Research Study Group Report
PDEs on Manifold

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1 Introduction

Functions of a biological cell are controlled by various mechanisms, both internal and external. One particular key component of a cell is a membrane that encompasses the cell. The cell membrane, as well as other membranes occurring in biology, have a structure of a bilayer and are comprised mainly of lipids and other amphiphilic molecules (which have both a water soluble, hydrophilic part and a water insoluble, hydrophobic part). Figure 1 depicts the structure of a bilayer.

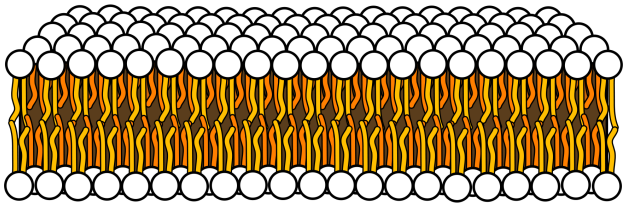

Figure 1: The structure of a bilayer. It consists of two layers of lipids. Each lipid consists of a hydrophilic head (white circles) and hydrophobic tails.

The ability to model the membrane mathematically is instrumental to understanding the shape and structure of the cell as well as its interactions with its environment.

It is important to note that the bilayer structure of the membrane is very thin and highly flexible. It forms a closed surface without edges and its flexibility allows it to adapt to its environment. It is characterized by its shape and the composition of the lipids included in the bilayer.

Various models exist in literature with a popular model being the Helfrich model [7]. This has been built upon to include various additional aspects of the cell such as the lipid composition [15].

In this research study group we treat the membrane as an elastic body. The membrane is described by two functions (corresponding to the shape function u and the lipid composition function ϕ) and its stationary configuration corresponds to the minimisation of its free energy, which includes the coupling between the lipid composition and the shape function. We wish to focus on the effects of modelling the proteins contained within the membrane. This can be translated into mathematical terms as a constraint or a boundary condition for the surface.

The structure of the report is as follows: In Section 2 we describe the motivation of the protein inclusion problem. The review of the state of art and the derivation of the free energy, which minimiser determines the configuration of the membrane is presented in Section 3. In Section 4 we focus on mathematical formulation of the problem and prove the results regarding the existence and uniqueness of the exact solution as well as the solution to the discretised problem. In one of the types of boundary conditions we also prove the

convergence rate of the discretisation to the exact solution in the H^1 norm. The discretised problem is then solved by designing a finite element scheme, which is described in Section 6. The numerical scheme is Dune and it involves using a combination of Morley element (for the shape function u) and piecewise affine element (for the composition function ϕ). In Section 7 we use this scheme we to investigate various aspects of our model. In particular we look at the convergence of the numerical scheme and at the problem of modelling two inclusions. We study how the boundary conditions at the inclusions affect the minimum energy over the distance between two inclusions. The conclusion and possible further directions of the research study group are presented in Section 8.

2 Motivation

Both biologically and physically, proteins are important factors when considering the bilayer of a cell membrane. They are larger molecules that are used for a variety of functions involving the cell. The ones we will be interested in are those embedded into the membrane itself. While some proteins bond to the surface of the membrane [17], we are interested in those that are inserted directly into the surface. Due to the proteins' rigid structure, the surrounding membrane deforms to accommodate them (see Fig. 2).

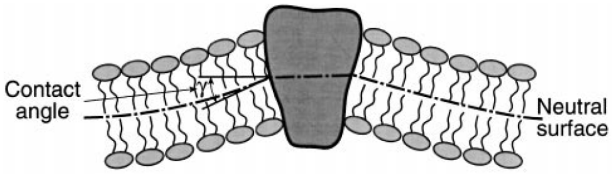

Figure 2: (from Hobbs [8]) The protein is included as part of the membrane and it deforms the shape and composition of the membrane around it.

Here we will consider vesicles as our model for cell membranes. These have a lipid bilayer but do not have the internal structure of the cell; for instance they lack nucleui, Golgi apparatus and cytoskeletons. Furthermore they can easily be created in a lab for the purpose of experiments.

The problem of modelling the cell's morphology is important to understanding how the cell interacts with its environment. Transmembrane proteins are embedded in the membrane [19, 5] and play an important role in transport, adhesion and signalling.

We will look at the effect that protein insertions into a cell membrane have on the membrane's shape. By examining the energy associated with these interactions, we are able to find how much the membrane is displaced by proteins.

Here we use a simplified model for the cell membrane, as a construction of pairs of lipids. Due to the relative size of the proteins and the width of the lipid bilayer to the overall cell, we will consider the bilayer as a surface.

3 State of art

In recent years a wide variety of models have been produced to attempt to understand different aspects of modelling cell membranes. For example [17] includes the analysis of interactions between protein scaffolds and [15] presents a model for protein inclusions. There are also models that include no proteins and instead try to gain a deep mathematical understanding of the behaviour of the bilayer [3]. The most relevant results to our topic are presented in [15] and in [3]. Proteins diffusing through the cell membrane are studied in [16] and an analysis of phase transition (e.g. a change of lipid concentration in the bilayer) is studied in [14] and [1].

In the paper by Grunau et al. [3] the authors investigate the Willmore equation with Dirichlet boundary conditions. Such techniques can be applied to our framework of vesicles. The surface is taken to be rotationally symmetric on which, given a smooth immersed surface $f : M \to \mathbb{R}^3$, the authors define the Willmore functional

$$W(f) = \int_{f(M)} H^2 dA, \tag{1}$$

where M is the reference manifold and H is the mean curvature on $f(M) = \Gamma$. The problem is reformulated in the hyperbolic half-plane and then the existence of a minimum to this problem together with certain properties of the minimiser are proved. It turns out that solutions to this must satisfy the Willmore equation

$$\Delta_\Gamma H + 2H(H^2 - K) = 0 \quad \text{on } \Gamma.$$

Turner's model [15] is a linearised model of a single protein inclusion, and its effect on the membrane (i.e. its deformation). It is concerned with a single inclusion located at the origin (see Fig. 3). The two functions describing the membrane are u (the height of the membrane) and φ (the composition difference of the lipids of the membrane).

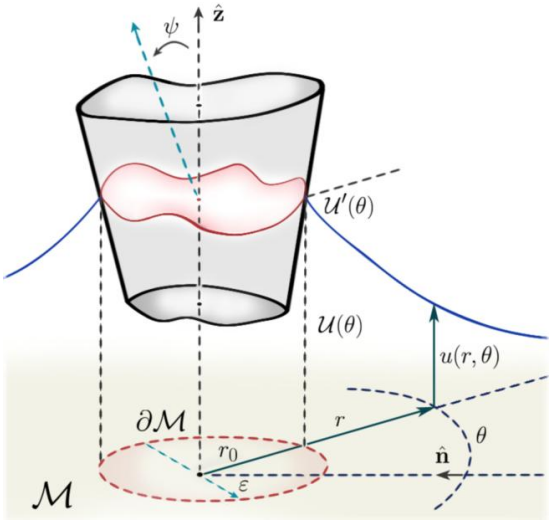

Figure 3: (from [15]) Illustration of the model of the inclusion of the protein considered in [15]. Here, u is the height of the membrane and the boundary conditions for u corresponding to the protein inclusions are described by functions $U(\theta)$ and $U'(\theta)$.

The energy functional $\mathcal{F}$ considered in [15] (labelled by (1) and (2) in the paper) consists of two parts. The first one, $\mathcal{F}_u$, is related to the bending energy of the lipids and the second one, $\mathcal{F}_\varphi$, their local compositional difference (a physical quality of the molecules). To see how the form of $\mathcal{F}_u$ is derived, we first consider the Helfrich energy of the surface Γ:

$$E = \int_\Gamma \frac{\kappa}{2} H^2 \, dA,$$

where, κ is the bending rigidity and H is the mean curvature. We will use the graph representation of Γ by writing $\Gamma = \{(x, y, u(x, y)) : (x, y) \in \Omega \subset \mathbb{R}^2\}$. This is known as the Monge gauge. In this form the mean curvature H in is given in local coordinates x, y by

$$H = \operatorname{div} \frac{\nabla u}{\sqrt{1 + |\nabla u|^2}}.$$

The area element dA of the surface Γ is given by $dA = \sqrt{1+|\nabla u|^2}dxdy$. If we assume the variation of u to be small, we can use an approximation of the form $u = \epsilon h$ where $\epsilon > 0$ is small. Through some calculations, we can see that this allows us to come up with the approximations $H \approx \Delta u$ and $dA \approx (1 + \frac{1}{2}|\nabla u|^2)dxdy$. Excluding $O(\epsilon^4)$ terms, this gives us a linearised form of the bending energy

$$E = \int_\Omega \frac{\kappa}{2}|\Delta u|^2 \, dxdy. \tag{2}$$

This is the first term appearing in $\mathcal{F}_u$. The other term comes from incorporating surface tension, which is given by $\frac{\sigma}{2}|\nabla u|^2$, where σ is the surface tension coefficient. This gives us the following form of the energy

$$\mathcal{F}_u = \frac{1}{2}\int_\Omega \left(\kappa|\Delta u|^2 + \sigma|\nabla u|^2\right) dxdy. \tag{3}$$

On the other hand, the functional $\mathcal{F}_\varphi$ is given by

$$\mathcal{F}_\varphi = \frac{1}{2}\int_\Omega \left(a\varphi^2 + b|\nabla\varphi|^2 + 2c\varphi\Delta u\right) dxdy, \tag{4}$$

where a, b and c are physical constants and φ is the compositional difference of lipids. The sum $\mathcal{F} = \mathcal{F}_u + \mathcal{F}_\phi$ describes the total energy of the membrane.

4 Mathematical analysis of the linearised free energy minimisation problem

Having derived a model, we now focus on rigorous mathematical formulation and prove the results regarding existence and uniqueness of a solution. We will consider the energy functional

$$\mathcal{F}(u,\phi) := \frac{1}{2}\kappa\int_\Omega |\Delta u|^2 + \frac{1}{2}\sigma\int_\Omega |\nabla u|^2 + \frac{1}{2}a\int_\Omega \phi^2 + \frac{1}{2}b\int_\Omega |\nabla\phi|^2 + c\int_\Omega \phi\Delta u \tag{5}$$

and we will supplement the energy minimisation problem with two kinds of boundary conditions: Dirichlet boundary conditions (Section 4.1) and Navier boundary conditions (Section 4.2). We focus separately on each of these boundary conditions.

4.1 Dirichlet boundary conditions

The Dirichlet boundary conditions are:

$$\begin{cases} u|_{\partial\Omega} = g, \\ \frac{\partial u}{\partial\nu}\big|_{\partial\Omega} = f, \\ \phi|_{\partial\Omega} = p, \end{cases} \tag{6}$$

where ν is the unit normal vector to $\partial\Omega$. Let $\Omega \subset \mathbb{R}^3$ be an open set with Lipschitz boundary $\partial\Omega$, $g, p \in H^{1/2}(\partial\Omega)$ and

$$V := H^2_{g,f}(\Omega) \times H^1_p(\Omega),$$

where we denote $H^2_{g,f}(\Omega) := \{u \in H^2(\Omega) \,|\, u = g \text{ on } \partial\Omega\,,\ \frac{\partial u}{\partial\nu} = f \text{ on } \partial\Omega\}$. Clearly, V is a closed, convex set of a Hilbert space

$$H := H^2(\Omega) \times H^1(\Omega) \tag{7}$$

equipped with the norm $||(v,\psi)||_H^2 := ||v||_{H^2(\Omega)}^2 + ||\psi||_{H^1(\Omega)}^2$. We note that the function set V incorporates the boundary conditions (6). For $(u,\phi) \in V$ consider functional (5).

