Modeling and Simulation of Elastic Rods with Intrinsic Curvature and Twist Immersed in Fluid

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Abstract

Understanding the dynamics of thin elastic rods that are immersed in fluid is fundamental in explaining many problems that arise in biology, physics and engineering. Solving the coupled system of rod-fluid in 3D is usually very costly, however in case of low Reynolds number, the three-dimensional problem can be reduced a one-dimensional problem on the centerline of the rod. In this thesis we examine the method of regularized Stokeslets which is a numerical algorithm for an elastic rod immersed in viscous, incompressible fluid at zero Reynolds number governed by Stokes equations. In this method, the elastic rod is represented by a space curve corresponding to the centerline of the rod. In addition, an orthonormal triad is varying along the curve, with one vector being tangent to the curve, and the others describing the material twist. The model that is used for the elastic forces based on this, allows for natural configurations for the rods that are far from straight, as described by curvature and torsion. In this way, the basic or equilibrium configuration for the rod can be e.g. a helix. The linearity of Stokes equations allows us to evaluate the linear and angular fluid velocity only at centerline of the rod. We also examine the dependency to the numerical parameters together with the accuracy and convergence properties of the method. As a bench mark, we compare the numerical result of this method to those produced by the non-local slender body method for the case of elastic rods with no intrinsic curvature and twist inside a planar shear flow. We also present the simulation of the extension of helical rods when they are placed within a constant background flow and we provide a fast converging formula for the periodic summation of the fundamental solutions to the Stokes equations.
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I dedicate this thesis to my parents, Alireza and Homa, who never stopped believing in me.
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Chapter 1

Introduction

Modeling thin, rod-like flexible structures that are immersed in fluid can help in understanding many problems that arise in biology and physics. For example, the helical growth of filaments of the bacterium *Bacillus subtilis* [10] and in structural deformation and super-coiling of DNA [13, 14]. Kirchhoff’s rod theory [3] has been employed to study these phenomena. In this theory, the rod is described as a three-dimensional space curve together with an orthonormal triad at each material point that captures the local orientation of the material. While the fluid environment is considered in more recent studies [8, 11, 9, 2, 16], many related works focus on studying bent and twisted rods in the absence of any environment [4, 5, 15].

The above mentioned applications highlight the importance of including the interaction with viscous fluids in the modeling of rod dynamics. One method that has been employed to study the rod-fluid interactions is known as the Immersed Boundary method (IB) which was originally introduced by C. Peskin to study the flow patterns around heart valves. The method is based on a mixture of Eulerian scheme for discretizing the fluid equations and Lagrangian scheme for rod discretization [9, 8]. However, since the fluid is governed by the full Navier-Stokes equations, the cost of computation increases specially in three dimensional setting. In case of low Reynolds number this disadvantage can be overcome by considering the fundamental solutions to Stokes equations. The non-local slender body formulation is another method that was used for modeling fluid-filament interactions in zero Reynolds number [16]. In this method the three-dimensional problem is reduced to a one-dimensional problem on the centerline of the rod. The number of discretization points to obtain the desired resolution is much smaller than the IB method, yielding a lower computation cost. However, one drawback of this method is that the twist forces are neglected.

In this thesis we will consider the regularized Stokes model [8, 9, 13, 11, 2], where the structure of the immersed rod is described with a variation of Kirchhoff’s rod theory. The naturally bent and twisted rods are modeled in such a way that any deviation from the equilibrium configuration, produces internal forces and torques that drive the rod back to its natural shape. By using the linearity of Stokes
equations the local linear and angular velocity of the fluid can be represented as the superposition of regularized fundamental solutions. This will allow us to evaluate the linear and angular fluid velocity only at the centerline of the rod. The no-slip velocity conditions will then determine the linear and angular velocity of the rod. We will provide a comprehensive procedure to apply this method using test cases of relaxation of naturally bent and twisted open and closed rods.

This thesis is organized as following: Chapter 2 presents a mathematical model for the dynamics of the rod and discusses the coupling with the fluid using the regularized Stokeslets formulation. It then describes the non-dimensionalization of the coupled system. In Chapter 3 the discretization of equations for fluid-rod interaction is discussed and a step-by-step numerical scheme is presented. This chapter is continued with a validation of the method compared to the existing literature for relaxation of naturally twisted and curved open/closed rods. In chapter 4, as a benchmark, we compare the regularized Stokes method with non-local slender body formulation for the dynamics of elastic rods with no curvature and twist in planar shear flow. We will follow this chapter by investigating the extension of a helical rod in a constant background flow. In chapter 5 we will derive an Ewald summation formula for regularized fundamental solutions to Stokes equations in case of periodic array of point forces.
Chapter 2

Mathematical Model

The purpose of this chapter is to present a mathematical model that describes the dynamics of an elastic rod with intrinsic curvature and twist in an incompressible fluid at zero Reynolds number (Stokes flow). When the rod is not at its equilibrium state, elastic forces will be generated that drive the rod towards that state and the elastic rod will interact with the fluid and create a fluid flow around it. In the case of an externally imposed fluid flow, the elastic forces compete with the strength of the externally imposed flow to yield the resulting dynamics.

2.1 Dynamics of an elastic rod with intrinsic curvature and twist

To study the dynamics of an elastic rod immersed in fluid we will hire a variation of the Kirchhoff model for elastic rods developed in [11, 9, 8].

A rod can be represented as a space curve $X(s)$ in $\mathbb{R}^3$ along with associated orthonormal triads $\{D^1(s), D^2(s), D^3(s)\}$ where $0 \leq s \leq L$ is a Lagrangian parameter which is initialized as arclength and $L$ is the length of the unstressed rod. We also assume that the cross section of the rod is circular with constant radius. In the classical Kirchhoff rod model the triads $\{D^1(s), D^2(s), D^3(s)\}$ form a material frame, such that $D^i \cdot D^j = \delta_{ij}$, $i, j = 1, 2, 3$ and one of them (usually $D^3$) is constrained to be aligned with the tangent vector to the rod $\partial X/\partial s$. However in our model we allow slight perturbations by adding a penalty energy to the rod’s elastic energy, so the rod will fulfill these constraints as it tends to reach its equilibrium state.

We denote $F$ and $N$ to be the force and the moment transmitted across the cross section of the rod that can be obtained by averaging the stress acting across that section [8]. Also let $f$ and $n$ be the force and torque density applied from the
fluid on the rod respectively. Balance of momentum and angular momentum yield,

\[ 0 = f + \frac{\partial F}{\partial s}, \tag{2.1} \]
\[ 0 = n + \frac{\partial N}{\partial s} + \left( \frac{\partial X}{\partial s} \times F \right), \tag{2.2} \]

For a detailed derivation of these equations, see [8]. We may expand these forces in the curvilinear basis \( \{ D^1, D^2, D^3 \} \) as,

\[ F = F^1 D^1 + F^2 D^2 + F^3 D^3, \tag{2.3} \]
\[ N = N^1 D^1 + N^2 D^2 + N^3 D^3, \tag{2.4} \]
\[ f = f^1 D^1 + f^2 D^2 + f^3 D^3, \tag{2.5} \]
\[ n = n^1 D^1 + n^2 D^2 + n^3 D^3. \tag{2.6} \]

Following [11], \( N^i \) and \( F^i \) are given by,

\[ N^i = a_i \left( \frac{\partial D^j}{\partial s} \cdot D^k - \Omega_i \right), \tag{2.7} \]
\[ F^i = b_i \left( D^i \cdot \frac{\partial X}{\partial s} - \delta_{3i} \right). \tag{2.8} \]

Here \((i, j, k)\) is any cyclic permutation of \((1, 2, 3)\), \(a_1\) and \(a_2\) are the bending moduli about \(D^1\) and \(D^2\) respectively, and \(a_3\) is the twisting modulus of the rod. Note that since we assume that the rod has a circular cross section with axially symmetric material properties then \(a_1 = a_2\). More over \(b_3\) is the extension modulus and the shear moduli of the rod are \(b_1\) and \(b_2\). By knowing \(F\) and \(N\), which are determined by the shape of the rod, one can obtain \(f\) and \(n\) using equations (2.5) and (2.6).

The vector \((\Omega_1, \Omega_2, \Omega_3)\) is defined as the strain vector where the intrinsic curvature is given as \(\kappa = \sqrt{\Omega_1 + \Omega_2}\) and \(\Omega_3\) is the intrinsic twist of the rod. When the strain vector is \((0, 0, 0)\) the open rod is straight and untwisted at the relaxed state, while if both the intrinsic curvature and twist are nonzero, the equilibrium state is a helix. By not considering the variations under translation and rotation, the helical shape of a rod at relaxed state can be determined by the vector \((\kappa, \Omega_3)\).

As explained in [8] the relations above are obtained from a variational argument of the following elastic energy,

\[ E = \frac{1}{2} \int_0^L \left[ \sum_{i=1}^3 a_i \left( \frac{\partial D^j}{\partial s} \cdot D^k - \Omega_i \right)^2 + \sum_{i=1}^3 b_i \left( D^i \cdot \frac{\partial X}{\partial s} - \delta_{3i} \right)^2 \right] \tag{2.9} \]

It is observed that in contrast to Kirchhoff rod theory, we do not strictly enforce the constraint that \(D^3\) is to be aligned with the tangent vector to the rod. Instead, deviation of \(D^3\) from \(\partial X/\partial s\) is penalized, and the orthogonality of \(D^1\) and \(D^2\) to \(\partial X/\partial s\) is enforced in the same way, as seen in equation (2.9).
In addition to enforcing $D^3$ to align with $\partial X/\partial s$, equation (2.9) also enforces,

$$||\partial X/\partial s|| = 1.$$ 

Again, this is done with penalization, and will allow for small deviations. Hence, the standard Kirchhoff’s rod model will be obtained as $b_i \to \infty$.

In several studies of naturally straight elastic rods, i.e. of rods without intrinsic curvature and twist, the orthonormal triads are not introduced, and the rod is solely described by the coordinates of the centerline, $X(s,t)$ [16, 6]. In this case, the torque is set to zero, and the force is given as

$$f(s) = -\frac{\partial}{\partial s} \left( T(s) \frac{\partial}{\partial s} X(s) \right) + E \frac{\partial^4}{\partial s^4} X(s), \quad (2.10)$$

where $T$ is the line-tension of the rod, which acts as a Lagrange multiplier to enforce the in-extensibility. It can be shown that the Kirchoff rod model presented here reduces to this model for naturally straight rods $\Omega_1 = \Omega_2 = \Omega_3 = 0$, in the case of zero twist modulus ($a_3 = 0$), i.e. when the effect of twist is neglected. For more details see Appendix D.

## 2.2 Regularized Stokes formulation

Following the mathematical modeling of an elastic rod described in section 2.1, in this section we try to couple the rod with incompressible fluid. In the low Reynolds number regime, where viscous forces dominate, we may assume that the dynamics of the fluid is described by the incompressible Stokes equation. We then can use the linearity of these equations to derive the exact solution, described by the fundamental solutions namely *Stokelets, Rotlets* and *Doublets*. However, the fundamental solutions have singularities and the solution of associated integral equations require specialized quadrature. In this thesis, the method of regularized Stokeslets is used, which avoids this difficulty.

In this section we will derive the exact regularized solution to incompressible Stokes equations for a single immersed point force and torque in three dimensions similar to derivations in [11, 2] and then generalize it for the case of concentrated forces and torques along a curved rod.

We assume that the dynamics of the fluid is described by the incompressible Stokes equations,

$$0 = -\nabla p + \mu \Delta u + f^b, \quad (2.11)$$

$$0 = \nabla \cdot u. \quad (2.12)$$

Here $\mu$ is the fluid viscosity, $u$ is the fluid velocity, $p$ is the fluid pressure, and $f^b$ is the body force which is the force per unit volume applied to the fluid by the immersed body. Equation (2.12) enforces the incompressibility of the fluid.
Furthermore the local angular velocity of the fluid, \( w \), can be calculated from the local linear velocity using the following relation,

\[
w = \frac{1}{2} \nabla \times u.
\]  

(2.13)

The body force for a regularized point force and torque applied to the fluid has the following form:

\[
f^b(x) = f_0 \phi_\epsilon(x - X_0) + \frac{1}{2} \nabla \times n_0 \phi_\epsilon(x - X_0),
\]  

(2.14)

where \( f_0 \) and \( n_0 \) are the point force and point torque applied to the fluid at \( X_0 \). The cutoff function or blob function \( \phi_\epsilon \) is a radially symmetric and smooth approximation of the three-dimensional Dirac distribution centered at \( X_0 \), with the following property:

\[
\int_{\mathbb{R}^3} \phi_\epsilon(x - X_0) \, d^3x = 1,
\]  

(2.15)

The point force or torque is spread to a region centered at \( X_0 \) by the blob function \( \phi_\epsilon \). Here are examples of three-dimensional cut-off functions with infinite support which are used in this report,

\[
\phi_\epsilon(r) = \frac{15 \epsilon^4}{8 \pi (r^2 + \epsilon^2)^{7/2}},
\]  

(2.16)

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

(2.17)

Here \( r = ||x - X_0|| \) and the parameter \( \epsilon \) is a small parameter that controls the radius of the effective spreading region of the point force and torque. In figure 2.1, a graph of the blob function in equation (2.16) is presented for different values of \( \epsilon \). Note that due to the property given in equation (2.15), as \( \epsilon \) decreases the height of the blob function increases and we recover the Dirac delta function as \( \epsilon \to 0 \).

