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A formula for membrane mediated point particle interactions on near spherical biomembranes

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Abstract. We consider a model of a biomembrane with attached proteins. The membrane is represented by a near spherical continuous surface and attached proteins are described as discrete rigid structures which attach to the membrane at a finite number of points. The resulting surface minimises a quadratic elastic energy (obtained by a perturbation of the Canham–Helfrich energy) subject to the point constraints which are imposed by the attachment of the proteins. We calculate the derivative of the energy with respect to protein configurations. The proteins are constrained to move tangentially by translation and by rotation in the axis normal to a reference point. Previous studies have typically restricted themselves to a nearly flat membrane and circular inclusions. A numerically accessible representation of this derivative is derived and employed in some numerical experiments.

1. Introduction

The morphology of cell membranes and a variety of functions are well known to be regulated by the interplay between surface proteins and the curvature of the membrane. Biological membranes are composed of a lipid bilayer which is believed to act like a fluid in the lateral direction and elastically in the normal direction. This means that in principle, any proteins which may be embedded into or attached to the surface of the membrane may move freely; thus, not only can the proteins influence the shape of the membrane, but also the protein interaction will be membrane mediated.

Indeed, although direct protein-protein interactions are important, [20] demonstrated that the long range interactions are predominantly membrane mediated. An overview of membrane mediated interactions is given in [4]. An assumption of symmetry of the protein inclusion allows for either analytic representation or approximation by an asymptotic expansion of the interactions [10,19,29,37,39]. Frequently the studies of these interactions have been restricted to a nearly flat membrane with circular or single point inclusions. It is known that the shape of the inclusion has a significant impact on the interaction [30]. In the recent work of [35], a near spherical membrane which is deformed by particles which attach along segments of an ellipsoid or hyperbolid is considered; and in [23] arbitrary, sufficiently regular particle inclusions on a flat membrane are considered. Recent work

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has looked at shape formation of multiple smaller particles into larger structures [21, 36]. In [9], generic elastic energies on a manifold with embedded point particles which have a given interaction potential are considered. A variational formulation for equilibria of the surface and particle system is presented, along a discretisation. Numerical validations are given, and in particular, a Helfrich problem is presented. We further note the work of [5] which considers point constraints in a Kirchhoff plate—this bears a striking similarity to the biological problems of optimising the locations of constraints with respect to the elastic membrane energy.

It is widely accepted in the literature that the near stationary state of lipid membranes are minimisers of the Canham–Helfrich energy [6, 25],

$$\int_{\mathcal{M}} \left(\frac{\kappa}{2}(H - c_0)^2 + \sigma + \kappa_G K \right) \mathrm{d}\mathcal{M}, \tag{1.1}$$

where the membrane is assumed to be thin and well modelled by a two-dimensional surface $\mathcal{M}$. The quantities $\kappa > 0$, $\kappa_G \in \mathbb{R}$ are the bending rigidities associated to the mean and Gauss curvature respectively, and $\sigma \geq 0$ is the surface tension. For the principle curvatures of $\mathcal{M}$, κ_1, κ_2, we take $H := \kappa_1 + \kappa_2$ to be two times the usual value of the mean curvature and $K := \kappa_1 \kappa_2$ to be the typical Gauss curvature. The value $c_0 \in \mathbb{R}$ is the spontaneous curvature, which corresponds to a mismatch between the inner and outer layers of the membrane, for example, due to differing lipid composition.

We make some simplifying assumptions. The first is to set $c_0 = 0$, corresponding to a physical assumption that the mismatch between the layers is rather small. Another assumption is to neglect the Gauss curvature term. This may be justified by taking the rigidity κ_G to be constant and applying the Gauss–Bonnet theorem, which states that when $\mathcal{M}$ is closed, the quantity $\int_{\mathcal{M}} K$ depends only on the Euler characteristic of $\mathcal{M}$. As we are considering a fixed topology of near spherical membranes, we may ignore this constant. Thus, the energy (1.1) can be written as

$$\int_{\mathcal{M}} \left(\frac{\kappa}{2} H^2 + \sigma \right) \mathrm{d}\mathcal{M}. \tag{1.2}$$

It is natural to introduce a volume constraint corresponding to the membrane being impermeable and the fluid contained within the membrane being incompressible. Indeed, without the volume constraint, it is known that (1.2) is bounded below by $8\pi\kappa$ [38], and the degenerate sequence $\mathbb{S}^2(0, \frac{1}{n})$ for $n \to \infty$ is a minimising sequence. Further to this, we are interested in constraining $\mathcal{M}$ to contain a set of points, as this corresponds to a protein in a fixed location being attached to the membrane.

We assume that the attached proteins are rigid, that is to say, they do not bend and can only move by translations or rotations. It is of clear interest to consider the force that the membrane exerts on these attached proteins. This is relevant to, say, calculating locally minimising configuration of multiple proteins via a gradient flow, to estimate statistical quantities using over-damped Langevin Dynamics [32, Section 2.2.2], or as a step for a full model for the problem of particles in membranes. For further details on estimation of the free energy of a particle membrane, see [28].

The derivative of the energy with respect to particle location is calculated as a shape derivative in [14], and appears by use of a pull back method in [23], both in the case of large particles on a nearly flat membrane. We will follow many of the ideas of this second work, making use of methods from [7] to deal with the fact we are on a surface, rather than a flat domain.

One motivation for constructing a formula for the membrane mediated particle interactions may be seen from the following example. For $\bar{\mathcal{E}}(p)$, the total energy of the particle system (the membrane energy with electrostatic interaction) in configuration p, one might be interested in finding p^* such that $\bar{\mathcal{E}}(p^*)$ is minimal. One may choose to do this with a gradient descent algorithm in which an update step might be

$$p_{n+1} = p_n - \alpha_n \nabla_p \bar{\mathcal{E}}(p_n),$$

for some $\alpha_n > 0$ which may depend on n. Clearly one may approximate the derivative $\nabla_p \bar{\mathcal{E}}(p_n)$ by taking a difference quotient. However, this will be expensive, as one would require solving $3N + 1$ linear systems—the system associated to the state p_n and the $3N$ directions that ∇_p corresponds to. With the explicit formula we find, the algorithm to construct the gradient would require solving one linear system and evaluating $3N$ functionals, where these functionals are relatively cheap to evaluate compared to a linear solve for a fourth order PDE.

1.1. Outline

The quadratic energy approximating the general Canham–Helfrich energy (1.2) is presented in Section 2 along with precise definitions and notation for the attachments of particles to the membrane. The formula for the derivative of the minimising energy with respect to the location of the particles is derived in Section 3. Some numerical examples are presented in Section 4. In a finite element setting, we calculate and compare derivatives using the formula and a difference quotient of the energies for comparison.

1.2. Surface PDE preliminaries

For completion, we now provide several definitions and results on the topic of surface PDEs which we will later need. The results may be found in [11]. For Γ, a closed, sufficiently smooth, bounded, orientable hypersurface in $\mathbb{R}^3$ without boundary, there is a bounded domain $\Omega \subset \mathbb{R}^3$ such that $\Gamma = \partial\Omega$. The unit normal to Γ, ν, that points away from Ω is called the outwards unit normal. Define $P_\Gamma := \mathrm{I} - \nu \otimes \nu$ on Γ to be, at each point $x \in \Gamma$, the projection onto the tangent space at that point, $T_x\Gamma$, where I is the identity matrix and we define $a \otimes b := ab^T$, for $a, b \in \mathbb{R}^n$. For a differentiable function f on Γ, we define the tangential gradient

$$\nabla_\Gamma f := P_\Gamma \nabla \tilde{f},$$

where $\tilde{f}$ is a differentiable extension of f to an open neighbourhood of Γ in $\mathbb{R}^3$. Here ∇ is the standard derivative on $\mathbb{R}^3$. Lemma 2.4 of [11] shows this definition is independent

of the choice of extension $\tilde{f}$. We denote the components of the tangential gradient by

$$\underline{D}_i f := (\nabla_\Gamma f)_i .$$

The map $\mathcal{H} := \nabla_\Gamma \nu$ is called the extended Weingarten map, and is symmetric with eigenvalue zero in the normal direction. The mean curvature H is given as the trace of $\mathcal{H}$. For a twice differentiable function, the Laplace–Beltrami operator is defined to be

$$\Delta_\Gamma f := \nabla_\Gamma \cdot \nabla_\Gamma f = \sum_{i=1}^{3} \underline{D}_i \underline{D}_i f.$$

We write $D^2_\Gamma f$ to be the surface Hessian, and Lemma 2.6 in [11] shows that the surface Hessian is, in general, not symmetric with the relation

$$\underline{D}_i \underline{D}_j f - \underline{D}_j \underline{D}_i f = (\mathcal{H}\nabla_\Gamma f)_j \nu_i - (\mathcal{H}\nabla_\Gamma f)_i \nu_j . \tag{1.3}$$

It is well known [11, Lemma 2.8] that there is a small neighbourhood around Γ of width $\delta > 0$, $\mathcal{N}_\delta$, and maps $d\colon \mathcal{N}_\delta \to \mathbb{R}$ (the oriented distance function) and $\pi\colon \mathcal{N}_\delta \to \Gamma$ (the closest point projection), such that for any $\widetilde{X} \in \mathcal{N}_\delta$, we have the unique decomposition

$$\widetilde{X} = \pi(\widetilde{X}) + d(\widetilde{X})\nu(\pi(\widetilde{X})). \tag{1.4}$$

2. Membrane and particle model

We begin with models for the deformation of the membrane and for the particles together with their attachment to the membrane.

2.1. Membrane model

We now fix $\Gamma := \mathbb{S}^2(0, R)$ to be the 2-sphere of radius R, for a given $R > 0$. In light of this, we see that for $X \in \mathbb{R}^3 \setminus \{0\}$, we have $\pi(X) = R\frac{X}{|X|}$ and $d(X) = |X| - R$. We are interested in finding a surface which is a near spherical membrane of the form

$$\mathcal{M}(v) := \{x + \rho v(x)\nu(x) : x \in \Gamma\},$$

where ρ is small and v is sufficiently smooth. Thus, $\mathcal{M}(v)$ is a graph over Γ. We use the energy

$$J(v) := \frac{1}{2}\int_\Gamma \kappa(\Delta_\Gamma v)^2 + \Big(\sigma - \frac{2\kappa}{R^2}\Big)|\nabla_\Gamma v|^2 - \frac{2\sigma}{R^2}v^2 \tag{2.1}$$

derived in [12]. It is seen for $\int_\Gamma v = 0$ that $J(v)$ is the first non-trivial term of the Taylor expansion in ρ of the Lagrangian induced by the Canham–Helfrich energy, for surfaces with enclosed volume constrained to be $\frac{4}{3}\pi R^3$ around the critical point $(\Gamma, -\frac{\sigma}{R})$. This energy is analogous to the Monge gauge for a nearly flat membrane [14], which is formally obtained by taking the limit $R \to \infty$.

Definition 2.1. We define the bilinear form $a\colon H^2(\Gamma)\times H^2(\Gamma)\to\mathbb{R}$ to be

$$a(\eta,v):=\int_\Gamma \kappa\Delta_\Gamma\eta\Delta_\Gamma v+\Big(\sigma-\frac{2\kappa}{R^2}\Big)\nabla_\Gamma\eta\cdot\nabla_\Gamma v-\frac{2\sigma}{R^2}\eta v\quad\forall\eta,v\in H^2(\Gamma),\tag{2.2}$$

which is the bilinear form given by the first variation of (2.1). Furthermore, we define the space

$$U:=\left\{v\in H^2(\Gamma):\int_\Gamma v=0\right\}.$$

Remark 2.2. We note that under the small deformation methodology of [12], one may deal with appropriately small spontaneous curvature, denoted by c_0 in (1.1), as considered in [15, 17].

2.2. An energy minimising membrane subject to point constraints

With the above definitions, one may now write the following problem:

Problem 2.3. Given $Z\in\mathbb{R}^K$ and $\mathcal{C}=\{X_j\in\Gamma:\ j=1,\dots,K\}$, find $u\in U$ such that $J(u)$ is minimised subject to $u(X_j)=Z_j$ for $j=1,\dots,K$.

This defines K point constraints on u and is admissible for $u\in H^2(\Gamma)$ because of the well-known embedding for two dimensions, $H^2(\Gamma)\subset C(\Gamma)$ (see [1]).

We have the following well-posedness and regularity result. The well-posedness follows from [16, Theorem 5.1], while the regularity result may be found in Appendix C.

Theorem 2.4. *Suppose $K\geq 4$ and the points of $\mathcal{C}$ do not lie in a single plane. Then, there is a unique $u\in U$ which solves Problem 2.3. Moreover, for any $p\in(1,2)$, it holds that $u\in W^{3,p}(\Gamma)$.*

Remark 2.5.

- The fact the solution of Problem 2.3 has three weak derivatives will be used to give a more convenient representation of the derivative we calculate.
- A related problem has been considered in [12], where the authors consider the minimisation over a smaller space which enforces a fixed centre of mass for the membrane.
- The works [14, 22, 23] consider a larger solution space whereby the particles may, in some sense, tilt. The problem for this tilting on a sphere, or general domain, is of interest and may be studied in future work.
- An example of non-uniqueness for $K>4$ would be to consider $\mathcal{C}\subset\{x\in\Gamma:x_1=0\}$. Then, for a solution u of Problem 2.3, we see that $u+\alpha v_1\in U$ and $J(u+\alpha v_1)=J(u)$ for any $\alpha\in\mathbb{R}$.

2.3. A single particle model

We wish to model the attachment of proteins to a biomembrane. A protein is considered to be a rigid discrete structure which is attached to the membrane at a finite number of

fixed points. An example would be a protein such as FCHo2 F-BAR domains, where it is understood that a small number of atoms are more likely to attach to the membrane [26, 27]. This is in contrast to the case mainly considered in [22], where the protein is modelled as being embedded in the membrane and attached along a curved boundary. The protein-biomembrane interaction is modelled by attachment at these points.