4.1.1 Unique minimiser of the free energy functional

We have the following lemma

Lemma 1. If $c < \sqrt{\kappa a} + \sqrt{\sigma b}$, then $\mathcal{F}$ is α-convex on V.

Proof. If $c < \sqrt{\kappa a} + \sqrt{\sigma b}$ then there exists an $\epsilon > 0$ such that $\epsilon < \min\{\kappa, \sigma, a, b\}$ and

$$c \leq \sqrt{(\kappa-\epsilon)(a-\epsilon)} + \sqrt{(\sigma-\epsilon)(b-\epsilon)}.$$

We first note that, for all $v \in H^2(\Omega)$, $\psi \in H_0^1(\Omega)$, we have

$$\begin{aligned}
c\int_\Omega \psi\Delta v\,dx &\leq c\left|\int_\Omega \psi\Delta v\,dx\right| \\
&\leq \sqrt{(\kappa-\epsilon)(a-\epsilon)}\left|\int_\Omega \psi\Delta v\,dx\right| + \sqrt{(\sigma-\epsilon)(b-\epsilon)}\left|\int_\Omega \psi\Delta v\,dx\right| \\
&\leq \sqrt{(\kappa-\epsilon)(a-\epsilon)}||\psi||_{L^2}||\Delta v||_{L^2} \\
&\quad +\sqrt{(\sigma-\epsilon)(b-\epsilon)}\left|-\int_\Omega \nabla\psi\cdot\nabla v\,dx + \int_{\partial\Omega}\underbrace{\psi}_{=0}\frac{\partial v}{\partial\nu}\,dS(x)\right| \\
&\leq \sqrt{(\kappa-\epsilon)(a-\epsilon)}||\psi||_{L^2}||\Delta v||_{L^2} + \sqrt{(\sigma-\epsilon)(b-\epsilon)}||\nabla\psi||_{L^2}||\nabla v||_{L^2} \\
&\leq \frac{\kappa-\epsilon}{2}||\Delta v||_{L^2}^2 + \frac{a-\epsilon}{2}||\psi||_{L^2}^2 + \frac{\sigma-\epsilon}{2}||\nabla v||_{L^2}^2 + \frac{b-\epsilon}{2}||\nabla\psi||_{L^2}^2. \qquad (8)
\end{aligned}$$

Moreover, for any bilinear, symmetric form $a(\cdot,\cdot)$, using the identity $\lambda^2 - \lambda = (1-\lambda)^2 - (1-\lambda)$ we have

$$\begin{aligned}
& a(\lambda u_1 + (1-\lambda)u_2, \lambda u_1 + (1-\lambda)u_2) \\
= \;& \lambda^2 a(u_1,u_1) + (1-\lambda)^2 a(u_2,u_2) + 2\lambda(1-\lambda)a(u_1,u_2) \\
= \;& \lambda a(u_1,u_1) + (1-\lambda)a(u_2,u_2) + (\lambda^2-\lambda)(a(u_1,u_1)+a(u_2,u_2)) \\
& +2\lambda(1-\lambda)a(u_1,u_2) \\
= \;& \lambda a(u_1,u_1) + (1-\lambda)a(u_2,u_2) + (\lambda^2-\lambda)a(u_1-u_2,u_1-u_2). \qquad (9)
\end{aligned}$$

We also recall the Poincaré inequality:

$$||v||_{L^2} \leq C||\nabla v||_{L^2} \qquad \forall v \in H_0^1(\Omega), \qquad (10)$$

where $C > 0$ is a constant dependent only on the domain Ω. Moreover, for any $v \in H_{0,0}^2(\Omega)$, we have $\nabla v = 0$ on $\partial\Omega$ (because both the normal derivative and the tangent derivative vanish) and

$$||\Delta v||_{L^2} = |v|_{H^2}. \qquad (11)$$

The last statement follows from the following argument. Take $v \in C_0^\infty(\Omega)$ and write

$$\begin{aligned} ||\Delta v||_{L^2}^2 &= \int_\Omega \sum_{i,j=1}^3 \frac{\partial^2 v}{\partial x_i^2}\frac{\partial^2 v}{\partial x_j^2} dx = \sum_{i,j=1}^3 \left(-\int_\Omega \frac{\partial v}{\partial x_i}\frac{\partial^3 v}{\partial x_i \partial x_j^2} dx + \int_{\partial\Omega} \underbrace{\frac{\partial v}{\partial x_i}}_{=0} \frac{\partial^2 v}{\partial x_j^2} \right) \\ &= \sum_{i,j=1}^3 \left(\int_\Omega \frac{\partial^2 v}{\partial x_i \partial x_j}\frac{\partial^3 v}{\partial x_i \partial x_j} dx - \int_{\partial\Omega} \underbrace{\frac{\partial v}{\partial x_i}}_{=0} \frac{\partial^2 v}{\partial x_i \partial x_j} \right) = |v|_{H^2}^2. \end{aligned}$$

Using the fact that $H^2_{0,0}(\Omega) = \overline{C_0^\infty(\Omega)}^{||\cdot||_{H^2}}$ we can use the density argument to get (11).

We now let $\lambda \in [0,1]$ and consider a convex combination $\lambda(u_1,\phi_1)+(1-\lambda)(u_2,\phi_2) = (\lambda u_1+(1-\lambda)u_2, \lambda\phi_1+(1-\lambda)\phi_2)$. Applying the identity (9) to $\frac{1}{2}\kappa\int_\Omega \Delta u\,\Delta v\,dx$, $\frac{1}{2}\sigma\int_\Omega \nabla u\cdot\nabla v\,dx$, $\frac{1}{2}a\int_\Omega \phi\,\psi\,dx$, $\frac{1}{2}b\int_\Omega \nabla\phi\cdot\nabla\psi$ and using (8), we can write

$$\begin{aligned} & \mathcal{F}(\lambda(u_1,\phi_1)+(1-\lambda)(u_2,\phi_2)) \overset{(9)}{=} \lambda F(u_1,\phi_1)+(1-\lambda)F(u_2,\phi_2) \\ & -\frac{\lambda-\lambda^2}{2}(\kappa||\Delta u_1-\Delta u_2||_{L^2}^2+\sigma||\nabla u_1-\nabla u_2||_{L^2}^2+a||\phi_1-\phi_2||_{L^2}^2 \\ & +b||\nabla\phi_1-\nabla\phi_2||_{L^2}^2) - \lambda c\int_\Omega \phi_1\Delta u_1\,dx - (1-\lambda)c\int_\Omega \phi_2\Delta u_2 dx \\ & +c\int_\Omega (\lambda\phi_1+(1-\lambda)\phi_2)(\lambda\Delta u_1+(1-\lambda)\Delta u_2)dx \\ = \;& \lambda F(u_1,\phi_1)+(1-\lambda)F(u_2,\phi_2) \\ & -\frac{\lambda-\lambda^2}{2}(\kappa||\Delta u_1-\Delta u_2||_{L^2}^2+\sigma||\nabla u_1-\nabla u_2||_{L^2}^2+a||\phi_1-\phi_2||_{L^2}^2 \\ & +b||\nabla\phi_1-\nabla\phi_2||_{L^2}^2) - c(\lambda-\lambda^2)\int_\Omega (\phi_1-\phi_2)(\Delta u_1-\Delta u_2)dx \\ \overset{(8)}{\leq} \;& \lambda F(u_1,\phi_1)+(1-\lambda)F(u_2,\phi_2) \\ & -\frac{\epsilon(\lambda-\lambda^2)}{2}(||\Delta u_1-\Delta u_2||_{L^2}^2+||\nabla u_1-\nabla u_2||_{L^2}^2+||\phi_1-\phi_2||_{L^2}^2+||\nabla\phi_1-\nabla\phi_2||_{L^2}^2) \\ \overset{(10)}{\leq} \;& \lambda F(u_1,\phi_1)+(1-\lambda)F(u_2,\phi_2) \\ & -\frac{\epsilon(\lambda-\lambda^2)}{2}\left(\frac{1}{2}||\Delta u_1-\Delta u_2||_{L^2}^2+\frac{1}{2}||\nabla u_1-\nabla u_2||_{L^2}^2+\frac{1}{2C}||u_1-u_2||_{L^2}^2+||\phi_1-\phi_2||_{H^1}^2\right) \qquad (12) \\ \overset{(11)}{\leq} \;& \lambda F(u_1,\phi_1)+(1-\lambda)F(u_2,\phi_2)-\frac{\epsilon(\lambda-\lambda^2)}{4(1+C)}||(u_1,\phi_1)-(u_2,\phi_2)||_V^2. \end{aligned}$$

Hence α-convexity follows with $\alpha := \frac{\epsilon}{2(1+C)}$. □

Lemma 2. Consider the following minimisation problem:
Find $(u,\phi)\in V$, s.t.

$$\mathcal{F}(u,\phi) = \min_{(v,\psi)\in V} \mathcal{F}(v,\psi). \qquad (13)$$

If $c < \sqrt{\kappa a}+\sqrt{\sigma b}$, then this minimisation problem has a unique solution.

Proof. We note that K is a convex subset of V, which is a convex subset of $H^2(\Omega)\times H^1(\Omega)$, a Hilbert space. Hence the existence and uniqueness of a minimiser (u,ϕ) is a direct consequence of Theorem 2.7.1 from Elliott [4] and Lemma 1. □

4.1.2 Euler-Lagrange equations

Here we want to derive the Euler-Lagrange equations corresponding to the minimisation problem (13). We define $V_0 := H^2_{0,0}(\Omega) \times H^1_0(\Omega)$. Letting $(v, \psi) \in V_0$ and $t > 0$ we observe that $(u + tv, \phi + t\psi) \in V$. Hence

$$\mathcal{F}(u + tv, \phi + t\psi) - \mathcal{F}(u, \phi) \overset{(13)}{\geq} 0. \tag{14}$$

