A SURFACE INTEGRAL EQUATION BASED DERIVATION AND ALGORITHM FOR SIMULATING VESICLE FLOWS IN THREE DIMENSIONS

by

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ABSTRACT

We present a method for simulating the evolution of inextensible vesicles suspended in a Stokesian fluid flow. The flow model problem is reformulated as a coupled system of integro-differential equations relating the evolution of the vesicle membrane to the interfacial forces. Variational techniques are applied to derive an exact form for the interfacial forces on the vesicle. A super algebraic algorithm is presented to numerically evaluate weakly singular integrals which arise in the development of the simulation. Discretization of our coupled system of integro-differential equations is done using a fully discrete Galerkin method in space and an explicit scheme in time. This approach yields a high–order spatially accurate solution with relatively few degrees of freedom. Numerical results are given to demonstrate the effectiveness of the reformulation and the high–order algorithm.

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LIST OF SYMBOLS

Surface of a Vesicle	γ
Material Point on a Vesicle	$\mathbf{x}$
Free Space Green's Function for the Stokes Equations	$\mathbf{G}(\mathbf{x},\mathbf{y})$
Stokes Surface Integral Operator	$\mathcal{S}$
Bending Force	$\mathbf{f}_b$
Tension Force	$\mathbf{f}_\sigma$
First Fundamental Form	g_{ij}
Second Fundamental Form	b_{ij}
Riemannian Metric	w
Outward Unit Normal Vector	$\mathbf{n}$
Mean Curvature	H
Gaussian Curvature	K
Laplace–Beltrami Operator	∇_γ^2
Surface Divergence	div_γ
Surface Gradient	∇_γ
Spherical Harmonic	Y_{lm},Y_m^l
Vectorial Spherical Harmonic	Y_{lm}^k
Projection Operator	$\mathcal{L}_n$
Wigner 3–j Symbol	$d_{mj}^l(\beta)$
Spherical Morphism	$\mathbf{q}$
Point on the Unit Ball	$\mathbf{p}$

Rotation Operator . . . . $\mathcal{T}_{\mathbf{x}}$

Shear Rate . . . . χ

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To Jim and Lisa.

CHAPTER 1
INTRODUCTION

Our problem, at its core, is to model the evolving closed surface of a three dimensional vesicle suspended in a Stoksian fluid flow. The body of this work provides a mathematical and computational formulation of this problem. We begin with a look at vesicles. A vesicle, simply stated, is a sac filled with fluid. Perhaps the most familiar example of a vesicle is a water balloon. Biologically, a vesicle takes on a slightly more specific definition. That is, a biological vesicle is a phospholipid bilayer (double layer of tightly packed fat molecules) membrane which stores and transports cellular products [21]. Perhaps the most familiar example of a biological vesicle suspended in a fluid flow is a red blood cell [18, 19]. The main focus of the thesis work to is mathematically and computationally model biological vesicle flow.

The simulation of biological vesicles is important in designing vesicle based drug delivery systems and in the study of biomembrane mechanics [21]. Further, a good model for biological vesicles suspended in fluid flow could give good approximations to the time it takes for blood clots to move about the circulatory system and hence how long a medical professional may have to stop something like an infarction. It is for this reason we will focus on biological vesicle based models. Further, we will restrict our attention to the modeling of vesicle flows in large in the unbounded region exterior to the vesicle.

We now turn our attention to mathematical modeling of the problem. For a chosen time t, we may consider a vesicle to be a closed surface and henceforth we use $\gamma(t)$ [or simply γ] to represent the surface of the vesicle. The main aim of this thesis is to simulate $\gamma(t)$, given its initial shape and location $\gamma(0)$ in $\mathbb{R}^3$. The rate of change of $\gamma(t)$ will be modeled to be same as that the divergence-free velocity of the fluid (with constant viscosity contrast) in which the vesicle $\gamma(0)$ is suspended. As we will see, this aspect of the model falls from the physicality of the problem.

The velocity field and pressure of the fluid will be related through the Stokes's equations in $\mathbb{R}^3 \backslash \gamma(t)$ and, following [18,21], we use the surface inextensibility constraint by requiring the surface divergence of the velocity field to be zero on γ. A key part of the model is the efficient representation of each component of the coordinates of the vesicle. Following [21], we avoid the axisymmetric restriction on the vesicle assumed in [25], and use a general representation the vesicle surface in spherical coordinates that facilitates application of the fast, high-order surface integral algorithm developed and analyzed in [8], for wave propagation models.

More precisely, following [8, 21], we represent each coordinate of our surface, γ, in the spherical angles θ and ϕ as:

$$\gamma = \left\{ \begin{pmatrix} x1(\theta,\phi) \\ x2(\theta,\phi) \\ x3(\theta,\phi) \end{pmatrix} : \theta \in [0,\pi],\ \ \phi \in [0,2\pi] \right\}. \tag{1.1}$$

That is, we take

$$\gamma = \mathbf{x}(\theta,\phi), \qquad\qquad 0 \le \theta \le \pi,\ \ 0 \le \phi \le 2\pi.$$

In this thesis, we assume that $\mathbf{x}$ is a $\mathcal{C}^2$ function on the sphere. If our surface were allowed to have singularities, much of our numerical developments will not be of high–order. As in the case with most biological vesicles, the surface inextensibility assumption will ensure that during the evolution process the vesicle maintain a constant area and volume.

The problem of surfaces evolving in Stokesian flow has been studied extensively. Due to the linearity of the Stokes equations, analytic solutions have been developed for simple geometries. For instance, in reference [22], Stokes describes a method to find the flow field of a translating sphere by imposing a spherical coordinate system which yields the Stokes equations separable. This methodology, however, is not well suited to study the *evolution* of vesicles. Boundary integral reformulations can be a powerful tool to investigate Stokesian flows. Hence, the creeping flow model has been investigated by various researchers using boundary integral equation reformulation, see for example [18] and extensive references therein. Integral equation reformulation of the Stokes equations requires the evaluation of integrals with singularities. The so called *singularity method* is an analytic tool that can be used to evaluate integrals of this type. First described by Gray and Hancock in 1955 to study the motion of sea urchin spermatozoa [11], the singularity method involves moving the singularity field on a surface to some chosen space curve. While this method is, essentially, an approximation method, it has been used to derive exact solutions. Chwang and Wu present several such solutions in reference [3]. While the singularity method has its uses, analytic approximations may fail to capture the complex behavior of an evolving vesicle. Hence, we turn to numerical methods.

Mesh based methods (such as finite element and finite difference) have been used by several authors such as Feng and Klug in reference [7] for simulation of stationary vesicle dynamics such as equilibrium shapes. These methods, while useful in their own right, do not apply to vesicles suspended in a fluid flow which are of interest to us. Mesh based methods have been adapted to the fluid flow case (i.e. the high order b–spline method of [27]). Still, they require a discretization of the overall domain. Hence, one of the main advantages to surface integral formulations (such as the one used in [21]) is that only processes on the boundary of the vesicle need to be approximated. Reference [19] uses a gradient–augmented level set method to simulate 2D vesicle flows. The main advantage to this scheme is that it allows for finite Reynolds number flows. This method, however is still a 2D scheme and hence, somewhat less applicable to real world vesicle flows. Recent developments in 3D vesicle flow modeling have been made by Kumar and Graham in reference [16]. The authors present an efficient scheme to model the confined flow of multiple vesicles whose computational complexity scales linearly as the product of the degrees of freedom and the number of vesicles increases. The method presented in [16] is able to handle confined flows due the the use of a geometry dependent Green's function. Further, it is the first such work to employ this methodology.

In this thesis, we follow the recent algorithms developed in [8, 21] for the vesicle simulation. The main aim of this thesis is to describe an efficient mathematical and computational approach to understand the evolution process of a vesicle suspended in fluid flow. Reference

[21] presents a spectral method for vesicle simulation in 3D. As with the assumptions we made previously in this chapter, they represent each component of a vesicles pointing vector with a spherical, smooth parameterization. Further, they consider vesicles to be suspended in an unbounded Stokesian flow with no viscosity contrast. In reference [25], the same authors present a similar scheme to the one described in reference [21] that is specific to axissymetric vesicles. While the scheme presented in reference [25] is capable of dealing with vesicles of spherical or toroidal topology (not, however, vesicles which change topology) we wish to avoid the restriction to only axissymetric vesicles. Again the same authors consider the flow of 2D vesicles in reference [24] in which schemes that are higher order in time are presented. These schemes are adaptable to our method but infeasible due to the spatial complexity of our implementation. Still, the main drawback to the methods presented in [24] is that it is a 2D model of vesicle flow, which is inherently less realistic than a 3D one.

The remainder of this thesis is organized as follows. In Chapter 2, we derive the coupled integro–differential equation formulation of our model and derive a form for the interfacial forces on the surface of a vesicle. In Chapter 3, we present a novel algorithm, based on that of reference [8], for evaluating weakly singular integrals and describe an explicit in time, spectral in space scheme to model our vesicle flow problem. Further, Chapter 3 gives numerical results concerning the implementation of the aforementioned scheme. In Chapter 4, we reflect on the work done and give suggestions for furthering the developments presented in the body of the thesis. Finally, in Appendix A, we present some background material on Green's functions and potential theory and in Appendix B we present an in depth derivation of spherical harmonics.

CHAPTER 2

PROBLEM FORMULATION

In this chapter, we formulate the vesicle flow problem discussed in Chapter 1 as a system of integro–differential equations. Further, we derive an explicit form for the interfacial forces on the surface of a vesicle.

2.1 Deriving an Integral Equation

Our problem, at its core, is to describe the behavior of a vesicle suspended in an unbounded Stokesian flow. As one can imagine, most of the mathematical 'action' is happening on the boundary of the aforementioned vesicle. Hence, it seems reasonable to begin by finding a free space Green's function for the Stokes equations. Given this, we will, with a bit of work, be able to formulate our problem as a surface integral equation. In what follows, we base our work on that of [18]. Recall the homogeneous Stokes equations

$$\begin{aligned} -\nabla P + \mu \nabla^2 \mathbf{u} &= \mathbf{0}, \\ \nabla \cdot \mathbf{u} &= 0, \end{aligned} \tag{2.1}$$

where, henceforth, the Laplacian will act component–wise on a vector. Now, to derive the free space Green's function for the above equations, we consider the eventual settling of a particle placed in a Stokesian flow. That is, we examine the velocity field generated by a source placed at some point $\mathbf{y}$ with strength $\mathbf{g}$ [18, pg.19]. Mathematically, we seek a solution to the singularly forced Stokes equations

$$-\nabla P + \mu \nabla^2 \mathbf{u} = -\mathbf{g}\delta(\mathbf{x} - \mathbf{y}), \tag{2.2}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{2.3}$$

where $\mathbf{x}$ in (2.2) is an observation point and δ is the $3D$ Dirac-delta function. At this point, for compactness, we define $\mathbf{r} = \mathbf{x} - \mathbf{y}$. Recall the Green's function for Laplace's equation as $\frac{-1}{4\pi|\mathbf{r}|}$ such that

$$\nabla^2 \frac{-1}{4\pi|\mathbf{r}|} = \delta(\mathbf{r}).$$

For a detailed treatment of this, see appendix A. Using this, we rewrite (2.2) as

$$-\nabla P + \mu\nabla^2\mathbf{u} = -\mathbf{g}\nabla^2 \frac{-1}{4\pi|\mathbf{r}|}. \tag{2.4}$$

Taking the divergence of (2.4) gives

$$\begin{aligned}
\nabla\cdot(-\nabla P + \mu\nabla^2\mathbf{u}) &= \nabla\cdot(-\mathbf{g}\nabla^2\frac{-1}{4\pi|\mathbf{r}|}) \\
-\nabla\cdot\nabla P + \mu\nabla\cdot\nabla^2\mathbf{u} &= -\nabla\cdot\mathbf{g}\nabla^2\frac{-1}{4\pi|\mathbf{r}|} \\
-\nabla^2 P + \mu\nabla^2 \underbrace{(\nabla\cdot\mathbf{u})}_{=\ 0\ from\ (2.3)} &= -\nabla^2\left(\mathbf{g}\cdot\nabla\frac{-1}{4\pi|\mathbf{r}|}\right) \\
-\nabla^2 P &= -\nabla^2\left(\mathbf{g}\cdot\nabla\frac{-1}{4\pi|\mathbf{r}|}\right). \qquad (2.5)
\end{aligned}$$

Hence, from (2.5) we may take

$$P = \mathbf{g}\cdot\nabla\frac{-1}{4\pi|\mathbf{r}|} + \mathbf{H}(\mathbf{r}),$$

where $\mathbf{H}(\mathbf{r})$ is an arbitrary harmonic function. If we require that the pressure decay to zero as $|\mathbf{r}| \to \infty$, we see that,

$$\lim_{|\mathbf{r}|\to\infty} P = 0 \Rightarrow \lim_{|\mathbf{r}|\to\infty} \mathbf{g}\cdot\nabla\frac{-1}{4\pi|\mathbf{r}|} + \lim_{|\mathbf{r}|\to\infty}\mathbf{H}(\mathbf{r}) = 0 \Rightarrow \lim_{|\mathbf{r}|\to\infty}\mathbf{H}(\mathbf{r}) = 0.$$

As, $\mathbf{H}$, is harmonic and, $\lim_{|\mathbf{r}|\to\infty}\mathbf{H}(\mathbf{r}) = 0$, it must be bounded. Therefore, by Liouville's theorem [6, pg.30], $\mathbf{H}$ must be constant and as it vanishes at infinity, $\mathbf{H}$ must be zero. Hence, $\mathbf{H}(\mathbf{r}) = 0$ and

$$P = \mathbf{g}\cdot\nabla\frac{-1}{4\pi|\mathbf{r}|}.$$

With this, we may rewrite (2.4) as

$$\begin{aligned}
&-\nabla\left(\mathbf{g}\cdot\nabla\frac{-1}{4\pi|\mathbf{r}|}\right) + \mu\nabla^2\mathbf{u} = -\mathbf{g}\nabla^2\frac{-1}{4\pi|\mathbf{r}|} \\
&\Rightarrow \nabla^2\mathbf{u} = \nabla\left(\mathbf{g}\cdot\nabla\frac{-1}{4\pi|\mathbf{r}|}\right) - \mathbf{g}\nabla^2\frac{-1}{4\pi\mu|\mathbf{r}|} \\
&\Rightarrow \nabla^2\mathbf{u} = \frac{-1}{4\pi\mu}\mathbf{g}\cdot\left(\nabla\nabla - \mathbf{I}\nabla^2\right)\frac{1}{|\mathbf{r}|}, \qquad (2.6)
\end{aligned}$$

where $\nabla\nabla$ is defined by

$$\nabla\nabla = \begin{pmatrix} \frac{\partial^2}{\partial x_1^2} & \frac{\partial^2}{\partial x_1 \partial x_2} & \frac{\partial^2}{\partial x_1 \partial x_3} \\ \frac{\partial^2}{\partial x_2 \partial x_1} & \frac{\partial^2}{\partial x_2^2} & \frac{\partial^2}{\partial x_2 \partial x_3} \\ \frac{\partial^2}{\partial x_3 \partial x_1} & \frac{\partial^2}{\partial x_3 \partial x_2} & \frac{\partial^2}{\partial x_3^2} \end{pmatrix},$$

and

$$\mathbf{g} \cdot \nabla\nabla(f(x_1, x_2, x_3)) = \begin{pmatrix} g_1 \frac{\partial^2}{\partial x_1^2} f + g_2 \frac{\partial^2}{\partial x_1 \partial x_2} f + g_3 \frac{\partial^2}{\partial x_1 \partial x_3} f \\ g_1 \frac{\partial^2}{\partial x_2 \partial x_1} f + g_2 \frac{\partial^2}{\partial x_2^2} f + g_3 \frac{\partial^2}{\partial x_2 \partial x_3} f \\ g_1 \frac{\partial^2}{\partial x_3 \partial x_1} f + g_2 \frac{\partial^2}{\partial x_3 \partial x_2} f + g_3 \frac{\partial^2}{\partial x_3^2} f \end{pmatrix}.$$

Similarly,

$$\mathbf{g} \cdot \mathbf{I}\nabla^2(f(x_1, x_2, x_3)) = \mathbf{g}(\nabla^2 f(x_1, x_2, x_3)).$$

We adopt these conventions to simplify notation and prevent confusion concerning the action of the operators. Examining (2.6), it is reasonable to take

$$\mathbf{u} = \frac{1}{\mu}\mathbf{g} \cdot \left(\nabla\nabla - \mathbf{I}\nabla^2\right)\Psi, \tag{2.7}$$

where Ψ is a scalar function. We note that taking the divergence of the right hand side in the above expression yields

$$\begin{aligned} &\nabla \cdot \frac{1}{\mu}\mathbf{g} \cdot \left(\nabla\nabla - \mathbf{I}\nabla^2\right)\Psi \\ &= \frac{1}{\mu}\mathbf{g} \cdot \left(\nabla \cdot \nabla\nabla - \nabla \cdot \mathbf{I}\nabla^2\right)\Psi \\ &= \frac{1}{\mu}\mathbf{g} \cdot \left(\nabla \cdot \nabla\nabla - \nabla \cdot \mathbf{I}\nabla^2\right)\Psi \\ &= \frac{1}{\mu}\mathbf{g} \cdot \left(\begin{pmatrix} \frac{\partial^3}{\partial x_1^3} + \frac{\partial^3}{\partial x_1 \partial x_2^2} + \frac{\partial^3}{\partial x_1 \partial x_3^2} \\ \frac{\partial^3}{\partial x_1^2 \partial x_2} + \frac{\partial^3}{\partial x_2^3} + \frac{\partial^3}{\partial x_2 \partial x_3^2} \\ \frac{\partial^3}{\partial x_1^2 \partial x_3} + \frac{\partial^3}{\partial x_3 \partial x_2^2} + \frac{\partial^3}{\partial x_3^3} \end{pmatrix} - \begin{pmatrix} \frac{\partial^3}{\partial x_1^3} + \frac{\partial^3}{\partial x_1 \partial x_2^2} + \frac{\partial^3}{\partial x_1 \partial x_3^2} \\ \frac{\partial^3}{\partial x_1^2 \partial x_2} + \frac{\partial^3}{\partial x_2^3} + \frac{\partial^3}{\partial x_2 \partial x_3^2} \\ \frac{\partial^3}{\partial x_1^2 \partial x_3} + \frac{\partial^3}{\partial x_3 \partial x_2^2} + \frac{\partial^3}{\partial x_3^3} \end{pmatrix} \right)\Psi \\ &= 0. \end{aligned}$$

Hence, for any choice of the scalar function, Ψ, (2.3) is satisfied. Now, plugging our representation of $\mathbf{u}$, (2.7), into (2.6) yields

$$\nabla^2 \left[\frac{1}{\mu} \mathbf{g} \cdot \left(\nabla\nabla - \mathbf{I}\nabla^2 \right) \Psi \right] = \frac{-1}{4\pi\mu} \mathbf{g} \cdot \left(\nabla\nabla - \mathbf{I}\nabla^2 \right) \frac{1}{|\mathbf{r}|}$$
$$\Rightarrow \mathbf{g} \cdot \left(\nabla\nabla - \mathbf{I}\nabla^2 \right) \nabla^2 \Psi = \mathbf{g} \cdot \left(\nabla\nabla - \mathbf{I}\nabla^2 \right) \frac{-1}{4\pi|\mathbf{r}|}$$
$$\Rightarrow \mathbf{g} \cdot \left(\nabla\nabla - \mathbf{I}\nabla^2 \right) \left(\nabla^2 \Psi + \frac{1}{4\pi|\mathbf{r}|} \right) = 0,$$

and as $\mathbf{g}$ is arbitrary, we must have that

$$\left(\nabla\nabla - \mathbf{I}\nabla^2 \right) \left(\nabla^2 \Psi + \frac{1}{4\pi|\mathbf{r}|} \right) = 0.$$

The above is satisfied provided Ψ satisfies the Poisson equation

$$\nabla^2 \Psi = \frac{-1}{4\pi|\mathbf{r}|}.$$

Taking the Laplacian of both sides of the above equation yields

$$\nabla^2 \nabla^2 \Psi = \nabla^2 \frac{-1}{4\pi|\mathbf{r}|} = \delta(\mathbf{r}).$$

Hence, Ψ is the Green's function of the biharmonic equation. This is a well known function, $-|\mathbf{r}|/8\pi$ [18, pg.22]. To verify this, consider

$$\nabla^2 \frac{-|\mathbf{r}|}{8\pi} = \nabla \cdot \left(\nabla \frac{-|\mathbf{r}|}{8\pi} \right) = \frac{-1}{8\pi} \nabla \cdot \frac{\mathbf{r}}{|\mathbf{r}|}$$
$$= \frac{-1}{8\pi} \left(\frac{|\mathbf{r}|^2 - r_1^2}{|\mathbf{r}|^3} + \frac{|\mathbf{r}|^2 - r_2^2}{|\mathbf{r}|^3} + \frac{|\mathbf{r}|^2 - r_3^2}{|\mathbf{r}|^3} \right)$$
$$= \frac{-1}{8\pi} \frac{3|\mathbf{r}|^2 - |\mathbf{r}|^2}{|\mathbf{r}|^3} = \frac{-1}{8\pi} \frac{2}{|\mathbf{r}|} = \frac{-1}{4\pi|\mathbf{r}|},$$

and

$$\nabla^2 \frac{-1}{4\pi|\mathbf{r}|} = \delta(\mathbf{r}).$$

Hence, we take $\Psi(\mathbf{r}) = -|\mathbf{r}|/8\pi$. Plugging this into (2.7) gives

$$\mathbf{u} = \frac{1}{\mu} \mathbf{g} \cdot \left(\nabla\nabla - \mathbf{I}\nabla^2 \right) \frac{-|\mathbf{r}|}{8\pi} = \frac{1}{\mu} \mathbf{g} \cdot \left(\nabla\nabla \frac{-|\mathbf{r}|}{8\pi} - \mathbf{I}\nabla^2 \frac{-|\mathbf{r}|}{8\pi} \right)$$
$$= \frac{1}{\mu} \mathbf{g} \cdot \left(\nabla\nabla \frac{-|\mathbf{r}|}{8\pi} - \mathbf{I} \frac{-1}{4\pi|\mathbf{r}|} \right). \tag{2.8}$$

Now, we compute the term $\nabla\nabla \frac{-|\mathbf{r}|}{8\pi}$. For $i \neq j$,

$$\left[\nabla\nabla \frac{-|\mathbf{r}|}{8\pi} \right]_{i,j} = \frac{-1}{8\pi} \left[\nabla \frac{\mathbf{r}}{|\mathbf{r}|} \right]_{i,j} = \frac{-1}{8\pi} \frac{\partial}{\partial r_j} \frac{r_i}{|\mathbf{r}|} = \frac{r_i r_j}{|\mathbf{r}|^3}, \tag{2.9}$$

and for $i = j$,

$$\left[\nabla\nabla\frac{-|\mathbf{r}|}{8\pi}\right]_{i,i} = \frac{-1}{8\pi}\left[\nabla\frac{\mathbf{r}}{|\mathbf{r}|}\right]_{i,i} = \frac{-1}{8\pi}\frac{|\mathbf{r}|^2 - r_i^2}{|\mathbf{r}|^3} = \frac{1}{8\pi}\left(\frac{r_i^2}{|\mathbf{r}|^3} - \frac{1}{|\mathbf{r}|}\right). \tag{2.10}$$

Combining (2.10) and (2.9) we may write

$$\nabla\nabla\frac{-|\mathbf{r}|}{8\pi} = \frac{1}{8\pi}\left(\frac{\mathbf{r}\otimes\mathbf{r}}{|\mathbf{r}|^3} - \mathbf{I}\frac{1}{|\mathbf{r}|}\right).$$

Hence,

$$\begin{aligned}\mathbf{u} &= \frac{1}{\mu}\mathbf{g}\cdot\left(\nabla\nabla\frac{-|\mathbf{r}|}{8\pi} - \mathbf{I}\frac{-1}{4\pi|\mathbf{r}|}\right)\\ &= \frac{1}{8\pi\mu}\mathbf{g}\cdot\left(\left(\frac{\mathbf{r}\otimes\mathbf{r}}{|\mathbf{r}|^3} - \mathbf{I}\frac{1}{|\mathbf{r}|}\right) + \mathbf{I}\frac{2}{|\mathbf{r}|}\right) = \frac{1}{8\pi\mu}\left(\frac{\mathbf{r}\otimes\mathbf{r}}{|\mathbf{r}|^3} + \mathbf{I}\frac{1}{|\mathbf{r}|}\right)\mathbf{g}.\end{aligned}$$

For compactness of notation, from here on out we write

$$\left(\frac{\mathbf{r}\otimes\mathbf{r}}{|\mathbf{r}|^3} + \mathbf{I}\frac{1}{|\mathbf{r}|}\right) = \mathbf{G}(\mathbf{x},\mathbf{y}),$$

where $\mathbf{G}$ is the free space Greens function of the Stokes equations. Hence, we can express $\mathbf{u}$, in terms of a source point, $\mathbf{y}$, of strength $\mathbf{g}$, as

$$\mathbf{u}(\mathbf{x}) = \frac{1}{8\pi\mu}\mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{g}. \tag{2.11}$$

Now, we will prove a useful identity regarding $\mathbf{G}$.

Theorem 2.1. *For a vesicle with surface, γ, enclosing a volume, V, with normal vector, $\boldsymbol{n}$, suspended in a Stokesian flow,*

$$\int_\gamma \boldsymbol{G}(\boldsymbol{x},\boldsymbol{y})\boldsymbol{n}(\boldsymbol{x})dS(\boldsymbol{x}) = \boldsymbol{0}.$$

where $\boldsymbol{y}$ can be inside, outside, or on γ.

Proof. As we saw, the velocity of this vesicle can be expressed as

$$\mathbf{u}(\mathbf{x}) = \frac{1}{8\pi\mu}\mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{g}.$$

As $\mathbf{u}$ must be divergence free from (2.3), we know that

$$\nabla\cdot\mathbf{u}(\mathbf{x}) = \frac{1}{8\pi\mu}\nabla\cdot\mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{g} = 0 \Rightarrow \nabla\cdot\mathbf{G}(\mathbf{x},\mathbf{y}) = \mathbf{0}.$$

Integrating over the volume, V, taking $\mathbf{y}$ to be inside of γ, and using the divergence theorem gives

$$\int_V \nabla\cdot\mathbf{G}(\mathbf{x},\mathbf{y})dV(\mathbf{x}) = \mathbf{0} \Rightarrow \int_\gamma \mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{n}(\mathbf{x})dS(\mathbf{x}) = \mathbf{0}.$$

Now, the surface integral,

$$\int_\gamma \mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{n}(\mathbf{x})dS(\mathbf{x}),$$

can be recognized as a single layer potential with density 1 [18, pg.27]. Hence, this surface integral is continuous as $\mathbf{y}$ crosses γ. Our result follows. □

At this point it is convenient to introduce the notion of a stress tensor. The stress tensor is inherent to the mathematics and the physicality of our problem. We define the stress tensor, σ, as

$$\sigma_{ij} = -P\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right).$$

Henceforth, adopting the convention of summing over repeated indices, our previous work allows us to write the pressure field for the singularly forced flow as

$$P = g_j \nabla_j \frac{-1}{4\pi|\mathbf{r}|} = \frac{1}{8\pi}\left(2\frac{r_j}{|\mathbf{r}|^3}\right) g_j,$$

and

$$u_i(\mathbf{x}) = \frac{1}{8\pi\mu}\mathbf{G}_{ij}(\mathbf{x},\mathbf{y})g_j.$$

Hence, we may write the stress tensor for singularly forced flow as

$$\begin{aligned}\sigma_{ik} &= -\frac{1}{8\pi}\left(2\frac{r_j}{|\mathbf{r}|^3}\right) g_j\delta_{ik} + \mu\left(\frac{\partial \frac{1}{8\pi\mu}\mathbf{G}_{ij}(\mathbf{x},\mathbf{y})g_j}{\partial x_k} + \frac{\partial \frac{1}{8\pi\mu}\mathbf{G}_{kj}(\mathbf{x},\mathbf{y})g_j}{\partial x_i}\right)\\ &= \frac{1}{8\pi}\underbrace{\left(\left(-2\frac{r_j}{|\mathbf{r}|^3}\right)\delta_{ik} + \frac{\partial \mathbf{G}_{ij}(\mathbf{x},\mathbf{y})}{\partial x_k} + \frac{\partial \mathbf{G}_{kj}(\mathbf{x},\mathbf{y})}{\partial x_i}\right)}_{T_{ijk}(\mathbf{x},\mathbf{y})} g_j.\end{aligned}$$

We now seek to compute T_{ijk}

Theorem 2.2.

$$T_{ijk} = -6\frac{r_i r_j r_k}{|\boldsymbol{r}|^5}.$$

Proof. We proceed case-by-case. When $i \neq j \neq k$,

$$\left(-2\frac{r_j}{|\mathbf{r}|^3}\right)\delta_{ik} = 0,$$

and

$$\frac{\partial \mathbf{G}_{ij}(\mathbf{x},\mathbf{y})}{\partial x_k} = \frac{\partial}{\partial x_k}\frac{r_i r_j}{|\mathbf{r}|^3} = -3\frac{r_i r_j r_k}{|\mathbf{r}|^5} = \frac{\partial \mathbf{G}_{kj}(\mathbf{x},\mathbf{y})}{\partial x_i}.$$

Hence, in this case

$$T_{ijk} = -6\frac{r_i r_j r_k}{|\mathbf{r}|^5}.$$

When $i = k \neq j$,

$$\frac{\partial \mathbf{G}_{ij}(\mathbf{x}, \mathbf{y})}{\partial x_k} = \frac{\partial}{\partial x_i}\frac{r_i r_j}{|\mathbf{r}|^3} = \frac{r_j}{|\mathbf{r}|^3} - 3\frac{r_i^2 r_j}{|\mathbf{r}|^5} = \frac{\partial \mathbf{G}_{kj}(\mathbf{x}, \mathbf{y})}{\partial x_i},$$

and hence,

$$T_{ijk} = \left(-2\frac{r_j}{|\mathbf{r}|^3}\right)\delta_{ik} + 2\frac{r_j}{|\mathbf{r}|^3} - 6\frac{r_i^2 r_j}{|\mathbf{r}|^5} = -6\frac{r_i r_j r_k}{|\mathbf{r}|^5}.$$

When $i = j \neq k$,

$$\left(-2\frac{r_j}{|\mathbf{r}|^3}\right)\delta_{ik} = 0,$$

and

$$\frac{\partial \mathbf{G}_{ij}(\mathbf{x}, \mathbf{y})}{\partial x_k} = \frac{\partial}{\partial x_k}\left(\frac{r_i^2}{|\mathbf{r}|^3} + \frac{1}{|\mathbf{r}|}\right) = -3\frac{r_i^2 r_k}{|\mathbf{r}|^5} - \frac{r_k}{|\mathbf{r}|^3},$$

and

$$\frac{\partial \mathbf{G}_{kj}(\mathbf{x}, \mathbf{y})}{\partial x_i} = \frac{\partial}{\partial x_i}\frac{r_k r_i}{|\mathbf{r}|^3} = \frac{r_k}{|\mathbf{r}|^3} - 3\frac{r_i^2 r_k}{|\mathbf{r}|^5},$$

and hence,

$$T_{ijk} = \frac{r_k}{|\mathbf{r}|^3} - 3\frac{r_i^2 r_k}{|\mathbf{r}|^5} + -3\frac{r_i^2 r_k}{|\mathbf{r}|^5} - \frac{r_k}{|\mathbf{r}|^3} = -6\frac{r_i r_j r_k}{|\mathbf{r}|^5}.$$

A symmetry argument gives this same result for the case when $j = k \neq i$. Finally we consider the case when $i = j = k$. Now,

$$\frac{\partial \mathbf{G}_{ij}(\mathbf{x}, \mathbf{y})}{\partial x_k} = \frac{\partial \mathbf{G}_{kj}(\mathbf{x}, \mathbf{y})}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{r_i^2}{|\mathbf{r}|^3} + \frac{1}{|\mathbf{r}|}\right) = 2\frac{r_i}{|\mathbf{r}|^3} - 3\frac{r_i^3}{|\mathbf{r}|^5} - \frac{r_1}{|\mathbf{r}|^3} = \frac{r_i}{|\mathbf{r}|^3} - 3\frac{r_i^3}{|\mathbf{r}|^5}.$$

Hence,

$$T_{ijk} = -2\frac{r_j}{|\mathbf{r}|^3}\delta_{ik} + \frac{r_i}{|\mathbf{r}|^3} - 3\frac{r_i^3}{|\mathbf{r}|^5} + \frac{r_i}{|\mathbf{r}|^3} - 3\frac{r_i^3}{|\mathbf{r}|^5} = -6\frac{r_i r_j r_k}{|\mathbf{r}|^5}.$$

As we've exhausted all of the possible values of i,j, and, k, and arrived at the same result, we may express T in the compact form

$$T_{ijk} = -6\frac{r_i r_j r_k}{|\mathbf{r}|^5}.$$

□

Thus, we are left with a nice, compact form for the stress tensor of singularly forced flow,

$$\sigma_{ik} = \frac{1}{8\pi} T_{ijk}(\mathbf{x}, \mathbf{y}) g_j = \frac{1}{8\pi}\left(-6\frac{r_i r_j r_k}{|\mathbf{r}|^5}\right) g_j. \tag{2.12}$$

Let us return, for a moment, to the stress tensor for the homogeneous Stokes equations

$$\sigma_{ij} = -P\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) = -P\mathbf{I} + \mu\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right).$$

Taking the divergence of σ yields

$$\nabla \cdot \sigma = -\nabla \cdot P\mathbf{I} + \mu \nabla \cdot \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right) = -\nabla P + \mu\left(\nabla^2 \mathbf{u} + \nabla \underbrace{(\nabla \cdot \mathbf{u})}_{=\,0}\right) = -\nabla P + \mu \nabla^2 \mathbf{u},$$

which we recognize as the left hand side of the Stokes equation presented at the beginning of this section. Thus, for homogeneous stokes flow, we have

$$\nabla \cdot \sigma = 0. \tag{2.13}$$

Here we see one of the reasons that σ is so important. It contains all of the information from the Stokes equations. With our new representation for the left hand side of the Stokes equation, we may also derive a useful result concerning T_{ijk}.