To begin, we restrict ourselves to a single protein in order to establish notation. We describe the protein by a finite set of distinct points $\mathcal{G} := \{\widetilde{X}_i \in \mathbb{R}^3 : i = 1, \dots, M\}$. The points of $\mathcal{G}$ correspond to charged ends of the protein which attach to the membrane. The attachment constraint is the requirement that $\mathcal{G}$ is contained in the graph $\mathcal{M}(u)$, which we write as

$$\mathcal{G} \subset \mathcal{M}(u). \tag{2.3}$$

It follows that any $\widetilde{X} \in \mathcal{G}$ may be uniquely decomposed into

$$\widetilde{X} = \pi(\widetilde{X}) + d(\widetilde{X})\nu(\pi(\widetilde{X})) = R\frac{\widetilde{X}}{|\widetilde{X}|} + \big(|\widetilde{X}| - R\big)\frac{\widetilde{X}}{|\widetilde{X}|},$$

and condition (2.3) becomes

$$u(\pi(\widetilde{X})) = d(\widetilde{X}) \quad \forall \widetilde{X} \in \mathcal{G}. \tag{2.4}$$

For ease of notation, we write $X := \pi(\widetilde{X})$, $z := d(\widetilde{X})$ and index the points of $\mathcal{G}$ so that $\{\widetilde{X}_i\}_{i=1}^{M} = \mathcal{G}$, hence we may write (2.4) as

$$u(X_i) = z_i \quad \forall i = 1, \dots, M. \tag{2.5}$$

Definition 2.6. We write $\mathcal{C} := \{\pi(\widetilde{X}) : \widetilde{X} \in \mathcal{G}\} = \{X_i\}_{i=1}^{M}$ to be the reference points on Γ to the sites of attachment. Furthermore, we write

$$u|_{\mathcal{C}} = Z$$

as shorthand for (2.5).

2.4. Parameterisation of a single particle

We now parameterise the movement of a single particle. We attempt to keep our notation as similar as possible to that of [23], which deals with the movement of curves in a flat domain, in contrast to our points which move on a sphere.

The assumption that the protein is rigid is meant in the sense that any movement of $\mathcal{G}$ should preserve the orientation and the distance between points. There are six degrees of freedom by which $\mathcal{G}$ can be moved—this is translation and rotation. We further restrict to lateral (i.e. tangential) movement of $\mathcal{G}$ over the membrane. This means that the height of attachment above Γ, the values Z, will be independent of any movement. In the flat setting these lateral movements correspond to rotation perpendicular to the plane and translation within the plane. Although this is a strong restriction to make to the full model, it is important in this setting to avoid the particle moving out of the graph-like description.

The configuration of a single particle $\mathcal{G}$ is defined by a rigid transformation from a fixed position. We associate one point $X_{\mathcal{G}} \in \Gamma$ with $\mathcal{G}$. We call $X_{\mathcal{G}}$ the *centre* of $\mathcal{G}$. The configuration of the particle is defined by a rotation about the axis, which is defined by $\nu(X_{\mathcal{G}})$ together with a *tangential translation* of $X_{\mathcal{G}}$ along the surface of Γ. A rotation around $\nu(X_{\mathcal{G}})$ is characterised by an angle, $\alpha \in \mathbb{R}$. A tangential translation is characterised by a tangent vector $\tau \in T_{X_{\mathcal{G}}}\Gamma \cong \mathbb{R}^2$. For this tangent vector, the idea is to consider the transport of $X_{\mathcal{G}}$ along the geodesic defined by τ and that the other points should follow with a rigid transformation. In the setting of a sphere, this corresponds to rotating the points by angle $|\tau|$ in the axis perpendicular to both $\nu(X_{\mathcal{G}})$ and τ. Thus, for a particle with centre $X_{\mathcal{G}}$, this leads to the following definition of a particle configuration:

Definition 2.7. Given a particle $\mathcal{G} \subset \mathbb{R}^3$ with centre $X_{\mathcal{G}}$ and $p = (\alpha, \tau) \in \mathbb{R} \times T_{X_{\mathcal{G}}}\Gamma$, we write

$$\mathcal{G}(p) := \{\phi(p, \widetilde{X}) : \widetilde{X} \in \mathcal{G}\},$$

with

$$\phi(p, x) := R_T(\tau)R_n(\alpha)x \quad \forall x \in \mathbb{R}^3, \tag{2.6}$$

where $R_n(\alpha)$ is given by

$$R_n(\alpha)x := (\nu(X_{\mathcal{G}}) \otimes \nu(X_{\mathcal{G}}))x + \cos(\alpha)(\nu(X_{\mathcal{G}}) \times x) \times \nu(X_{\mathcal{G}}) + \sin(\alpha)(\nu(X_{\mathcal{G}}) \times x),$$

and for $\tau \neq 0$, define $\tilde{\tau} := \nu(X_{\mathcal{G}}) \times \frac{\tau}{|\tau|}$. Then, $R_T(\tau)$ is given by

$$R_T(\tau)x := (\tilde{\tau} \otimes \tilde{\tau})x + \cos(|\tau|)(\tilde{\tau} \times x) \times \tilde{\tau} + \sin(|\tau|)(\tilde{\tau} \times x),$$

and $R_T(0)x = x$. A diagram showing the transformations R_n and R_T may be found in Figure 1. Furthermore, write

$$\mathcal{C}(p) := \{\phi(p, X) : X \in \mathcal{C}\},$$

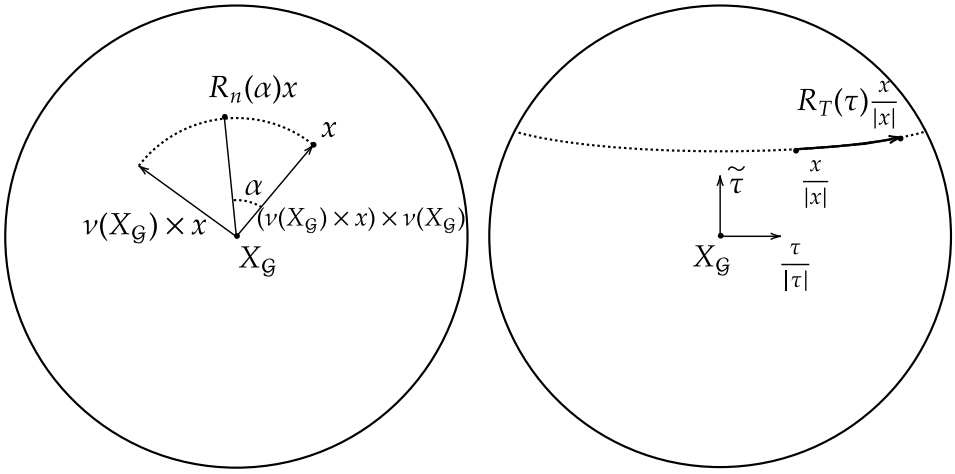
which coincides with the projection of $\mathcal{G}(p)$ onto Γ.

Remark 2.8. The choice that $\phi(p, x) := R_T(\tau)R_n(\alpha)x$ rather than $R_n(\alpha)R_T(\tau)x$ is arbitrary. It is clear that they will both generate the same family of configurations. In this setting, due to the symmetry of the surface, we see that the map $\phi(p, \cdot) = R_T(\tau)R_n(\alpha)$ is linear and has a matrix representation which lies in $SO(3)$.

We will, with an abuse of notation, identify $\mathcal{G}$ with $\mathcal{G}(0)$ and similarly $\mathcal{C}$ with $\mathcal{C}(0)$. Also note that p is periodic in the sense that, for $p = (\alpha, \tau)$, $\bar{p} = (\alpha + 2\pi, \tau)$ and $\tilde{p} = (\alpha, \tau + 2\pi\frac{\tau}{|\tau|})$, it holds that

$$\phi(p, \cdot) \equiv \phi(\bar{p}, \cdot) \equiv \phi(\tilde{p}, \cdot).$$

We note further that if $\mathcal{G}$ contains only one point, $\widetilde{X}_1$, and one sets $X_{\mathcal{G}} = X_1$, it is seen that α becomes a redundant parameter.



(a) Diagram for R_n. (b) Diagram for R_T.

Figure 1. Diagrams demonstrating the transformations R_n and R_T, both with $\nu(X_\mathcal{G})$ coming out of the page.

2.5. Configuration of particles

We now make the extension to multiple groups of particles.

Definition 2.9. Given discrete sets with finite number of points,

$$\mathcal{G}_1, \ldots, \mathcal{G}_N \subset \mathcal{N}_\delta \subset \mathbb{R}^3,$$

we write

$$\mathcal{C}_i := \{\pi(\widetilde{X}) : \widetilde{X} \in \mathcal{G}_i\} \quad \text{for } i = 1, \ldots, N,$$

which is the projection of $\mathcal{G}_i$ onto Γ. Let the $\mathcal{G}_1, \ldots, \mathcal{G}_N$ have centres $X_{\mathcal{G}_1}, \ldots, X_{\mathcal{G}_N}$, and let $p = (p_1, \ldots, p_N) \in \prod_{i=1}^N (\mathbb{R} \times T_{X_{\mathcal{G}_i}}\Gamma)$, where $p_i = (\alpha_i, \tau_i) \in \mathbb{R} \times T_{X_{\mathcal{G}_i}}\Gamma$. We define

$$\phi_i(p, x) := R_{T_i}(\tau_i) R_{n_i}(\alpha_i) x \quad \forall x \in \mathbb{R}^3,$$

where the operators $R_{T_i}(\tau_i)$, $R_{n_i}(\alpha_i)$ are defined relative to the centres $X_{\mathcal{G}_i}$, as in Definition 2.7.

Further define

$$\mathcal{G}_i(p) := \{\phi_i(p, \widetilde{X}) : \widetilde{X} \in \mathcal{G}_i\} \quad \text{for } i = 1, \ldots, N,$$
$$\mathcal{C}_i(p) := \{\phi_i(p, X) : X \in \mathcal{C}_i\} \quad \text{for } i = 1, \ldots, N,$$

the latter of which is the projection of $\mathcal{G}_i(p)$ onto Γ. Observe that

$$\mathcal{G}_i(0) = \mathcal{G}_i \quad \text{and} \quad \mathcal{C}_i(0) = \mathcal{C}_i, \qquad i = 1, \ldots, N.$$

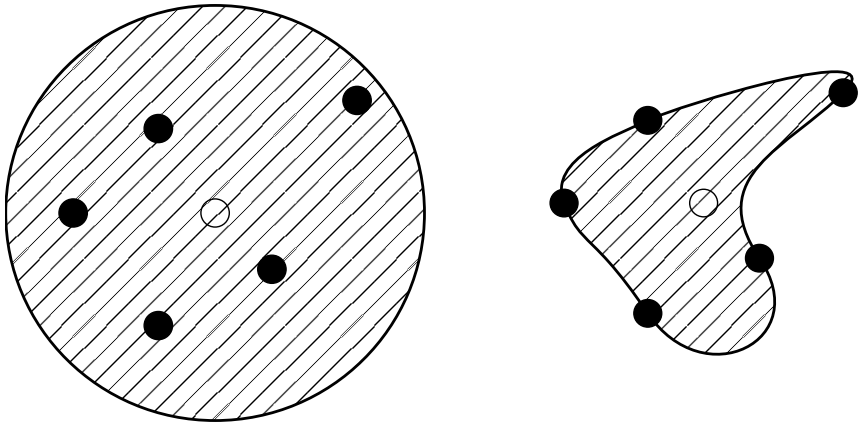


Figure 2. Diagram indicating the different areas which might be excluded from having part of another particle in for two identical particles. The left is the radius approach, on the right the area is given by the interior of a curve passing through all the points.

Definition 2.10. We define the set of feasible particle configurations to be

$$\Lambda^\circ := \left\{ p \in \prod_{i=1}^{N} (\mathbb{R} \times T_{X_{\mathscr{G}_i}}\Gamma) : \forall i,\ j = 1, \dots, N,\ i \neq j,\ \mathcal{C}_i(p) \cap \mathcal{C}_j(p) = \emptyset \right\}.$$

We define the closure of the set of feasible particle configuration by $\Lambda := \overline{\Lambda^\circ}$. Furthermore, for $p \in \Lambda$ we define

$$\Gamma(p) := \Gamma \setminus \bigcup_{i=1}^{N} \mathcal{C}_i(p).$$

We first note that $0 \in \prod_{i=1}^{N}(\mathbb{R} \times T_{X_{\mathscr{G}_i}})$ is not a distinguished configuration. Given any non-overlapping initial configuration of particles $\{\mathcal{C}_i\}_{i=1}^{N}$, it is clear that Λ° is the set of all possible configurations of particles which have been moved by the rigid motions parameterised by p described at the start of Section 2.4.

Remark 2.11. Notice that for $p \in \Lambda^\circ$, it may hold that the 'interiors' of particles overlap. As such, one might want to consider a subset of Λ° whereby one defines an appropriate interior of particles and assumes that the intersection of these is empty, or perhaps one may also assign a 'radius' to each particle and consider the set where there are no points from another particle which lie within this radius. Two ideas of these exclusion areas are shown in Figure 2. In this diagram, the clear dot is the centre of a particle and the black dots are the points of the particle. The exclusion area is signified by the hatched lines. The choice of this subset is of no importance when constructing the derivative, but is important when considering which particle configurations are admissible. Requiring that the particles do not overlap could be included as part of a Lennard-Jones potential, see (4.18) in [14],

where it could be seen that this discussion pertains to a choice of the distance function in their formula.

For each $p \in \Lambda^\circ$ we have a set of point constraints on elements of $H^2(\Gamma)$. This motivates of the parameterised trace operators which follow.

Definition 2.12. Let $p \in \Lambda^\circ$ be given.

