wavenumber is \( k = 2\pi/\lambda \) for wavelength \( \lambda \), the bending amplitude is \( b \), and \( \omega \) is the constant angular speed.

In the case of \( a \ll 1 \), we set \( a = 0 \) in Eq. (5.2) and approximate the cylinder with a centerline, representing a filament. At any given time \( t \geq 0 \), the velocity of the flagellum is calculated by

\[
u_x(s,t) = 0, \quad u_y(s,t) = -b\omega \cos(ks - \omega t), \quad u_z(s,t) = 0,
\]

(5.3)
where \( u_x, u_y, \) and \( u_z \) are the velocity components of \( x, y, \) and \( z, \) respectively. Note that we are in the frame of the swimmer. Fig. 5.1 (a) shows a sinusoidal swimmer of small thickness with the velocity fields along the centerline of the swimmer in the \( x-y \) plane. Whereas, Fig. 5.2 shows a sinusoidal swimmer with thickness \( a \) discretized by multiple cross-sections. The total velocity includes the velocity from the sinusoidal wave \( u_s(x) = (u_x, u_y, u_z), \) the translation \( U_0 = (U_0^x, U_0^y, U_0^z), \) and the rotation of the filament \( \Omega_0 = (\Omega_0^x, \Omega_0^y, \Omega_0^z) \) as:

\[
\mathbf{V} = u_s(x) + U_0 + \Omega_0 \times \mathbf{x}_k, \tag{5.4}
\]

where \( \mathbf{V} \) is defined similarly to Eq. (5.1) and for simplicity, we choose \( \mu = 1. \) Unless specified, the superscripts in translational and rotational velocity components are of the \( x, y, \) and \( z \) components, not the partial derivatives. We note that \( f_k, U_0, \) and \( \Omega_0 \) are constants at each time point which can be found by coupling Eq. (5.4) with the force-free and torque-free conditions. That is,

\[
\mathbf{V} - U_0 - \Omega_0 \times \mathbf{x}_k = u_s(x_k), \tag{5.5}
\]

\[
\sum_{k=1}^{N} f_k = 0, \tag{5.6}
\]

\[
\sum_{k=1}^{N} f_k \times \mathbf{x}_k = 0. \tag{5.7}
\]

In Eq. (5.5), for each value of \( k, M_k \) is a \( 3N \times 3N \) matrix while the coefficients for \( U_0 \) and \( \Omega_0 \) form \( 3 \times 3N \) matrices. The coefficient matrices in Eq. (5.6) and Eq. (5.7) are \( (3N + 6) \times 3. \) To determine \( U_0, \Omega_0, \) and \( f, \) we solve Eq. (5.5)–(5.7) which can be written in terms of a matrix
We can then compute pressure using the regularized version of Eq. (3.3). In Fig. 5.1(b), the pressure in the $x$-$y$ plane is shown where we note larger variations in pressure close to the filament.

The numerical results for the translational velocity $U_0$ are used to compare to the asymptotic swimming speed $U_\infty$ derived in Eq. (2.37). Hereinafter, we set $t = 2\pi$ and $\omega = 2\pi$. We first study the case of a finite-length filament satisfying $b \ll a$, i.e. the cylinder thickness is larger than the amplitude. We discretize the cylinder with $m_b = 10$ points on each cross section and fix the thickness at $a = 0.4$ and vary amplitude $b$ from 0.01 to 0.05. In Fig. 5.3(a), we observe that for $\gamma = 1$, the numerical data (marker points) have good agreement with the asymptotic analysis (dashed line) with a longer length ($L = 40$). Similar results are observed as $\gamma$ is varied. In Fig. 5.3(b), the finite-length swimmer has a wavelength of $\lambda = 20$ or $ka \approx 0.1$ and the numerical data also matches up well with the asymptotic solutions. In addition, the radius of the circular cross-section also affects the overall performance of the swimmer. As observed in Fig. 5.3(c), the asymptotic swimming speed decreases as the thickness $a$ increases. The numerical results are able to capture this trend and agree with the analytical solutions for radii $a = 0.2$, 0.3, 0.4 with $L = 40$, $\gamma = 1$, and $\lambda = 5$. 

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Figure 5.3: Cylinder swimming speeds: The comparison between the asymptotic swimming speed of the thick cylinder with $a = 0.4$ (dashed line) with the numerical data (marker points) for different amplitudes with permeability $\gamma = 1$ when (a) $\lambda = 5$ and $\varepsilon = 0.01$ and (b) $\lambda = 20$ and $\varepsilon = 0.12$. (c) The resulting swimming speed of the cylinder as thickness $a$ is varied for $\gamma = 1$ and $\lambda = 5$ with $\varepsilon = 0.01$.

Figure 5.4: Filament swimming speeds (centerline approximation): (a) The swimming speed of the filament ($a \ll 1$) for $\gamma = 1$ where numerical data is given with marker points and the asymptotic speed is shown with a solid line. The difference between the asymptotic values with the numerical results for different amplitudes, and different lengths for (b) $\gamma = 10$, (c) $\gamma = 0.01$, and (d) $\gamma = 0.1$.

We note that most microorganisms do not satisfy $b \ll a$ and we wish to understand how well the asymptotic swimming speed approximates the actual swimming speed of organisms.
with small thickness $a$. For these simulations, since $a \ll 1$, we use a centerline approximation of the filament. In Fig. 5.4(a) the numerical data (marker points) also have good agreement with the asymptotic analysis (solid line) with a longer length ($L = 50$). We also plot the difference between the asymptotic values with the numerics for different lengths and different amplitudes when $\gamma = 10$ as shown in Fig. 5.4(b). As the length increases, the differences decrease. This shows that finite-length swimmers swim slower than the asymptotic predictions and this difference decreases for smaller amplitude $b$ (with fixed $\omega$ and $\lambda$). Also, the difference increases as $b$ increases since the asymptotic analysis assumes that $b/a \ll 1$. We note that the error is slightly larger for smaller permeability as in Fig. 5.4(c) for $\gamma = 0.01$ and in Fig. 5.4(d) for $\gamma = 0.1$. Thus, the infinite-length cylinder swimming speed captures the swimming speed of a finite-length swimmer with more accuracy for larger permeability.

In addition to the translational velocity, we can calculate the angular velocity for different parameters. We again use a centerline approximation assuming small thickness and look at five different bending amplitudes and five different permeabilities. Fig. 5.5(a) shows that the angular velocity when $L = 5$ increases linearly as the amplitude increases. We capture the same behavior for longer swimmers (at $L = 10$ in Fig. 5.5(b) and $L = 50$ in Fig. 5.5(c)). We note that the angular velocity is much larger in the case of small length; in order for a swimmer of shorter length to achieve a prescribed amplitude, the angular velocity increases.

5.1.2 Helical Bending

For this test case, we calculate the external torque exerted on the filament by the surrounding fluid. Consider the right-handed helix where the configuration is parameterized by the 3D space
Figure 5.6: Plot of a helix with different types of approximation is shown. (a) Centerline for a right-handed helix immersed in a Brinkman fluid with, $r_1 = 0.25$, $L = 20$ and $\lambda = 5$. The flow field is shown at $z = 0$ and $z = 10$. (b) Right-handed helix with thickness $a = 0.4$ is discretized with 121 cross-sections with $m_b = 15$, $L = 30$ and $\lambda = 10$.

\[
x(s, t) = r_1 \cos(ks + \omega t) + a \cos(\theta), \quad y(s, t) = r_1 \sin(ks + \omega t) + a \sin(\theta), \quad z(s, t) = r_2 s + Ut,
\]

for $s, k, \theta, \omega$ defined as above, $r_1$ is the radius of the helix (or the amplitude), $r_2$ is a constant defined as $r_2 = \cos \theta = \sqrt{1 - k^2 r_1^2}$ where $\theta$ is the pitch angle, and $U$ is the constant propulsion velocity. The prescribed helical configuration, in the frame of the swimmer, gives the velocity of the helix as

\[
   u(s, t) = -r_1 \omega \sin(ks + \omega t), \quad v(s, t) = r_1 \omega \cos(ks + \omega t), \quad w(s, t) = U. \quad (5.8)
\]

The centerline of a helix when $a = 0$ is shown in Fig. 5.6(a) where the velocity is shown on marker points in two planes and is calculated using Eq. (5.4) where $u_s$ is prescribed by Eq. (5.8). When $a > 0$, a helix with thickness $a$ is shown in Fig. 5.6(b) with 121 cross-sections and 15
points on each cross-section. The torque is calculated as

\[ T = \int_{\Gamma} \mathbf{g}_k \times \mathbf{x}_k \, ds, \]  \hspace{1cm} (5.9) 

where \( \Gamma \) is the helix (surface of the spiral cylinder or centerline of the flagella) and \( \mathbf{g}_k \) is the surface force (traction) applied on the filament. The torque is then numerically approximated by

\[ T = \sum_{k=1}^{N} (\mathbf{g}_k \times \mathbf{x}_k) \Delta s, \]  \hspace{1cm} (5.10) 

which we compare with the analytical solution \( T_\infty \) in (2.60).

\[ \begin{array}{c}
\text{Amplitude, } \gamma = 0.01 \\
\text{Torque}
\end{array} \]

\[ \begin{array}{c}
\text{Amplitude, } \gamma = 1 \\
\text{Torque}
\end{array} \]

\[ \begin{array}{c}
\text{Amplitude, } \gamma = 10 \\
\text{Torque}
\end{array} \]

Figure 5.7: The comparison between the asymptotic velocity (dash-line) and the numerical data (marker points) for \( \lambda = 5 \). (a) Total torque on the surface of a cylinder with \( a = 0.4 \) and \( \gamma = 10 \) where \( b \) is varied from 0.06 to 0.1. Total torque using a centerline approximation when \( a = 0.05 \ll 1 \) for (b) \( \gamma = 0.01, \varepsilon = 0.01 \), (c) \( \gamma = 1, \varepsilon = 0.0055 \) and \( \gamma = 10, \varepsilon = 0.005 \) with \( b \) between 0.05 and 0.15.

In Fig. 5.7(a), we present results for a thick cylinder with \( a = 0.4 \) and \( b \ll a \). For this case, we discretize the surface of the cylinder with \( m_b = 10 \) points on each cross section. In Fig. 5.7(a), the asymptotic value for the torque is shown with a dashed line and the marker points
are the simulation results for three different cylinder lengths using $\gamma = 10$ and $\epsilon = 0.12$. As the length and amplitude increase, there is an increase in torque and better agreement between the asymptotics and the numerical results. Similar results are observed when permeability $\gamma$ is varied. In Fig. 5.7(b), at permeability $\gamma = 0.01$ and $\epsilon = 0.01$, the torque for a thin cylinder ($a \ll 1$) using a centerline approximation compares well to the asymptotic results for a cylinder of radius $a = 0.05$ for longer lengths. We note that similar to the swimming speeds for the case of planar bending, the asymptotics greatly overestimate the torque for shorter length filaments. Similarly, for the cases of $\gamma = 1$ and $\gamma = 10$, the analytical results for an infinite-length spiral cylinder overestimate the torque for the finite-length spiral filament of small radius. We note that previous computational studies using the MRB have observed that the optimal numerical regularization parameter $\epsilon$ varies for each $\gamma$ and can be sensitive for torque calculations [45]. We also observed this sensitivity and decreased the regularization parameter as permeability increased.

5.2 Kirchhoff Rod Model Test Cases

In this Section, we study the effect of the fluid resistance on the behavior and overall performance of an open elastic rod and a planar bending sinusoidal flagellum using the Brinkman KR model as detailed in Section 4.4. Unless stated differently, all the simulations are done using the approach of regularizing the fundamental solutions for the MRB (Section 4.3.1).

5.2.1 Open Elastic Rod

In the first test case, we study an open rod, a classical test case in elastic rod theory [68, 50]. We assume that the KR is immersed in an incompressible Brinkman fluid. The configuration of the rod depends on the 3D space curve $X(s,t)$ and the corresponding orthonormal triad $\{D^1(s,t), D^2(s,t), D^3(s,t)\}$. The rod is initialized as a straight rod with a small perturbation $\xi = 0.001$ so that it does not start from an equilibrium configuration

\[
X(s) = (0, 0, (1 + \xi)s),
\]

\[
D^1(s) = (1, 0, 0), \quad D^2(s) = (0, \cos \xi, -\sin \xi), \quad D^3(s) = (0, \sin \xi, \cos \xi).
\]
The intrinsic bend and twist of an untwisted, straight rod are \( \{\Omega_1, \Omega_2, \Omega_3\} = (0, 0, 0) \) while the non-zero and constant strain-twist vector represents a helical shape. The characteristics of the rod are also defined by the choice of the material stiffness coefficients (SC) \( a_i \) (bending and twisting moduli) and \( b_i \) (shearing and stretching moduli). In Table 5.2, we present different values of \( a_i \) and \( b_i \) for two sets of stiffness parameters, labeled SC1 and SC2 taken from [50] and [73], respectively. Unless mentioned otherwise we utilize the SC1 parameter set. As defined in Table 5.2 we set the length of the rod to be \( L = 6 \mu m \) with 76 immersed boundary points and set \( \{\Omega_1, \Omega_2, \Omega_3\} = (1.3, 0, \pi) \). The viscosity \( \mu \), the time step \( \Delta t \) and the spacing \( \Delta s \) are also shown in Table 5.2. The number of turns, \( q \), of the helix can be determined by the equation [50, 49]:

\[
q = \frac{\Omega_3 L}{2\pi} = 3 \text{ (turns)}.
\]

For the first test case, we initialize the rod as straight and give it a preferred curvature and twist corresponding to a helix. The moments as described in Section 4.1 correspond to differences between the actual configuration of the rod and the prescribed one. This results in the rod

![Figure 5.8: The rod is initialized as a perturbed, straight rod and achieves the preferred configuration of a helix. The deformation of the rod is shown at different time points with the permeability }\gamma=0.1.\]

(a) t=0.001s, (b) t=0.002s, (c) t=0.003s, (d) t=0.005s, (e) t=0.01s
moving and interacting with the fluid until it reaches the prescribed configuration.

Fig. 5.8 shows different time lapses when the straight rod deforms into a helix in a fluid with permeability $\gamma = 0.1$ and the regularization parameter is $\varepsilon = 7\Delta s$. We want to investigate the effect of the permeability on the behavior of the rod. As mentioned, the smaller $\gamma$ is, the more resistance presented in the fluid, which makes it harder for the rod to achieve its desired configuration. The statement is supported by the numerical results shown in Fig. 5.9 for $\varepsilon = 7\Delta s$ with five different permeabilities $\gamma = 0.01$, $\gamma = 0.1$, $\gamma = 1$, $\gamma = 10$, and $\gamma = 100$ corresponding to $\alpha = 10$, $\alpha = \sqrt{10}$, $\alpha = 1$, $\alpha = 1/\sqrt{10}$, and $\alpha = 0.1$, respectively. That is, the rod is still a straight configuration at time $t = 0.01$ s when the permeability is small, $\gamma = 0.01$, as shown in Fig. 5.9(a). We observe that in Fig. 5.9(b) the rod has more bend and twist along its length when compared to the case of $\gamma = 0.01$. It deforms more toward a helix in Figs. 5.9(c)–(d) for larger permeabilities. At the same time, for a larger permeability $\gamma = 100$, the rod in Fig. 5.9(e) has a more complete helical configuration compared to the other cases. The energy profiles in Fig. 5.10 are obtained from the energy penalty equation given in (4.7). Figs. 5.10(a)–(b) shows that the bending and twisting energy decrease for increased permeability. In addition, we know from elastic rod theory that as the rod reaches its equilibrium configuration, the energy decreases to zero. We observe that it takes an increased amount of time to reach the equilibrium configuration for decreased permeability (increased fluid resistance). We observe that the rod for decreased permeability requires more bending and twisting energy.

![Figure 5.9](image)

Figure 5.9: The rod is initialized as a straight, untwisted rod at $t = 0$. The deformation of the rod is captured with various permeability at $t = 0.01s$ where the rod is given a preferred curvature and twist corresponding to a helix. The regularization parameter is $\varepsilon = 7\Delta s$.

The regularization parameter $\varepsilon$ also affects the dynamics of the rod as it moves and interacts.
Figure 5.10: Energy plots with various permeability values using SC1 set of stiffness coefficients with the regularization parameter $\epsilon = 7\Delta s$. (a): Bending Energy, (b): Twisting Energy.