Theorem 2.3.

$$\nabla \cdot T_{ijk}(\boldsymbol{x} - \boldsymbol{y}) = -8\pi\delta(\boldsymbol{x} - \boldsymbol{y}).$$

Proof. We begin with the singularly forced Stokes equation

$$-\nabla P + \mu \nabla^2 \mathbf{u} = -\mathbf{g}\delta(\mathbf{x} - \mathbf{y}).$$

Rewriting this in terms of σ gives

$$\nabla \cdot \sigma = -\mathbf{g}\delta(\mathbf{x} - \mathbf{y}).$$

Using the form we derived earlier for σ in a singularly forced system gives

$$\nabla \cdot \frac{1}{8\pi} T_{ijk}(\mathbf{x}, \mathbf{y})\mathbf{g} = -\mathbf{g}\delta(\mathbf{x} - \mathbf{y}).$$

As $\mathbf{g}$ is arbitrary, we may discard it. Further, multiplying both sides by 8π gives our result.

□

Now, let us consider two solutions to the Stokes equations, $\mathbf{u}$, and $\mathbf{u}'$ with associated stress tensors, σ, and σ'. Let $\mathbf{u}$ be a solution to the homogeneous Stokes equations, (2.1) and $\mathbf{u}'$ be a solution to the singularly forced Stokes equations. We know from (2.11) that

$$\mathbf{u}' = \frac{1}{8\pi\mu}\mathbf{G}(\mathbf{x}, \mathbf{y})\mathbf{g},$$

and from (2.12), we have

$$\sigma' = \frac{1}{8\pi}T_{ijk}\mathbf{g}.$$

Let us now consider the expression

$$\nabla \cdot (\mathbf{u}'\sigma - \mathbf{u}\sigma').$$

Using the above forms for $\mathbf{u}'$ and σ' we derive a useful identity (note that in what follows, for a column vector $\mathbf{v}$ and a matrix M, $\mathbf{v} \cdot M = M\mathbf{v}$ where we have adopted this convention to keep with the presentation of this result in [18])

$$\begin{aligned}
&\nabla \cdot (\mathbf{u}' \cdot \sigma - \mathbf{u} \cdot \sigma') = \nabla \cdot \left(\frac{1}{8\pi\mu}\mathbf{G}(\mathbf{x}, \mathbf{y})\mathbf{g} \cdot \sigma - \mathbf{u} \cdot \frac{1}{8\pi}T_{ijk}(\mathbf{x}, \mathbf{y})\mathbf{g} \right) \\
&= \nabla \cdot \left(\frac{1}{8\pi\mu}\mathbf{G}(\mathbf{x}, \mathbf{y})\mathbf{g} \cdot \sigma \right) - \nabla \cdot \left(\mathbf{u} \cdot \frac{1}{8\pi}T_{ijk}(\mathbf{x}, \mathbf{y})\mathbf{g} \right) \\
&= \frac{1}{8\pi\mu}\left(\underbrace{(\nabla \cdot \mathbf{G}(\mathbf{x}, \mathbf{y})\mathbf{g})}_{=\ 0\ by (2.1)}\sigma + \mathbf{G}(\mathbf{x}, \mathbf{y})\mathbf{g} \cdot \underbrace{(\nabla \cdot \sigma)}_{=\ 0\ by\ defn} \right) \\
&- \frac{1}{8\pi}\left(\underbrace{(\nabla \cdot \mathbf{u})}_{=\ 0\ by\ (2.1)} \cdot T_{ijk}(\mathbf{x}, \mathbf{y})\mathbf{g} + \mathbf{u} \cdot \underbrace{(\nabla \cdot T_{ijk}(\mathbf{x}, \mathbf{y}))}_{=\ -8\pi\delta(\mathbf{x}-\mathbf{y})\ by\ (2.3)}\ \mathbf{g} \right) \\
&= \mathbf{u} \cdot \delta(\mathbf{x} - \mathbf{y})\mathbf{g}.
\end{aligned}$$

Hence,

$$\nabla \cdot \left(\frac{1}{8\pi\mu}\mathbf{G}(\mathbf{x}, \mathbf{y})\mathbf{g} \cdot \sigma - \mathbf{u} \cdot \frac{1}{8\pi}T_{ijk}(\mathbf{x}, \mathbf{y})\mathbf{g} \right) = \mathbf{u} \cdot \delta(\mathbf{x} - \mathbf{y})\mathbf{g}.$$

Now, if we take the source point, $\mathbf{y}$, and our observation point, $\mathbf{x}$, to be in the interior, V, of a vesicle with boundary, γ. We may integrate both sides of the above expression over the volume, V, to obtain

$$\int_V \nabla \cdot \left(\frac{1}{8\pi\mu}\mathbf{G}(\mathbf{x}, \mathbf{y})\mathbf{g} \cdot \sigma - \mathbf{u} \cdot \frac{1}{8\pi}T_{ijk}(\mathbf{x}, \mathbf{y})\mathbf{g} \right) dV(\mathbf{y}) = \int_V \mathbf{u}(\mathbf{y}) \cdot \delta(\mathbf{x} - \mathbf{y})\mathbf{g} dV(\mathbf{y}) = \mathbf{u}(\mathbf{x}) \cdot \mathbf{g}.$$

Using the divergence theorem on the left hand side of the above expression gives

$$\int_\gamma \left(\frac{1}{8\pi\mu} \mathbf{G}(\mathbf{x},\mathbf{y})\sigma\mathbf{n} - \frac{1}{8\pi} \mathbf{u}(\mathbf{y}) T_{ijk}(\mathbf{x},\mathbf{y})\mathbf{n} \right) \cdot \mathbf{g} dS(\mathbf{y}) = \mathbf{u}(\mathbf{x}) \cdot \mathbf{g}.$$

Now, as $\mathbf{g}$ is arbitrary, we may discard it giving the boundary integral formulation of the stokes equations as

$$\frac{1}{8\pi\mu} \int_\gamma \mathbf{G}(\mathbf{x},\mathbf{y}) \left(\sigma\mathbf{n}\right) dS(\mathbf{y}) - \frac{1}{8\pi} \int_\gamma \mathbf{u}(\mathbf{y}) T_{ijk}(\mathbf{x},\mathbf{y})\mathbf{n} dS(\mathbf{y}) = \mathbf{u}(\mathbf{x}).$$

It is convenient to adopt the notation $\sigma\mathbf{n} = \mathbf{f}$ as $\sigma\mathbf{n}$ is the surface force, or traction, exerted on the vesicle [18, pg.27]. Thus, for a source point, $\mathbf{y}$ in the interior of a vesicle, the velocity of the vesicle at an interior point $\mathbf{x}$ can be found by solving

$$\frac{1}{8\pi\mu} \int_\gamma \mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{f} dS(\mathbf{y}) - \frac{1}{8\pi} \int_\gamma \mathbf{u}(\mathbf{y}) T_{ijk}(\mathbf{x},\mathbf{y})\mathbf{n} dS(\mathbf{y}) = \mathbf{u}(\mathbf{x}). \tag{2.14}$$

Note that in the above representation, the left hand side is a sum of a single and double layer potentials. For a detailed discussion of these, see appendix A.

Now notice that if we take our observation point $\mathbf{x}$ to be outside of the vesicle γ while our observation point remains in the interior, the integral

$$\int_V \mathbf{u}(\mathbf{y}) \cdot \delta(\mathbf{x}-\mathbf{y})\mathbf{g} dV(\mathbf{y}),$$

vanishes. By a similar process to above, we see that

$$\frac{1}{8\pi\mu} \int_\gamma \mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{f} dS(\mathbf{y}) - \frac{1}{8\pi} \int_\gamma \mathbf{u}(\mathbf{y}) T_{ijk}(\mathbf{x},\mathbf{y})\mathbf{n} dS(\mathbf{y}) = 0,$$

or

$$\frac{1}{\mu} \int_\gamma \mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{f} dS(\mathbf{y}) = \int_\gamma \mathbf{u}(\mathbf{y}) T_{ijk}(\mathbf{x},\mathbf{y})\mathbf{n} dS(\mathbf{y}), \tag{2.15}$$

for $\mathbf{y}$ outside of γ.

We now consider the case of interest to us, a vesicle suspended in a Stokesian flow. In this case, we may split the velocity $\mathbf{u}$ into two parts, an undisturbed component, $\mathbf{u}^\infty$, and a disturbance component, $\mathbf{u}^D$ which admit surface forces $\mathbf{f}^\infty$, and $\mathbf{f}^D$, respectively. These components are such that $\mathbf{u} = \mathbf{u}^\infty + \mathbf{u}^D$. On γ, $\mathbf{u}^\infty = \mathbf{u}^D$ [18, pg.32]. With this, we write the two boundary integral equations for the two velocity components. For the integral equation of the disturbance component, we take $\mathbf{x}_{In}$ to be inside of γ and for the undisturbed component, we take $\mathbf{x}_{Out}$ to be outside of γ. This seems natural as we would like to view the effect of the disturbance from the vesicle's 'point of view' and we wouldn't like this for the undisturbed portion. Thus, we write

$$\frac{1}{8\pi\mu}\int_{\gamma}\mathbf{G}(\mathbf{x}_{In},\mathbf{y})\mathbf{f}^{D}dS(\mathbf{y})-\frac{1}{8\pi}\int_{\gamma}\mathbf{u}^{D}(\mathbf{y})T_{ijk}(\mathbf{x}_{In},\mathbf{y})\mathbf{n}dS(\mathbf{y})=\mathbf{u}^{D}(\mathbf{x}_{In}), \tag{2.16}$$

form (2.14), and

$$\frac{1}{\mu}\int_{\gamma}\mathbf{G}(\mathbf{x}_{Out},\mathbf{y})\mathbf{f}^{\infty}dS(\mathbf{y})=\int_{\gamma}\mathbf{u}^{\infty}(\mathbf{y})T_{ijk}(\mathbf{x}_{Out},\mathbf{y})\mathbf{n}dS(\mathbf{y}), \tag{2.17}$$

from (2.15). As $\mathbf{u}^{\infty}=\mathbf{u}^{D}$ on γ, we may rewrite (2.17) as

$$\frac{1}{\mu}\int_{\gamma}\mathbf{G}(\mathbf{x}_{Out},\mathbf{y})\mathbf{f}^{\infty}dS(\mathbf{y})=\int_{\gamma}\mathbf{u}^{D}(\mathbf{y})T_{ijk}(\mathbf{x}_{Out},\mathbf{y})\mathbf{n}dS(\mathbf{y}). \tag{2.18}$$

At this point, we take the limit as $\mathbf{x}_{Out}$ and $\mathbf{x}_{In}$ approach the same boundary point, $\mathbf{x}$. As

$$\int_{\gamma}\mathbf{u}^{D}(\mathbf{y})T_{ijk}(\mathbf{x}_{In/Out},\mathbf{y})\mathbf{n}dS(\mathbf{y})$$

is a double layer potential, a minor modification of the results given in appendix A can be used to show that

$$\lim_{\mathbf{x}_{In/Out}\to\mathbf{x}}=\pm4\pi\mathbf{u}^{D}(\mathbf{x})+⨍_{\gamma}\mathbf{u}^{D}(\mathbf{y})T_{ijk}(\mathbf{x},\mathbf{y})\mathbf{n}dS(\mathbf{y}), \tag{2.19}$$

where the $\pm$ depends on whether $\mathbf{x}_{In}$ is approaching $\mathbf{x}$ (+) or $\mathbf{x}_{In}$ (-), and $⨍$ is the Cauchy principal value integral. Note that this result is also given in [18, pg.27]. Using (2.19) in (2.18), and noting that the left hand side is a single layer potential (and hence continuous across γ), we have that

$$\frac{1}{\mu}\int_{\gamma}\mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{f}^{\infty}dS(\mathbf{y})+4\pi\mathbf{u}^{D}(\mathbf{x})=⨍_{\gamma}\mathbf{u}^{D}(\mathbf{y})T_{ijk}(\mathbf{x},\mathbf{y})\mathbf{n}dS(\mathbf{y}). \tag{2.20}$$

Similarly, using (2.19) in (2.16), we have

$$\frac{1}{4\pi\mu}\int_{\gamma}\mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{f}^{D}dS(\mathbf{y})-\frac{1}{4\pi}⨍_{\gamma}\mathbf{u}^{D}(\mathbf{y})T_{ijk}(\mathbf{x},\mathbf{y})\mathbf{n}dS(\mathbf{y})=\mathbf{u}^{D}(\mathbf{x}). \tag{2.21}$$

Putting (2.20) into (2.21) eliminates the double layer potential giving

$$\frac{1}{8\pi\mu}\int_{\gamma}\mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{f}^{D}dS(\mathbf{y})-\frac{1}{8\pi\mu}\int_{\gamma}\mathbf{G}(\mathbf{x},\mathbf{y})\mathbf{f}^{\infty}dS(\mathbf{y})=\mathbf{u}^{D}(\mathbf{x}).$$

Hence, by adding $\mathbf{u}^{\infty}(\mathbf{x})$ to both sides, we arrive at

$$\frac{1}{8\pi\mu}\int_{\gamma}\mathbf{G}(\mathbf{x},\mathbf{y})\left(\mathbf{f}^{D}-\mathbf{f}^{\infty}\right)dS(\mathbf{y})+\mathbf{u}^{\infty}(\mathbf{x})=\mathbf{u}(\mathbf{x}). \tag{2.22}$$

Note that this equation is valid no matter where we take our observation point, $\mathbf{x}$, as the integral operator is a single layer potential. Still, as it will serve us well to restrict our attention to the surface of our vesicle, we will take $\mathbf{x} \in \gamma$. Finally, we adopt a more compact notation for the single layer integral operator on the left hand side of (2.22), $\mathcal{S}$, such that

$$\mathcal{S}[\mathbf{R}](\mathbf{x}) = \frac{1}{8\pi\mu} \int_{\gamma} \mathbf{G}(\mathbf{x}, \mathbf{y}) \mathbf{R}(\mathbf{y}) dS(\mathbf{y}). \tag{2.23}$$

Hence, using (2.23), we may write (2.22), in a much nicer form, as

$$\mathcal{S}\left[\mathbf{f}^D - \mathbf{f}^\infty\right](\mathbf{x}) + \mathbf{u}^\infty(\mathbf{x}) = \mathbf{u}(\mathbf{x}). \tag{2.24}$$

2.2 Finding the Force

In section (2.1) we developed an integral equation formulation of our problem in the form of (2.22). While this formulation will serve us well, we're not quite done yet. We are seeking to characterize the shape of a vesicle and hence need to relate everything in (2.22) to γ. We've seen in section 1 that we can represent γ with a vectorial parameterization $\gamma = \mathbf{x}(\theta, \phi)$. Now, we see that our equation of motion, (2.22), relates the velocity, $\mathbf{u}(\mathbf{x})$, to the traction force $\mathbf{f}(\mathbf{y}) = \mathbf{f}^D(\mathbf{y}) - \mathbf{f}^\infty(\mathbf{y})$. From here on out, we will adopt the notation $\mathbf{f}^D(\mathbf{y}) = \mathbf{f}_\sigma$ and $\mathbf{f}^\infty(\mathbf{y}) = \mathbf{f}_b$. This is because these forces will be known as the tension and bending forces respectively. Now, we see that $\mathbf{u}$ and $\mathbf{f}$ depend on $\mathbf{x}$ (or equivalently $\mathbf{y}$) and hence the shape of our vesicle. This is well and good but we now need to focus on how these quantities relate to our vesicle if we are to have any hope of using (2.22) to solve for the shape of our vesicle. By requiring that the velocity of the vesicle be equal to the velocity at a material point (a reasonable assumption made in reference [21, pg.3]), we have that

$$\frac{d}{dt}\mathbf{x} = \mathbf{u}(\mathbf{x}),$$

and hence a relation between $\mathbf{u}$ and the shape of our vesicle. Putting this together with (2.24), we may reformulate the integral equation governing our problem as

$$\mathcal{S}\left[\mathbf{f}_\sigma - \mathbf{f}_b\right](\mathbf{x}) + \mathbf{u}^\infty(\mathbf{x}) = \frac{d}{dt}\mathbf{x}. \tag{2.25}$$

We now need to describe the relation between the traction force, $\mathbf{f}$, and our membrane, $\mathbf{x}$. Fortunately, this is a much more interesting endeavor. It has been shown by [14] that the bending energy on a vesicle is given by the functional

$$\mathcal{E} = \int_{\gamma} \frac{\kappa_b}{2} H^2 + \sigma d\gamma.$$

Here, κ_b is the bending modulus (a constant parameter value), H is the mean curvature of γ, and σ is the tension (a Lagrange function to maintain the constant area constraint). The above is often referred to as the Willmore functional. To find an expression for the traction force on our vesicle, we must take the negative variational derivative of $\mathcal{E}$ with respect to the surface [19, sec.2]. In other words

$$\mathbf{f} = -\frac{\delta \mathcal{E}}{\delta \mathbf{x}}.$$

We begin this endeavor by defining some important geometric quantities. Let $\partial_1 = \partial_\theta$, $\partial_2 = \partial_\phi$. Now, for $i, j \in 1, 2$,

$$\mathbf{x}_i = \partial_i \mathbf{x}, \quad \mathbf{x}_{ij} = \partial_i \partial_j \mathbf{x}.$$

Hence, we define the first fundamental form matrix by

$$g_{ij} = \mathbf{x}_i \cdot \mathbf{x}_j = \begin{pmatrix} E & F \\ F & G \end{pmatrix}. \tag{2.26}$$

Now, the metric on our surface is given by

$$w = det(g) = EG - F^2.$$

With this, we define the inverse of g as

$$g^{-1} = g_{ij}^{-1} = g^{ij} = \frac{1}{w} \begin{pmatrix} G & -F \\ -F & E \end{pmatrix}.$$

We now define the outward-facing unit normal vector as

$$\mathbf{n} = \frac{\mathbf{x}_1 \times \mathbf{x}_2}{\|\mathbf{x}_1 \times \mathbf{x}_2\|} = \frac{\mathbf{x}_1 \times \mathbf{x}_2}{\sqrt{\|\mathbf{x}_1\|^2 \|\mathbf{x}_2\|^2 - (\mathbf{x}_1 \cdot \mathbf{x}_2)^2}} = \frac{\mathbf{x}_1 \times \mathbf{x}_2}{\sqrt{w}}. \tag{2.27}$$

With this, we may define the second fundamental form matrix

$$b_{ij} = \mathbf{x}_{ij} \cdot \mathbf{n} = \begin{pmatrix} L & M \\ M & N \end{pmatrix}. \tag{2.28}$$

Now, if we let

$$p = det(b) = LN - M^2,$$

we may define

$$b^{-1} = b_{ij}^{-1} = b^{ij} = \frac{1}{p} \begin{pmatrix} N & -M \\ -M & L \end{pmatrix}.$$

Now, with these, we have clean, nice definitions of the mean curvature H, and the Gaussian curvature, K, as

$$H = \frac{1}{2}g^{ij}b_{ij} = \frac{EN - 2FM + GL}{2g} = \frac{EN - 2FM + GL}{2(EG - F^2)},$$
$$K = \frac{p}{w} = \frac{LN - M^2}{EG - F^2}, \tag{2.29}$$

where, in the above, and in what follows, we have adopted the convention that repeated indices imply summation over them. Now, to begin our computation of the first variational derivative, we must consider a slight perturbation of our surface in the normal direction as per [26]. Hence, let

$$\mathbf{x}' = \mathbf{x} + \delta\mathbf{x} = \mathbf{x} + \psi(\theta, \phi)\mathbf{n},$$

where we assume ψ is sufficiently small and smooth in θ and ϕ. With this we may define the derivative of $\mathbf{x}'$ as,

$$\mathbf{x}'_i = \partial_i(\mathbf{x} + \psi(\theta, \phi)\mathbf{n}) = \mathbf{x}_i + \psi_i\mathbf{n} + \psi\mathbf{n}_i. \tag{2.30}$$

Notice, however, that our expression in (2.30) involves a derivative of $\mathbf{n}$. To characterize this derivative, we turn to the Weingarten Equations [15, pg.138]:

$$\mathbf{n}_i = -b_{ij}g^{jk}\mathbf{x}_k. \tag{2.31}$$

Notice the equations in (2.31) imply that $\mathbf{n}_i$ is in the tangent space of $\mathbf{x}$. As such, we will reserve the use of equation (2.31) in (2.30) until we have exploited the orthogonality of $\mathbf{n}$ and $\mathbf{n}_i$ (for notational brevity). We may now compute the local variation of g_{ij}.

$$\begin{aligned}
\delta g_{ij} &= \mathbf{x}'_i \cdot \mathbf{x}'_j - \mathbf{x}_i \cdot \mathbf{x}_j = (\mathbf{x}_i + \psi_i\mathbf{n} + \psi\mathbf{n}_i) \cdot (\mathbf{x}_j + \psi_j\mathbf{n} + \psi\mathbf{n}_j) - \mathbf{x}_i \cdot \mathbf{x}_j \\
&= \mathbf{x}_i \cdot \mathbf{x}_j + \underbrace{\mathbf{x}_i \cdot (\psi_j\mathbf{n})}_{=0} + \mathbf{x}_i \cdot (\psi\mathbf{n}_j) + \underbrace{\mathbf{x}_j \cdot (\psi_i\mathbf{n})}_{=0} + \psi_i\psi_j \underbrace{\mathbf{n} \cdot \mathbf{n}}_{=1} \\
&+ \underbrace{(\psi_i\mathbf{n}) \cdot (\psi\mathbf{n}_j)}_{=0} + \psi\mathbf{n}_i \cdot \mathbf{x}_j + \underbrace{\psi\mathbf{n}_i \cdot \psi_j\mathbf{n}}_{=0} + \psi\mathbf{n}_i \cdot \psi\mathbf{n}_j - \mathbf{x}_i \cdot \mathbf{x}_j \\
&= \psi(\mathbf{x}_i \cdot \mathbf{n}_j) + \psi_i\psi_j + \psi(\mathbf{n}_i \cdot \mathbf{x}_j) + \psi^2(\mathbf{n}_i \cdot \mathbf{n}_j).
\end{aligned} \tag{2.32}$$

Now, as we have exploited the orthogonality relationship mentioned above, we will substitute (2.31) into (2.32). Additionally, as we are only concerned with the first variation, we may discard any terms in ψ which are higher than first order. Hence, (2.32) becomes

$$
\begin{aligned}
\delta g_{ij} &= \psi(\mathbf{x}_i \cdot -b_{jl}g^{lk}\mathbf{x}_k) + \psi(-b_{il}g^{lk}\mathbf{x}_k \cdot \mathbf{x}_j) = \psi(-b_{jl}g^{lk}(\mathbf{x}_i \cdot \mathbf{x}_k) - b_{il}g^{lk}(\mathbf{x}_k \cdot \mathbf{x}_j)) \\
&= \psi(-b_{jl}\underbrace{g^{lk}g_{ki}}_{=\,\delta_{li}} - b_{il}\underbrace{g^{lk}g_{kj}}_{=\,\delta_{lj}}) = \psi(-b_{jl}\delta_{li} - b_{il}\delta_{lj}) = \psi(-b_{ji} - b_{ij}) \\
&= -2\psi b_{ij}.
\end{aligned} \tag{2.33}
$$

Note that the last equality in (2.33) is due to the symmetry in the second fundamental form. The use of Jacobi's formula for differentiating a determinant may now be used to find the first variation on w [4, pg.19]. This formula gives that

$$
\delta w = wg^{ij}(\delta g_{ij}) + \mathcal{O}(\psi^2) = wg^{ij}(-2\psi b_{ij}) = -2\psi w g^{ij} b_{ij} = -4\psi w H. \tag{2.34}
$$

We will now find the a form for the first variation of g^{ij}. We begin with a creative use of the product rule. Consider,

$$
\begin{aligned}
0 = \delta I = \delta(g^{-1}g) &= \delta(g^{-1})g + g^{-1}\delta(g) + \underbrace{\delta(g^{-1})\delta(g)}_{\mathcal{O}(\psi^2)} = \delta(g^{-1})g + g^{-1}\delta(g) \\
\Rightarrow -\delta(g^{-1})g &= g^{-1}\delta(g) \Rightarrow \delta(g^{-1}) = -g^{-1}\delta(g)g^{-1}.
\end{aligned} \tag{2.35}
$$

Now, using (2.33), we may simplify (2.35) as

$$
\begin{aligned}
\delta(g^{-1}) &= -g^{-1}(-2\psi b)g^{-1} = 2\psi g^{-1} b g^{-1} \\
&= 2\psi \frac{1}{w^2} \begin{pmatrix} G & -F \\ -F & E \end{pmatrix} \begin{pmatrix} L & M \\ M & N \end{pmatrix} \begin{pmatrix} G & -F \\ -F & E \end{pmatrix} \\
&= 2\psi \frac{1}{w^2} \begin{pmatrix} \begin{matrix} G^2L - 2GFM + F^2N \\ +(ENG - ENG) \end{matrix} & \begin{matrix} F^2M - FGL + GME - EFN \\ +(F^2M - F^2M) \end{matrix} \\ \begin{matrix} F^2M - FGL + GME - EFN \\ +(F^2M - F^2M) \end{matrix} & \begin{matrix} F^2L - 2FME + E^2N \\ +(EGL - EGL) \end{matrix} \end{pmatrix} \\
&= 2\psi \frac{1}{w^2} \left(\underbrace{(EN - 2FM + GL)}_{2wH} \underbrace{\begin{pmatrix} G & -F \\ -F & E \end{pmatrix}}_{wg^{-1}} - \underbrace{(EG - F^2)}_{w} \underbrace{\begin{pmatrix} N & -M \\ -M & L \end{pmatrix}}_{pb^{-1}} \right) \\
&= 2\psi \frac{1}{w^2}(2w^2 H g^{-1} - wpb^{-1}) = 2\psi(2Hg^{-1} - Kb^{-1}).
\end{aligned}
$$

Hence,

$$
\delta g^{ij} = 2\psi(2Hg^{ij} - Kb^{ij}). \tag{2.36}
$$

We now turn our attention to the local variation of the normal vector. For brevity, we will now adopt the notation $b_i^k = b_{ik}g^{kj}$. This allows us to write $\mathbf{n}_i = -b_{ij}g^{jk}\mathbf{x}_k = -b_i^k\mathbf{x}_k$. Now, consider,

$$\begin{aligned}\mathbf{x}_1' \times \mathbf{x}_2' &= (\mathbf{x}_1 + \psi_1\mathbf{n} + -\psi b_1^k\mathbf{x}_k) \times (\mathbf{x}_2 + \psi_2\mathbf{n} + -\psi b_2^k\mathbf{x}_k) \\ &= \underbrace{(\mathbf{x}_1 \times \mathbf{x}_2)}_{=\sqrt{g}\mathbf{n}} + \psi_1(\mathbf{n} \times \mathbf{x}_2) - \psi(b_1^k\mathbf{x}_k \times \mathbf{x}_2) \\ &\quad + \psi_2(\mathbf{x}_1 \times \mathbf{n}) - \psi(\mathbf{x}_1 \times b_2^k\mathbf{x}_k) + \mathcal{O}(\psi^2). \end{aligned} \tag{2.37}$$

While the expression in (2.37) is lovely, its real utility is not seen until we simplify a bit. Consider,

$$\begin{aligned}\mathbf{n} \times \mathbf{x}_2 &= \frac{\mathbf{x}_1 \times \mathbf{x}_2}{\sqrt{g}} \times \mathbf{x}_2 = -\mathbf{x}_2 \times (\frac{\mathbf{x}_1}{\sqrt{w}} \times \mathbf{x}_2) \\ &= \mathbf{x}_2(\mathbf{x}_2 \cdot \frac{\mathbf{x}_1}{\sqrt{w}}) - \frac{\mathbf{x}_1}{\sqrt{w}}(\mathbf{x}_2 \cdot \mathbf{x}_2) = \mathbf{x}_2\frac{F}{\sqrt{w}} - \mathbf{x}_1\frac{G}{\sqrt{w}}. \end{aligned} \tag{2.38}$$