- For $i = 1, \dots, N$, define the maps $\gamma_i(p)\colon H^2(\Gamma) \to \mathbb{R}^{|\mathcal{C}_i|}$ by

$$\gamma_i(p)\colon v \mapsto (v \circ \phi_i(p, \cdot))\,|_{\mathcal{C}_i},$$

  where $\phi_i(p, \cdot)|_{\mathcal{C}_i}$ is meant as in Definition 2.6.
- For $v \in H^2(\Gamma)$, $Z \in \prod_{i=1}^N \mathbb{R}^{|\mathcal{C}_i|}$, we say $\gamma(p)v = Z$ when

$$\gamma_i(p)v = Z_i \in \mathbb{R}^{|\mathcal{C}_i|} \quad \text{for } i = 1, \dots, N,$$

  where Z is given by the particles $\mathcal{G}_1, \dots, \mathcal{G}_N$.
- Define the following subsets of $H^2(\Gamma)$ by

$$U(p) := \{v \in U : \gamma(p)v = Z\},$$
$$U_0(p) := \{v \in U : \gamma(p)v = 0\}.$$

Assumption 2.13. Henceforth, we assume that there is l with $1 \le l \le N$ such that $\mathcal{C}_l$ is not coplanar.

Definition 2.14 (Membrane configurational energy). Given $p \in \Lambda^\circ$, we define $u(p) \in U(p)$ by

$$u(p) := \operatorname*{arg\,min}_{v \in U(p)} J(v)$$

and we define the membrane configurational energy $\mathcal{E}\colon \Lambda^\circ \to \mathbb{R}$ by

$$\mathcal{E}(p) := J(u(p)).$$

By a trivial extension to Theorem 2.4, it is clear that $u(p)$ exists, is unique, and satisfies $u(p) \in W^{3,2-\delta}(\Gamma)$ for any $\delta \in (0, 1)$. For $p \in \partial\Lambda^\circ$ we do not necessarily have that a $u(p)$ exists—this is due to $U(p)$ possibly being empty.

Remark 2.15. Notice that $\mathcal{E}$ may not be the total energy associated to the particle-membrane configuration. For example, $\mathcal{E}$ may be augmented with a pairwise interaction between particles modelling direct forces between different particles.

3. Gradient of the energy with respect to configuration changes

In this section we find a formula for the derivative of $\mathcal{E}(p)$ with respect to changes in the configuration p.

Definition 3.1 (Derivative of the configurational energy). The configurational energy is differentiable at $p \in \Lambda^\circ$ in the direction $e \in \prod_{i=1}^N (\mathbb{R} \times T_{X_{\mathscr{g}_i}} \Gamma)$ if the derivative

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}(p + te)|_{t=0}$$

exists. We denote this derivative by $\partial_e \mathcal{E}(p)$.

The difficulty lies in the implicit definition of the energy $\mathcal{E}(p)$ in terms of the minimisation of the quadratic energy $J(v)$ over the configurational space $U(p)$. This is because it requires the evaluation of the evaluation of $\frac{\mathrm{d}}{\mathrm{d}t} J(u(p + te))|_{t=0}$ which involves the minimisation of $J(\cdot)$ over $U(p + te)$. In order to achieve this, we fix p and employ suitable local isomorphisms on the vector spaces $U(p)$ via appropriate diffeomorphisms of the domain $\Gamma(p)$. This is applied locally to transform the energy (2.1) and the related minimisation problems over a reference function space.

We begin with the existence of a sufficiently regular family of diffeomorphisms.

Lemma 3.2. *Let $k \geq 3$. For each $p \in \Lambda^\circ$ there exists an open ball $\mathcal{B} \subset \prod_{i=1}^N (\mathbb{R} \times T_{X_{\mathscr{g}_i}} \Gamma)$ containing 0 and a family of C^k-diffeomorphisms $\chi \colon \mathcal{B} \times \Gamma \to \Gamma$ such that*

$$\chi(0, \cdot) \text{ is the identity on } \Gamma;$$

and for all $q \in \mathcal{B}$, $p + q \in \Lambda^\circ$ and

$$v \circ \chi(q, \cdot)^{-1} \in U(p + q) \iff v \in U(p). \tag{3.1}$$

The proof of this lemma is given in Section 3.3, where we give an explicit construction of the maps. We note that it is possible to construct the family to be infinitely differentiable.

We now define what we mean by the derivative of χ with respect to e.

Definition 3.3. Given $q \in \mathcal{B}$ and $e \in \prod_{i=1}^N (\mathbb{R} \times T_{X_{\mathscr{g}_i}} \Gamma)$, for each $x \in \Gamma$, the derivative of $\chi(\cdot, x)$ at q in direction e is defined to be

$$\partial_e \chi(q, x) := \frac{\mathrm{d}}{\mathrm{d}t} \chi(q + te, x)|_{t=0}.$$

Remark 3.4. Notice that:

- The dependence on p of $\mathcal{B}$ and χ has been suppressed.
- For our purposes, we will not require full knowledge of the diffeomorphism χ, only of the derivative $\partial_e \chi(0, \cdot)$.
- The fact that Λ may be identified as a subset of the finite dimensional space $\mathbb{R}^{3\times N}$ will be exploited to reduce the problem of differentiability of $\mathcal{E}$ to be an application of the Implicit Function Theorem applied to a reformulated interaction energy.
- The condition (3.1) may be decomposed into three parts: $\gamma(p + q)\left(v \circ \chi^{-1}\right) = \gamma(p)v$ for all $v \in H^2(\Gamma)$, $\int_\Gamma v \circ \chi^{-1} = \int_\Gamma v$ for all $v \in H^2(\Gamma)$ and $v \in H^2(\Gamma) \iff v \circ \chi^{-1} \in H^2(\Gamma)$.

- The condition on χ that $\int_\Gamma v \circ \chi(q,\cdot)^{-1} = \int_\Gamma v$ for all $v \in H^2(\Gamma)$ is equivalent to requiring that $\det(\nabla_\Gamma \chi(q,\cdot) + \nu(\cdot) \circ \chi(q,\cdot) \otimes \nu(\cdot)) = 1$ on Γ. As such, it is sufficient to have $\partial_e \det(\nabla_\Gamma \chi(q,\cdot) + \nu(\cdot) \circ \chi(q,\cdot) \otimes \nu(\cdot)) = 0$ for any $e \in \prod_{i=1}^N (\mathbb{R} \times T_{X_{\mathscr{G}_i}}\Gamma)$. We will later see that, for $q = 0$, this is the same as requiring $\operatorname{div}_\Gamma \partial_e \chi(0,\cdot)$ vanishes.

3.1. The transformed functional and its derivative

Using the χ in Lemma 3.2, we have the following functional.

Definition 3.5. Let $J^*\colon \mathcal{B} \times U(p) \to \mathbb{R}$ be given by

$$J^*\colon (q,v) \mapsto J(v \circ \chi^{-1}(q,\cdot)), \quad J^*(0,v) = J(v) \qquad \forall v \in U(p).$$

We call $J^*(\cdot, v)$ the transformed membrane energy. Given $e \in \prod_{i=1}^N (\mathbb{R} \times T_{X_{\mathscr{G}_i}})$, if, for any $v \in U(p)$, the derivative

$$\frac{\mathrm{d}}{\mathrm{d}t} J^*(te, v)|_{t=0}$$

exists, then we denote the derivative by $\partial_e J^*(0,v)$.

We now define some terms which appear in [7] which are useful to give an explicit representation of J^*.

Definition 3.6. Given $q \in \mathcal{B}$, we define on Γ the matrices and determinant

$$\begin{aligned} B &= B(q,\cdot) := \nabla_\Gamma \chi(q,\cdot) + \nu(\cdot) \circ \chi(q,\cdot) \otimes \nu(\cdot), \\ G &= G(q,\cdot) := B(q,\cdot)^T B(q,\cdot), \\ b &= b(q,\cdot) := \det(B(q,\cdot)). \end{aligned}$$

The following convenient representation of J^* is immediate from Lemmas A.1 and A.2 in the appendix.

Lemma 3.7. *Given $v \in U(p)$, $q \in \mathcal{B}$, it holds that*

$$J^*(q,v) = \frac{\kappa}{2} \int_\Gamma \frac{1}{b} \left(div_\Gamma (bG^{-1}\nabla_\Gamma v)\right)^2 + \left(\frac{\sigma}{2} - \frac{\kappa}{R^2}\right) \int_\Gamma b \nabla_\Gamma v \cdot G^{-1} \nabla_\Gamma v - \frac{\sigma}{R^2} \int_\Gamma b v^2. \tag{3.2}$$

Note that we wish to differentiate J^* with respect to q and that the q-dependence is located in the coefficients $B(q)$.

Lemma 3.8. *Suppose $\mathcal{B} \subset \prod_{i=1}^N (\mathbb{R} \times T_{X_{\mathscr{G}_i}}\Gamma)$ is sufficiently small with $0 \in \mathcal{B}$ and $\chi \in C^k(\mathcal{B} \times \Gamma; \Gamma)$. Then, $J^* \in C^{k-2}(\mathcal{B} \times U(p); \mathbb{R})$.*

Proof. It is clear from the expression for J^* that it depends on B, the derivative of B and smoothly (in $H^2(\Gamma)$) on v. Since $B(0) = \mathrm{I}$, the identity matrix, B depends continuously on q and det is a continuous map, thus for a sufficiently small neighbourhood $\mathcal{B} \ni 0$, $\det(B(q)) > c > 0$, and it holds that B is non-singular. Thus, by smoothness of the integrand, we may apply the dominated convergence theorem to obtain $J^* \in C^{k-2}(\mathcal{B} \times U(p); \mathbb{R})$. ∎

Theorem 3.9. *There exists an open neighbourhood $\hat{\mathcal{B}}$ of 0 in $\prod_{i=1}^{N}(\mathbb{R}\times T_{X_{\mathscr{E}_i}}\Gamma)$ such that $\mathcal{E}(p+\cdot)\in C^{k-2}(\hat{\mathcal{B}};\mathbb{R})$. In particular, for $k\geq 3$ and $u=\arg\min_{v\in U(p)}J(v)$,*

$$\partial_e\mathcal{E}(p)=\partial_e J^*(0,u).$$

Proof. In what follows, we suppress the dependence on p and write $u=u(p), U_0=U_0(p)$. Define $\mathcal{J}\in C^{k-2}(\mathcal{B}\times U_0;\mathbb{R})$ by $\mathcal{J}(q,v):=J^*(q,u+v)$ for $(q,v)\in\mathcal{B}\times U_0$. For fixed q, $\mathcal{J}(q,\cdot)$ is a quadratic functional and by the definition of u, we have that the minimiser of the functional $\mathcal{J}(0,v)$ over U_0 is given by $v=0$. Define $F\in C^{k-2}(\mathcal{B}\times U_0;U_0^*)$ by $F(q,v):=D_v\mathcal{J}(q,v)$ where, for fixed q, $D_v\mathcal{J}$ is the first variation of $\mathcal{J}(q,\cdot)$ over U_0. For each (q,v), $F(q,v)$ is a linear functional. Since $J(0,v)$ attains minima at $v=0$, it follows that $F(0,0)=D_v\mathcal{J}(0,0)=0\in U_0^*$. Furthermore, the first variation of F at $(0,0)$,

$$D_vF(0,0)\colon(\xi,\eta)\in U_0\times U_0\mapsto D_vF(0,0)[\xi,\eta]=D_{vv}\mathcal{J}(0,0)[\xi,\eta]=a(\xi,\eta),$$

is a strictly coercive bilinear form over $U_0\times U_0$. As a consequence, it follows that the map $U_0\ni v\mapsto D_vF(0,v)\in U_0^*$ is invertible.

It therefore holds that we may apply the Implicit Function Theorem, Theorem B.1, to $f=F$, with $(a,b)=(0,0)$, $\mathcal{X}=\prod_{i=1}^{N}(\mathbb{R}\times T_{X_{\mathscr{E}_i}}\Gamma)$, $\mathcal{Y}=U_0$, $\mathcal{Z}=\mathcal{Y}^*$ and $\Omega=\mathcal{B}\times\mathcal{Y}$. As such, there is a neighbourhood of 0, $\hat{\mathcal{B}}=V\subset\mathcal{B}$ and a function $\hat{v}\in C^{k-2}(\hat{\mathcal{B}};U_0(p))$ such that $\hat{v}(0)=0$ and $F(q,\hat{v}(q))=0$, that is to say $J_v^*(q,\hat{v}(q)+u)=0$, so $\hat{v}(q)+u$ is a critical point of $J^*(q,\cdot)$. By coercivity of $J^*(q,\cdot)$ over $U(p)$, $\hat{u}(q):=\hat{v}(q)+u$ is the unique minimiser. Hence,

$$\mathcal{E}(p+q)=\min_{\eta\in U(p+q)}J(\eta)=\min_{\eta\in U(p)}J^*(q,\eta)=J^*(q,\hat{u}(q)).$$

Since $\hat{u}\in C^{k-2}(\hat{\mathcal{B}};U(p))$, $J^*\in C^{k-2}(\mathcal{B}\times U(p);\mathbb{R})$, and it follows that $\mathcal{E}(p+\cdot)\in C^{k-2}(\hat{\mathcal{B}};\mathbb{R})$. Taking the derivative of $\mathcal{E}$ gives

$$\partial_e\mathcal{E}(p)=\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(p+te)|_{t=0}=\frac{\mathrm{d}}{\mathrm{d}t}J^*(te,u)|_{t=0}+\frac{\mathrm{d}}{\mathrm{d}t}J^*(0,\hat{u}(te))|_{t=0}=\partial_eJ^*(0,u),$$

where $\frac{\mathrm{d}}{\mathrm{d}t}J^*(0,\hat{u}(te))|_{t=0}=D_vJ^*(0,u)[\frac{\mathrm{d}}{\mathrm{d}t}\hat{u}(te)|_{t=0}]$ vanishes since $D_vJ^*(0,u)=0$. ∎

Remark 3.10. Although J^* depends on the choice of χ, the derivative $\partial_e\mathcal{E}(p)$ is independent of the choice of χ. One may consider a different diffeomorphism, say, $\tilde{\chi}$ with energy $\widetilde{J}^*$. One would then have that

$$\min_{\eta\in U(p+q)}J^*(q,\eta)=\min_{\tilde{\eta}\in U(p+q)}\widetilde{J}^*(q,\tilde{\eta}),$$

and arrive at $\partial_e\mathcal{E}(p)=\partial_e\widetilde{J}^*(0,u)=\partial_eJ^*(0,u)$.