For any given blob function we can define the corresponding regularized Green’s functions,

\[
\Delta^2 B_\epsilon(r) = \Delta G_\epsilon(r) = \phi_\epsilon(r).
\]  

(2.18)

By taking the divergence of equation 2.11 we get:

\[
0 = -\Delta p + \nabla \cdot (\mu \Delta u) + \nabla \cdot (f_0 \phi_\epsilon(r)) + \nabla \cdot \left( \frac{1}{2} \nabla \times n_0 \phi_\epsilon(r) \right)
\]

\[
= -\Delta p + \nabla \cdot (f_0 \phi_\epsilon(r))
\]

\[
= -\Delta p + f_0 \cdot \nabla \phi_\epsilon(r)
\]

Here we used the fact that \( u \) is divergence free and also \( \nabla \cdot (\nabla \times A) = 0 \) for any vector field \( A \). Now by substituting the latter in equation (2.18) and using the fact that \( f_0 \) is a constant vector, will get,
2.2. REGULARIZED STOKES FORMULATION

\[ \Delta p = f_0 \cdot \nabla (\Delta G_\epsilon(r)) = \Delta (f_0 \cdot \nabla G_\epsilon(r)), \]  

\text{(2.19)}

And hence,

\[ p = f_0 \cdot \nabla G_\epsilon(r) + C_1, \]  

\text{(2.20)}

where \( C_1 \) is the integral constant. Since it is the relative change of the pressure that is important for us, for simplicity we may assume that \( C_1 = 0 \). Now we can solve for the fluid velocity and angular velocity by substituting the particular solution for the pressure into equation (2.11) and then equation (2.13). For detailed derivations, see Appendix A. We obtain,

\[ \mu u = (-\Delta I + \nabla \nabla) B_\epsilon(r) f_0 - \frac{1}{2} (\nabla \times) G_\epsilon(r) n_0 + C_2, \]  

\text{(2.21)}

\[ \mu w = -\frac{1}{2} (\nabla \times) G_\epsilon(r) f_0 - \frac{1}{4} (-\Delta I + \nabla \nabla) G_\epsilon(r) n_0, \]  

\text{(2.22)}

where \( \Delta I \), \( \nabla \nabla \) and \( \nabla \times \) are matrix differential operators applied on a vector field and are given by,

\[ \Delta I = \begin{pmatrix} \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} & 0 & 0 \\ 0 & \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} & 0 \\ 0 & 0 & \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \end{pmatrix}, \]  

\text{(2.23)}

\text{Figure 2.1.} Blob function given in equation (2.16) for different values of the regularization parameter \( \epsilon \).
\[ \nabla \nabla = \begin{pmatrix} \frac{\partial^2}{\partial x^2} & \frac{\partial^2}{\partial y^2} & \frac{\partial^2}{\partial z^2} \\ \frac{\partial^2}{\partial x\partial y} & \frac{\partial^2}{\partial y\partial x} & \frac{\partial^2}{\partial y\partial z} \\ \frac{\partial^2}{\partial x\partial z} & \frac{\partial^2}{\partial y\partial z} & \frac{\partial^2}{\partial z^2} \end{pmatrix}, \quad (2.24) \]

\[ \nabla \times = \begin{pmatrix} 0 & -\frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & 0 \end{pmatrix}, \quad (2.25) \]

and \( C_2 \) is a constant three dimensional vector. Again we may assume that \( C_2 \) is the zero vector since we are interested in the relative difference in the velocity. Now define,

\[ S_\epsilon (r) = 8\pi (\Delta I + \nabla \nabla) B_\epsilon (r), \quad (2.26) \]
\[ R_\epsilon (r) = 4\pi (\nabla \times) G_\epsilon (r), \quad (2.27) \]
\[ D_\epsilon (r) = 4\pi (\Delta I + \nabla \nabla) G_\epsilon (r), \quad (2.28) \]

where \( S_\epsilon (r), R_\epsilon (r) \) and \( D_\epsilon (r) \) are called the regularized Stokeslets, Rotlets and Doublets respectively. The velocity and angular velocity of the fluid with a single point force \( f_0 \), and torque \( n_0 \) located at \( X_0 \) can now be written as,

\[ u(x) = \frac{1}{8\pi \mu} S_\epsilon (r)f_0 - \frac{1}{8\pi \mu} R_\epsilon (r)n_0, \quad (2.29) \]
\[ w(x) = -\frac{1}{8\pi \mu} R_\epsilon (r)f_0 - \frac{1}{16\pi \mu} D_\epsilon (r)n_0, \quad (2.30) \]

where \( x \) is any point in the fluid including points on the rod and \( r = |x - X_0| \). These expressions can be written as,

\[ u(x) = \frac{1}{\mu} (H_1(r)I + H_2(r) \vec{r} \otimes \vec{r})f_0 + \frac{1}{2\mu} (Q(r) (\vec{r} \times))n_0, \quad (2.31) \]
\[ w(x) = \frac{1}{2\mu} (Q(r) (\vec{r} \times))f_0 + \frac{1}{4\mu} (D_1(r)I + D_2(r) \vec{r} \otimes \vec{r})n_0, \quad (2.32) \]

where \( \vec{r} = x - X_0 \) and \( I \) is a 3 \times 3 identity matrix. The vector product \( \otimes \) is the tensor product defined by \( \vec{v}_1 \otimes \vec{v}_2 = \vec{v}_1 \vec{v}_2^T \) and \( (\vec{r} \times) \) is a 3 \times 3 matrix such that, \( (\vec{r} \times) \vec{v}_3 = \vec{r} \times \vec{v}_3 \), for any vertical vectors \( v_1, v_2 \) and \( v_3 \) in \( \mathbb{R}^3 \). Moreover the functions \( H_1, H_2, D_1, D_2 \) and \( Q \) are given as,

\[ H_1(r) = -\frac{B'_\epsilon (r)}{r} - B''_\epsilon (r), \quad (2.33) \]
\[ H_2(r) = \frac{B''_\epsilon (r)}{r^2} - \frac{B'_\epsilon (r)}{r^3}, \quad (2.34) \]
\[ Q(r) = -\frac{G'_\epsilon (r)}{r}, \quad (2.35) \]
\[ D_1(r) = \frac{G'_\epsilon (r)}{r} + G''_\epsilon, \quad (2.36) \]
\[ D_2(r) = -\frac{G''_\epsilon (r)}{r^2} + \frac{G'_\epsilon (r)}{r^3}. \quad (2.37) \]
2.3. REGULARIZED STOKES FORMULATION FOR AN ELASTIC ROD WITH CURVATURE AND TWIST

The dependency of the method on the choice of blob function \( \phi \) will be discussed in section 3.3.

2.3 Regularized Stokes formulation for an elastic rod with curvature and twist

In section 2.1 we used Kirchhoff’s rod model to develop dynamics of an elastic rod with curvature and twist. Moreover in section 2.2 we presented the exact solution to the incompressible Stokes equations with a single immersed regularized point force and torque. In this section we shall first generalize a single point force and torque to a set of point forces and torques concentrated along a curve in three dimensions and then describe the movement of the rod using the no-slip condition for the velocity. It is worth to mention that as the rod moves in the fluid the exerted forces and torques to the fluid will change with time, hence in this section we will assume that the forces and torques are also a function of time in addition to space.

In the moving rod formulation the body force in equation (2.11) will correspond to an integration of point forces and torques distributed along the centerline of the rod:

\[
f^b(x,t) = \int_0^L (-f(s,t)) \phi_\epsilon(r) \, ds + \frac{1}{2} \nabla \times \int_0^L (-n(s,t)) \phi_\epsilon(r) \, ds,
\]

(2.38)

where \( f(s,t) \) and \( n(s,t) \) are the point force and torque located at \( X(s,t) \) and \( \phi_\epsilon \) is the regularized kernel introduced in section 2.2. Due to the linearity of Stokes equation, we can generalize the regularized solution in equations (2.29) and (2.30) to a superposition of fundamental solutions of multiple body forces concentrated along the centerline of the rod.

Lastly to close the system, we present the equations that describes the movement of the rod:

\[
\frac{\partial}{\partial t} X(s,t) = u(X(s,t), t),
\]

(2.39)

\[
\frac{\partial}{\partial t} D^i(s,t) = w(X(s,t), t) \times D^i(s,t), \quad i = 1, 2, 3,
\]

(2.40)

Equation (2.39) makes sure that the linear velocity of any point on the rod is equal to the local linear velocity of the fluid at that point. This condition is also known as the no-slip condition for the velocity. Similarly equation (2.40) represents the no-slip condition for the angular velocity which states that the rotation of the orthonormal triads is a rigid rotation corresponding to the local angular velocity of the fluid at that point. For more details, see [11].

2.4 Non-dimensionalization

We non-dimensionalize the problem using the rod length \( L \) as the characteristic length. Assume that we have a characteristic velocity \( u_0 \). The characteristic time
will be \( T = L/u_0 \). The suitable characteristic velocity/time depends on the problem, and we will get back to this shortly. We can define the following dimensionless variables,

\[
\begin{align*}
 s^* &= \frac{s}{L}, & X^* &= \frac{X}{L}, & x^* &= \frac{x}{L}, & r^* &= \frac{r}{L}, \\
u^* &= \frac{\nu}{u_0},
\end{align*}
\] (2.41)

\[
\begin{align*}
 f^* &= \frac{L^3}{a} f, & n^* &= \frac{L^2}{a} n, \\
 F^* &= \frac{L^2}{a} F, & N^* &= \frac{L}{a} N,
\end{align*}
\] (2.42)

\[
\begin{align*}
t^* &= \frac{L}{u_0} t
\end{align*}
\] (2.45)

and the following dimensionless parameters,

\[
\begin{align*}
 \epsilon^* &= \frac{\epsilon}{L}, & b_i^* &= \frac{L^2}{a} b_i, & a_i^* &= 1, & \Omega_i^* &= \frac{\Omega_i}{L}, & \text{for } i = 1, 2, 3.
\end{align*}
\] (2.46)

Here we assumed \( a_1 = a_2 = a_3 = a \). Now by substituting these variables and parameters into the equations presented chapter 2 we can derive the dimension-less equations for the velocity and angular velocity of the fluid.

\[
\begin{align*}
 8\pi\mu u_0 L^3/a u^*(x^*) &= \int_0^1 f^*(X^*)S_\epsilon(r^*) \, ds^* - \int_0^1 n^*(X^*)R_\epsilon(r^*) \, ds^*, \\
 8\pi\mu u_0 L^3/a w^*(x^*) &= -\int_0^1 f^*(X^*)R_\epsilon(r^*) \, ds^* - \frac{1}{2} \int_0^1 n^*(X^*)D_\epsilon(r^*) \, ds^*,
\end{align*}
\] (2.47) (2.48)

where \( \mu \) is the viscosity of the fluid. The dimensionless parameter \( \bar{\mu} = (8\pi\mu u_0 L^3)/a \) is the effective viscosity which relates the characteristic speed of the fluid to the elastic force of the rod. Now we will have,

\[
\begin{align*}
 \bar{\mu} u(x) &= \int_0^1 f(X)S_\epsilon(r) \, ds - \int_0^1 n(X)R_\epsilon(r) \, ds, \\
 \bar{\mu} w(x) &= -\int_0^1 f(X)R_\epsilon(r) \, ds - \frac{1}{2} \int_0^1 n(X)D_\epsilon(r) \, ds.
\end{align*}
\] (2.49) (2.50)

In the case of a background shear flow, it is natural to take the characteristic time as \( T = 1/\dot{\gamma} \), where \( \dot{\gamma} \) is the shear rate. A natural characteristic velocity is then \( u_0 = L/T \). This yields,

\[
\bar{\mu} = \frac{8\pi\mu \dot{\gamma} L^4}{a}
\] (2.51)

In the case of a uniform background flow with speed \( U \), we simply set \( u_0 = U \), and hence \( T = L/U \). Then the effective viscosity becomes,
\[ \bar{\mu} = \frac{8\pi \mu UL^3}{a} \quad (2.52) \]

Considering the case when there is no external flow, a characteristic time scale can be defined as \( T = 8\pi \mu L^4/a \). With this choice, \( u_0 = L/T = a/(8\pi \mu L^3) \) and,

\[ \bar{\mu} = \frac{8\pi \mu L^3}{a} \frac{a}{8\pi \mu L^3} = 1. \quad (2.53) \]

Hence, in the case of no external flow, there are no parameters left, except for \( b_i \) which is a numerical parameter to keep the triad aligned. This means that the dynamics of a relaxing rod in an otherwise quiescent fluid will not depend on the ratio of the viscosity and the bending modulus. The dynamics will be the same independent of the physical parameters, i.e. the rod will relax in the same way. Only the time it takes will differ.
Chapter 3

Implementation and Validation

In chapter 2 we introduced a mathematical model that describes the dynamics of an elastic rod in a fluid. Deviations from the equilibrium shape of the rod produces forces and torques, that act on the fluid. To derive these forces, a Kirchoff rod model allowing for rods with intrinsic curvature and twist was used, and a regularized Stokeslet method was used to derive the equations of the fluid flow. The system was closed by imposing no-slip velocity conditions, determining the translational and angular velocity of the rod.