Similarly,

$$\mathbf{x}_1 \times \mathbf{n} = \mathbf{x}_1\frac{F}{\sqrt{w}} - \mathbf{x}_2\frac{E}{\sqrt{w}}. \tag{2.39}$$

Further,

$$\begin{aligned} b_1^k\mathbf{x}_k \times \mathbf{x}_2 &= (b_1^1\mathbf{x}_1 + b_1^2\mathbf{x}_2) \times \mathbf{x}_2 = (b_1^1\mathbf{x}_1 \times \mathbf{x}_2 + b_1^2\underbrace{\mathbf{x}_2 \times \mathbf{x}_2}_{=0}) \\ &= b_1^1\underbrace{\mathbf{x}_1 \times \mathbf{x}_2}_{\mathbf{n}\sqrt{w}} = \frac{-FM + GL}{w}\mathbf{n}\sqrt{w}. \end{aligned} \tag{2.40}$$

Similarly,

$$\begin{aligned} \mathbf{x}_1 \times b_2^k\mathbf{x}_k &= \mathbf{x}_1 \times (b_2^1\mathbf{x}_1 + b_2^2\mathbf{x}_2) = (b_2^1\underbrace{\mathbf{x}_1 \times \mathbf{x}_1}_{=0} + b_2^2\underbrace{\mathbf{x}_1 \times \mathbf{x}_2}_{=\mathbf{n}\sqrt{w}}) \\ &= \frac{-FM + EN}{w}\mathbf{n}\sqrt{w}. \end{aligned} \tag{2.41}$$

Now, plugging (2.38), (2.39), (2.40), and (2.41) into (2.37), we have

$$
\begin{aligned}
\mathbf{x}_1' \times \mathbf{x}_2' &= \sqrt{w}\mathbf{n} + \psi_1 \left(\mathbf{x}_2 \frac{F}{\sqrt{w}} - \mathbf{x}_1 \frac{G}{\sqrt{w}} \right) - \psi \left(\frac{-FM + GL}{w} \mathbf{n} \sqrt{w} \right) \\
&+ \psi_2 \left(\mathbf{x}_1 \frac{F}{\sqrt{w}} - \mathbf{x}_2 \frac{E}{\sqrt{w}} \right) - \psi \left(\frac{-FM + EN}{w} \mathbf{n} \sqrt{w} \right) \\
&= \sqrt{w}\mathbf{n} \left(1 - \psi \underbrace{\frac{EN - 2FM + GL}{w}}_{=\ 2H} \right) - \sqrt{w}\mathbf{x}_i g^{ij} \psi_j \\
&= \sqrt{w} \left(\mathbf{n} \left(1 - \psi 2H \right) - \mathbf{x}_i g^{ij} \psi_j \right). \qquad (2.42)
\end{aligned}
$$

Now, a simple application of the chain rule, combined with the result of (2.34), gives us

$$
\delta \sqrt{w} = \frac{1}{2} \frac{1}{\sqrt{w}} (\delta w) = \frac{1}{2} \frac{1}{\sqrt{w}} (-4\psi w H) = -2\psi \sqrt{w} H. \qquad (2.43)
$$

Hence,

$$
\sqrt{w}' = \sqrt{w} + \delta \sqrt{w} = \sqrt{w} - 2\psi \sqrt{w} H. \qquad (2.44)
$$

Following [4, pg.22], we may now compute $\delta \mathbf{n}$ as

$$
\delta \mathbf{n} = \frac{\mathbf{x}_1' \times \mathbf{x}_2'}{\sqrt{w}'} - \mathbf{n}.
$$

Using (2.42) and (2.44), we write

$$
\begin{aligned}
\delta \mathbf{n} &= \frac{\mathbf{x}_1' \times \mathbf{x}_2'}{\sqrt{w}'} - \mathbf{n} = \frac{\sqrt{w} \left(\mathbf{n} \left(1 - \psi 2H \right) - \mathbf{x}_i g^{ij} \psi_j \right)}{\sqrt{w} - 2\psi \sqrt{w} H} - \mathbf{n} \\
&= \left(\mathbf{n} \left(1 - \psi 2H \right) - \mathbf{x}_i g^{ij} \psi_j \right) \underbrace{\frac{1}{1 - 2\psi H}}_{=\ 1 + 2\psi H + \mathcal{O}(\psi^2)\ \textit{from geo. series}} - \mathbf{n} \\
&= \left(\mathbf{n} \left(1 - \psi 2H \right) - \mathbf{x}_i g^{ij} \psi_j \right) \left(1 + 2\psi H \right) - \mathbf{n} \\
&= \mathbf{n} - 2\psi H \mathbf{n} - \mathbf{x}_i g^{ij} \psi_j + 2\psi H \mathbf{n} + \mathcal{O}(\psi^2) - \mathbf{n} = -\mathbf{x}_i g^{ij} \psi_j. \qquad (2.45)
\end{aligned}
$$

Proceeding according to [4, pg.24], we may find the variation of the second fundamental form as

$$
\delta b_{ij} = \delta(\mathbf{x}_{ij} \cdot \mathbf{n}) = (\delta \mathbf{n}) \cdot \mathbf{x}_{ij} + \mathbf{n} \cdot (\partial_i \delta \mathbf{x}_j) + \underbrace{(\delta \mathbf{n}) \cdot (\partial_i \delta \mathbf{x}_j)}_{=\ \mathcal{O}(\psi^2)}. \qquad (2.46)
$$

We must now compute the individual terms of (2.46) to arrive at a nice, compact form. We begin with

$$\partial_i \delta \mathbf{x}_j = \partial_i(-\psi b_j^k \mathbf{x}_k + \psi_j \mathbf{n}) = -\psi_i b_j^k \mathbf{x}_k - \psi \left((\partial_i b_j^k)\mathbf{x}_k + b_j^k \mathbf{x}_{ki} \right) + \psi_{ij}\mathbf{n} + \psi_j(\mathbf{n}_i),$$

and hence,

$$\begin{aligned}
\mathbf{n} \cdot (\partial_i \delta \mathbf{x}_j) &= n \cdot \left(-\psi_i b_j^k \mathbf{x}_k - \psi \left((\partial_i b_j^k)\mathbf{x}_k + b_j^k \mathbf{x}_{ki} \right) + \psi_{ij}\mathbf{n} + \psi_j(\mathbf{n}_i) \right) \\
&= -\psi_i b_j^k \underbrace{(\mathbf{x}_k \cdot \mathbf{n})}_{=\,0} - \psi \left((\partial_i b_j^k) \underbrace{(\mathbf{x}_k \cdot \mathbf{n})}_{=\,0} + b_j^k \underbrace{(\mathbf{x}_{ki} \cdot \mathbf{n})}_{=\,b_{ki}} \right) + \psi_{ij} \underbrace{(\mathbf{n} \cdot \mathbf{n})}_{=\,1} + \psi_j \underbrace{(\mathbf{n}_i \cdot \mathbf{n})}_{=\,0} \\
&= -\psi b_j^k b_{ki} + \psi_{ij}. \qquad (2.47)
\end{aligned}$$

Now, $b_j^k b_{ki} = b_{jl} g^{lk} b_{ki}$. So, consider,

$$\begin{aligned}
& b g^{-1} b \\
&= \frac{1}{w} \begin{pmatrix} L & M \\ M & N \end{pmatrix} \begin{pmatrix} G & -F \\ -F & E \end{pmatrix} \begin{pmatrix} L & M \\ M & N \end{pmatrix} \\
&= \frac{1}{w} \begin{pmatrix} \begin{matrix} GL^2 - 2LFM + EM^2 \\ +(ENL - ENL) \end{matrix} & \begin{matrix} GLM - FLN + MNE - FM^2 \\ +(FM^2 - FM^2) \end{matrix} \\ \begin{matrix} GLM - FLN + MNE - FM^2 \\ +(FM^2 - FM^2) \end{matrix} & \begin{matrix} GM^2 - 2FNM + N^2E \\ +(NGL - NGL) \end{matrix} \end{pmatrix} \\
&= \underbrace{\frac{EN - 2FM + GL}{w}}_{2H} \begin{pmatrix} L & M \\ M & N \end{pmatrix} - \underbrace{\frac{LN - M^2}{w}}_{K} \begin{pmatrix} E & F \\ F & G \end{pmatrix} \\
&= 2Hb - Kg.
\end{aligned}$$

Hence, $b_j^k b_{ki} = 2Hb_{ij} - Kg_{ij}$ and we may write (2.47) as

$$\mathbf{n} \cdot (\partial_i \delta \mathbf{x}_j) = -\psi(2Hb_{ij} - Kg_{ij}) + \psi_{ij}. \qquad (2.48)$$

Now, we introduce some new, temporary notation. Following [26], we may express $\mathbf{x}_{ij}$ in terms of its tangential and normal components (via an equation of Gauss [15, pg.138])as

$$\mathbf{x}_{ij} = \Gamma_{ij}^k \mathbf{x}_k + b_{ij}\mathbf{n}. \qquad (2.49)$$

In (2.49), Γ^k_{ij} is the Christoffel symbol of the second kind. There is no need to formally define this, as we will only be using it as a sort of 'notational place holder' (i.e we will eventually be getting rid of it). With this convenient new expression, we may use (2.45) and (2.49) to compute

$$\begin{aligned}\delta\mathbf{n}\cdot\mathbf{x}_{ij} &= (-\mathbf{x}_i g^{il}\psi_l)\cdot(\Gamma^k_{ij}\mathbf{x}_k + b_{ij}\mathbf{n}) = -\Gamma^k_{ij}\underbrace{(\mathbf{x}_k\cdot\mathbf{x}_i)}_{g_{ki}}g^{il}\psi_l - b_{ij}\Gamma^k_{ij}\underbrace{(\mathbf{x}_k\cdot\mathbf{n})}_{=\,0} \\ &= -\Gamma^k_{ij}\underbrace{g_{ki}g^{il}}_{\delta_{kl}}\psi_l = -\Gamma^k_{ij}\delta_{kl}\psi_l = -\Gamma^k_{ij}\psi_k. \end{aligned} \tag{2.50}$$

Plugging (2.48) and (2.50) into (2.46) gives the variation of the second fundamental form as

$$\delta b_{ij} = -\psi(2Hb_{ij} - Kg_{ij}) + \psi_{ij} - \Gamma^k_{ij}\psi_k. \tag{2.51}$$

We are finally ready to compute the local variation of H. We compute this variation via the product rule and (2.51), (2.36). This gives

$$\begin{aligned}\delta H &= \frac{1}{2}\delta(g^{ij}b_{ij}) = \frac{1}{2}\delta(g^{ij})b_{ij} + \frac{1}{2}g^{ij}\delta(b_{ij}) + \frac{1}{2}\underbrace{\delta(g^{ij})\delta(b_{ij})}_{=\,\mathcal{O}(\psi^2)} \\ &= \frac{1}{2}2\psi(2Hg^{ij} - Kb^{ij})b_{ij} + \frac{1}{2}g^{ij}(-\psi(2Hb_{ij} - Kg_{ij}) + \psi_{ij} - \Gamma^k_{ij}\psi_k) \\ &= \psi(2H\underbrace{g^{ij}b_{ij}}_{=\,2H} - K\underbrace{b^{ij}b_{ij}}_{=\,2}) - \psi(H\underbrace{g^{ij}b_{ij}}_{=\,2H} - \frac{1}{2}K\underbrace{g^{ij}g_{ij}}_{=\,2}) + \frac{1}{2}g^{ij}\psi_{ij} - \frac{1}{2}g^{ij}\Gamma^k_{ij}\psi_k \\ &= \psi(2H^2 - K) + \frac{1}{2}g^{ij}\psi_{ij} - \frac{1}{2}g^{ij}\Gamma^k_{ij}\psi_k. \end{aligned} \tag{2.52}$$

With this, we may now compute the global variation of

$$\frac{1}{2}\kappa_b\int_\gamma H^2 d\gamma = \frac{1}{2}\kappa_b\int_\gamma H^2\sqrt{w}d\theta d\phi.$$

Following reference [26], we proceed as such,

$$\begin{aligned}\delta\frac{1}{2}\kappa_b\int_\gamma H^2\sqrt{w}d\theta d\phi &= \frac{1}{2}\kappa_b\left(\int_\gamma \delta(H^2)\sqrt{w} + H^2(\delta\sqrt{w})d\theta d\phi\right) \\ &= \frac{1}{2}\kappa_b\left(\int_\gamma 2H\delta(H)\sqrt{w} + H^2(\delta\sqrt{w})d\theta d\phi\right). \end{aligned}$$

Now, from (2.52) and (2.43), we may write

$$
\begin{aligned}
&\frac{1}{2}\kappa_b \left(\int_\gamma 2H\delta(H)\sqrt{w} + H^2(\delta\sqrt{w}) d\theta d\phi \right) \\
&= \frac{1}{2}\kappa_b \left(\int_\gamma 2H(\psi(2H^2 - K) + \frac{1}{2}g^{ij}\psi_{ij} - \frac{1}{2}g^{ij}\Gamma^k_{ij}\psi_k)\sqrt{w} + H^2(-2\psi H\sqrt{w}) d\theta d\phi \right) \\
&= \frac{1}{2}\kappa_b \left(\int_\gamma (\psi 4H^3 - 2\psi HK + Hg^{ij}\psi_{ij} - Hg^{ij}\Gamma^k_{ij}\psi_k)\sqrt{w} - 2\psi H^3\sqrt{w} d\theta d\phi \right) \\
&= \frac{1}{2}\kappa_b \left(\int_\gamma (2\psi H(H^2 - K) + Hg^{ij}\psi_{ij} - Hg^{ij}\Gamma^k_{ij}\psi_k)\sqrt{w} d\theta d\phi \right) \\
&= \frac{1}{2}\kappa_b \int_\gamma 2\psi H(H^2 - K)\sqrt{w} d\theta d\phi + \frac{1}{2}\kappa_b \int_\gamma Hg^{ij}\psi_{ij}\sqrt{w} d\theta d\phi - \frac{1}{2}\kappa_b \int_\gamma Hg^{ij}\Gamma^k_{ij}\psi_k\sqrt{w} d\theta d\phi.
\end{aligned}
$$

Integrating the second and third terms by parts with respect to ψ and discarding the additional terms that this will create (as they will involve evaluating ψ on γ which will be very small), we have

$$
\begin{aligned}
&\frac{1}{2}\kappa_b \int_\gamma 2\psi H(H^2 - K)\sqrt{w} d\theta d\phi + \frac{1}{2}\kappa_b \int_\gamma \psi \partial_i\partial_j(Hg^{ij}\sqrt{w})\frac{\sqrt{w}}{\sqrt{w}} d\theta d\phi \\
&\qquad\qquad - \frac{1}{2}\kappa_b \int_\gamma \psi \partial_k(H\Gamma^k_{ij}g^{ij}\sqrt{w})\frac{\sqrt{w}}{\sqrt{w}} d\theta d\phi \\
&= \frac{1}{2}\kappa_b \int_\gamma \psi \left(2H(H^2 - K) + \frac{1}{\sqrt{w}}\partial_i\partial_j(Hg^{ij}\sqrt{w}) - \frac{1}{\sqrt{w}}\partial_k(H\Gamma^k_{ij}g^{ij}\sqrt{w}) \right) d\gamma \\
&= \frac{1}{2}\kappa_b \int_\gamma \psi \Big(2H(H^2 - K) + \frac{1}{\sqrt{w}}\partial_i(\partial_j(g^{ij}\sqrt{w})H) \\
&\qquad\qquad + \frac{1}{\sqrt{w}}\partial_i((g^{ij}\sqrt{w})\partial_j H) + \frac{1}{\sqrt{w}}\partial_k(H\Gamma^k_{ij}g^{ij}\sqrt{w}) \Big) d\gamma.
\end{aligned}
$$

Now, using the result that $\partial_i[(\partial_j g^{ij}\sqrt{w})H] = -\partial_k(\Gamma^k_{ij}g^{ij}\sqrt{w}H)$, given in [26], we may write

$$
\begin{aligned}
&\frac{1}{2}\kappa_b \int_\gamma \psi \Big(2H(H^2 - K) + \frac{1}{\sqrt{w}} \underbrace{\partial_i(\partial_j(g^{ij}\sqrt{w})H)}_{= \, -\partial_k(\Gamma^k_{ij}g^{ij}\sqrt{w}H)} \\
&\qquad + \frac{1}{\sqrt{w}}\partial_i((g^{ij}\sqrt{w})\partial_j H) + \frac{1}{\sqrt{w}}\partial_k(H\Gamma^k_{ij}g^{ij}\sqrt{w}) \Big) d\gamma = \\
&\frac{1}{2}\kappa_b \int_\gamma \psi \left(2H(H^2 - K) + \frac{1}{\sqrt{w}}\partial_i((g^{ij}\sqrt{w})\partial_j H) \right) d\gamma.
\end{aligned} \tag{2.53}
$$

We now require a brief diversion to define some fundamental operators. For a scalar function f, and a vector field $\mathbf{F}$, we define

$$\nabla_\gamma^2 f = \frac{1}{\sqrt{w}}\partial_i((g^{ij}\sqrt{w})\partial_j f), \quad \nabla_\gamma f = (g^{ij}\mathbf{x}_j)\partial_i f, \quad div_\gamma \mathbf{F} = (g^{ij}\partial_j \mathbf{F})\cdot \mathbf{x}_i. \tag{2.54}$$

We refer to these operators as the Laplace–Beltrami, surface gradient, and surface divergence. In (2.53), we may recognize $\frac{1}{\sqrt{w}}\partial_i((g^{ij}\sqrt{w})\partial_j H)$ as $\nabla_\gamma^2 H$. Hence,

$$\frac{1}{2}\kappa_b \int_\gamma \psi \left(2H(H^2-K) + \frac{1}{\sqrt{w}}\partial_i((g^{ij}\sqrt{w})\partial_j H)\right) d\gamma =$$
$$\frac{1}{2}\kappa_b \int_\gamma \psi \left(2H(H^2-K) + \nabla_\gamma^2 H\right) d\gamma. \tag{2.55}$$

Now, (2.55) is the first variation of the functional $(1/2)\kappa_b \int_\gamma H^2 d\gamma$. We note that this variation is entirely in the normal direction (as tangential variation would only re–parameterize this functional [4]). Further, for notational convenience, we will redefine $\kappa_b/2$ as κ_b. Hence, we may represent the L^2 gradient of $\kappa_b \int_\gamma H^2 d\gamma$ as

$$\frac{\delta\left(\kappa_b \int_\gamma H^2 d\gamma\right)}{\delta \mathbf{x}} = \kappa_b \int_\gamma \psi \left(2H(H^2-K) + \nabla_\gamma^2 H\right) \mathbf{n} \; d\gamma. \tag{2.56}$$

We now seek to compute the L^2-gradient of

$$\int_\gamma \sigma d\gamma.$$

In this case, there is also a tangential component to $\frac{\delta\left(\int_\gamma \sigma d\gamma\right)}{\delta \mathbf{x}}$ which relates to the variation of σ. Note that we require this term to ensure the local surface inextensibility condition. Since σ is arbitrary but depends on $\mathbf{x}$, we say that the local L^2 gradient must simply be the surface gradient defined in (2.54). We take this gradient to be negative (acceptable as it remains the variation in the tangent space) to fit with the convention of [21]. The normal component of this variation can be computed from (2.43). Hence,

$$\frac{\delta\left(\int_\gamma \sigma d\gamma\right)}{\delta \mathbf{x}} = \int_\gamma \delta(\sigma\sqrt{w})\mathbf{n} d\theta d\phi = \int_\gamma \sigma(-2H\psi)\mathbf{n} d\gamma - \int_\gamma (\nabla_\gamma \sigma)\psi d\gamma.$$

In the above, $2H\mathbf{n} = \nabla_\gamma^2 \mathbf{x}$ from the mean-curvature-normal definition of the Laplace-Beltrami operator [4]. Hence,

$$\frac{\delta\left(\int_\gamma \sigma d\gamma\right)}{\delta \mathbf{x}} = -\int_\gamma (\sigma \nabla_\gamma^2 \mathbf{x} + \nabla_\gamma \sigma)\phi d\gamma. \tag{2.57}$$

Putting (2.57) and (2.56) together, we may write that for

$$\mathcal{E} = \int_\gamma \frac{\kappa_b}{2} H^2 + \sigma d\gamma,$$

we have

$$\mathbf{f} = \mathbf{f}_\sigma - \mathbf{f}_b = -\frac{\delta \mathcal{E}}{\delta \mathbf{x}} = -\int_\gamma \kappa_b \left(2H(H^2 - K) + \nabla_\gamma^2 H\right) \mathbf{n}\psi \; d\gamma + \int_\gamma (\sigma \nabla_\gamma^2 \mathbf{x} + \nabla_\gamma \sigma)\psi d\gamma,$$

and we may define

$$\mathbf{f}_b = \kappa_b \left(2H(H^2 - K) + \nabla_\gamma^2 H\right) \mathbf{n}, \quad \mathbf{f}_\sigma = \sigma \nabla_\gamma^2 \mathbf{x} + \nabla_\gamma \sigma. \tag{2.58}$$

Now, we required a tangential variation of σ to ensure a local surface inextensibility condition. We now seek to formulate this condition mathematically. Inextensibility typically translates to 'divergence free' velocity. As this condition applies to the surface, we expect to use the 'surface divergence' operator defined in (2.54). This condition is tantamount to requiring that our surface maintain constant surface area. Hence, following [21], we require that

$$div_\gamma \frac{\partial}{\partial t} \mathbf{x} = 0 \tag{2.59}$$

Now, plugging (2.25) into (2.59), we have

$$\begin{aligned}
&div_\gamma \left(\mathcal{S}\left[\mathbf{f}_\sigma - \mathbf{f}_b\right](\mathbf{x}) + \mathbf{u}^\infty(\mathbf{x})\right) = 0 \\
&div_\gamma \mathcal{S}\left[\mathbf{f}_\sigma\right](\mathbf{x}) + div_\gamma \left(\mathbf{u}^\infty(\mathbf{x}) - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x})\right) = 0 \\
&div_\gamma \mathcal{S}\left[\mathbf{f}_\sigma\right](\mathbf{x}) = -div_\gamma \left(\mathbf{u}^\infty(\mathbf{x}) - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x})\right).
\end{aligned}$$

Hence we may outline an algorithm to solve this problem as:

$$\textit{Step } 1: \tag{2.60}$$

solve

$$div_\gamma \mathcal{S}\left[\mathbf{f}_\sigma\right](\mathbf{x}) = -div_\gamma\left(\mathbf{u}^\infty(\mathbf{x}) - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x})\right)$$

for $\mathbf{f}_\sigma$.

$$\textit{Step } 2: \tag{2.61}$$

use $\mathbf{f}_\sigma$ in

$$\mathcal{S}\left[\mathbf{f}_\sigma - \mathbf{f}_b\right](\mathbf{x}) + \mathbf{u}^\infty(\mathbf{x}) = \frac{\partial}{\partial t}\mathbf{x}$$

to update the surface for a new time.

CHAPTER 3

A HIGH ORDER ALGORITHM TO SIMULATE VESICLE FLOW

In this chapter we outline a numerical algorithm to solve the problem formulated in Chapter 2. We begin by examining some tools we will need in our numerical developments.

3.1 The Harmony of Spherical Harmonics

Spherical harmonics will be central to the development of our numerical methods. For a detailed derivation of spherical harmonics see appendix B. As our definition of spherical harmonics we take

$$Y_{lm}(\theta,\phi) = (-1)^{\frac{m+|m|}{2}} \sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}} e^{im\phi} P^l_{|m|}(\cos(\theta)), \tag{3.1}$$

where P^l_m is an associated Legendre polynomial. We use (3.1) to ensure orthonormality, i.e

$$\int_{S^2} Y^l_m(\mathbf{x}) \overline{Y^{l'}_{m'}(\mathbf{x})} dS(\mathbf{x}) = \delta_{mm'}\delta_{ll'}. \tag{3.2}$$

As with most classes of orthogonal functions, one of the main utilities of spherical harmonics is that some functions may be represented as linear combinations of them. For a function, $f(\theta,\phi) \in L^1(S^2)$, we have that f may be written as [2, pg. 26]

$$f(\theta,\phi) = \sum_{l=0}^{\infty} \sum_{|m|\le l} c^l_m Y_{lm}(\theta,\phi), \tag{3.3}$$

where the coefficients, c^l_m, are given by

$$c^l_m = \int_{S^2} f(\theta,\phi) \overline{Y_{lm}(\theta,\phi)} dS^2.$$

The above form for the coefficients is easily verified assuming the form for f given in (3.3), multiplying both sides of the equality by $\overline{Y_{m'l'}(\theta,\phi)}$, integrating over the surface of a sphere, and using (3.2). It will be convenient, at this point, to introduce the notation of the L^2 inner product over the unit ball S^2 as

$$\int_{S^2} f\overline{g} dS^2 = \langle f, g\rangle .$$

With this, we write,

$$c^l_m = \langle f, Y_{lm}\rangle .$$

Hence we may approximate some spherical function, f, by truncating its series representation at some, finite, maximum value of l, say, L. Precisely,

$$f(\theta,\phi) \approx \sum_{l=0}^{L} \sum_{|m|\leq l} c_m^l Y_{lm}(\theta,\phi).$$

We represent this using a projection operator, $\mathcal{L}_L$, such that,

$$f(\theta,\phi) \approx \mathcal{L}_L(f) = \sum_{l=0}^{L} \sum_{|m|\leq l} c_m^l Y_{lm}(\theta,\phi). \tag{3.4}$$

Before we begin a new investigation, we will give formulas for the partial derivatives of spherical harmonics. Rather than deriving them we will simply present them as their derivation is straightforward given the definitions we have already seen. Following [21], the formulas are as follows:

$$\begin{aligned}
\frac{\partial^k}{\partial^k \phi} Y_{lm}(\theta,\phi) &= (im)^k Y_{lm}(\theta,\phi) \\
\frac{\partial}{\partial \theta} Y_{lm}(\theta,\phi) &= \sqrt{(l-m)(l+m+1)} e^{-i\phi} Y_{l(m+1)}(\theta,\phi) + m\cot(\theta) Y_{lm}(\theta,\phi) \\
\frac{\partial^2}{\partial^2 \theta} Y_{lm}(\theta,\phi) &= (l+m+1)\sqrt{(l-m)(l+m+2)} e^{-2i\phi} Y_{l(m+2)}(\theta,\phi) \\
&\quad + (2m+1)\sqrt{(l-m)(l+m+1)} e^{-i\phi} \cot(\theta) Y_{l(m+1)}(\theta,\phi) - m^2 Y_{lm}(\theta,\phi).
\end{aligned} \tag{3.5}$$

These will be invaluable to us as many of our numerical schemes will hinge on the ability to compute derivatives of functions represented as a spherical harmonic series.