From here we can see that $\frac{d}{dt^+} [\mathcal{F}(u + tv, \phi + t\psi)]_{t=0} \geq 0$. Analogously, taking $-t$ instead of t in (14) we get $0 \leq \frac{d}{dt^+} [\mathcal{F}(u - tv, \phi - t\psi)]_{t=0} = \frac{d}{dt^-} [\mathcal{F}(u + tv, \phi + t\psi)]_{t=0}$. Hence

$$\begin{aligned} 0 &= \frac{d}{dt} [\mathcal{F}(u + tv, \phi + t\psi)]_{t=0} \\ &= \kappa \int_\Omega \Delta u \, \Delta v + \sigma \int_\Omega \nabla u \cdot \nabla v + a \int_\Omega \phi\psi + b \int_\Omega \nabla\phi \cdot \nabla\psi + c \int_\Omega \phi \Delta v + c \int_\Omega \psi \Delta u \\ &=: a((u, \phi), (v, \psi)), \end{aligned}$$

which is the weak formulation of the Euler-Lagrange equations. Consider a problem
Find $(u, \phi) \in V$ such that

$$a((u, \phi), (v, \psi)) = 0 \qquad \forall (v, \psi) \in V_0. \tag{15}$$

Then the solution $(u, \phi) \in V$ of (15) is the minimiser of $\mathcal{F}$ over V. Indeed, take any $(v, \psi) \in V$. From convexity of $\mathcal{F}$ we have $\mathcal{F}(tv + (1-t)u, t\psi + (1-t)\phi) \leq t\mathcal{F}(v, \psi) + (1-t)\mathcal{F}(u, \phi)$, which gives

$$\begin{aligned} \mathcal{F}(v, \psi) - \mathcal{F}(u, \phi) \quad &\geq \quad \frac{1}{t} [\mathcal{F}(u + t(v-u), \phi + t(\psi - \phi)) - \mathcal{F}(u, \phi)] \\ &\overset{t \to 0^+}{\longrightarrow} \quad a((u, \phi), (v - u, \psi - \phi)) = 0, \end{aligned}$$

where the inequality holds as $(v - u, \psi - \phi) \in V_0$.
In order to derive the PDE corresponding to the weak formulation (15), we formally integrate by parts to get

$$\begin{aligned} 0 &= -\kappa \int_\Omega \nabla\Delta u \cdot \nabla v + \kappa \int_{\partial\Omega} \underbrace{\frac{\partial v}{\partial \nu}}_{=0} \Delta u - \sigma \int_\Omega \Delta u \, v + \sigma \int_{\partial\Omega} \frac{\partial u}{\partial \nu} \underbrace{v}_{=0} + a \int_\Omega \phi\psi \\ &\quad - b \int_\Omega \Delta\phi \, \psi + b \int_{\partial\Omega} \frac{\partial \phi}{\partial \nu} \underbrace{\psi}_{=0} - c \int_\Omega \nabla\phi \cdot \nabla v + c \int_{\partial\Omega} \underbrace{\frac{\partial v}{\partial \nu}}_{=0} \phi + c \int_\Omega \psi \Delta u \\ &= \kappa \int_\Omega \Delta^2 u \, v - \kappa \int_{\partial\Omega} \frac{\partial(\Delta u)}{\partial \nu} \underbrace{v}_{=0} - \sigma \int_\Omega \Delta u \, v + a \int_\Omega \phi\psi - b \int_\Omega \Delta\phi \, \psi + c \int_\Omega \Delta\phi \, v \\ &\quad - c \int_{\partial\Omega} \frac{\partial \phi}{\partial \nu} \underbrace{v}_{=0} + c \int_\Omega \psi \Delta u \\ &= \int_\Omega \left(\kappa\Delta^2 u - \sigma\Delta u + c\Delta\phi\right) v + \int_\Omega \left(a\phi - b\Delta\phi + c\Delta u\right) \psi. \end{aligned}$$

Hence the Euler-Lagrange equations are

$$\begin{cases} \kappa\Delta^2 u - \sigma\Delta u + c\Delta\phi = 0, \\ a\phi - b\Delta\phi + c\Delta u = 0 \end{cases} \tag{16}$$

and they are equipped with boundary conditions (6).

4.1.3 What if $c \geq \sqrt{\kappa a} + \sqrt{\sigma b}$?

Suppose that $c \geq \sqrt{\kappa a} + \sqrt{\sigma b}$ and $\Omega := (0, 2\pi)^2$ and consider the functional (5) with $\kappa = a$ and $\sigma = b$. One can then show that $\mathcal{F}(\alpha(u_0, u_0))$ is concave with respect to α when $u_0(x, y) = \sin x \sin y$. Indeed, $\Delta u_0 = -2u_0$ and one can calculate that $\mathcal{F}(\alpha(u_0, u_0)) = -\alpha^2 \epsilon ||u_0||^2_{H^1}$ for some $\epsilon > 0$, which is a concave function of α. Hence such a $\mathcal{F}$ is not convex on $\{u \in H^2(\Omega) : u|_{\partial\Omega} = 0\} \times H^1_0(\Omega)$. In fact, $\mathcal{F}$ is not bounded below on this space, so the minimiser does not exist. As for the function set V, it is not clear how analyse it convexity (and hence the existence of the minimiser) for such c.

On the other hand suppose $\Omega' = \mathbb{R}^2 \setminus \overline{B(0,1)}$. The approach applied in Turner [15] uses modified Bessel functions $K_n(\cdot)$ to write the explicit form of the solution (u, ϕ) of the Euler-Lagrange equations (16) in Ω' (see (8), (9) in Turner [15]). In the stability region (i.e. when $c < \sqrt{\kappa a} + \sqrt{\sigma b}$) one can use the approximation $K_n(\rho) \approx \mathrm{e}^{-\rho}(\pi\rho/2)^{-1/2}$ when $\rho \gg n$ to obtain the asymptotic behaviour (i.e. for large $|x|$) of u

$$u(x) \sim \frac{1}{\sqrt{r}} \mathrm{e}^{-\lambda(\mathrm{r}-1)} \cos(\omega \mathrm{r} + \vartheta), \tag{17}$$

where ϑ depends only on the parameters σ, κ, a, b, c and λ and ω are given by the real and imaginary parts of

$$k_\pm = \frac{1}{2\sqrt{\kappa b}} \left(\sqrt{(\sqrt{\kappa a} + \sqrt{\sigma b})^2 - c^2} \pm \sqrt{(\sqrt{\kappa a} - \sqrt{\sigma b})^2 - c^2} \right).$$

(the numbers $k^2_\pm$ are the solutions of the characteristic equation $r^2(\kappa b) + r(c^2 - \sigma b - a\kappa) + \sigma a = 0$)
One can observe that λ becomes negative when c crosses the stability threshold $\sqrt{\kappa a} + \sqrt{\sigma b}$, from where the asymptotic approximation (17) suggests a blowup of u as $|x|$ tends to ∞. This is an unphysical behaviour and the region $c > \sqrt{\kappa a} + \sqrt{\sigma b}$ is called *Leiber unstable regime* (see e.g. Leiber [11], [12]).

4.2 Navier boundary conditions

Here we consider Navier boundary conditions:

$$\begin{cases} u|_{\partial\Omega} = g, \\ \Delta u|_{\partial\Omega} = f, \\ \phi|_{\partial\Omega} = p, \end{cases} \tag{18}$$

where $g, f, p \in H^{1/2}(\partial\Omega)$. As the second of the above boundary conditions is a *natural boundary condition* (rather than an *essential boundary condition*) we have to modify the energy functional (5) by adding the respective boundary terms $-\int_{\partial\Omega}(\kappa f + cp)\frac{\partial u}{\partial \nu} dS(x)$. These terms correspond to the energy required to impose the boundary conditions on the solution. Hence we will consider the energy functional of the form

$$\overline{\mathcal{F}}(u, \phi) := \mathcal{F}(u, \phi) - \int_{\partial\Omega} (\kappa f + cp) \frac{\partial u}{\partial \nu} dS(x). \tag{19}$$

We will consider the function set

$$W := \{v \in H^2(\Omega) \,|\, v|_{\partial\Omega} = g\} \times H^1_p(\Omega),$$

which is a convex, closed subset of Hilbert space $H^2(\Omega) \times H^1(\Omega)$. The respective energy minimisation problem is:

Find $(u,\phi)\in W$ such that

$$\overline{\mathcal{F}}(u,\phi)=\inf_{(v,\psi)\in W}\overline{\mathcal{F}}(v,\psi). \tag{20}$$

Our aim is to find a solution to the above minimisation problem. We have the following lemma:

Lemma 3. Suppose that $c<\sqrt{\kappa a}+\sqrt{\sigma b}$. Then the functional $\overline{\mathcal{F}}$ is α-convex W and the minimisation problem (20) has a unique solution.

Proof. The proof proceeds in the similar way as the in the case of Dirichlet boundary conditions (see proof of Lemma 1), except for the equivalence (11). In order to get a similar equivalence we use the C^2 regularity of $\partial\Omega$ and the elliptic regularity result (see e.g. Theorem 4 on p. 334 of Evans [6]) to write

$$||v||_{H^2(\Omega)}\leq C\left(||\Delta v||_{L^2(\Omega)}+||v||_{L^2(\Omega)}\right) \tag{21}$$

for $v\in H_0^1(\Omega)\cap H^2(\Omega)$ (this is because one can write that $v\in H_0^1(\Omega)$ is a solution to a (trivial) PDE $\Delta v=\Delta v$). Using (21) one obtains α-convexity in a similar way as in the proof of Lemma 1. The second part of the claim follows from Lemma 2. □

4.2.1 Euler-Lagrange equations

Let $W_0:=H_0^1(\Omega)\cap H^2(\Omega)\times H_0^1(\Omega)$Similarly as in Section 4.1.2, one can derive the Euler-Lagrange equations of the problem (20):

$$\overline{a}((u,\phi),(v,\psi))=0\qquad\forall(v,\psi)\in W_0, \tag{22}$$

where $(u,\phi)\in W$ is the minimiser of (20) and

$$\begin{aligned}\overline{a}((u,\phi),(v,\psi)) \;:=\; & \kappa\int_\Omega\Delta u\,\Delta v+\sigma\int_\Omega\nabla u\cdot\nabla v+a\int_\Omega\phi\psi+b\int_\Omega\nabla\phi\cdot\nabla\psi\\ & +c\int_\Omega\phi\Delta v+c\int_\Omega\psi\Delta u-\int_{\partial\Omega}(\kappa f+cp)\frac{\partial v}{\partial\nu}dS(x)\end{aligned} \tag{23}$$

We note that if $(u,\phi)\in W$ is a solution to (22) then it is also a solution to (20) (because $\overline{\mathcal{F}}$ is convex on W). We shall now focus on finding the solution to (22). We will find the solution by formal integration by parts some of the terms appearing in (23) and considering the substitution $w=\Delta u$ (the precise meaning will be given in the next section). This will enable us to simplify the Euler-Lagrange equations to the equation not involving u and we will find u by considering the following Dirichlet problem:

$$\begin{cases}\Delta u=w & \text{in }\Omega,\\ u|_{\partial\Omega}=g.\end{cases}$$

4.2.2 Existence of the solution (u,ϕ)

Let us consider the following problem: Find $w\in H_f^1(\Omega)$, $\phi\in H_p^1(\Omega)$ such that

$$\begin{aligned}0 \;=\; & \kappa\int_\Omega\nabla w\cdot\nabla v\,dx+\sigma\int_\Omega w\,v\,dx+a\int_\Omega\phi\,\psi\,dx+b\int_\Omega\nabla\phi\cdot\nabla\psi\,dx\\ & +c\int_\Omega\nabla\phi\cdot\nabla v\,dx+c\int_\Omega\psi\,w\,dx\qquad\qquad\forall v,\psi\in H_0^1(\Omega).\end{aligned} \tag{24}$$

We note that this problem comes up when one by integration by parts in (22) and substitution $w := \Delta u$. From here we define $u \in H^1_g$ to be the solution of

$$\int_\Omega \nabla u \cdot \nabla v \, dx = \int_\Omega w \, v \, dx \qquad \forall v \in H^1_0(\Omega). \tag{25}$$

In what follows we are going to show that, if $c^2 < 2\min\{\kappa b, \sigma a\}$, then (24) has a unique solution $(w, \phi) \in H^1_f(\Omega) \times H^1_p(\Omega)$ and that, given w, (25) has a unique solution $u \in H^1_g$. This will, in particular, give us the pair of functions $u \in H^1_g$, $\phi \in H^1_p(\Omega)$. We will then show that this pair of functions is the solution to the Euler-Lagrange equations (22).