<table>
<thead>
<tr>
<th>Stiffness Coefficients</th>
<th>SC1</th>
<th>SC2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bending modulus, $a = a_1 = a_2$ (g $\mu$m$^3$ s$^{-2}$)</td>
<td>$3.5 \times 10^{-3}$</td>
<td>$1.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>Twisting modulus, $a_3$ (g $\mu$m$^3$ s$^{-2}$)</td>
<td>$3.5 \times 10^{-3}$</td>
<td>$1.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>Shearing modulus, $b = b_1 = b_2$ (g $\mu$m s$^{-2}$)</td>
<td>$8.0 \times 10^{-1}$</td>
<td>$6.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>Stretching modulus, $b_3$ (g $\mu$m s$^{-2}$)</td>
<td>$8.0 \times 10^{-1}$</td>
<td>$6.0 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

Table 5.2: Table of stiffness coefficients of the rod taken from [50] (SC1) and [73] (SC2).

with the fluid. The energy profiles for bending and twisting energy for different choices of $\epsilon = 5\Delta s$, $6\Delta s$, $7\Delta s$, $8\Delta s$ are shown in Fig. 5.11. The rod has a decreased bending energy and twisting energy when the regularization parameter decreases, Fig. 5.11(a)–(b), respectively. The regularization parameter can also be thought of as a physical parameter describing the radius of the rod since it controls the region where the majority of the force is spread. It makes sense that a rod of larger radius might take longer to reach its equilibrium configuration and have an increased energy.

We also want to study the effect of the stiffness coefficients on the energy performance of the rod. We use two sets of stiffness coefficients, SC1 and SC2, to simulate the test cases. The bending moduli and twisting modulus in SC1 are smaller than the ones in SC2. This means that the rod is less stiff and that deviations from the preferred curvature are not penalized as strongly (lead to a smaller magnitude of the torque). As we can see in Fig. 5.12(a)–(b) the SC2 stiffness coefficients have an increased bending energy and twisting energy initially and approach zero in a shorter time period than for the SC1 parameters. This means the straight rod in the case of SC2 becomes a helix much faster than in the case of SC1. However, if the
stiffness coefficients are increased higher, the rod becomes too stiff to bend and twist in the fluid.

Figure 5.11: Energy plots with different regularization parameters using SC1 (Table. 5.2) with $\gamma = 0.1$. (a): Bending Energy, (b): Twisting Energy.

Figure 5.12: (a) Bending enery and (b) Twisting energy when using the different stiffness coefficients in Table. 5.2

5.2.2 Cylinder with Planar Bending

In this test case, we want to look at the motion of the cylindrical tail propagating planar bending waves. The waves in the $y$ plane travel along the filament in the $z$ direction whose spatial coordinates are $x(s, t) = 0$, $y(s, t) = b \sin(ks + \sigma t)$, and $z(s, t) = s$ with the corresponding curvatures and twist

$$\Omega_1 = -bk^2 \sin(ks + \sigma t), \quad \Omega_2 = 0, \quad \Omega_3 = 0,$$
where \( b \) is the amplitude, \( U \) is the velocity of the propagating waves, and the wavenumber is \( k = \frac{2\pi}{\lambda} \) where \( \lambda \) is the wavelength. We note that this is a preferred curvature where the achieved amplitude is an emergent property. This is in contrast to Section 5.1.1 where we exactly prescribed the motion.

Suppose \( U_\infty \) is the asymptotic swimming speed for the cylinder propagating planar bending waves, then from Chapter 2 the second order nondimensional swimming speed \( U_\infty/U \) to the second order solution is given as

\[
\frac{U_\infty}{U} = \frac{1}{2} b^2 k^2 \left\{ \frac{(1 - \chi^2)K_0(\zeta_1) + \chi^2 \log \chi}{(1 - \chi^2)K_0(\zeta_1) - (2 - \chi^2) \log \chi} \right\}, \tag{5.11}
\]

where \( K_0 \) is the modified Bessel function of the second kind of order zero, \( \chi = \sqrt{1 + \frac{\alpha^2}{k^2}} \) with \( \alpha = \frac{1}{\sqrt{\gamma}} \) and \( \zeta_1 = ka \ll 1 \). To compare it with the numerical results, we rewrite the above equation in dimensional units as

\[
U_\infty = \frac{1}{2} b^2 k \sigma \left\{ \frac{(1 - \chi^2)K_0(\zeta_1) + \chi^2 \log \chi}{(1 - \chi^2)K_0(\zeta_1) - (2 - \chi^2) \log \chi} \right\},
\]

where \( \sigma \) is the beat frequency of the cylinder.

First, we study the planar bending wave solutions of the rod numerically for the case of \( L = 40 \) and \( L = 80 \). The results are plotted in Fig. 5.13. For the case of \( L = 40 \), the rod is discretized by 600 points while the rod with \( L = 80 \) is discretized with 1200 points with \( \varepsilon = 7\Delta s \) and permeability \( \gamma = 100 \) or \( \alpha = 0.1 \). The rod is prescribed with five different

---

**Figure 5.13:** Fitting the numerical data (marker points) with the asymptotic swimming speed (dashed lines) for (a) \( L = 40 \mu m \) with 600 points and (b) \( L = 80 \mu m \) with 1200 points for various frequencies for \( \varepsilon = 7\Delta s \) and permeability \( \gamma = 100 \).
amplitudes \( b = 0.05, 0.075, 0.1, 0.125 \) and 0.15. As the frequency \( \sigma \) is varied from 250 − 500 Hz, the swimming speed of the rod is calculated. The numerical results show that for different frequencies, the swimming speed scales quadratically with respect to the amplitude. For \( L = 40 \), Fig. 5.13(a) shows that the numerics (marker points) are validated by the asymptotic solutions (dashed lines) although the rod cannot achieve the preferred amplitude in this time interval. As mentioned earlier, there is a time dependent preferred curvature at each point along the rod. Therefore, the emergent curvature and amplitude vary based on the permeability and other parameters in the model. Similar to the case of \( L = 40 \), the numerical data match up well with the analytical results modeled for the rod of length \( L = 80 \). In this case, the rod is able to achieve an amplitude that is closer to the preferred amplitude than that of the \( L = 40 \) rod. To see if the length might be a factor in achieving the preferred amplitudes, we run another simulation for \( L = 160 \). We see that in the case of \( \sigma = 350 \) Hz in Fig. 5.14(a), the achieved amplitude of \( L = 160 \) is better than the case of \( L = 40 \), but not as good as \( L = 80 \).

Additionally, we study the performance of the cylinder using the two different approaches presented in Chapter 4. The numerical results are obtained from regularizing the fundamental solutions (Section 4.3.1) with the regularization parameter \( \varepsilon_1 = 7\Delta s \) and from choosing the blob function (Section 4.3.2) with \( \varepsilon_2 = 0.909\varepsilon_1 \). We see in Fig. 5.14(b) for the case of \( L = 40 \), numerical results from both approaches match up well with the asymptotic analysis. For the stiffness parameter used, the achieved amplitude is closer to the desired amplitude for the case of choosing a blob function.

### 5.2.3 Emergent Waveforms of a Kirchhoff Rod

Next, we study the emergent waveforms of a swimmer for different permeability with \textit{slightly different} stiffness coefficients from Table 5.2. In this test case, the swimmers are initialized as straight rods. The waveforms arise due to a described configuration given in the form of a sinusoidal curve \( x(s,t) = 0, y(s,t) = b\sin(ks + \sigma t), \) and \( z(s,t) = s \) with a preferred planar curvature

\[
\Omega_1 = -bk^2 \sin(ks + \sigma t), \quad \Omega_2 = 0, \quad \Omega_3 = 0.
\]

The emergent amplitude and swimming speed depend on the resistance \( \alpha \) in the fluid. The numerical study of a sinusoidal waveform with planar bending is motivated by experimental

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Figure 5.14: Comparisons of achieved amplitudes for (a) different lengths, L = 40 µm, L = 80 µm, and L = 160 µm and (b) different approaches. The approaches in (b) include choosing the blob function in Section 4.3.3 and regularizing the fundamental solutions in Section 4.3.1 for L = 40 µm. The simulations are done using SC1 set with frequency σ = 350 Hz and γ = 100.

results of human sperm shown to exhibit a sinusoidal curvature in time [4]. Typically, the length of the human sperm flagellum is between 50 − 55 µm [4, 21]. The wavelengths are between 10 − 60 µm. Depending on the fluid environment, the beat frequency ranges from 10 − 20 Hz, [4], and the mean amplitude can be as large as 5.9 µm [74].

For all the simulations, we fix the length of the rod to be L = 50 µm and the amplitude to be b = 4 µm. The rod is discretized using a centerline approximation with 301 points. The fluid linear and angular velocity are computed using the method of choosing a blob function (Section 4.3.1). Thus, the regularization parameter is ε = 0.1 for ε = 6Δs. The time step is Δt = 10^-6 s while the beat frequency is 20 Hz, giving σ = 20(2π). The permeabilities are varied with γ = 0.01, 0.1, 1, 10, 100. The stiffness parameters used are listed in Table 5.3. Previous experiments on sea urchin sperm have estimated that the interdoublet bending resistance of the flagellum is 1 × 10^8 pN nm^2/rad and the shear resistance is 6 pN/rad [73]. Converting pN nm^2 to g µm^3 s^-2 and pN to g µm s^-2, we are in the range of SIMS1. Mammalian sperm also have a series of outer dense fibers that surround the 9+2 axonemal structure (Fig. 1.5). Thus, mammalian sperm are stiffer than marine invertebrate sea urchin sperm [73, 22] and the SIMS3 parameters are more representative of human sperm.

In the first set of simulations (SIMS1), the stiffness coefficients taken from Table 5.3 are a_i = 0.1 and b_i = 0.06, for i = 1, 2, 3. The wavelength is chosen to be λ = 20 µm. Four
different snapshots of the swimmers in time are shown in Fig. 5.15 with the $x$–axis indicating the location of the rod. We note that the results from Fig. 5.15 are four different simulations placed in the same figure for comparison. The endpoint of each rod is also tracked and plotted. At $t = 0.0012s$ in Fig. 5.15(a), the sine waves start forming for higher permeabilities while the rod in the case of $\gamma = 0.01$ is still a straight line. Fig. 5.15(b) at $t = 0.12s$ shows that the filaments with higher permeabilities swim away from the initial locations. The additional fluid resistance is preventing the swimmers from generating the preferred amplitude. For the permeability of $\gamma = 100$ and $\gamma = 10$, the rods reach closer to the desired amplitude than the case of $\gamma = 1$. For $\gamma = 0.1$, the rod forms a more obvious sine wave and the emergent amplitude is much smaller than the desired amplitude. The rod with permeability $\gamma = 0.01$ starts moving although it does not have much waving interaction due to the increased resistance in the fluid. At time $t = 0.36s$, Fig. 5.15(c) shows that although the rod in the case of $\gamma = 1$ has not fully achieved the desired amplitude, it seems to swim faster than the other filaments. At time $t = 0.6s$, the emergent waveforms of the rods in the cases of $\gamma = 100$ and $\gamma = 10$ seem to get closer to the preferred amplitude. We notice that the swimmer in the case of $\gamma = 10$ can swim faster than the one when $\gamma = 100$. Although the rod in the case $\gamma = 1$ does not seem to achieve the required amplitude, it swims faster than the other four rods. There is a small amount of waving at the end of the filament in the case of $\gamma = 0.1$ and we see that the rod translates away from the initial location. On the other hand, we record limited movement for the rod with permeability of $\gamma = 0.01$. In the case of $\gamma = 100, 10, 1$ and $\gamma = 0.1$ (when zooming in), the endpoints of these rods exhibit figure-of-eight motions. No figure-of-eight motions are recorded at any other points along the rod except the endpoint. The rods in all the cases move with a linear trajectory and seem to have symmetrical waveforms.

In the second set of simulations (SIMS2), the wavelength of the swimmer is chosen to be $\lambda = 40 \mu m$. The length $L$, the amplitude $b$, the stiffness coefficients $a_i$ and $b_i$ and the beat frequency of the rod are the same as in SIMS1 (Table 5.3). The regularization parameter $\varepsilon_2$
Figure 5.15: Snapshots of the swimming flagellum in a Brinkman fluid for five simulations with different permeabilities at (a) $t = 0.0012s$, (b) $t = 0.12s$, (c) $t = 0.36s$ and (d) $t = 0.6s$. The endpoints of the swimmers are also tracked and plotted with a dark blue line. The length of the rod is $L = 50 \mu m$, the amplitude is $b = 4 \mu m$ and the wavelength is $\lambda = 20 \mu m$.

Figure 5.16: Swimming filaments in the case where $a_i = 0.1$ and $b_i = 0.06$. The length of the rod is $L = 50 \mu m$ with wavelength $\lambda = 40 \mu m$ and amplitude $b = 4 \mu m$. Two separate simulations are combined for comparison at (a) $t = 0.0012s$, (b) $t = 0.6s$ and (c) $t = 1.2s$. The green and red filaments represent rods in a Brinkman fluid with $\gamma = 100$ and $\gamma = 1$, respectively. The endpoints of the swimmers (in blue) are also tracked.
and the time step $\Delta t$ are also the same as before. For this test case, we just consider two permeabilities $\gamma = 100$ (dashed green line) and $\gamma = 1$ (solid red line) corresponding to $\alpha = 0.1$ and $\alpha = 1$, respectively. Two separate simulations are put together in the same figure for comparison. The motion at the endpoint of the rod is tracked and plotted in the same figure as the rods. Fig. 5.16 shows the development of the waveforms of filaments in a Brinkman fluid at different time points. When $t = 0.0012s$, the two rods in Fig. 5.16(a) seem to show little to no movement along the length. After a longer time, when $t = 0.6s$ in Fig. 5.16(b), the rod in the case of $\gamma = 100$ displays a sinusoidal curve and the emergent amplitude does not get close to the preferred amplitude. In the case of $\gamma = 1$, the rod has small curvature and the trajectory indicates little forward motion. Even at time $t = 1.2s$, the two rods in Fig. 5.16(c) display limited forward motion as well as bending along the length. The problem may be that the stiffness coefficients for SIMS2 could be too small. That is, the preferred curvature function is not being enforced strongly and the swimmer is “floppy” and unable to propagate the curvature wave for this particular choice of wavelength and amplitude.

![Figure 5.16](image)

**Figure 5.16:** Swimming filaments in the case where $a_i = 1$ and $b_i = 0.6$. Two separate simulations are combined for comparison at (a) $t = 0.0012s$, (b) $t = 0.24s$ and (c) $t = 0.6s$. The green filament represents a rod in a Brinkman fluid with $\gamma = 1$. The red filament corresponds to a rod in a Brinkman fluid with $\gamma = 0.1$. The length of the rod is $L = 50 \mu m$ with wavelength $\lambda = 40 \mu m$ and amplitude $b = 4 \mu m$.

We repeat the same simulations as in SIMS2 but the stiffness coefficients are now set as
As opposed to SIMS2, the rods in this case show movement at a much earlier time point. We observe in Fig. 5.17(a) that at \( t = 0.0012 \) s, the rods start forming a sine wave where the rod in the case of \( \gamma = 100 \) exhibits higher curvature bending than the one in the case of \( \gamma = 1 \). At time \( t = 0.24 \) s, the rods translate away from the initial locations, display more bending, but have not yet achieved the preferred amplitude as shown in Fig. 5.17(b). The rod in green (\( \gamma = 100 \)) swims ahead of the red rod (\( \gamma = 1 \)). When \( t = 0.6 \) s in Fig. 5.17(c), we observe that the rod in the case of \( \gamma = 100 \) swim faster than the one with \( \gamma = 0.1 \). The waveforms of the rods are less symmetric. For instance, at \( t = 0.6 \) s the endpoint of the green curve reaches up to 3.32 while the first point is at -1.08. The amplitudes of the upper and lower peaks are recorded at 2.18 and -2.77, respectively. Although the flagella exhibit asymmetrical bending along the length, they swim with a linear trajectory. We also see the figure-of-eight motions at the endpoint (not plotted) of the filaments. Different from SIMS2, the figure-of-eight motions are also observed in SIMS3 for the material points that are located toward the end of the filaments.