Now, as we will be primarily concerned with vector valued functions in our later developments, it is sensible, at this point to introduce a vector analogue of the spherical harmonics discussed earlier. The simplest, and possibly most natural, way to develop a concept of a vector valued spherical harmonic is to take our scalar harmonics and multiply them by a standard basis vector $\mathbf{e}_k$. Hence we arrive at the Euclidean vector harmonics, $Y_{lm}^k(\theta,\phi)$, defined by

$$Y_{lm}^k(\theta,\phi) = Y_{lm}(\theta,\phi)\mathbf{e}_k.$$

We note that these vector harmonics are orthogonal in a natural way, i.e.

$$\int_{S^2} Y_{lm}^k(\theta,\phi)\cdot\overline{Y_{l'm'}^{k'}(\theta,\phi)}dS^2 = \int_{S^2} \underbrace{\mathbf{e}_k\cdot\mathbf{e}_{k'}}_{=\,\delta_{kk'}} Y_{lm}(\theta,\phi)\overline{Y_{l'm'}(\theta,\phi)}dS^2 = \delta_{kk'}\delta_{ll'}\delta_{mm'}.$$

Hence, given a vector valued function, $\mathbf{F}(\theta,\phi)$, we may define, in much the same way as (3.3), an expansion in terms of our new vector harmonics as

$$\mathbf{F}(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{|m|\leq l}\sum_{k=1}^{3} c_{lm}^k Y_{lm}^k(\theta,\phi),$$

with the coefficients given by

$$c_{lm}^k = \int_{S^2}\mathbf{F}(\theta,\phi)\cdot\overline{Y_{l'm'}^{k'}(\theta,\phi)}dS^2 = \left\langle \mathbf{F}, Y_{l'm'}^{k'}\right\rangle.$$

We now turn our attention to the rotation of functions defined on a sphere. This is a concept that will become exceedingly valuable to us in our numerical algorithms. It will become very important for us to represent functions defined on a sphere as a truncated spherical harmonic series. Hence, our problem of rotating a spherical function may be simplified to the problem of rotating a given spherical harmonic. When we think of rotations of a point on on a sphere, it is natural to turn to the Euler angles (α,β,γ). If we wish to take the standard Cartesian axes and transform them to new, rotated axes, we may rotate the z-axis counterclockwise by and angle α which takes the y-axis to a position called *the line of nodes* [17, App. C]. If we then rotate the y-axis, about the line of nodes, counterclockwise by an angle β we have taken the z axes to its new location. If we then rotate counterclockwise by an angle γ about the new z-axis we will have taken the y-axis to its new location and completed our transformation. It is clear then, that the Euler angels (α,β,γ) represent a rotational isometry on the surface of a sphere. Now, given a spherical harmonic of degree l, we may represent it as a non-trivial linear combination of spherical harmonics of the same degree [2, pg.21]. Hence, we expect that the rotation (α,β,γ) applied to a spherical harmonic of degree l and order m may be expressed as

$$Y_m^l(\theta',\phi') = \sum_{|j|\leq l} D_{mj}^l(\alpha,\beta,\gamma)Y_j^l(\theta,\phi),$$

where (θ,ϕ) are our original coordinates, (θ',ϕ') are coordinates in our rotated system and

$D^l_{mj}(\alpha, \beta, \gamma)$ is a coefficient indexed by m, j, l and dependent on (α, β, γ). As α and β both represent rotations about a z-axis and as the angle a spherical harmonic takes with the z-axis, ϕ, only appears in a complex exponential, these transformations admit a simple representation as $e^{-ij\alpha}$ and $e^{-im\gamma}$. Now, we may write

$$Y^l_m(\theta', \phi') = \sum_{|j| \leq l} e^{-ij\alpha} d^l_{mj}(\beta) e^{-im\gamma} Y^l_j(\theta, \phi). \tag{3.6}$$

The new coefficient $d^l_{mj}(\beta)$, however, does not have a similarly nice representation. Referred to as the Wigner 3-j symbol [17, App. C], the coefficient $d^l_{mj}(\beta)$ has a known form

$$d^l_{mj}(\beta) = (-1)^{m+j} \sqrt{\frac{(l+j)!(l-j)!}{(l+m)!(l-m)!}} cos^{j+m}(\frac{1}{2}\beta) sin^{j-m}(\frac{1}{2}\beta) P^{(j-m, j+m)}_{l-j}(\cos(\beta)), \tag{3.7}$$

where $P^{(a,b)}_N(x)$ is a Jacobi polynomial defined by

$$P^{(a,b)}_n(x) = \frac{1}{2^n} \sum_{k=0}^{n} \binom{n+a}{n-k} \binom{n+b}{k} (x-1)^k (x+1)^{n-k}. \tag{3.8}$$

Hence, we have a representation for the rotation of a given spherical harmonic. At this point, it is worthy to note the special case when $\beta = \frac{\pi}{2}$ gives [8]

$$d^l_{mj}(\frac{\pi}{2}) = (-1)^{m+j} 2^j \sqrt{\frac{(l+j)!(l-j)!}{(l+m)!(l-m)!}} P^{(j-m, j+m)}_{l-j}(0),$$

which fall immediately from the definition. Using this, [8] gives a computationally efficient implementation of $d^l_{mj}(\beta)$ as

$$d^l_{mj}(\beta) = e^{i(m-j)\frac{\pi}{2}} \sum_{|k| \leq l} d^l_{jk}(\frac{\pi}{2}) d^l_{mk}(\frac{\pi}{2}) e^{ik\beta}. \tag{3.9}$$

Another special case of the Wigner 3-j symbol will provide a concise proof of a famous theorem for us. We examine, for a moment, the Jacobi polynomials. Much like for the associated Legendre polynomials, we may write a definition of Jacobi polynomials which is equivalent to (3.8) using Rodrigues' formula [5]

$$P^{(a,b)}_n(x) = \frac{(-1)^n}{2^n n!} (1-x)^{-a} (1+x)^{-b} \frac{d^n}{dx^n} \left((1-x)^a (1+x)^b (1-x^2)^n \right). \tag{3.10}$$

Using this, we may derive a useful form for $d^l_{0j}(\beta)$. From (3.7), we have that

$$
\begin{aligned}
d^l_{0j}(\beta) &= (-1)^j \sqrt{\frac{(l+j)!(l-j)!}{l!l!}} cos^j(\frac{1}{2}\beta) sin^j(\frac{1}{2}\beta) P^{(j,j)}_{l-j}(\cos(\beta)) \\
&= (-1)^j \sqrt{\frac{(l+j)!(l-j)!}{l!l!}} \left(\frac{1}{2}\sin(\beta)\right)^j \frac{(-1)^{l-j}}{2^{l-j}(l-j)!}(1-cos^2(\beta))^{-j} \\
&\qquad \frac{d^{l-j}}{d(\cos(\beta))^{l-j}}(1-cos^2(\beta))^l,
\end{aligned}
$$

and making the substitution $x = \cos(\beta)$

$$
\begin{aligned}
&= \sqrt{\frac{(l+j)!(l-j)!}{l!l!}} \left(1-x^2\right)^{j/2} \frac{(-1)^l}{2^l(l-j)!}(1-x^2)^{-j}(-1)^l \frac{d^{l-j}}{dx^{l-j}}(x^2-1)^l \\
&= \sqrt{\frac{(l+j)!(l-j)!}{l!l!}} \left(1-x^2\right)^{-j/2} \frac{1}{2^l(l-j)!} \frac{d^{l-j}}{dx^{l-j}}(x^2-1)^l.
\end{aligned}
$$

By (B.14) (see appendix B)

$$
\begin{aligned}
&= \sqrt{\frac{(l+j)!(l-j)!}{l!l!}} \left(1-x^2\right)^{-j/2} \frac{1}{2^l(l-j)!} \frac{d^{l-j}}{dx^{l-j}}(x^2-1)^l \\
&= \sqrt{\frac{(l+j)!(l-j)!}{l!l!}} \frac{l!}{(l-j)!} P^l_{-j}(x),
\end{aligned}
$$

and by (B.20) (see appendix B)

$$
\begin{aligned}
&= \sqrt{\frac{(l+j)!(l-j)!}{l!l!}} \frac{l!}{(l-j)!}(-1)^j \frac{(l-j)!}{(l+j)!} P^l_j(x) \\
&= (-1)^j \sqrt{\frac{(l+j)!}{(l-j)!}} P^l_j(x) \\
&= (-1)^j \sqrt{\frac{(l+j)!}{(l-j)!}} P^l_j(\cos(\beta)).
\end{aligned}
$$

Hence, we may write

$$
D^l_{0j}(\alpha,\beta,\gamma) = e^{-ij\alpha} d^l_{0j}(\beta) = (-1)^j \sqrt{\frac{(l+j)!}{(l-j)!}} e^{-ij\alpha} P^l_j(\cos(\beta)) = \sqrt{\frac{4\pi}{2l+1}} \overline{Y^l_j(\beta,\alpha)}. \quad (3.11)
$$

With this, we are ready to prove the addition theorem for spherical harmonics.

Theorem 3.4. *Given two points on a the surface of a unit sphere, say, (θ,ϕ) and (θ',ϕ'), whose pointing vectors ($\boldsymbol{x}$ and $\boldsymbol{x}'$ respectively) make an angle η with each other,*

$$P_l(\cos(\eta)) = \frac{4\pi}{2l+1} \sum_{|m|\leq l} \overline{Y_j^l(\theta, \phi)} Y_j^l(\theta', \phi').$$

Proof. If we rotate the sphere that our points exist on so that $\mathbf{x}'$ is aligned with the z-axis, we see that γ becomes the polar angle of $\mathbf{x}$ in the new rotated system. We form this system from the Euler angles $(\phi', \theta', -\phi')$. For convenience, we will define ϕ_r to be the azimuthal angle of $\mathbf{x}$ in this rotated system. Hence, by (3.6)

$$Y_m^l(\eta, \phi_r) = \sum_{|j|\leq l} D_{mj}^l(\phi', \theta', -\phi') Y_j^l(\theta, \phi).$$

Plugging in $m = 0$ and using (3.11), we have

$$\begin{aligned}
Y_0^l(\eta, \phi_r) &= \sum_{|j|\leq l} D_{0j}^l(\phi', \theta', -\phi') Y_j^l(\theta, \phi) \Rightarrow \\
\sqrt{\frac{2l+1}{4\pi}} P_0^l(\cos(\eta)) &= \sum_{|j|\leq l} \sqrt{\frac{4\pi}{2l+1}} \overline{Y_j^l(\theta', \phi')} Y_j^l(\theta, \phi) \Rightarrow \\
P_l(\cos(\eta)) &= \frac{4\pi}{2l+1} \sum_{|j|\leq l} \overline{Y_j^l(\theta', \phi')} Y_j^l(\theta, \phi).
\end{aligned}$$

Further, note that as $\mathbf{x}$ and $\mathbf{x}'$ are unit vectors, $\cos(\eta) = \mathbf{x} \cdot \mathbf{x}'$ and hence an alternate formulation of the addition theorem using pointing vector notation is

$$P_l(\mathbf{x} \cdot \mathbf{x}') = \frac{4\pi}{2l+1} \sum_{|j|\leq l} \overline{Y_j^l(\mathbf{x}')} Y_j^l(\mathbf{x}).$$

□

3.2 Projection and Quadrature on the Sphere

At many points in the numerical implementation of the algorithm presented in section (2.2), as (2.60) and (2.61), we will be required to numerically compute integrals involving spherical harmonics over the unit sphere. Hence, we require a spectrally accurate numerical integration scheme. We begin our discussion of quadrature with the Gauss-Legendre quadrature scheme. For this scheme, the N quadrature points, t_i, are given as the roots to the N^{th} degree Legendre polynomial, and the weights are given as $\eta_i = \frac{-2}{(N+1)P_{N+1}(t_i)P_N'(t_i)}$, with $i = 1, 2, \ldots, N$. It can be shown, [23, pg.290] that this scheme will exactly integrate any polynomial of degree $2N-1$ or lower. Further, reference [23, pg.290] gives a $\mathcal{O}(N^2)$ algorithm for computing the Gauss-Legendre weights and nodes as finding the Eigen–system of a symmetric tridiagonal matrix, J, given by

$$J_{i,i} = 0, \qquad\qquad i = 1, \dots, N$$

and

$$J_{i,i-1} = J_{i-1,i} = \frac{i}{\sqrt{4i^2-1}}, \qquad\qquad i = 2, \dots, N$$

where the Eigenvalues of this matrix are the Gauss-Legendre nodes and the first entry of each of the normalized Eigenvectors is the corresponding weight. It should be noted that the form of this matrix is derived from the monic recurrence relation for Legendre polynomials [23, pg.290].

We now describe a quadrature scheme for numerically integrating over the surface of a sphere. As we will often be concerned with integrating spherical harmonics or functions involving spherical harmonics, we seek a quadrature scheme which is exact for spherical harmonics of a given degree and lower. Specifically, we want to use the quadrature scheme to find the coefficients of a spherical harmonic expansion of the form (3.3). Say, for instance, that we had a spherical function, $f(\theta,\phi)$, which could be represented exactly as a finite linear combination of spherical harmonics in the form of (3.3). We would then wish to find the coefficients, c_{lm}, of this function exactly using a quadrature scheme. Consider the form of these coefficients,

$$c_{l'm'} = \int_0^{2\pi}\int_0^{\pi} f(\theta,\phi)\overline{Y_{l'm'}(\theta,\phi)}\sin(\theta)d\theta d\phi.$$

As f can be represented exactly as a finite linear combination of spherical harmonics, we have

$$c_{l'm'} = c_{lm}\sum_{l=0}^{L}\sum_{|m|\le l}\int_0^{2\pi}\int_0^{\pi} Y_{lm}(\theta,\phi)\overline{Y_{l'm'}(\theta,\phi)}\sin(\theta)d\theta d\phi,$$

and by the orthogonality of spherical harmonics, we have that

$$c_{lm} = c_{lm}\int_0^{2\pi}\int_0^{\pi} Y_{lm}(\theta,\phi)\overline{Y_{lm}(\theta,\phi)}\sin(\theta)d\theta d\phi.$$

Now, from the definition of spherical harmonics (3.1), the above integrand is a polynomial, say, Q, in $\cos(\theta)$ of degree $2l$ which is at most of degree $2L$. Hence, we seek a quadrature scheme which evaluates integrals of the form

$$\int_0^\pi Q(\cos(\theta))\sin(\theta)d\theta$$

exactly, where Q is a polynomial of degree at most $2L$. If we make a change of variables, $t = \cos(\theta)$, we may rewrite the above integral as,

$$\int_{-1}^{1} Q(t)dt. \tag{3.12}$$

As we have seen Gauss–Legendre quadrature is exact for polynomials of degree $2L-1$ or lower. Hence, an $L+1$ point Gaussian quadrature scheme will suffice to numerically calculate integrals of the form (3.12) exactly. As we performed a change of variables, to arrive at (3.12), we may take our theta nodes, θ_i to be $cos^{-1}(t_i)$ where t_i is the i^{th} Gauss-Legendre node. The theta weights for this quadrature remain the Gauss-Legendre weights. Now for a quadrature scheme in the ϕ direction, we again look for accuracy in integrating spherical harmonics. The ϕ dependence in a given spherical harmonic is periodic (i.e is $e^{im\phi}$). Hence, following [21], we use a $2(L+1)$ node trapezoidal rule in ϕ. Specifically, the ϕ nodes are given by $\left\{\phi_k = \frac{\pi k}{L}\right\}_{k=0}^{2L+1}$ and the weights by $\xi_k = \frac{\pi}{L}$.

To summarize, the quadrature nodes and weights we will be using throughout our numerical explorations are

$$\left\{\phi_k = \frac{\pi k}{L}\right\}_{k=0}^{2L+1}, \qquad \xi_k = \frac{\pi}{L}, \tag{3.13}$$

and for t_i as the i^{th} root of the $(L+1)^{th}$ degree Legendre polynomial,

$$\left\{\theta_i = cos^{-1}(t_i)\right\}_{i=0}^{L}, \qquad \left\{\eta_i = \frac{-2}{(L+1)P_{L+1}(t_i)P_L'(t_i)}\right\}_{i=0}^{L}. \tag{3.14}$$

To illustrate the exactness in the use of this quadrature for numerical integration of spherical harmonics, we present results from the following test. Analytically, we know that the $(L+1)^2 \times (L+1)^2$ Gramian matrix,

$$[\mathbf{Y}]_{lm,l'm'} = \langle Y_{lm}, Y_{l'm'} \rangle,$$

must equal the $(L+1)^2 \times (L+1)^2$ identity matrix by the orthogonality of spherical harmonics. Table 3.1 gives the matrix 2-norm error between $\mathbf{Y}$ and I where the entries of $\mathbf{Y}$ are computed using the $2((L+1)+1)^2$ point quadrature rule described above for several values of L.

Table 3.1: Error in Gramian matrix of spherical harmonics

L	$\|\mathbf{Y}-I\|$
1	4.7837e-16
5	4.2274e-15
10	1.7147e-14
15	4.7234e-14
20	4.3524e-14
25	1.2996e-13

This test serves to give an estimate of the global error in using our quadrature to compute integrals involving only spherical harmonics. For instance, those which arise as the coefficients of functions which admit representations as a finite linear combination of spherical harmonics. We see that the error in the above table is extremely low for all values of L presented. However, the error does rise slightly as L increases due to round-off error [21]. As we have motivated, one of the utilities of this quadrature scheme is that it will find, exactly, the coefficients in a *finite* spherical harmonic expansion of degree L provided an expansion of this form exists. If such an expansion does not exist, we seek to approximate a function, f, by a finite linear combination of spherical harmonics. We recall (3.4) in which we defined an projection operator, $\mathcal{L}_L$, that approximated spherical functions as linear combinations of spherical harmonics up to the L^{th} degree. The coefficients of this linear combination are given by an integral of the form

$$\int_{S^2} f(\theta,\phi)\overline{Y_{lm}}dS^2,$$

which is itself of the form

$$\int_{S^2} g(\theta,\phi)dS^2,$$

where g is not necessarily a spherical polynomial. In this case, [21], shows that the quadrature scheme we presented is super–algebraically convergent with L. Because this quadrature scheme has everything we might want, we will seek to solve our problem numerically on a mesh of the nodes of this scheme.

3.2.1 Results Concerning the Numerical Representation of Surfaces

Here, we present results concerning the accuracy achieved in the approximation of some surfaces using our $\mathcal{L}$ operator defined in equation (3.4). To this end, we will present examples that highlight the strengths and pitfalls of our methods to numerically represent surfaces. For our first example, we examine the surface defined by

$$\mathbf{x}(\theta, \phi) = \left(1 + e^{-3Re[Y_2^3(\theta,\phi)]}\right) [\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)]^T. \tag{3.15}$$

We approximate this, on a grid of our quadrature nodes (θ_i, ϕ_j), for several values of L as

$$\mathbf{x}(\theta, \phi) \approx \sum_{l=0}^{L} \sum_{|m|\leq l} \sum_{k=1}^{3} \omega_{l,m}^k Y_{l,m}^k(\theta_i, \phi_j) = \tilde{\mathbf{x}}(\theta_i, \phi_j),$$

where

$$\omega_{l,m}^k = \sum_{i=1}^{(L+1)+1} \sum_{j=1}^{2(L+1)+2} \eta_i \xi_j \mathbf{x}(\theta_i, \phi_j) \cdot \overline{Y_{l,m}^k(\theta_i, \phi_j)}. \tag{3.16}$$

Below is a table of the relative L^2 error in our approximation to (3.15) for various values of L:

Table 3.2: relative L^2 error in approximation of (3.15)

L	$\|\mathbf{x} - \tilde{\mathbf{x}}\| / \|\mathbf{x}\|$
1	4.6824e-01
10	1.8603e-03
20	2.1803e-07
30	1.7323e-11
40	1.3267e-14

Further, using the coefficients, ω, computed in the style of (3.16), we plot our approximations to this surfaces using a mesh of 50 equally spaced in θ and 100 equally spaced points in ϕ (to make them look nicer for smaller values of L) in Figure 3.1. From Table 3.2 and Figure 3.1 we see that our approximation of the surface $\mathbf{x}$ defined in (3.15) can be represented fairly accurately with a finite linear combination of spherical harmonics. It is worth to note that the surface defined in (3.15) has a number of good properties. Firstly, it is smooth (i.e. has no sharp peaks or folds). Further, the surface is not highly oscillatory. Surfaces of this type require high degree spherical harmonics which our numerical schemes are not well equip

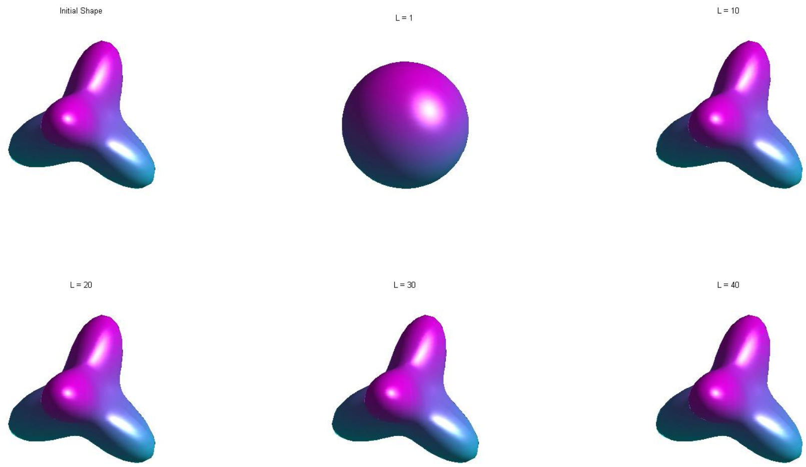

Figure 3.1: A plot of approximations to the surface, $\mathbf{x}$, defined in (3.15), for various values of L where the upper left–hand plot is the exact surface.

to handle. While we have ruled out the use of singular surfaces in Chapter 1, we wish to demonstrate, numerically, why we made this restriction. Hence, we present results for the following two, singular surfaces. Consider,

$$\mathbf{P}(\theta, \phi) = e^{\theta}[\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)]^T, \quad (3.17)$$

and

$$\mathbf{F}(\theta, \phi) = \left(1 + \frac{\sin(5\theta)}{5}\right)[\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)]^T. \quad (3.18)$$

Where $\mathbf{P}$ has two sharp peaks at the north and south poles and $\mathbf{F}$ has sharp folds around the north and south poles. To see this, we present the following figures showing the surfaces and our approximations to them for various values of L. We see in Figure 3.2 that the peak at the south pole of the surface is never accurately captured, and in Figure 3.3 all of the features of the surface at the north and south poles are not captured. Further, in Figure 3.3 we see that some oscillatory features are added in our approximations which are not present in the original surface.

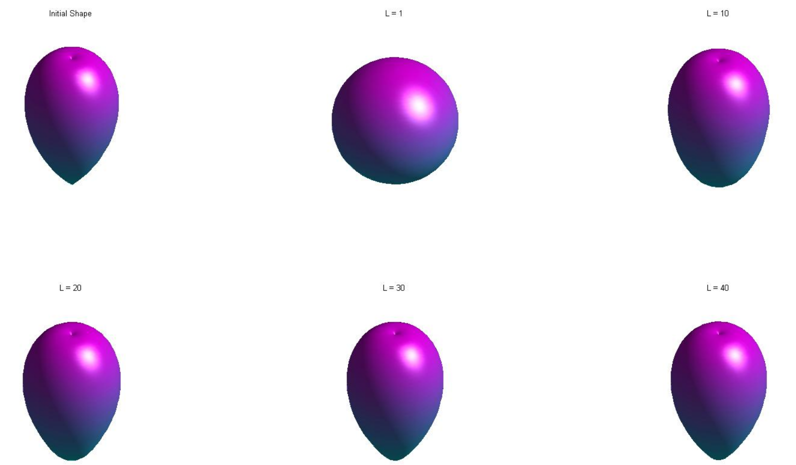

Figure 3.2: A plot of approximations to the surface, **P**, defined in (3.17), for various values of L where the upper left–hand plot is the exact surface.

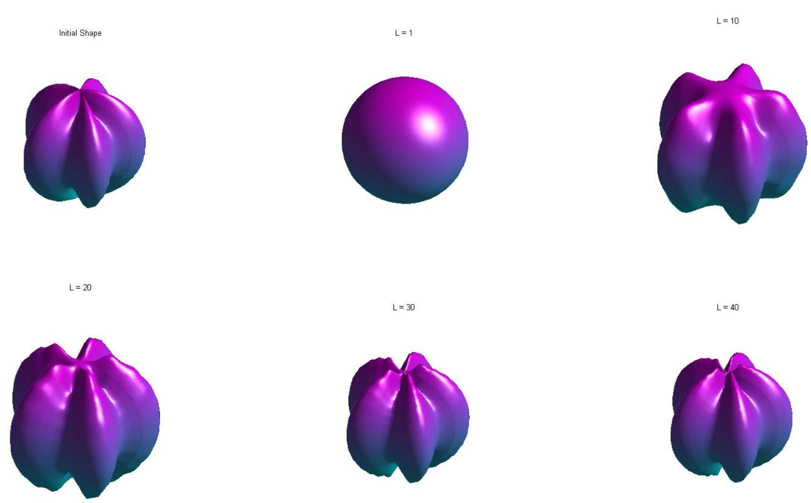

Figure 3.3: A plot of approximations to the surface, **F**, defined in (3.18), for various values of L where the upper left–hand plot is the exact surface.

3.3 Discretizing the Stokes Operator

Recall that step one of our vesicle simulation algorithm (2.60) is to solve

$$div_\gamma \mathcal{S}_\gamma [f_\sigma] = -div_\gamma (\mathbf{u}^\infty - \mathcal{S}_\gamma [f_b]) \tag{3.19}$$

for f_σ where $\mathcal{S}_\gamma$ is the weakly singular integral operator defined by

$$\mathcal{S}_\gamma [\Psi] (\mathbf{x}) = \int_\gamma G(\mathbf{x},\mathbf{y})\ \Psi(\mathbf{y})\ d\gamma(\mathbf{y}), \qquad G(\mathbf{x},\mathbf{y}) = \frac{1}{8\pi}\left(\frac{1}{|\mathbf{x}-\mathbf{y}|}\mathbf{I} + \frac{(\mathbf{x}-\mathbf{y})\otimes(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3}\right),$$

and f_b is the bending force (a known quantity defined in equation (2.58)). We seek to find a computationally efficient method of discretizing the action of the Stokes operator ($\mathcal{S}_\gamma$) on a vector field. We will see in the next section that our discretizations of these operators admit an efficient Galerkin scheme for solving (3.19).

We begin our discretization of $\mathcal{S}_\gamma$ by noting that the kernel of $\mathcal{S}_\gamma$, $G(\mathbf{x},\mathbf{y})$ admits a factorization of the form

$$G(\mathbf{x},\mathbf{y}) = \frac{1}{|\mathbf{x}-\mathbf{y}|}\left(\frac{1}{8\pi}\mathbf{I} + \frac{1}{8\pi}\frac{(\mathbf{x}-\mathbf{y})\otimes(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2}\right) = \frac{1}{|\mathbf{x}-\mathbf{y}|}\left(m_1(\mathbf{x},\mathbf{y}) + m_2(\mathbf{x},\mathbf{y})\right),$$

with $m_1(\mathbf{x},\mathbf{y}) = \frac{1}{8\pi}\mathbf{I}$ and $m_2(\mathbf{x},\mathbf{y}) = \frac{1}{8\pi}\frac{(\mathbf{x}-\mathbf{y})\otimes(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2}$ in accordance with [8]. In this representation, m_1 is clearly in $C^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ and hence, non-singular. While it may seem that m_2 is singular, the double pole (seen in the denominator at $\mathbf{x}=\mathbf{y}$) is 'canceled' by the double zero from the numerator. Hence, m_2 is, in fact, non-singular. As m_1 and m_2 are both non-singular, the above representation of $G(\mathbf{x},\mathbf{y})$ effectively factors out its weakly singular component.

We now turn our attention to the surface, γ which $\mathcal{S}_\gamma$ is taken over. As γ is an arbitrary domain, computing an integral over it could be cumbersome. In our problem, γ represents the surface of our vesicle which, as per section 1, we require to be diffeomorphic to the surface of a sphere. Thus, we know that there is a smooth, bijective coordinate mapping, say, $\mathbf{q}: S^2 \to \gamma$, taking the boundary of a unit sphere to our surface. Still, we saw in sections 3.1 and 3.2.1 that maps of this kind can be accurately approximated by a truncated spherical harmonic series. As our surface is changing with time and hence, in general, has no analytic representation, we will implement this mapping $\mathbf{q}$ as the truncated spherical harmonic series representation of our surface γ. The mapping, $\mathbf{q}$, allows us to represent our integral operator, $\mathcal{S}_\gamma$, as

$$\mathcal{S}_\gamma\left[\Psi\right](\mathbf{x}) = \int_\gamma G(\mathbf{x},\mathbf{y})\ \Psi(\mathbf{y})\ d\gamma(\mathbf{y}) = \int_{\partial S^2} G(\mathbf{q}(\hat{\mathbf{x}}),\mathbf{q}(\hat{\mathbf{y}}))\ \Psi(\mathbf{q}(\hat{\mathbf{y}}))\ J(\hat{\mathbf{y}})\ ds(\hat{\mathbf{y}}),$$

where $J(\mathbf{y})$ is the Jacobian of $\mathbf{q}$ and $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ are coordinates on the unit sphere of the form $[\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)]^T$. We seek to evaluate integrals of this type with the spherical quadrature described in section 3.2. This, however, creates a minor numerical complication. This quadrature has the spherical Jacobian, $W = \sin(\theta)$, built into it. Thus, numerically, we implement the Jacobian of $\mathbf{q}$ as $J(\hat{\mathbf{y}}) = J(\theta,\phi)/\sin(\theta)$ to cancel out the now-unwanted spherical Jacobian introduced by our quadrature.

While this coordinate transformation, $\mathbf{q}$, certainly eliminates much of the difficulty and uncertainty in dealing with integrals over an arbitrary surface, it also creates some numerical challenges. Let us examine the two form

$$\begin{aligned} &G(\mathbf{q}(\hat{\mathbf{x}}),\mathbf{q}(\hat{\mathbf{y}}))\ \Psi(\mathbf{q}(\hat{\mathbf{y}}))\ J(\hat{\mathbf{y}})\ ds(\hat{\mathbf{y}}) = \\ &\frac{1}{|\mathbf{q}(\hat{\mathbf{x}})-\mathbf{q}(\hat{\mathbf{y}})|}\left(m_1(\mathbf{q}(\hat{\mathbf{x}}),\mathbf{q}(\hat{\mathbf{y}})) + m_2(\mathbf{q}(\hat{\mathbf{x}}),\mathbf{q}(\hat{\mathbf{y}}))\right)\ \Psi(\mathbf{q}(\hat{\mathbf{y}}))\ J(\hat{\mathbf{y}})\ ds(\hat{\mathbf{y}}). \end{aligned} \tag{3.20}$$

In (3.20), we see that while $1/\left|\mathbf{q}(\hat{\mathbf{x}})-\mathbf{q}(\hat{\mathbf{y}})\right|$ is now the only singular 'bit' of our kernel, it still has infinitely many singularities (i.e whenever $\mathbf{q}(\hat{\mathbf{x}}) = \mathbf{q}(\hat{\mathbf{y}})$). Thus, we turn our attention to the removal of these singularities.

As we've reformed our integral operator to act over the surface of a sphere, we now seek to exploit the symmetry which this admits. We note that integrals taken with respect to the surface measure of a sphere are invariant under rotation (due to the isometry property of $SO(3)$). The weakly singular factor in our kernel, $\left|\mathbf{q}(\hat{\mathbf{x}})-\mathbf{q}(\hat{\mathbf{y}})\right|^{-1}$, may have many singularities, however, following [8–10], we will show that cleaver use of rotations which will not effect the value of our integral, will coalesce the singularities in our kernel to the north pole. Consider a point on the surface of a sphere defined by its polar and azimuthal angles (θ,ϕ). If we rotate this point clockwise about the z-axis by ϕ radians, the point will lie on the great circle of the $x - z$ plane. Thus, a clockwise rotation about the y-axis by θ radians will place our point at the north pole of the unit sphere. We may represent this transformation as a product of rotation matrices. Note that, to perform our rotation, we only rotated about the y and z axes. Thus, we consider the basis elements of $SO(3)$ which correspond to these rotations; namely

$$P(\psi) = \begin{pmatrix} \cos(\psi) & -\sin(\psi) & 0 \\ \sin(\psi) & \cos(\psi) & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

which corresponds to a counter clockwise rotation about the z-axis by ψ radians, and

$$Q(\xi) = \begin{pmatrix} \cos(\xi) & 0 & \sin(\xi) \\ 0 & 1 & 0 \\ -\sin(\xi) & 0 & \cos(\xi) \end{pmatrix},$$

which corresponds to a counter clockwise rotation about the y-axis by ξ radians. Hence, the matrix

$$T(\theta, \phi) = Q(-\theta)P(-\phi) = \begin{pmatrix} \cos(\theta) & 0 & -\sin(\theta) \\ 0 & 1 & 0 \\ \sin(\theta) & 0 & \cos(\theta) \end{pmatrix} \begin{pmatrix} \cos(\phi) & \sin(\phi) & 0 \\ -\sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

represents the transformation of a point, (θ, ϕ), on the surface of a sphere, onto the north pole. We note that the coordinates of the north pole are independent of the azimuth, ϕ, and hence, we must return this angle to its original value while maintaining the result of the above transformation in order to gain unique invertability of this transformation. Thus, we may write

$$T(\theta, \phi) = P(\phi)Q(-\theta)P(-\phi) =$$

$$\begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos(\theta) & 0 & -\sin(\theta) \\ 0 & 1 & 0 \\ \sin(\theta) & 0 & \cos(\theta) \end{pmatrix} \begin{pmatrix} \cos(\phi) & \sin(\phi) & 0 \\ -\sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Hence, for a point $\hat{\mathbf{x}} = [\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)]^T$ on the boundary of a sphere, we have that

$$T(\theta, \phi)\hat{\mathbf{x}} = [0, 0, 1]^T = \hat{\mathbf{n}}. \tag{3.21}$$

As $P, Q \in SO(3)$, $T \in SO(3)$, and has an orthogonal inverse, T^T. Hence, we may rearrange

(3.21) to arrive at

$$\hat{\mathbf{x}} = T(\theta,\phi)^T[0,0,1]^T = T(\theta,\phi)^T\hat{\mathbf{n}}. \tag{3.22}$$

As the notation $T(\theta,\phi)$ is a bit tedious, following [8], we will adopt the notation $T_{\hat{\mathbf{x}}}$ (as per [8]) to describe the transformation which carries a point $\hat{\mathbf{x}}$ on the surface of a sphere to the north pole. With this notation in hand, we define a smooth linear transformation, $\mathcal{T}_{\hat{\mathbf{x}}}$ on continuous functions, Ψ, defined on the unit ball,

$$\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\hat{\mathbf{z}}) = \Psi(T_{\hat{\mathbf{x}}}^T\hat{\mathbf{z}}).$$

With this, a bivariate analogue of $\mathcal{T}_{\hat{\mathbf{x}}}$ can be defined for continuous function of two variables on the unit ball,

$$\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\hat{\mathbf{z}},\hat{\mathbf{w}}) = \Psi(T_{\hat{\mathbf{x}}}^T\hat{\mathbf{z}}, T_{\hat{\mathbf{x}}}^T\hat{\mathbf{w}}).$$

Now, let us turn our attention to the function $K(\hat{\mathbf{x}},\hat{\mathbf{y}}) = 1/\left|\hat{\mathbf{x}}-\hat{\mathbf{y}}\right|$ (The Harmonic Kernel). Given that $T_{\hat{\mathbf{x}}}\hat{\mathbf{y}} = \hat{\mathbf{z}}$ for some $\hat{\mathbf{z}}$ on the surface of a sphere, the result of (3.22) allow us to write

$$K(\hat{\mathbf{x}},\hat{\mathbf{y}}) = \frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|} = \frac{1}{|T_{\hat{\mathbf{x}}}^T\hat{\mathbf{n}} - T_{\hat{\mathbf{x}}}^T\hat{\mathbf{z}}|} = \frac{1}{|T_{\hat{\mathbf{x}}}^T(\hat{\mathbf{n}}-\hat{\mathbf{z}})|} = \frac{1}{|T_{\hat{\mathbf{x}}}^T|\,|(\hat{\mathbf{n}}-\hat{\mathbf{z}})|} = \frac{1}{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|}. \tag{3.23}$$

Hence, using our new transformation, we have that integrals over the sphere, with kernel $K(\hat{\mathbf{x}},\hat{\mathbf{y}})$, of some function Ψ, may be rewritten as

$$\int_{\partial S^2}\frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|}\Psi(\hat{\mathbf{y}})ds(\hat{\mathbf{y}}) = \int_{\partial S^2}\frac{1}{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|}\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\hat{\mathbf{z}})ds(\hat{\mathbf{z}}).$$

Here, the transformation $\mathcal{T}_{\hat{\mathbf{x}}}$ allows us to exploit the result found in (3.23) while maintaining the use of one consistent 'dummy' integration variable (i.e $\hat{\mathbf{z}}$). Imposing the standard spherical coordinates, (θ,ϕ), in the above integral reveals a surprising cancellation.