Suppose $c^2 < 2\min\{\kappa b, \sigma a\}$. Then problem (24) has a unique solution. Indeed, writing $w = w_0 + w_f$ and $\phi = \phi_0 + \phi_p$, where $w_f \in H^1_f(\Omega)$, $\phi_p \in H^1_p(\Omega)$ are fixed, we can reformulate (24) as follows:
Find $(w_0, \phi_0) \in (H^1_0(\Omega))^2$ such that

$$A((w_0, \phi_0), (v, \psi)) = l(v, \psi) \qquad \forall (v, \psi) \in (H^1_0(\Omega))^2, \tag{26}$$

where

$$\begin{aligned} A((w_0, \phi_0), (v, \psi)) &:= \kappa \int_\Omega \nabla w_0 \cdot \nabla v \, dx + \sigma \int_\Omega w_0 \, v \, dx + a \int_\Omega \phi_0 \, \psi \, dx + b \int_\Omega \nabla \phi_0 \cdot \nabla \psi \, dx \\ &\quad + c \int_\Omega \nabla \phi_0 \cdot \nabla v \, dx + c \int_\Omega \psi \, w_0 \, dx, \\ l(v, \psi) &:= -A((w_f, \phi_p), (v, \psi)). \end{aligned}$$

Noting that $A(\cdot, \cdot)$ is a symmetric, bounded, bilinear form on $(H^1_0(\Omega))^2 \times (H^1_0(\Omega))^2$ and that $l(\cdot)$ is a bounded linear functional on $(H^1_0(\Omega))^2$ we only need to check coercivity of $A(\cdot, \cdot)$ on $(H^1_0(\Omega))^2$. For $c^2 < 2\min\{\kappa b, \sigma a\}$ we can write that $c^2 \leq 2\min\{(\kappa - \epsilon)(b - \epsilon), (\sigma - \epsilon)(a - \epsilon)\}$ for some $\epsilon > 0$. We have

$$\begin{aligned} A((v, \psi), (v, \psi)) &= \kappa |v|^2_{H^1} + \sigma ||v||^2_{L^2} + b|\psi|^2_{H^1} + a||\psi||^2_{L^2} + c \int_\Omega \nabla \psi_0 \cdot \nabla v \, dx + c \int_\Omega \psi \, v \, dx \\ &\geq \kappa |v|^2_{H^1} + \sigma ||v||^2_{L^2} + b|\psi|^2_{H^1} + a||\psi||^2_{L^2} - \sqrt{2(\kappa - \epsilon)(b - \epsilon)}|\psi|_{H^1}|v|^2_{H^1} \\ &\quad - \sqrt{2(\sigma - \epsilon)(a - \epsilon)}||\psi||_{L^2}||v||_{L^2} \\ &\geq \kappa |v|^2_{H^1} + \sigma ||v||^2_{L^2} + b|\psi|^2_{H^1} + a||\psi||^2_{L^2} - (\kappa - \epsilon)|v|^2_{H^1} - (b - \epsilon)|\psi|^2_{H^1} \\ &\quad - (\sigma - \epsilon)||v||^2_{L^2} - (a - \epsilon)||\psi||^2_{L^2} \\ &= \epsilon(||v||^2_{H^1} + ||\psi||^2_{H^1}), \end{aligned} \tag{27}$$

where we have used Cauchy-Schwarz inequality and Young's inequality. Hence the bilinear form $A(\cdot, \cdot)$ is coercive and Lax-Milgram theorem gives existence and uniqueness of solution $(w_0, \phi_0) \in (H^1_0(\Omega))^2$ to the problem (26) and hence the existence of solution $(w, \phi) \in H^1_f(\Omega) \times H^1_p(\Omega)$ to the problem (24). The uniqueness can be proved as follows: Suppose there exist $(w_1, \phi_1), (w_2, \phi_2) \in H^1_f(\Omega) \times H^1_p(\Omega)$ solving (24). Then $(w_1 - w_2, \phi_1 - \phi_2) \in (H^1_0(\Omega))^2$ satisfies $A((w_1 - w_2, \phi_1 - \phi_2), (v, \psi)) = 0$ for all $(v, \psi) \in H^1_0(\Omega)$ and hence, taking $(v, \psi) := (w_1 - w_2, \phi_1 - \phi_2)$, we have

$$0 = A((w_1 - w_2, \phi_1 - \phi_2), (w_1 - w_2, \phi_1 - \phi_2)) \overset{(27)}{\geq} \epsilon(||w_1 - w_2||^2_{H^1} + ||\phi_1 - \phi_2||^2_{H^1}) \geq 0,$$

which implies that $w_1 = w_2$, $\phi_1 = \phi_2$ and hence establishes uniqueness.

Also, problem (25) has a unique solution. Indeed, writing $u = u_0 + u_g$, where $u_0 \in H^1_0(\Omega)$ and $u_g \in H^1_g(\Omega)$ is a fixed function (by the surjectivity of the trace operator), gives $\int_\Omega \nabla u_0 \cdot \nabla v \, dx = \int_\Omega wv \, dx - \int_\Omega \nabla u_g \cdot \nabla v \, dx$, from where we use the Poincaré inequality to show the coercivity of the associated bilinear, symmetric and bounded form and get the existence and uniqueness of the solution $u_0 \in H^1_0(\Omega)$ by usual argument using Lax-Milgram theorem. This gives the existence of the solution $u \in H^1_g(\Omega)$ to the problem (25). Suppose there are two solution u_1, u_2 to (25). Then $u_1 - u_2 \in H^1_0(\Omega)$ satisfies $\int_\Omega \nabla(u_1 - u_2) \cdot \nabla v \, dx = 0$ for all $v \in H^1_0(\Omega)$ and, taking $v := u_1 - u_2$, we may write

$$0 = \int_\Omega \nabla(u_1 - u_2) \cdot \nabla(u_1 - u_2) \, dx = ||\nabla(u_1 - u_2)||^2_{L^2}.$$

Hence $\nabla(u_1 - u_2) = 0$ in Ω, which implies that $u_1 - u_2 = const$. From homogeneous boundary conditions we get $u_1 = u_2$. Hence the solution $u \in H^1_g(\Omega)$ to the problem (25) is unique.

We will now prove that the solution (u, ϕ) obtained by solving equations (25), (24) is in fact the solution of the problem (22). Firstly, using the interior regularity of the weak solutions to elliptic PDEs (see e.g. Theorem 1 and the following Remark on pp. 327,328 of Evans [6]) we note that (25) gives $u \in H^2_{loc}(\Omega)$, $\Delta u = w$ almost everywhere in Ω and $||\Delta u||_{L^2} = ||w||_{L^2} < \infty$. Hence $(u, \phi) \in W$. Noting that $W_0 \subset (H^1_0(\Omega))^2$, we write, for $(v, \psi) \in W_0$,

$$\begin{aligned}
0 \overset{(24)}{=} \; & \kappa \int_\Omega \nabla w \cdot \nabla v \, dx + \sigma \int_\Omega w \, v \, dx + a \int_\Omega \phi \, \psi \, dx + b \int_\Omega \nabla \phi \cdot \nabla \psi \, dx \\
& + c \int_\Omega \nabla \phi \cdot \nabla v \, dx + c \int_\Omega \psi \, w \, dx \\
\overset{(25)}{=} \; & -\kappa \int_\Omega \underbrace{w}_{=\Delta u} \Delta v \, dx + \kappa \int_{\partial\Omega} \frac{\partial v}{\partial \nu} \underbrace{w}_{=f} \, dS(x) - \sigma \int_\Omega \nabla u \cdot \nabla v \, dx + a \int_\Omega \phi \, \psi \, dx \\
& + b \int_\Omega \nabla \phi \cdot \nabla \psi \, dx + c \int_\Omega \nabla \phi \cdot \nabla v \, dx - c \int_\Omega \nabla u \cdot \nabla \psi \, dx \\
= \; & -\kappa \int_\Omega \Delta u \, \Delta v \, dx + \kappa \int_{\partial\Omega} \frac{\partial v}{\partial \nu} f \, dS(x) - \sigma \int_\Omega \nabla u \cdot \nabla v \, dx + a \int_\Omega \phi \, \psi \, dx + b \int_\Omega \nabla \phi \cdot \nabla \psi \, dx \\
& - c \int_\Omega \phi \Delta v \, dx + c \int_{\partial\Omega} \underbrace{\phi}_{=p} \frac{\partial v}{\partial \nu} dS(x) + c \int_\Omega \psi \Delta u \, dx - \int_{\partial\Omega} \frac{\partial u}{\partial \nu} \underbrace{\psi}_{=0} \, dS(x),
\end{aligned}$$

which, after taking $-v$ in place of v, gives (22). This together with Lemma 3 proves that (u, ϕ) obtained by solving the system of equations (25), (24) is the unique solution of the minimisation problem (20).

Remark 1. Here we have assummed a C^2 regularity of $\partial\Omega$, but the result is still true when $\partial\Omega$ is only Lipschitz. In fact, in the case of Lipschitz boundary one could replace Lemma 3 with stating only strict convexity of $\overline{\mathcal{F}}$ on W and hence the uniqueness of the solution. The existence of the solution follows from solving problems (24), (25).

5 Numerical approximation of the solution

Here we want to find a discretized approximations of problems (13) (corresponding to the Dirichlet boundary conditions) and (20) (corresponding to the Navier boundary conditions). In both cases we will use the finite element method. We will use non-conforming Morley elements together with piecewise affine elements for solving the Dirichlet boundary problem and piecewise affine elements for solving the Navier boundary problem. In the discretisation we commit a variational crime of assuming that $\Omega = \Omega_h$ (where Ω_h is the

computational domain), where in fact Ω_h is going to be a polyhedral approximation.

5.1 Dirichlet boundary problem

5.1.1 Morley elements

Now that we have existence for our problem we would like to solve it numerically. For this we use finite element method. We will be using a combination of Morley elements (for u) and piecewise affine elements (for ϕ). The Morley elements are non-conforming ones, which means that the discretised function space is not a subspace of the original space. In fact, the solution of the discretised problem may not even be continuous. However, the advantage of this approach is that we can use lower order polynomial basis functions in each triangle, which makes the implementation of the numerical scheme much easier.

The Morley element is used widely throughout different elliptic PDE problems (see e.g. [22], [18], [20]). However, there are no results known to authors where a combination of Morley elements and piecewise affine elements is used in the same system.

We approximate Ω by a polyhedral domain Ω_h. For a subset $T \subset \Omega_h$ let $P^2(T)$ denote the space of quadratic polynomials on T. Let $\mathcal{T}$ be a triangulation of the computational domain Ω_h.

Definition 1. The Morley Element is the triple $(T, P^2(T), \mathcal{N})$ where T is a triangular element, $P^2(T)$ is the space of quadratic polynomials defined on T, and $\mathcal{N} = \{\mathcal{N}_1, \mathcal{N}_2, \mathcal{N}_3, \mathcal{N}_4, \mathcal{N}_5, \mathcal{N}_6\}$ is the set of nodal variables, where

$$\begin{aligned}
\mathcal{N}_1(u_h) &:= u_h(z_1), \qquad \mathcal{N}_4(u_h) := \frac{\partial u_h}{\partial \nu} u_h(z_4), \\
\mathcal{N}_2(u_h) &:= u_h(z_2), \qquad \mathcal{N}_5(u_h) := \frac{\partial u_h}{\partial \nu} u_h(z_5), \\
\mathcal{N}_3(u_h) &:= u_h(z_3), \qquad \mathcal{N}_6(u_h) := \frac{\partial u_h}{\partial \nu} u_h(z_6).
\end{aligned}$$

More details about the Morley element can be found in [10] and [21]. From here we can define the discretised function set.