We conclude from this numerical study that the emergent waveform may be different from the preferred waveform due to the resistance \( \alpha \) of the Brinkman fluid and the rigidity of the rod. For higher permeability (less resistance), the rod achieves a more obvious sinusoidal configuration and the emergent amplitude gets closer to the preferred one. If the rod is too stiff or too much resistance is present in the fluid, the rod shows little to no forward motion. The bending along its length is less likely to occur. We observe symmetrical waveforms for rods with smaller stiffness coefficients, whereas, rods with higher stiffness coefficients seem to display asymmetrical waveforms.
Chapter 6

Calcium Concentration Model

Calcium dynamics is the subject of many studies in mathematical modeling since it plays an important role in muscle mechanics and cardiac electrophysiology \[75, 76\]. Cell movement and the beating patterns of cilia and flagella are also controlled by \(Ca^{2+}\) concentration ([\(Ca^{2+}\)]) \[21, 75, 18\]. For instance, spermatozoa can alter their beatform from symmetrical to asymmetrical in response to an increase in the intracellular [\(Ca^{2+}\)] as shown in Figs. 3(a)–(c) \[14\]. This change in flagellar bending is required in order for the sperm to successfully navigate along the female reproductive tract \[74, 17\]. The CatSper channels allows \(Ca^{2+}\) to enter the flagellum when they are open. They are located on the plasma membrane of the principal piece of the largest segment of the flagellum as shown in Fig. 6.1. Experiments have shown that \(Ca^{2+}\) is stored in a region called the redundant nuclear envelop (RNE) located in the neck of the flagellum \[79, 17, 78\]. This release of \(Ca^{2+}\) from the RNE is dependent on the local concentration of inositol 1,4,5 –

![Diagram of a human sperm with different regions and dimensional values](image)

Figure 6.1: Illustration of a human sperm with different regions and their dimensional values, which include the head (≈ 5 µm), the neck (≈ 2 µm), the midpiece (≈ 4 µm), the principal piece (≈ 50 µm), and the endpiece (≈ 3 µm). The image also shows the CatSper channel along the principal piece and the Redundant Nuclear Envelope in the neck of the sperm. The figure is recreated from Olson et al. \[78\].

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trisphosphate (IP_3) and modulated by the receptor IP_3R. Since previous studies have developed a model of Ca^{2+} dynamics and flagellar curvature, we use this model to understand how Ca^{2+} changes emergent trajectories and waveforms of the swimmer modeled as a KR.

6.1 Calcium Model

In this section, we summarize the system of 1D reaction-diffusion equations that models the [Ca^{2+}] and its release from the RNE via IP_3. The model was previously developed by Olson et al. [18]. We denote C (µM) as the calcium concentration and P (µM) as the IP_3 concentration where µM is micro moles per liter. The Ca^{2+} and IP_3 are coupled as follows

\[
\begin{align*}
\frac{\partial C}{\partial t} &= D_C \frac{\partial^2 C}{\partial s^2} + J_{CAT}^C - J_{PMCA}^C + J_{PP,\text{leak}}^C + J_{RNE,\text{out}}^C - J_{RNE,\text{in}}^C, \\
\frac{\partial P}{\partial t} &= D_P \frac{\partial^2 P}{\partial s^2} + J_{\text{prod}}^P - J_{\text{deg}}^P,
\end{align*}
\]  

(6.1)

where \( D_C (\mu m^2 s^{-1}) \) and \( D_P (\mu m^2 s^{-1}) \) are the diffusion coefficients for Ca^{2+} and IP_3 concentrations, respectively. The reaction terms \( J_{CAT}^C (\mu M s^{-1}) \) and \( J_{\text{prod}}^P (\mu M s^{-1}) \) are taken from previous models and experiments and are detailed below. The reaction terms \( J_{CAT}^C \) can be understood as local sinks and sources of Ca^{2+}, where Ca^{2+} may be entering or exiting from a channel on the flagellum or from the RNE. Here, we categorize the reaction terms in Eq. (6.1) by five different types of fluxes including the flux going through the CatSper channel, \( J_{CAT}^C \), the flux going out of the sperm via a plasma membrane channel denoted \( J_{PMCA}^C \), the leak of Ca^{2+} getting into the sperm through the surrounding environment, namely \( J_{PP,\text{leak}}^C \), the flux that pumps excess Ca^{2+} into the RNE store called \( J_{RNE,\text{in}}^C \) and the flux \( J_{RNE,\text{out}}^C \) is the outflow of calcium from the RNE. The first three fluxes are examined only at the principal part while the last two fluxes are studied in the neck region of the spermatozoa.

The reaction term \( J_{CAT}^C \) is modeled as

\[
J_{CAT}^C = \begin{cases} 
0, & \text{if } x \notin PP \\
 k_{CAT} \cdot O(t) \cdot C_{\text{ext}}, & \text{if } x \in PP 
\end{cases}
\]  

(6.3)

This equation represents the Ca^{2+} pumped into the flagellum via the CatSper channel located in the plasma membrane of the principal piece (PP) of the sperm with constant rate, \( k_{CAT} (s^{-1}) \).
The amount of $Ca^{2+}$ pumped in is controlled by cyclic adenosine monophosphate (cAMP), which facilitates the opening of CatSper channels. The $Ca^{2+}$ in the surrounding environment $C_{ext}$ also affects the flux through the channels. The fraction of open CatSper channels, $O(t)$, is given by

$$\frac{dO}{dt} = \nu_1 A(1 - O) - \nu_2 O,$$

where $0 \leq O \leq 1$. The rate constant $\nu_1 (s^{-1})$ is the concentration depaopening rate and $\nu_2 (s^{-1})$ is the closing rate. In addition, $O(t)$ depends on the local cAMP concentration $A(t)$ ($\mu M$) modeled by the following first order differential equation

$$\frac{dA}{dt} = -\beta_{deg} A,$$

where $\beta_{deg}$ is the degradation rate.

Experiments have shown that the fundamental mechanism for removal of $Ca^{2+}$ from the sperm flagellum is via the plasma membrane $Ca^{2+}$ ATPase or PMCA [17, 18]. The main role of the PMCA is to export excess cytoplasmic $Ca^{2+}$ out in exchange for one or two extracellular protons brought into the cytosol. Here, we make an assumption that the clearance mode is modeled only for the principal piece of the spermatozoa. It is known that the flux of PMCA, $J_{PMCA}^C$, is modeled based on the Hill function [17, 75] as

$$J_{PMCA}^C = \begin{cases} 
0, & \text{if } x \notin PP \\
V_{PMCA} \frac{C^{n_{PMCA}}_{PMCA}}{C^{n_{PMCA}}_{PMCA} + k_{1/2}^{PMCA}}, & \text{if } x \in PP
\end{cases}$$

(6.6)

where $V_{PMCA}$ is the maximal rate of $Ca^{2+}$ movement by the PMCA, $k_{1/2}^{PMCA}$ is the $[Ca^{2+}]$ when the PMCA is at half activation, and $n_{PMCA}$ is the Hill coefficient. On the other hand, a secretory pathway $Ca^{2+}$-ATPase (SPCA) is responsible for refilling sperm intracellular stores and therefore affects RNE stores. Excess $Ca^{2+}$, $J_{RNE, in}^C$, is pumped back into the RNE and is modeled using the Hill function as

$$J_{RNE, in}^C = \begin{cases} 
0, & \text{if } x \notin Neck \\
V_{SPCA} \frac{C^{n_{sp}}_{sp}}{C^{n_{sp}}_{sp} + k_{SPCA}^{sp}}, & \text{if } x \in Neck
\end{cases}$$

(6.7)
where $V_{SPCA}$ is the maximal rate of $Ca^{2+}$ movement by the SPCA, $k_{SPCA}^{n_{sp}}$ is the $[Ca^{2+}]$ when the SPCA is at half activation, and $n_{sp}$ is the Hill coefficient.

If there is an increase in $Ca^{2+}$ in the neck and head regions, $Ca^{2+}$ is released out of the RNE through $IP_3$ gated channels and is modeled as

$$J_{RNE, out}^C = \begin{cases} 
0, & \text{if } x \not\in \text{Neck} \\
V_{RNE} Pr_{IP_3 R} + V_{RNE, leak}, & \text{if } x \in \text{Neck}
\end{cases} \quad (6.8)$$

where $V_{RNE, leak}$ is the leak across the RNE membrane and is assumed to be constant at all time.

In this model, we consider three binding domains that may be in an activated or unactivated state. One binds $IP_3$ and the other two bind $Ca^{2+}$. Each domain may have more than one binding site. The probability of the $IP_3$ receptors being opened, $Pr_{IP_3 R}$, is modeled as

$$Pr_{IP_3 R} = p_1 p_2 p_3 = \left[ \frac{P_{n_p}}{P_{n_p} + k_{1_p}^{n_p}} \right] \left[ p_b + \frac{(1 - p_b)C}{k_2 + C^2} \right] h, \quad (6.9)$$

where $p_1$ and $p_2$ are the functions describing the binding and activation of domain 1 and domain 2, respectively and $p_3$ represents the inactivation of the receptors in domain 3. Here, $p_1$ is given as a function of local $IP_3$ concentration with respect to time and space as a Hill function for a half-maximal binding constant $k_1$ and $n_p$ is the Hill coefficient given in Table 6.1. The term $p_2$ is modeled as an increasing function when $Ca^{2+}$ is low and $p_b$ is regarded as the fraction of activated $IP_3$ receptors when $[Ca^{2+}] = 0$. The last term, $p_3 = h$ represents an inactivation of the receptors and is modeled as

$$\tau_h \frac{\partial h}{\partial t} = \frac{k_3^2}{k_3^2 + C^2} - h, \quad (6.10)$$

for time constant $\tau_h$ and $k_3$ is the concentration of $Ca^{2+}$ where inactivation of $IP_3$ by $Ca^{2+}$ is half-maximal. The steady state of $h$ is $k_3^2/(k_3^2 + C^2)$, which is a decreasing function with respect to the $[Ca^{2+}]$. That is, as the $[Ca^{2+}]$ increases, $h$ decreases to a steady state with time constant $\tau_h$.

Furthermore, there is also a flux due to the leak of $Ca^{2+}$ out of the principal piece of the sperm flagellum. The leak flux $J_{PP, leak}^C$ is modeled as a constant value.

When $Ca^{2+}$ enters the cytosol via the CatSper channel, it is hypothesized that there is an
<table>
<thead>
<tr>
<th>Parameters</th>
<th>Explanation</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>CatSper</strong></td>
<td>Basal rate of CatSper</td>
<td>$3.5 \times 10^{-4} \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$k_{CAT}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\nu_1$</td>
<td>Opening rate</td>
<td>$0.005 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$\nu_2$</td>
<td>Closed rate</td>
<td>$0.07 \text{ s}^{-1}$</td>
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<tr>
<td><strong>PMCA</strong></td>
<td>Maximal velocity of PMCA</td>
<td>$0.75 \mu\text{Ms}^{-1}$</td>
</tr>
<tr>
<td>$V_{PMCA}$</td>
<td>Calcium concentration activation</td>
<td>$0.2 \mu\text{M}$</td>
</tr>
<tr>
<td>$k_{PMCA}$</td>
<td>Hill coefficient</td>
<td>$2$</td>
</tr>
<tr>
<td>$n_{pm}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>**Ca}^{2+}</td>
<td>$Ca}^{2+}$ leak into cytosol via PP</td>
<td>$0.15 \mu\text{Ms}^{-1}$</td>
</tr>
<tr>
<td>$J_{PP,\text{leak}}$</td>
<td>Diffusion coefficient for $Ca}^{2+}$</td>
<td>$20 \mu\text{m}^2\text{s}^{-1}$</td>
</tr>
<tr>
<td>$D_{Ca}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>**Ca}^{2+}</td>
<td>$Ca}^{2+}$ in the surrounding medium</td>
<td>$2000 \mu\text{M}$</td>
</tr>
<tr>
<td>$Ca}_{\text{Ext}}$</td>
<td>Resting calcium</td>
<td>$0.1 \mu\text{M}$</td>
</tr>
<tr>
<td><strong>cAMP</strong></td>
<td>Rate of cAMP degradation</td>
<td>$0.1 \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$\beta_{deg}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A^*$</td>
<td>$[\text{cAMP}]$ in cytosol at $t=5s$</td>
<td>$100 \mu\text{M}$</td>
</tr>
<tr>
<td>**IP}^{3}$</td>
<td>Diffusion Coefficient for $IP}^{3}$</td>
<td>$300 \mu\text{ms}^{-1}$</td>
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<td>$D_{IP}$</td>
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<tr>
<td>$v_s$</td>
<td>Production Rate of $IP}^{3}$ production</td>
<td>$0.015 \mu\text{Ms}^{-1}$</td>
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<td>$\rho_{deg}$</td>
<td>Degradation rate of $IP}^{3}$</td>
<td>$2.5 \text{ s}^{-1}$</td>
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<td>$P^*$</td>
<td>Resting concentration of $IP}^{3}$</td>
<td>$0 \mu\text{M}$</td>
</tr>
<tr>
<td><strong>Ca}^{2+} Sensitivity</strong></td>
<td>Sensitivity of PLC to calcium</td>
<td>$0.7 \mu\text{M}$</td>
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<tr>
<td>$k_{PLC}$</td>
<td>Maximal calcium flux</td>
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<td>$V_{RNE,\text{leak}}$</td>
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</tr>
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<td><strong>IP}^{3}R</strong></td>
<td>Hill coefficient $IP}^{3} \text{ binding}$</td>
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</tr>
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<td>$n_p$</td>
<td>$K_m$ for $IP}^{3}$ binding to its $R$</td>
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</tr>
<tr>
<td>$k_1$</td>
<td>Fraction of act $IP}^{3}R$</td>
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</tr>
<tr>
<td>$b$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$k_2$</td>
<td>$K_m$ for act of $IP}^{3}R$ by $Ca}^{2+}$</td>
<td>$0.7 \mu\text{M}$</td>
</tr>
<tr>
<td>$\tau_h$</td>
<td>Time for $IP}^{3}R$ inact by $Ca}^{2+}$</td>
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</tr>
<tr>
<td>$k_3$</td>
<td>$K_m$ for inact of $R$ by $Ca}^{2+}$</td>
<td>$0.7 \mu\text{M}$</td>
</tr>
<tr>
<td><strong>SPCA</strong></td>
<td>Maximal velocity for SPCA</td>
<td>$0.3 \mu\text{Ms}^{-1}$</td>
</tr>
<tr>
<td>$V_{SPCA}$</td>
<td>Hill coefficient for SPCA</td>
<td>$1$</td>
</tr>
<tr>
<td>$n_{sp}$</td>
<td>calcium level of SPCA</td>
<td>$0.1\mu\text{M}$</td>
</tr>
</tbody>
</table>

Table 6.1: Parameters for $Ca}^{2+} - IP}^{3}$ reaction-diffusion equations. The first column corresponds to the notation presented in the model description. The second column is the explanation of each parameter. The third column includes the values of each parameter with their corresponding units. The values are taken from Olson et al. [78].
increase in $IP_3$ concentration \[80\] \[81\]. The mechanism to generate $IP_3$ is triggered by cAMP and is sensitive to $[Ca^{2+}]$. The production of the $IP_3$ decreases with time due to a decrease of cAMP concentration, $A(t)$ as modeled in Eq. (6.5). Thus, the flux of production of $IP_3$, $J_{prod}$, is modeled using the Hill function as

$$J_{prod}^P = \begin{cases} 0, & \text{if } x \notin \text{Neck} \\ v_s \cdot A(t) \cdot \frac{C}{C + k_{PLC}}, & \text{if } x \in \text{Neck} \end{cases} \quad (6.11)$$

where $v_s$ is the maximal rate of $IP_3$ production, $A(t)$ is the concentration of cAMP and $k_{PLC}$ is the threshold of $[Ca^{2+}]$ for synthesizing $IP_3$ production.

The last flux term controlling the $IP_3$ concentration is $J_{deg}$ representing the degradation of $IP_3$ and is modeled as a linear function with respect to $P(x, t)$ \[82\] as

$$J_{deg}^P = p_{deg} P(x, t), \quad (6.12)$$

where $p_{deg}$ is the degradation rate.