In this chapter we describe the numerical methods that we used to to solve this system of equations and present the solutions in case of open and closed rods with different intrinsic curvature and twist. Further on, we investigate the accuracy of the method in time and space in addition to the numerical stability analysis of the method. Finally we compare the effect of different blob function and also the effect of the regularization parameter $\epsilon$ on the solution.

3.1 Numerical Scheme

The spatial discretization of the centerline of the rod $X(s)$ is obtained by introducing a fixed uniform interval $\Delta s$ of the Lagrangian variable $s$. We then introduce $s_k = k\Delta s$ for $k = 1, 2, \ldots, M$ where $M\Delta s$ is the length of an unstressed rod, $L$. Other Lagrangian variables, $X, D^1, D^2, D^3, F, N, f$ and $n$ will be defined at points $s_k$ and for this purpose we use the notation $X_k = X(k\Delta s)$. We shall need, however, to define the orthonormal triads $D^i_{k\pm \frac{1}{2}}$ for $k = 1, 2, \ldots, M$.

Now we can discretize the body force given in equation (2.38) in space using the trapezoidal rule to obtain,

$$f^b(x, t) = \sum_{k=1}^{M} -f_k\Delta s\phi_e(x - X_k) + \frac{1}{2} \nabla \times \sum_{k=1}^{M} -n_k\Delta s\phi_e(x - X_k), \quad (3.1)$$

Note that this discretization means that we approximated the concentrated point forces and torques along a curve with a set of $M$ immersed boundary points. The
strength of the point force and torque located at \(X_k\) is equal to \(f_k \Delta s\) and \(n_k \Delta s\) respectively for \(k = 1, 2, \ldots, M\) and correspond to \(f_0\) and \(n_0\) used in section 2.2.

Now we can compute the triads in the point \(s_k + \frac{1}{2}\) using the triad located at \(s_k\) and \(s_{k+1}\). To do this we need to find the linear rotation that maps \(D^1_k, D^2_k\) and \(D^3_k\) onto \(D^1_{k+1}, D^2_{k+1}\) and \(D^3_{k+1}\) respectively. Note that this is a linear interpolation, and other interpolation techniques can also be used.

The orthonormal rotation matrix \(A\) that maps the triad \(D^i_k\) to the triad \(D^i_{k+1}\) for \(i = 1, 2, 3\) can be uniquely defined as,

\[
A = \sum_{i=1}^{3} D^i_{k+1} (D^i_k)^T
\]

(3.2)

Where the superscript \(T\) denotes the matrix transpose and \(D^i\) is a \(3 \times 1\) vector.

Furthermore, in order to compute \(D^1_{k+1/2}, D^2_{k+1/2}\) and \(D^3_{k+1/2}\), we can take the principle square root \((\sqrt{A} \times \sqrt{A} = A)\) of the matrix \(A\), which means the rotation about the same axis with half the angel,

\[
D^i_{k+1/2} = \sqrt{A} D^i_k,
\]

(3.3)

In order to compute the forces and moments that are transmitted across the section of the rod we discretize equations (2.7) and (2.8) using second order finite differences schemes at half points to obtain,

\[
F^1_{k+1/2} = b_1 D^1_{k+1/2} \frac{X_{k+1} - X_k}{\Delta s},
\]

(3.4)

\[
F^2_{k+1/2} = b_2 D^2_{k+1/2} \frac{X_{k+1} - X_k}{\Delta s},
\]

(3.5)

\[
F^3_{k+1/2} = b_3 \left( D^3_{k+1/2} \frac{X_{k+1} - X_k}{\Delta s} - 1 \right),
\]

(3.6)

\[
N^1_{k+1/2} = a_1 \left( \frac{D^2_{k+1} - D^2_k}{\Delta s}, D^3_{k+1/2} - \Omega_1 \right),
\]

(3.7)

\[
N^2_{k+1/2} = a_2 \left( \frac{D^3_{k+1} - D^3_k}{\Delta s}, D^1_{k+1/2} - \Omega_2 \right),
\]

(3.8)

\[
N^3_{k+1/2} = a_3 \left( \frac{D^1_{k+1} - D^1_k}{\Delta s}, D^2_{k+1/2} - \Omega_3 \right),
\]

(3.9)

Now we may use equations (2.3) and (2.4) to get,

\[
F_{k+1/2} = \sum_{i=1}^{3} F^i_{k+1/2} D^i_{k+1/2},
\]

(3.10)

\[
N_{k+1/2} = \sum_{i=1}^{3} N^i_{k+1/2} D^i_{k+1/2},
\]

(3.11)
3.1. NUMERICAL SCHEME

The next step is to compute the force and torque density applied from the rod to the fluid by discretizing equations (2.1) and (2.2),

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

(3.12)

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

(3.13)

Here we used central finite differences schemes for equation (3.12). In equation (3.13) the first term on the right hand side is approximated with central finite differences and we use an average of the approximation at the two half points to the left and the right. It is worth to mention that the shape of the rod should be taken into account while discretizing the end points of the rod, which will be discussed more in sections 3.1.1 and 3.1.2.

Now that we have estimated the force an torque exerted by the rod we can compute the velocity and angular velocity of the fluid using superposition of equations (2.29) and (2.30),

\[
u(x) = \frac{1}{8\pi\mu} \sum_{k=1}^{M} -f_k \Delta s S_e(x - X_k) - \frac{1}{8\pi\mu} \sum_{k=1}^{M} -n_k \Delta s R_e(x - X_k),
\]

(3.14)

\[
w(x) = -\frac{1}{8\pi\mu} \sum_{k=1}^{M} -f_k \Delta s R_e(x - X_k) - \frac{1}{8\pi\mu} \sum_{k=1}^{M} -n_k \Delta s D_e(x - X_k),
\]

(3.15)

Now we can update the position of the rod and proceed in time. In order to do this we need to compute the velocity and angular velocity of the fluid at \(X_k\) for \(k = 1, \ldots, M\) and use the no slip condition to move forward in time. By using the forward Euler method we will have,

\[
\frac{X_k^{n+1} - X_k^n}{\Delta t} = u(X_k^n),
\]

(3.16)

Where the superscript indicates the time step index, so that \(X_k^n = X(s_k, n\Delta t)\). Note that there is a forth order constraint on the time step \((\Delta t/(\Delta s)^4 < \mathcal{O}(1))\). This means that very small time steps is required to obtain stability and there is no need for higher order time stepping method since spatial errors dominate. Now let \(R(e, \theta)\) be the orthogonal matrix that describes a rotation with angel \(\theta\) about the axis of the unit vector \(e\) which is explicitly [8] given by,

\[
R(e, \theta) = (\cos \theta)I + (1 - \cos \theta)ee^T + (\sin \theta)(e \times),
\]

(3.17)

Finally we update the orthonormal triad by rotating it in terms of \(R\),

\[
(D_k^n)^{n+1} = R \left( \frac{W_k^{n+1}}{|W_k^{n+1}|}, |W_k^{n+1}|\Delta t \right) (D_i^n)^{n+1},
\]

(3.18)
Table 3.1. Computational parameters for simulation of open and closed elastic rods

<table>
<thead>
<tr>
<th></th>
<th>Open</th>
<th>Closed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unstressed rod, $L(\mu m)$</td>
<td>6</td>
<td>15.708</td>
</tr>
<tr>
<td>Immersed Boundary points, $M$</td>
<td>76</td>
<td>200</td>
</tr>
<tr>
<td>Mesh width, $\Delta s(\mu m)$</td>
<td>0.0785</td>
<td>0.0785</td>
</tr>
<tr>
<td>Time step, $\Delta t(s)$</td>
<td>$10^{-6}$</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>Regularization parameter, $\epsilon(\mu m)$</td>
<td>$5\Delta s - 8\Delta s$</td>
<td>$3\Delta s - 6\Delta s$</td>
</tr>
</tbody>
</table>

where $i = 1, 2, 3$. The latter equation indicates that each triad is rotated at the locally averaged angular velocity of the fluid for an amount of time equal to $\Delta t$ [8]. Now the time step is complete. A summery of one time step of the method is the following,

1. Compute force and moment that are transmitted across the section of the rod at half points using equations (3.4) to (3.9).

2. Expand the force and torque vectors in the basis of triads using equations (3.10) and (3.11).

3. Compute triad vectors at half points using equations (3.2) and (3.3).

4. Compute force and torque exerted by the fluid at the material point $s_k$ using equations (3.12) and (3.13)

5. Compute the local linear velocity of the fluid at points $X(s, t)$ using equation (3.14).

6. Compute the local angular velocity of the fluid at points $X(s, t)$ using equation (3.15).

7. Update the position of the rod and triads using equations (3.16) and (3.18).

We regenerated the results in [11] for open and closed elastic rods. The computational and the material parameters used for this simulation and in [11] are presented in Tables 3.1 and 3.2 respectively.

Note that in this set up we assumed that there is no external flow, hence one can consider the non-dimensionalized form. As discussed in sections 2.4, All the material parameters can be removed using the effective viscosity defined in equation (2.53). And the dimensionless numerical parameter $b_i$ may be computed from equation (2.46).

### 3.1.1 Open Elastic Rod

As discussed in chapter 2 an elastic rod is represented by a three dimensional space-curve together with orthonormal triad \{ $X(s, t), D^1(s, t), D^2(s, t), D^3(s, t)$ \}. In case
Table 3.2. Material parameters for simulation of open and closed elastic rods

<table>
<thead>
<tr>
<th></th>
<th>Open</th>
<th>Closed</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>$3.5 \times 10^{-3}$</td>
</tr>
<tr>
<td>Twist modulus, $a_3 (g \mu m^3 s^{-2})$</td>
<td>$3.5 \times 10^{-3}$</td>
<td>$3.5 \times 10^{-3}$</td>
</tr>
<tr>
<td>Shear modulus, $b = b_1 = b_2 (g \mu m^3 s^{-2})$</td>
<td>$8.0 \times 10^{-1}$</td>
<td>$8.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>Stretch modulus, $b_3 (g \mu m^3 s^{-2})$</td>
<td>$8.0 \times 10^{-1}$</td>
<td>$8.0 \times 10^{-1}$</td>
</tr>
<tr>
<td>Perturbation parameter, $\zeta$</td>
<td>0.0001</td>
<td>1</td>
</tr>
<tr>
<td>Twist vector, $(\Omega_1, \Omega_2, \Omega_3) (\mu m^{-1})$</td>
<td>varied</td>
<td>varied</td>
</tr>
<tr>
<td>Fluid viscosity, $\mu (g \mu m^{-1} s^{-1})$</td>
<td>$10^{-6}$</td>
<td>$10^{-6}$</td>
</tr>
</tbody>
</table>

Further on we carry out the discretization introduced in section 3.1. Since the end points of the rod is moving freely in the fluid the internal force and moment at the end points of the rod are zero. This leads to the following boundary conditions:

\[
F_{1/2} = F_{M+1/2} = 0, \\
F_{1/2} = F_{M+1/2} = 0.
\]

To treat the boundary points in equation (3.13) we need to introduce ghost points $X_0$ and $X_{M+1}$. This can be obtained by extrapolating $\{X_i\}_{i=1}^M$ with respect to $s$. Linear extrapolation would then give,

\[
X_0 = 2X_1 - X_2, \\
X_{M+1} = 2X_M - X_{M-1}.
\]

By setting the intrinsic curvature and twist $(\kappa, \Omega_3)$ one can follow the procedure presented in section 3.1 and proceed in time. According to the Kirchhoff’s rod theory any perturbation of an open rod with the twist vector $(\Omega_1, \Omega_2, \Omega_3) = (0, 0, 0)$ will relax to a stable equilibrium state that is straight and untwisted [11]. This was tested and verified through our simulations using various initial perturbation including the one introduced in this report, but we do not present the numerical results for this case. Moreover for any positive intrinsic curvature $\kappa$ if the twist value is greater than a critical twist value, a straight rod will become unstable and
bifurcate into a stable helix configuration [11]. The critical twist value depends on the material parameters of the rod, as well as the strain twist vector [11]. The geometric properties of an open rod, such as number of turns along the rod, can be determined as [11],

\[ q = \frac{\Omega_3 L}{2\pi}, \]  

(3.28)

where \( q \) is the number of turns along the rod, \( \Omega_3 \) is the intrinsic twist and \( L \) is the length of unstressed rod. In Figure 3.1 the results of the regularized Stokes formulation are presented with each row corresponding to a different intrinsic twist. In both cases the twist is large enough to cause the rod to move away from its initial straight shape to reach its equilibrium state which is a stable helix. Each instance shows the time profile of the rod between \( t = 0.001s \) and \( t = 0.005s \) as the rod evolves toward its equilibrium configuration. The length of the rod is given as \( L = 6 \ \mu m \), the intrinsic twist is given as \( \Omega_3 = \pi/2 \) and \( \Omega_3 = \pi \) for the first and second simulation respectively. Note that the characteristic time introduced in section 3.1 is given by \( T = 8\pi \mu L^4/a \approx 9.3063 \). It can be observed that by using equation (3.28) theoretically the number of turns would be \( q = 1.5 \) and \( q = 3 \) for the first and second simulation respectively which matches our results in figure 3.1. The results in 3.1 match the ones presented in [11] in sense of shape of the rod and the time scale.