Let us examine $|\hat{\mathbf{n}}-\hat{\mathbf{z}}|$ in spherical coordinates.

$$
\begin{aligned}
&|\hat{\mathbf{n}} - \hat{\mathbf{z}}|^2 \\
&= \left|[0,0,1]^T - [\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)]^T\right|^2 \\
&= \left|[-\sin(\theta)\cos(\phi), -\sin(\theta)\sin(\phi), 1-\cos(\theta)]^T\right|^2 \\
&= sin^2(\theta)cos^2(\phi) + sin^2(\theta)sin^2(\phi) + 1 - 2\cos(\theta) + cos^2(\theta) \\
&= sin^2(\theta)(cos^2(\phi) + sin^2(\phi)) + 1 - 2\cos(\theta) + cos^2(\theta) \\
&= sin^2(\theta) + cos^2(\theta) + 1 - 2\cos(\theta) \\
&= 2(1-\cos(\theta)) = 4sin^2(\theta/2).
\end{aligned} \tag{3.24}
$$

Hence, $|\hat{\mathbf{n}} - \hat{\mathbf{z}}| = 2\sin(\theta/2)$ (for $\theta \in [0,\pi]$). This result with the fact that on a sphere, $ds = \sin(\theta)d\theta d\phi$ allow us to write

$$
\begin{aligned}
&\int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|} \mathcal{T}_{\hat{\mathbf{x}}}\Psi(\hat{\mathbf{z}})ds(\hat{\mathbf{z}}) \\
&= \int_{\partial S^2} \frac{1}{|[0,0,1]^T - [\sin(\theta)\cos(\phi), \sin(\theta)\cos(\phi), \cos(\theta)]^T|} \mathcal{T}_{\hat{\mathbf{x}}}\Psi(\theta,\phi)\sin(\theta)d\theta d\phi \\
&= \int_{\partial S^2} \frac{\sin(\theta)}{2\sin(\theta/2)} \mathcal{T}_{\hat{\mathbf{x}}}\Psi(\theta,\phi)d\theta d\phi \\
&= \int_{\partial S^2} \frac{2\sin(\theta/2)\cos(\theta/2)}{2\sin(\theta/2)} \mathcal{T}_{\hat{\mathbf{x}}}\Psi(\theta,\phi)d\theta d\phi \\
&= \int_{\partial S^2} \cos(\theta/2)\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\theta,\phi)d\theta d\phi.
\end{aligned} \tag{3.25}
$$

The resulting integrand, $\cos(\theta/2)\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\theta,\phi)$, is non-singular provided $\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\theta,\phi)$ is smooth. Hence, we see that our rotation scheme can effectively remove the singularity from integral of the above type. Unfortunately, the integral we're concerned with is not quite of this type. As we saw earlier, the singular factor in our kernel is $1/\left|\mathbf{q}(\hat{\mathbf{x}}) - \mathbf{q}(\hat{\mathbf{y}})\right|$. While this may look similar to the harmonic kernel, it does not admit a nice representation in spherical coordinates (which was the crux of our singularity canceling method). We may, however, use an old trick to eliminate this problem. Consider

$$\int_{\partial S^2} \frac{1}{|\mathbf{q}(\hat{\mathbf{x}}) - \mathbf{q}(\hat{\mathbf{y}})|} \underbrace{(m_1(\mathbf{q}(\hat{\mathbf{x}}), \mathbf{q}(\hat{\mathbf{y}})) + m_2(\mathbf{q}(\hat{\mathbf{x}}), \mathbf{q}(\hat{\mathbf{y}})))}_{m(\hat{\mathbf{x}}, \hat{\mathbf{y}})} \; \Psi(\mathbf{q}(\hat{\mathbf{y}})) \; J(\hat{\mathbf{y}}) \; ds(\hat{\mathbf{y}})$$
$$= \int_{\partial S^2} \frac{1}{|\hat{\mathbf{x}} - \hat{\mathbf{y}}|} \frac{|\hat{\mathbf{x}} - \hat{\mathbf{y}}|}{|\mathbf{q}(\hat{\mathbf{x}}) - \mathbf{q}(\hat{\mathbf{y}})|} m(\hat{\mathbf{x}}, \hat{\mathbf{y}}) \Psi(\mathbf{q}(\hat{\mathbf{y}})) \; J(\hat{\mathbf{y}}) \; ds(\hat{\mathbf{y}})$$
$$= \int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|} \mathcal{T}_{\hat{\mathbf{x}}} \frac{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|}{|\mathbf{q}(\hat{\mathbf{n}}) - \mathbf{q}(\hat{\mathbf{z}})|} \mathcal{T}_{\hat{\mathbf{x}}} m(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}})) \; \mathcal{T}_{\hat{\mathbf{x}}} J(\hat{\mathbf{z}}) \; ds(\hat{\mathbf{z}}).$$

At this point, we may proceed by our earlier methodology to remove the singularity in $1/|\hat{\mathbf{n}} - \hat{\mathbf{z}}|$ through the imposition of spherical coordinates. We will have that the entire integrand is non-singular if

$$\mathcal{T}_{\hat{\mathbf{x}}} \frac{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|}{|\mathbf{q}(\hat{\mathbf{n}}) - \mathbf{q}(\hat{\mathbf{z}})|}, \; \mathcal{T}_{\hat{\mathbf{x}}} m(\hat{\mathbf{n}}, \hat{\mathbf{z}}), \; \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}})), \; \mathcal{T}_{\hat{\mathbf{x}}} J(\hat{\mathbf{z}}),$$

all admit non-singular representations in spherical coordinates. As we've already seen that $m(\hat{\mathbf{x}}, \hat{\mathbf{y}})$ and $J(\hat{\mathbf{y}})$ are smooth, they certainly admit smooth representations when rotated in spherical polars. Further, as Ψ is an arbitrary function, we may simply require that it be non-singular when rotated in spherical polar coordinates. Thus, it remains to show that $\mathcal{T}_{\hat{\mathbf{x}}}(|\hat{\mathbf{n}} - \hat{\mathbf{z}}|/|\mathbf{q}(\hat{\mathbf{n}}) - \mathbf{q}(\hat{\mathbf{z}})|)$ is non-singular. We begin this by proving a lemma.

Lemma 3.1. *A function of the form $p(x)/q(x)$ is in $\mathcal{C}^\infty(\mathbb{R})$ if $p, q \in \mathcal{C}^\infty(\mathbb{R})$ and q does not vanish for all $x \in \mathbb{R}$.*

Proof. The assumption that $p, q \in \mathcal{C}^\infty(\mathbb{R})$ allows us to write

$$\frac{d}{dx}\frac{p(x)}{q(x)} = \frac{q(x)p'(x) - p(x)q'(x)}{q^2(x)} = \frac{\tilde{p}(x)}{\tilde{q}(x)}.$$

We note that $\tilde{p}(x)$ inherits smoothness form p and q. Further, as q does not vanish, $\tilde{q}$ does not vanish. Thus, $\tilde{p}(x)/\tilde{q}(x)$ fits all of the criteria of the lemma and our result follows inductively. □

With this, we may prove a result from [9, pg.794]

Theorem 3.5. *The mapping $(\theta, \phi) \mapsto \mathcal{T}_{\hat{\boldsymbol{x}}} \frac{|\hat{\boldsymbol{n}} - \hat{\boldsymbol{z}}|}{|\boldsymbol{q}(\hat{\boldsymbol{n}}) - \boldsymbol{q}(\hat{\boldsymbol{z}})|}$ is $\mathcal{C}^\infty$ on ∂S^2.*

Proof. We begin by noting that this mapping provides a representation of $\hat{\mathbf{z}}$ in spherical coordinates of the form $\hat{\mathbf{z}} = \mathbf{p}(\theta, \phi) = [\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta)]^T$. We may also introduce the notation $\mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi) = \mathbf{q}(T_{\hat{\mathbf{x}}}^T \mathbf{p}(\theta, \phi))$ to make the proceeding work cleaner. Note that as $\mathbf{q}$ is assumed to be smooth, $\mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)$ inherits this property (as $T_{\hat{\mathbf{x}}}^T$ is a smooth map as well). Now,

$$\mathcal{T}_{\hat{\mathbf{x}}} \frac{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|}{|\mathbf{q}(\hat{\mathbf{n}}) - \mathbf{q}(\hat{\mathbf{z}})|} = \frac{\left|T_{\hat{\mathbf{x}}}^T \hat{\mathbf{n}} - T_{\hat{\mathbf{x}}}^T \mathbf{p}(\theta, \phi)\right|}{|\mathbf{q}(T_{\hat{\mathbf{x}}}^T \hat{\mathbf{n}}) - \mathbf{q}(T_{\hat{\mathbf{x}}}^T \mathbf{p}(\theta, \phi))|}$$
$$= \frac{\left|T_{\hat{\mathbf{x}}}^T\right| |\hat{\mathbf{n}} - \mathbf{p}(\theta, \phi)|}{|\mathbf{Q}(\hat{\mathbf{x}}, 0, 0) - \mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)|},$$

and by the result of (3.24), we may continue the above work as

$$\frac{\left|T_{\hat{\mathbf{x}}}^T\right| |\hat{\mathbf{n}} - \mathbf{p}(\theta, \phi)|}{|\mathbf{Q}(\hat{\mathbf{x}}, 0, 0) - \mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)|} = \frac{2\sin(\theta/2)}{|\mathbf{Q}(\hat{\mathbf{x}}, 0, 0) - \mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)|} = \Phi(\theta, \phi).$$

We now note that the smoothness of $\Phi(\theta, \phi)$ is equivalent to the smoothness of $\Phi^2(\theta, \phi)$. Now, consider

$$\Phi^2(\theta, \phi) = \frac{4sin^2(\theta/2)}{|\mathbf{Q}(\hat{\mathbf{x}}, 0, 0) - \mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)|^2} = \frac{(\sin(\theta/2)/(\theta/2))^2}{|\mathbf{Q}(\hat{\mathbf{x}}, 0, 0) - \mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)|^2 /\theta^2}.$$

Hence, as $(\sin(\theta/2)/(\theta/2))^2 = sinc^2(\theta/2)$, it is entire. Our result follows by Lemma (3.1) provided $|\mathbf{Q}(\hat{\mathbf{x}}, 0, 0) - \mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)|^2 /\theta^2$ is smooth with respect to θ (as we expect no problems from ϕ) and does not vanish for all values of θ. Thus, it remains to show that $|\mathbf{Q}(\hat{\mathbf{x}}, 0, 0) - \mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)|^2 /\theta^2$ is smooth and non-zero for all values of θ. As coordinates of the north pole of a sphere are independent of the value of ϕ, we may write $\mathbf{Q}(\hat{\mathbf{x}}, 0, 0) = \mathbf{Q}(\hat{\mathbf{x}}, 0, \phi)$. With this, we realize that $\mathbf{Q}(\hat{\mathbf{x}}, 0, \phi)$ is homotopically equivalent to $\mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi)$ under the map $\mathbf{Q}(\hat{\mathbf{x}}, (1-t)\theta, \phi)$ for $t \in [0, 1]$. Thus, we may write

$$\mathbf{Q}(\hat{\mathbf{x}}, 0, \phi) - \mathbf{Q}(\hat{\mathbf{x}}, \theta, \phi) = \int_0^1 \frac{d}{dt} \mathbf{Q}(\hat{\mathbf{x}}, (1-t)\theta, \phi) dt.$$

By the chain rule,

$$\int_0^1 \frac{d}{dt} \mathbf{Q}(\hat{\mathbf{x}}, (1-t)\theta, \phi) dt = -\theta \int_0^1 \frac{d}{d\theta} \mathbf{Q}(\hat{\mathbf{x}}, (1-t)\theta, \phi) dt.$$

Hence,

$$
\begin{aligned}
&|\mathbf{Q}(\hat{\mathbf{x}},0,\phi)-\mathbf{Q}(\hat{\mathbf{x}},\theta,\phi)|^2\\
&=\theta^2\int_0^1 \frac{d}{d\theta}\mathbf{Q}(\hat{\mathbf{x}},(1-t)\theta,\phi)^T dt\int_0^1 \frac{d}{d\theta}\mathbf{Q}(\hat{\mathbf{x}},(1-t)\theta,\phi)dt.
\end{aligned}
$$

With this, we see that the denominator of $\Phi^2(\theta,\phi)$ can be written as

$$
\int_0^1 \frac{d}{d\theta}\mathbf{Q}(\hat{\mathbf{x}},(1-t)\theta,\phi)^T dt\int_0^1 \frac{d}{d\theta}\mathbf{Q}(\hat{\mathbf{x}},(1-t)\theta,\phi)dt,
$$

which is clearly smooth and non-negative for $\theta \neq 0$ (as Q is smooth for all θ,ϕ). Thus, we need only show that $\frac{d}{d\theta}\mathbf{Q}(\hat{\mathbf{x}},(1-t)\theta,\phi)$ does not vanish at $\theta=0$. Which is equivalent to showing that $\frac{d}{d\theta}\mathbf{Q}(\hat{\mathbf{x}},\theta,\phi)$ does not vanish at $\theta=0$. From our definition of $\mathbf{Q}$,

$$
\frac{d}{d\theta}\mathbf{Q}(\hat{\mathbf{x}},\theta,\phi)=\frac{d}{d\theta}\mathbf{q}(T_{\hat{\mathbf{x}}}^T\mathbf{p}(\theta,\phi)).
$$

Now, as we've seen, there is a Jacobian matrix, $\mathbf{J}$ associated with the mapping $\mathbf{q}$. Thus, by [10, pg.308]

$$
\begin{aligned}
\frac{d}{d\theta}\mathbf{q}(T_{\hat{\mathbf{x}}}^T\mathbf{p}(\theta,\phi)) &= \mathbf{J}(T_{\hat{\mathbf{x}}}^T\mathbf{p}(\theta,\phi))T_{\hat{\mathbf{x}}}^T\frac{d}{d\theta}\mathbf{p}(\theta,\phi)\\
&= \mathbf{J}(T_{\hat{\mathbf{x}}}^T\mathbf{p}(\theta,\phi))T_{\hat{\mathbf{x}}}^T[\cos(\theta)\cos(\phi),\cos(\theta)\sin(\phi),-\sin(\theta)]^T,
\end{aligned}
$$

and hence,

$$
\begin{aligned}
\frac{d}{d\theta}\,\mathbf{Q}(\hat{\mathbf{x}},\theta,\phi)|_{\theta=0} &= \mathbf{J}(T_{\hat{\mathbf{x}}}^T\mathbf{p}(0,\phi))T_{\hat{\mathbf{x}}}^T[\cos(\phi),\sin(\phi),0]^T\\
&= \mathbf{J}(T_{\hat{\mathbf{x}}}^T\hat{\mathbf{n}})T_{\hat{\mathbf{x}}}^T[\cos(\phi),\sin(\phi),0]^T\\
&= \mathbf{J}(\hat{\mathbf{x}})T_{\hat{\mathbf{x}}}^T[\cos(\phi),\sin(\phi),0]^T.
\end{aligned}
$$

Now, as $\mathbf{q}$ is a smooth mapping, its Jacobian $\mathbf{J}$ is full rank. Further, as $[\cos(\phi),\sin(\phi),0]^T \neq \mathbf{0}$,

$$
\frac{d}{d\theta}\,\mathbf{Q}(\hat{\mathbf{x}},\theta,\phi)|_{\theta=0} = \mathbf{J}(\hat{\mathbf{x}})T_{\hat{\mathbf{x}}}^T[\cos(\phi),\sin(\phi),0]^T \neq \mathbf{0},
$$

our desired result follows. $\square$

With this result, we see that the only singular factor in

$$
\int_{\partial S^2}\frac{1}{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|}\mathcal{T}_{\hat{\mathbf{x}}}\frac{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|}{|\mathbf{q}(\hat{\mathbf{n}})-\mathbf{q}(\hat{\mathbf{z}})|}\mathcal{T}_{\hat{\mathbf{x}}}m(\hat{\mathbf{n}},\hat{\mathbf{z}})\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\hat{\mathbf{z}}))\ \mathcal{T}_{\hat{\mathbf{x}}}J(\hat{\mathbf{z}})\ ds(\hat{\mathbf{z}})
$$

is $|\hat{\mathbf{n}}-\hat{\mathbf{z}}|^{-1}$. Hence, for brevity, we will adopt the notation of [8]

$$\mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}}) = \mathcal{T}_{\hat{\mathbf{x}}} \frac{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|}{|\mathbf{q}(\hat{\mathbf{n}}) - \mathbf{q}(\hat{\mathbf{z}})|} \mathcal{T}_{\hat{\mathbf{x}}} m(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} J(\hat{\mathbf{z}}).$$

We note that, as all of its constituents are smooth, $\mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}})$ is smooth. Now, using the technique developed in (3.25), it is clear that the singularity in

$$\int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|} \mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}}))\ ds(\hat{\mathbf{z}})$$

can be removed.

As our goal is to create a discretized version of the Stokes operator, we must also consider how we will discretize the vector field on which it acts. Through our previous work, we have established that the continuous stokes operator can be written as

$$\mathcal{S}_\gamma [\Psi] (\mathbf{x}) = \int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|} \mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}}))\ ds(\hat{\mathbf{z}}),$$

wherein Ψ is the vector field on which $\mathcal{S}_\gamma$ acts. Using the projection operator defined earlier in (3.4), we will seek to approximate Ψ in the space of n^{th} degree vector-valued spherical polynomials $\mathbf{P}^n$ by

$$\Psi(\mathbf{x}) \approx \mathcal{L}_n \{\Psi(\mathbf{x})\}.$$

As we have seen, accuracy in spherical polynomial approximation is largely dependent on n. Thus, if we seek to approximate the factor

$$\mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}})),$$

in our integral representation of $\mathcal{S}$, we must seek a higher degree of accuracy than that sought in our approximation of just Ψ to establish a reasonable degree of accuracy in discretizing the action of $\mathcal{S}$ [8, pg.12]. Hence, we hyper interpolate the aforementioned factor to approximate it in $\mathbf{P}^{n'}$, where $n' > n$. For scalability of our discretization, we require that n' depend on n. For our implementation, we take $n' = 2n$. With this, we may write

$$\mathcal{S}_\gamma [\Psi] (\mathbf{x}) \approx \int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}} - \hat{\mathbf{z}}|} \mathcal{L}_{n'} \{\mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}}))\}\ ds(\hat{\mathbf{z}}),$$

where a bit of manipulation and the definition of $\mathcal{L}_{n'}$ gives us

$$
\begin{aligned}
&\int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|}\mathcal{L}_{n'}\left\{\mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}},\hat{\mathbf{z}})\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\hat{\mathbf{z}}))\right\}\ ds(\hat{\mathbf{z}}) \\
&= \int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|}\sum_{l=0}^{n'}\sum_{|m|\le l}\sum_{k=1}^{3}\left\langle \mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}},\hat{\mathbf{z}})\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\hat{\mathbf{z}})), Y^k_{l,m}(\hat{\mathbf{z}})\right\rangle\ Y^k_{l,m}(\hat{\mathbf{z}})ds(\hat{\mathbf{z}}) \\
&= \sum_{l=0}^{n'}\sum_{|m|\le l}\sum_{k=1}^{3}\left\langle \mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}},\hat{\mathbf{z}})\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\hat{\mathbf{z}})), Y^k_{l,m}(\hat{\mathbf{z}})\right\rangle\ \int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|} Y^k_{l,m}(\hat{\mathbf{z}})ds(\hat{\mathbf{z}}) \\
&= \sum_{l=0}^{n'}\sum_{|m|\le l}\sum_{k=1}^{3}\left\langle \mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}},\hat{\mathbf{z}})\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\hat{\mathbf{z}})), Y^k_{l,m}(\hat{\mathbf{z}})\right\rangle\ \mathbf{e}_k \int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|} Y_{l,m}(\hat{\mathbf{z}})ds(\hat{\mathbf{z}}).
\end{aligned} \tag{3.26}
$$

We may further simplify (3.26) with the following theorem

Theorem 3.6.

$$
\int_{\partial S^2} \frac{1}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|} Y_{l,m}(\hat{\boldsymbol{y}})ds(\hat{\boldsymbol{y}}) = \frac{4\pi}{2l+1} Y_{l,m}(\hat{\boldsymbol{x}}).
$$

Proof. We begin by recalling the result (A.4) from appendix (A). That is, given a harmonic function, u, defined on Ω and a function v defined on $\partial\Omega$, such that

$$
\begin{aligned}
\nabla^2 u &= 0 \qquad \textit{in}\ \ \Omega, \\
u &= v \qquad \textit{on}\ \ \partial\Omega,
\end{aligned}
$$

we have that

$$
\underbrace{\frac{1}{4\pi}\int_{\partial\Omega} \frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|}\left(\frac{\partial}{\partial\hat{\mathbf{n}}} v(\hat{\mathbf{y}})\right) ds(\hat{\mathbf{y}})}_{\mathcal{W}\left(\frac{\partial}{\partial\hat{\mathbf{n}}} v\right)} - \underbrace{\frac{1}{4\pi}\int_{\partial\Omega}\left(\frac{\partial}{\partial\hat{\mathbf{n}}}\frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|}\right) v(\hat{\mathbf{y}})ds(\hat{\mathbf{y}})}_{\mathcal{Z}(v)} = \frac{1}{2}v(\hat{\mathbf{x}}).
$$

Now, in our case, $\Omega = S^2$. Thus, at a point $\hat{\mathbf{y}}$ on ∂S^2, the normal vector is simply $\hat{\mathbf{y}}$. This allows us to compute

$$
\begin{aligned}
\frac{\partial}{\partial\hat{\mathbf{n}}}\frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|} &= \hat{\mathbf{n}}\cdot\frac{\hat{\mathbf{x}}-\hat{\mathbf{y}}}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|^3} = \frac{\hat{\mathbf{y}}\cdot(\hat{\mathbf{x}}-\hat{\mathbf{y}})}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|^3} \\
&= \frac{\hat{\mathbf{y}}\cdot\hat{\mathbf{x}}-|\hat{\mathbf{y}}|}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|^2\,|\hat{\mathbf{x}}-\hat{\mathbf{y}}|} = \frac{\hat{\mathbf{y}}\cdot\hat{\mathbf{x}}-|\hat{\mathbf{y}}|}{(|\hat{\mathbf{x}}|-2\hat{\mathbf{x}}\cdot\hat{\mathbf{y}}+|\hat{\mathbf{y}}|)\,|\hat{\mathbf{x}}-\hat{\mathbf{y}}|}.
\end{aligned}
$$

Now, as $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ exist on the unit ball, we know that $|\hat{\mathbf{y}}| = |\hat{\mathbf{x}}| = 1$. Hence,

$$
\frac{\partial}{\partial\hat{\mathbf{n}}}\frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|} = \frac{\hat{\mathbf{y}}\cdot\hat{\mathbf{x}}-|\hat{\mathbf{y}}|}{(|\hat{\mathbf{x}}|-2\hat{\mathbf{x}}\cdot\hat{\mathbf{y}}+|\hat{\mathbf{y}}|)\,|\hat{\mathbf{x}}-\hat{\mathbf{y}}|} = \frac{\hat{\mathbf{y}}\cdot\hat{\mathbf{x}}-1}{2(1-\hat{\mathbf{x}}\cdot\hat{\mathbf{y}})\,|\hat{\mathbf{x}}-\hat{\mathbf{y}}|} = -\frac{1}{2}\frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|}.
$$

With this, and (A.4) we may write that for some function v defined on the surface of a sphere,

$$
\begin{aligned}
&\mathcal{W}\left(\frac{\partial}{\partial \hat{\mathbf{n}}} v\right) - \mathcal{Z}(v) \\
&= \frac{1}{4\pi}\int_{\partial S^2} \frac{1}{|\hat{\mathbf{x}} - \hat{\mathbf{y}}|}\left(\frac{\partial}{\partial \hat{\mathbf{n}}} v(\hat{\mathbf{y}})\right) ds(\hat{\mathbf{y}}) - \frac{1}{4\pi}\int_{\partial S^2}\left(\frac{\partial}{\partial \hat{\mathbf{n}}}\frac{1}{|\hat{\mathbf{x}} - \hat{\mathbf{y}}|}\right) v(\hat{\mathbf{y}}) ds(\hat{\mathbf{y}}) \\
&= \frac{1}{4\pi}\int_{\partial S^2} \frac{1}{|\hat{\mathbf{x}} - \hat{\mathbf{y}}|}\left(\frac{\partial}{\partial \hat{\mathbf{n}}} v(\hat{\mathbf{y}})\right) ds(\hat{\mathbf{y}}) + \frac{1}{2}\frac{1}{4\pi}\int_{\partial S^2} \frac{1}{|\hat{\mathbf{x}} - \hat{\mathbf{y}}|} v(\hat{\mathbf{y}}) ds(\hat{\mathbf{y}}) \\
&= \mathcal{W}\left(\frac{\partial}{\partial \hat{\mathbf{n}}} v\right) + \frac{1}{2}\mathcal{W}(v) = \frac{1}{2} v(\hat{\mathbf{x}}).
\end{aligned} \tag{3.27}
$$

Now, we note that $u(\hat{\mathbf{x}}) = r^l Y_{l,m}(\theta, \phi)$ solves Laplace's equation in a sphere with $u = Y_{l,m}(\theta, \phi)$ on ∂S^2. We now compute

$$
\begin{aligned}
&\frac{\partial}{\partial \hat{\mathbf{n}}} u = \nabla u \cdot \hat{\mathbf{n}} \\
&= \left(\frac{\partial}{\partial r} u \mathbf{e}_r + \frac{1}{r}\frac{\partial}{\partial \theta} u \mathbf{e}_\theta + \frac{1}{r\sin(\theta)}\frac{\partial}{\partial \phi} u \mathbf{e}_\phi\right) \cdot \mathbf{e}_r \\
&= \left(\frac{\partial}{\partial r} u(\mathbf{e}_r \cdot \mathbf{e}_r) + \frac{1}{r}\frac{\partial}{\partial \theta} u(\mathbf{e}_\theta \cdot \mathbf{e}_r) + \frac{1}{r\sin(\theta)}\frac{\partial}{\partial \phi} u(\mathbf{e}_\phi \cdot \mathbf{e}_r)\right) \\
&= \frac{\partial}{\partial r} u = l r^{l-1} Y_{l,m}(\theta, \phi).
\end{aligned}
$$

Thus, on the boundary of a sphere,

$$
\frac{\partial}{\partial \hat{\mathbf{n}}} u = \frac{\partial}{\partial \hat{\mathbf{n}}} Y_{l,m}(\theta, \phi) = l Y_{l,m}(\theta, \phi).
$$

Using this and (3.27), we have

$$
\begin{aligned}
&\mathcal{W}\left(\frac{\partial}{\partial \hat{\mathbf{n}}} v\right) + \frac{1}{2}\mathcal{W}\left(v\right) = \frac{1}{2} v(\hat{\mathbf{x}}) \Rightarrow \\
&\mathcal{W}\left(\frac{\partial}{\partial \hat{\mathbf{n}}} Y_{l,m}\right) + \frac{1}{2}\mathcal{W}\left(Y_{l,m}\right) = \frac{1}{2} Y_{l,m} \Rightarrow \\
&\mathcal{W}\left(lY_{l,m}\right) + \frac{1}{2}\mathcal{W}\left(Y_{l,m}\right) = \frac{1}{2} Y_{l,m} \Rightarrow \\
&l\mathcal{W}\left(Y_{l,m}\right) + \frac{1}{2}\mathcal{W}\left(Y_{l,m}\right) = \frac{1}{2} Y_{l,m} \Rightarrow \\
&\frac{2l+1}{2}\mathcal{W}\left(Y_{l,m}\right) = \frac{1}{2} Y_{l,m} \Rightarrow \\
&\frac{1}{4\pi}\int_{\partial S^2} \frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|} Y_{l,m}(\hat{\mathbf{y}}) ds(\hat{\mathbf{y}}) = \frac{1}{2l+1} Y_{l,m}(\hat{\mathbf{x}}) \Rightarrow \\
&\int_{\partial S^2} \frac{1}{|\hat{\mathbf{x}}-\hat{\mathbf{y}}|} Y_{l,m}(\hat{\mathbf{y}}) ds(\hat{\mathbf{y}}) = \frac{4\pi}{2l+1} Y_{l,m}(\hat{\mathbf{x}}).
\end{aligned}
$$