### 6.2 System of 1D Reaction-Diffusion Equations for a Fixed Domain

In this section, we present some numerical results of the system of reaction-diffusion equations in Eq. (6.1) and Eq. (6.2). We use no-flux boundary conditions for our model as

$$\frac{\partial C}{\partial x} \bigg|_{x=0,L} = \frac{\partial P}{\partial x} \bigg|_{s=0,L} = 0. \quad (6.13)$$

The initial conditions of $C$ and $P$ are given as

$$C(x, 0) = C^*, \quad P(x, 0) = P^*, \quad (6.14)$$

where $C^* = 0.1 \, (\mu M)$ is taken from \[78\] and $P^* = 0$ represents the resting level of $IP_3$. Also, the initial condition for the fraction of open CatSper channels, $O(0)$ and the initial condition
for the inactivation of the receptors, \( h(0) \) are

\[
O(0) = 0, \quad h(0) = 1.
\]

The concentration of cAMP, \( A(t) \), is set up such that there is \( A(t) \) when \( t > 5s \). That is, there are no CatSper channels open before the application of \( A(t) \) at \( t = 5s \). Thus, \( A(t) \) is

\[
A(t) = \begin{cases} 
0, & t < 5s \\
A^*, & t = 5s
\end{cases}
\]

\[ (6.15) \]

where \( A^* = 100 \ \mu M \) is estimated from experiments \[83\]. All other model parameters are listed in Table 6.1. The value of each parameter is based on previous models and experiments. The length of the spermatozoa is set to be \( L = 120 \ \mu m \), which is the length scale for the mouse sperm where \( x = 0 \) is the starting point on the head and \( x = 120 \) is the end point on the tail of the sperm. The sperm is divided into five different regions: head = 10 \( \mu m \), neck = 2 \( \mu m \), midpiece = 20 \( \mu m \), principal piece = 80 \( \mu m \), and endpiece = 8 \( \mu m \). We note that these values are the measurements of a mouse sperm taken from previous experiments \[84, 85\].

We use the Crank–Nicolson method \[86\] with explicit representations of the reaction terms to discretize Eqs. (6.1)–(6.2) as

\[
\frac{C_{k}^{n+1} - C_{k}^{n}}{\Delta t} = D_C \left[ \frac{C_{k-1}^{n+1} - 2C_{k}^{n+1} + C_{k+1}^{n+1}}{2\Delta x^2} + \frac{C_{k-1}^{n} - 2C_{k}^{n} + C_{k+1}^{n}}{2\Delta x^2} \right] + \left( \sum_{i} J_{C_i}^{n} \right)_{k}^{n}, \quad (6.16)
\]

\[
\frac{P_{k}^{n+1} - P_{k}^{n}}{\Delta t} = D_P \left[ \frac{P_{k-1}^{n+1} - 2P_{k}^{n+1} + P_{k+1}^{n+1}}{2\Delta x^2} + \frac{P_{k-1}^{n} - 2P_{k}^{n} + P_{k+1}^{n}}{2\Delta x^2} \right] + \left( \sum_{j} J_{P_j}^{n} \right)_{k}^{n}, \quad (6.17)
\]

where \( J_{C_i} \) and \( J_{P_j} \) correspond to the fluxes. The spacing size is \( \Delta x \) and \( \Delta t \) is the time-step size.

We note that \( k \) corresponds to the \( k^{th} \) spatial location and \( (n+1) \) is the new time step. We wish to solve Eqs. (6.16)–(6.17) for \( C_{k}^{n+1} \) and \( P_{k}^{n+1} \) for \( k = 1, \ldots, N \) where \( N \) is the number of points on a fixed 1D domain \( x = [0, N\Delta s = L] \). The Neumann boundary conditions are expanded up to the second order in space using the one-sided expansion as

\[
\frac{\partial C}{\partial x} \bigg|_{x=0} = \frac{1}{2\Delta x} \left( -3C_{1}^{n+1} + 4C_{2}^{n+1} - C_{3}^{n+1} \right) = 0,
\]

\[ (6.18) \]
\[ \frac{\partial C}{\partial x} \bigg|_{x=L} = \frac{1}{2\Delta x} \left( C_{k+1}^{n+1} - 4C_k^{n+1} + 3C_k^{n+1} \right) = 0. \quad (6.19) \]

The same scheme can be applied to the boundary conditions for \( P \).

The numerical simulation is done using five different grids \( \Delta x = 1/8, 1/16, 1/32, 1/64, 1/128 \) and \( 1/256 \) with \( \Delta x = 1/256 \) (\( \mu \text{m} \)) as the reference grid. For each grid, the equations are solved at each time step, \( \Delta t = 0.01 s \) for a total time of \( t = 100 s \). We compute the \( L_2 \)-norm error between the reference solution \( C_{\text{ref}} = C_{1/256} \) with the solutions from the coarser grids. Also, suppose \( p \) is the order of convergence of the method, then the formula to calculate \( p \) is given as

\[ p = \log_2 \left( \frac{\| C_{\Delta x} - C_{\text{ref}} \|_2}{\| C_{\Delta x/2} - C_{\text{ref}} \|_2} \right). \quad (6.20) \]

The error and order of convergence results are shown in Table 6.2. We see in Table 6.2 that as the grid is refined, the error decreases. The order of convergence for the 1D reaction-diffusion \( \text{Ca}^{2+} - \text{IP}_3 \) model is around 1.5 since we are using explicit representations for the reaction terms.

<table>
<thead>
<tr>
<th>( \Delta x )</th>
<th>( | C - C_{\text{ref}} |_2 )</th>
<th>Order of Convergence</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/8</td>
<td>( 1.545 \times 10^{-4} )</td>
<td>–</td>
</tr>
<tr>
<td>1/16</td>
<td>( 7.488 \times 10^{-5} )</td>
<td>1.0458</td>
</tr>
<tr>
<td>1/32</td>
<td>( 3.497 \times 10^{-5} )</td>
<td>1.0988</td>
</tr>
<tr>
<td>1/64</td>
<td>( 1.499 \times 10^{-5} )</td>
<td>1.2222</td>
</tr>
<tr>
<td>1/128</td>
<td>( 4.998 \times 10^{-6} )</td>
<td>1.5849</td>
</tr>
</tbody>
</table>

Table 6.2: Table of error and order of convergence for the 1D reaction-diffusion \( \text{Ca}^{2+} - \text{IP}_3 \) model. The first column is the grid. The second column is the \( L_2 \)-norm error between the solutions of the coarser grid and the solution of the reference grid. The last column is the order of convergence.

In addition, we plot the \([\text{Ca}^{2+}]\) up to time \( t = 100 s \) at the head (green solid line), the principal piece (red dashed line), and the midpiece (blue line) in Fig. 6.2(a). We observe that there is an increase in \([\text{Ca}^{2+}]\) in the head of the sperm after the 8-Br-cAMP is released at \( t = 5 s \). This higher \([\text{Ca}^{2+}]\) in the head agrees with the observation made by Olson et al. [78]. The increases in concentration are also seen for the midpiece and principal piece. Similarly, we observe in Fig. 6.2(b) the same patterns of increase and decrease in concentration along the length of the sperm. This is a good comparison between our simulations and the previously published model results in [78].
Figure 6.2: The $[Ca^{2+}]$ of the sperm is plotted. (a) The $[Ca^{2+}]$ of the head (TrackH), the midpiece (TrackMP), and the principal piece (TrackPP) up to time $t = 100s$ are shown. (b) The $[Ca^{2+}]$ along the sperm for different times is shown. In both simulations, the time step is $\Delta t = 0.01$.

6.3 System of 1D Transport-Diffusion Equations for a Moving Interface

To understand the effects of $[Ca^{2+}]$ on sperm motility, we study the solutions of a swimming flagellum immersed in a fluid numerically. The sperm is assumed to be a moving interface in space where the centerline is modeled as $X(s,t)$ depending on time $t$ and arclength $s$. The flagellum alters local bending due to the local $[Ca^{2+}]$, which is determined by solving the coupled system of reaction-diffusion equations described in Section 6.2. However, since we consider a moving filament, we have to rewrite Eqs. (6.1)–(6.2) in terms of $X(s,t)$ and this is a transport-diffusion equation.

In this Section, we extend our model from Section 6.2 where reaction-diffusion was considered on a fixed 1D line. Here, the transport-reaction-diffusion equation is on a moving interface that is the swimming flagellum. We summarize the derivations to obtain the transport-diffusion equation. The reaction terms are added later. The transport equation has been previously derived and is detailed in [87].

6.3.1 Transport-Diffusion Equation

Let $L(s)$ be an interfacial segment where the concentration is defined. Suppose there is no passive diffusion and no transport due to a moving interface. Thus, the mass on the segment is
conserved and is calculated as
\[ \frac{d}{dt} \int_{L(s)} C(s,t) ds = 0, \] (6.21)

where \( s \) is the arclength of the filament. The integral is rewritten in terms of the initial configuration of the flagellum as
\[ \frac{d}{dt} \int_{L(0)} C(s,t) \left\| \frac{\partial X}{\partial s} \right\| ds = 0, \] (6.22)

where \( X(s,t) = (X(s,t), Y(s,t)) \). Bringing the time derivative inside the integral, we have
\[
\int_{L(0)} \left( \frac{\partial C}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| + C \frac{\partial}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| \right) ds = 0, \]
(6.23)

where \( \| \cdot \| \) is the norm of a function and \( \| \partial X/\partial s \| \) is the stretching or compression factor. The first term (I) in Eq. (6.23) represents the material derivative and the second term (II) is the time derivative accounting for changes in material surface elements due to stretching. We note that both the interface and the concentration are tracked in a Lagrangian manner. Next, we calculate the rate of the stretching of the interfacial segments. Consider the following relation
\[
\left\| \frac{\partial X}{\partial s} \right\| = \sqrt{\left( \frac{\partial X}{\partial s} \right)^2 + \left( \frac{\partial Y}{\partial s} \right)^2}.
\]

Then, the second term of Eq. (6.23) becomes
\[
\frac{\partial}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| = \frac{1}{\| \partial X/\partial s \|} \left[ \frac{\partial X}{\partial s} \left( \frac{\partial X}{\partial t} \right) + \frac{\partial Y}{\partial s} \left( \frac{\partial Y}{\partial t} \right) \right].
\]

Rewriting using \( u = \frac{\partial X}{\partial t} = (u, v) \), then
\[
\frac{\partial}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| = \frac{1}{\| \partial X/\partial s \|} \left[ \frac{\partial X}{\partial s} \left( \frac{\partial u}{\partial s} + \frac{\partial Y}{\partial s} \right) + \frac{\partial Y}{\partial s} \left( \frac{\partial u}{\partial s} + \frac{\partial Y}{\partial s} \right) \right],
\]
\[
= \frac{1}{\| \partial X/\partial s \|} \left[ \frac{\partial X}{\partial s} \left( \nabla u \cdot \frac{\partial X}{\partial s} \right) + \frac{\partial Y}{\partial s} \left( \nabla v \cdot \frac{\partial X}{\partial s} \right) \right].
\]

Consider the tangent vector \( \tau = \frac{\partial X/\partial s}{\| \partial X/\partial s \|} \), then
\[
\frac{\partial}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| = \tau \cdot \left( \nabla u \cdot \frac{\partial X}{\partial s}, \nabla v \cdot \tau \left\| \frac{\partial X}{\partial s} \right\| \right),
\]
87
\[
\frac{\partial}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| = (\nabla_s \cdot \mathbf{u}) \left\| \frac{\partial X}{\partial s} \right\|.
\]

(6.24)

Here, the term \((\nabla_s \cdot \mathbf{u})\) is the surface divergence. Substituting the time derivative of the stretching term back into (6.23) and since the material segment is arbitrary, then

\[
\frac{\partial C}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| + \frac{\partial C}{\partial s} \left\| \frac{\partial X}{\partial s} \right\| = 0.
\]

(6.25)

If we allow diffusion in the system, we obtain the following equation

\[
\frac{\partial C}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| + C \frac{\partial C}{\partial s} \left\| \frac{\partial X}{\partial s} \right\| = D_C \frac{\partial}{\partial s} \left( \frac{\partial C/\partial s}{\left\| \frac{\partial X}{\partial s} \right\|} \right).
\]

(6.26)

where \(D_C\) is the diffusion coefficient of the concentration \(C\). Similarly, the transport-diffusion equation of \(IP_3\) is written as

\[
\frac{\partial P}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| + P \frac{\partial P}{\partial s} \left\| \frac{\partial X}{\partial s} \right\| = D_P \frac{\partial}{\partial s} \left( \frac{\partial P/\partial s}{\left\| \frac{\partial X}{\partial s} \right\|} \right).
\]

(6.27)

The 3D case can easily be extended by adding a third component to the derivations.

### 6.3.2 Discretization of Transport-Diffusion Equation

We discretize Eq. (6.26) without the reaction part. We denote a collection of discrete points \(s_k = k\Delta s, k = 1, \ldots, N\) as the immersed interface such that Lagrangian markers are denoted by \(X_k = X(s_k) = (X_k, Y_k)\). The concentration \(C\) defined at half-integer points is written as \(s_{k+1/2} = (k+1/2)\Delta s\). In addition, the derivative approximation for an arbitrary function, \(\Theta(s)\), defined on the interface:

\[
\frac{\partial \Theta}{\partial s} \approx D_s \Theta(s) = \frac{\Theta(s + \Delta s/2) - \Theta(s - \Delta s/2)}{\Delta s}.
\]

(6.28)

We rewrite the equations Eqs. (6.26)–(6.27) by replacing the term \(\nabla_s \cdot \mathbf{u}\) with \(\frac{\partial}{\partial t} \left\| \frac{\partial X}{\partial s} \right\|\), then

\[
\frac{\partial C}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| + C \frac{\partial C}{\partial s} \left\| \frac{\partial X}{\partial s} \right\| = D_C \frac{\partial}{\partial s} \left( \frac{\partial C/\partial s}{\left\| \frac{\partial X}{\partial s} \right\|} \right),
\]

(6.29)

\[
\frac{\partial P}{\partial t} \left\| \frac{\partial X}{\partial s} \right\| + P \frac{\partial P}{\partial s} \left\| \frac{\partial X}{\partial s} \right\| = D_P \frac{\partial}{\partial s} \left( \frac{\partial P/\partial s}{\left\| \frac{\partial X}{\partial s} \right\|} \right).
\]

(6.30)
For illustration, we discretize Eq. (6.29) using the Crank-Nicolson scheme and the derivative approximation in Eq. (6.28):

\[
\frac{C_{k+1}^{n+1} - C_k^{n+1}}{\Delta t} = \frac{1}{2 \Delta s} \left( \frac{(C_{k+1}^{n+1} - C_k^{n+1})/\Delta s}{(||D_s X_{k+1}^{n+1}|| + ||D_s X_k^{n+1}||)/2} - \frac{(C_{k}^{n+1} - C_{k-1}^{n+1})/\Delta s}{(||D_s X_k^{n+1}|| + ||D_s X_{k-1}^{n+1}||)/2} \right) + \frac{D_C}{2 \Delta s} \left( \frac{(C_{k+1}^{n} - C_k^{n})/\Delta s}{(||D_s X_{k+1}^{n}|| + ||D_s X_k^{n}||)/2} - \frac{(C_{k}^{n} - C_{k-1}^{n})/\Delta s}{(||D_s X_k^{n}|| + ||D_s X_{k-1}^{n}||)/2} \right). 
\]

(6.31)

The expression on the left hand side is

\[
LHS = \frac{C_{k+1}^{n+1} - C_k^{n+1}}{\Delta t} \cdot \frac{||D_s X_{k+1}^{n+1}|| + ||D_s X_k^{n+1}||}{2} + \frac{||D_s X_k^{n+1}||}{2} \cdot \frac{C_{k+1}^{n+1} + C_k^{n}}{2},
\]

\[
= \frac{1}{\Delta t} C_k^{n+1} (||D_s X_{k+1}^{n+1}|| + ||D_s X_k^{n+1}||) - \frac{1}{\Delta t} C_k^n (||D_s X_k^{n+1}|| + ||D_s X_n^{n}||) + \frac{1}{\Delta t} C_k^n (||D_s X_k^{n+1}|| - ||D_s X_n^{n}||) + \frac{1}{\Delta t} C_k^n (||D_s X_k^{n}|| - ||D_s X_n^{n}||),
\]

\[
= \frac{1}{\Delta t} ||D_s X_{k+1}^{n+1}|| C_k^{n+1} - \frac{1}{\Delta t} ||D_s X_k^{n+1}|| C_k^n.
\]