We have also examined the change of the elastic energy of the rod which is given in equation (2.9) to see how the rod interacts with the fluid to reach its equilibrium configuration under different regularization parameters \( \epsilon \). In figure 3.2 each curve shows the elastic energy evolution of a rod with twist vector \((\Omega_1, \Omega_2, \Omega_3) = (1.3, 0, \pi)\) with four different values of \( \epsilon \) in the range \( 5\Delta s - 7\Delta s \). It is observed from figure 3.2 that the elastic energy that is initially stored in the rod decrease rapidly at first and then the decay slows down as the rod reaches its equilibrium configuration, however the process is monotonic. In [11] different comparisons between the results of regularized Stokes formulation and generalized immersed boundary method (gIB) is presented. By reducing the effect of the periodic copies, gIB shows similar behavior as the regularized Stokes formulation. For more information consider [11, 8].

### 3.1.2 Closed Elastic Rod

In this section we discuss the dynamics of a closed elastic rod with intrinsic curvature and twist immersed in viscous fluid. For initial configuration, we apply sinusoidal perturbation to a circular rod in a horizontal plane. In this case the length of the rod will be \( L = 2\pi r_0 \), which is the circumference of an unstressed circular rod with radius \( r_0 \). Similar to the derivation in [11] the initial configuration of the rod is
\((\Omega_1, \Omega_2, \Omega_3) = (1.3, 0, \pi/2)\)

\[(\Omega_1, \Omega_2, \Omega_3) = (1.3, 0, \pi)\]

\[t = 0.000 \text{ s} \quad t = 0.001 \text{ s} \quad t = 0.002 \text{ s} \quad t = 0.003 \text{ s} \quad t = 0.004 \text{ s}\]

**Figure 3.1.** Result of regularized Stokes formulation where an open rod is initialized as perturbation of a straight rod. The top row corresponds to the twist vector \((1.3, 0, \pi/2)\) and the bottom row corresponds to the twist vector \((1.3, 0, \pi)\). In both rows the evolution of the rod is shown at each 0.001s as it moves toward its equilibrium configuration. The regularization parameter is set to be \(\epsilon = 6\Delta s\).

given by,

\[X(s) = r_0 r \left( \frac{s}{r_0} \right), \quad (3.29)\]

\[D^1(s) = \cos \left( \zeta \sin \frac{s}{r_0} \right) z + \sin \left( \zeta \sin \frac{s}{r_0} \right) r \left( \frac{s}{r_0} \right), \quad (3.30)\]

\[D^2(s) = -\sin \left( \zeta \sin \frac{s}{r_0} \right) z + \cos \left( \zeta \sin \frac{s}{r_0} \right) r \left( \frac{s}{r_0} \right), \quad (3.31)\]

\[D^3(s) = \theta \left( \frac{s}{r_0} \right) \quad (3.32)\]

Where \(\zeta\) is the perturbation parameter and \((r, \theta, z)\) are the cylindrical coordinate. Now the discretization introduced in section 3.1 can be carried out. In case
of closed rod we should apply periodic boundary condition,

\[ X_1 = X_{M+1}, \]

(3.33)

Where \( M \) is the number of immersed boundary points. Also we will have the following conditions on force and moment,

\[ F_{1/2} = F_{M+1/2}, \]  \hspace{1cm} (3.34)

\[ N_{1/2} = N_{M+1/2}. \]  \hspace{1cm} (3.35)

The values chosen for the perturbation parameter and the length of the unstressed rod can be found in table 3.1. It is worth to mention that a relaxed circular rod with no twist has a natural curvature given by \( 1/r_0 \). Hence a perturbed circular rod with intrinsic curvature \( \kappa = 1/r_0 \) and intrinsic twist \( \Omega_3 = 0 \) will relax to a stable equilibrium state that is an untwisted circle. This was tested and verified through our simulations using various initial perturbation including the one introduced in this report, but we do not present the numerical results for this case.

In Figure 3.3 the result of regularized Stokes formulation for the closed rod is presented with each row corresponding to a different intrinsic twist. In both cases
3.2. CONVERGENCE AND ACCURACY

\[(\Omega_1, \Omega_2, \Omega_3) = (1.2, 0, 0.6)\]

\[(\Omega_1, \Omega_2, \Omega_3) = (1.2, 0, 0.5)\]

\[t = 0.03 \, s \quad t = 0.04 \, s \quad t = 0.05 \, s \quad t = 0.07 \, s \quad t = 0.1 \, s\]

**Figure 3.3.** Result of regularized Stokes formulation where an closed rod is initialized as sinusoidal perturbation of a circular rod. The top row corresponds to the twist vector \((1.2, 0, 0.6)\) and the bottom row corresponds to the twist vector \((1.2, 0, 0.5)\). In both rows the evolution of the rod is shown between \(t = 0.03s\) and \(t = 0.1\) as it moves toward its equilibrium coiled configuration. The regularization parameter is set to be \(\epsilon = 4\Delta s\).

the rod evolves toward a coiled configuration which is different than the helical shape as for the open rods. The intrinsic twist for the first row of figure 3.3 is set to be \(\Omega_3 = 0.6\) and for the second row \(\Omega_3 = 0.5\). It is observed that as the intrinsic twist is increased the rod become less coiled in their equilibrium configuration. Note that as the closed rod do not have free ends, it takes significantly longer time to reach its equilibrium configuration compared to an open rod. The results of gIB was compared to regularized Stokes formulation for closed rod in [11] and they match if the effect of periodic copies is reduced. The results in 3.3 match the ones presented in [11] in sense visual shape, number of twists and the time scale.

3.2 Convergence and Accuracy

To compute the convergence rate of the numerical method, we performed the same runs of a non-dimensionalized rod with strain vector \((\Omega_1^* \Omega_2^* \Omega_3^*) = (7.8, 0, 3\pi)\) using a fixed time-step and different number of immersed boundary points \(M = 50, M = 100\) and \(M = 200\). The set up of the run was similar to section 3.1.1 i.e. the straight rod is used as the initial configuration. The convergence rate was computed as 2.08 which was based on the ratios of norm of error in the Euclidean distance between the discrete points of consecutive solutions,

\[
\frac{||\hat{X}_{\Delta s} - \hat{X}_{\Delta s/2}||}{||\hat{X}_{\Delta s/2} - \hat{X}_{\Delta s/4}||} = 2^p + O(\Delta s). \tag{3.36}
\]

Here, \(\Delta s\) is the length of the space discretization, \(\hat{X}\) is a specific point on the rod and \(p\) is the order of the accuracy. Figure 3.4 illustrates how the solutions converge as the step size \(\Delta s\) decreases.
Comparison between solutions from run with a rod with strain vector 
\((\Omega_1^*, \Omega_2^*, \Omega_3^*) = (7.8, 0, 3\pi)\) and different number of immersed boundary points \(M = 50, M = 100\) and \(M = 200\). The convergence rate based on successive solutions is 2.08.

Since in-extensibility is formulated as an added penalty to the energy in equation (2.9), it is interesting to examine the length error of the rod during the simulation. As the rod is initially set to have length \(L = 1\), the initial error in length is zero. We expect to have some error in the length as the rod moves away from the initial configuration and maintain its original length as it moves closer to its equilibrium configuration and minimizes its elastic energy. In figure 3.5 the absolute values of the length errors as a function of time have been plotted for different number of immersed boundary points. As it is observed the rod is extended up to 0.2% of its original length and the length error tends to zero as the rod is relaxed.
3.3. Regularization parameter and the choice of blob function

In this section we will examine the effect of regularization on the numerical solution. Regularization can be controlled either by the choice of the blob function or the parameter $\epsilon$ which controls the effective radius if the region where the blob function supports [2]. In figure 3.6, We used the two blob function introduced in equations (2.16) and (2.17) in the set up of simulations presented in section 3.1.1. The parameters used in the run are $M = 75$, $(\Omega_1, \Omega_2, \Omega_3) = (1.3, 0, \pi)$ and $\epsilon = 4\Delta s$. It is observed that the effect of different blob functions is minor on the numerical solution since we use small values of $\epsilon$. However, the decay properties and the compactness of the support is important in picking the right blob function for the problem.

We also examined the effect of the regularization parameter $\epsilon$ on the numerical solution. In figure 3.7 we varied $\epsilon$ from $5\Delta s$ to $8\Delta s$. The other parameters are the same as in section 3.1.1 with strain vector $(1.3, 0, \pi/2)$. As it is observed the difference is not negligible. Note that the equilibrium configuration of the rod is independent of the parameter $\epsilon$ and the differences in figure 3.7 shows the latency in reaching the equilibrium configuration.

Figure 3.5. The length error of an elastic rod with strain vector $(\Omega_1^*, \Omega_2^*, \Omega_3^*) = (7.8, 0, 3\pi)$ and straight initial configuration plotted for different resolution $M = 50$, $M = 100$ and $M = 200$.
Figure 3.6. The effect of different blob functions on the solution. The blob function in equation (2.16) is presented with the solid line and the blob function in equation (2.16) is presented with the dotted line. The parameters used are $M = 75$, $(\Omega_1, \Omega_2, \Omega_3) = (1.3, 0, \pi)$ and $\epsilon = 4\Delta s$ and the solution is plotted at $t = 0.005s$. 
3.3. REGULARIZATION PARAMETER AND THE CHOICE OF BLOB FUNCTION

Figure 3.7. The effect of different regularization parameter on the numerical solution. The parameters used are $M = 75$, $(\Omega_1, \Omega_2, \Omega_3) = (1.3, 0, \pi)$ and $\epsilon = 4\Delta s$ and the solution is plotted at $t = 0.005s$. 
Chapter 4

Applications

In this chapter we will use the mathematical model in chapter 2 in two physical problems. In section 4.1 we will examine the dynamics of an elastic rod with no curvature and twist placed in a shear-flow and in section 4.2 we will inspect the behavior of a helical rod while being extended in a constant background flow.

4.1 Planar flow

The study of motion of ellipsoidal particles immersed in viscous fluid is important and has been studied before [6]. "Jeffry orbits" refer to the rotation of rigid particles about its axis when placed in a shear flow [6]. As a straight non-flexible rod is placed in a planar shear flow, it will rotate about its centerline. However if the rod is flexible and the shear rate is high enough, it will become unstable to buckling [16]. Numerical solutions of Jeffry orbits of a straight flexible rod is studied in [16] which is based on non-local slender body theory, requiring the solution of an integral equation. As a bench mark, we shall formulate the Jeffry orbits of a flexible straight rod with no intrinsic curvature and twist using regularized Stokeslets model and compare the results to those presented in [16].

We may use the dimensionless form of regularized Stokeslets method using effective viscosity given in section 2.4,

\[ \bar{\mu} = \frac{8\pi \mu \dot{\gamma} L^2}{E/L^2} \]  

(4.1)

A straight rod is placed vertically in the \( xy \)-plane with the following shear-flow,

\[ U_0(x) = \dot{\gamma}(0, x_1, 0), \]  

(4.2)

with rod’s center point at \((0,0,0)\). Here, \( x = (x_1, x_2, x_3) \in \mathbb{R}^3 \) and \( \dot{\gamma} \) is the strength of the shear flow. Due to the linearity of the Stokes equation we can now modify the no-slip condition given in equation (2.39) to obtain the velocity of the fluid,

\[ \frac{\partial}{\partial t} X(s, t) = u(X(s, t), t) + U_0(X). \]  

(4.3)
Figure 4.1. The buckling of elastic rod with no intrinsic curvature and twist in a shear flow for $\bar{\mu} = 1.4 \times 10^4$

For initial configuration of the rod, similar to [16], we apply a small perturbation to the rod so that it is not exactly straight,

\begin{align}
X(s) &= \sin(\theta_0)(s - 1)/2 + d_y s^4(1 - s)^4, \quad (4.4) \\
Y(s) &= \cos(\theta_0)(s - 1)/2. \quad (4.5)
\end{align}

Here, $\theta_0 \approx 0.9936\pi$ is the initial angle of the rod with the $-y$ axis, and $d_y = -10^{-4}$ is the magnitude of the nonlinear perturbation. Note that this is a small disturbance compared to a straight rod. More over we use the following perturbation for the
4.1. PLANAR FLOW

Figure 4.2. The buckling of elastic rod with no intrinsic curvature and twist in a shear flow for $\bar{\mu} = 2.4 \times 10^4$


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where $\zeta$ is a small perturbation parameter. The numerical parameters for the simulation are $M = 200$, $\epsilon = 6\Delta s$ and $b_1 = b_2 = b_3/2 = 8228.57$.

If a flexible rod is placed on a shear flow while having a small initial angle with the y-axis, it will start to rotate slowly. If the strength of the shear flow is strong
enough the rod will start buckling and becoming compressed. As the horizontal line is passed, the rod will then start to extend and retrieve its straight shape.

Figure 4.1 and 4.2 show the evolution of an rod placed in the shear flow for different effective viscosities. It is seen that as $\bar{\mu}$ is increased, the amount of buckling also increases.