□

Now, Using this result in (3.26), we obtain

$$
\begin{aligned}
&\sum_{l=0}^{n'} \sum_{|m|\le l} \sum_{k=1}^{3} \left\langle \mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}})), Y_{l,m}^k(\hat{\mathbf{z}}) \right\rangle \ \mathbf{e}_k \int_{\partial S^2} \frac{1}{|\hat{\mathbf{n}}-\hat{\mathbf{z}}|} Y_{l,m}(\hat{\mathbf{z}}) ds(\hat{\mathbf{z}}) \\
&= \sum_{l=0}^{n'} \sum_{|m|\le l} \sum_{k=1}^{3} \left\langle \mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}})), Y_{l,m}^k(\hat{\mathbf{z}}) \right\rangle \ \mathbf{e}_k \frac{4\pi}{2l+1} Y_{l,m}(\hat{\mathbf{n}}) \\
&= \sum_{l=0}^{n'} \sum_{|m|\le l} \sum_{k=1}^{3} \left\langle \mathcal{T}_{\hat{\mathbf{x}}} M(\hat{\mathbf{n}}, \hat{\mathbf{z}}) \mathcal{T}_{\hat{\mathbf{x}}} \Psi(\mathbf{q}(\hat{\mathbf{z}})), Y_{l,m}^k(\hat{\mathbf{z}}) \right\rangle \ \frac{4\pi}{2l+1} Y_{l,m}^k(\hat{\mathbf{n}}). \qquad (3.28)
\end{aligned}
$$

Approximating the inner product in (3.28), using the quadrature rule (3.13) and (3.14) described in section (3.2), we may write

$$
\begin{aligned}
&\sum_{l=0}^{n'}\sum_{|m|\leq l}\sum_{k=1}^{3}\left\langle \mathcal{T}_{\hat{\mathbf{x}}}M(\hat{\mathbf{n}},\hat{\mathbf{z}})\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\hat{\mathbf{z}})), Y^k_{l,m}(\hat{\mathbf{z}})\right\rangle \ \frac{4\pi}{2l+1}Y^k_{l,m}(\hat{\mathbf{n}})\\
&=\sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\sum_{l=0}^{n'}\sum_{|m|\leq l}\sum_{k=1}^{3}\\
&\qquad\left(\overline{Y^k_{l,m}(\mathbf{p}(\theta_{s'},\phi_{r'}))}^T\mathcal{T}_{\hat{\mathbf{x}}}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\mathbf{p}(\theta_{s'},\phi_{r'})))\right)\frac{4\pi}{2l+1}Y^k_{l,m}(\hat{\mathbf{n}})\\
&=\sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\underbrace{\sum_{k=1}^{3}\mathbf{e}_k\mathbf{e}_k^T}_{=\ I}\\
&\qquad(\mathcal{T}_{\hat{\mathbf{x}}}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\mathbf{p}(\theta_{s'},\phi_{r'}))))\sum_{l=0}^{n'}\sum_{|m|\leq l}\frac{4\pi}{2l+1}\overline{Y_{l,m}(\mathbf{p}(\theta_{s'},\phi_{r'}))}Y_{l,m}(\hat{\mathbf{n}})\\
&=\sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\mathcal{T}_{\hat{\mathbf{x}}}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\mathbf{p}(\theta_{s'},\phi_{r'})))\\
&\qquad\underbrace{\sum_{l=0}^{n'}\sum_{|m|\leq l}\frac{4\pi}{2l+1}\overline{Y_{l,m}(\mathbf{p}(\theta_{s'},\phi_{r'}))}Y_{l,m}(\hat{\mathbf{n}})}_{\alpha^{n'}_{s'}}.
\end{aligned}
$$

By the addition theorem for spherical harmonics (Theorem 3.4), we have that

$$
\begin{aligned}
\alpha^{n'}_{s'} &= \sum_{l=0}^{n'}\sum_{|m|\leq l}\frac{4\pi}{2l+1}\overline{Y_{l,m}(\mathbf{p}(\theta_{s'},\phi_{r'}))}Y_{l,m}(\hat{\mathbf{n}})\\
&=\sum_{l=0}^{n'}\mathcal{P}_l(\hat{\mathbf{n}}\cdot\mathbf{p}(\theta_{s'},\phi_{r'})) = \sum_{l=0}^{n'}\mathcal{P}_l\cos(\theta_{s'}).
\end{aligned}
$$

Hence,

$$
\mathcal{S}_\gamma\left[\Psi\right](\mathbf{x}) \approx \sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\alpha^{n'}_{s'}\mathcal{T}_{\hat{\mathbf{x}}}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathcal{T}_{\hat{\mathbf{x}}}\Psi(\mathbf{q}(\mathbf{p}(\theta_{s'},\phi_{r'}))).
$$

At this point, we seek a suitable approximation of Ψ in the space of n^{th} degree spherical polynomials. Thus, we write

$$
\sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\alpha^{n'}_{s'}\mathcal{T}_{\hat{\mathbf{x}}}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathcal{T}_{\hat{\mathbf{x}}}\mathcal{L}_n\left\{\Psi(\mathbf{q}(\mathbf{p}(\theta_{s'},\phi_{r'})))\right\}.
$$

If we assume that $\mathcal{L}_n\left\{\Psi(\mathbf{q}(\mathbf{p}(\theta_{s'},\phi_{r'})))\right\}$ has a representation of the form

$$\mathcal{L}_n\left\{\Psi(\mathbf{q}(\mathbf{p}(\theta_{s'},\phi_{r'})))\right\} = \sum_{l=0}^{n}\sum_{|m|\le l}\sum_{k=1}^{3}\omega_{l,m}^{k}Y_{l,m}^{k}(\theta_{s'},\phi_{r'}),$$

we may write

$$\mathcal{S}_\gamma\left[\Psi\right](\mathbf{x}) \approx \sum_{l=0}^{n}\sum_{|m|\le l}\sum_{k=1}^{3}\omega_{l,m}^{k}\sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\alpha_{s'}^{n'}\mathcal{T}_{\hat{\mathbf{x}}}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathcal{T}_{\hat{\mathbf{x}}}Y_{l,m}^{k}(\theta_{s'},\phi_{r'}).$$

We may now write this as a linear system by forming an inner product of $\mathcal{S}$ with $Y_{l',m'}^{k'}(\hat{\mathbf{x}})$, giving

$$\mathcal{S}_\gamma\left[\Psi\right](\mathbf{x}) \approx \mathbf{M}\boldsymbol{\omega},$$

where $\boldsymbol{\omega}$ is a vector of the coefficients found by taking a truncated euclidean vector harmonic expansion of Ψ, and $\mathbf{M}$ is a matrix whose entries are given by

$$\begin{aligned}\mathbf{M}_{l'm'k',lmk} &= \left\langle \sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\alpha_{s'}^{n'}\mathcal{T}_{\hat{\mathbf{x}}}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathcal{T}_{\hat{\mathbf{x}}}Y_{l,m}^{k}(\theta_{s'},\phi_{r'}), Y_{l',m'}^{k'}(\hat{\mathbf{x}})\right\rangle_n \\ &= \sum_{r=0}^{2n+1}\sum_{s=1}^{n+1}\mu_r\nu_s\sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\alpha_{s'}^{n'} \\ &\qquad \overline{Y_{l',m'}^{k'}}^{T}(\theta_s,\phi_r)\mathcal{T}_{\mathbf{p}(\theta_s,\phi_r)}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathcal{T}_{\mathbf{p}(\theta_s,\phi_r)}Y_{l,m}^{k}(\theta_{s'},\phi_{r'}) \\ &= \sum_{r=0}^{2n+1}\sum_{s=1}^{n+1}\mu_r\nu_s\sum_{r'=0}^{2n'+1}\sum_{s'=1}^{n'+1}\xi_{r'}\eta_{s'}\alpha_{s'}^{n'} \\ &\qquad \overline{Y_{l',m'}}(\theta_s,\phi_r)\mathbf{e}_{k'}^{T}\mathcal{T}_{\mathbf{p}(\theta_s,\phi_r)}M(\hat{\mathbf{n}},\mathbf{p}(\theta_{s'},\phi_{r'}))\mathbf{e}_{k}\mathcal{T}_{\mathbf{p}(\theta_s,\phi_r)}Y_{l,m}(\theta_{s'},\phi_{r'}).\end{aligned}$$

We know from section 3.1, that the factor $\mathcal{T}_{\mathbf{p}(\theta_s,\phi_r)}Y_{l,m}(\theta_{s'},\phi_{r'})$ can be represented as a linear combination of spherical harmonics of the same degree. Following the notation of [8] and using (3.9), we give a computationally efficient implementation of this linear combination as

$$\mathcal{T}_{\mathbf{p}(\theta_s,\phi_r)}Y_{l,m}(\theta_{s'},\phi_{r'}) = \sum_{|\tilde{m}|\le l}F_{sl\tilde{m}m}e^{i(m-\tilde{m})\phi_r}Y_{l,\tilde{m}}(\theta_{s'},\phi_{r'}),$$

where

$$F_{sl\tilde{m}m} = e^{i(m-\tilde{m})\frac{\pi}{2}}\sum_{|j|\le l}d_{\tilde{m},j}^{l}(\frac{\pi}{2})d_{m,j}^{l}(\frac{\pi}{2})e^{ij\theta_s}.$$

Thus, introducing the notation $\mathbf{x}_{rs} = \mathbf{p}(\theta_s,\phi_r)$ and $\mathbf{y}_{rs}^{r's'} = T_{\mathbf{p}(\theta_s,\phi_r)}^{T}\mathbf{p}(\theta_{s'},\phi_{r'})$, we may write

$$\mathbf{M}_{l'm'k',lmk} =$$

$$= \sum_{r=0}^{2n+1} \sum_{s=1}^{n+1} \mu_r \nu_s \sum_{r'=0}^{2n'+1} \sum_{s'=1}^{n'+1} \xi_{r'} \eta_{s'} \alpha_{s'}^{n'} \overline{Y_{l',m'}}(\theta_s, \phi_r) \mathbf{e}_{k'}^T M(\mathbf{x}_{rs}, \mathbf{y}_{rs}^{r's'}) \mathbf{e}_k$$

$$\sum_{|\tilde{m}| \leq l} F_{sl\tilde{m}m} e^{i(m-\tilde{m})\phi_r} Y_{l,\tilde{m}}(\theta_{s'}, \phi_{r'}). \quad (3.29)$$

3.4 An Explicit Time–Stepping Scheme

In the previous section, we outlined a method to discretize the action of the Stokes operator $\mathcal{S}$ on a vector field $\mathbf{F}$ as a matrix vector system

$$\mathcal{S}[\mathbf{F}] \approx \mathbf{M}\boldsymbol{\omega},$$

where $\boldsymbol{\omega}$ is an $3(n+1)^2 \times 1$ vector of the coefficients given by taking $\mathcal{L}_n(\mathbf{F})$. With this, we look back at the algorithm, (2.60) and (2.61) ,outlined in section 2.2, i.e.

$$Step\ 1:$$

solve

$$div_\gamma \mathcal{S}\left[\mathbf{f}_\sigma\right](\mathbf{x}) = -div_\gamma\left(\mathbf{u}^\infty(\mathbf{x}) - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x})\right)$$

for $\mathbf{f}_\sigma$.

$$Step\ 2:$$

use $\mathbf{f}_\sigma$ in

$$\mathcal{S}\left[\mathbf{f}_\sigma - \mathbf{f}_b\right](\mathbf{x}) + \mathbf{u}^\infty(\mathbf{x}) = \frac{\partial}{\partial t}\mathbf{x}$$

We now seek a fully discrete version this algorithm. We begin by elaborating on $Step 1$.

$$Modified\ Step\ 1:$$

Take a fixed time step Δt, so that at some time $n\Delta t$ the points on the surface of our vesicle are given by $\mathbf{x}^n(\theta, \phi)$. We may take $\mathbf{x}^n$ on a grid of the quadrature nodes described in section 3.2. Thus, we use $\mathbf{x}^n(\theta_i, \phi_j)$ as our discretized version of $\mathbf{x}^n$. We approximate $\mathbf{x}^n(\theta_i, \phi_j)$ using $\mathcal{L}_L(\mathbf{x}^n)$ giving

$$\mathbf{x}^n(\theta_i, \phi_j) \approx \sum_{l=0}^{L} \sum_{|m| \leq l} \sum_{k=1}^{3} c_{l,m}^k Y_{l,m}^k(\theta_i, \phi_j),$$

where

$$c_{l,m}^k = \sum_i \sum_j \xi_j \eta_i (\mathbf{x}^n(\theta_i, \phi_j) \cdot \overline{Y_{lm}^k}(\theta_i, \phi_j)).$$

Using this approximation of $\mathbf{x}^n$ in the space of L^{th} degree vector spherical harmonics, we may make use of our formulas for the derivatives of spherical harmonics, (3.5) to approximate partial derivatives of $\mathbf{x}^n$ as

$$D^\alpha \mathbf{x}^n(\theta_i, \phi_j) \approx \sum_{l=0}^{L} \sum_{|m|\leq l} \sum_{k=1}^{3} c_{l,m}^k \left(D^\alpha Y_{l,m}^k(\theta_i, \phi_j) \right),$$

where α is a multi-index. As we now have a suitable means of discretizing derivatives of $\mathbf{x}^n$, we may use these to find suitable discretizations of the first and second fundamental forms defined in the beginning of section 2.2 in (2.26) and (2.28). With these, it is straight forward to find a discretization of $\mathbf{f}_b$ as

$$\mathbf{f}_b(\theta_i, \phi_j) = \left[\kappa_b \left(2H(H^2 - K) + \nabla_\gamma^2 H\right) \mathbf{n}\right](\theta_i, \phi_j),$$

using the definitions (2.29), (2.27) and, (2.54). Hence, with discretization of $\mathbf{f}_b$ we may find an approximation of $\mathbf{f}_b$ in the space of L^{th} degree vector spherical harmonics, i.e

$$\mathbf{f}_b(\theta_i, \phi_j) \approx \sum_{l=0}^{L} \sum_{|m|\leq l} \sum_{k=1}^{3} a_{l,m}^k Y_{l,m}^k(\theta_i, \phi_j),$$

where

$$a_{l,m}^k = \sum_i \sum_j \xi_j \eta_i (\mathbf{f}_b(\theta_i, \phi_j) \cdot \overline{Y_{lm}^k}(\theta_i, \phi_j)).$$

We now use the method outlined in section (3.3) to find and save the matrix $\mathbf{M}$ representing $\mathcal{S}$. We note that the computation of $\mathbf{M}$ requires the use of $\mathbf{x}^n$ on our current grid (θ_i, ϕ_j) and a larger, hyper interpolation grid, $(\theta_{r'}, \phi_{s'})$. We may find $\mathbf{x}^n(\theta_{r'}, \phi_{s'})$ by using

$$\mathbf{x}^n(\theta_{r'}, \phi_{s'}) \approx \sum_{l=0}^{L} \sum_{|m|\leq l} \sum_{k=1}^{3} c_{l,m}^k Y_{l,m}^k(\theta_{r'}, \phi_{s'}).$$

Now, with $\mathbf{M}$ computed, we may write

$$\mathcal{L}\left\{\mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x}^n)\right\}_L \approx \mathbf{Ma}.$$

Now, given type of flow which we are concerned with, we may define a suitable discretization of $\mathbf{u}^\infty(\mathbf{x}^n)$. This will be discussed in some detail later on in this section. For now, let us assume a discretization of $\mathbf{u}^\infty$ and we write

$$\mathbf{u}^{\infty}(\theta_i,\phi_j) \approx \sum_{l=0}^{L}\sum_{|m|\le l}\sum_{k=1}^{3} b_{l,m}^{k} Y_{l,m}^{k}(\theta_i,\phi_j),$$

where the coefficients $b_{l,m}^{k}$ are computed similarly to $a_{l,m}^{k}$ and $c_{l,m}^{k}$. Hence,

$$\mathcal{L}\left\{\mathbf{u}^{\infty}(\mathbf{x}^n) - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x}^n)\right\}_L \approx \mathbf{b} - \mathbf{Ma},$$

and

$$\mathbf{u}^{\infty}(\mathbf{x}^n) - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x}^n) \approx \sum_{l=0}^{L}\sum_{|m|\le l}\sum_{k=1}^{3}[\mathbf{b} - \mathbf{Ma}]_{lm}^{k} Y_{l,m}^{k}(\theta_i,\phi_j).$$

With this, we have that

$$-div_{\gamma}\left(\mathbf{u}^{\infty}(\mathbf{x}^n) - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x}^n)\right) \approx \sum_{l=0}^{L}\sum_{|m|\le l}\sum_{k=1}^{3} -[\mathbf{b} - \mathbf{Ma}]_{lm}^{k}\, div_{\gamma}(Y_{l,m}^{k}(\theta_i,\phi_j)),$$

where $div_{\gamma}(Y_{l,m}^{k}(\theta_i,\phi_j))$ is straightforward to compute using our definitions for the derivatives of spherical harmonics and the surface divergence, (3.5) and (2.54). Hence, we have a discretization for the right hand side of the equation in *Step* 1. As it is now a known quantity, for brevity, we will adopt a new notation for the right hand side

$$f(\theta_i,\phi_j) = \sum_{l=0}^{L}\sum_{|m|\le l}\sum_{k=1}^{3} -[\mathbf{b} - \mathbf{Ma}]_{lm}^{k}\, div_{\gamma}(Y_{l,m}^{k}(\theta_i,\phi_j)).$$

Now, we look at the left hand side of the equation in *Step* 1,

$$div_{\gamma}\mathcal{S}\left[\mathbf{f}_{\sigma}\right](\mathbf{x}^n).$$

The aim of *Step* 1 is to solve for $\mathbf{f}_{\sigma}$. Now, we approximate $\mathbf{f}_{\sigma}$ in the space of L^{th} degree vector spherical harmonics. Proceeding to solve the equation in *Step* 1 with this assumption, using the Galerkin method, we will have to solve a $3(L+1)^2 \times 3(L+1)^2$ system. We may, however, reduce the dimensionality of this system by a factor of 9 by using the from we derived for $\mathbf{f}_{\sigma}$, (2.58), in section 2.2

$$\mathbf{f}_{\sigma} = \sigma\nabla_{\gamma}^{2}\mathbf{x}^n + \nabla_{\gamma}\sigma.$$

If we assume that σ has an approximation in the space of L^{th} degree scalar spherical harmonics,

$$\sigma \approx \sum_{l=0}^{L}\sum_{|m|\le l} s_{lm} Y_{lm},$$

we may write

$$\mathbf{f}_\sigma \approx \sum_{l=0}^{L} \sum_{|m|\le l} s_{lm} \left(\nabla_\gamma^2 \mathbf{x}^n Y_{lm} + \nabla_\gamma Y_{lm}\right).$$

Further, we make the approximation

$$\nabla_\gamma^2 \mathbf{x}^n Y_{lm} + \nabla_\gamma Y_{lm} \approx \sum_{l=0}^{L} \sum_{|m|\le l} \sum_{k=1}^{3} d_{lm}^k Y_{l,m}^k.$$

With this,

$$\mathcal{L}\left\{\mathcal{S}\left[\mathbf{f}_\sigma\right](\mathbf{x}^n)\right\} \approx \sum_{l=0}^{L} \sum_{|m|\le l} s_{lm} \mathcal{L}\left\{\mathcal{S}\left[\nabla_\gamma^2 \mathbf{x}^n Y_{lm} + \nabla_\gamma Y_{lm}\right]\right\} \approx \sum_{l=0}^{L} \sum_{|m|\le l} s_{lm} (\mathbf{Md}),$$

and thus,

$$div_\gamma \mathcal{S}\left[\mathbf{f}_\sigma\right](\mathbf{x}^n) \approx \sum_{l=0}^{L} \sum_{|m|\le l} s_{lm}\, div_\gamma \left(\sum_{l'=0}^{L} \sum_{|m'|\le l'} \sum_{k'=1}^{3} [\mathbf{Md}]_{l'm'}^{k'} Y_{l',m'}^{k'} \right).$$

Hence, we may rewrite *Step* 1 as: solve

$$\sum_{l=0}^{L} \sum_{|m|\le l} s_{lm} \sum_{l'=0}^{L} \sum_{|m'|\le l'} \sum_{k'=1}^{3} [\mathbf{Md}]_{l'm'}^{k'}\, div_\gamma \left(Y_{l',m'}^{k'}\right) = f$$

for $\mathbf{s}$. We may do this through the Galerkin scheme by forming inner products on both sides with $Y_{\tilde{l}\tilde{m}}$ giving

$$\sum_{l=0}^{L} \sum_{|m|\le l} s_{lm} \sum_{l'=0}^{L} \sum_{|m'|\le l'} \sum_{k'=1}^{3} [\mathbf{Md}]_{l'm'}^{k'} \left\langle div_\gamma \left(Y_{l',m'}^{k'}\right), Y_{\tilde{l}\tilde{m}} \right\rangle = \left\langle f, Y_{\tilde{l}\tilde{m}} \right\rangle.$$

Where, for instance,

$$\left\langle f, Y_{\tilde{l}\tilde{m}} \right\rangle = \sum_i \sum_j \xi_j \eta_i f(\theta_i, \phi_j) \overline{Y_{\tilde{l}\tilde{m}}}(\theta_i, \phi_j).$$

Thus, we arrive at the $(L+1)^2 \times (L+1)^2$ linear system

$$\mathbf{Ws} = \mathbf{f}, \tag{3.30}$$

where

$$[\mathbf{W}]_{\tilde{l}\tilde{m},lm} = \sum_{l'=0}^{L} \sum_{|m'|\le l'} \sum_{k'=1}^{3} [\mathbf{Md}]_{l'm'}^{k'} \left\langle div_\gamma \left(Y_{l',m'}^{k'}\right), Y_{\tilde{l}\tilde{m}} \right\rangle, \qquad [\mathbf{f}]_{\tilde{l}\tilde{m}} = \left\langle f, Y_{\tilde{l}\tilde{m}} \right\rangle.$$

Using, $\mathbf{s}$, we may find $\mathbf{f}_\sigma$ and *Step* 1 is complete. Now, to solve (3.30), we use a direct solver. It should be noted that reference [21] uses a preconditioned GMRES method. As their preconditioner, reference [21], considers the inverse of a diagonal matrix of the eigenvalues of the operator $\mathcal{N}$ (discussed later in this Chapter in Theorem 3.8) say N^{-1}. Using this, they take their preconditioner, P as

$$P = \mathcal{F}^{-1} N^{-1} \mathcal{F}$$

where $\mathcal{F}$ is the discrete Fourier transform matrix.

We now elaborate a bit on *Step* 2 of our algorithm.

$$Modified\ Step\ 2:$$

Currently, *Step* 2 reads: use

$$\mathcal{S}\left[\mathbf{f}_\sigma - \mathbf{f}_b\right](\mathbf{x}) + \mathbf{u}^\infty(\mathbf{x}) = \frac{\partial}{\partial t}\mathbf{x}$$

to update the position. To approach this, we use a forward difference approximation for $\frac{\partial}{\partial t}\mathbf{x}$, giving

$$\mathcal{S}\left[\mathbf{f}_\sigma - \mathbf{f}_b\right](\mathbf{x}^n) + \mathbf{u}^\infty(\mathbf{x}) = \frac{1}{\Delta t}\left(\mathbf{x}^{n+1} - \mathbf{x}^n\right).$$

As we now have a means to compute $\mathbf{f}_\sigma$ and $\mathbf{f}_b$, we may approximate $\mathbf{f}_\sigma - \mathbf{f}_b$ in the space of L^{th} degree vector spherical harmonics as

$$\mathbf{f}_\sigma - \mathbf{f}_b \approx \sum_{l=0}^{L} \sum_{|m|\le l} \sum_{k=1}^{3} p_{l,m}^k Y_{l,m}^k,$$

and hence,

$$\mathcal{L}\left\{\mathcal{S}\left[\mathbf{f}_\sigma - \mathbf{f}_b\right](\mathbf{x}^n)\right\}_L \approx \mathbf{M}\mathbf{p}.$$

Thus, adopting the notation

$$S(\theta_i, \phi_j) = \sum_{l=0}^{L} \sum_{|m|\le l} \sum_{k=1}^{3} [\mathbf{M}\mathbf{p}]_{l,m}^k Y_{l,m}^k(\theta_i, \phi_j),$$

we may rewrite the equation in *Step* 2 as

$$S(\theta_i, \phi_j) + \mathbf{u}^\infty(\mathbf{x}^n(\theta_i, \phi_j)) = \frac{1}{\Delta t}\left(\mathbf{x}^{n+1}(\theta_i, \phi_j) - \mathbf{x}^n(\theta_i, \phi_j)\right).$$

Thus, we solve for $\mathbf{x}^{n+1}$ as

$$\mathbf{x}^{n+1}(\theta_i, \phi_j) = \Delta t\left[S(\theta_i, \phi_j) + \mathbf{u}^\infty(\mathbf{x}^n(\theta_i, \phi_j))\right] + \mathbf{x}^n(\theta_i, \phi_j).$$

Now to address a few concerns which may have arisen in the exposition of our algorithm. Firstly, we used a forward in time scheme to discretize $\frac{\partial}{\partial t}\mathbf{x}$ in *Step* 2. Hence, we expect there to be some stability conditions on Δt. Indeed there are. Reference [21] conjectures that the stability conditions on Δt are related to the degree of the spherical harmonic projection by $\Delta t \sim \mathcal{O}(L^{-3})$. To make sense of this, we must look at the conditioning of our problem. We begin by defining

$$\begin{aligned} \mathbf{V}^l_m &= \nabla_\gamma Y_{lm} - (l+1)Y_{lm}\mathbf{n}, \\ \mathbf{W}^l_m &= \nabla_\gamma Y_{lm} - lY_{lm}\mathbf{n}. \end{aligned} \tag{3.31}$$

These vector fields are important to us as they are eigenfunctions of $\mathcal{S}[\cdot]$.

Theorem 3.7. *For* $\mu = 1$,

$$\begin{aligned} \mathcal{S}[\boldsymbol{V}^l_m](S^2) &= \frac{l}{(2l+1)(2l+3)}\boldsymbol{V}^l_m, \\ \mathcal{S}[\boldsymbol{W}^l_m](S^2) &= \frac{l+1}{(2l-1)(2l+1)}\boldsymbol{W}^l_m. \end{aligned}$$

A proof of this result is given in [21, App. A]. We have chosen not to include it here as it is lengthy and a bit cumbersome. Note that the $\mu = 1$ criteria is only to allow for a nice representation of this equality. A similar result holds when $\mu \neq 1$. Now, looking at the left hand side of *Step* 1, we see that we must compute $div_\gamma \mathcal{S}[\sigma \nabla^2_\gamma \mathbf{x}^n + \nabla_\gamma \sigma](\mathbf{x})$. As σ is the unknown, we may think of this as one linear operator and define

$$\mathcal{N}_{\mathbf{x}}(\sigma) = div_\gamma \mathcal{S}[\sigma \nabla^2_\gamma \mathbf{x} + \nabla_\gamma \sigma](\mathbf{x}).$$

We now give a result concerning the spectrum of this operator.

Theorem 3.8. *When* $\mu = 1$,

$$\mathcal{N}_{S^2}(Y_{lm}) = -\frac{l(l+1)(2l^2+2l-1)}{(2l-1)(2l+1)(2l+3)}Y_{lm}.$$

Proof. We begin by noting that

$$Y_{lm}\nabla^2_{S^2}\hat{\mathbf{x}} + \nabla_{S^2}Y_{lm} = \frac{(l+2)\mathbf{V}^l_m + (l-1)\mathbf{W}^l_m}{2l+1}.$$

Hence,

$$\mathcal{S}[Y_{lm}\nabla^2_{S^2}\hat{\mathbf{x}} + \nabla_{S^2}Y_{lm}](S^2) = \frac{l+2}{2l+1}\mathcal{S}[\mathbf{V}^l_m](S^2) + \frac{l-1}{2l+1}[\mathbf{W}^l_m](S^2),$$

and by Theorem 3.7,

$$= \frac{l+2}{2l+1}\frac{l}{(2l+1)(2l+3)}\mathbf{V}^l_m + \frac{l-1}{2l+1}\frac{l+1}{(2l-1)(2l+1)}\mathbf{W}^l_m$$
$$= \frac{l(l+2)}{(2l+1)^2(2l+3)}\mathbf{V}^l_m + \frac{(l-1)(l+1)}{(2l+1)^2(2l-1)}\mathbf{W}^l_m.$$

now,

$$div_{S^2}\mathbf{V}^l_m = div_{S^2}\nabla_\gamma Y_{lm} - (l+1)\,div_{S^2}Y_{lm}\mathbf{n} = \nabla^2_{S^2}Y_{lm} - (l+1)\,div_{S^2}Y_{lm}\mathbf{x},$$

by construction, we have that $\nabla^2_{S^2}Y_{lm} = -l(l+1)Y_{lm}$. Hence,

$$= -l(l+1)Y_{lm} - (l+1)\,div_{S^2}Y_{lm}\mathbf{x} = -l(l+1)Y_{lm} - (l+1)2Y_{lm} = -(l+1)(l+2)Y_{lm}.$$

Similarly,

$$div_{S^2}\mathbf{W}^l_m = -l(l+1)Y_{lm}.$$

Hence,

$$\mathcal{N}_{S^2}(Y_{lm}) = -\frac{l(l+2)}{(2l+1)^2(2l+3)}(l+1)(l+2)Y_{lm} - \frac{(l-1)(l+1)}{(2l+1)^2(2l-1)}l(l+1)Y_{lm}.$$

and our result follows $\square$

Now, in the left hand side of the equation in *Step* 2 we must compute

$$\mathcal{S}[\mathbf{f}_b](\mathbf{x}).$$

Now, [21] gives that $\mathbf{f}_b$ is dominated by $\nabla^4_\gamma\mathbf{x}$. Hence, we define an operator

$$\mathcal{B}_\gamma[\mathbf{f}] = \mathcal{S}[\nabla^4_\gamma\mathbf{f}](\mathbf{x}).$$

With this, we present a theorem

Theorem 3.9. *When $\mu = 1$,*

$$\mathcal{B}_{S^2}[\boldsymbol{V}^l_m] = \frac{l^3(l-1)^2}{(2l+1)(2l+3)}\,\boldsymbol{V}^l_m.$$

Proof. It is straightforward to compute

$$\nabla^2_{S^2}\mathbf{V}^l_m = -l(l-1)\mathbf{V}^l_m.$$

Hence

$$\nabla^4_{S^2}\mathbf{V}^l_m = l^2(l-1)^2\mathbf{V}^l_m,$$

and by Theorem 3.7

$$\mathcal{S}[\nabla^4_{S^2}\mathbf{V}^l_m] = l^2(l-1)^2\frac{l}{(2l+1)(2l+3)}\mathbf{V}^l_m.$$

□

From Theorems 3.9 and 3.8, we see that the eigenvalues of $\mathcal{N} \sim \mathcal{O}(l)$ and the eigenvalues of $\mathcal{B} \sim \mathcal{O}(l^3)$. Hence, the condition number of the matrix obtained in the Galerkin scheme used in *Step* 1 is $\mathcal{O}(L^3)$. Now, we imagine a greatly simplified version of *Step* 2. We may argue that the equation in *Step* 2 is of the from $\partial_t\Psi = -c\Psi$ where c is an eigenvalue of $\mathcal{B}$ such that $c \sim \mathcal{O}(L^3)$ from Theorem 3.9. Thus, using a forward difference to approximate $\partial_t\Psi$ we have $\frac{1}{\Delta t}[\Psi^{n+1} - \Psi^n] = -c\Psi^n$. Rearranging this gives $\Psi^{n+1} = [1 - \Delta tc]\Psi^n$. For this to be stable, we need $|1 - \Delta tc| \leq 1$ and hence [21]'s choice to use $\Delta t = \mathcal{O}(L^{-3})$.