The right hand side expression is

\[
RHS = \frac{D_C}{(\Delta s)^2} \left[ \frac{C_{k+1}^{n+1} - C_k^{n+1}}{||D_s X_{k+1}^{n+1}|| + ||D_s X_k^{n+1}||} - \frac{C_k^{n+1} - C_{k-1}^{n+1}}{||D_s X_k^{n+1}|| + ||D_s X_{k-1}^{n+1}||} \right] + \frac{D_C}{(\Delta s)^2} \left[ \frac{C_k^{n+1} - C_k^{n}}{||D_s X_k^{n+1}|| + ||D_s X_k^{n}||} - \frac{C_k^{n} - C_{k-1}^{n}}{||D_s X_k^{n}|| + ||D_s X_{k-1}^{n}||} \right],
\]

\[
= \frac{\eta_1}{||D_s X_{k+1}^{n+1}|| + ||D_s X_k^{n+1}||} C_k^{n+1} - \eta_1 \left( \frac{1}{||D_s X_{k+1}^{n+1}|| + ||D_s X_k^{n+1}||} + \frac{1}{||D_s X_k^{n+1}|| + ||D_s X_{k-1}^{n+1}||} \right) + \frac{\eta_1}{||D_s X_k^{n+1}|| + ||D_s X_{k-1}^{n+1}||} C_k^{n+1} + \frac{\eta_1}{||D_s X_k^{n}|| + ||D_s X_{k-1}^{n}||} C_k^{n+1} - \eta_1 \left( \frac{1}{||D_s X_k^{n}|| + ||D_s X_{k-1}^{n}||} + \frac{1}{||D_s X_k^{n}|| + ||D_s X_{k-1}^{n}||} \right),
\]

for \( \eta_1 = D_C/(\Delta s)^2 \). The final form of Eq. (6.31) is

\[
= - \frac{\eta}{||D_s X_{k+1}^{n+1}|| + ||D_s X_k^{n+1}||} C_{k+1}^{n+1} - \frac{\eta}{||D_s X_k^{n+1}|| + ||D_s X_{k-1}^{n+1}||} C_{k+1}^{n+1} + \frac{\eta}{||D_s X_k^{n}|| + ||D_s X_{k-1}^{n}||} C_k^{n+1} + \frac{\eta}{||D_s X_k^{n}|| + ||D_s X_{k-1}^{n}||} C_k^{n+1}.
\]
for $\eta = D_C \Delta t / (\Delta s)^2$. We can rewrite the equation in terms of the matrix–vector system as follows

$$
\begin{pmatrix}
  a_{11} & a_{12} \\
  a_{21} & a_{22} & a_{23} \\
  \vdots & \vdots & \vdots \\
  a_{N-1,N-2} & a_{N-1,N-1} & a_{N-1,N} \\
  a_{N,N-1} & a_{NN}
\end{pmatrix}
\begin{pmatrix}
  C_1^{n+1} \\
  C_2^{n+1} \\
  C_3^{n+1} \\
  \vdots \\
  C_{N-1}^{n+1} \\
  C_N^{n+1}
\end{pmatrix}
= 
\begin{pmatrix}
  0 \\
  b_2 C_1^n + c_2 C_2^n + d_2 C_3^n \\
  b_3 C_2^n + c_3 C_3^n + d_3 C_4^n \\
  \vdots \\
  b_{N-2} C_{N-3}^n + c_{N-2} C_{N-2}^n + d_{N-2} C_{N-1}^n \\
  b_{N-1} C_{N-2}^n + c_{N-1} C_{N-1}^n + d_{N-1} C_N^n \\
  0
\end{pmatrix},
$$

where $a_{11}, a_{12}, a_{N,N-1}$, and $a_{NN}$ depend on the Neumann boundary condition

$$
a_{k,k-1} = -\frac{\eta}{\|D_s X_k^n\| + ||D_s X_{k-1}^n||},
$$

$$
a_{k,k} = \|D_s X_k^n\| + \frac{\eta}{\|D_s X_k^n\| + ||D_s X_{k+1}^n||} + \frac{\eta}{\|D_s X_k^n\| + ||D_s X_{k-1}^n||},
$$

$$
a_{k,k+1} = -\frac{\eta}{\|D_s X_{k+1}^n\| + ||D_s X_k^n||},
$$

with

$$
b_k = \|D_s X_k^n\| + ||D_s X_{k-1}^n||,
$$

$$
c_k = \|D_s X_k^n\| - \frac{\eta}{\|D_s X_{k+1}^n\| + ||D_s X_k^n||} - \frac{\eta}{\|D_s X_k^n\| + ||D_s X_{k-1}^n||},
$$

$$
d_k = \|D_s X_{k+1}^n\| + ||D_s X_k^n||,
$$

for $k = 2, \ldots, N-1$. Since we are using the no-flux boundary condition, the total mass of the concentration is conserved numerically and the following equation is satisfied,

$$
\sum_k C_k^{n+1} \|D_s X_k^n\| \Delta s = \sum_k C_k^n \|D_s X_k^n\| \Delta s. \quad (6.32)
$$

The discretization of Eq. (6.30) can be done in a similar fashion.

Next, we validate our simulations by studying mass conservation on a moving interface using the transport-diffusion equation. Since the KR model is 3D and is mainly planar for sinusoidal
bending waves, we use a simple curve as a test case. The curve is parameterized as

\[ X(s, t) = s, \quad Y(s, t) = b \sin(ks - \sigma t), \quad Z(s, t) = 0, \]

where \( b \) is the amplitude, \( k \) is the wavenumber, \( \sigma \) is the frequency, and the arclength is \( 0 < s < L \) where \( L \) is the length of the curve. For simplicity, we choose \( b = 1, k = 1 \) and \( \omega = 1 \). We set \( L = 15 \, \mu\text{m} \) and \( s \) is discretized with spacing \( \Delta s \).

We evaluate Eq. (6.32) for four time steps \( \Delta t = 10^{-3} - 10^{-6} \) and different spacings \( \Delta s = 1/32, 1/64, 1/128 \). The calculations are done up to time \( t = 1 \) s and \( t = 5 \) s. The results are presented in Table 6.3 where we report the mean of the mass differences over the total time.

As mentioned earlier, we want to conserve the total mass over time because of the no-flux boundary condition and no reaction terms. Thus, mass should be conserved since it is neither created or destroyed along the interface and it is not leaving at the boundaries. We study the problem with three different grids \( \Delta s = 1/32, 1/64, 1/128 \) and four different time steps \( \Delta t \) ranging from \( 10^{-3} - 10^{-6} \). The evaluations of mass conservation are computed up to time \( t = 1 \) s and \( t = 5 \) s. The results are presented in Table 6.3, where we report the mean of the mass differences over the total time using Eq. (6.32). As \( \Delta t \) decreases, the mass conservation is more strictly enforced. We also observe a decrease in mass difference when \( \Delta s \) decreases and when the calculations are done with a longer time (\( t = 1 \) s versus \( t = 5 \) s). We also show the log–log plot in Fig. 6.3 of the results presented in Table 6.3. The \( x \)-axis indicates the decreasing time steps while the \( y \)-axis shows the mean difference in the mass over time \( t = 1 \) s (solid lines) and \( t = 5 \) s (dashed lines). We can see clearly that the differences in mass decrease when \( \Delta s \) is decreased from 1/32 to 1/128.

Table 6.3: Table of mean mass differences calculated using Eq. (6.32) for four time steps \( \Delta t = 10^{-3} - 10^{-6} \) and different spacings \( \Delta s = 1/32, 1/64, 1/128 \). The calculations are done up to \( t = 1 \) s and \( t = 5 \) s.

<table>
<thead>
<tr>
<th>( \Delta x )</th>
<th>1/32</th>
<th>1/64</th>
<th>1/128</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta t )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( 10^{-3} )</td>
<td>9.59×10^{-7}</td>
<td>7.44×10^{-7}</td>
<td>4.75×10^{-7}</td>
</tr>
<tr>
<td>( 10^{-4} )</td>
<td>9.45×10^{-8}</td>
<td>7.41×10^{-8}</td>
<td>4.61×10^{-8}</td>
</tr>
<tr>
<td>( 10^{-5} )</td>
<td>9.43×10^{-9}</td>
<td>7.41×10^{-9}</td>
<td>4.59×10^{-9}</td>
</tr>
<tr>
<td>( 10^{-6} )</td>
<td>9.43×10^{-10}</td>
<td>7.40×10^{-10}</td>
<td>4.59×10^{-10}</td>
</tr>
</tbody>
</table>
Figure 6.3: Mass conservation of the transport-diffusion equation is observed at time $t = 1s$ (solid lines) and $t = 5s$ (dashed lines) for $\Delta t = 10^{-3} - 10^{-6}$. The grids are set at $\Delta s = 1/32$ (blue), $\Delta s = 1/64$ (red), $\Delta s = 1/128$ (green). The lines correspond to the mean mass differences calculated from Eq. (6.32).

### 6.3.3 Transport-Reaction-Diffusion Equation

The full transport-reaction-diffusion equations of $Ca^{2+}$ and $IP_3$ are

\[
\frac{\partial C}{\partial t} \frac{\partial X}{\partial s} + C \frac{\partial}{\partial t} \left( \frac{\partial X}{\partial s} \right) = D_C \frac{\partial}{\partial s} \left( \frac{\partial C}{\partial s} \right) + \sum_i J^C_i, \tag{6.34}
\]

\[
\frac{\partial P}{\partial t} \frac{\partial X}{\partial s} = P \frac{\partial}{\partial t} \left( \frac{\partial X}{\partial s} \right) = D_P \frac{\partial}{\partial s} \left( \frac{\partial P}{\partial s} \right) + \sum_j J^P_j. \tag{6.35}
\]

To validate our implementation, we simulate a test case of a moving filament coupled with the transport-reaction-diffusion equations. The parameterized curve has the same form as in Eq. (6.33). The transport-diffusion parts of Eqs. (6.34) – (6.35) are discretized using the Crank-Nicolson method as in Section 6.3.2. Whereas, the reaction terms, described in Section 6.1, are expanded explicitly.

For this test case, the grid is $\Delta s = 1/64$ and the time step is $\Delta t = 0.01$. The simulation is done up to time $t = 100s$. The length of the filament is $L \approx 62 \mu m$, which includes the head $\approx 5 \mu m$, the neck $\approx 2\mu m$, the principal piece $\approx 50\mu m$, and the end piece $\approx 3\mu m$. The location $s = 0$ and $s = 62$ represent the tip of the head and the end of the tail, respectively. These values are analogous to the measurements of a human sperm [21]. The resulting $[Ca^{2+}]$ along the filament is plotted for different times as shown in Fig. 6.4. At $t = 1s$ in Fig. 6.4(a), the concentration is still at the resting (basal) level. After the 8-Br-cAMP is released at $t = 5s$,
the CatSper channels are open. Then, an increase in $[Ca^{2+}]$ is observed along the sperm length where the maximum concentration is recorded in the head region. The $[Ca^{2+}]$ for later times are also plotted in Fig. 6.4(b). It shows that when CatSper channels are closed, the clearance mechanism brings the $[Ca^{2+}]$ down and back to the resting level. Compared to Fig. 6.2 the solution curves in Fig. 6.4 vary more locally, which is due to the moving interface.

6.4 A Kirchhoff Rod with Calcium Model

In this Section, we study the swimming trajectories and beating patterns of a filament immersed in a Brinkman fluid coupled with the $Ca^{2+}$ model. The filament is discretized at the centerline using the KR model presented in Chapter 4. The emergent waveform is due to a preferred curvature function as

$$\Omega_1(s, t) = -bk^2 \sin(ks - \sigma t), \quad \Omega_2(s, t) = 0, \quad \Omega_3(s, t) = 0,$$  \hspace{1cm} (6.36)

where $k$ is the wavenumber, $\sigma$ is the frequency, and $b$ is the amplitude. As previously mentioned, the swimming pattern of spermatozoa is affected by the presence of $Ca^{2+}$ in the flagellum. To incorporate the $Ca^{2+}$ into our model, we modify the amplitude $b$ as a $Ca^{2+}$ dependent function as

$$b = b_m \frac{C(s, t)}{C(s, t) + k_A},$$  \hspace{1cm} (6.37)
where $C(s,t)$ represents the $[Ca^{2+}]$, $b_m$ is the maximum amplitude and is assumed to be a positive constant. The coefficient $k_A$ is determined as follows

$$k_A = \begin{cases} 
  k_+, & \Omega_1(s,t) > 0 \\
  k_-, & \Omega_1(s,t) < 0 
\end{cases} \quad (6.38)$$

where $k_{\pm}$ are positive constants. The way $k_A$ is set up allows the rod to have an asymmetry in the bending. The KR is, thus, able to bend with a larger amplitude in one direction. We use the transport-reaction-diffusion equations in Eqs. (6.34) to (6.35) to model the $[Ca^{2+}]$ and $IP_3$ concentration. This preferred amplitude and curvature with $Ca^{2+}$ dependence has previously been used for an Euler elastic in a Stokes fluid [17].

### 6.4.1 Algorithm

The numerical algorithm of a KR model is detailed in Section 4.4. Here, we modify the algorithm to include $Ca^{2+}$ and $IP_3$ in the system. The rod is initialized as a straight configuration $X(s,t)$ and is discretized using a centerline approximation with $N$ immersed boundary points. We denote $(\cdot)^n_k$ to be the variable $(\cdot)$ at the $n^{th}$ time step and $k^{th}$ point where $k = 1, \cdots, N$.

Given $X^n, C^n$ and $P^n$:

1. Evaluate the curvature function using Eq. (6.36).

2. Calculate the internal torque and internal force as in Eqs. (4.36) to (4.37) and evaluate the torque and force exerted on the fluid by the rod using Eqs. (4.39) to (4.40).

3. Solve the local linear and angular fluid velocity using Eqs. (4.41) to (4.42).

4. Update the location of the rod $X^{n+1}_k$ and its orthonormal triads as in Eqs. (4.43) to (4.44).

5. Solve $C^{n+1}_k$ and $P^{n+1}_k$ using the transport-reaction-diffusion equations in Eqs. (6.34) to (6.35).

### 6.4.2 Numerical Study

In this section, we study the effects of $[Ca^{2+}]$ on the swimming patterns of a sperm flagellum idealized as a KR. The length of the rod is $L = 62\mu$m and is discretized using a centerline approximation with 311 immersed boundary points. The stiffness coefficients are $a_i = 0.1$ and
b_i = 0.06. The wavelength is chosen to be \( \lambda = 20 \ \mu m \) and the permeability is \( \gamma = 1 \). The initial [Ca^{2+}] is 1 \( \mu M \). The maximum amplitude \( b_m = 4.5 \ \mu m \) and the coefficient \( k_A \) is equal to 0.3 \( \mu m \) when \( \Omega_1(s,t) < 0 \) and 0.5 \( \mu m \) when \( \Omega_1(s,t) > 0 \). All others parameters of the Ca^{2+} model are shown in Table 6.1. The 8-Br-cAMP is released at \( t = 10^{-4} s \).

Figure 6.5: The locations of a swimmer at three different time points including \( t = 0.01 s \) (solid blue line), \( t = 1 s \) (dashed red line), and \( t = 2 s \) (solid green line). The length of the rod is \( L = 62 \ \mu m \), the wavelength is \( \lambda = 20 \ \mu m \), and the permeability is \( \gamma = 1 \). The black circle corresponds to the head of the swimmer showing the swimming direction.