To understand how the rod is interacting with the fluid we also examined the elastic energy of the rod as it rotates in a shear-flow. Figure 4.3 shows the energy evolution of the rod with configuration of figure 4.2. It can be observed that the most elastic energy is stored in the rod as it is passing the horizontal line ($x$-axis).

The effective viscosity used in [16] is slightly higher, also the shape of buckling appears to be different. These could be due to the fact that we are imposing a numerical thickness to the elastic rod in the regularized Stokeslets mode. However, the time scale for the rotation of the elastic rod matches in both methods and also matches the analytical solution presented in [16].

### 4.2 Extension of a helical rod in a constant flow

In this section we will examine the behavior of an elastic rod placed inside a fluid with constant flow while having one anchored point i.e. a fixed point that does not move with the flow. We introduce a constant background flow in the positive $z$-direction given by,

$$U = U_0(0, 0, 1),$$

where $U_0$ is the strength of the flow. To formulate the anchored point of the rod we need to modify the no-slip condition in equation (2.39) to allow a certain slip since in this case the background flow will slip by the rod. Let $S(s, t)$ be the slip
velocity of the background flow at time $t$ and $X(s, t)$. Then due to the linearity of Stokes equations we can modify equation (2.39) to have,

$$\frac{\partial}{\partial t} X(s, t) = U - S(s, t), \quad (4.10)$$

Now to compute the amount of the slip, assume that $X(0)$ is anchored, then the slip of the background flow at any point $X(s)$ on the rod will be equal to the relative velocity of this point to $X(0)$ in the absence of any background flow. This means that if in the absence of any background flow the velocity of $X(s, t)$ is $u^*$ relative to $X(0)$ then by applying the background flow, due to linearity of Stokes equations, the velocity of $X(s, t)$ will become $U - u^*$. So we will have,

$$S(s, t) = u(X(0, t), t) - u(X(s, t), t), \quad (4.11)$$

where $u$ is given by the equation (2.29). Note that since there are no background angular velocity, we do not need to modify equation (2.30).

To formulate the anchored point, we set the background flow to be zero at $X(0, t)$. However, to obtain a smooth and continues vector field of the background flow, we smoothly increase the strength of the flow from zero to $U_0$ over a small interval around $X(0)$. Now the formulation of the background flow in equation (4.9) will be modified to,

$$U(x) = D(|x - X(0)|) (0, 0, 1), \quad (4.12)$$

where $D$ is the damping function defined as,

$$D(r) = \begin{cases} 
U_0 \sin^2 \left( \frac{r\pi}{0.1} \right), & r < 0.05, \\
U_0, & r \geq 0.05.
\end{cases} \quad (4.13)$$

Note that the ball $|x - X(0)| < 0.05$ is small compared to the length of the rod.

We desire to have a helical shape for the rod as the initial configuration. However, formulating a consistent initial triad for a helical rod can be very complicated. Instead we can use the result of the simulation in section 3.1.1 which are the position and the triad of each immersed boundary point and all the numerical parameters, and use it as the initial configuration of the simulation of extension of a helical rod in a constant flow. The numerical parameters parameter for the runs are $M = 200$, $\epsilon = 6\Delta s$, $b_1 = b_2 = b_3/2 = 8228.57$ and $(\Omega_1^*, \Omega_2^*, \Omega_3^*) = (7.8, 0, 6\pi)$.

Figures 4.4 and 4.5 show the extension of a helical rod in constant flow with different values for of effective viscosity. In these figures the most bottom point of the rod is anchored and the constant background flow is in the direction of positive $z$. It is observed that the rods tends to become straight at the fixed end and remain curled near the free end. The amount of curvature is reduced as the strength of the shear flow is increased.
Figure 4.4. The extension of a helical rod with strain vector $(\Omega_1^*, \Omega_2^*, \Omega_3^*) = (7.8, 0, 6\pi)$ with $\bar{\mu} = 3.5 \times 10^4$. The most bottom point is anchored and the flow is in the positive $z$ direction.
Figure 4.5. The extension of a helical rod with strain vector \((\Omega_1^*, \Omega_2^*, \Omega_3^*) = (7.8, 0, 6\pi)\) with \(\bar{\mu} = 7 \times 10^4\). The most bottom point is anchored and the flow is in the positive \(z\) direction.
Chapter 5

Numerical Solution of Periodic Stokes Flow

In chapter 4 we examined the simulation of two physical problems. The investigation of larger problems e.g. the simulation of multiple twisted and curved rods, require an efficient numerical method since the method of Regularized Stokeslets becomes computationally expensive. In case of periodic array of point forces and torques, some challenges appears in development of an efficient numerical method. In particular, in three spatial dimensions, flow arising from a single point force, as given by the Stokeslet, decay as $1/r$, where $r$ denotes the distance from the point force [7]. This means that the direct sum of Stokeslets over a periodic array of point forces diverges.

To overcome this challenge, it is assumed that there is a pressure gradient that balances the forces and the method of Ewald summation is used. The idea is to split a slowly and conditionally convergent series into a sum of two exponentially decaying series, one in real space and one in Fourier space, while the convergence of each sum is controlled by a single parameter. This method is computationally slow as a sum over over the $M$ immersed boundary points and all of their periodic images gives $O(M^2)$ complexity. To boost the complexity, Fourier-based particle-mesh methods are used that reduces the complexity to $O(M \log M)$ [7].

Another difficulty that arises, as discussed in chapter 2, is the singularity of fundamental solutions, Stokeslets, Rotlets and Doublets. To overcome this difficulty one could use the regularization method like what was presented previously in this report. However, carrying out the Fourier part of Ewald summation for the fundamental solutions, requires calculations of complicated integrals, even with a careful choice of the blob function. Leinderman et al. [7], came up with a way to avoid the Fourier sum of the regularized Stokeslets while maintaining the fast convergence, by using the linearity of the Stokes equations and tuning the blob function. A similar trick can also be used to carry out the Ewald summation for the Rotlets and the Doublets.

In this chapter following the derivations in [12, 7], we derive an Ewald summation
formula for the Rotlets, which to our knowledge, was not done before. Then by using the same trick in [7] we limit the Ewald summation of the regularized fundamental solutions to the real space while keeping the fast convergence. We do not focus on reducing the $O(M^2)$ complexity and it is left for future work.

5.1 Green’s function for periodic Stokes flow

In this section we will review the formulation presented in [12, 7] for the Stokeslets and extend it to Rotlets and Doublets. First we derive the Ewald summation for the case of point forces and torques, then in section 5.2 we present the fast convergent series of the regularized point forces and torques.

Consider the steady motion of Stokes fluid past a triply-periodic array of point forces and torques located at the vertices of a three-dimensional lattice defined by the vectors,

$$X_n = i_1 a_1 + i_2 a_2 + i_3 a_3, \quad (i_1, i_2, i_3 \in \mathbb{Z}).$$  (5.1)

Here $a_1, a_2$ and $a_3$ are the basis vectors that indicate the lattice. As discussed in chapter 2 and 3 we can write the motion of the fluid as,

$$-\nabla p + \mu \Delta u = -\sum_k f_k \delta(\hat{x}_k) - \frac{1}{2} \nabla \times \sum_k n_k \delta(\hat{x}_k),$$  (5.2)

$$\nabla \cdot u = 0.$$  (5.3)

where summation over $k$ indicates summation over the infinite lattice extending in all periodic directions and $\hat{x}_k = x - x_0 - X_k$. Here $x_0$ is the location of one point force and torque and the $k$-th point force and torque, $f_k$ and $n_k$, are located at $x_k = x_0 + X_k$. We would like to emphasize again that the point forces and torques are not regularized, hence the blob function $\phi_\epsilon$, is now replaced by $\lim_{\epsilon \to 0} \phi_\epsilon = \delta$, which is the Dirac’s delta function.

Similar to derivations in chapter 2 we can derive fluid’s velocity and angular velocity in terms of fundamental solutions.

$$\mu u(x) = \frac{1}{8\pi} \sum_k S(\hat{x}_k)f_k - \frac{1}{8\pi} \sum_k R(\hat{x}_k)n_k,$$  (5.4)

$$\mu w(x) = -\frac{1}{8\pi} \sum_k R(\hat{x}_k)f_k - \frac{1}{16\pi} \sum_k D(\hat{x}_k)n_k.$$  (5.5)

where,

$$S(\hat{x}_k) = 8\pi(-\Delta I + \nabla \nabla)B(r) = \frac{J}{r} + \frac{\hat{x}_k \otimes \hat{x}_k}{r^3},$$  (5.6)

$$R(\hat{x}_k) = 4\pi(\nabla \times)G(r) = \frac{(\hat{x}_k \times)}{r^3},$$  (5.7)

$$D(\hat{x}_k) = 4\pi(-\Delta I + \nabla \nabla)G(r) = \frac{J}{r^3} - 3 \frac{\hat{x}_k \otimes \hat{x}_k}{r^3},$$  (5.8)
5.1. GREEN’S FUNCTION FOR PERIODIC STOKES FLOW

Note that $r = ||\hat{x}_k|| = ||x - x_0 - X_k||$ and the Green’s functions for the Laplacian and Biharmonic operators are given as,

$$G(r) = -\frac{1}{4\pi r}, \quad B(r) = -\frac{r}{8\pi}. \quad (5.9)$$

By looking at equations (5.4) and (5.6) we see that fundamental difficulty in the summation is the $1/r$ decay so that the direct sum over the lattice is divergent. However, direct summation can be avoided. Following the method presented in [12], $S(\hat{x})$ may be decomposed using the Beenakker decomposition [1, 12] as,

$$S(\hat{x}) = 8\pi (-\Delta I + \nabla \nabla) [B(r) \text{erfc}(\xi r) + \text{erf}(\xi r)] \frac{\Theta_S(\hat{x})}{\Phi_S(\hat{x})}. \quad (5.10)$$

Here, erf and erfc are Gauss error function and Gauss complementary error function and $\xi$ is an arbitrary positive splitting parameter which indicates the contribution from each sum. As $\xi$ tends to zero, there is larger contribution from $\Theta_S(\hat{x})$ and as $\xi$ grows larger than 1, there is larger contribution from $\Phi_S(\hat{x})$. Now if we apply the differential operator in $\Theta_S$ we will have,

$$\Theta_S(\hat{x}_k) = C(\xi r) \frac{I}{r} + D(\xi r) \frac{\hat{x}_k \otimes \hat{x}_k}{r^3}, \quad (5.11)$$

where,

$$C(\chi) = \text{erfc}(\chi) + \frac{2\chi}{\sqrt{\pi}} (2\chi^2 - 3) \exp(-\chi^2), \quad (5.12)$$

$$D(\chi) = \text{erfc}(\chi) + \frac{2\chi}{\sqrt{\pi}} (1 - 2\chi^2) \exp(-\chi^2). \quad (5.13)$$

We can observe that $\Theta_S$ decays in Gaussian manner as the observation point $x$ moves far from the location of the point forces. This indicates that the slow decay of $S$ is contained in the $\Phi_S$ term. However since this term is smooth and does not contain any singularity [7], we can instead sum the Fourier transform of $\Phi_S$ over the reciprocal lattice in Fourier space with the transformation variable $k$, given as,

$$k = j_1 b_1 + j_2 b_2 + j_3 b_3, \quad k.a_l = j_l, \quad (l = 1, 2, 3), \quad (5.14)$$

where $a_1$, $a_2$ and $a_3$ are the basis vectors introduced in equation (5.1) and $b_1$, $b_2$ and $b_3$ are the reciprocal base vectors defined as,

$$b_1 = \frac{2\pi}{r} a_2 \times a_3, \quad b_2 = \frac{2\pi}{r} a_3 \times a_1, \quad b_2 = \frac{2\pi}{r} a_1 \times a_2, \quad (5.15)$$
and \( \tau = (a_1 \times a_2) \cdot a_3 \) is the volume of a periodic cell in physical space. Now consider the Poisson’s summation formula stating that for any function \( F \) defined over vertices of a three dimensional lattice,

\[
\sum_{k=0}^{\infty} F(X_k) = \frac{1}{\tau} \sum_{m=0}^{\infty} \hat{F}(k_m),
\tag{5.16}
\]

where \( \hat{F}(k) \) is the three-dimensional Fourier transform of \( F \) with respect to \( X \). Following derivations in [12] the three-dimensional Fourier transformation of \( \Phi_S \) with respect to \( X \) is,

\[
\hat{\Phi}_S(k, \hat{x}_0) = \frac{8\pi}{|k|^2} \left[ \left( 1 + \frac{|k|^2}{4\xi^2} + \frac{|k|^4}{8\xi^4} \right) \exp \left( -\frac{|k|^2}{4\xi^2} \right) \right] \left( k \otimes k - I \right) \exp(ik.\hat{x}_0).
\tag{5.17}
\]

The sum of this function over the reciprocal lattice will lead to an expression for the sum in physical space using the Poisson’s formula in equation (5.16). We can also observe that the sum of this function has the Gaussian decay. Now by combining equations (B.9), (5.11) and (5.18) we are able to write,

\[
\sum_k S(\hat{x}_k) = \sum_k \Theta_S(\hat{x}_k) + \frac{1}{\tau} \sum_{|k_m| \neq 0} \hat{\Phi}_S(k_m, \hat{x}_0).
\tag{5.18}
\]

The first summation on the right hand side is in the physical space and the second summation is in reciprocal space. Note that the sum of \( \Phi_S \) in Fourier space contains no singularity and that \( \Theta_S \) contains the entire singularity of \( 1/r \). For more information consider [12, 7].