3.2. An explicit formula for the derivative

It is convenient to define the following.

Definition 3.11. Define the tangential vector field $V\colon \prod_{i=1}^{N}(\mathbb{R}\times T_{X_{\mathscr{G}_i}}\Gamma)\times\Gamma\to\mathbb{R}^3$ by

$$V(e,x) := \partial_e \chi(0,x),$$

which is tangential in the sense that $V(e,x)\in T_x\Gamma$ for all $(e,x)\in\prod_{i=1}^{N}(\mathbb{R}\times T_{X_{\mathscr{G}_i}}\Gamma)\times\Gamma$.

Proposition 3.12. *Given $e\in\prod_{i=1}^{N}(\mathbb{R}\times T_{X_{\mathscr{G}_i}}\Gamma)$, set $\mathcal{A} := (div_\Gamma V)I - (\nabla_\Gamma V + \nabla_\Gamma V^T)$. Then, for $\eta\in H^2(\Gamma)$ it holds that*

$$\begin{aligned}\partial_e J^*(0,\eta) = \kappa\int_\Gamma (\mathcal{A} : D^2_\Gamma\eta - \Delta_\Gamma V\cdot\nabla_\Gamma\eta)\Delta_\Gamma\eta \\ - \frac{\kappa}{R^2}\int_\Gamma (V\cdot\nabla_\Gamma\eta + \frac{1}{2}div_\Gamma V\Delta_\Gamma\eta)\Delta_\Gamma\eta \\ + \Big(\frac{\sigma}{2}-\frac{\kappa}{R^2}\Big)\int_\Gamma \nabla_\Gamma\eta\cdot\mathcal{A}\nabla_\Gamma\eta - \frac{\sigma}{R^2}\int_\Gamma div_\Gamma V\eta^2.\end{aligned}$$

Proof. We will make use of the fact that $B(0)=\mathrm{I}$ and $\det(B(0))=1$. To simplify notation when taking the derivative ∂_e, we assume that we are evaluating at $q=0$, if there is no argument given. The product rule gives

$$\begin{aligned}\partial_e J^*(0,\eta) = \frac{\kappa}{2}\int_\Gamma 2\mathrm{div}_\Gamma\frac{\mathrm{d}}{\mathrm{d}t}(\det(B(te))G(te)^{-1}\nabla_\Gamma\eta)|_{t=0}\Delta_\Gamma\eta \\ - (\Delta_\Gamma\eta)^2\frac{\mathrm{d}}{\mathrm{d}t}\det(B(te))|_{t=0} \\ + \Big(\frac{\sigma}{2}-\frac{\kappa}{R^2}\Big)\int_\Gamma\nabla_\Gamma\eta\cdot\frac{\mathrm{d}}{\mathrm{d}t}(\det(B(te))G(te)^{-1})|_{t=0}\nabla_\Gamma\eta \\ - \frac{\sigma}{R^2}\int_\Gamma\frac{\mathrm{d}}{\mathrm{d}t}\det(B(te))|_{t=0}\eta^2,\end{aligned}\tag{3.3}$$

where we calculate

$$\begin{aligned}\partial_e B &= \nabla_\Gamma V + (\mathcal{H}V)\otimes\nu,\\ \partial_e\det(B) &= \mathrm{div}_\Gamma V,\\ \partial_e B^{-1} &= -\nabla_\Gamma V - (\mathcal{H}V)\otimes\nu.\end{aligned}$$

Since $G := B^TB$, one has

$$\frac{\mathrm{d}}{\mathrm{d}t}(\det(B(te))G(te)^{-1})|_{t=0} = (\mathrm{div}_\Gamma V)\,\mathrm{I} - \nabla_\Gamma V - (\mathcal{H}V)\otimes\nu - \nabla_\Gamma V^T - \nu\otimes(\mathcal{H}V).$$

We are also required to calculate the surface divergence of the above quantity:

$$\begin{aligned}&\mathrm{div}_\Gamma\partial_e(\det(B)G^{-1})\\ &\quad= \mathrm{div}_\Gamma\left((\mathrm{div}_\Gamma V)\,\mathrm{I} - \nabla_\Gamma V - (\mathcal{H}V)\otimes\nu - \nabla_\Gamma V^T - \nu\otimes(\mathcal{H}V)\right)\end{aligned}$$

$$= \sum_{k=1}^{n+1} (\nabla_\Gamma \underline{D}_k - \underline{D}_k \nabla_\Gamma) V_k - \Delta_\Gamma V - \mathrm{div}_\Gamma((\mathcal{H}V) \otimes \nu + \nu \otimes (\mathcal{H}V))$$

$$= -\Delta_\Gamma V - H\mathcal{H}V + \sum_{k=1}^{n+1} (\mathcal{H}\nabla_\Gamma V_k)_k \nu - (\mathcal{H}\nabla_\Gamma V_k)\nu_k - \underline{D}_k(\nu(\mathcal{H}V)_k).$$

It can be seen that

$$\sum_{k=1}^{n+1} (\mathcal{H}\nabla_\Gamma V_k)_k = \mathcal{H} : \nabla_\Gamma V,$$

similarly,

$$\sum_{k=1}^{n+1} (\mathcal{H}\nabla_\Gamma V_k)_j \nu_k = -(\mathcal{H}^2 V)_j.$$

Moreover,

$$\sum_{k=1}^{n+1} \underline{D}_k(\nu(\mathcal{H}V)_k) = \mathcal{H}^2 V + (\mathcal{H} : \nabla_\Gamma V + (\nabla_\Gamma \cdot \mathcal{H}) \cdot V)\nu.$$

Together, this gives

$$\mathrm{div}_\Gamma(\partial_e(\det(B)G^{-1})) = -\Delta_\Gamma V - \nu(\nabla_\Gamma \cdot \mathcal{H}) \cdot V - H\mathcal{H}V,$$

where the middle term will vanish when multiplied against a tangential vector field. We are left with

$$\partial_e(\det(B(q))G^{-1}) : D_\Gamma^2 \eta = \mathcal{A} : D_\Gamma^2 \eta - (\mathcal{H}V) \otimes \nu : D_\Gamma^2 \eta - \nu \otimes (\mathcal{H}V) : D_\Gamma^2 \eta,$$

where one may recall that for vectors b, c and matrix A, $A : (b \otimes c) = b^T A c$. Thus,

$$\partial_e(\det(B)G^{-1}) : D_\Gamma^2 \eta = \mathcal{A} : D_\Gamma^2 \eta + \mathcal{H}^2 \nabla_\Gamma \eta \cdot V,$$

which gives the desired result when evaluating H and $\mathcal{H}$ for a sphere. ∎

By Theorem 3.9, when evaluating this at the solution of Problem 2.3, we will obtain the derivative we seek. Notice that it might be convenient to integrate by parts to remove the surface Hessian. This will give an alternate formula which is better suited for the numerical methods considered in [13, 16].

Corollary 3.13. *Under the assumptions of Proposition 3.12 it may be seen that, for $p < 2$ and $\eta \in W^{3,p}(\Omega)$,*

$$\partial_e J^*(q, \eta)|_{q=0} = -\kappa \int_\Gamma \frac{1}{2} (div_\Gamma V) (\Delta_\Gamma \eta)^2 + \nabla_\Gamma \Delta_\Gamma \eta \cdot \mathcal{A} \nabla_\Gamma \eta + \frac{1}{2}\left(\sigma - \frac{2\kappa}{R^2}\right) \int_\Gamma \nabla_\Gamma \eta \cdot \mathcal{A} \nabla_\Gamma \eta - \frac{\sigma}{R^2} \int_\Gamma (div_\Gamma V)\, \eta^2. \tag{3.4}$$

Proof. This follows from integration by parts in (3.3) and following through with the above proof. The integration by parts is admissible by the regularity of η. ∎

By the additional regularity shown in Theorem 2.4, we see that we may pick $\eta = \arg\min_{v\in U(p)} J(v)$ in the above. This gives the main result of the work which follows from the previous results.

Theorem 3.14. *Let* $p \in \Lambda^\circ$, $u = \arg\min_{v\in U(p)} J(v)$ *and* $\mathcal{A} := (div_\Gamma V)I - \nabla_\Gamma V - \nabla_\Gamma V^T$. *Then,*

$$\partial_e \mathcal{E}(p) = -\kappa \int_\Gamma \frac{1}{2}\,(div_\Gamma V)\,(\Delta_\Gamma u)^2 + \nabla_\Gamma \Delta_\Gamma u \cdot \mathcal{A}\nabla_\Gamma u + \frac{1}{2}\Big(\sigma - \frac{2\kappa}{R^2}\Big)\int_\Gamma \nabla_\Gamma u \cdot \mathcal{A}\nabla_\Gamma u - \frac{\sigma}{R^2}\int_\Gamma (div_\Gamma V)\,u^2. \tag{3.5}$$

Proof. This is an application of Theorem 3.9 and Corollary 3.13. ∎

Example 3.15. Let $N = 1$. Then $\partial_e \mathcal{E}(p) = 0$ for all $p \in \Lambda^\circ$ and directions $e \in \mathbb{R} \times T_{X_\mathcal{G}}\Gamma$. This follows from the symmetry of the sphere and the invariance of J under rotations and translations.

3.3. Proof of Lemma 3.2 by construction

Here, we prove Lemma 3.2 by constructing χ.

3.3.1. Rotation of a single particle. This example pertains to a simple rotation. The example we consider is rotating a single particle whose centre X_G is taken to be the North pole $N := (0, 0, R)^T$, without loss of generality. The points of the particle are contained in the set $B_r(N) := \{x : x_3 > R - r\}$ around the North pole, and all other points are contained in the set $B_{r+\varepsilon}(N)^C := \{x : x_3 < R - r - \varepsilon\}$.

Since this is a one-parameter family of transformations, we write, with an abuse of notation, $\chi(\alpha, \cdot) = \chi(q, \cdot)$ for the diffeomorphism.

We may then explicitly write

$$\chi(\alpha, x) = \zeta(x)\Big((0, 0, x_3)^T + \cos(\alpha)\Big(\frac{N}{R} \times x\Big) \times \frac{N}{R} + \sin(\alpha)\Big(\frac{N}{R} \times x\Big)\Big) + (1 - \zeta(x))x,$$

where $\zeta\colon \Gamma \to \mathbb{R}$ is a C^k-smooth cut off function such that $\zeta = 1$ on $B_r(N)$, $\zeta = 0$ on $B_{r+\varepsilon}(N)^C$, and depends only on x_3.

It is clear that this χ is C^k-smooth with $\chi(\alpha, \cdot)$ having inverse $\chi(-\alpha, \cdot)$, and that it moves the points of the particle based at the North pole as required, while others remain stationary. Furthermore, for each fixed x_3 it is essentially a two-dimensional rotation about $(0, 0, 1)^T$, so the volume element induced by χ is constantly equal to 1.

It is convenient to calculate the derivative $\partial_e \chi(0, x)$ for $e = (1, 0)$:

$$\partial_e \chi(0, x) = \partial_s(\chi(s, x))|_{s=0} = \zeta(x)\Big(\frac{N}{R} \times x\Big).$$

One may also verify that $\mathrm{div}_\Gamma \partial_e \chi(0,\cdot) = 0$. This follows by calculating

$$\mathrm{div}_\Gamma \partial_e \chi(0,x) = \frac{1}{R}(\nabla_\Gamma \zeta(x)\cdot(N\times x) + \zeta(x)\mathrm{div}_\Gamma(N\times x)).$$

Since ζ depends only on x_3, one sees that the first term is some scalar function multiplied by $P_\Gamma(x)N\cdot(N\times x)$, which vanishes. For the second term, one calculates, by extending to a small neighbourhood of the surface (as in the definition of surface derivatives),

$$\mathrm{div}_\Gamma(N\times x) = \sum_{i=1}^{3} \underline{D}_i (N\times x)_i = \sum_{i,j=1}^{3} \Big(\delta_{ij} - \frac{x_i x_j}{R^2}\Big)\partial_j (N\times x)_i.$$

We see that this vanishes, since $\delta_{ij}\partial_j(N\times x)_i = 0$ for any $i, j = 1,2,3$, and

$$\sum_{i=1}^{3} \frac{x_i x_j}{R^2}\partial_j (N\times x)_i = \sum_{i=1}^{3} \frac{x_j}{R^2}\partial_j (x_i (N\times x)_i) = 0$$

for any $j = 1,2,3$.

3.3.2. A general χ. Since the set $\bigcup_{i=1}^N \mathcal{C}_i(p)$ is a finite union of points, we know there is a strictly positive distance separating each pair of points. It follows that we may assume that the family of sets $\bigcup_{i=1}^N \mathcal{C}_i(p+tq)$ for $(t,q)\in[0,1]\times\mathcal{B}$ also satisfy this condition, and set $\varepsilon > 0$ to be the smallest separation between the points of $\bigcup_{i=1}^N \mathcal{C}_i(p+tq) =: K$, that is,

$$\varepsilon = \inf_{(t,q)\in[0,1]\times\mathcal{B}} \inf_{x\in K} \inf_{\substack{y\in K,\\ y\neq x}} |x-y|.$$

Definition 3.16 ([34, equation (2.6)]). We define the vector surface curl of a C^1 function $\psi\colon\Gamma\to\mathbb{R}$ by

$$\mathrm{curl}_\Gamma \psi := \nu\times\nabla_\Gamma\psi.$$

Definition 3.17. Given $\delta\in(0,\varepsilon)$, define $\mathcal{V}\colon[0,1]\times\mathcal{B}\times\Gamma\to\mathbb{R}^3$ by

$$\mathcal{V} := \mathrm{curl}_\Gamma \psi,$$

where for each $(t,q)\in[0,1]\times\mathcal{B}$ and $x\in\bigcup_{i=1}^N \mathcal{C}_i(p+tq)$, the function $\psi\colon[0,1]\times\mathcal{B}\times\Gamma\to\mathbb{R}$ is locally given by

$$\psi(t,q,y) = \zeta(|x-y|)y\cdot(\partial_s\big(\phi_i(p+sq,\cdot)\circ\phi_i(p+tq,\cdot)^{-1}(y)\big)|_{s=t}\times\nu(x))$$

for $y\in\Gamma\cap B_{\varepsilon/2}(x)$, otherwise $\psi = 0$, where $\zeta\colon\mathbb{R}\to\mathbb{R}$ is a C^{k+1}-smooth cut off function such that

$$\begin{cases}\zeta(s) = 1 & |s|\le\delta/4,\\ \zeta(s) = 0 & |s|\ge\delta/2.\end{cases}$$

Example 3.18. We now give a calculation of $\partial_s(\phi_i(p+sq,\cdot)\circ\phi_i(p+tq,\cdot)^{-1}(y))|_{s=t}$. For simplicity, we set $p=0$ and $t=0$ and neglect any i subscripts.