Three snapshots of a moving filament are captured at \( t = 0.02 s \) (solid blue line), \( t = 1 s \) (dashed red line), and \( t = 2 s \) (solid green line) as shown in Fig. 6.5. The head of the sperm is at \( s = 0 \) and the tail is at \( s = 62 \). We note that the first point on the rod is enlarged to show the swimming direction which is initially set from right to left. At \( t = 0.02 s \), the rod becomes a sine wave but it still stays at the initial location. At \( t = 1 s \), the rod moves in the south-west direction relative to the original position. This indicates that the swimming trajectory of the sperm is no longer linear. When the simulation reaches \( t = 2 s \), the rod heads south even further. The trace of the first point of a swimming rod is shown in Fig. 6.6 which clearly indicates that it is not a
linear trajectory. The final time is at $t = 5s$. We also plot the pressure and the directional flow of the fluid at $t = 0.02s$ (Fig. 6.7(a)), $t = 1s$ (Fig. 6.7(b)), and $t = 2s$ (Fig. 6.7(c)). We can see the bending amplitude is different on one side of the rod versus the other. By looking at the segment in Fig. 6.7(b), we can see that the maximum of the concave part is higher compared to the minimum (in magnitude) of the convex curve. In Fig. 6.7(c), the amplitude of the first peak is smaller, in magnitude, compared to the amplitude of the second peak. The rod seems to have a flat segment right after the second peak. These observations indicate the asymmetrical bending along the length of the flagellum.

Next, we study the role of permeability in affecting the behavior of a sperm flagellum with an increased intracellular $[Ca^{2+}]$. The 8-Br-cAMP is released at $t = 10^{-4}s$, allowing $Ca^{2+}$ to enter the flagellum via the CatSper channel. The resulting swimming progression is shown in Fig. 6.8 for five different permeabilities including $\gamma = 0.01$ (dashed black line), $\gamma = 0.1$ (solid red line), $\gamma = 1$ (solid-dotted green line), $\gamma = 10$ (solid blue line), and $\gamma = 100$ (dashed orange line) at $T = 0.6s$. We note that results simulated are done separately and superimposed into the same figure for comparison. We observe that there is minimal movement in the cases of $\gamma = 0.01$ and $\gamma = 0.1$. Nevertheless, sinusoidal formation with very small amplitude can be seen

![Graphs showing flow field at different times](image)

(a) $t = 0.02s$  
(b) $t = 1s$  
(c) $t = 2s$

Figure 6.7: The flow field of a KR immersed in a Brinkman fluid with $Ca^{2+}$ is plotted for different times with (a) $t = 0.02s$, (b) $t = 1s$, and (c) $t = 2s$. The color bar represents the pressure. The head indicates the swimming direction of the rod.
when zooming in. The rods in these cases still stay at the initial location. In the other three cases ($\gamma = 100, 10, 1$), the emergent waveforms get closer to the preferred configuration and break away from the original position. These three rods head south and swim at different rates. The rod with $\gamma = 10$ seems to move faster than the other cases while the head of the rod with $\gamma = 100$ is at the lowest position compared to other rods. In all the cases, a nonlinear swimming trajectory is recorded and shown in Fig. 6.9. It shows that in the cases of $\gamma = 100$ and $\gamma = 10$, the rods are seen to have higher emergent amplitudes compared to the other cases. Minimal swimming progression is seen for the cases of $\gamma = 0.01$ (in black) and $\gamma = 0.1$ (in red) although the trajectory of the rod with $\gamma = 0.1$ indicates a nonlinear propulsion. These observations show that the resistance plays a big role in preventing and enhancing the progression of a swimmer. That is, for a larger resistance (a smaller permeability), a rod can only make small motions and can not reach a preferred configuration even if there is an increased $[Ca^{2+}]$ in the flagellum.

The rod of length $L = 62 \mu m$ and wavelength $\lambda = 50 \mu m$ is simulated for five different permeabilities at $t = 0.6 s$. The $8$-Br-cAMP is released at $t = 10^{-4} s$. The 8-Br-cAMP is released at $t = 0.6 s$. The rods of five different permeabilities are captured at $t = 0.6 s$ including $\gamma = 0.01$ (dashed black line), $\gamma = 0.1$ (solid red line), $\gamma = 1$ (solid-dotted green line), $\gamma = 10$ (solid blue line), and $\gamma = 100$ (dashed orange line) at $t = 0.6 s$. The 8-Br-cAMP is released at $t = 10^{-4} s$.

Figure 6.8: Rods of five different permeabilities are captured at $t = 0.6 s$ including $\gamma = 0.01$ (dashed black line), $\gamma = 0.1$ (solid red line), $\gamma = 1$ (solid-dotted green line), $\gamma = 10$ (solid blue line), and $\gamma = 100$ (dashed orange line) at $t = 0.6 s$. The 8-Br-cAMP is released at $t = 10^{-4} s$.

Figure 6.9: Nonlinear trajectory of rods with five different permeabilities at time $t = 0.6 s$. Simulations are done separately and put together for comparison including $\gamma = 0.01$ (in black), $\gamma = 0.1$ (in red), $\gamma = 1$ (in green), $\gamma = 10$ (in blue), and $\gamma = 100$ (in orange).
permeabilities ranging from 0.01 to 100. The stiffness coefficients $a_i = 0.1$ and $b_i = 0.06$ (CAL1) and $a_i = 1$ and $b_i = 0.6$ (CAL2) are used. As described in Section 5.2.3, these stiffness coefficients are representative of different species of sperm. We compare the behavior of the flagella for two different sets of stiffness coefficients in the case of $\gamma = 100$ (or $\alpha = 0.01$) as shown in Fig. 6.10. The 8-Br-cAMP is also released at $t = 10^{-4}$ s in all the simulations. We denote L1 and L2 to be rods with stiffness coefficients CAL1 and CAL2, respectively. At $t = 0.012$s (Fig. 6.10(a)), L1 shows no movement along the length while L2 starts having some bending that forms the sinusoidal pattern. In Fig. 6.10(b) at $t = 0.12$s, we can clearly see the sine curve formed for L2 while there is minimal movement for L1. The emergent waveform of L2 is rather asymmetrical, with the maximum amplitude of the peak near the head being smaller than the maximum amplitude of the peak near the tail. Both rods are still at the initial location at this time point. At $t = 0.6$s, L2 breaks away from the initial position and heads south with
a nonlinear trajectory recorded and shown in Fig. 6.11. It shows that the trajectory of L2 is nonlinear while there is insignificant movement for L1. That means, the stiffness coefficients affect the swimming pattern of rods with added \([Ca^{2+}]\). In addition to the nonlinear swimming progression, we also see that the rod with \(\gamma = 100\) makes a figure-of-eight motion at the first point, which is interesting since we did not observe this phenomenon for the cases of swimming flagella with no \([Ca^{2+}]\) dependence.
Chapter 7

Discussion and Future Research

7.1 Discussion

In this dissertation, we have analyzed the swimming speeds of an infinite-length cylinder propagating planar and spiral bending waves. The cylinder is immersed in a fluid governed by the Brinkman equation which is used to describe the flow in a porous medium. Our model is motivated by the undulatory locomotion of microscopic organisms such as spermatozoa. Thus, we focus our analysis on the case where the sperm radius is smaller than the distance between the fibers embedded in the medium. These fiber networks or obstacles are also assumed to be stationary and of low volume fraction. The solutions are derived asymptotically where the amplitude is assumed to be much smaller than the radius of the circular cross-section of the cylinder. We find that up to second order expansions, the propulsion in the planar and spiral bending cases are enhanced with larger fluid resistance for specific combinations of wavenumber, cylinder thickness, and permeability. We also include the biological applications in Section 2.4 that show swimming enhancement for different species of spermatozoa. We see that the mesh spacing is larger than the thickness of the cylinder, allowing enough room for the swimmer to navigate between stationary fibers. We note that the corresponding swimming speeds in Stokes flow are recovered when the resistance approaches zero [34].

In addition, we compare the ratio of the swimming speeds of the 3D cylinder with the 2D sheet in a Brinkman fluid. We found that the ratio varies greatly decreasing from 0.8 to 0.1 as the scaled resistance increases. The greater the scaled resistance $\alpha/k$ is, the more significant it affects the swimming speed of the 3D cylinder (in comparison to the 2D sheet). The analysis is
important in understanding the potential contributions of the rotational effects into the overall swimming velocity and the differences between 2D and 3D swimming.

We also examine the ratio of the 3D cylinder in a Brinkman fluid with the one in Stokes flow. We see that the ratio is inversely proportional to an increase of the scaled resistance. That means, the stationary obstacles within the Brinkman fluid enhance the swimming velocity relative to the Stokes case. Leshansky [31] also observed an enhancement in swimming speeds of a 2D sheet in a Brinkman fluid compared to the Stokes case. In contrast to a viscoelastic fluid, the swimming speeds of the sheet and cylinder are slower relative to the Stokes case [42, 43, 44].

In this asymptotic analysis, we have assumed prescribed kinematics. When the cylinder thickness satisfies the inequality in Eq. (2.66), the cylinder requires more work to maintain planar bending for a larger resistance or smaller permeability. An increase in work done is an important factor in designing artificial microswimmers in a porous medium [88]. This could also be a constraint on reaching higher swimming speeds in fluids with larger resistance. Since the asymptotic analysis was based on prescribed kinematics, it is possible to obtain higher swimming speeds in fluids with more fibers (small permeability $\gamma$). However, in reality, it may not be possible because microorganisms are not able to produce that much work to maintain their bending at such small permeability. Thus, we want to look at the swimming speeds when the work is fixed. From Eq. (2.45) we let $W_\infty = W/\mu \pi U^2$ be the nondimensional work, then Eq. (2.37) can be written in terms of $W_\infty$ as

$$\frac{U_\infty}{U} = \frac{1}{2} W_\infty \left[ k_0(\zeta_1) - \frac{1}{2} \left( \frac{k^2}{\alpha^2} + 1 \right) \log \left( 1 + \frac{\alpha^2}{k^2} \right) \right].$$

We fix $\zeta_1$ to be $\zeta_1 = 0.03 \ll 1$ and consider three different fixed values of $W_\infty$ as 0.15, 0.2, 0.25. Fig. 7.1 shows the relation between the nondimensional swimming speed $U_\infty/U$ and the scaled resistance $\alpha/k$. We observe that for fixed values of work, as the work increases, the swimming speeds also increase. However, as the scaled resistance increases, the swimming speed decreases. This is different from what we have observed in Chapter 2 where for small permeability (large resistance) the swimming speed must increase. This is not a contradiction to our analysis. Rather, it gives a different perspective that swimmers in fluids with small permeability can not swim faster if a significant increase in work can not be generated by the swimmers.

We have compared our asymptotic solutions to computational results of finite-length swim-
mers with prescribed kinematics using the MRB. The asymptotic swimming speeds match well with the computations for cylinders of longer length. Although the asymptotic analysis is able to capture the trends of swimming speed in terms of the dependence on permeability and amplitude, it overestimates the swimming speed for shorter length filaments. This is important to consider when using asymptotic swimming speeds to make predictions of the behavior of finite-length swimmers. We have also observed that the analytical results overestimate the torque for a finite-length filament with a helical propagating wave.

For the computational study of a finite-length filament undergoing prescribed bending, we observed a large increase in angular velocity as the swimmer length decreases. Additionally, angular velocity increased linearly as amplitude increased for a fixed beat frequency. Sperm cells have been observed to ‘roll’ as they swim (simultaneous rotation of the sperm cell body and flagellum) \[89, 4\]. Specifically, human sperm were found to increase rolling from 1.5 Hz to 10 Hz and decrease amplitude as the viscosity of methylcellulose solutions was decreased \[4\]. In our computational study, angular rotation (rolling) varies linearly with amplitude and is much smaller than the experimental data. However, we are not accounting for the dynamics of a cell body and have prescribed kinematics. A study of 3D computational models of finite-length swimmers with cell bodies and emergent kinematics is of interest in the future to fully understand swimming speed and angular velocity as a function of the permeability.

In this dissertation, we also derive the linear and angular velocity of a KR immersed in a Brinkman fluid using the MRB. This is an extension of previous work for the case of a KR immersed in a Stokes fluid derived in \[50\]. This method allows the study of 3D finite-
length swimmers represented as a KR (neglecting the cell body). We find that the swimming speed depends on the resistance parameter $\alpha$. The evaluations of the velocity can be done by regularizing the fundamental solutions or by choosing a blob function. The velocity of a KR in Stokes flow are recovered as the resistance goes to zero.

The dynamics of an open elastic rod is studied using the KR model. The deformation of the rod varies due to the presence of the resistance parameter. In this implementation of the KR model, the preferred curvature and twist are chosen and deviations from the preferred configuration and the current rod configuration generate force and torque along the centerline of the rod. In the case of an elastic rod with a preferred helical configuration, larger resistances or smaller permeabilities make it more difficult for a rod to deform and achieve its preferred configuration. More bending and twisting energy are also required for rods with smaller permeability to reach the equilibrium configuration. In the case when $\alpha$ goes to zero, the behavior of the rod is the same as in Stokes flow [50]. Additionally, we find that the regularization parameter $\varepsilon$ can affect the performance of an elastic rod. For smaller $\varepsilon$, less bending and twisting energy are used to reach the equilibrium configuration. The regularization parameter is analogous to the radius of the rod. That means, a rod with smaller radius deforms to a preferred configuration faster. Stiffness coefficients also play a role in controlling the dynamics of the rod. Larger stiffness coefficients lead to a larger magnitude in the torque. Thus, the energy approaches zero faster than the rod with smaller stiffness coefficients. However, if the rod is too stiff, no motion is recorded.

In the case of a cylinder with a preferred curvature corresponding to a propagating sine wave, we match the asymptotic solutions of an infinite-length swimmer with a finite KR for various frequencies. The numerical swimming speed scales quadratically and matches well with the asymptotic solutions derived in Chapter 2. Depending on the length of the rod, the emergent amplitudes can get closer to the preferred amplitudes. Different methods to calculate the linear and angular velocity (regularizing the fundamental solutions and choosing a blob function) also give different results on emergent amplitudes with the latter method achieving an amplitude closer to the preferred amplitude.

Using a KR model, we next study the emergent waveforms of an idealized swimmer. We use parameters characteristic of human sperm and study a swimmer with a preferred curvature corresponding to a propagating planar sinusoidal wave. We use a preferred curvature that is
planar in our test cases because in experiments swimmers are observed to have a fairly planar waveform [21]. The study shows that for larger resistance, a rod is less likely to reach a preferred curvature or move away from the initial location. For a specific wavelength, the emergent waveforms can be different due to a specific combination of stiffness coefficients, permeability, and the wavelength of the rod. A figure-of-eight pattern at the end of the flagellum is observed for different permeabilities and different wavelengths. This pattern of movement is similar to previous experimental studies by Gray [90]. Rods with higher stiffness coefficients are more likely to display asymmetrical waveforms than rods that are less stiff. The swimming trajectory is linear for all the cases, which agrees with previous experiments by Ho et al. [14]. We also check that when initialized as a planar swimmer, the rod stays planar and does not go out of the plane. This is due to the fact that the blob is spread symmetrically along the rod.

We observe that the rod of wavelength $\lambda = 20\mu m$ in a Brinkman fluid with $\gamma = 1$ swims faster than other rods (Fig. 5.15). This is an interesting observation and may be explained as follows. In the fluid with high permeability (no fibers or $\gamma \to \infty$ or Stokes flow), the rods swim freely in a purely viscous fluid. When there is a small amount of fibers in the fluid, the fibers allow the sperm to work with the local flow in a way that gives an extra push to enhance the swimming velocity. As the permeability $\gamma$ gets smaller, the flow decays in a smaller region due to the screening length $\sqrt{\gamma} = 1/\alpha$. However, due to the incompressibility condition, the flow is larger in magnitude. In turn, it changes the magnitude of the vorticity. For instance, we use the numerical results in Section 5.2.3 to look at the vorticity of the flow in the $x$ direction for the cases of $\gamma = 100$ and $\gamma = 1$ as shown in Fig. 7.2. Notice that the color bar of the plots are at different scales representing different magnitudes of the vorticity. Clearly, the vorticity of flow when $\gamma = 1$ is stronger (in magnitude) than the one in the case of $\gamma = 100$. This is one reason why the rod in the fluid of $\gamma = 1$ achieves a higher swimming velocity compared to the flow of $\gamma = 100$. We note that the term $-\frac{5}{\gamma} \mathbf{u}$ in Eq. (1.4) is also called the damping force stress term [91]. When $\gamma$ is further decreased, the damping stress becomes dominant and the viscous shear stress effect is negligible [92]. This prevents forward progression of the swimmers. In addition, the screening length ($\sqrt{\gamma} = 1/\alpha$) is defined as a length around a swimmer over which a disturbance to the velocity would decay [36]. Thus, as the resistance $\alpha$ increases, $\sqrt{\gamma}$ decreases and the shear stress is generated over a very short distance [91]. This is one reason preventing swimmers in fluids with small permeabilities from reaching the preferred configuration.
Figure 7.2: The vorticity of the flow (in color) in the $x$ direction for the case of $\gamma = 100$ (left figure) and $\gamma = 1$ (right figure) at time $t = 0.36s$. The flow field (black arrows) is also plotted.