We now discuss the issue of the undisturbed velocity $\mathbf{u}^\infty$. First, we define some important non-dimensional parameters. Given the area, A, and the volume V of the initial shape of our vesicle (whose points are given by $\mathbf{x}^0$), following [21] we define

$$\begin{aligned} &\textit{length scale}: && R_0 = \sqrt{\frac{A}{4\pi}}, \\ &\textit{time scale}: && \tau = \frac{\mu R_0^3}{\kappa_b}, \\ &\textit{shear rate}: && \chi = \dot{\lambda}\tau. \end{aligned} \tag{3.32}$$

We note that simple shear flows are completely characterized by the quantities χ and τ

defined in (3.32). Given these, we may find $\dot{\lambda}$ and define a few possibilities for $\mathbf{u}^\infty$. Firstly, if we want our vesicle to be suspended in a linear shear flow, we have that

$$linear: \qquad \mathbf{u}^\infty(\mathbf{x}^n) = \dot{\lambda}\begin{pmatrix} x_3^n \\ 0 \\ 0 \end{pmatrix}.$$

Similarly, if we want our vesicle suspended in a parabolic shear flow, we have

$$parabolic: \qquad \mathbf{u}^\infty(\mathbf{x}^n) = \dot{\lambda}\begin{pmatrix} (x_3^n)^2 \\ 0 \\ 0 \end{pmatrix}.$$

Further, if we want our vesicle suspended in an extensional shear flow,

$$extensional: \qquad \mathbf{u}^\infty(\mathbf{x}^n) = \dot{\lambda}\begin{pmatrix} x_1^n \\ -x_2^n \\ 0 \end{pmatrix}.$$

With these, we may derive an exact form for σ under certain circumstances.

Theorem 3.10. *If $\mu = 1$ and the initial shape of our vesicle is a unit sphere, in a linear shear flow,*

$$\boldsymbol{u}^\infty(\boldsymbol{x}^n) = \dot{\lambda}\begin{pmatrix} x_3^0 \\ 0 \\ 0 \end{pmatrix} = \dot{\lambda}\begin{pmatrix} \cos(\theta) \\ 0 \\ 0 \end{pmatrix},$$

we have that

$$\sigma = \dot{\lambda}\frac{35}{22}\sqrt{\frac{2\pi}{15}}\left(Y_{-1}^2(\theta,\phi) - Y_1^2(\theta,\phi)\right).$$

Proof. For the unit sphere, by (2.26), we have that

$$E = 1,\ F = 0,\ G = sin^2(\theta),\ w = \sin(\theta).$$

Further, a simple computation gives that

$$H = -1,\ K = 1.$$

Given these quantities, we may compute

$$\mathbf{f}_b = \kappa_b\left(\nabla_{S^2}^2 H + 2H(H^2 - K)\right)\mathbf{n} = \kappa_b\left(\nabla_{S^2}^2(-1) + 2(-1)(1-1)\right)\mathbf{n} = 0,$$

hence,

$$div_{S^2}\left(\mathcal{S}[\mathbf{f}_b](S^2)\right) = div_{S^2}\left(\mathcal{S}[0](S^2)\right) = div_{S^2}(0) = 0. \tag{3.33}$$

Now, looking at the equation in *Step* 1, we have

$$div_{S^2}\mathcal{S}\left[\mathbf{f}_\sigma\right](\mathbf{x}) = -div_{S^2}\left(\dot{\lambda}\begin{pmatrix}\cos(\theta)\\0\\0\end{pmatrix} - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x})\right).$$

Now, using (3.33) the right hand side can be simplified as

$$-\, div_{S^2}\left(\dot{\lambda}\begin{pmatrix}\cos(\theta)\\0\\0\end{pmatrix} - \mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x})\right) =$$
$$-\, div_{S^2}\left(\dot{\lambda}\begin{pmatrix}\cos(\theta)\\0\\0\end{pmatrix}\right) + div_{S^2}\left(\mathcal{S}\left[\mathbf{f}_b\right](\mathbf{x})\right) = -div_{S^2}\left(\dot{\lambda}\begin{pmatrix}\cos(\theta)\\0\\0\end{pmatrix}\right).$$

Now, using (2.54), we have that

$$-div_{S^2}\left(\dot{\lambda}\begin{pmatrix}\cos(\theta)\\0\\0\end{pmatrix}\right) = \dot{\lambda}\sin(\theta)\cos(\theta)\cos(\phi),$$

which we may rewrite as

$$\dot{\lambda}\sin(\theta)\cos(\theta)\cos(\phi) = -\dot{\lambda}\sqrt{\frac{2\pi}{15}}\left(Y_1^2(\theta,\phi) - Y_{-1}^2(\theta,\phi)\right). \tag{3.34}$$

Now, if we assume a spherical harmonic expansion for σ of the form

$$\sigma = \sum_{l=0}^{L}\sum_{|m|\leq l} a_m^l Y_m^l(\theta,\phi),$$

and plug this into the left hand side of *Step* 1, we have that

$$div_{S^2}\mathcal{S}\left[\mathbf{f}_\sigma\right](\mathbf{x}) = \mathcal{N}_{S^2}(\sigma) = \sum_{l=0}^{L}\sum_{|m|\leq l} a_m^l \mathcal{N}_{S^2}(Y_m^l(\theta,\phi)),$$

and by (3.8)

$$\sum_{l=0}^{L}\sum_{|m|\leq l} a_m^l \mathcal{N}_{S^2}(Y_m^l(\theta,\phi)) = \sum_{l=0}^{L}\sum_{|m|\leq l} -a_m^l \frac{l(l+1)(2l^2+2l-1)}{(2l-1)(2l+1)(2l+3)} Y_m^l(\theta,\phi). \tag{3.35}$$

Now, equating (3.35) and (3.34) gives

$$\sum_{l=0}^{L}\sum_{|m|\leq l} -a_m^l \frac{l(l+1)(2l^2+2l-1)}{(2l-1)(2l+1)(2l+3)} Y_m^l(\theta,\phi) = -\dot{\lambda}\sqrt{\frac{2\pi}{15}}\left(Y_1^2(\theta,\phi) - Y_{-1}^2(\theta,\phi)\right).$$

Equating the coefficients of this equation gives

$$a_m^l = 0 \text{ for } l \neq 2 \text{ and } m \neq 1, -1,$$

and

$$a_1^2 = \dot{\lambda}\frac{35}{22}\sqrt{\frac{2\pi}{15}},\ a_{-1}^2 = -\dot{\lambda}\frac{35}{22}\sqrt{\frac{2\pi}{15}}.$$

Our result follows. □

3.4.1 Numerical Results Concerning the Explicit Scheme

In section 3.2.1, we saw some results concerning the accuracy of our projection operator $\mathcal{L}_L$. We now present result concerning the accuracy of our approximation to the curvature of a surface, our discretization of the Stokes operator, and our scheme on the whole. We begin by looking at the accuracy of our discrete Stokes operator. As a means of demonstrating that our numerical implementation the Stokes operator functions properly, we turn to the eigenfunction relationship of Theorem 3.7. This theorem gives us an exact form for the action of the Stokes operator on $\mathbf{W}_m^l(\theta,\phi)$ and $\mathbf{V}_m^l(\theta,\phi)$. Hence, for $L=3$, we present a table of relative L^2 error in our numerical approximation of $\mathcal{S}[\mathbf{W}_m^l](S^2)$, i.e,

$$Stokes\ Error = \frac{\left\|\mathcal{S}[\mathbf{W}_m^l](S^2) - \frac{l+1}{(2l-1)(2l+1)}\mathbf{W}_m^l\right\|_{L^2}}{\left\|\frac{l+1}{(2l-1)(2l+1)}\mathbf{W}_m^l\right\|_{L^2}},$$

where

$$\mathcal{S}[\mathbf{W}_m^l](S^2)$$

is computed using the matrix $\mathbf{M}$ described in section 3.3 and by projecting $\mathbf{W}_m^l$ using $\mathcal{L}_3$. Hence we also present the relative L^2 error in our approximation of $\mathbf{W}_m^l$, i.e

$$\mathbf{W}_m^l\ Error = \frac{\left\|\mathbf{W}_m^l - \mathcal{L}_3(\mathbf{W}_m^l)\right\|_{L^2}}{\left\|\mathbf{W}_m^l\right\|_{L^2}}.$$

From Table 3.3, we see that given a numerically exact vector of spherical harmonic expansion coefficients, our discretization of the Stokes operator reproduces the desired eigenfunction relationship exactly. Hence, we see that our discretization of the Stokes operator works accurately. However, there is another side to the story. Table 3.4 shows the run times for computing the discretization of the Stokes operator, $\mathbf{M}$, for various values of L on a 2.93 GHz Processor. With this, we conjecture that the runtime for computing $\mathbf{M}$ is $\mathcal{O}(L^4)$. This is

Table 3.3: relative L^2 error in approximation of the action of the Stokes operator

l	m	$\mathbf{W}_m^l$ Error	Stokes Error
1	-1	7.61e-16	1.48e-15
1	0	8.24e-16	8.52e-16
1	1	7.62e-16	1.45e-15
2	-2	7.31e-16	1.69e-15
2	-1	6.88e-16	1.78e-15
2	0	6.63e-16	1.67e-15
2	1	6.50e-16	1.82e-15
2	2	7.44e-16	1.71e-15
3	-3	8.48e-16	2.05e-15
3	-2	7.73e-16	2.87e-15
3	-1	7.91e-16	3.40e-15
3	0	7.90e-16	2.58e-15
3	1	8.31e-16	3.40e-15
3	2	7.04e-16	3.14e-15
3	3	8.58e-16	1.99e-15

Table 3.4: Run times for computing **M** for various values of L

L	Run Time (s)
1	.5
2	4
3	22
4	80
5	260
6	700
7	1600
8	3700

prohibitively large. As the computation of $\mathbf{M}$ clearly dominate the complexity of our overall algorithm, for $L = 8$ it would take about a day to run 20 steps of our explicit scheme. We will show, however, that for relatively simple initial vesicle shapes, our algorithm maintains a reasonable degree of accuracy for relatively low values of L.

We now turn our focus to the accuracy with which we compute derivatives. As we use explicit formulas for the partial derivative of spherical harmonics, we expect that the accuracy of our derivatives be contingent on the accuracy of our spherical harmonic expansions. There is however, a bit of hitch to this. One major component of our algorithm is the computation of the mean and Gaussian curvature of a surface. This computation requires the use of every partial derivative of our surface's pointing vector up to order two. Still, while it may be possible to accurately represent our surfaces pointing vector with a linear combination of vector spherical harmonics up to degree L, this does not necessarily imply that the mean or Gaussian curvature can be accurately approximated by spherical harmonics up to degree L. Still, we present results which indicate that this may not be a problem for relatively simple geometries. Consider the spheroid parameterized in spherical coordinates by

$$\mathbf{x}(\theta, \phi) = \begin{pmatrix} \sin(\theta)\cos(\phi) \\ \sin(\theta)\sin(\phi) \\ 2\cos(\theta) \end{pmatrix},$$

shown in Figure 3.4 We may analytically find the mean and Gaussian curvatures of this

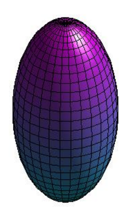

Figure 3.4: prolate spheroid

surface as

$$H(\theta, \phi) = \sqrt{2}\frac{(3\cos(2\theta) - 7)}{(5 - 3\cos(2\theta))^{3/2}}, \quad K(\theta, \phi) = \frac{16}{(5 - 3\cos(2\theta))^2}. \tag{3.36}$$

Table 3.5 gives the L^2 error in our approximation of the curvature of this spheroid. For this

Table 3.5: Relative L^2 error in computing mean and Gaussian Curvature of a prolate spheroid.

L	Relative L^2 Error in Approximating the surface	$\frac{\|H-H_{approx.}\|_{L^2}}{\|H\|_{L^2}}$	$\frac{\|K-K_{approx.}\|_{L^2}}{\|K\|_{L^2}}$
1	9.07e-16	1.64e-16	5.06e-16
2	6.23e-16	9.18e-16	1.10e-15
3	9.23e-16	2.07e-15	5.36e-15
4	2.11e-15	6.62e-15	1.98e-14
5	2.85e-15	1.60e-14	4.84e-14
6	2.27e-15	1.53e-14	1.90e-14
7	3.70e-15	4.35e-14	1.33e-13

spheroid, our algorithm computes mean and Gaussian curvature to near machine accuracy. Hence, for this simple case of the spheroid, the problem of accurate projection of curvature onto the space of L^{th} degree spherical harmonics seems to be averted. One way to avert this problem in general is to always use a larger value of L than seems necessary. Still, a more efficient way to address this issue is outlined in Chapter 4.

Finally, we present the results of the full explicit scheme. We consider the prolate spheroid defined by

$$\mathbf{x}(\theta, \phi) = \begin{pmatrix} \sin(\theta)\cos(\phi) \\ \sin(\theta)\sin(\phi) \\ 2\cos(\theta) \end{pmatrix},$$

suspended in a linear shear flow with shear rate $\chi = 20$ and dynamic viscosity $\mu = 1$. We use a vectorial spherical harmonic approximation of this surface up to degree $L = 4$ and hence, taking our time step to be $2L^{-3}$ (in accordance with the stability results derived in section 3.4). As reference [21] suggests, we take the bending modulus of our vesicle to be $\kappa_b = 1e - 2$. Figure 3.5 shows our vesicle after every 14 time steps on a grid of 30 equally spaced points in the θ and ϕ directions up to 112 time steps. To ensure that the constant surface area condition was being maintained in this evolution, we compute the maximum relative error in the surface area of the vesicle as it evolves as

$$\max_n \frac{|A - A_{n\Delta t}|}{|A|} = 0.0034.$$

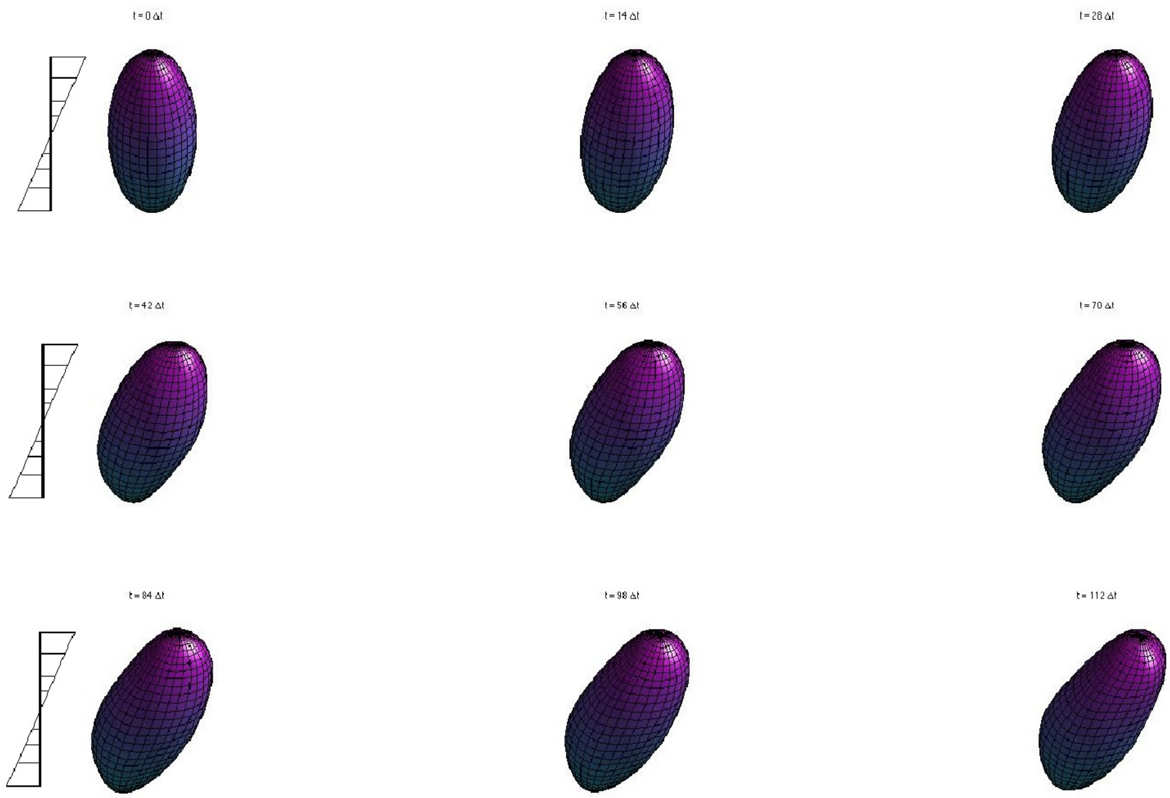

Figure 3.5: A prolate spheroid suspended in a linear shear flow

Further, under the same criteria as the simulation for the prolate spheroid, we present results for a sphere suspended in a linear shear flow. Taking $L = 4$ we have that the relative L^2 error in σ after the first step of the evolution of the sphere versus the exact solution derived in section 3.4 is $6.43e-16$. In Figure 3.6, we give a plot of the relative error in the vesicle's surface area as it evolves. Further, Figure 3.7 shows the sphere's evolution after every 25 time steps up to 125 time steps.

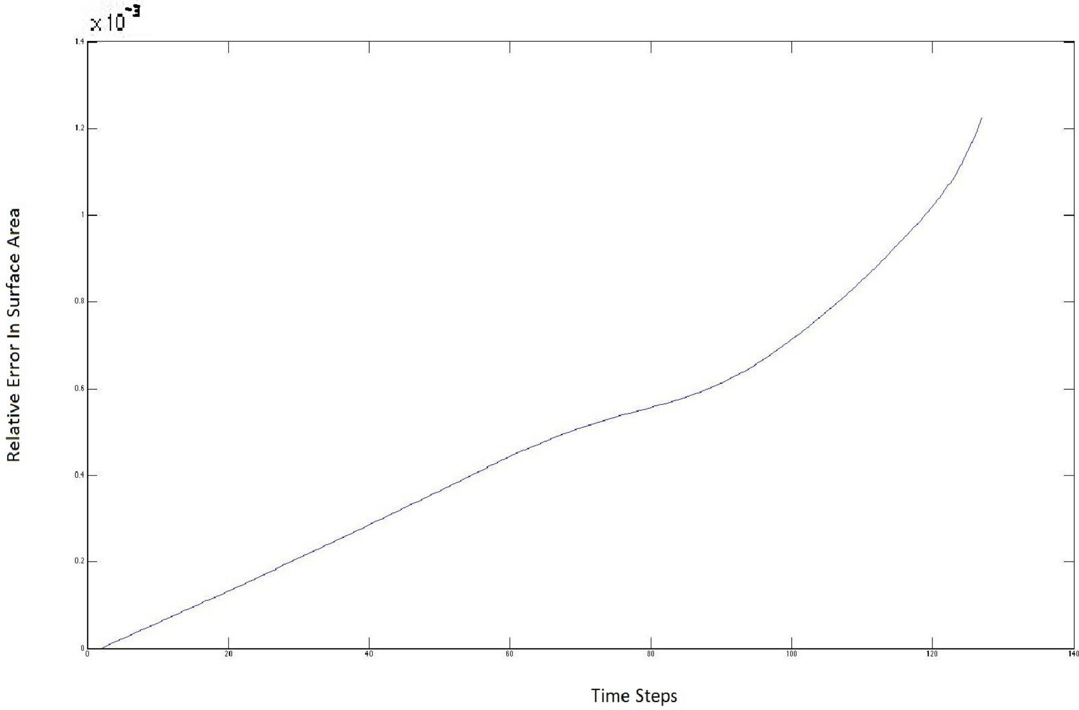

Figure 3.6: Relative error in the surface area of a sphere plotted against time

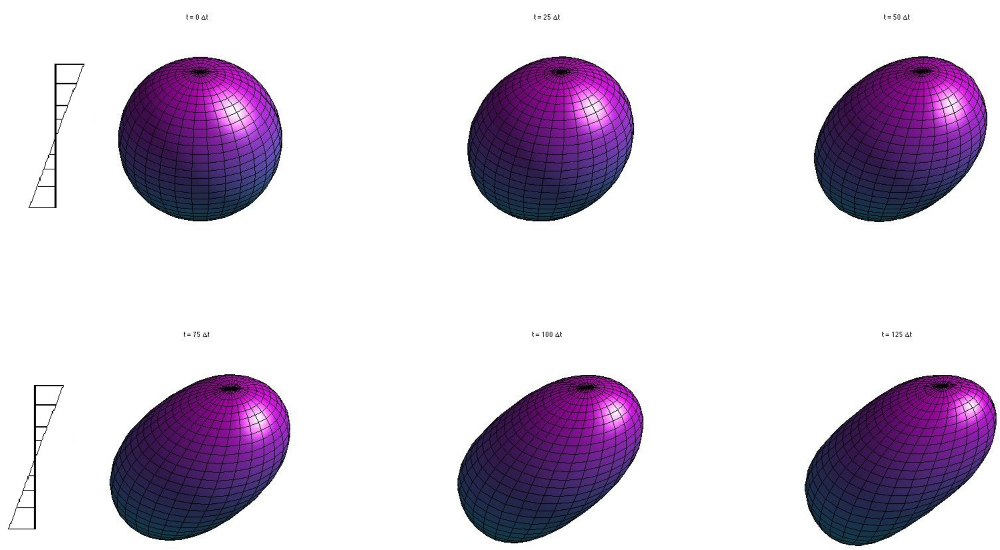

Figure 3.7: A sphere suspended in a linear shear flow

CHAPTER 4

CONCLUSIONS AND FUTURE WORK

We saw in Section 3.4.1 many of the strengths and failings of the presented method. In this chapter we will address these and give suggestions for improvements in our methodology. The first thing we will address is our discretization of the Stokes operator. In Section 3.4.1, we saw that while our discretization of the Stokes operator is accurate, our implementation of the scheme to generate its entries is so computationally intensive that it cripples the speed of our overarching explicit scheme. This limits the initial vesicle shapes which we consider to those which may be accurately represented by linear combinations of very low degree vector spherical harmonics. As mentioned in [8], we may use FFT's to speed up calculations of rotation coefficients and sums in the ϕ direction seen in 3.29. This improvement would bring the complexity of our algorithm down to $\mathcal{O}(L^5)$ as opposed to our current *time* complexity of $\mathcal{O}(L^4)$ [8].

Now, in Section 3.4.1 we mentioned that our current method for computing the mean and Gaussian curvature of a surface may have problems if the mean or Gaussian curvature, in order to be represented accurately, require higher degree spherical harmonics than we use to approximate our surface. We did not require a solution to this problem as the time complexity of the computation of our discrete Stokes operator limited the vesicles which we considered to those for which there is no problem in our scheme's ability to compute mean and Gaussian curvatures. Reference [21] addresses this concern with an up–sampling scheme. By this, we mean that once we have a degree L approximation of our surface on a mesh of $2(L+1)^2$ points, we take $L' = 2L$ and evaluate our spherical harmonic approximation on a mesh of $2(L'+1)^2$ points, use this to compute the mean and Gaussian curvatures. With this, we are able to approximate our mean and Gaussian curvature in the space of L' degree spherical harmonics, we then throw out higher frequency terms to return to an approximation in the space of L degree spherical harmonic. We may then evaluate this on our original mesh.

In Section 3.4 we described an explicit scheme to simulate a vesicle suspended in a Stokes flow. This scheme came with a somewhat restrictive stability condition of the form $\Delta t \sim \mathcal{O}(L^{-3})$, where L maximum degree of the spherical harmonic approximation we use to represent our vesicle. This stability condition, however, is not terribly restrictive for our implementation as time complexity of our discretization of the Stokes operator limits us to small values of L. Were this not to be the case (i.e we had an efficient implementation of the discretization of the Stokes operator), reference [21] describes a semi–implicit time stepping scheme with no restrictions on the time step and only a modest increase computational complexity from the explicit scheme. The idea of this scheme is to consider a modified version of the algorithm we presented in Section 2.2 and fleshed out in Section 3.4. That is,

Step 1 :

solve

$$div_\gamma \mathcal{S}\left[\mathbf{f}_\sigma^{n+1}\right](\mathbf{x}^n) = -div_\gamma\left(\mathbf{u}^\infty(\mathbf{x}^n) - \mathcal{S}\left[\mathbf{f}_b^n\right](\mathbf{x}^n)\right)$$

for $\mathbf{f}_\sigma^{n+1}$.

Step 2 :

use $\mathbf{f}_\sigma^{n+1}$ in

$$\mathcal{S}\left[\mathbf{f}_\sigma^{n+1} - \mathbf{f}_b^{n+1}\right](\mathbf{x}^n) + \mathbf{u}^\infty(\mathbf{x}^n) = \frac{1}{\Delta t}\left(\mathbf{x}^{n+1} - \mathbf{x}^n\right)$$

to solve for $\mathbf{x}^{n+1}$, where

$$\mathbf{f}_b^{n+1} = \kappa_b\left(\nabla_\gamma^2 H^{n+1} + 2H^{n+1}((H^n)^2 - K^n)\right)\mathbf{n}^n,$$

and

$$H^{n+1} = \frac{1}{2(W^n)^2}(E^n\mathbf{x}_{\phi\phi}^{n+1} - 2F^n\mathbf{x}_{\phi\theta}^{n+1}G^n\mathbf{x}_{\theta\theta}^{n+1})\cdot\mathbf{n}^n.$$

Additionally, reference [21] proposes a scheme in which multiple vesicles may be simulated. This scheme, however, requires a reparameterization scheme to maintain grid quality. Hence, the implementation of this scheme requires an exposition outside the scope of the work presented here. Further, reference [16] presents a scheme to model multiple vesicles in a more realistic confined flow.

One of the limitations of the methods presented in this work is that we assume there is no viscosity contrast across our vesicle membrane. To account for this, our methods may be extended to include a double layer potential in the integral equation formulation of our problem presented in Section 2.1 [18]. The numerical treatment of this double layer potential may be done in a similar manner to singular integration scheme described in Section 3.3. To the best of our knowledge, no work has been done to model vesicles suspended in a fluid flow which undergo a change in their topology. Additionally, to the best of our knowledge, no methods exist to model 3D vesicles in finite Reynolds number flows. Hence, there is much work to be done in these areas.

We have shown that the method presented in this work to simulate single vesicle flows in three dimensions is viable for vesicles with a 'simple' spherical topology. While there are certainly things which can be done to improve the efficiency and robustness of our algorithm, the intention of this work was not to contribute to the field in this way. Our intention was to provide a thorough exposition of the coalescence of concepts and techniques involved in 3D simulations of vesicle flows.