5.1.2 The discretised function set

Let $\mathcal{T} = (T_1, \ldots, T_M)$ be a triangulation of the computational domain Ω_h. Let each triangle $T \in \mathcal{T}$ be eqiupped with the anti-clockwise local numbering V_1^T, V_2^T, V_3^T of vertices. For $k \in \{1, 2, 3\}$ we will denote by V_{k+1}^T the neighbouring (in the anti-clockwise direction) vertex of the vertex V_k^T in the triangle $T \in \mathcal{T}$ (in particular we identify $V_4^T = V_1^T$). We will say that the triangle $T_1 \in \mathcal{T}$ *adjoins* to the triangle $T_2 \in \mathcal{T}$ (denoted by $T_1 \parallel T_2$) if they have a common edge, i.e. if there exist $k, m \in \{1, 2, 3\}$ s.t. $V_k^{T_1} V_{k-1}^{T_1} = V_m^{T_2} V_{m+1}^{T_2}$ (cf. Figure 4), where $AB \subset \mathbb{R}^2$ denotes the interval with endpoints $A, B \in \mathbb{R}^2$. If $T_1 \parallel T_2$, we also denote $M^{T_1 T_2} := (V_k^{T_1} + V_{k-1}^{T_1})/2 = (V_m^{T_2} + V_{m+1}^{T_2})/2$ (cf. Figure 4).

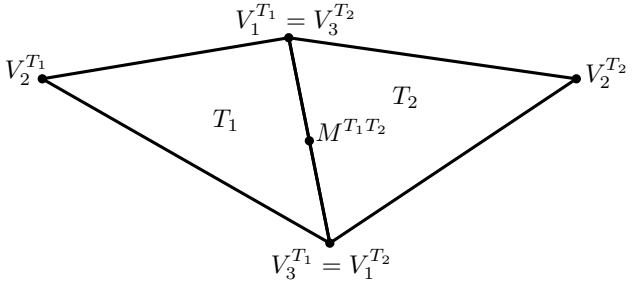

Figure 4: The adjoining triangles T_1 and T_2 (here $k = 1$, $m = 3$).

Let u, ϕ be functions defined on Ω_h such that $u|_T \in \mathcal{P}^2(T)$, $\phi|_T \in \mathcal{P}^1(T)$ for all $T \in \mathcal{T}$, where $\mathcal{P}^n(T)$ denotes the space of polynomials of degree n on $T \subset \mathbb{R}^2$. Let $T_i \parallel T_j$ for some $i, j \in \{1, \ldots, M\}$. We say that u *agree on the common edge* $V_k^{T_1} V_{k-1}^{T_1} = V_m^{T_2} V_{m+1}^{T_2}$ of T_i and T_j (denoted by $u|_{T_i} \doteq u|_{T_j}$) if

$$\begin{cases} u|_{T_1}(V_k^{T_1}) = u|_{T_2}(V_m^{T_2}), \\ u|_{T_1}(V_{k-1}^{T_1}) = u|_{T_2}(V_{m+1}^{T_2}). \end{cases}$$

In other words, $u|_{T_i} \doteq u|_{T_j}$ if the values of u agrees at the endpoints of the common edge of T_i and T_j. Furthermore, we will say that u *and its normal derivative at the midpoint agree on the common edge*$V_k^{T_1} V_{k-1}^{T_1} = V_m^{T_2} V_{m+1}^{T_2}$ of T_i and T_j (denoted by $u|_{T_i} \fallingdotseq u|_{T_j}$) if $u|_{T_i} \doteq u|_{T_j}$ and

$$\frac{\partial\, u|_{T_1}}{\partial \nu_k^{T_1}}(M^{T_1 T_2}) = -\frac{\partial\, u|_{T_2}}{\partial \nu_{m+1}^{T_2}}(M^{T_1 T_2}),$$

where n_k^T is the normal vector to $V_k^T V_{k-1}^T$ pointing outwards T. In other words, $u|_{T_i} \fallingdotseq u|_{T_j}$ if the values of u agrees at the endpoints of the common edge of T_i and T_j and the outward normal derivative at the midpoint $M^{T_i T_j}$ from the side of T_1 agrees with the inward normal derivative at the same point from the side of T_2.
Let

$$\begin{aligned} V_h \;:=\; \Big\{ & (u,\phi) : \overline{\Omega_h} \to \mathbb{R}^2 \;:\; u|_T \in \mathcal{P}^2(T),\, \phi|_T \in \mathcal{P}^1(T) \;\; \forall T \in \mathcal{T}, \\ & u|_{T_i} \fallingdotseq u|_{T_j} \;\text{ and }\; \phi|_{T_i} \doteq \phi|_{T_j} \;\text{ whenever } T_i \parallel T_j \Big\} \end{aligned}$$

be the discretized function space equipped with the norm defined by

$$||(u,\phi)||_{V_h}^2 := \sum_{T \in \mathcal{T}} \left(||u||_{H^2(T)}^2 + ||\phi||_{H^1(T)}^2 \right).$$

We note V_h is the cartesian product of the Morley element space (for u) and the piecewise linear element space (for ϕ).

5.1.3 Mathematical analysis of the discretisation

Consider a symmetric, bilinear form $\widehat{a}(\cdot,\cdot) : V_h \times V_h \to \mathbb{R}$ defined by

$$\begin{aligned} \widehat{a}((u,\phi),(v,\psi)) \;:=\; & \sum_{T \in \mathcal{T}} \Big(\kappa \int_T \Delta u\, \Delta v\, dx + \sigma \int_T \nabla u \cdot \nabla v\, dx + a \int_T \phi\, \psi\, dx + b \int_T \nabla \phi \cdot \nabla \psi\, dx \\ & + c \int_T \phi \Delta v\, dx + c \int_T \psi \Delta u\, dx \Big). \end{aligned}$$

We note that $\widehat{a}(\cdot,\cdot)$ is bounded on $V_h \times V_h$. Indeed,

$$\begin{aligned} |\widehat{a}((u,\phi),(v,\psi))| \;\le\; & \sum_{T \in \mathcal{T}} \big(\kappa ||\Delta u||_{L^2(T)} ||\Delta v||_{L^2(T)} + \sigma ||\nabla u||_{L^2(T)} ||\nabla v||_{L^2(T)} + a ||\phi||_{L^2(T)} ||\psi||_{L^2(T)} \\ & + b ||\nabla \phi||_{L^2(T)} ||\nabla \psi||_{L^2(T)} + c ||\phi||_{L^2(T)} ||\Delta v||_{L^2(T)} + c ||\psi||_{L^2(T)} ||\Delta u||_{L^2(T)} \big) \\ \le\; & C(\kappa,\sigma,a,b,c) \left(||(u,\phi)||_{V_h} ||(v,\psi)||_{V_h} \right). \end{aligned}$$

Now, let $V_1, \ldots, V_N$ denote the nodes of the triangulation that are located on the boundary of Ω_h and let $M_1, \ldots, M_N$ denote the midpoints of the edges located at the boundary of $\partial\Omega_h$.
Let

$$V_h^{f,g,p} := \left\{ (u,\phi) \in V_h \,:\, u(V_i) = g_i,\ \phi(V_i) = p_i,\ \frac{\partial u}{\partial \nu_i}(M_i) = f_i,\ i = 1, \ldots, N \right\},$$

where $g_i = g(V_i)$, $f_i = f(M_i)$, $p_i = p(V_i)$ and n_i is the outward normal vector to V_iV_{i+1}, $i = 1, \ldots, N$. The discretisation of the problem (4.1.2) problem is:
Find $(u,\phi) \in V_h^{f,g,p}$ such that

$$\widehat{a}((u,\phi),(v,\psi)) = 0 \qquad \forall (v,\psi) \in V_h^{0,0,0}. \tag{28}$$

This problem has a unique solution if $c \leq \sqrt{\kappa a}$. We note that this is a weaker condition than $c < \sqrt{\kappa a} + \sqrt{\sigma b}$ considered in Lemma 1, but we hope that this result could be improved. For the proof of this result note that we can decompose u into $u_{g,f} + u_{0,0}$ and ϕ into $\phi_p + \phi_0$, where $(u_{g,f}, \phi_p) \in V_h^{f,g,p}$ and $(u_{0,0}, \phi_0) \in V_h^{0,0,0}$ (this can be done by writing u as a linear combination of the Morley nodal basis functions corresponding to the appropriate degrees of freedom in the triangles located at the boundary edges, and similarly for ϕ with piecewise linear nodal basis functions). We can then rewrite (28) in the form:
Find $(u_{0,0}, \phi_0) \in V_h^{0,0,0}$ such that

$$\widehat{a}((u_{0,0},\phi_0),(v,\psi)) = l(\,(v,\psi)\,) \qquad \forall (v,\psi) \in V_h^{0,0,0}, \tag{29}$$

where $l(\,(v,\psi)\,) := -\widehat{a}((u_{g,f},\phi_p),(v,\psi))$. Clearly $l(\cdot)$ is a bounded linear functional on V_h (this is because $\widehat{a}(\cdot,\cdot)$ is a bounded bilinear form on $V_h \times V_h$). What is more $\widehat{a}(\cdot,\cdot)$ is an inner product on the space $V_h^{0,0,0}$. For this, we only need to show that $\widehat{a}(\cdot,\cdot)$ is non-degenerate. Clearly $\widehat{a}((u,\phi),(u,\phi)) \geq 0$ for all $(u,\phi) \in V_h^{0,0,0}$. Suppose now that $(u,\phi) \in V_h^{0,0,0}$ is such that $\widehat{a}((u,\phi),(u,\phi)) = 0$. We then have

$$\begin{aligned}
0 &= \sum_{T\in\mathcal{T}} \left(\kappa ||\Delta u||^2_{L^2(T)} + \sigma ||\nabla u||^2_{L^2(T)} + a||\phi||^2_{L^2(T)} + b||\nabla\phi||^2_{L^2(T)} + 2c\int_T \phi \Delta u \, dx \right) \\
&\geq \sum_{T\in\mathcal{T}} \left(\kappa ||\Delta u||^2_{L^2(T)} + \sigma ||\nabla u||^2_{L^2(T)} + a||\phi||^2_{L^2(T)} + b||\nabla\phi||^2_{L^2(T)} - 2\sqrt{\kappa}||\Delta u||_{L^2(T)}\sqrt{a}||\phi||_{L^2(T)} \right) \\
&\geq \sum_{T\in\mathcal{T}} \left(\sigma ||\nabla u||^2_{L^2(T)} + b||\nabla\phi||^2_{L^2(T)} \right) \geq 0,
\end{aligned}$$

which implies that $\nabla u = \nabla\phi = 0$ in every $T \in \mathcal{T}$. This means that u is constant in each $T \in \mathcal{T}$ and from the fact that values of u agree at the vertices of every two neighbouring triangles (i.e. $u|_{T_i} \doteq u|_{T_j}$ whenever $T_i \parallel T_j$) we get that u is constant in Ω_h. From the fact that $u(V_i) = 0$ for any $V_i \in \partial\Omega_h$ we get $u \equiv 0$. By the same argument we show that $\phi \equiv 0$. Hence $\widehat{a}(\cdot,\cdot)$ is an inner product on $V_h^{(0,0,0)} \times V_h^{(0,0,0)}$. Consequently, the existence of the solution of the problem (29) follows from the Riesz Representation Theorem (see e.g. Yosida [23], p. 90). Hence the existence of a solution to the problem (28). The uniqueness of solution to (28) follows from the observation that if (u_1,ϕ_1), (u_2,ϕ_2) satisfy (28) then $(u_1 - u_2, \phi_1 - \phi_2) \in V_h^{(0,0,0)}$ satisfy $\widehat{a}((u_1 - u_2, \phi_1 - \phi_2),(v,\psi)) = 0$ for all $(v,\psi) \in V_h^{(0,0,0)}$. Therefore in particular $\widehat{a}((u_1 - u_2, \phi_1 - \phi_2),(u_1 - u_2, \phi_1 - \phi_2)) = 0$ and non-degeneracy of $\widehat{a}(\cdot,\cdot)$ implies $(u_1,\phi_1) = (u_2,\phi_2)$.