Let $q = (\alpha, \tau) \in \mathbb{R} \times T_{X_{\mathscr{G}}}$. We then have

$$\phi(sq, x) = R_T(s\tau) R_n(s\alpha) x,$$

therefore

$$\partial_s \left(\phi(sq, x)\right)|_{s=0} = \left(\nu(X_{\mathscr{G}}) \times \tau\right) \times x + \alpha \left(\nu(X_{\mathscr{G}}) \times x\right).$$

It is clear that the first term corresponds to the translation and the second term, the rotation.

Lemma 3.19. *The function $\mathcal{V}$ given in Definition 3.17 satisfies*

- $\mathcal{V} \in C^k$;
- $div_\Gamma \mathcal{V} = 0$;
- $\mathcal{V}(t, 0, x) = 0$ *for all* $(t, x) \in [0, 1] \times \Gamma$;
- *For each* $i = 1, \ldots, N$,

$$\mathcal{V}(t, q, \cdot) = \partial_s \left(\phi_i(p + tq, \cdot) \circ \phi_i(p + sq, \cdot)^{-1}\right)|_{s=t}$$

  on $\mathcal{C}_i(p + tq)$, *for each* $(t, q) \in [0, 1] \times \mathcal{B}$; *and*
- $\partial_e \mathcal{V}(t, 0, x) = \mathcal{V}(0, e, x)$ *for all* $t \in [0, 1]$, $e \in \prod_{i=1}^N (T_{X_{\mathscr{G}_i}} \times \mathbb{R})$, *and* $x \in \Gamma$.

Proof. Smoothness and that $\mathcal{V}(\cdot, 0, \cdot)$ vanishes is clear by construction, divergence-free follows from $\mathcal{V}$ being the curl of another function [34, Lemma 2.1]. For the point conditions, we evaluate at $y \in \Gamma$ such that $|x - y| < \frac{\delta}{4}$ for some $x \in \mathcal{C}_i(p + tq)$,

$$\begin{aligned}\operatorname{curl}_\Gamma \psi(t, q, y) &= \operatorname{curl}_\Gamma \left(y \cdot \left(\partial_s \left(\phi_i(p + sq, \cdot) \circ \phi_i(p + tq, \cdot)^{-1}(y)\right)|_{s=t}\right) \times \nu(x)\right) \\ &= \nu(y) \times \left(\nabla_\Gamma y \cdot \left(\partial_s \left(\phi_i(p + sq, \cdot) \circ \phi_i(p + tq, \cdot)^{-1}(y)\right)|_{s=t} \times \nu(x)\right)\right)\end{aligned}$$

for each $(t, q) \in [0, 1] \times \mathcal{B}$, $i = 1, \ldots, N$. This, upon evaluation at $x \in \mathcal{C}_i(p + tq)$ for any $(t, q) \in [0, 1] \times \mathcal{B}$ and $i = 1, \ldots, N$, leaves us with

$$\operatorname{curl}_\Gamma \psi(t, q, x) = \partial_s \left(\phi_i(p + sq, \cdot) \circ \phi_i(p + tq, \cdot)^{-1}\right)|_{s=t}(x).$$

The final condition takes a little bit of work. We show the condition holds near the 'special points' of $\bigcup_{i=1}^N \mathcal{C}_i(p)$. Given $i = 1, \ldots, N$, for $x \in \mathcal{C}_i(p)$ and y near x, we see that

$$\begin{aligned}\partial_e \mathcal{V}(t, 0, y) &= \partial_s \mathcal{V}(t, se, y)|_{s=0} \\ &= \partial_s \left(\mathcal{V}(t, se, \phi_i(p + se, \cdot) \circ \phi_i(p, \cdot)^{-1}(y))\right)|_{s=0} \\ &\quad + \partial_s \left(\mathcal{V}(t, se, x) - \mathcal{V}(t, se, \phi_i(p + se, \cdot) \circ \phi_i(p, \cdot)^{-1}(y))\right)|_{s=0} \\ &= \partial_s \left(\mathcal{V}(t, se, \phi_i(p + se, \cdot) \circ \phi_i(p, \cdot)^{-1}(y))\right)|_{s=0} \\ &\quad + \partial_s \left(\mathcal{V}(t, se, y) - \mathcal{V}(t, se, \phi_i(p + se, \cdot) \circ \phi_i(p, \cdot)^{-1}(y))\right)|_{s=0}.\end{aligned}$$

This first term we may see is equal to $\mathcal{V}(0, e, x)$. For the remaining terms,

$$\begin{aligned}&\partial_s \left(\mathcal{V}(t, se, \phi_i(p + se, \cdot) \circ \phi_i(p, \cdot)^{-1}(y)) \mathcal{V}(t, se, y)\right)|_{s=0} \\ &\quad = \partial_s \left(\nabla_\Gamma \mathcal{V}(t, se, y) \cdot \left(\phi_i(p + se, \cdot) \circ \phi_i(p, \cdot)^{-1}(y)\right) - y\right)|_{s=0},\end{aligned}$$

which we see vanishes due to the fact that $\nabla_\Gamma \mathcal{V}(\cdot, se, \cdot) \to 0$ as $s \to 0$ on $[0,1] \times \Gamma$ and also $\phi_i(p + se, \cdot) \circ \phi_i(p, \cdot)^{-1}(y) - y \to 0$ as $s \to 0$. ∎

We will construct χ in the following way.

Definition 3.20.

(1) Let $\eta\colon [0,1] \times \mathcal{B} \times \Gamma \to \Gamma$ be the solution of the family of ODEs

$$\partial_t \eta(t, q, x) = \mathcal{V}(t, q, \eta(t, q, x)), \quad \eta(0, q, x) = x$$

for all $(q, x) \in \mathcal{B} \times \Gamma$.

(2) Let $\chi\colon \mathcal{B} \times \Gamma \to \Gamma$ be defined by $\chi(q, x) = \eta(1, q, x)$ for all $(q, x) \in \mathcal{B} \times \Gamma$.

It is clear by standard ODE theory [24] that η exists and is smooth. Moreover, $\eta(1, q, \cdot)$ is a diffeomorphism.

Proposition 3.21. *The map $\chi\colon \mathcal{B} \times \Gamma \to \Gamma$, $(q, x) \mapsto \eta(1, q, x)$ satisfies the conditions in Lemma 3.2.*

Proof. This follows from the properties of $\mathcal{V}$ in Lemma 3.19. The smoothness of χ follows from the smoothness of $\mathcal{V}$ and standard ODE theory [24], as does the existence and smoothness of an inverse. The condition that $\mathcal{V}(\cdot, 0, \cdot) = 0$ gives that $\chi(0, \cdot)$ is the identity.

The condition $v \circ \chi(q, \cdot)^{-1} \in U(p + q)$ if and only if $v \in U(p)$ has three parts:

- $v \circ \chi(q, \cdot) \in H^2(\Gamma)$ if and only if $v \in H^2(\Gamma)$,
- $\int_\Gamma v = \int_\Gamma v \circ \chi(q, \cdot)$ for all $v \in H^2(\Gamma)$, and
- $\gamma(p + q)\left(v \circ \chi^{-1}\right) = \gamma(p) v$ for all $v \in H^2(\Gamma)$.

The first condition follows from two applications of Lemma A.2 with $X = \chi(q, \cdot)$ and $X = \chi(q, \cdot)^{-1}$, and the smoothness of these maps. The second condition follows from the fact that $\operatorname{div}_\Gamma \mathcal{V} = 0$. The final condition follows from the point conditions on $\mathcal{V}$. By considering the ODE that η solves, we see that χ satisfies

$$\chi(q, \cdot) = \phi_i(p + q, \cdot) \circ \phi_i(p, \cdot)^{-1} \quad \text{on } \mathcal{C}_i(p),$$

for each $i = 1, \dots, N$, which gives, recalling the definition of γ in Definition 2.12,

$$\begin{aligned} \gamma_i(p + q) v &= v \circ \phi_i(p + q, \cdot)|_{\mathcal{C}_i} \\ &= v \circ \phi_i(p + q, \cdot) \circ \phi_i(p, \cdot)^{-1} \circ \phi_i(p, \cdot)|_{\mathcal{C}_i} \\ &= \gamma_i(p)(v \circ \chi(q, \cdot)). \end{aligned}$$

Hence, the desired result follows. ∎

We now wish to calculate $\partial_e \chi(0, \cdot)$ on Γ.

Proposition 3.22. *For each $e \in \prod_{i=1}^N (T_{X_{g_i}} \times \mathbb{R})$, the following holds:*

$$\partial_e \chi(0, \cdot) = \mathcal{V}(0, e, \cdot) \quad \text{on } \Gamma.$$

Proof. It is clear that $\partial_e \chi(0,\cdot) = \partial_e \eta(1,0,\cdot)$. From the ODE solved by η, one may see that $\eta_e(t,x) := \partial_e \eta(t,0,x)$ for $(t,x) \in [0,1] \times \Gamma$ satisfies

$$\partial_t \eta_e(t,x) = \partial_e \mathcal{V}(t,0,\eta(t,0,x)) + \nabla_\Gamma \mathcal{V}(t,0,\eta(t,0,x))\eta_e(t,x),$$

for all $(t,x) \in [0,1] \times \Gamma$. Recall that $\mathcal{V}(t,0,x) = 0$ for all $(t,x) \in [0,1] \times \Gamma$, so the second term in the above ODE vanishes and one has that $\eta(t,0,x) = x$ for all $(t,x) \in [0,1] \times \Gamma$. By applying the final condition of Lemma 3.19, one has that

$$\partial_t \eta_e(t,x) = \mathcal{V}(0,e,x),$$

hence, $\partial_e \chi(0,\cdot) = \eta_e(1,\cdot) = \mathcal{V}(0,e,\cdot)$ on Γ. ∎

4. Numerical experiments

To begin, we discuss the approximation errors which arise in numerical simulations.

Proposition 4.1. *Let $\tilde{u} \in W^{1,\infty}(\Gamma)$ with $-\Delta_\Gamma \tilde{u} \in W^{1,2-\delta}(\Gamma)$ for any $\delta > 0$. Then, for any $\varepsilon \in (0,1)$, $p \in (1,2)$, and $q = p^*$ there is $C > 0$ such that*

$$\begin{aligned}|\partial_e J^*(0,\tilde{u}) - \partial_e \mathcal{E}(p)| \leq C\|\nabla_\Gamma V\|_{0,\infty}\big(&\|\Delta_\Gamma(u-\tilde{u})\|_{1,p}\|\nabla_\Gamma u\|_{1,q} \\ &+ \|\Delta_\Gamma(u-\tilde{u})\|_{0,2}\left(\|\Delta_\Gamma \tilde{u}\|_{0,2} + \|\Delta_\Gamma u\|_{0,2}\right) \\ &+ \|\nabla_\Gamma(u-\tilde{u})\|_{0,\frac{2-\varepsilon}{1-\varepsilon}}\|\Delta_\Gamma \tilde{u}\|_{1,2-\varepsilon} \\ &+ \|\nabla_\Gamma(u-\tilde{u})\|_{1,2}(\|\nabla_\Gamma u\|_{1,2} + \|\nabla_\Gamma \tilde{u})\|_{1,2})\big).\end{aligned}$$

Proof. This follows from the form $\partial_e J^*$ takes in (3.5) and making use of Hölder inequalities. ∎

The particular form for the estimate above is chosen so that one may apply the error estimates of [16], making use of a split formulation to approximate u and $-\Delta_\Gamma u + u$ with linear finite elements. There may be different estimates one wishes to show which relate to the formula of Proposition 3.12, for example, if one were to use a higher order discretisation of the membrane problem such as the method of [31], which deals with a biharmonic problem on surfaces.

4.1. Experiments

The numerical experiments are chosen to illustrate the formula and that the method of difference quotients may be unreliable. It is clear that the difference quotient will be slower—one would have to solve (at least) two algebraic systems, whereas when using the formula, a single algebraic system is solved and a functional evaluated.

For all of the experiments, the values $\kappa = \sigma = R = 1$ are taken. The optimal membrane shape, $u(p)$, is approximated by solving a penalised finite element problem denoted by $u_h(p)$. The penalisation weakly enforces the point constraints and is done in order to ease

the linear algebra. Second order splitting is used and linear finite elements are employed following [16], where the error due to using a penalty formulation is shown to be well controlled. All of the experiments have been implemented under the Distributed and Unified Numerics Environment (DUNE) [2, 3]. The finite element discretisation is defined as follows.