In a similar fashion, we can split the summation of Rotlets and Doublets into two fast converging sums, one in the physical space and one in the Fourier space. For the Rotlets we will have,

\[
\sum_k R(\hat{x}_k) = \sum_k \Theta_R(\hat{x}_k) + \frac{1}{\tau} \sum_{|k_m| \neq 0} \hat{\Phi}_R(k_m, \hat{x}_0),
\tag{5.19}
\]

where,

\[
\Theta_R(\hat{x}_k) = E(\xi r) \frac{(\hat{x}_k \times)}{r^3},
\tag{5.20}
\]

\[
E(\chi) = \text{erfc}(\chi) + \frac{2\chi}{\sqrt{\pi}} \exp(-\chi^2),
\tag{5.21}
\]

and,

\[
\hat{\Phi}_R(k, \hat{x}_0) = \frac{4\pi i}{|k|^2} \exp \left( -\frac{|k|^2}{4\xi^2} \right) (\hat{k} \times) \exp(ik.\hat{x}_0).
\tag{5.22}
\]

Here \( i = \sqrt{-1} \). Also for the Doublets we will have,

\[
\sum_k D(\hat{x}_k) = \sum_k \Theta_D(\hat{x}_k) + \frac{1}{\tau} \sum_{|k_m| \neq 0} \hat{\Phi}_D(k_m, \hat{x}_0),
\tag{5.23}
\]
5.2. REGULARIZATION METHOD FOR PERIODIC STOKES FLOW

where,

\[ \Theta_D(\hat{x}_k) = \bar{C}(\xi_r) \frac{I}{r^3} - 3\bar{D}(\xi_r) \frac{\hat{x}_k \otimes \hat{x}_k}{r^5}, \] (5.24)

\[ \bar{C}(\chi) = \text{erf}(\chi) + \frac{2\chi}{\sqrt{\pi}} (1 + 2\chi^2) \exp(-\chi^2), \] (5.25)

\[ \bar{D}(\chi) = \text{erf}(\chi) + \frac{2\chi}{\sqrt{\pi}} (1 + \frac{2}{3}\chi^2) \exp(-\chi^2). \] (5.26)

and,

\[ \hat{\Phi}_D(k, \hat{x}_0) = -4\pi \exp \left( -\frac{|k|^2}{4\xi_r^2} \right) \left( I - \frac{k \otimes k}{|k|^2} \right) \exp(ik \cdot \hat{x}_0). \] (5.27)

For detailed derivations of Ewald sums for the Rotlets and Doublets, see Appendix B.

5.2 Regularization method for periodic Stokes flow

When calculating the velocity and angular velocity of fluid at the location point, forces and torques, the fundamental solutions presented in section 5.1 become singular. To overcome this difficulty, similar to what we had in chapter 2, we may use a regularized method. Instead of equations (5.2) and (5.2), we may now consider,

\[ -\nabla p + \mu \Delta u = -\sum_k f_k \phi_\epsilon(\hat{x}_k) - \frac{1}{2} \nabla \times \sum_k n_k \phi_\epsilon(\hat{x}_k), \] (5.28)

\[ \nabla \cdot u = 0. \] (5.29)

The summation over \( k \) again indicates the summation over the infinite lattice extending in all periodic directions and \( \Phi_\epsilon \) is the blob function introduced in chapter 2 i.e. a radially symmetric and smooth approximation of the three-dimensional Dirac distribution centered at \( x_k \). The direct decomposition of regularized Stokeslets would be \( S_\epsilon(\hat{x}) = 8\pi (-\Delta I + \nabla \nabla) B_\epsilon(r) = \Theta_{S_\epsilon}(\hat{x}) + \Phi_{S_\epsilon}(\hat{x}) \) where,

\[ \Theta_{S_\epsilon}(\hat{x}) = 8\pi (-\Delta I + \nabla \nabla)[B_\epsilon(r) \text{erfc}(\xi_r)], \] (5.30)

\[ \Phi_{S_\epsilon}(\hat{x}) = 8\pi (-\Delta I + \nabla \nabla)[B_\epsilon(r) \text{erfc}(\xi_r)]. \] (5.31)

Again we would have the Gaussian decay in \( \Theta_{S_\epsilon} \) and \( \Phi_{S_\epsilon} \) will contain the \( 1/r \) decay in physical space. However, to determine the convergence rate of \( \Phi_{S_\epsilon}(\hat{x}) \) in Fourier space one must deal with calculation of complicated integrals, even if the blob function is chosen with caution. Following the method presented in [7], this can be avoided.

Instead of the direct decomposition, we split equations (5.28) and (5.29) into the following system of equations,
\[
\begin{cases}
- \nabla p_1 + \mu \Delta u_1 = - \sum_n f \delta(\hat{x}_n) - \frac{1}{2} \nabla \times \sum_n n \delta(\hat{x}_n), \\
\nabla \cdot u_1 = 0, \\
w_1 = \frac{1}{2} \nabla \times u_1.
\end{cases}
\] (5.32)

And,

\[
\begin{cases}
- \nabla p_2 + \mu \Delta u_2 = - \sum_n f[\phi_n(\hat{x}_n) - \delta(\hat{x}_n)] - \frac{1}{2} \nabla \times \sum_n n[\phi_n(\hat{x}_n) - \delta(\hat{x}_n)], \\
\nabla \cdot u_2 = 0, \\
w_2 = \frac{1}{2} \nabla \times u_2.
\end{cases}
\] (5.33)

Because of linearity of Stokes equation we will have,

\[
u = u_1 + u_2,
\] (5.34)

\[
w = w_1 + w_2,
\] (5.35)

\[
p = p_1 + p_2,
\] (5.36)

where \(u, w\) and \(p\) are the solution to equations (5.28) and (5.29). Note that \(u_1\) and \(w_1\) are the solution to equations (5.2) and (5.3) and the singularity of \(u_1\) and \(w_1\) is contained entirely in the physical space part of the decomposition \((\Theta_S, \Theta_R\) and \(\Theta_D)\) while there is no singularity within the Fourier space calculation since \(\Phi_S, \Phi_R\) and \(\Phi_D\) are smooth. The goal is to remove the singularity and replace it with a regularized term all within the physical space sum without changing the summation in the Fourier space. Following equations (5.34) and (5.35) we will have,

\[
u = u_1 + \frac{1}{8\pi\mu} \sum_k [S_\epsilon(\hat{x}_k) - S(\hat{x}_k)] f_k - \frac{1}{8\pi\mu} \sum_k [R_\epsilon(\hat{x}_k) - R(\hat{x}_k)] n_k,
\] (5.37)

\[
w = w_1 - \frac{1}{8\pi\mu} \sum_k [R_\epsilon(\hat{x}_k) - R(\hat{x}_k)] f_0 - \frac{1}{16\pi\mu} \sum_k [D_\epsilon(\hat{x}_k) - D(\hat{x}_k)] n_k,
\] (5.38)

Now consider the periodic Green’s functions \(S_p, R_p\) and \(D_p\),

\[
u = \frac{1}{8\pi\mu} S_p - \frac{1}{8\pi\mu} R_p, \quad w = - \frac{1}{8\pi\mu} R_p - \frac{1}{16\pi\mu} D_p.
\] (5.39)
Using the decomposition in section 5.1 we can now write,

\[
S_p(\hat{x}) = \sum_k (S(\hat{x}_k) + S_\epsilon(\hat{x}_k) - S(\hat{x}_k))
\]

\[
= \sum_k (\Theta S(\hat{x}_k) + \Phi S(\hat{x}_k) + S_\epsilon(\hat{x}_k) - S(\hat{x}_k)) + \frac{1}{r} \sum_{|k_m| \neq 0} \hat{\Phi}_S(k_m, \hat{x}_0)
\]

By excluding \( n = 0 \) from \( \Theta S_p \) which contains the entire singularity we will have,

\[
\Theta S_p = \sum_k \left( C(\xi r_k) \frac{I}{r_k} + D(\xi r_k) \frac{\hat{x}_k \otimes \hat{x}_k}{r_k^3} + 8\pi H_1(r_k) I + 8\pi H_2(r_k) \frac{\hat{x}_k \otimes \hat{x}_k - I}{r_k^3} \right)
\]

\[
= \sum_{k \neq 0} \left( C(\xi r_k) \frac{I}{r_k} + D(\xi r_k) \frac{\hat{x}_k \otimes \hat{x}_k}{r_k^3} + (8\pi H_1(r_k) - \frac{1}{r_k}) I + 8\pi (H_2(r_k) - \frac{1}{r_k^3}) \hat{x}_k \otimes \hat{x}_k \right) +
\]

\[
+ \left( C(\xi r_0) - \frac{1}{r_0} \right) I + \frac{D(\xi r_0) - 1}{r_0^3} \hat{x}_0 \otimes \hat{x}_0 +
\]

\[
+ 8\pi H_1(r_0) I + 8\pi H_2(r_0) \frac{\hat{x}_0 \otimes \hat{x}_0}{r_0^3}
\]

Here, \( H_1 \) and \( H_2 \) are given by equations (2.33) and (2.34). We want the sums to converge fast so that we can truncate the summation while keeping the accuracy. In order not to destroy the original convergence properties of equation (5.30), we want \( S - S_\epsilon \) to decay as fast \( \Theta S \) i.e. with Gaussian decay. But since we have \( S - S_\epsilon = 8\pi (\Delta I + \nabla \nabla \nabla)(B_c - B(r)) \) we can guarantee Gaussian decay by carefully tuning the blob function. We will discuss conditions on the blob function later on in this section. It can be checked that \( \Theta_S \) does not contain any singularity. The only terms left to consider is \( [(C(\xi r_0) - 1)/r_0 I + [(D(\xi r_0) - 1)/r_0^3] \hat{x}_k \otimes \hat{x}_k \) which can be easily proven to be non-singular,

\[
\lim_{r \to 0} \frac{C(\xi r) - 1}{r} = -\frac{8\xi}{\sqrt{\pi}},
\]

\[
\lim_{r \to 0} \frac{D(\xi r) - 1}{r^3} = 0,
\]

For more information, see [7]. In the same fashion we can decompose regularized Rotlets and Doublets as follow,
\[ Rp(\hat{x}) = \sum_{k} \left( \Theta_{R}(\hat{x}_k) + \Phi_{R}(\hat{x}_k) + R_{e}(\hat{x}_k) - R(\hat{x}_k) \right) \]
\[ = \sum_{k} \left( \Theta_{R}(\hat{x}_k) + R_{e}(\hat{x}_k) - R(\hat{x}_k) \right) + \frac{1}{\tau} \sum_{|k_m| \neq 0} \Phi_{R}(k_m, \hat{x}_0) \tag{5.44} \]

\[ Dp(\hat{x}) = \sum_{k} \left( \Theta_{D}(\hat{x}_k) + \Phi_{D}(\hat{x}_k) + D_{e}(\hat{x}_k) - D(\hat{x}_k) \right) \]
\[ = \sum_{k} \left( \Theta_{D}(\hat{x}_k) + D_{e}(\hat{x}_k) - D(\hat{x}_k) \right) + \frac{1}{\tau} \sum_{|k_m| \neq 0} \Phi_{D}(k_m, \hat{x}_0) \tag{5.45} \]

And again by excluding the cell containing \( x_0 \) (represented by \( n = 0 \)), we will have,

\[ \Theta_{R_p} = \sum_{k} \left( E(\xi r_k)(\hat{x}_k \times \frac{\hat{x}_k \times}{r_k^3}) + \frac{(\hat{x}_k \times)}{r_k^3} \right) \]
\[ = \sum_{k \neq 0} \left( E(\xi r_k)(\hat{x}_k \times \frac{\hat{x}_k \times}{r_k^3}) + (4\pi Q(r_k) - \frac{1}{r_k^3})(\hat{x}_k \times) \right) + \left( \frac{E(\xi r_0) - 1}{r_0^3} (\hat{x}_0 \times) + 4\pi Q(r_0) - (\hat{x}_0 \times) \right), \tag{5.46} \]

\[ \Theta_{D_p} = \sum_{k} \left( C(\xi r_k) \frac{I_{r_k}}{r_k^3} - 3D(\xi r_k) \frac{\hat{x}_k \otimes \hat{x}_k}{r_k^3} + \frac{3\hat{x}_k \otimes \hat{x}_k}{r_k^3} + 4\pi D_{1}(r_k) I + 4\pi D_{2}(r_k) \hat{x}_k \otimes \hat{x}_k - \frac{I}{r_k^3} + \frac{3\hat{x}_k \otimes \hat{x}_k}{r_k^3} \right), \tag{5.47} \]
\[ = \sum_{k \neq 0} \left( C(\xi r_k) \frac{I_{r_k}}{r_k^3} - 3D(\xi r_k) \frac{\hat{x}_k \otimes \hat{x}_k}{r_k^3} + (4\pi D_{1}(r_k) - \frac{1}{r_k^3}) I + (4\pi D_{2}(r_k) + \frac{3}{r_k^3}) \hat{x}_k \otimes \hat{x}_k \right) + \left( \frac{C(\xi r_0) - 1}{r_0^3} I - \frac{3D(\xi r_0) - 3}{r_0^3} \hat{x}_0 \hat{x}_0 + 4\pi D_{1}(r_0) I + 4\pi D_{2}(r_0) \hat{x}_0 \otimes \hat{x}_0 \right). \]