We do not prove convergence of the solution to the discretised problem to the exact solution. Some results regarding convergence of the Morley element method can be found in [20], [18], [9], [13] and [22], but the analysis of the convergence of the combination of Morley elements and piecewise affine elements exceeded the time-frame of the research study group. Instead we will present the numerical convergence results.

5.2 Navier boundary problem

5.2.1 Piecewise linear elements

Suppose that $\mathcal{T} = (T_1, \ldots, T_M)$ is a triangulation of the computational domain Ω_h. In the case of Navier boundary conditions one can consider piecewise affine elements for w, ϕ and u. Let $V_1, \ldots, V_K$ be the nodes of the triangulation with $V_1, \ldots, V_N$ being the nodes in the interior of Ω_h and $V_{N+1}, \ldots, V_K$ being the nodes on the boundary. Let

$$W_h := \left\{ u_h \in H^1(\Omega_h) \,:\, u_h|_T \in \mathcal{P}^1(T) \;\; \forall T \in \mathcal{T} \right\}$$

be the discretized function space. This is the space corresponding to the the standard piecewise linear finite element basis functions. Let also, for $g \in C(\partial\Omega)$,

$$W_h^g := \{ u_h \in W_h \,:\, u_h(V_{N+i}) = g(V_{N+1}) \;\; \forall i = 1, \ldots K - N \} .$$

We note that $W_h^0 \subset H_0^1(\Omega_h)$.

5.2.2 Mathematical analysis of the discretisation

We write the discretizations of the problems (24) and (25):

1. Find $(w_h, \phi_h) \in W_h^f \times W_h^p$ such that

$$A((w_h, \phi_h), (v_h, \psi_h)) = 0 \qquad \forall (v_h, \psi_h) \in (W_h^0)^2. \tag{30}$$

2. Find $u_h \in W_h^g$ such that

$$\int_{\Omega_h} \nabla u_h \cdot \nabla v_h \, dx = \int_{\Omega_h} w_h \, v_h \, dx \qquad \forall v_h \in W_h^0. \tag{31}$$

The existence and uniqueness of solutions $(w_h, \phi_h) \in W_h^f(\Omega) \times W_h^p$, $u \in W_h^g$ to the problems (30) and (31), respectively, follows by the similar argument as presented in Section 4.2.2. Indeed, here the discretized function spaces are subspaces of the respective Hilbert spaces considered in Section 4.2.2. Hence the boundedness and coercivity of the respective bilinear forms and the boundedness of the respective linear functional follows in the similar way as presented in Section 4.2.2.

5.2.3 Convergence rate of the approximation

We will prove the convergence rate in the case $c^2 < 2\min\{\kappa b, \sigma a\}$ (we note that this is the weaker condition than the condition $c < \sqrt{\kappa a} + \sqrt{\sigma b}$ considered in Lemma 3). If this condition is satisfied then $c^2 < 2\min\{(\kappa - \epsilon)(b - \epsilon), (\sigma - \epsilon)(a - \epsilon)\}$ for every $\epsilon > 0$ such that

$$\epsilon \leq \frac{1}{2} \min\{(\kappa + b - \sqrt{(\kappa - b)^2 + 2c^2}), (\sigma + a - \sqrt{(\sigma - a)^2 + 2c^2})\}.$$

It is important to note that the bilinear form $A(\cdot, \cdot)$ is coercive on $H_0^1(\Omega)$ with such an ϵ (cf. (27)).These interactions seems to suggest a attractive/repulsive relationship exists between inclusions. Inclusions of the same type desire to be a certain distance from each other. This is in contrast to the case of inclusions with oposite Neumann values. Here the inclusions only repeal each other, the slight increases seen at long distances are due to the inclusions being closer to the boundary of the whole domain. These ideal distances are likely a result of the paramter conditions. We do not know if the paramter values we have taken are

biologically accurate. For this we need to make several assumptions. We assume $\Omega = \Omega_h$. In other words we will derive an error bound between u_h, ϕ_h solving (31), (30) and u, ϕ solving (25), (24), but in the domain Ω_h instead of Ω (as considered in Section 4.2). This is one of the variational crimes. We also take f, g, p to be constant functions on each components of the boundary $\partial\Omega_h$ and assume that $u \in H^1_g(\Omega_h)$, $w \in H^1_f(\Omega_h)$, $\phi \in H^1_p(\Omega_h)$ solving (25), (24) belong to the function space $H^2(\Omega_h)$.
Let $\mathcal{T}$ be such that $\max_{T\in\mathcal{T}} \operatorname{diam} T \leq h$ for some $h > 0$. Let $(w_h, \phi_h) \in W^f_h \times W^p_h$ be the (unique) solution to (30) and let $u \in W^g_h$ be the (unique) solution to (31) (with the right hand side depending on w_h).
Let also $(w, \phi) \in H^1_f(\Omega_h) \times H^1_p(\Omega_h)$ be the (unique) solution to (24) and let $u \in H^1_g(\Omega_h)$ be the (unique) solution to (25) (with the right hand side depending on w). We note that $w - w_h, \phi - \phi_h, u - u_h \in H^1_0(\Omega_h)$ (because f, g, p are constant on each component of $\partial\Omega_h$). Taking $v := v_h \in W^0_h$ and $\phi = \phi_h \in W^0_h$ in (24) and subtracting (30) we obtain the following Galerkin orthogonality relation:

$$A((w - w_h, \phi - \phi_h), (v_h, \psi_h)) = 0 \qquad \forall (v_h, \psi_h) \in W^0_h. \tag{32}$$

We write, for all $(v_h, \psi_h) \in W^0_h$,

$$\begin{aligned}
\epsilon(||w - w_h||^2_{H^1} + ||\phi - \phi_h||^2_{H^1}) &\leq A((w - w_h, \phi - \phi_h), (w - w_h, \phi - \phi_h)) \\
&\overset{(32)}{=} A((w - w_h, \phi - \phi_h), (w - v_h, \phi - \psi_h)) \\
&\leq C_0 \sqrt{||w - w_h||^2_{H^1} + ||\phi - \phi_h||^2_{H^1}} \sqrt{||w - v_h||^2_{H^1} + ||\phi - \psi_h||^2_{H^1}},
\end{aligned}$$

where C_0 is the boundedness coefficient of $A(\cdot, \cdot)$. Taking $\min_{(v_h,\psi_h)\in(W^0_h)^2}$ in the above inequality we obtain the Cea's lemma of the form

$$\sqrt{||w - w_h||^2_{H^1} + ||\phi - \phi_h||^2_{H^1}} \leq \frac{C_0}{\epsilon} \min_{(v_h,\psi_h)\in(W^0_h)^2} \sqrt{||w - v_h||^2_{H^1} + ||\phi - \psi_h||^2_{H^1}}. \tag{33}$$

Now using the interpolation result

$$\min_{v_h \in W^0_h} ||w - v_h||_{H^1(\Omega_h)} \leq \overline{C} h |w|_{H^2(\Omega_h)}, \tag{34}$$

which holds for some positive constant C (see e.g. Theorem 4.4.20 on p. 108 of Brenner & Ridgway Scott [2] for the proof), we get

$$||w - w_h||^2_{H^1(\Omega_h)} + ||\phi - \phi_h||^2_{H^1(\Omega_h)} \leq \left(\frac{C_0\,\overline{C}}{\epsilon}\right)^2 h^2 (|w|^2_{H^2(\Omega_h)} + |\phi|^2_{H^2(\Omega_h)}), \tag{35}$$

which is an error bound for w_h and ϕ_h. In particular we get

$$||w - w_h||_{L^2(\Omega_h)} \leq \frac{C_0\,\overline{C}}{\epsilon} h \sqrt{|w|^2_{H^2(\Omega_h)} + |\phi|^2_{H^2(\Omega_h)}}. \tag{36}$$

Now let $u_h \in W^g_h$ be the (unique) solution to (31) and $u \in H^1_g(\Omega)$ be the (unique) solution to (25). Take $v := v_h \in W^0_h$ in (25) and subtract (31) to get

$$\int_{\Omega_h} (\nabla u - \nabla u_h) \cdot \nabla v_h \, dx = \int_{\Omega_h} (w - w_h) v_h \, dx \tag{37}$$

We can see that we don't get the Galerkin orthogonality relation in this case. This is because of the variational crime (note that the right hand side functional is different in (25) and in (31)) and in what follows we will need to make use of the error bound (36) to get an error bound for u_h. Similarly as before we note that

$u - u_h \in H_0^1(\Omega_h)$. Hence, using the Poincaré inequality (10), we can write, for all $v_h \in W_h^0$,

$$\begin{aligned}
\frac{1}{1+C}||u-u_h||_{H^1}^2 &\overset{(10)}{\leq} ||\nabla u - \nabla u_h||_{H^1}^2 = \int_{\Omega_h} (\nabla u - \nabla u_h)\cdot(\nabla u - \nabla u_h)\,dx \\
&\overset{(37)}{=} \int_{\Omega_h} (\nabla u - \nabla u_h)\cdot(\nabla u - \nabla v_h) - \int_{\Omega_h} (w - w_h)(u_h - v_h)\,dx \\
&\leq ||\nabla u - \nabla u_h||_{L^2}||\nabla u - \nabla v_h||_{L^2} + ||w - w_h||_{L^2}||u_h - v_h||_{L^2} \\
&\leq ||u-u_h||_{H^1}||\nabla u - \nabla v_h||_{L^2} + ||w-w_h||_{L^2}(||u-u_h||_{H^1} + ||u-v_h||_{H^1}).
\end{aligned}$$

Hence

$$\frac{1}{1+C}||u-u_h||_{H^1} \leq ||u-v_h||_{H^1} + ||w-w_h||_{L^2} + ||w-w_h||_{L^2}\frac{||u-v_h||_{H^1}}{||u-u_h||_{H^1}}$$

and taking $\min_{v_h \in W_h^0}$ of this inequality gives

$$\begin{aligned}
||u-u_h||_{H^1} &\leq (1+C)\min_{v_h\in W_h^0}||u-v_h||_{H^1} + (1+C)||w-w_h||_{L^2}\left(1 + \underbrace{\min_{v_h\in W_h^0}\frac{||u-v_h||_{L^2}}{||u-u_h||_{L^2}}}_{\leq 1}\right) \\
&\overset{(34),(36)}{\leq} (1+C)\overline{C}\,h\left(|u|_{H^2(\Omega_h)} + \frac{C_0}{\epsilon}\sqrt{|w|_{H^2(\Omega_h)}^2 + |\phi|_{H^2(\Omega_h)}^2}\right).
\end{aligned}$$