Definition 4.2. Let Γ_h be a connected, polygonal surface approximating Γ and $\mathcal{S}_h$ be the space of linear finite element functions on Γ_h. Given $v_h \in \mathcal{S}_h$, a finite element function, let $w_h \in \mathcal{S}_h$ satisfy

$$\int_{\Gamma_h} \nabla_{\Gamma_h} v_h \cdot \nabla_{\Gamma_h} \eta_h + v_h \eta_h = \int_{\Gamma_h} w_h \eta_h$$

for all $\eta_h \in \mathcal{S}_h$. We define

$$J_h(v_h) := \frac{1}{2} \int_{\Gamma_h} \kappa (w_h - v_h)^2 + \Big(\sigma - \frac{2\kappa}{R^2}\Big) |\nabla_{\Gamma_h} v_h|^2 - \frac{2\sigma}{R^2} v_h^2,$$

which is the discrete analogue of (2.1). Define

$$\mathcal{E}_h(p) := J_h(u_h(p)),$$

which is the discrete analogue of Definition 2.14, where $u_h(p)$ is the minimiser of J_h over $\mathcal{S}_h$ such that $\int_{\Gamma_h} u_h(p) = 0$ and $\gamma(p)(u_h^l(p)) = Z$.

Let $V_h = I_h V$, where V is as in Definition 3.11 and $I_h \colon C(\Gamma) \to \mathcal{S}_h$ is the interpolation map. Then define $\mathcal{A}_h := I(\mathrm{div}_{\Gamma_h} V_h) - \nabla_{\Gamma_h} V_h - \nabla_{\Gamma_h} V_h^T$ and

$$\begin{aligned}(\partial_e J^*)_h(v_h) := -\kappa \int_{\Gamma_h} \frac{1}{2} (\mathrm{div}_{\Gamma_h} V)(v_h - w_h)^2 + \nabla_{\Gamma_h}(v_h - w_h) \cdot \mathcal{A}_h \nabla_{\Gamma_h} v_h \\ + \frac{1}{2}\Big(\sigma - \frac{2\kappa}{R^2}\Big) \int_{\Gamma_h} \nabla_{\Gamma_h} v_h \cdot \mathcal{A}_h \nabla_{\Gamma_h} v_h - \frac{\sigma}{R^2} \int_{\Gamma_h} (\mathrm{div}_{\Gamma_h} V) v_h^2,\end{aligned}$$

which is the discrete analogue of (3.4).

Remark 4.3. Note that $(\partial_e J^*)_h$ is not necessarily the derivative of $\mathcal{E}_h$. The difference quotients with respect to particle configurations will be approximations of the derivative of $\mathcal{E}_h$.

The first experiment is for a fixed particle configuration and a sequence of refined meshes. This is followed by some experiments on a fixed grid and varying the particle configurations. The experiments demonstrate that applying the formula to the finite element approximation is superior to using difference quotients. Since exact values of approximated quantities are unknown, the error at level h is estimated by the difference between the value at level h and the value on the most refined grid. Thus, for quantity F_h and smallest grid size h^*, we say the error E_h is given by $|F_h - F_{h^*}|$. For two grids with size h_1 and h_2, we say the EOC of F_h is given by $\log(E_{h_1}/E_{h_2})/\log(h_1/h_2)$, and we take h_1 and h_2 to be from successively refined grids.

For the first three experiments, $V(\cdot,\cdot) = \mathcal{V}(0,\cdot,\cdot)$, as in the construction in Definition 3.17; and δ is taken to be roughly h, so that the interpolation of V has support on a small, fixed number of vertices. This makes the evaluation of the functional very quick. For the remaining experiments, V is constructed as in Section 3.3.1, where the r and ε we use for the cut off function are taken to be $r = 0.75$ and $\varepsilon = 0.15$.

4.1.1. Convergence experiment. In this experiment we consider a fixed configuration that has six particles each consisting of a single point with locations and constraints given by

$$\begin{aligned} X_1 &= (0,0,1)^T, \quad Z_1 = 1; & X_2 &= (0,0,-1)^T, \quad Z_2 = 0;\\ X_3 &= (0,1,0)^T, \quad Z_3 = 0; & X_4 &= (0,-1,0)^T, \quad Z_4 = 0;\\ X_5 &= (1,0,0)^T, \quad Z_5 = 0.1; & X_6 &= (-1,0,0)^T, \quad Z_6 = 0. \end{aligned}$$

Approximate evaluations of the energy together with the derivative in the direction $e = (1,0,0)^T \in T_{X_1}\Gamma$ are computed. For each finite element mesh size h, we calculate

$$\mathcal{E}_h(0), \quad \mathcal{E}_h(\theta(\delta_h)), \quad \mathcal{E}_h(-\theta(\delta_h)), \quad (\partial_e J^*)_h(u_h).$$

Here, $\mathcal{E}_h(\theta(\delta))$ denotes the energy where the point X_1 is replaced by the point

$$X_1(\theta(\delta)) := (\sin(\theta(\delta)), 0, \cos(\theta(\delta)))^T, \text{ with } \theta(\delta) := \arcsin\left(\frac{\delta}{\sqrt{\delta^2 + (\delta-1)^2}}\right).$$

Another approximation to $\partial_e \mathcal{E}(0)$ is given by the difference quotient

$$DQ_h := \frac{(\mathcal{E}_h(\theta(\delta_h)) - \mathcal{E}_h(-\theta(\delta_h)))}{(\theta(\delta_h) - \theta(-\delta_h))}$$

of the energies. The function θ and the values of δ_h are chosen so that $X_1(\pm\theta(\delta_h))$ lie on a vertex of the grid. The results are tabulated in Table 1. Observe that they indicate convergence of the energy $\mathcal{E}_h(0)$, the difference quotient DQ_h, and the derivative $(\partial_e J^*)_h(u_h)$ as $h \to 0$. The experimental order of convergence of the derivative quantities are displayed in Table 2.

4.1.2. Experiment for simple particles lying on vertices. For this experiment, approximations of the energy and the derivative are calculated on a sequence of configurations parameterised by the location of one point, $X_1(t)$. The configuration is defined for each t by

$$X_1(t) = (\sin(\theta(t)), 0, \cos(\theta(t)))^T, \quad Z_1 = 0.1,$$

and

$$\begin{aligned} X_2 &= (0,0,-1)^T, \ Z_2 = 0; & X_3 &= (0,1,0)^T, \quad Z_3 = 0;\\ X_4 &= (0,-1,0)^T, \ Z_4 = 0; & X_5 &= (-1,0,0)^T, \ Z_5 = 0, \end{aligned}$$

h	δ_h	$\mathcal{E}_h(-\theta(\delta_h))$	$\mathcal{E}_h(0)$	$\mathcal{E}_h(\theta(\delta_h))$	$(\partial_e J^*)_h(u_h)$	DQ_h
0.301511	0.25	16.7958	17.199	16.3577	−1.2195	−1.5438
0.152499	0.125	15.524	15.5781	15.3318	−1.33257	−1.4439
0.0764719	0.0625	15.0356	15.0309	14.945	−1.37356	−1.40516
0.0382639	0.03125	14.8615	14.8509	14.8174	−1.38244	−1.39168
0.0191355	0.0078125	14.8006	14.7929	14.7788	−1.38464	−1.38720

Table 1. Calculated quantities for experiment in Section 4.1.1.

h	$E_{\partial_e J_h^*}$	E_{DQ_h}	$\mathrm{EOC}_{\partial_e J_h^*}$	EOC_{DQ_h}
0.301511	0.165134	0.156597	–	–
0.152499	0.0520672	0.0567013	1.69327	1.49032
0.0764719	0.0110707	0.0179647	2.24306	1.66523
0.0382639	0.00219195	0.00448579	2.33893	2.00384
0.0191355	–	–	–	–

Table 2. Derived quantities for experiment in Section 4.1.1.

where θ is again defined by

$$\theta(t) := \arcsin\left(\frac{t}{\sqrt{t^2+(t-1)^2}}\right).$$

With this choice of θ, the points $X_1, \ldots, X_5$ lie on vertices of our chosen grid for each evaluation of t. We calculate $\mathcal{E}_h(t)$ and $(\partial_e J^*)_h(u_h(t))$ for $t \in \left\{\frac{m}{2^6} : m \in \mathbb{N}_0, m \leq 2^6\right\}$. Figure 3 displays $\mathcal{E}_h(t)$ whilst the values $(\partial_e J^*)_h(u_h(t))$ with the difference quotient of $\mathcal{E}_h(t)$, and the difference between them, are shown in Figure 4. One may calculate that the relative error has a maximum of 2% at the boundary and is below 1% for the interior.

4.1.3. Experiment for simple particles not lying on vertices of the grid. This experiment demonstrates that when the constraint points do not lie on the vertices of the grid, the difference quotient becomes a less reliable method. We choose $t \in \{\frac{m}{100} : m \in \mathbb{N}_0, m \leq 100\}$. The plot of the resulting $\mathcal{E}_h(t)$ in Figure 5 has the same characteristic shape as the plot in the previous experiment. For Figure 6, we plot $(\partial_e J^*)_h(u_h(t))$ with the difference quotient of $\mathcal{E}_h(t)$, and the difference between them. We notice that here, the difference quotient does not match the formula as well as it did in the previous experiment.

4.1.4. Experiment for non-trivial particles. This experiment concerns two non-trivial particles for which there is little chance of the points lying on vertices unless, one tailors the grid to the points. The base of the particle $\mathcal{C}_1$ has centre $X_{\mathcal{G}_1} = (0,0,1)^T$ and $\mathcal{C}_1 = \{X_i\}_{i=1}^8$, where

$$X_1 = (0.5, 0, \sqrt{1-0.5^2})^T,$$

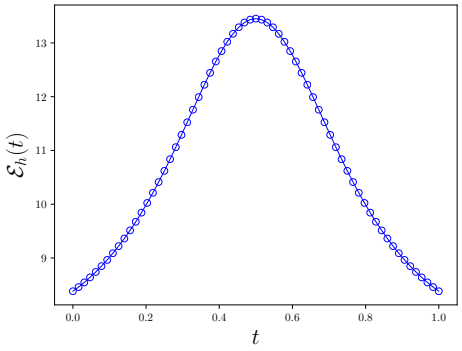
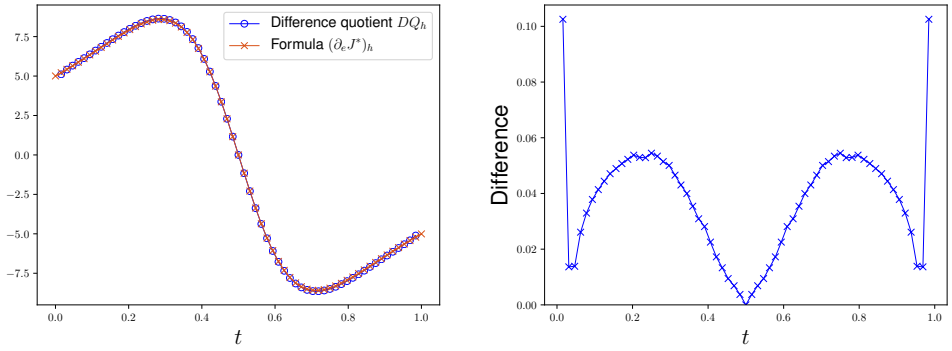


Figure 3. Energy $\mathcal{E}_h(t)$ for experiment in Section 4.1.2.



(a) $(\partial_e J^*)_h$ and DQ_h (b) $|(\partial_e J^*)_h - DQ_h|$

Figure 4. Graphs of quantities from experiment in Section 4.1.2.

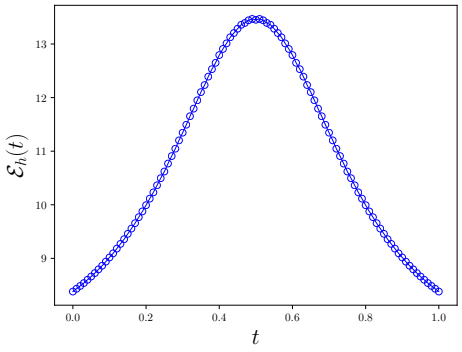


Figure 5. Energy $\mathcal{E}_h(t)$ for experiment in Section 4.1.3.

$$
\begin{aligned}
X_2 &= (-0.5, 0, \sqrt{1-0.5^2})^T,\\
X_3 &= (0.25, 0.25, \sqrt{1-0.25^2-0.25^2})^T,\\
X_4 &= (-0.25, 0.25, \sqrt{1-0.25^2-0.25^2})^T,\\
X_5 &= (0.25, -0.25, \sqrt{1-0.25^2-0.25^2})^T,\\
X_6 &= (-0.25, -0.25, \sqrt{1-0.25^2-0.25^2})^T,\\
X_7 &= (0, 0.125, \sqrt{1-0.125^2})^T,\\
X_8 &= (0, -0.125, \sqrt{1-0.125^2})^T,
\end{aligned}
$$

and $(Z_1)_i = 1 - \frac{1}{5}(X_i)_1^2$, for $i = 1, \ldots, 8$. The second particle is

$$\mathcal{C}_2 := \{x = (x_1, x_2, x_3)^T \in \Gamma : (x_1, x_3, -x_2)^T \in \mathcal{C}_1\},$$

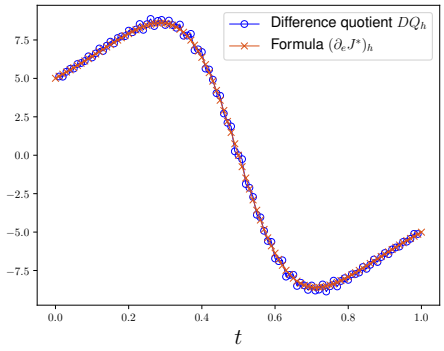
with $(Z_2)_i = 1 - \frac{1}{5}(X_i)_1^2$ for $i = 1, \ldots, 8$.

Particle $\mathcal{C}_1$ is rotated about the North pole so that we consider the particle configuration in the state $((\frac{\pi}{2}t, 0), (0, 0))$, recalling Definition 2.9. The quantities $\mathcal{E}_h(t)$ and $(\partial_e J^*)_h(u_h(t))$ are calculated for $t \in \{\frac{m}{2^5} : m \in \mathbb{N}_0, m \leq 2^6\}$. The quantities $\mathcal{E}(t)$, $(\partial_e J^*)_h(u_h(t))$, and the central difference quotient for $\mathcal{E}_h(t)$ are plotted in Figure 7 and Figure 8. The results show that the difference quotients become highly unreliable.