In the case of the preferred curvature model, as observed in Fig. 5.15, the rod in a fluid with permeability $\gamma = 1$ swims faster than other rods. On the other hand, we see that swimmers with prescribed kinematics have higher swimming velocity in a fluid with small permeability (Chapter 2). As observed in previous studies, the swimming speeds for finite-length swimmers undergo non-monotonic changes for planar swimmers where there is an increasing fluid resistance [45, 93]. In these studies, finite-length swimmers were not able to achieve large amplitude bending as the permeability is decreased. In addition, experimental studies in [4, 13] have shown that the emergent waveforms and swimming speeds vary greatly depending on the fluid environment. Thus, it is important to put the asymptotic results in the context of finite-length swimmers where certain ranges of bending kinematics are not observed in gels or fluids with small volume fractions of fibers. In addition, the efficiency of the swimmers in both of these models is of interest. The efficiency can be approximated by the square of the swimming speed over the power [51]. Further comparisons between the asymptotic solutions and KR swimmers in terms of efficiency, power, and velocity are of interest in the future.

We note that the KR in all the test cases are discretized using a centerline approximation. The use of the MRB allows the force to be spread in a small region around the rod creating a 3D cylinder with circular cross-section whose radius depends on $\varepsilon$. That means $\varepsilon$ can play the role of a numerical parameter (regularization parameter) or a physical parameter as the radius of the cylinder. Changing the permeability $\gamma$ or the resistance $\alpha$ also affects the performance of the solutions since the regulation function depends on $\gamma$ (or $\alpha$).
We discuss the effects of blob functions, regularization parameters, and resistances in detail as follows. The blob is a radially symmetrical function. It is more concentrated as $r \to 0$ and decays to zero as $r \to \infty$. We observe in Fig. 7.2 that the velocity field is more concentrated near the structure. Because our model assumes a 3D flow in an infinite fluid domain, the velocity decays to zero in the far field at a rate that is proportional to $\gamma / r^3$. In addition, the solution of the fluid velocity depends on the choice of a blob function and the regularization parameter $\varepsilon$. Different blob functions may give different results on and off the structure. In fact, when using two different blob functions, we spread the forces differently; thus, we expect to record different solutions for the velocity field. Cortez et al. [45] compared the numerical results obtained from a study of a sphere in a uniform Brinkman flow to the exact solution for two different blob functions with various resistances. The regularization parameters were chosen in the study such that the comparison between the two blob functions are fair [45]. The study showed that for a small $\alpha$, the numerical solutions do not have much difference on and off the structure and match up well with the analytical result. As the resistance grows, numerical solution from one blob function agrees better with the exact solution than the other. There are also differences between the numerical solutions from the two blob functions near the structure although both solutions decays to zero in the far field.

In general, the velocity field of the MRB is given in Eq. (5.1). This equation represents the superposition of the flow velocity generated by $N$ forces exerted on the fluid by a swimming filament. These forces are located along the filament. In this case, the velocity can be written in terms of an integral as [45]

$$u(x) = \int_{\Gamma} M_\varepsilon (x - x(s)) f(s) ds,$$

where $\Gamma$ represents the filament and $s$ is a segment along $\Gamma$. Eq. (5.1) can be seen as an approximation to the integral using a quadrature rule. Thus, in addition to a discretization error, the evaluation of the integral also introduces a quadrature error [48, 45]. A study of a translating sphere using the Method of Regularized Stokeslets by Cortez et al. [48] showed that when varying $\varepsilon$ and fixing the grid spacing $\Delta s$, the error is more accurate in the far field and less accurate near the sphere. A recent study on a 2D flow past a cylinder using the MRB showed the error of the velocity field depends on both $\varepsilon$ and the resistance $\alpha$ [46].
minimum computed error increases as $\alpha$ increases. We also make an observation that the error starts decreasing but ultimately grows larger as $\varepsilon$ increases \cite{10}. The study also investigated the effect of the regularized solutions $H_1^\varepsilon(r)$ and $H_2^\varepsilon(r)$ versus the singular solutions $H_1$ and $H_2$ on the computed errors. It would be interesting to further investigate the errors (discretization error and quadrature error) on and off a structure of a 3D test case with an exact solution to the Brinkman flow for different blob functions, regularization parameters, and permeabilities $\gamma$ (different test cases from \cite{45}). In the KR model, we want to study how $H_i^\varepsilon(r)$, $Q_i^\varepsilon(r)$, and $D_i^\varepsilon(r)$ ($i = 1, 2$) would affect the errors.

The swimming pattern of the sperm flagellum can also be determined by the presence of $[Ca^{2+}]$ along its length. In this dissertation, we also implement the 1D reaction-diffusion equations to account for the $Ca^{2+}$ and $IP_3$ to the preferred curvature. The swimming pattern and swimming trajectory of rods in fluids with different permeabilities are studied using the KR model. A nonlinear swimming trajectory is observed for all the simulations. The rod exhibits asymmetrical bending along its length. We also see that larger permeabilities allow the rods to swim and get to a preferred configuration easier. For smaller permeabilities (larger resistances), the flagella display little to no movement along the length. Stiffness coefficients also affect the behavior of rods with added $[Ca^{2+}]$. In the case of a rod with a longer wavelength, increasing stiffness coefficients allow the rod to deform and achieve a preferred configuration easier.

In terms of coding practice, it is sufficient to discretize the reaction-diffusion equations and transport-reaction-diffusion equations using the Crank-Nicolson method. However, the codes we created can be improved in terms of computational time. Thus, we are interested in exploiting the method of lines with stiff MATLAB solvers, which are optimally vectorized, to compare with our solutions. On the other hand, the discretization of these equations results in an implicit system that has to be solved at every time step. In addition, the solutions can not be computed in parallel. This can be very expensive for large systems. Therefore, to speed up the process, we need to look at other implicit methods. One such method is the Implicit Integration Factor (IIF) method \cite{94}. The IIF method is used to implement the reaction-diffusion equations. The method is shown to be robust and of second-order convergence, even with a very large time-step $\Delta t$ \cite{95,94}.
7.2 Future Research

The swimming trajectory and swimming pattern of an individual swimming flagellum are affected by the combination of wavelength, stiffness coefficients, the permeability of the Brinkman flow, and $[Ca^{2+}]$. Additionally, swimmers interact and feel each other through the flow. Synchronization of flagellar waveforms and attraction of swimmers have been observed and recorded [96]. Flagellar synchronization has also been studied asymptotically and numerically for Stokes flow [33, 97, 98, 99] and for a viscoelastic fluid [100]. Thus, it is interesting to investigate the swimming pattern and swimming trajectory of two or more swimming flagella in a Brinkman fluid. Here, we present some preliminary results of two swimming rods immersed in a Brinkman fluid for two different permeabilities. Two rods with length $L = 50 \mu m$ are discretized as straight configurations using the KR model. The vertical distance $d$ between the two rods is initialized at $d = 5 \mu m$ apart from one another with a phase shift equal to zero (two rods are swimming in-phase). The distance in time between the heads of the two swimmers is calculated and shown in Fig. 7.3 for $\gamma = 1$ (green solid line) and $\gamma = 100$ (blue solid line). The rods in the case of $\gamma = 100$ start attracting faster than the case of $\gamma = 1$. When time reaches $0.06s$, the distance $d$ in the case of $\gamma = 100$ gets smaller compared to the distance of the rods with $\gamma = 1$. This preliminary result shows that the permeability, in fact, affects the attraction of swimming flagella. Further numerical studies are needed to fully investigate attraction in a Brinkman fluid. In this test case, the two rods are placed in the same plane. After $t = 0.06s$, we observe no out-of-plane motion.

Figure 7.3: Distance between the first points of two rods for $t = 0 - 0.06s$ where the solid blue line represents a rod with $\gamma = 100$ and solid green line corresponds to a rod with $\gamma = 1$.

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We also run another simulation where three rods are positioned in a way that the endpoints form a triangle in the $X−Y$ plane as shown in Fig. 7.4. The simulation is done in a Brinkman fluid with $\gamma = 100$. The rods are discretized as straight configurations using the KR model with the same preferred planar sine curve. The initialization of the rods are such that the swimming and bending directions are in the $z$-axis and $y$-axis, respectively. After a short time ($t = 6 \times 10^{-4}$ s), the rods feel the presence of each other and start moving out of the plane. We draw this conclusion based on the non zero $x$ component of each of the three rods. The three rods continue displaying out-of-plane motion at later time points. This test case provides

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure7.4.png}
\caption{Three rods in a Brinkman fluid with $\gamma = 100$ are positioned such that the endpoints form a triangle in the $X−Y$ plane.}
\end{figure}

motivation for future work to understand how multiple swimmers react when positioned on two different planes that are perpendicular to one another. Further simulations should also be carried out when rods are initialized as sinusoidal curves instead of straight configurations.

Also in the future, we want to study the effects of phase shifts on the synchronization of the swimmers. The effects of $[Ca^{2+}]$ on the synchronization of the swimmers are also interesting to examine numerically. A recent study using the Method of Regularized Stokeslets has shown that the synchronization of 2D sheets occurs faster than 3D filaments in the case of a symmetric beatform [51]. We also want to look at the same problem using the MRB. In addition to numerical studies, we want to analyze the synchronization of the swimmers asymptotically for idealized 2D sheets and 3D cylinders.
Appendix A

A.1 Vector Calculus Identities

The following vector identities are used in the derivation of the regularized Brinkman equation for the KR model. We note that $\phi_\varepsilon(r)$ is the blob function, $B_\varepsilon(r)$ and $G_\varepsilon(r)$ relate to $\phi_\varepsilon(r)$ through Eq. (3.12). Also, $f_0$ and $m_0$ are the point force and point torque, respectively.

$$\nabla \cdot (f_0 \phi_\varepsilon) = \phi_\varepsilon \nabla \cdot f_0 + f_0 \cdot \nabla \phi_\varepsilon = f_0 \cdot \nabla \phi_\varepsilon. \quad (f_0 \text{ is a constant vector})$$

$$\frac{1}{2} \nabla \cdot [\nabla \times (m_0 \phi_\varepsilon)] = \frac{1}{2} \nabla \cdot (\phi_\varepsilon \nabla \times f_0 + \nabla \phi_\varepsilon \times f_0) = 0.$$ 

$$\nabla \times (m_0 B_\varepsilon(r)) = B_\varepsilon(r) \nabla \times m_0 + \nabla B_\varepsilon(r) \times m_0 = \nabla B_\varepsilon(r) \times m_0.$$ 

$$\nabla \times (m_0 G_\varepsilon(r)) = G_\varepsilon(r) \nabla \times m_0 + \nabla G_\varepsilon(r) \times m_0 = \nabla G_\varepsilon(r) \times m_0 = 0.$$ 

$$\nabla \times [(f_0 \cdot \nabla) \nabla B_\varepsilon(r)] = (f_0 \cdot \nabla) \nabla \times (\nabla B_\varepsilon(r)) + \nabla (f_0 \cdot \nabla) \nabla B_\varepsilon(r).$$ 

$$\nabla \times (f_0 \Delta B_\varepsilon(r)) = \nabla \times [f_0 \left( \alpha^2 B_\varepsilon(r) + G_\varepsilon(r) \right)] =$$ 

$$\alpha^2 \nabla \times (f_0 B_\varepsilon(r)) + \nabla \times (f_0 G_\varepsilon(r)),$$

$$= \alpha^2 (B_\varepsilon(r) f_0 + \nabla B_\varepsilon(r) \times f_0) + G_\varepsilon(r) f_0 + \nabla G_\varepsilon(r) \times f_0,$$

$$= \alpha^2 \nabla B_\varepsilon(r) \times f_0 + \nabla G_\varepsilon(r) \times f_0.$$ 

$$\nabla \times (\nabla B_\varepsilon(r) \times m_0) = \nabla \cdot (m_0 \nabla B_\varepsilon(r)) - \Delta B_\varepsilon(r) m_0.$$ 

$$\nabla \times (\nabla G_\varepsilon(r) \times m_0) = \nabla \cdot (m_0 \nabla G_\varepsilon(r)) - \Delta G_\varepsilon(r) m_0.$$
A.2 Finding $H_\epsilon^2(r)$ and $H_\epsilon'(r)$ from $B_\epsilon(r)$ in 3D Case

Consider the function $B_\epsilon(r) = \frac{1 - e^{\alpha R}}{4\pi \alpha^2 R^3}$. The first derivative $B_\epsilon'(r)$ is of the form

$$B_\epsilon'(r) = \frac{re^{-\alpha R}}{4\pi \alpha^2 R^3} (\alpha R - e^{\alpha R} + 1).$$

The second derivative is calculated as follows

$$B_\epsilon''(r) = -\frac{e^{-\alpha R}}{4\pi \alpha^2 R^5} \left[ \alpha^2 r^2 R^2 + (\varepsilon^2 - 2r^2)(e^{\alpha R} - 1) + \alpha R(2r^2 - \varepsilon^2) \right],$$

$$= -\frac{e^{-\alpha R}}{4\pi \alpha^2 R^5} \left[ \alpha^2 r^2 R^2 + R^2 e^{\alpha R} - 3r^2 e^{\alpha R} - R^2 + 3r^2 + 3\alpha r^2 R - \alpha R^3 \right],$$

$$= -\frac{e^{-\alpha R}}{4\pi \alpha^2 R^5} \left[ r^2 \left( \alpha^2 R^2 - 3e^{\alpha R} + 3 + 3\alpha R \right) + R^2 \left( e^{\alpha R} - 1 - \alpha R \right) \right].$$

We first need to calculate the value of $H_\epsilon^2(r)$ and then $H_\epsilon'(r)$. $H_\epsilon^2(r)$ in 3D has the form

$$H_\epsilon^2(r) = \frac{r B_\epsilon''(r) - B_\epsilon'(r)}{r^3},$$

$$= -\frac{e^{-\alpha R}}{4\pi \alpha^2 R^5 r^2} \left[ r^2 \left( \alpha^2 R^2 - 3e^{\alpha R} + 3 + 3\alpha R \right) + R^2 \left( e^{\alpha R} - 1 - \alpha R \right) \right] - \frac{1}{r^3} \frac{r e^{-\alpha R}}{4\pi \alpha^2 R^3} (\alpha R - e^{\alpha R} + 1),$$

$$= -\frac{e^{-\alpha R}}{4\pi \alpha^2 R^5} \left( \alpha^2 R^2 - 3e^{\alpha R} + 3 + 3\alpha R \right).$$

Then,

$$H_\epsilon'(r) = -\frac{e^{-\alpha R}}{4\pi \alpha^2 R^3} \left( \frac{3}{\alpha^2 R^2} + \frac{3}{\alpha R} + 1 \right) + \frac{3}{4\pi \alpha^2 R^5}.$$

Similarly, $H_\epsilon^1(r)$ can be written as

$$H_\epsilon^1(r) = -\frac{r B_\epsilon''(r) + B_\epsilon'(r)}{r},$$

$$= \frac{e^{-\alpha R}}{4\pi \alpha^2 R^5} \left[ r^2 \left( \alpha^2 R^2 - 3e^{\alpha R} + 3 + 3\alpha R \right) + R^2 \left( e^{\alpha R} - 1 - \alpha R \right) \right] - \frac{e^{-\alpha R}}{4\pi \alpha^2 R^3} (\alpha R - e^{\alpha R} + 1),$$

$$= -\frac{e^{-\alpha R}}{4\pi \alpha^2 R^5} \left( \alpha^2 R^2 - 3e^{\alpha R} + 3 + 3\alpha R \right) \varepsilon^2 + \frac{e^{-\alpha R}}{4\pi \alpha^2 R^5} R^2 \left( \alpha^2 R^2 - 3e^{\alpha R} + 3 + 3\alpha R \right)$$

$$- 2\frac{e^{-\alpha R}}{4\pi \alpha^2 R^5} R^2 \left( -e^{\alpha R} + 1 + \alpha R \right),$$

$$= \varepsilon^2 H_\epsilon^2 + \frac{e^{-\alpha R}}{4\pi \alpha^2 R^3} \left( \alpha^2 R^2 - e^{\alpha R} + 1 + \alpha R \right).$$
Then,

\[ H_1^\varepsilon(r) = \varepsilon^2 H_2^\varepsilon + \frac{e^{-\alpha R}}{4\pi \alpha^2 R} \left( \frac{1}{\alpha^2 R^2} + \frac{1}{\alpha R} + 1 \right) - \frac{1}{4\pi \alpha^2 R^3}. \]

### A.3 Coefficients

Since the velocity and the angular velocity depend on the choice of the blob function or the regularized version of \( B_\varepsilon(r) \), the explicit formula for \( u \) and \( \omega \) can be derived as follows. First, consider the linear velocity equation in (4.13)

\[ \mu u = (f_0 \cdot \nabla) \nabla B_\varepsilon - f_0 \Delta B_\varepsilon - \frac{1}{2} \alpha^2 \nabla B_\varepsilon \times m_0 - \frac{1}{2} \nabla G_\varepsilon \times m_0. \]

Each term on the RHS of \( u \) is calculated explicitly using \( \frac{\partial r}{\partial \hat{x}} = \hat{x} \) for \( \hat{x} = x - X_0 \) and \( r = |x - X_0| \).