Here \( Q, D_{1} \) and \( D_{2} \) are given by equations (2.35) to (2.37). With a similar argument we had for the Stokeslets, in order not to destroy the original convergence properties, we need \( R_{e} - R \) and \( D_{e} - D \) to have Gaussian decay. This is possible
by the right choice of the blob function. To prove that $\Theta_{R_p}$ and $\Theta_{D_p}$ are non-singular we only need to consider the main lattice box where $n = 0$. Since $Q$, $D_1$ and $D_2$ are constructed to be non-singular, we only have to prove that the terms $[(E(\xi r_0) - 1)/r_0^3](\hat{x}_k \times)$ and $[(C(\xi r_0) - 1)/r_0^3]I + [(D(\xi r_0) - 1)/r_0^5]\hat{x}_k \otimes \hat{x}_k$ are non-singular. For this consider the following,

$$\lim_{r \to 0} E(\xi r) - 1 \frac{1}{r^3} = \frac{-4\xi^4}{3\sqrt{\pi}}, \quad (5.48)$$

$$\lim_{r \to 0} \bar{C}(\xi r) - 1 \frac{1}{r^3} = \frac{8\xi^3}{3\sqrt{\pi}}, \quad (5.49)$$

$$\lim_{r \to 0} \bar{D}(\xi r) - 1 \frac{1}{r^5} = 0, \quad (5.50)$$

We will finish this section by presenting the required conditions on the blob function so that $S_{\epsilon} - S$, $R_{\epsilon} - R$ and $D_{\epsilon} - D$ contain Gaussian decay as the observer point moves away from the point forces and torques. The following theorem, which is an extension to the theorem presented in [7], will guarantee these decay conditions.

**Second moment theorem.** Let $\phi_{\epsilon}$ be a continuous bounded function that satisfies the following conditions:

1. $\phi_{\epsilon}(r)$ is radially symmetric.

2. $\phi_{\epsilon}(r)$ has the decay property $|\phi_{\epsilon}(r)| \leq C r^m \exp(-\xi^2 r^2)$ for some integer $m > 0$ and some constants $C > 0$ and $\xi > 0$.

3. $\int_0^\infty r^2 \phi_{\epsilon}(r) dr = \frac{1}{\pi r}.$

4. $\int_0^\infty r^4 \phi_{\epsilon}(r) dr = 0.$

Then,

$$|8\pi H_1(r) - 1/r| \leq C_1 r^m \exp(-\xi^2 r^2), \quad (5.51)$$

$$|8\pi H_2(r) - 1/r^3| \leq C_2 r^{m-2} \exp(-\xi^2 r^2), \quad (5.52)$$

$$|4\pi Q(r) - 1/r^3| \leq C_3 r^{m-2} \exp(-\xi^2 r^2), \quad (5.53)$$

$$|4\pi D_1(r) - 1/r^3| \leq C_4 r^m \exp(-\xi^2 r^2), \quad (5.54)$$

$$|4\pi D_2(r) - 1/r^5| \leq C_5 r^{m-2} \exp(-\xi^2 r^2). \quad (5.55)$$

For detailed proof, see Appendix C.
Chapter 6

Conclusion and Discussion

In this thesis we presented the mathematical modeling of an elastic rod with natural curvature and twist placed within a viscous fluid with zero Reynolds number. The dependency of the method to the numerical parameters together with the accuracy and convergence properties of the method was examined in chapter 3 along with the validation of the method for the test case of relaxation of naturally bent and twisted open/closed rods. We then compared the regularized Stokelets method with non-local slender body formulation for the case of elastic rods with no intrinsic curvature and twist inside a planar shear flow. In chapter 4 we also examined the extension of helical rods when they are immersed in a constant background flow. Finally in chapter 5 we derived an Ewald summation for regularized fundamental solutions to Stokes equations to obtain fast converging summations over a periodic array of point forces.

The motivation of using the regularized Stokes method to model zero Reynolds applications compared to the other methods is the reduction of complexity while taking into account the curvature and the twist of the rod. Also because the discretization of the fluid is avoided, the method can be easily adopted to various applications. The test cases of relaxation, extension and interactions of the fluid with various external flows in this thesis, are examples of such.

Through several numerical examples and applications, this method has been derived, implemented and verified. However there are many other applications that are interesting to investigate. One exciting example would be the investigation of the Jeffry orbits of twisted and bent rods since many theoretical and numerical modeling of this phenomena can be found in the existing literature. Another set of application can also be examined are the swimming rods. The idea is to make intrinsic curvature and twist time dependent so that the rod obtain a natural movement. This motion would then help the rod to swim inside the fluid environment. Following the derivations for an Ewald sums for the fundamental solutions in chapter 5, the truncation error is to be examined. Then by truncating the summation in the physical space and using fast methods for efficient computation of the summation in reciprocal space we can reduce the complexity from $O(M^2)$ to $O(M \log M)$.
or even $\mathcal{O}(M)$. 
Appendix A

Derivation of solution to incompressible Stokes equations

Consider the regularized Green’s functions for $\phi_\epsilon$ in equation (2.18). To derive the linear velocity of the fluid we substitute a particular solution for the pressure in equation (2.20) into equation (2.11). We have,

$$\mu \Delta u = \nabla p - f_0 \phi_\epsilon - \frac{1}{2} \nabla \times (n_0 \phi_\epsilon) \tag{A.1}$$

$$= \nabla (f_0 \cdot \nabla G_\epsilon) - f_0 \phi_\epsilon - \frac{1}{2} \nabla \phi_\epsilon \times n_0$$

$$= \nabla (f_0 \cdot \nabla (\Delta B_\epsilon)) - f_0 \Delta^2 B_\epsilon - \frac{1}{2} \nabla (\Delta G_\epsilon) \times n_0.$$

Now the solution of regularized Stokes equation for a given point force and torque is,

$$\mu u = \nabla (f_0 \cdot \nabla B_\epsilon) - f_0 \Delta B_\epsilon - \frac{1}{2} \nabla G_\epsilon \times n_0 + C_2. \tag{A.2}$$

where $C_2$ is the integral constant. To evaluate the angular velocity of the fluid, we use equations (A.2) and (2.13) to write,

$$\mu w = \frac{1}{2} \nabla \times (\mu u) \tag{A.3}$$

$$= \frac{1}{2} \nabla \times [\nabla (f_0 \cdot \nabla B_\epsilon)] - \frac{1}{2} \nabla \times [f_0 \Delta B_\epsilon] - \frac{1}{4} \nabla \times [\nabla G_\epsilon \times n_0]$$

$$= 0 - \frac{1}{2} (\Delta G_\epsilon) \times f_0 - \frac{1}{4} \nabla \times [\nabla \times (n_0 G_\epsilon)]$$

$$= -\frac{1}{2} (\Delta G_\epsilon) \times f_0 - \frac{1}{4} \nabla (n_0 \cdot \nabla G_\epsilon) + \frac{1}{4} n_0 \Delta G_\epsilon.$$

Here we used the vector identities that $\nabla \times (\nabla g) = 0$ and $\nabla \times (\nabla \times A) = \nabla (\nabla \cdot A) - \Delta A$ for any scalar function $g$ and any vector field $A$. With some modifications
to equations (A.2) and (A.3) we obtain,

\[
\begin{align*}
\mu u &= (-\Delta I + \nabla \nabla) B_\epsilon(r) f_0 - \frac{1}{2} (\nabla \times) G_\epsilon(r) n_0 + C_2, \\
\mu w &= -\frac{1}{2} (\nabla \times) G_\epsilon(r) f_0 - \frac{1}{4} (-\Delta I + \nabla \nabla) G_\epsilon(r) n_0,
\end{align*}
\]  

(A.4) (A.5)

where \( \Delta I, \nabla \nabla \) and \( (\nabla \times) \) are given in equations (2.23) - (2.25).
Appendix B

Ewald sums for the Routlets and the Doublets

Following the derivation of Ewald summation of the Stokeslets in chapter 5, we derive the Ewald summation for the Rotlets and Doublets given in equations (5.7) and (5.8). We may decompose $R(\hat{x})$ using the Beenakker decomposition as,

$$
R(\hat{x}) = 4\pi(\nabla \times)G(r)
\begin{align*}
&= 4\pi(\nabla \times) [G(r)\text{erfc}(\xi r) + \text{erf}(\xi r)] \\
&= 4\pi(\nabla \times) [G(r)\text{erfc}(\xi r)] + 4\pi(\nabla \times) [G(r)\text{erf}(\xi r)].
\end{align*}
$$

If we apply the differential operator in $\Phi_R$ we will have,

$$
\Phi_R(\hat{x}) = E(\xi r)\frac{(\hat{x} \times) r}{r^3},
$$

where,

$$
E(\chi) = \text{erf}(\chi) + \frac{2\chi}{\sqrt{\pi}} \exp(-\chi^2).
$$

Here $\hat{x} = x - x_0 - X$. To use the Poisson’s summation formula given in equation (5.16), we need to compute the three-dimensional Fourier transformation of $\Phi_R$ with respect to $X$. We have,

$$
\hat{\Phi}_R(k, \hat{x}_0) = \int_{\mathbb{R}^3} \exp(ik \cdot X)\Phi(\hat{x}) \, d^3X
\begin{align*}
&= \int_{\mathbb{R}^3} \exp(ik \cdot X)(\nabla \times) \left(\frac{-\text{erf}(\xi r)}{r}\right) \, d^3X \\
&= i(k \times) \int_{\mathbb{R}^3} \exp(ik \cdot X) \left(\frac{\text{erf}(\xi r)}{r}\right) \, d^3X.
\end{align*}
$$
Here we used integration by parts to move the differential operator and applied it on $\exp(ik.X)$. Note that $r = |x - x_0 - X|$. To evaluate the last integral, call it $Q$, we use spherical coordinates to write,

\[
Q = \exp(ik.\hat{x}_0) \int_{\mathbb{R}^3} \exp(ik \cdot (X - \hat{x}_0)) \left( \frac{\text{erf}(\xi r)}{r} \right) d^3X
\]

\[
= 2\pi \exp(ik.\hat{x}_0) \int_0^{2\pi} \int_0^\infty \exp(i|k| r \cos \theta) \text{erf}(\xi r) r \sin \theta \, d\theta \, dr
\]

Performing the integration with respect to $\theta$ we obtain,

\[
Q = \exp(ik.\hat{x}_0) \frac{4\pi}{|k|} \int_0^\infty \sin(|k| r) \text{erf}(\xi r) \, dr.
\]

The last integration is computed in [12] and is given by,

\[
\int_0^\infty \sin(|k| r) \text{erf}(\xi r) \, dr = \frac{1}{|k|} \exp(-\frac{|k|^2}{4\xi^2}).
\]

By substituting this into $Q$ and then into equation (B.4) we obtain the Fourier transformation of $\Phi_R$ given as,

\[
\hat{\Phi}_R(k, \hat{x}_0) = \frac{4\pi i}{|k|^2} \exp \left( -\frac{|k|^2}{4\xi^2} \right)(\vec{k} \times) \exp(ik.\hat{x}_0).
\]

Now we will derive the decomposition of the Doublets given in equation (5.8) which is based on private notes of A. Tornberg. The Doublets may be decomposed as follow,

\[
D(\hat{x}) = 4\pi(-\Delta I + \nabla \nabla)G(r) = 4\pi(-\Delta I + \nabla \nabla)G(r)[\text{erf}(\xi r) + \text{erf}(\xi r)]
\]

\[
\Theta_D(\hat{x}) \equiv \frac{\Theta_D(\hat{x})}{\Phi_D(\hat{x})}
\]

If we apply the differential operator in $\Theta_D$ we obtain,

\[
\Theta_D(\hat{x}) = \tilde{C}(\xi r) \frac{I}{r^3} - 3\tilde{D}(\xi r) \frac{\hat{x} \otimes \hat{x}}{r^5},
\]

where,

\[
\tilde{C}(\chi) = \text{erf}(\chi) + \frac{2\chi}{\sqrt{\pi}}(1 + 2\chi^2) \exp(-\chi^2),
\]

\[
\tilde{D}(\chi) = \text{erf}(\chi) + \frac{2\chi}{\sqrt{\pi}}(1 + \frac{2}{3}\chi^2) \exp(-\chi^2).
\]

Now we derive the Fourier part of this decomposition. The Doublets may be expressed in terms of Stokeslets as follow,
\[ D(\hat{x}) = -\frac{1}{2} \Delta S(\hat{x}). \] (B.13)

It can be easily checked that,
\[
\frac{1}{2} \Delta \left( r \text{ erfc}(\xi r) - \frac{1}{\sqrt{\pi \xi}} \exp(-\xi^2 r^2) - \frac{1}{2\xi^2} \frac{\text{erf}(\xi r)}{r} \right) = \frac{\text{erfc}(\xi r)}{r}. \] (B.14)

This means that the screening function is \( \gamma(r) = \xi^3 \pi^{-3/2} \exp(-\xi^2 r^2) \) with the Fourier transform \( \hat{\gamma}(k) = \exp(-|k|^2/(4\xi^4)) \). This would yield,
\[
\hat{\Phi}_D(k, \hat{x}_0) = -4\pi \exp \left( -\frac{|k|^2}{4\xi^2} \right) \left( I - \frac{k \otimes k}{|k|^2} \right) \exp(ik.\hat{x}_0). \] (B.15)
Appendix C

Proof for the Second Moment Theorem

Here we provide the proof to the second moment theorem which was presented in chapter 5. The proof is an extension to the derivations in [7].