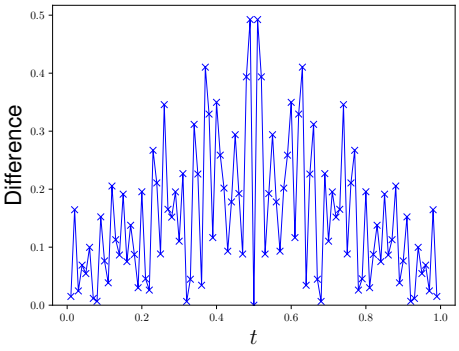
4.1.5. Experiment to observe the numerical error of a trivial system. The difference quotient in the previous experiment is extremely noisy. In this experiment, we consider a perturbation of the above experiment, where we remove $\mathcal{C}_2$ so that, in light of Example 3.15, we are approximating zero. The quantities from this experiment are plotted in Figure 9, where the exact values are independent of t and equal to zero. Note that the oscillations in Figure 9(a) indicate that using a difference quotient will be an unreliable way of calculating the derivative. On the other hand, one sees in Figure 9(b) that the error in the discrete formula for the derivative is bounded by 10^{-4}.

4.1.6. Application of formula. In this experiment we consider two particles which are not axi-symmetric. The idea of the experiment is to show how orientation may affect the membrane mediated forces. We consider a particle based at a pole and a particle based at the equator and calculate the derivative of the energy for a displacement of the particle at the pole in the direction of the particle at the equator. A negative derivative implies that the energy decreases and indicates an attractive force, whereas a positive derivative indicates the opposite. This calculation is repeated after rotating the particle at the pole by $\frac{\pi}{2}$. The particle $\mathcal{C}_1 = \{X_i\}_{i=1}^8$ is defined by

$$
\begin{aligned}
X_1 &= (0.3, 0, \sqrt{1-0.3^2})^T,\\
X_2 &= (-0.3, 0, \sqrt{1-0.3^2})^T,\\
X_3 &= (0.15, 0.15, \sqrt{1-0.15^2-0.15^2})^T,\\
X_4 &= (-0.15, 0.15, \sqrt{1-0.15^2-0.15^2})^T,
\end{aligned}
$$



(a) $(\partial_e J^*)_h$ and DQ_h



(b) $|(\partial_e J^*)_h - DQ_h|$

Figure 6. Graphs of quantities from experiment in Section 4.1.3.

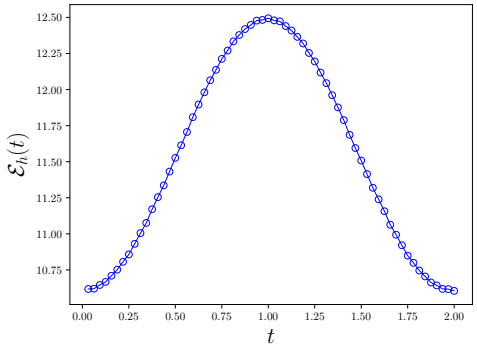
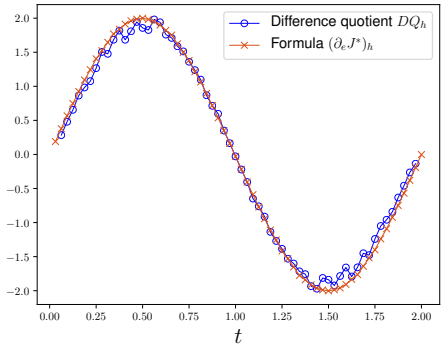
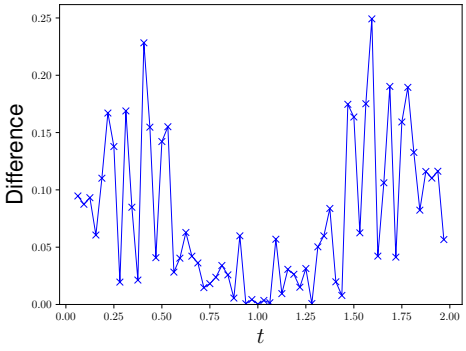


Figure 7. Energy $\mathcal{E}_h(t)$ for experiment in Section 4.1.4.

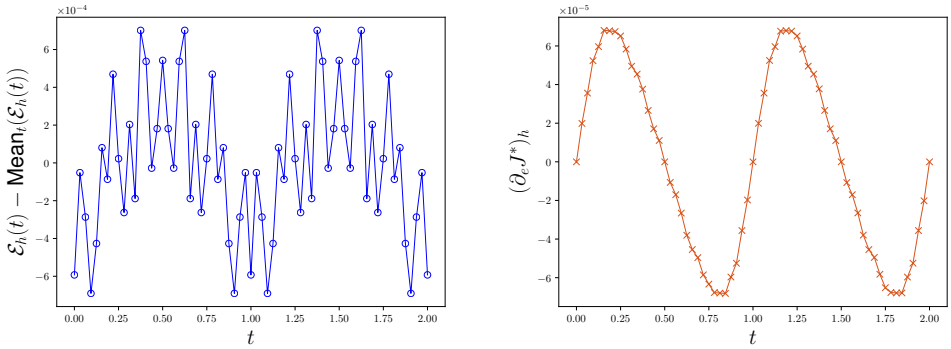


(a) $(\partial_e J^*)_h$ and DQ_h



(b) $|(\partial_e J^*)_h - DQ_h|$

Figure 8. Graphs of quantities from experiment in experiment in Section 4.1.4.



(a) Deviation from average of $\mathcal{E}_h(t)$ (b) $(\partial_e J^*)_h$

Figure 9. Graphs for experiment in Section 4.1.5.

$$X_5 = (0.15, -0.15, \sqrt{1 - 0.15^2 - 0.15^2})^T,$$
$$X_6 = (-0.15, -0.15, \sqrt{1 - 0.15^2 - 0.15^2})^T,$$
$$X_7 = (0, 0.075, \sqrt{1 - 0.075^2})^T,$$
$$X_8 = (0, -0.075, \sqrt{1 - 0.075^2})^T,$$

and $(Z_1)_i = 1 - 10(X_i)_1^2$, for $i = 1, \ldots, 8$, and centre $X_{\mathcal{G}_1} := (0, 0, 1)^T$. We define $\mathcal{C}_2$ by

$$\mathcal{C}_2 := \{x = (x_1, x_2, x_3)^T \in \Gamma : (x_1, x_3, -x_2)^T \in \mathcal{C}_1\},$$

with $(Z_2)_i = 1 - 10(X_i)_1^2$, for $i = 1, \ldots, 8$, and centre $X_{\mathcal{G}_2} = (0, 1, 0)^T$. We let $\tau = (0, 1, 0)^T \in T_{X_{\mathcal{G}_1}}$. The derivative at $0 \in \prod_{i=1}^2 (\mathbb{R} \times T_{X_{\mathcal{G}_i}} \Gamma)$ in direction $e = ((0, \tau), (0, 0))$ is calculated. We recall that the direction e represents a translation of $\mathcal{C}_1$ in the direction τ. We then rotate the particle at the pole by $\frac{\pi}{2}$, so that the particle system is in configuration $p = ((\frac{\pi}{2}, 0), (0, 0))$, and calculate the derivative in the same direction e.

The calculated values are

$$(\partial_e J^*)_h(0) \approx -10.6729 \quad \text{and} \quad (\partial_e J^*)_h(p) \approx 18.5636,$$

which show that different orientations may have different signs of the derivative so that one orientation is attractive and the other repulsive. The discrete displacements, $u_h(0)$ and $u_h(p)$, of the membrane are displayed in Figure 10.

5. Conclusion

In this article we have shown the differentiability of $\mathcal{E}(p)$, the membrane mediated interaction energy for a near spherical membrane with particles attached at points which depend

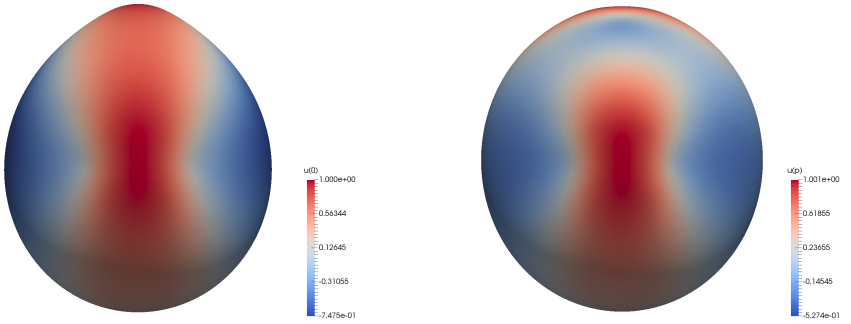


Figure 10. The rescaled graphs of the membranes from experiment in Section 4.1.6, left $0.1\,u(0)$, right $0.1\,u(p)$, both with $(0,1,0)^T$ coming out of the page and $(0,0,1)^T$ pointing up. The colours represent the magnitude of the deformation.

smoothly on p. Further to showing the differentiability, we have given an explicit formula to calculate the derivative and given numerical examples which show that this formula is more robust than a difference quotient approach. It would be of interest to extend this analysis for particles which are able to move more generally, tilting and moving out from the surface. Furthermore, it is desirable to consider the problem for inequality constraints on the 'interior' of a particle. Finally, one could analyse higher order derivatives of the energy so that one could determine the stability of a given configuration.

A. The pullback to a reference domain

We give some general results on the calculation of the composition of pullbacks and derivatives, where we consider that the image and domain of the diffeomorphism need not be the same. As we are working with different surfaces, it is necessary to make clear to which surface geometric quantities belong to. This is achieved by using a superscript of the surface, e.g. H^{Γ_1} is the mean curvature of Γ_1, and H^{Γ_0} the mean curvature of Γ_0. Consider the case of Γ_0 and Γ_1 being C^k, compact surfaces, with $\mathrm{X}\colon \Gamma_0 \to \Gamma_1$ a C^k-diffeomorphism, where we require $k \geq 2$.

Given some function $u\colon \Gamma_1 \to \mathbb{R}$, we wish to obtain expressions for $(\nabla_{\Gamma_1} u) \circ \mathrm{X}$ and $(\underline{D}^2_{\Gamma_1} u) \circ \mathrm{X}$. The first part of this is developed in [7], where also the trace of the second quantity, the Laplace–Beltrami, is calculated. Although the surface Hessian is not required for the model we consider in this work, we compute it for completion as it may arise in other elastic type models, where the Hessian regularly arises. This is carried out using a method which avoids integration by parts, so that surfaces with boundary may be considered.

Lemma A.1. *Let $u \in H^1(\Gamma_1)$. Then $u \circ \mathrm{X} \in H^1(\Gamma_0)$ and*

$$(\nabla_{\Gamma_1} u) \circ \mathrm{X} = \left(\nabla_{\Gamma_0}\mathrm{X} + \nu^{\Gamma_1} \circ \mathrm{X} \otimes \nu^{\Gamma_0}\right)^{-T} \nabla_{\Gamma_0}(u \circ \mathrm{X}) = \nabla_{\Gamma_0}\mathrm{X} G_{\Gamma_0}^{-1} \nabla_{\Gamma_0}(u \circ \mathrm{X}),$$

where $G_{\Gamma_0} := \nabla_{\Gamma_0}\mathrm{X}^T \nabla_{\Gamma_0}\mathrm{X} + \nu^{\Gamma_0} \otimes \nu^{\Gamma_0}$.

The proof is shown in Lemma 3.2 of [7]. We write $B := \nabla_{\Gamma_0}\mathrm{X} + \nu^{\Gamma_1} \circ \mathrm{X} \otimes \nu^{\Gamma_0}$, which satisfies

$$B^T B = G_{\Gamma_0}.$$

This gives a simpler form of the above lemma, where

$$(\nabla_{\Gamma_1} u) \circ \mathrm{X} = B^{-T} \nabla_{\Gamma_0}(u \circ \mathrm{X}).$$

Lemma A.2. *Let $u \in H^2(\Gamma_1)$. Then, $u \circ \mathrm{X} \in H^2(\Gamma_0)$ and for $i, j = 1, \ldots, n+1$, we have*

$$\begin{aligned}(\underline{D}_i^{\Gamma_1} \underline{D}_j^{\Gamma_1} u) \circ \mathrm{X} = \frac{1}{b} \mathrm{div}_{\Gamma_0}\left(b B^{-1}(B^{-T} \nabla_{\Gamma_0} \hat{u})_j\right)_i \\ + (H^{\Gamma_1} \circ \mathrm{X} - H^{\Gamma_0})(\nu_i^{\Gamma_1} \circ \mathrm{X})(B^{-T} \nabla_{\Gamma_0} \hat{u})_j,\end{aligned}$$

where $b = \det(B)$, $b_{ij} = B_{ij}$ and $b^{ij} = (B^{-1})_{ij}$.