Then,

\[
(f_0 \cdot \nabla) \nabla B_\varepsilon = f_0 \cdot \frac{\partial}{\partial \hat{x}} \left( \frac{\partial B_\varepsilon(r)}{\partial \hat{x}} \right) = f_0 \cdot \frac{\partial}{\partial \hat{x}} \left( B'_\varepsilon \frac{\hat{x}}{r} \right),
\]

\[
= f_0 \cdot \left( \hat{x} B''_\varepsilon(r) - \frac{\hat{x}}{r} B'_\varepsilon(r) \right),
\]

\[
= (f_0 \cdot \hat{x}) \frac{r B''_\varepsilon(r) - B'_\varepsilon(r)}{r} + f_0 \frac{B'_\varepsilon(r)}{r},
\]

\[
f_0 \Delta B_\varepsilon = f_0 \left( B''_\varepsilon(r) + \frac{2}{r} B'_\varepsilon(r) \right),
\]

\[
\nabla B_\varepsilon = B'_\varepsilon \frac{\hat{x}}{r},
\]

\[
\nabla G_\varepsilon = G'_\varepsilon \frac{\hat{x}}{r}.
\]

Substituting these evaluations into the linear velocity equation, we have

\[
\mu u = (f_0 \cdot \hat{x}) \hat{x} \frac{r B''_\varepsilon(r) - B'_\varepsilon(r)}{r^3} + f_0 \frac{B'_\varepsilon(r)}{r} - f_0 \left( B''_\varepsilon(r) + \frac{2}{r} B'_\varepsilon(r) \right)
\]

\[
- \frac{1}{2} \alpha^2 B'_\varepsilon(r) \frac{\hat{x}}{r} \times m_0 - \frac{1}{2} G'_\varepsilon(r) \frac{\hat{x}}{r} \times m_0,
\]

\[
= (f_0 \cdot \hat{x}) \hat{x} \frac{r B''_\varepsilon(r) - B'_\varepsilon(r)}{r^3} + f_0 \left( -B''_\varepsilon(r) - B'_\varepsilon(r) \right)
\]

\[
+ \frac{1}{2} \alpha^2 \left( m_0 \times \hat{x} \right) \frac{B'_\varepsilon(r)}{r} + \frac{1}{2} \left( m_0 \times \hat{x} \right) G'_\varepsilon(r) \frac{\hat{x}}{r}.
\]
Let,
\[ H_1^5(r) = -\frac{rB_z''(r) + B_z'(r)}{r}, \quad H_2^5(r) = \frac{rB_z''(r) - B_z'(r)}{r^3}, \]
\[ Q_1^5(r) = \frac{G_z'(r)}{r}, \quad Q_2^5(r) = \frac{B_z'(r)}{r}. \]

The linear velocity is
\[ \mu u = f_0H_1^5(r) + (f_0 \cdot \hat{x})\hat{x}H_2^5(r) + \frac{1}{2}(m_0 \times \hat{x}) [Q_1^5(r) + \alpha^2Q_2^5(r)]. \]

By following the same techniques used above for linear velocity, the angular velocity from (4.14) becomes
\[
\begin{align*}
\mu \omega &= \frac{1}{2} \alpha^2 f_0 \times \nabla B_z + \frac{1}{2} f_0 \times \nabla G_z - \frac{1}{4} \alpha^2(m_0 \cdot \nabla)\nabla B_z + \frac{1}{4} \alpha^2 \Delta B_z m_0 - \frac{1}{4} (m_0 \cdot \nabla)\nabla G_z + \frac{1}{4} \Delta G_z m_0,
\end{align*}
\]
\[
= \frac{1}{2} \alpha^2 (f_0 \times \hat{x}) \frac{B_z'(r)}{r} + \frac{1}{2} (f_0 \times \hat{x}) \frac{G_z'(r)}{r} - \frac{1}{4} \alpha^2 (m_0 \cdot \hat{x}) \hat{x} \frac{rB_z''(r) - B_z'(r)}{r^3}
+ \frac{1}{4} \alpha^2 \left( B_z''(r) + \frac{B_z(r)}{r} \right) m_0 - \frac{1}{4} (m_0 \cdot \hat{x}) \hat{x} \frac{rG_z''(r) - G_z'(r)}{r^3}
+ \frac{1}{4} \left( \phi_z - \frac{G_z'(r)}{r} \right) m_0 - (m_0 \cdot \hat{x}) \hat{x} \frac{rG_z''(r) - G_z'(r)}{r^3},
\]
Let
\[ D_1^5(r) = \phi_z(r) - \frac{G_z'(r)}{r} = \phi_z(r) - Q_1^5(r), \quad D_2^5(r) = -\frac{rG_z''(r) - G_z'(r)}{r^3}.
\]
Then,
\[
\begin{align*}
\mu \omega &= \frac{1}{2} (f_0 \times \hat{x}) [Q_1^5(r) + \alpha^2Q_2^5(r)] - \frac{1}{4} \alpha^2 [m_0H_1^5(r) + (m_0 \cdot \hat{x})\hat{x}H_2^5(r)] + \frac{1}{4} [m_0D_1^5(r) + (m_0 \cdot \hat{x})\hat{x}D_2^5(r)].
\end{align*}
\]
A.4 The Linear and Angular Velocity and Coefficients When $\alpha \rightarrow 0$

The equations of the linear and angular velocity of a KR in a Brinkman fluid are given in Chapter 4 as

$$\mu u = f_0 H_1^\varepsilon (r) + (f_0 \cdot \hat{x}) \hat{x} H_2^\varepsilon (r) + \frac{1}{2} (m_0 \times \hat{x}) \left[ Q_1^\varepsilon (r) + \alpha^2 Q_2^\varepsilon (r) \right],$$
$$\mu \omega = \frac{1}{2} (f_0 \times \hat{x}) \left[ Q_1^\varepsilon (r) + \alpha^2 Q_2^\varepsilon (r) \right] - \frac{1}{4} \alpha^2 [m_0 H_1^\varepsilon (r) + (m_0 \cdot \hat{x}) \hat{x} H_2^\varepsilon (r)] + \frac{1}{4} [m_0 D_1^\varepsilon (r) + (m_0 \cdot \hat{x}) \hat{x} D_2^\varepsilon (r)],$$

where the coefficients $H_i^\varepsilon (r)$, $Q_i^\varepsilon (r)$, and $D_i^\varepsilon (r)$ for $i = 1, 2$ are given as

$$H_1^\varepsilon (r) = - \frac{r B''_1 (r) + B'_1 (r)}{r}, \quad H_2^\varepsilon (r) = \frac{r B''_2 (r) - B'_2 (r)}{r^3},$$
$$Q_1^\varepsilon (r) = \frac{G'_1 (r)}{r}, \quad Q_2^\varepsilon (r) = \frac{B'_1 (r)}{r},$$
$$D_1^\varepsilon (r) = \phi_r (r) - \frac{G'_1 (r)}{r} = \phi_r (r) - Q_1^\varepsilon (r), \quad D_2^\varepsilon (r) = - \frac{r G''_2 (r) - G'_2 (r)}{r^3}.$$ 

As previously mentioned, the coefficients can be calculated in two different ways either by regularizing the fundamental solutions as in Section 3.2 or by selecting an appropriate blob function presented in Section 3.3. When $\alpha \rightarrow 0$, the linear and angular velocity become

$$\mu u = f_0 H_1^\varepsilon (r) + (f_0 \cdot \hat{x}) \hat{x} H_2^\varepsilon (r) + \frac{1}{2} (m_0 \times \hat{x}) Q_1^\varepsilon (r),$$
$$\mu \omega = \frac{1}{2} (f_0 \times \hat{x}) Q_1^\varepsilon (r) + \frac{1}{4} [m_0 D_1^\varepsilon (r) + (m_0 \cdot \hat{x}) \hat{x} D_2^\varepsilon (r)].$$

These two equations are precisely the linear and angular velocity of a KR immersed in Stokes flow, which were previously derived in [50]. We now use two approaches to calculate the remaining coefficients in the velocity equations

A.4.1 Regularizing the Fundamental Solutions

When $\alpha \rightarrow 0$, the coefficients in Section 4.3.1 become

$$H_1^\varepsilon (r) = \frac{r^2 + 2 \varepsilon^2}{8 \pi (r^2 + \varepsilon^2)^{3/2}}, \quad H_2^\varepsilon (r) = \frac{1}{8 \pi (r^2 + \varepsilon^2)^{3/2}}, \quad Q_1^\varepsilon (r) = \frac{2 \varepsilon^2 + 5 \varepsilon^2}{8 \pi (r^2 + \varepsilon^2)^{3/2}}.$$


\[
D_1^\varepsilon(r) = \frac{-2r^4 - 7r^2\varepsilon^2 + 10\varepsilon^4}{8\pi(r^2 + \varepsilon^2)^{7/2}}, \quad D_2^\varepsilon(r) = \frac{3(2r^2 + 7\varepsilon^2)}{8\pi(r^2 + \varepsilon^2)^{7/2}}.
\]

These coefficients are the same as those derived in [50]. That means, when \( \alpha \to 0 \), the problem is to solve the linear and angular velocity of a KR in Stokes flow by selecting the blob function of the form

\[
\psi_\varepsilon(r) = \frac{15\varepsilon^4}{8\pi(r^2 + \varepsilon^2)^{7/2}}
\]
as in [50].

### A.4.2 Selecting a Blob Function

When \( \alpha \to 0 \), the coefficients in Section 4.3.2 become

\[
H_1^\varepsilon(r) = \begin{cases} 
\frac{1}{4\pi^{3/2}} e^{-r^2/\varepsilon^2} + \frac{1}{8\pi} \text{erf}\left(\frac{r}{\varepsilon}\right) & r > 0 \\
\frac{1}{2\pi^{3/2}} & r = 0
\end{cases},
\]

\[
H_2^\varepsilon(r) = \begin{cases} 
\frac{1}{8\pi^{3/2}} \left[ -\frac{2r}{\varepsilon} e^{-r^2/\varepsilon^2} + \sqrt{\pi} \text{erf}\left(\frac{r}{\varepsilon}\right) \right] & r > 0 \\
\frac{1}{6\pi^{3/2}} & r = 0
\end{cases},
\]

\[
Q_1^\varepsilon(r) = \begin{cases} 
\frac{e^{-r^2/\varepsilon^2}}{4\pi^{3/2} \varepsilon^3} (-2r\varepsilon^2 + 2r^3) + \frac{1}{4\pi r^3} \text{erf}\left(\frac{r}{\varepsilon}\right), & r > 0 \\
\frac{5}{6\pi^{3/2} \varepsilon^3} & r = 0
\end{cases},
\]

\[
D_1^\varepsilon(r) = \begin{cases} 
\frac{-e^{-r^2/\varepsilon^2}}{4\pi^{3/2} \varepsilon^3 \varepsilon^5} (-2r\varepsilon^4 - 8r^3\varepsilon^2 + 4r^5) - \frac{1}{4\pi r^3} \text{erf}\left(\frac{r}{\varepsilon}\right), & r > 0 \\
\frac{5}{3\pi^{3/2} \varepsilon^3} & r = 0
\end{cases},
\]

\[
D_2^\varepsilon(r) = \begin{cases} 
\frac{e^{-r^2/\varepsilon^2}}{4\pi^{3/2} \varepsilon^3 \varepsilon^5} (-6r\varepsilon^4 - 4r^3\varepsilon^2 + 4r^5) + \frac{3}{4\pi r^3} \text{erf}\left(\frac{r}{\varepsilon}\right), & r > 0 \\
\frac{7}{5\pi^{3/2} \varepsilon^3} & r = 0
\end{cases}.
\]

This means, when \( \alpha \to 0 \), the problem becomes solving the linear and angular velocity of a KR in Stokes flow by selecting the blob function of the form

\[
\phi_\varepsilon(r) = \frac{1}{\pi^{3/2} \varepsilon^2} \left( \frac{5}{2} - \frac{r^2}{\varepsilon^2} \right) e^{-r^2/\varepsilon^2}.
\]

### A.5 A Rotation Matrix: Rodrigues Formula

We want to rederive an axis-angle rotation matrix \( R(e, \theta) \). This matrix is called the Rodrigues rotation matrix, which maps one vector to another around the \( e \)-axis and about an angle \( \theta \) [71].
Both $e$ and $\theta$ depend on the angular velocity as
\[
e = \frac{\omega (X^n_k)}{\|\omega (X^n_k)\|}, \quad \theta = \|\omega (X^n_k)\| \Delta t.
\]

Without loss of generality, we only illustrate the rotation on $(D^1_k)^n$, vector $D^1$ at $n^{th}$ time step and $k^{th}$ point. The rotations for other vectors can be carried out in a similar fashion. For simplicity, we let $r_n = (D^1_k)^n$ and $r_{n+1} = (D^1_k)^{n+1}$. The rotation from $r_n$ to $r_{n+1}$ as shown in Fig. A.1a) is written as
\[
r_{n+1} = r_n + v,
\]
where $v$ can be determined as follows.

*Figure A.1: (a) The plot of a rotation from vector $r_n$ to $r_{n+1}$. (b) A closer view of the triangle ABC.*

From Fig. A.1b), $v$ is decomposed into the tangential ($v_\parallel$) and normal ($v_\perp$) components as $v = v_\parallel + v_\perp$. Each component can be written explicitly as
\[
v_\parallel = \frac{\|v_\parallel\|}{\|e \times r_n\|} (e \times r_n),
\]
where $\|v_\parallel\| = R \sin \theta$ for $R$ is the length of the segment $BC$. The segments $BC$ and $AC$ have
the same length $R$. But, from Fig. A.1(a), $\|e \times r_n\| = \|r_n\| \sin \theta = R$. Thus, $v_\parallel$ becomes

$$v_\parallel = \sin \theta (e \times r_n).$$

Also, from Fig. A.1, the normal component of $v$ is written as

$$v_\perp = \frac{\|v_\perp\|}{\|e \times r_n\|} (e \times (e \times r_n)).$$

But, $\|e \times r_n\| = R$ and $\|v_\perp\| = R(1 - \cos \theta)$, then

$$v_\perp = (1 - \cos \theta) (e \times (e \times r_n)).$$

Substituting $v = v_\parallel + v_\perp$ back to Eq. (A.1) and considering the identity $(e \times (e \times r_n)) = (e \cdot r_n)e - r_n$, we have

$$r_{n+1} = r_n + \sin \theta (e \times r_n) + (1 - \cos \theta) ((e \cdot r_n)e - r_n),$$

$$= \cos \theta r_n + (1 - \cos \theta)(e \cdot r_n)e + \sin \theta (e \times r_n),$$

$$= \cos \theta r_n + (1 - \cos \theta)ee^T r_n + \sin \theta (e \times r_n),$$

$$r_{n+1} = R(e, \theta)r_n.$$  

Or,

$$\begin{align*}
(D^k)^{n+1} &= R(e, \theta)(D^1)^n, \\
\end{align*}$$

where $R(e, \theta) = (\cos \theta)I + (1 - \cos \theta)ee^T + \sin \theta(e \times)$ and $I$ is the $3 \times 3$ identity matrix.
Bibliography