Hence we have proved the following result:

Theorem 1. Suppose that $c^2 < 2\min\{\kappa b, \sigma a\}$, $\Omega = \Omega_h$, each of the functions $f, g, p : \partial\Omega \to \mathbb{R}$ is constant on each component of $\partial\Omega$ and that the $u, w, \phi \in H^2(\Omega_h)$. Then if the functions u, w, ϕ solve the system of equations (25), (24), then the following error bounds hold:

$$\begin{aligned}
||u-u_h||_{H^1} &\leq (1+C)\overline{C}\,h\left(|u|_{H^2(\Omega_h)} + \frac{C_0}{\epsilon}\sqrt{|w|_{H^2(\Omega_h)}^2 + |\phi|_{H^2(\Omega_h)}^2}\right), \\
\sqrt{||w-w_h||_{H^1(\Omega_h)}^2 + ||\phi-\phi_h||_{H^1(\Omega_h)}^2} &\leq \frac{C_0\,\overline{C}}{\epsilon}h\sqrt{|w|_{H^2(\Omega_h)}^2 + |\phi|_{H^2(\Omega_h)}^2}
\end{aligned}$$

for all $\epsilon > 0$ such that $\epsilon \leq \frac{1}{2}\min\{(\kappa + b - \sqrt{(\kappa-b)^2 + 2c^2}), (\sigma + a - \sqrt{(\sigma-a)^2+2c^2})\}$.

6 Numerical Implementation

6.1 Introduction

In the numerical implementation we are going to focus on the Dirichlet boundary conditions (4.1) only. They are more interesting because the convergence rate is unknown and the numerical scheme requires use of two different elements in the same problem. The aim is hence to use the above numerical scheme to compute u_h and ϕ_h. Our software is Dune, which uses C++ coding, and MATLAB. Firstly we need to generate a computational mesh.

6.2 Grid Generation

Recall that we wish to simulate the effect of protein inclusions on a small patch of the surface of a cell. We will take our computational domain to be a square $(-1,1)^2$ with inner circular boundaries representing inclusions. We then can triangulate this domain to get a macro triangulation. We create the mesh using the PDE toolbox in MATLAB (see Figure 5).

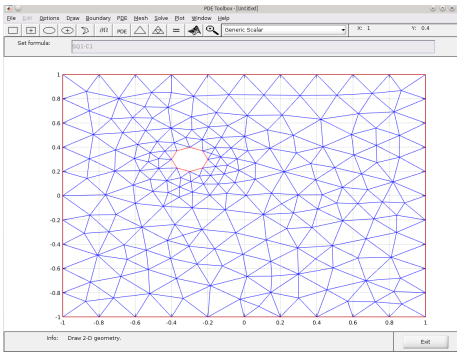

Figure 5: An example of a mesh created using MATLAB's PDE toolbox.

In order to get more accurate results the macro triangulation needs to be refined, which can be also done in MATLAB. In the refinement we pay special attention to the circular inclusion. When a new vertex is created on a boundary edge it is projected onto the of the non-polyhedral domain inner boundary of Ω (see Figure 6). This reduces the variational crime of the domain Ω by the polyhedral computational domain Ω_h. The mesh can be then applied in the numerical solution implemented in Dune.

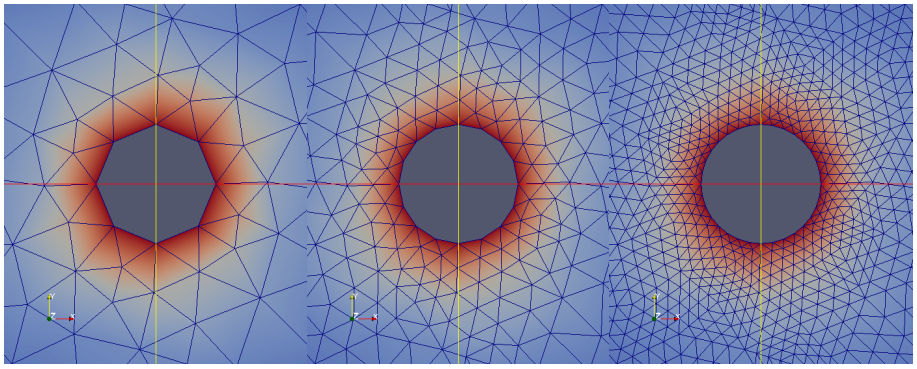

Figure 6: Example of projecting onto the inclusion boundary the new vertices, which are created during the refinement process

6.3 Matrix Vector formulation of the Model

We now have to rewrite the numerical scheme (29) in a matrix formulation. Let θ_i, $i = 1, \dots, 6M$, where M is the number of triangles in triangulation $\mathcal{T}$, denote the nodal basis functions related to the i^{th} degree of freedom of the function u_h and let η_k, $k = 1, \dots, 3M$ denote the nodal basis functions related to the k^{th} degree of freedom for the piecewise affine ϕ_h. By taking in turn $v_h := \theta_i$, $i = 1, \dots, 6M$, $\psi_h := \eta_k$, $k = 1, \dots, 3M$ in (28) we obtain

$$0 \quad = \quad \sum_{T \in \mathcal{T}} \left(\kappa \int_T \Delta u_h \, \Delta \theta_i + \sigma \int_T \nabla u_h \cdot \nabla \theta_i + a \int_T \phi_h \eta_k + b \int_T \nabla \phi_h \cdot \nabla \eta_k + c \int_T \phi_h \Delta \theta_i + c \int_T \eta_k \Delta u_h \right)$$

for $i = 1, \ldots, 6M$, $k = 1, \ldots, 3M$. Now writing u_h and ϕ_h as linear combinations of nodal basis functions θ_i and η_k we can get

$$\begin{aligned} 0 &= \sum_{T\in\mathcal{T}} \sum_{j=1}^{6M} U_j \left(\int_T \kappa \Delta\theta_j \, \Delta\theta_i + \sigma \int_T \nabla\theta_j \cdot \nabla\theta_i + c \int_T \eta_k \Delta\theta_j \right) \\ &\quad + \sum_{T\in\mathcal{T}} \sum_{l=1}^{3M} \Phi_l \left(a \int_T \eta_l \eta_k + b \int_T \nabla\eta_l \cdot \nabla\eta_k + c \int_T \eta_l \Delta\theta_i \right) \end{aligned}$$

for $i = 1, \ldots, 6M$, $k = 1, \ldots, 3M$. We can rewrite this in the following block-matrix form: of as a set of block matrices which then represents the discretised PDE system. We want to have a matrix of the following form,

$$\left(\begin{array}{c|c} \kappa L + \sigma K & cD \\ \hline cD^T & aM + bN \end{array} \right) \begin{pmatrix} U \\ \Phi \end{pmatrix} = \mathbf{0},$$

where $L, K \in \mathbb{R}^{6M\times 6M}$, $M, N \in \mathbb{R}^{3M\times 3M}$ and $D \in \mathbb{R}^{6M\times 3M}$ are defined as follows,

$$\begin{aligned} L_{i,j} &= \sum_{T\in\mathcal{T}} \int_T \Delta\theta_i \Delta\theta_j, \quad K_{i,j} = \sum_{T\in\mathcal{T}} \int_T \nabla\theta_i \nabla\theta_j, \quad D_{i,j} = \sum_{T\in\mathcal{T}} \int_T \Delta\theta_i \eta_j, \\ M_{i,j} &= \sum_{T\in\mathcal{T}} \int_T \eta_i \eta_j, \quad N_{i,j} = \sum_{T\in\mathcal{T}} \int_T \nabla\eta_i \nabla\eta_j \end{aligned}$$

and U, Φ are vectors of coefficients of u_h, ϕ_h, respectively. We note that each of the block matrices L, K, D, M, N is sparse since the entries are only non-zero for adjacent elements. For the sake of using less memory, we only store those entries that are non-zero.

6.4 Boundary Conditions

Next, we want to incorporate the boundary conditions into the system. Denote $\partial\Omega_h = \partial\Omega_0 \cup \Gamma_1 \cup \Gamma_2$, where Γ denote the inclusions' boundaries and $\Omega_0 = (-1, 1)^2$. We need to impose boundary values for both $\partial\Omega_0$ and Γ. Specifically we have the Dirichlet condition for ϕ on both boundaries and the Dirichlet and Neumann conditions u on the same boundaries.

To introduce these into the system, we check row by row on the matrix whether the corresponding basis function relates to an edge (only for Morley elements) or vertex of an element lying on any of the boundaries. In the case that this is true, the process in the code is to:

1. Set the entire row of the matrix to zero,
2. For each entry of the right hand side vector, say RHS_j, subtract $A_{i,j} * BC$, where i is the row number and BC is the imposed boundary value,
3. Set the entire column to zero,
4. Set the diagonal entry to one,
5. Finally set RHS_i to be equal to the imposed boundary value.

6.5 Solving the system and generating the output

Once the boundary conditions have been imposed, the system can be solved for U and Φ by inverting the matrix. This is done using the conjugate gradient method. The assumption that the matrix is symmetric is

trivial and positive definiteness follows from the coercivity of the bilinear form $\widehat{a}(\cdot,\cdot)$. The solution can be visualised using the program Para-View.

7 Simulations

7.1 Convergence

We would like to observe the convergence of the scheme. One possible option is to adjust the right hand side of the Euler-Lagrange equations (16) so that the exact solution is a function of our choice. Taking $\Omega = B_1(0)\backslash B_{0.5}(0)$ and considering the functions $u(\mathbf{x}) = 1 - |x|^4$ and $\phi(\mathbf{x}) = 1 - |x|^2$ we can get the following strong form of the Euler-Lagrange equations:

$$\begin{cases} \kappa\Delta^2 u - \sigma\Delta u + c\Delta\phi = 16\sigma|\mathbf{x}|^2 - 4c - 64\kappa, \\ a\phi - b\Delta\phi + c\Delta u = -(a+16c)|\mathbf{x}|^2 + 4b + a. \end{cases} \tag{38}$$

Solving the discretised problem corresponding to these Euler Lagrange equations allows us to compare the discrete solution u_h and the exact solution u (see Fig. 7).

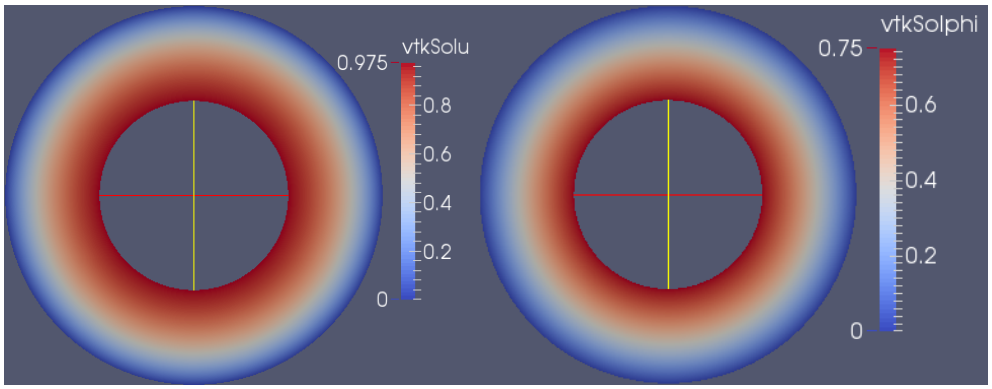

Figure 7: The approximate solution u_h (left), ϕ_h (right) to (38) with BCs of the exact solution u, ϕ.