Proof. We write $\hat{u} := u \circ \mathrm{X}$ and where indices are repeated in a product, summation is assumed. We now make use of the preceding lemma to obtain

$$\underline{D}_i^{\Gamma_1} \underline{D}_j^{\Gamma_1} u \circ \mathrm{X} = b^{li} \underline{D}_l^{\Gamma_0}\left(b^{kj} \underline{D}_k^{\Gamma_0} \hat{u}\right).$$

Then, we write this as something similar to a divergence form:

$$\begin{aligned}\underline{D}_i^{\Gamma_1} \underline{D}_j^{\Gamma_1} u \circ \mathrm{X} = \frac{1}{b} \underline{D}_l^{\Gamma_0}\left(b b^{li} b^{kj} \underline{D}_k^{\Gamma_0} \hat{u}\right) - \frac{1}{b} \underline{D}_l^{\Gamma_0}(b) b^{li} b^{kj} \underline{D}_k^{\Gamma_0} \hat{u} \\ - \underline{D}_l^{\Gamma_0}\left(b^{li}\right) b^{kj} \underline{D}_k^{\Gamma_0} \hat{u}.\end{aligned}$$

In [7], it is shown that

$$\underline{D}_l^{\Gamma_0} b^{li} = -b^{lm} \underline{D}_l^{\Gamma_0} b_{mf} b^{fi}, \quad \frac{1}{b} \underline{D}_l^{\Gamma_0} b = b^{fm} \underline{D}_l^{\Gamma_0} b_{mf}.$$

Inserting these into the above gives

$$\begin{aligned}\underline{D}_i^{\Gamma_1} \underline{D}_j^{\Gamma_1} u \circ \mathrm{X} = \frac{1}{b} \underline{D}_l^{\Gamma_0}\left(b b^{li} b^{kj} \underline{D}_k^{\Gamma_0} \hat{u}\right) - b^{fm} \underline{D}_l^{\Gamma_0} b_{mf} b^{li} b^{kj} \underline{D}_k^{\Gamma_0} \hat{u} \\ + b^{lm} \underline{D}_l^{\Gamma_0} b_{mf} b^{fi} b^{kj} \underline{D}_k^{\Gamma_0} \hat{u}.\end{aligned}$$

Since we are summing over f, k, l and m in the above, it is possible to swap the indices, in particular we swap f and l in the second term. We now consider the terms

$$\begin{aligned}b^{lm} \underline{D}_l^{\Gamma_0} b_{mf} b^{fi} b^{kj} \underline{D}_k^{\Gamma_0} \hat{u} - b^{lm} \underline{D}_f^{\Gamma_0} b_{ml} b^{fi} b^{kj} \underline{D}_k^{\Gamma_0} \hat{u} \\ = b^{lm} b^{fi}\left(b^{kj} \underline{D}_k^{\Gamma_0} \hat{u}\right)\left(\underline{D}_l^{\Gamma_0} b_{mf} - \underline{D}_f^{\Gamma_0} b_{ml}\right).\end{aligned} \tag{A.1}$$

We now wish to use the definition of B in order to simplify equation A.1. To this end, we want to swap the order of the derivatives. As in [7], one calculates

$$\begin{aligned}\underline{D}_l^{\Gamma_0} b_{mf} - \underline{D}_f^{\Gamma_0} b_{ml} = \big(\underline{D}_l^{\Gamma_0}(\nu_m^{\Gamma_1} \circ \mathrm{X}) - (\mathcal{H}^{\Gamma_0} \nabla_{\Gamma_0} \mathrm{X}_m)_l\big)\nu_f^{\Gamma_0} \\ + \big((\mathcal{H}^{\Gamma_0} \nabla_{\Gamma_0} \mathrm{X}_m)_f - \underline{D}_f^{\Gamma_0}(\nu_m^{\Gamma_1} \circ \mathrm{X})\big)\nu_l^{\Gamma_0}.\end{aligned}$$

We now use this to simplify (A.1). We make use of the relation $b^{ki}\nu_k^{\Gamma_0} = \nu_i^{\Gamma_1} \circ \mathrm{X}$ to calculate each part:

$$\begin{aligned}b^{lm}b^{fi}\underline{D}_l^{\Gamma_0}(\nu_m^{\Gamma_1} \circ \mathrm{X})\nu_f^{\Gamma_0} &= (\nu_i^{\Gamma_1} \circ \mathrm{X})(B^{-T}(\nabla_{\Gamma_1}\nu_m) \circ \mathrm{X})_m \\ &= (H^{\Gamma_1}\nu_i^{\Gamma_1}) \circ \mathrm{X}, \\ b^{lm}b^{fi}(\mathcal{H}^{\Gamma_0}\nabla_{\Gamma_0}\mathrm{X}_m)_l\nu_f^{\Gamma_0} &= b^{lm}b^{fi}\mathcal{H}_{lk}^{\Gamma_0}\underline{D}_k^{\Gamma_0}\mathrm{X}_m\nu_f^{\Gamma_0} \\ &= b^{lm}b^{fi}\mathcal{H}_{lk}^{\Gamma_0}b_{mk}\nu_f^{\Gamma_0} \\ &= H^{\Gamma_0}(\nu_i^{\Gamma_1} \circ \mathrm{X}), \\ b^{lm}b^{fi}(\mathcal{H}^{\Gamma_0}\nabla_{\Gamma_0}\mathrm{X}_m)_f\nu_l^{\Gamma_0} &= b^{lm}b^{fi}\mathcal{H}_{fk}^{\Gamma_0}\underline{D}_k^{\Gamma_0}\mathrm{X}_m\nu_l^{\Gamma_0} \\ &= b^{lm}b^{fi}\mathcal{H}_{fk}^{\Gamma_0}b_{mk}\nu_l^{\Gamma_0} \\ &= b^{fi}\mathcal{H}_{fl}^{\Gamma_0}\nu_l^{\Gamma_0} \\ &= 0, \\ b^{lm}b^{fi}(\nu_m^{\Gamma_1} \circ \mathrm{X})\nu_l^{\Gamma_1} &= (\nu_m^{\Gamma_1} \circ \mathrm{X})(B^{-T}\nabla_{\Gamma_0}(\nu^{\Gamma_1} \circ \mathrm{X}))_i \\ &= (\nu_m^{\Gamma_1} \circ \mathrm{X})\mathcal{H}_{mi}^{\Gamma_1} \circ \mathrm{X} \\ &= 0.\end{aligned}$$

This then gives

$$\begin{aligned}b^{lm}b^{fi}\big(b^{kj}\underline{D}_k^{\Gamma_0}\hat{u}\big)\big(\underline{D}_l^{\Gamma_0}b_{mf} - \underline{D}_f^{\Gamma_0}b_{ml}\big) \\ = ((H^{\Gamma_1} \circ \mathrm{X}) - H^{\Gamma_0})\big(\nu_i^{\Gamma_1} \circ \mathrm{X}\big)\big(B^{-T}\nabla_{\Gamma_0}\hat{u}\big)_j,\end{aligned}$$

which completes the result. ∎

Remark A.3. By taking the trace of $\underline{D}_{\Gamma_1}^2 u \circ \mathrm{X}$, one obtains

$$(\Delta_{\Gamma_1} u) \circ \mathrm{X} = \frac{1}{b}\mathrm{div}_{\Gamma_0}(bG_{\Gamma_0}^{-1}\nabla_{\Gamma_0}(u \circ \mathrm{X})).$$

B. Implicit function theorem

We give the version of the implicit function theorem we use in Theorem 3.9, which is taken from [8, Theorem 7.13-1].

Theorem B.1. *Let $\mathcal{X}$ be a normed vector space and $\mathcal{Y}$ and $\mathcal{Z}$ Banach spaces with $\Omega \subset \mathcal{X} \times \mathcal{Y}$ open and $(a,b) \in \Omega$. Let $f \in C(\Omega;\mathcal{Z})$ such that $f(a,b) = 0$; the derivative $\frac{\partial f}{\partial y}(x,y) \in \mathcal{L}(\mathcal{Y};\mathcal{Z})$ exists at all points $(x,y) \in \Omega$; $\frac{\partial f}{\partial y} \in C(\Omega;\mathcal{L}(\mathcal{Y};\mathcal{Z}))$; and $\frac{\partial f}{\partial y}(a,b)$ is a bijection, so that $(\frac{\partial f}{\partial y}(a,b))^{-1} \in \mathcal{L}(\mathcal{Z};\mathcal{Y})$.*

(1) *Then, there is an open neighbourhood V of a in $\mathcal{X}$, a neighbourhood W of b in $\mathcal{Y}$, and $g \in C(V;W)$ such that $V \times W \subset \Omega$ and $\{(x,y) \in V \times W : f(x,y) = 0\} = \{(x,y) \in V \times W : y = g(x)\}$.*

(2) *Assume in addition that f is differentiable at $(a,b) \in \Omega$. Then, f is differentiable at a and*

$$g'(a) = \left(\frac{\partial f}{\partial y}(a,b)\right)^{-1} \frac{\partial f}{\partial x}(a,b) \in \mathcal{L}(\mathcal{X};\mathcal{Y}).$$

(3) *Assume in addition that $f \in C^k(\Omega;\mathcal{Z})$ for some $k \geq 1$. Then, there is an open neighbourhood $\widetilde{V} \subset V$ of a in $\mathcal{X}$ and neighbourhood $\widetilde{W} \subset W$ of b in $\mathcal{Y}$ such that $\frac{\partial f}{\partial y}(x,y) \in \mathcal{L}(\mathcal{Y};\mathcal{Z})$ is a bijection, so that $(\frac{\partial f}{\partial y}(x,y))^{-1} \in \mathcal{L}(\mathcal{Z};\mathcal{Y})$ at each $(x,y) \in \widetilde{V} \times \widetilde{W}$, $g \in C^k(\widetilde{V};\mathcal{Y})$ and $g'(x) = -(\frac{\partial f}{\partial y}(x,g(x)))^{-1} \frac{\partial f}{\partial x}(x,g(x)) \in \mathcal{L}(\mathcal{X};\mathcal{Y})$ for each $x \in \widetilde{V}$.*

C. Elliptic regularity

We first show, for arbitrary surfaces, that $\Delta_\Gamma u \in W^{1,p}(\Gamma)$ for $p \leq 2$ gives $u \in W^{3,p}(\Gamma)$.

Proposition C.1. *Suppose $u \in H^1(\Gamma)$ with $\Delta_\Gamma u \in W^{1,p}(\Gamma)$ for some $p \in (1,2]$ and Γ is a C^3 surface. Then, there is a constant $C > 0$ independent of u such that for each $i,j = 1,2,3$,*

$$\|\underline{D}_i \underline{D}_j u\|_{1,p} \leq C\left(\|\underline{D}_j \Delta_\Gamma u\|_{0,p} + \|\Delta_\Gamma u\|_{0,2} + \|\nabla_\Gamma u\|_{0,2}\right).$$

Proof. We make use of the following inf-sup condition, shown in [13]:

$$\exists \gamma > 0 : \gamma \|\xi\|_{1,p} \leq \sup_{\eta \in W^{1,q}(\Gamma)} \frac{\int_\Gamma \nabla_\Gamma \eta \cdot \nabla_\Gamma \xi + \eta\xi}{\|\eta\|_{1,q}} \quad \forall \xi \in W^{1,p}(\Gamma).$$

Since Γ has finite measure, it holds that $\|\underline{D}_i \underline{D}_j u\|_{0,p} \leq C \|\underline{D}_i \underline{D}_j u\|_{0,2}$, which we know is controlled by $\|\Delta_\Gamma u\|_{0,2} + \sqrt{\|\mathcal{H} H - 2\mathcal{H}^2\|_{0,\infty}} \|\nabla_\Gamma u\|_{0,2}$ (see [11]). It is then sufficient to show that $\int_\Gamma \nabla_\Gamma \underline{D}_i \underline{D}_j u \cdot \nabla_\Gamma \eta$ is bounded appropriately.

$$\begin{aligned}\int_\Gamma \nabla_\Gamma \underline{D}_i \underline{D}_j u \cdot \nabla_\Gamma \eta = &\int_\Gamma \underline{D}_j \Delta_\Gamma u \underline{D}_i \eta \\ &+ \left((\mathcal{H}\nabla_\Gamma \underline{D}_k u)_j \nu_k - (\mathcal{H}\nabla_\Gamma \underline{D}_k u)_k \nu_i - \underline{D}_k\left[(\mathcal{H}\nabla_\Gamma u)_k \nu_j\right]\right)\underline{D}_i \eta \\ &- \underline{D}_k \underline{D}_j u (\mathcal{H}\nabla_\Gamma \eta)_k \nu_i - (\mathcal{H}\nabla_\Gamma \underline{D}_j u)_k \nu_i \underline{D}_k \eta.\end{aligned}$$

This follows from repeatedly applying integration by parts and swapping the order of derivatives. Applying Hölder's inequality, we immediately obtain the result. ∎

Proposition C.2. *Let $u \in H^2(\Gamma)$ be the unique solution of Problem 2.3. Then, it holds that for any $p < 2$, $u \in W^{3,p}(\Gamma)$.*

Proof. By [18, Theorem 2.34] and the arguments presented in [16, Section 5], it is clear that there is $\bar{p} \in \mathbb{R}$ and $\lambda \in \mathbb{R}^K$ such that

$$a(u, v) + \bar{p} \int_\Gamma v + \lambda \cdot v|_{\mathcal{E}} = 0 \quad \forall v \in H^2(\Gamma).$$

Let $\eta := -\Delta_\Gamma u - \frac{2}{R^2} u \in L^2(\Gamma)$. Then, for any $v \in H^2(\Gamma)$,

$$a(u, v) = \int_\Gamma (-\kappa \Delta_\Gamma v + \sigma v)\eta = -\lambda \cdot v|_{\mathcal{E}} - \bar{p} \int_\Gamma v.$$

Let $\phi \in C^\infty(\Gamma)$ and consider the inverse Laplace type map $G : L^2(\Gamma) \to H^2(\Gamma)$ such that $G : \phi \mapsto v$, where $-\kappa \Delta_\Gamma v + \sigma v = \phi$. Via a local argument, it may be seen that for any $q > 2$, $\|v\|_{0,\infty} \leq C \|\phi\|_{-1,q}$ (see [33]). Hence,

$$\begin{aligned} \langle \phi, \eta \rangle = \int_\Gamma \phi \eta &= \int_\Gamma (-\kappa \Delta_\Gamma v + \sigma v)\eta \\ &= -\lambda \cdot v|_{\mathcal{E}} - \bar{p} \int_\Gamma v \\ &\leq \|\lambda\|_{\mathbb{R}^M} \|v\|_{0,\infty} + |\bar{p}| \|v\|_{0,1} \\ &\leq C \|\phi\|_{-1,q}. \end{aligned}$$

Thus, we have shown that η represents a bounded linear operator on $W^{-1,q}(\Gamma)$, and in turn we have shown that $-\Delta_\Gamma u - \frac{2}{R^2} u \in W^{1,q^*}(\Gamma)$. In particular, by Proposition C.1, it holds that $u \in W^{3,q^*}(\Gamma)$. Since $q^* < 2$ is arbitrary, the result is complete. ∎

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