Second moment theorem. Let \( \phi_\epsilon \) be a continuous bounded function that satisfies the following conditions:

1. \( \phi_\epsilon (r) \) is radially symmetric.
2. \( \phi_\epsilon (r) \) has the decay property \( |\phi_\epsilon (r)| \leq Cr^m \exp(-\xi^2 r^2) \) for some integer \( m > 0 \) and some constants \( C > 0 \) and \( \xi > 0 \).
3. \( \int_0^\infty r^2 \phi_\epsilon (r) \, dr = \frac{1}{4\pi} \).
4. \( \int_0^\infty r^4 \phi_\epsilon (r) \, dr = 0 \).

Then,

\[
|8\pi H_1 (r) - 1/r| \leq C_1 r^m \exp(-\xi^2 r^2), \quad (C.1)
\]
\[
|8\pi H_2 (r) - 1/r^3| \leq C_2 r^{m-2} \exp(-\xi^2 r^2), \quad (C.2)
\]
\[
|4\pi Q (r) - 1/r^3| \leq C_3 r^{m-2} \exp(-\xi^2 r^2), \quad (C.3)
\]
\[
|4\pi D_1 (r) - 1/r^3| \leq C_4 r^m \exp(-\xi^2 r^2), \quad (C.4)
\]
\[
|4\pi D_2 (r) - 1/r^5| \leq C_5 r^{m-2} \exp(-\xi^2 r^2). \quad (C.5)
\]

Proof. Let \( M_n = \int_0^\infty r^{n+2} \phi_\epsilon (r) \, dr \) for \( n = 0, 1, 2 \), where \( \phi_\epsilon \) is a function satisfying the conditions above. Also consider the corresponding regularized Green’s functions,

\[
\Delta^2 B_\epsilon (r) = \Delta G_\epsilon (r) = \phi_\epsilon (r). \quad (C.6)
\]
Since \( \phi_e \) is radially symmetric, the function must satisfy the following ordinary differential equations,

\[
G_e''(r) + \frac{2}{r} G_e'(r) = \frac{1}{r} (r G_e(r)) = \phi_e(r), \tag{C.7}
\]
\[
B_e''(r) + \frac{2}{r} B_e'(r) = \frac{1}{r} (r B_e(r)) = G_e(r). \tag{C.8}
\]

Note that by the definition of \( \phi_e(r) \), \( B_e(0) \) and \( G_e(0) \) are bounded and also,

\[
\lim_{r \to \infty} G_e(r) + \frac{r}{4\pi} = 0, \tag{C.9}
\]
\[
\lim_{r \to \infty} B_e(r) + \frac{r}{8\pi} = 0. \tag{C.10}
\]

Equations (C.7) and (C.8) can be solved by integrating \( rG_e(r) \) and \( rB_e(r) \) twice and using integration by parts to obtain,

\[
G_e(r) = - \frac{1}{r} M_0 - \int_r^\infty s \phi_e(s) \, ds + \frac{1}{r} \int_r^\infty s^2 \phi_e(s) \, ds, \tag{C.11}
\]
\[
B_e(r) = - \frac{r}{2} M_0 - \frac{r^2}{6} \int_r^\infty s \phi_e(s) \, ds + \frac{r}{2} \int_r^\infty s^2 \phi_e(s) \, ds \tag{C.12}
- \frac{1}{2} \int_r^\infty s^3 \phi_e(s) \, ds - \frac{1}{6r} \left( M_2 - \int_r^\infty s^4 \phi_e(s) \, ds \right).
\]

Conditions 3 and 4 of the theorem indicate that \( M_0 = 1/(4\pi) \) and \( M_2 = 0 \). We are interested in the decay of the following functions,

\[
E(r) = \frac{8\pi}{r} - \frac{1}{r^3} = - \frac{8\pi B_e''(r)}{r} - \frac{8\pi B_e'(r)}{r^3} - \frac{1}{r^3}, \tag{C.13}
\]
\[
F(r) = \frac{8\pi}{r} - \frac{1}{r^3} = \frac{4\pi G_e''(r)}{r} - \frac{4\pi G_e'(r)}{r^3} - \frac{1}{r^3}, \tag{C.14}
\]
\[
H(r) = \frac{4\pi}{r} - \frac{1}{r^3} = \frac{4\pi G_e''(r)}{r} - \frac{4\pi G_e'(r)}{r^3} - \frac{1}{r^3}, \tag{C.15}
\]
\[
\bar{E}(r) = \frac{4\pi}{r^3} = - \frac{4\pi G_e''(r)}{r^4} + \frac{4\pi G_e'(r)}{r^3} - \frac{1}{r^5}, \tag{C.16}
\]
\[
\bar{F}(r) = \frac{4\pi}{r^3} = - \frac{4\pi G_e''(r)}{r^4} + \frac{4\pi G_e'(r)}{r^3} - \frac{1}{r^5}. \tag{C.17}
\]

Using the expressions for \( G_e(r) \) and \( B_e(r) \) in equations (C.11) and (C.12) we
\[
E(r) = \frac{16\pi}{3} \int_r^\infty s\phi_\varepsilon(s) \, ds - \frac{4\pi}{r} \int_r^\infty s^2\phi_\varepsilon(s) \, ds - \frac{4\pi}{3r^3} \int_r^\infty s^4\phi_\varepsilon(s) \, ds, \tag{C.18}
\]
\[
F(r) = -\frac{4\pi}{r^3} \int_r^\infty s^2\phi_\varepsilon(s) \, ds + \frac{4\pi}{r^5} \int_r^\infty s^4\phi_\varepsilon(s) \, ds, \tag{C.19}
\]
\[
H(r) = \frac{4\pi}{r^3} \int_r^\infty s^2\phi_\varepsilon(s) \, ds, \tag{C.20}
\]
\[
\bar{E}(r) = 4\pi\phi_\varepsilon(r) - \frac{4\pi}{r^3} \int_r^\infty s^2\phi_\varepsilon(s) \, ds, \tag{C.21}
\]
\[
\bar{F}(r) = \frac{4\pi}{r^2} \phi_\varepsilon - \frac{4\pi}{r^5} \int_r^\infty s^2\phi_\varepsilon(s) \, ds. \tag{C.22}
\]

Note that for \( n \geq 1 \), condition 2 in the theorem implies that,
\[
\int_r^\infty s^n\phi_\varepsilon(s) \, ds \leq \int_r^\infty s^n s^{n+m} \exp(-\xi^2 s^2) \, ds \tag{C.23}
\]
\[
= C\xi^{-(n+m+1)} \int_{\xi r}^\infty z^{n+m} \exp(-z^2) \, dz \leq \tilde{C}\xi^{-2r^{n+m-1}} \exp(-\xi^2 r^2).
\]

This inequality along with equations (C.18) to (C.22) will guarantee the decays in equations (C.1) to (C.5). \( \square \)
Appendix D

Comments on the Equilibrium Equations of the Rod

The following derivations are based on private notes of Charles S. Peskin. Consider an axially symmetric rod with zero twist modulus i.e. $a_1 = a_2 = a$ and $a_3 = 0$. In this case it can be shown that,

$$\frac{\partial N}{\partial s} = D^3 \times a \frac{\partial^2 D^3}{\partial s^2}. \quad (D.1)$$

Note that in the equilibrium state $\partial X/\partial s = D^3$ so the latter equation can be written as,

$$\frac{\partial N}{\partial s} = \frac{\partial X}{\partial S} \times a \frac{\partial^3 D^3}{\partial s^3}. \quad (D.2)$$

The in extensibility of the rod yields,

$$\frac{\partial X}{\partial s} \cdot \frac{\partial X}{\partial s} = 1, \quad (D.3)$$
$$\frac{\partial X}{\partial s} \cdot \frac{\partial^2 X}{\partial s^2} = 0, \quad (D.4)$$
$$\frac{\partial^2 X}{\partial s^2} \cdot \frac{\partial^2 X}{\partial s^2} + \frac{\partial X}{\partial s} \cdot \frac{\partial^3 X}{\partial s^3} = 0. \quad (D.5)$$

By inserting equation (D.2) into equation (2.1) and (2.2) we obtain,

$$0 = f + \frac{\partial F}{\partial s}, \quad (D.6)$$
$$0 = n + \frac{\partial X}{\partial s} \times \left( a \frac{\partial^3 D^3}{\partial s^3} + F \right). \quad (D.7)$$

We can decompose $n = n^{\perp} + n^{\parallel}$ where $n^{\parallel}$ is in the direction of $\partial X/\partial s$ and $n^{\perp}$ is in the perpendicular plane to $\partial X/\partial s$. Then from equation (D.7) it can be observed
that $n^\parallel = (\partial X/\partial s) \cdot n = 0$, and so $n = n^\perp$. We wish to eliminate $n^\perp$. Define,

$$G = \frac{\partial X}{\partial s} \times n^\perp,$$  \hspace{1cm} (D.8)

$$g = -\frac{\partial G}{\partial s}. \hspace{1cm} (D.9)$$

By using equation (D.7) we have,

$$G = \frac{\partial X}{\partial s} \times n^\perp = \frac{\partial X}{\partial s} \times \left( \frac{\partial X}{\partial s} \times \left( a \frac{\partial^3 D}{\partial s^3} + F \right) \right). \hspace{1cm} (D.10)$$

Let $b = a \frac{\partial^3 D}{\partial s^3} + F$, then,

$$G = -\frac{\partial X}{\partial s} \times \frac{\partial X}{\partial s} \times b \hspace{1cm} (D.11)$$

$$= -\left( \frac{\partial X}{\partial s} \cdot b \right) \frac{\partial X}{\partial s} - \left( \frac{\partial X}{\partial s} \cdot \frac{\partial X}{\partial s} \right) b$$

$$= b - \left( \frac{\partial X}{\partial s} \cdot b \right) \frac{\partial X}{\partial s}$$

$$= b^\perp.$$  \hspace{1cm} (D.12)

Here we used equation (D.3). Hence,

$$G = a \left( \frac{\partial^3 X}{\partial s^3} \right)^\perp + F^\perp. \hspace{1cm} (D.13)$$

Note that,

$$\left( \frac{\partial^3 X}{\partial s^3} \right)^\perp = \frac{\partial^3 X}{\partial s^3} - \left( \frac{\partial X}{\partial s} \cdot \frac{\partial^3 X}{\partial s^3} \right) \frac{\partial X}{\partial s}. \hspace{1cm} (D.14)$$

By inserting equation (D.5) into (D.13) and then into (D.12) we get,

$$G = a \frac{\partial^3 X}{\partial s^3} + a \left| \frac{\partial^2 X}{\partial s^2} \right|^2 \frac{\partial X}{\partial s} + F^\perp, \hspace{1cm} (D.15)$$

and also from equation (D.9),

$$0 = g + \frac{\partial G}{\partial s} = g + a \frac{\partial^4 X}{\partial s^4} + a \frac{\partial}{\partial s} \left( \left| \frac{\partial^2 X}{\partial s^2} \right|^2 \right) + \frac{\partial F^\perp}{\partial s}. \hspace{1cm} (D.16)$$
Now subtract equation (D.15) from (D.6),
\[0 = f - g - a \frac{\partial^4 X}{\partial s^4} - a \frac{\partial}{\partial s} \left( \frac{\partial X}{\partial s} \left| \frac{\partial^2 X}{\partial s^2} \right|^2 \right) + \frac{\partial}{\partial s} (F - F^\perp).\] (D.16)

Note that from equation (2.3), \(F - F^\perp = F^3 D^3 = F^3 (\partial X/\partial s)\). Hence,
\[0 = (f - g) - a \frac{\partial^4 X}{\partial s^4} + \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right),\] (D.17)
with,
\[T = F^3 - a \left| \frac{\partial^2 X}{\partial s^2} \right|^2.\] (D.18)

This means that in the case \(n = n^\perp\), we can remove \(n\) by modifying \(f\). In other words, the transverse components of torque can be changed to an equivalent distribution of applied force. In the previous setting \(F\) was an unknown vector needed to enforce \(\partial X/\partial s = D^3\). However in this setting one component remains, which is now denoted \(T\), that must be determined such that equation (D.3) holds.

The modified force \(\tilde{f}\) that comes out of this derivations is given by,
\[\tilde{f} = f - g = a \frac{\partial^4 X}{\partial s^4} - \frac{\partial}{\partial s} \left( T \frac{\partial X}{\partial s} \right).\] (D.19)

This is formulation of the force given in equation (2.10).
Bibliography