We also plot the total energy $\mathcal{F}$ of the approximate solution u_h, ϕ_h versus number of nodes in the triangulation (Fig. 8).

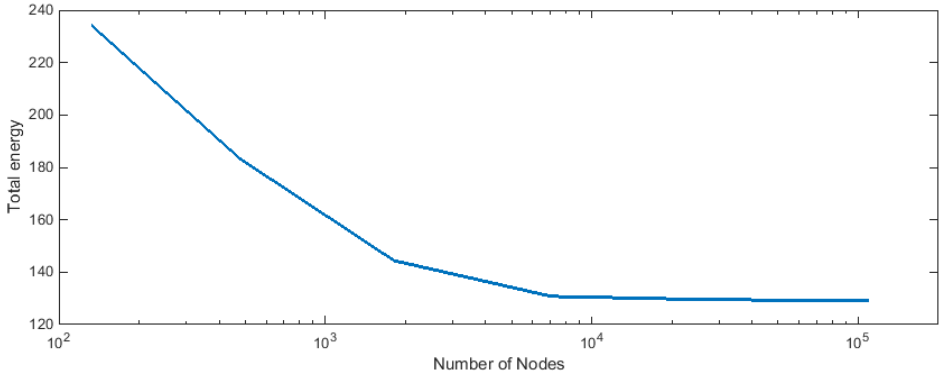

Figure 8: The total energy of the system vs. number of nodes.

We can see that the energy seems to be tending to a constant value. This suggests that the numerical scheme seems to converge. While we don't have proof of convergence we believe this test is a strong indication of convergence. Following this we can now look to investigate the interactions in our model.

7.2 Moving Inclusions

Here we consider two inclusions in the membrane. Let us denote $\partial\Omega_h = \partial\Omega_0 \cup \Gamma_1 \cup \Gamma_2$, where Γ_1, Γ_2 denote the inclusions' boundaries, $\Omega_0 = (-1,1)^2$ and each inclusion has diameter 0.22.
We set $u_h|_{\partial\Omega_h} = \frac{\partial u_h}{\partial \nu}\big|_{\partial\Omega_0} = \phi_h|_{\partial\Omega_0} = 0$ and $\phi_h|_{\Gamma_1} = \phi_h|_{\Gamma_2} = 1$. We consider two cases

1. Here we consider boundary conditions $\frac{\partial u_h}{\partial \nu}\big|_{\Gamma_1} = \frac{\partial u_h}{\partial \nu}\big|_{\Gamma_2} = 1$. We solve the system for several values of the distance between inclusions (see Figure 9). For each experiment we can compute the energy of the system (Fig. 10) , which describes the interaction between inclusions.

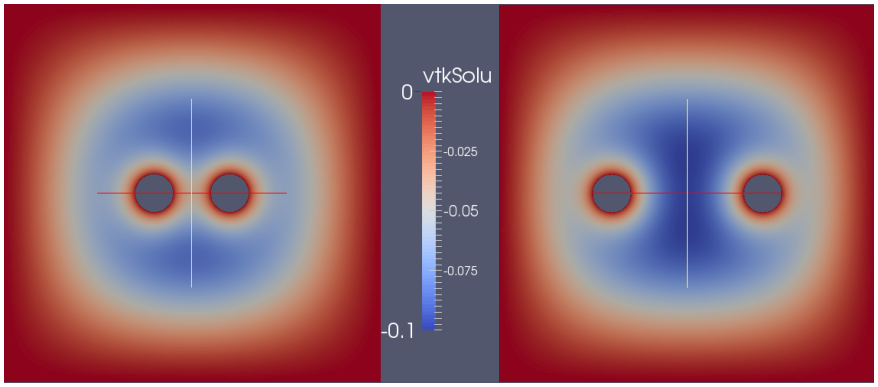

Figure 9: Plot of u_h for different distances (0.3 on the left and 0.6 on the right) between inclusions (3990 and 4047 nodes respectively).

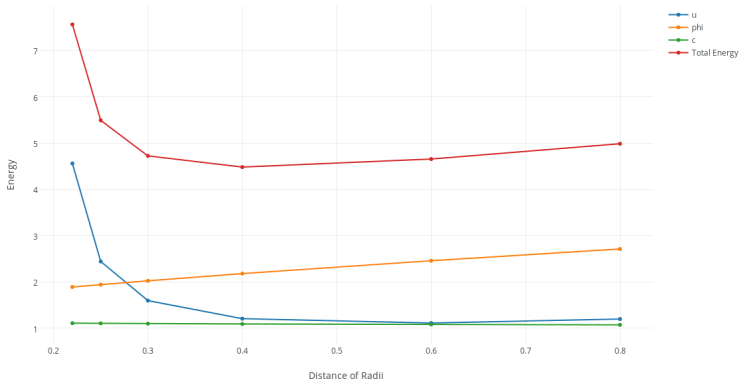

Figure 10: The energy of the system vs. distance between inclusions (with $O(10^3)$ nodes). The red curve corresponds to the total energy (i.e. (5), while the other curves corresponds to its components (i.e. terms with coefficients κ, σ for the blue curve, terms with coefficients a, b for the yellow curve and the coupling term for the green curve.

The smaller the distance between the inclusions the bigger deformation of the membrane between the inclusions and hence the larger energy of the system. The increase of total energy for distances > 0.5 may be justified by the inclusions approaching the boundary of the square $(-1,1)$. From here we can see that the total energy of the system attains its maximum at some distance (≈ 0.4), which corresponds to the

equilibrium state, i.e. the distance which would attained between inclusions if they were allowed to move freely in the horizontal direction.

2. Here we consider boundary conditions $\frac{\partial u_h}{\partial \nu}\big|_{\Gamma_1} = 1$, $\frac{\partial u_h}{\partial \nu}\big|_{\Gamma_2} = -1$. We run similar experiments as in the case 1 and plot the respective results on Fig. 11, 12.

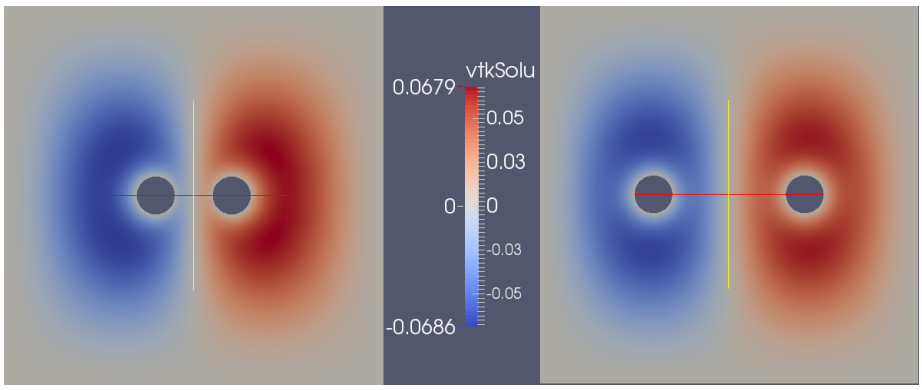

Figure 11: Plot of u_h for different distances between inclusions (3990 and 4047 nodes respectively).

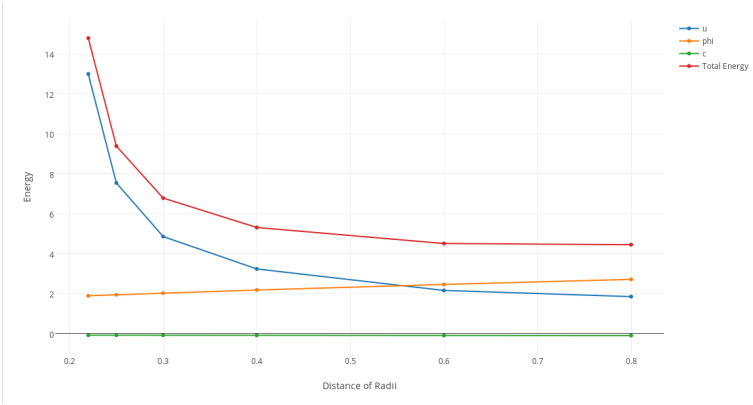

Figure 12: The energy of the system vs. distance between inclusions (with $O(10^3)$ nodes).

In this case (i.e. when $\frac{\partial u_h}{\partial \nu}\big|_{\Gamma}$ has a different sign at Γ_1 and at Γ_2) we observe the decrease of the energy as distance increases.

These interactions seems to suggest a attractive/repulsive relationship exists between inclusions. Inclusions of the same type desire to be a certain distance from each other. This is in contrast to the case of inclusions with opposite Neumann values. Here the inclusions only repeal each other, the slight increases seen at long distances are due to the inclusions being closer to the boundary of the whole domain. These ideal distances are likely a result of the parameter conditions. We do not know if the parameter values we have taken are biologically accurate.

8 Conclusion and Further Directions

8.1 Moving forward

The model could be extended in several ways. A more accurate description of the lipid composition would be to consider the double well potential as outlined in the proposal. This could be potentially analysed using

a gradient flow scheme which could be designed by making suitable changes to our existing code. We would then have implemented non-linear terms. The lipid concentrations should then exhibit phase separation around the inclusions. Ideally we would also like to solve the fully non-linear problem (i.e. not considering the linearised form (2) of energy E) but this is much more difficult.

Another point would be to analyse the current model with non constant boundary conditions. While these may seem to represent the biological system best, there may be such inclusions that do not bind uniformly to the surrounding membrane. Another model assumption that could be dropped is the graphical representation of the membrane. This would be a more realistic model of a membrane if the work was to be extended to outside of a small patch of the cell or to consider closed surfaces.

One could also modify the model to use Neumann boundary conditions for ϕ (see e.g. Turner [15]). This would biologically relate to having no outflow of ϕ. This would allow for direct comparison of the two models with one inclusion. As for the Navier boundary conditions (4.2), we could also implement the respective numerical scheme and compare the experimental results with the convergence rate derived in Section 5.2.3. We could also seek a relationship between the distance between inclusions and the boundary conditions of the inclusions.

8.2 Conclusion

We have analysed a model for the biological membrane with the protein inclusions. We have considered the model with various boundary conditions and found a restriction on the value of c for the existence of a unique solution. A similar restriction was found in the discrete case but we suspect this result may not be sharp. We have implemented the numerical scheme in the case of Dirichlet boundary conditions and investigated the effect of distance between two inclusions on the total energy of the system in the two cases of prescribed boundary values. The scheme was implemented in Dune using a combination of Morley element (for u) and affine elements (for ϕ). From this we have seen that for inclusions of the same type (same boundary conditions at the edge of inclusion) we observe an equilibrium distance between them. For inclusions of the opposite type we instead see only a repulsion between the two proteins. This suggests that biologically proteins of a similar type may naturally try to group with other proteins of the same type.

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