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APPENDIX A - GREEN'S FUNCTIONS

Green's function are functions which satisfy the singularly forced version of a given PDE. By this we mean, given differential operator, say, L, which governs a PDE in some volume, $V \subset \mathbb{R}^3$, with boundary, $S \subset \mathbb{R}^2$, over a vector field, $\mathbf{U}(\mathbf{x})$,

$$\begin{aligned} L\{\mathbf{U}(\mathbf{x})\} &= \mathbf{F}(\mathbf{x}), && in \;\; V, \\ \mathbf{U}(\mathbf{x}) &= \mathbf{H}(\mathbf{x}). && on \;\; S \end{aligned}$$

The Green's function, $\mathbf{G}$ of this PDE satisfies

$$\begin{aligned} L\{\mathbf{G}(\mathbf{x},\mathbf{x}_0)\} &= \delta(\mathbf{x}-\mathbf{x}_0) && in \;\; V, \\ \mathbf{G}(\mathbf{x},\mathbf{x}_0) &= 0 && on \;\; S, \end{aligned}$$

where $\mathbf{x}_0$ is some fixed location in V. When V is the whole space, we call $\mathbf{G}$ a *fundamental solution*. To see how we might find one of these, let us consider the familiar Poisson equation in all of $\mathbb{R}^3$,

$$\nabla^2 G(\mathbf{x},\mathbf{x}_0) = \delta(\mathbf{x}-\mathbf{x}_0) \tag{A.1}$$

with the condition that $G \to 0$ as $|\mathbf{x}-\mathbf{x}_0| \to \infty$. Now, let us consider a spherical volume, S_R, of radius $R \geq |\mathbf{x}-\mathbf{x}_0|$, centered at $\mathbf{x}_0$. Integrating (A.1) over S_R gives

$$1 = \int_{S_R} \delta(\mathbf{x}-\mathbf{x}_0)dV = \int_{S_R} \nabla^2 G(\mathbf{x},\mathbf{x}_0)dV = \int_{S_R} \nabla \cdot (\nabla G(\mathbf{x},\mathbf{x}_0))dV$$

Using the divergence theorem, we have

$$1 = \int_{\partial S_R} \frac{\partial G(\mathbf{x},\mathbf{x}_0)}{\partial \mathbf{n}} dS$$

As the surface is a sphere, $\mathbf{n}$ is simply the unit radial vector, r, hence we may write that $\mathbf{n} \cdot (\nabla G(\mathbf{x},\mathbf{x}_0)) = G'(r)$. Hence,

$$1 = \int_{\partial S_R} G'(r)dS = G'(R)\int_{\partial S_R} dS = G'(R)4\pi R^2$$

Hence, we choose $R = |\mathbf{x}-\mathbf{x}_0|$ to arrive at

$$1 = G'(|\mathbf{x}-\mathbf{x}_0|)4\pi|\mathbf{x}-\mathbf{x}_0|^2$$

Hence

$$G'(|\mathbf{x}-\mathbf{x}_0|) = \frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|^2}$$

and

$$G(|\mathbf{x}-\mathbf{x}_0|) = \frac{-1}{4\pi|\mathbf{x}-\mathbf{x}_0|} + c$$

where c is a constant. But, as we require that $G \to 0$ as $|\mathbf{x}-\mathbf{x}_0| \to \infty$, it must be that $c = 0$. Hence,

$$G(\mathbf{x},\mathbf{x}_0) = \frac{-1}{4\pi|\mathbf{x}-\mathbf{x}_0|} \tag{A.2}$$

is the Fundamental solution of the Poisson equation. Continuing along these lines, consider Laplace's equation in some volume V bounded by a closed smooth surface, with non-zero Dirichlet boundary conditions

$$\begin{aligned} \nabla^2 u(\mathbf{x}) &= 0 \qquad && \textit{in } V, \\ u(\mathbf{x}) &= g(\mathbf{x}) \qquad && \textit{on } \partial V \end{aligned} \tag{A.3}$$

Now Green's second theorem gives that for two twice continuously differentiable functions over a volume V', v and w,

$$\int_{V'} w\nabla^2 v - v\nabla^2 w dV = \int_{\partial V'} w\frac{\partial v}{\partial \mathbf{n}} - v\frac{\partial w}{\partial \mathbf{n}} dS$$

plugging in u form (A.3) as w in Greens second theorem gives

$$\int_V u\nabla^2 v dV = \int_{\partial V} \left[u\frac{\partial v}{\partial \mathbf{n}} - v\frac{\partial u}{\partial \mathbf{n}}\right] dS$$

taking v in the above expression as $G(\mathbf{x},\mathbf{x}_0) = \frac{-1}{4\pi|\mathbf{x}-\mathbf{x}_0|}$ (where again $\mathbf{x}_0$ is a point in the interior of V) and replacing any occurrences of u on the right hand side with g (as the integral is taken over the boundary) gives

$$\int_V u(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}_0) dV = \int_{\partial V} G(\mathbf{x},\mathbf{x}_0)\frac{\partial u}{\partial \mathbf{n}} - g\frac{\partial G(\mathbf{x},\mathbf{x}_0)}{\partial \mathbf{n}} dS$$

or

$$u(\mathbf{x}_0) = \int_{\partial V} G(\mathbf{x},\mathbf{x}_0)\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS - \int_{\partial V} g(\mathbf{x})\frac{\partial G(\mathbf{x},\mathbf{x}_0)}{\partial \mathbf{n}} dS$$

Note that Laplace's Equation is homogeneous and thus, multiplying G by negative one will maintain all of the properties of this Green's function. Hence, we take $G(\mathbf{x},\mathbf{x}_0) = \frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|}$

and write,

$$u(\mathbf{x}_0) = \int_{\partial V} \frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS - \int_{\partial V} g(\mathbf{x})\frac{\partial}{\partial \mathbf{n}}\frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|} dS$$

Note that we obtained this expression by assuming that $\mathbf{x}_0$ was inside the volume V. This assumption, leads to an interesting dilemma. What if we were to take the limit of the above expression as $\mathbf{x}_0$ tends toward the boundary from the inside. Let us examine a sequence of points $\mathbf{y}_k$ in the interior of V tending toward a point on ∂V, say, $\mathbf{y}$. Now let us examine

$$\int_{\partial V} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}_k|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS$$

we note that the factor $\frac{1}{4\pi|\mathbf{x}-\mathbf{y}_k|}$ will become singular at $\mathbf{y}$ in the limit. So, we indent the volume over which this integral is taken by a hemisphere of radius ϵ, centered at $\mathbf{y}$. We will call this hemispherical surface H_ϵ and we will denote the indented volume by V_ϵ. Hence, we may write

$$\int_{\partial V_\epsilon} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}_k|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS = \int_{\partial V \backslash H_\epsilon} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}_k|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS + \int_{H_\epsilon} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}_k|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS$$

And we may now take the limit as $\mathbf{y}_k$ goes to $\mathbf{y}$ without issue. Further, noting that over H_ϵ, $\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} = \frac{1}{4\pi\epsilon}$, gives

$$\int_{\partial V_\epsilon} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS = \int_{\partial V \backslash H_\epsilon} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS + \int_{H_\epsilon} \frac{1}{4\pi\epsilon}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS$$

and

$$\int_{H_\epsilon} \frac{1}{4\pi\epsilon}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS = \frac{2\pi\epsilon^2 u(\mathbf{y})}{4\pi\epsilon}$$

Now this term clearly goes to zero in the limit as $\epsilon \to 0$. Hence, as $\epsilon \to 0$, we have that

$$⨍_{\partial V} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS = \int_{\partial V} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}\frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS$$

where $⨍$ is the Cauchy principle value integral. Hence,

$$\int_{\partial V} \frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|}\frac{\partial g(\mathbf{x})}{\partial \mathbf{n}} dS$$

is continuous as $\mathbf{x}_0$ crosses the boundary from the interior of V. A similar argument gives that this integral is continuous as $\mathbf{x}_0$ crosses the boundary from the exterior of V. Integrals operators of this type are referred to as *single layer potentials* [12, pg.158]. Now, we again consider a sequence of interior points $\mathbf{y}_k$ approaching a boundary point $\mathbf{y}$ and look at

$$\int_{\partial V} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}_k|} dS$$

using the same methodology as with the single layer potential, we arrive at

$$\int_{\partial V_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS = \int_{\partial V \setminus H_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS + \int_{H_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS$$

where

$$\int_{H_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS = \int_{H_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \epsilon} \frac{1}{4\pi\epsilon} dS = g(\mathbf{y}) \frac{-2\pi\epsilon^2}{4\pi\epsilon^2} dS = \frac{-1}{2} g(\mathbf{y})$$

Hence,

$$\int_{\partial V_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS = \int_{\partial V \setminus H_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS - \frac{1}{2} g(\mathbf{y})$$

Now, taking the limit as $\epsilon \to 0$ gives

$$⨍_{\partial V} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS = \int_{\partial V \setminus H_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS - \frac{1}{2} g(\mathbf{y})$$

A similar argument in which we take a limit of exterior points going to the boundary and take our ϵ indentation to be outward, gives

$$⨍_{\partial V} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS = \int_{\partial V \setminus H_\epsilon} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} dS + \frac{1}{2} g(\mathbf{y})$$

Integral operators of this type are known as *double layer potentials* [12, pg.158]. This phenomenon of gaining a $\pm\frac{1}{2}$ when an observation point approaches the boundary is called a *jump*. Now, looking at

$$u(\mathbf{x}_0) = \int_{\partial V} \frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|} \frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS - \int_{\partial V} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|} dS$$

we see that taking the limit as $\mathbf{x}_0$ approaches the boundary gives

$$\frac{1}{2} u(\mathbf{x}_0) = \int_{\partial V} \frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|} \frac{\partial u(\mathbf{x})}{\partial \mathbf{n}} dS - \int_{\partial V} g(\mathbf{x}) \frac{\partial}{\partial \mathbf{n}} \frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|} dS \tag{A.4}$$

APPENDIX B - DERIVATION OF SPHERICAL HARMONICS

Spherical harmonics are a orthogonal functions on the unit sphere whose properties are so vast and impactful that they will be at the heart of the work presented in this thesis. Consider the familiar 3D Laplace's equation in rectangular coordinates,

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0$$

Recall that functions, u, which satisfy this equation are called harmonics. Hence, from the name, one might expect that spherical harmonics are functions which satisfy Laplace's equation in spherical coordinates. While this is not quite the whole story, spherical harmonics do arise from solutions to Laplace's equation in spherical coordinates. The form of Laplace's equation in spherical coordinates is rather arduous to derive. Luckily, a full and detailed derivation is given in [20]. Hence, for brevity and our sanity, we will simply state that Laplace's equation in spherical coordinates is given by

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial u}{\partial \theta}\right) + \frac{1}{r^2 sin^2(\theta)}\frac{\partial^2 u}{\partial \phi^2} = 0$$

Multiplying this equation by r^2 gives the equivalent formulation,

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial u}{\partial \theta}\right) + \frac{1}{sin^2(\theta)}\frac{\partial^2 u}{\partial \phi^2} = 0 \tag{B.1}$$

We proceed to solve this equation via separation of variables. We assume that our solution, u, can be written as $u(r,\theta,\phi) = R(r)Y(\theta,\phi)$ and plug this into (B.1) to arrive at

$$Y\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{R}{\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial Y}{\partial \theta}\right) + \frac{R}{sin^2(\theta)}\frac{\partial^2 Y}{\partial \phi^2} = 0$$

Now, dividing this expression by $R(r)Y(\theta,\phi)$ and rearranging

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) = -\frac{1}{Y}\frac{1}{\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial Y}{\partial \theta}\right) - \frac{1}{Y}\frac{1}{sin^2(\theta)}\frac{\partial^2 Y}{\partial \phi^2}$$

We see that the left and right hand sides of this equation depend on different variables and hence must equal a constant. Thus,

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) = -\frac{1}{Y}\frac{1}{\sin(\theta)}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial Y}{\partial \theta}\right) - \frac{1}{Y}\frac{1}{sin^2(\theta)}\frac{\partial^2 Y}{\partial \phi^2} = \lambda \tag{B.2}$$

We now turn our attention to the radial part of this equation. Rewriting gives

$$r^2\frac{\partial^2 R}{\partial r^2} + 2r\frac{\partial R}{\partial r} - \lambda R = 0 \tag{B.3}$$

Proceeding by the method of Frobenius, we guess a solution of the form $R(r) = \sum_{n=0}^{\infty} a_n r^{n+\nu}$ and plug this in to (B.3). This gives

$$r^2 \sum_{n=0}^{\infty} a_n (n+\nu)(n+\nu-1) r^{n+\nu-2} + 2r \sum_{n=0}^{\infty} a_n (n+\nu) r^{n+\nu-1} - \lambda \sum_{n=0}^{\infty} a_n r^{n+\nu} = 0$$
$$\Rightarrow \sum_{n=0}^{\infty} a_n [(n+\nu)(n+\nu+1) - \lambda] r^{n+\nu} = 0$$

Hence, the indicial equation gives the form of λ as

$$\nu(\nu+1) = \lambda$$

Now, we return to (B.3). We may recognize this equation as being of the Cauchy-Euler type [13]. Hence, plugging our form for lambda into (B.3), and guessing a solution of the form $R(r) = r^{\alpha}$ gives

$$r^{\alpha}(\alpha(\alpha-1) + 2\alpha - \nu(\nu+1)) = 0 \Rightarrow \alpha = \nu, -(\nu+1)$$

Hence, $R(r) = Ar^{\nu} + Br^{-(\nu+1)}$. Requiring that our solution be regular at the origin gives that $B = 0$ and $\nu \geq 0$. Hence, $R(r) = Ar^{\nu}$ and $\lambda = \nu(\nu+1) \geq 0$. We now return our attention to (B.2), specifically, the angular portion. We have that

$$-\frac{1}{Y}\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial Y}{\partial\theta}\right) - \frac{1}{Y}\frac{1}{sin^2(\theta)}\frac{\partial^2 Y}{\partial\phi^2} = \nu(\nu+1) \quad \text{(B.4)}$$

Now, guessing a separated solution to (B.4) of the form $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$ and multiplying by $Ysin^2(\theta)$, we have

$$-\Theta\frac{\partial^2\Phi}{\partial\phi^2} = \nu(\nu+1)\Theta\Phi sin^2(\theta) + \sin(\theta)\Phi\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Theta}{\partial\theta}\right)$$

and hence,

$$-\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} = \nu(\nu+1)sin^2(\theta) + \sin(\theta)\frac{1}{\Theta}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Theta}{\partial\theta}\right) = \mu \quad \text{(B.5)}$$

where μ is the separation constant. We now turn our attention to the Φ component of (B.5), i.e

$$-\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} = -\mu$$

Using techniques from ordinary differential equations, we know that Φ must be of the form $\Phi(\phi) = Ae^{i\sqrt{\mu}\phi} + Be^{-i\sqrt{\mu}\phi}$. As we are dealing with spherical functions, we require that Φ

be periodic with a period which evenly divides 2π. Hence, $\sqrt{\mu} = m$ for some integer m and $\Phi(\phi)$ must be a linear combination of complex exponentials of the form $e^{im\phi}$.

We must now consider the final constituent of (B.1), the Θ equation. Looking at (B.5) we see that the equation governing Θ can now be rewritten (using the result derived above, that $\mu = m^2$) as

$$\nu(\nu+1)sin^2(\theta) + \sin(\theta)\frac{1}{\Theta}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Theta}{\partial\theta}\right) = m^2$$

and with a bit of rearranging,

$$\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\Theta}{\partial\theta}\right) + \left(\nu(\nu+1) - \frac{m^2}{sin^2(\theta)}\right)\Theta = 0 \tag{B.6}$$

We now make the change of variables $t = \cos(\theta)$. As $\theta \in [0, \pi]$, $t \in [-1, 1]$. Further, by the chain rule, $\frac{\partial}{\partial\theta} = -\sin(\theta)\frac{\partial}{\partial t}$. Thus, we write (B.6) as

$$\frac{\partial}{\partial t}\left((1-t^2)\frac{\partial\Theta}{\partial t}\right) + \left(\nu(\nu+1) - \frac{m^2}{1-t^2}\right)\Theta = 0 \tag{B.7}$$

If $m = 0$, (B.7) becomes the familiar Legendre equation in, say, $P(t)$ [13, pg.338].

$$\frac{\partial}{\partial t}\left((1-t^2)\frac{\partial P(t)}{\partial t}\right) + \nu(\nu+1)P(t) = 0 \tag{B.8}$$

Hence, we guess a power series solution of the form $P(t) = \sum_{n=0}^{\infty} a_n t^n$ and plug it in to (B.8). following [20], this will give, for the coefficients a_n, the recurrence relation of the form

$$a_{n+2} = \frac{n(n+1) - \nu(\nu+1)}{(n+1)(n+2)}a_n \tag{B.9}$$

We see that for large n, this recurrence relation gives that $a_{n+2} \approx a_n$. Hence, for large n our power series for $P(t)$ is approximately geometric and thus will diverge for $t = -1, 1$. Therefor, for regularity of our solution at our boundary values of t (and hence the poles of our sphere), we must require that a_n vanish for some n. This will only happen if ν is an integer, say, l. This fact combined with the recurrence relation (B.9) gives a form for the power series representation of $P(t)$ in terms of the constant l. This function is known as the Legendre polynomial, denoted by $P_l(t)$ [13, pg.338]. Hence we have that

$$\frac{\partial}{\partial t}\left((1-t^2)\frac{\partial P_l(t)}{\partial t}\right) + l(l+1)P_l(t) = 0$$

or equivalently,

$$(1-t^2)\frac{\partial^2 P_l(t)}{\partial t^2} - 2t\frac{\partial P_l(t)}{\partial t} + l(l+1)P_l(t) = 0 \qquad \text{(B.10)}$$

We now take the m^{th} derivative of (B.10) with respect to t (where m is the same as in (B.7)), and by the generalized product rule,

$$\frac{\partial^m}{\partial t^m}\left((1-t^2)\frac{\partial^2 P_l(t)}{\partial t^2} - 2t\frac{\partial P_l(t)}{\partial t} + l(l+1)P_l(t) = 0\right) \Rightarrow$$
$$(1-t^2)\frac{\partial^2}{\partial t^2}\frac{\partial^m P_l(t)}{\partial t^m} + m(-2t)\frac{\partial^2}{\partial t^2}\frac{\partial^{m-1} P_l(t)}{\partial t^{m-1}} - 2\frac{m(m-1)}{2}\frac{\partial^2}{\partial t^2}\frac{\partial^{m-2} P_l(t)}{\partial t^{m-2}}$$
$$-2t\frac{\partial}{\partial t}\frac{\partial^m P_l(t)}{\partial t^m} - 2m\frac{\partial}{\partial t}\frac{\partial^{m-1} P_l(t)}{\partial t^{m-1}} + l(l+1)\frac{\partial^m P_l(t)}{\partial t^m} = 0 \Rightarrow$$
$$(1-t^2)\frac{\partial^2}{\partial t^2}\frac{\partial^m P_l(t)}{\partial t^m} - 2t(m+1)\frac{\partial}{\partial t}\frac{\partial^m P_l(t)}{\partial t^m} + \left(l(l+1) - m(m+1)\right)\frac{\partial^m P_l(t)}{\partial t^m} = 0$$

Defining $\frac{\partial^m P_l(t)}{\partial t^m} = Q^l_m(t)$, we may write

$$(1-t^2)\frac{\partial^2}{\partial t^2}Q^l_m(t) - 2t(m+1)\frac{\partial}{\partial t}Q^l_m(t) + \left(l(l+1) - m(m+1)\right)Q^l_m(t) = 0 \qquad \text{(B.11)}$$

Now, we make a substitution of $Q^l_m(t) = (1-t^2)^{-m/2}P^l_m(t)$ into (B.11), where $P^l_m(t)$ is an arbitrary function which is regular on $[-1,1]$. We will perform this term by term.

$$(1-t^2)\frac{\partial^2}{\partial t^2}Q^l_m(t) = (1-t^2)\frac{\partial^2}{\partial t^2}((1-t^2)^{-m/2}P^l_m(t)) =$$
$$(1-t^2)^{-m/2}(1-t^2)\frac{\partial^2}{\partial t^2}P^l_m(t) + 2mt(1-t^2)^{-m/2}\frac{\partial}{\partial t}P^l_m(t)$$
$$+ m(1-t^2)^{-m/2-1}(1+(1+m)t^2)P^l_m(t) \qquad \text{(B.12)}$$

and

$$-2t(m+1)\frac{\partial}{\partial t}Q^l_m(t) = -2t(m+1)\frac{\partial}{\partial t}((1-t^2)^{-m/2}P^l_m(t)) =$$
$$-2t(m+1)(1-t^2)^{-m/2}\frac{\partial}{\partial t}P^l_m(t) - 2t^2m(m+1)(1-t^2)^{-m/2-1}P^l_m(t) \qquad \text{(B.13)}$$

Putting (B.12) and (B.13) into (B.11) gives

$$
\begin{aligned}
0 =&(1-t^2)^{-m/2}(1-t^2)\frac{\partial^2}{\partial t^2}P^l_m(t) + 2mt(1-t^2)^{-m/2}\frac{\partial}{\partial t}P^l_m(t)\\
&+ m(1-t^2)^{-m/2-1}(1+(1+m)t^2)P^l_m(t) - 2t(m+1)(1-t^2)^{-m/2}\frac{\partial}{\partial t}P^l_m(t)\\
&- 2t^2m(m+1)(1-t^2)^{-m/2-1}P^l_m(t) - m(1+m)(1-t^2)^{-m/2}P^l_m(t)\\
&+ l(l+1)(1-t^2)^{-m/2}P^l_m(t)
\end{aligned}
$$

$$\Rightarrow$$

$$
\begin{aligned}
0 =&(1-t^2)^{-m/2}(1-t^2)\frac{\partial^2}{\partial t^2}P^l_m(t) + (1-t^2)^{-m/2}\left(2mt - 2t(m+1)\right)\frac{\partial}{\partial t}P^l_m(t)\\
&+ \left(m(1-t^2)^{-m/2-1}P^l_m(t) - m(1+m)(1-t^2)^{-m/2-1}P^l_m(t)\right)P^l_m(t)\\
&+ l(l+1)(1-t^2)^{-m/2}P^l_m(t)
\end{aligned}
$$

$$\Rightarrow$$

$$
0 =(1-t^2)^{-m/2}\left((1-t^2)\frac{\partial^2}{\partial t^2}P^l_m(t) - 2t\frac{\partial}{\partial t}P^l_m(t) + \left(l(l+1) - \frac{m^2}{1-t^2}\right)P^l_m(t)\right)
$$

$$\Rightarrow$$

$$
0 =(1-t^2)\frac{\partial^2}{\partial t^2}P^l_m(t) - 2t\frac{\partial}{\partial t}P^l_m(t) + \left(l(l+1) - \frac{m^2}{1-t^2}\right)P^l_m(t)
$$

Hence, P^l_m solves (B.7). Tracing our definitions backwards, we have $P^l_m(t) = (1-t^2)^{m/2}Q^l_m(t) = (1-t^2)^{m/2}\frac{\partial^m P_l(t)}{\partial t^m}$. In this representation, it is clear that our definition of $P^l_m(t)$ is only valid if m is positive (as negative derivatives don't make sense) and only non-trivial if $m \leq l$ (as $P_l(t)$ is an l^{th} degree polynomial). The positive restriction on m can be alleviated through the application of Rodrigues' formula [13, pg.340]

$$
P_l(t) = \frac{1}{2^l l!}\frac{\partial^l}{\partial t^l}(t^2-1)^l
$$

Which gives

$$
P^l_m(t) = \frac{1}{2^l l!}(1-t^2)^{m/2}\frac{\partial^{m+l}}{\partial t^{m+l}}(t^2-1)^l \tag{B.14}
$$

as a definition for $P^l_m(t)$ valid for all m such that $|m| \leq l$. Recalling our original goal, we have that, $\Theta(\theta) = P^l_m(\cos(\theta))$ must solve (B.6) with $\nu = l$ such that $l = 0, 1, 2, ...$ and $|m| \leq l$. Putting this together with our results that $R(r) = Ar^\nu = Ar^l$ and $\Phi(\phi) = Be^{im\phi}$, by superposition, we have that the general solution to Laplace's equation in spherical coordinates can be expressed as

$$u(r,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{|m|\leq l} a_m^l r^l e^{im\phi} P_m^l(\cos(\theta)) \tag{B.15}$$

In (B.15), the angular factor, $e^{im\phi}P_m^l(\cos(\theta))$, is referred to as a *spherical harmonic* of degree l and order m and typically denoted as $Y_m^l(\theta,\phi)$ or $Y_l^m(\theta,\phi)$.

The real utility of spherical harmonics is seen in their orthogonality relationship. To prove this, we begin with a lemma concerning the associated Legendre polynomials

Lemma B.2.

$$\int_{-1}^{1} P_m^l(t) P_m^{l'}(t)dt = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'}$$

Proof. Without a loss of generality, let us assume that $l' \leq l$. This is acceptable as our problem is symmetric. Now, we have, by (B.14) that

$$\int_{-1}^{1} P_m^l(t) P_m^{l'}(t)dt = \frac{1}{2^{l'}l'!}\frac{1}{2^l l!}\int_{-1}^{1}(1-t^2)^m \frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\left(\frac{\partial^{m+l}}{\partial t^{m+l}}(t^2-1)^l\right)dt$$

Now, integrating the right hand side of the above equality by parts, taking $u = (1-t^2)^m \frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}$ and $dv = \frac{\partial^{m+l}}{\partial t^{m+l}}(t^2-1)^l$, we have

$$\begin{aligned}
&\frac{1}{2^{l+l'}l'!l!}\int_{-1}^{1}(1-t^2)^m \frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\left(\frac{\partial^{m+l}}{\partial t^{m+l}}(t^2-1)^l\right)dt \\
&= \frac{1}{2^{l+l'}l'!l!}\left[(1-t^2)^m \frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\left(\frac{\partial^{m+l-1}}{\partial t^{m+l-1}}(t^2-1)^l\right)\right]_{-1}^{1} \\
&- \frac{1}{2^{l+l'}l'!l!}\int_{-1}^{1}\frac{\partial}{\partial t}\left((1-t^2)^m \frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\right)\left(\frac{\partial^{m+l-1}}{\partial t^{m+l-1}}(t^2-1)^l\right)dt
\end{aligned}$$

In the above, the bracketed term vanishes as $(1-t^2)^m = 0$ at $t = -1, 1$. We see that integrating by parts $m+l-1$ more times will give

$$\begin{aligned}
&\frac{1}{2^{l+l'}l'!l!}\int_{-1}^{1}(1-t^2)^m \frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\left(\frac{\partial^{m+l}}{\partial t^{m+l}}(t^2-1)^l\right)dt \\
&= (-1)^{m+l}\frac{1}{2^{l+l'}l'!l!}\int_{-1}^{1}(t^2-1)^l \frac{\partial^{m+l}}{\partial t^{m+l}}\left((1-t^2)^m \frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\right)dt
\end{aligned} \tag{B.16}$$

We now examine the $\frac{\partial^{m+l}}{\partial t^{m+l}}\left((1-t^2)^m \frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\right)$ factor. Using the generalized product rule, we have

$$\frac{\partial^{m+l}}{\partial t^{m+l}}\left((1-t^2)^m\frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\right)=$$
$$\sum_{n=0}^{l+m}\binom{l+m}{n}\underbrace{\frac{\partial^n}{\partial t^n}(1-t^2)^m}_{\substack{\neq 0\ if\\ n\leq 2m}}\ \underbrace{\frac{\partial^{l'+l+2m-n}}{\partial t^{l'+l+2m-n}}(t^2-1)^{l'}}_{\substack{\neq 0\ if\\ l'+l+2m-n\leq 2l'}}$$

Hence, the above expression will only be non-zero if $n = 2m$ and $l = l'$ (as we have assumed that $l' \leq l$). Hence, we may write

$$\frac{\partial^{m+l}}{\partial t^{m+l}}\left((1-t^2)^m\frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\right)=\delta_{ll'}\binom{l+m}{2m}\frac{\partial^{2m}}{\partial t^{2m}}(1-t^2)^m\frac{\partial^{2l}}{\partial t^{2l}}(t^2-1)^l$$
$$\delta_{ll'}\binom{l+m}{2m}(-1)^m(2m)!(2l)!=\delta_{ll'}(-1)^m(2l)!\frac{(l+m)!}{(l-m)!}$$

Hence, plugging this into (B.16) gives

$$(-1)^{m+l}\frac{1}{2^{l+l'}l'!l!}\int_{-1}^{1}(t^2-1)^l\frac{\partial^{m+l}}{\partial t^{m+l}}\left((1-t^2)^m\frac{\partial^{m+l'}}{\partial t^{m+l'}}(t^2-1)^{l'}\right)dt=$$
$$\delta_{ll'}(-1)^l\frac{(2l)!}{2^{2l}(l!)^2}\frac{(l+m)!}{(l-m)!}\int_{-1}^{1}(t^2-1)^l dt \tag{B.17}$$

Now, for the remaining integral, we make the substitution $s = \frac{t+1}{2}$. this gives

$$\int_{-1}^{1}(t^2-1)^l dt = 2^{2l+1}(-1)^l\int_0^1 s^l(1-s)^l ds = 2^{2l+1}(-1)^l\mathcal{B}(l+1,l+1) = 2^{2l+1}(-1)^l\frac{(l!)^2}{(2l+1)!}$$

where in the above, $\mathcal{B}(x,y)$ is the beta function. Now, putting this together with (B.17) gives

$$\delta_{ll'}(-1)^l\frac{(2l)!}{2^{2l}(l!)^2}\frac{(l+m)!}{(l-m)!}\int_{-1}^{1}(t^2-1)^l dt=$$
$$\delta_{ll'}(-1)^l\frac{(2l)!}{2^{2l}(l!)^2}\frac{(l+m)!}{(l-m)!}2^{2l+1}(-1)^l\frac{(l!)^2}{(2l+1)!}=\delta_{ll'}\frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}$$

and hence our result is proven. □

Now then, with this lemma, we may investigate the orthogonality of the spherical harmonics, $Y^l_m(\theta,\phi)$. First, however, it is convenient, at this point, to introduce an alternative notation for $Y_{lm}(\theta,\phi)$. As (θ,ϕ) corresponds to the spherical coordinates of a point on the unit ball, this point must also have a Cartesian pointing vector of length one. If we call this pointing vector $\mathbf{x}$, we may write

$$Y_{lm}(\theta,\phi) = Y_{lm}(\mathbf{x})$$

This pointing vector notation will be ideal to present some ideas later on and hence will be used interchangeably with the (θ,ϕ) notation as needed. Now, consider,

$$\int_{S^2} Y^l_m(\mathbf{x})\overline{Y^{l'}_{m'}(\mathbf{x}} dS(\mathbf{x}) = \int_0^{\pi}\int_0^{2\pi} Y^l_m(\theta,\phi)\overline{Y^{l'}_{m'}(\theta,\phi)}\sin(\theta)d\theta d\phi \tag{B.18}$$

using our current definition of spherical harmonics into (B.18), we have that

$$\begin{aligned}
&\int_0^{\pi}\int_0^{2\pi} Y^l_m(\theta,\phi)\overline{Y^{l'}_{m'}(\theta,\phi)}\sin(\theta)d\theta d\phi\\
&= \int_0^{\pi}\int_0^{2\pi} e^{im\phi}P^l_m(\cos(\theta))e^{-im'\phi}P^{l'}_{m'}(\cos(\theta))\sin(\theta)d\theta d\phi\\
&= \int_0^{2\pi} e^{im\phi}e^{-im'\phi}d\phi\int_0^{\pi} P^l_m(\cos(\theta))P^{l'}_{m'}(\cos(\theta))\sin(\theta)d\theta\\
&= 2\pi\delta_{mm'}\int_0^{\pi} P^l_m(\cos(\theta))P^{l'}_{m'}(\cos(\theta))\sin(\theta)d\theta =
\end{aligned}$$

making the change of variables $t = \cos(\theta)$, $dt = -\sin(\theta)$ and noting that the presence of $\delta_{mm'}$ allows us to use m and m' interchangeably, using (B.2),

$$\begin{aligned}
&2\pi\delta_{mm'}(-1)\int_1^{-1} P^l_m(t)P^{l'}_m(t)dt\\
&= 2\pi\delta_{mm'}\int_{-1}^{1} P^l_m(t)P^{l'}_m(t)dt\\
&= \delta_{mm'}\delta_{ll'}\frac{4\pi}{2l+1}\frac{(l+m)!}{(l-m)!}
\end{aligned}$$

Hence, we may refine our definition of spherical harmonics as

$$Y^l_m(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}e^{im\phi}P^l_m(\cos(\theta))$$

so that

$$\int_{S^2} Y^l_m(\mathbf{x})\overline{Y^{l'}_{m'}(\mathbf{x})}dS(\mathbf{x}) = \delta_{mm'}\delta_{ll'} \tag{B.19}$$

and hence our spherical harmonics are *orthonormal* in l and m on the unit ball. Further, as we've only changed our definition by a multiplicative constant, spherical harmonics remain as the angular factor in our solution of Laplace's equation in spherical polars. For computational efficiency, some adopt the Condon-Shortley phase factor of $(-1)^m$ in their definition of spherical harmonics [1, pg.682]. As we will be concerned with a computationally efficient implementation of spherical harmonics, we shall also adopt this phase factor. Hence,

$$Y_m^l(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} e^{im\phi} P_m^l(\cos(\theta))$$

It is straight forward to show that this does not effect the orthogonality relationship we have demonstrated in (B.19). We now seek to further the computational efficiency in our definition of spherical harmonics by exploiting a symmetry property. Reference [17, pg.67] give the relationship that for positive values of m,

$$P_{-m}^l(t) = (-1)^m \frac{(l-m)!}{(l+m)!} P_m^l(t) \tag{B.20}$$

Hence, for positive m, we have that

$$\begin{aligned} Y_{-m}^l(\theta,\phi) &= (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}} e^{-im\phi} (-1)^m \frac{(l-m)!}{(l+m)!} P_m^l \\ &= \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} e^{-im\phi} P_m^l(t) \end{aligned}$$

Hence, we will adopt a new notation, introduced in [8], Y_{lm}, for our new, computationally efficient definition of spherical harmonics, given by

$$Y_{lm}(\theta,\phi) = (-1)^{\frac{m+|m|}{2}} \sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}} e^{im\phi} P_{|m|}^l(\cos(\theta)) \tag{B.21}$$

This definition is convenient as it allows for the computation of the associated Legendre polynomials of positive order to be reused for those of negative order. It should be noted that our new phase factor of $(-1)^{\frac{m+|m|}{2}}$ accounts for the absence of a phase for negative values of m and the standard Condon-Shortley phase factor for positive values of m.