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THE SHAPE DERIVATIVE OF THE GAUSS CURVATURE

ANÍBAL CHICCO-RUIZ, PEDRO MORIN, AND M. SEBASTIAN PAULETTI

Abstract. We present a review of results about the shape derivatives of scalar- and vector-valued shape functions, and extend the results from Doğan and Nochetto [*ESAIM Math. Model. Numer. Anal.* 46 (2012), no. 1, 59–79] to more general surface energies. In that article, Doğan and Nochetto consider surface energies defined as integrals over surfaces of functions that can depend on the position, the unit normal and the mean curvature of the surface. In this work we present a systematic way to derive formulas for the shape derivative of more general geometric quantities, including the Gauss curvature (a new result not available in the literature) and other geometric invariants (eigenvalues of the second fundamental form). This is done for hyper-surfaces in the Euclidean space of any finite dimension. As an application of the results, with relevance for numerical methods in applied problems, we derive a Newton-type method to approximate a minimizer of a shape functional. We finally find the particular formulas for the first and second order shape derivatives of the area and the Willmore functional, which are necessary for the aforementioned Newton-type method.

1. Introduction

Energies that depend on the domain appear in applications in many areas, from materials science, to biology, to image processing. Examples when the domain dependence of the energy occurs through surfaces include the minimal surface problem, the study of the shape of droplets (surface tension), image segmentation and shape of bio-membranes, to name a few. In the language of the shape derivative theory [27, 8, 16, 30], these energies are called shape functionals. This theory provides a solid mathematical framework to pose and solve minimization problems for such functionals.

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For most of the problems of interest, the energy (shape functional) can be cast as

$$\int_\Gamma F(\text{geometric quantities}),$$

where "geometric quantities" stands for quantities such as the normal $\boldsymbol{n}$, the mean curvature κ, the Gauss curvature κ_g, or in general any quantity that is well defined for a surface Γ as a geometric object, i.e., independent of the parametrization. For example, $F = 1$ in the case of a minimal surface; $F = F(x, \boldsymbol{n})$ is used in the modeling of crystals [2, 1, 29, 28] in materials science. The Willmore functional corresponds to $F = \frac{1}{2}\kappa^2$ [31]—where κ is the mean curvature—and the related spontaneous curvature functional to $F = \frac{1}{2}(\kappa - \kappa_0)^2$; they are used in models for the bending energy of membranes, particularly in the study of biological vesicles [15, 20, 19, 26]. In these cases a term with the Gaussian curvature κ_G is part of the energy which is essential when dealing with membranes with boundaries (not closed). The modified form of the Willmore functional, which corresponds to $F = g(x)\kappa^2$, is used to model bio-membranes when the concentration or composition of lipids changes spatially [3, 6].

The minimization of these energies requires the knowledge of their (shape) derivatives with respect to variations of the domain and has motivated researchers to seek formulas for the shape derivative of the normal and the mean curvature. The shape derivative of the normal is simple and can be found in [8, 30] among other references. Particular cases of $F = F(x, n)$ are derived in [4, 22, 28]. The shape derivative of the mean curvature or particular cases of $F = F(\kappa)$ can also be found in [32, 17, 25, 11, 10, 9, 30], where the shape derivative is computed from scratch; some using parametrizations, others in a more coordinate-free setting using the oriented distance function, but in general the same computations are repeated each time a new functional dependent on the mean curvature appears. A more systematic approach to the computations is found in [9], where Doğan and Nochetto propose a formula for the shape derivative of a functional of the form $F = F(x, \boldsymbol{n}, \kappa)$, that relies on knowing the shape derivatives of $\boldsymbol{n}$ and κ. They rightfully assert that by having this formula at hand, it wouldn't be necessary to redo all the computations every time a new functional depending on these quantities appears.

The main motivation of this article was to find such a formula when F also depends on the Gauss curvature κ_g which, as far as we know, has not been presented elsewhere. With this goal in mind we performed a thorough review of existing results in the literature and briefly summarize them in this article, hoping that it will be a useful reference for future works. In the course of our research we faced the need to compute shape derivatives of tangential differential operators, so our results allow us to compute shape derivatives of surface invariants. These are important when second order shape derivatives are necessary in Newton-type methods for minimizing functionals. We have also discovered that the different definitions of shape derivative of boundary-based and domain-based functionals have led to some misunderstandings and confusion in the past. We hope to clarify this issue in the present article.

Our new results (Section 7) allow us to develop a more systematic approach to compute shape derivatives of integrands that are functional relations of geometric quantities. The method, starting from the shape derivative of the normal as the base case, provides a recursive formula for the shape derivative of higher order tangential derivatives of geometric quantities. In particular we give a nice formula for the shape derivative of the Gaussian curvature and extend the results of [9] to more generals integrands.

Outline. The outline of this article is as follows. Sections 2–5 contain a review of known results which we have put together from different sources and hope that can be useful for future reference, besides making the article more self-contained. Those readers who are familiar with the existing results about shape differentiation can skip these sections and jump to Sections 7–9 where the new results are stated and proved. Except for a few minor results, all the statements in Sections 2–5 can be found in the literature, but not all of them together in one reference.

In Section 2 we state some preliminary concepts and elements of basic tangential calculus. In Section 3 we recall the concept of shape differentiable functionals through the velocity method. In Section 4 we motivate and introduce the concept of shape derivative of functions involved in the definition of shape functionals, and we point out an important difference between the definition of shape derivative for domain functions and for boundary functions, which has led to some confusion in previous works. In Section 5 we explore some properties of shape differentiation of (shape) functions, such as the relationship between the shape derivative of domain functions and the classical derivative operators. Also we obtain the boundary shape derivative of the normal and the mean curvature.

In Section 7 we look into the relationship between the shape derivative of boundary functions and the tangential derivative operators, obtaining the main results of this article.

We end with Sections 8 and 9 where we apply the newly obtained results to find the shape derivatives of the Gauss curvature, the geometric invariants and introduce a quasi-Newton method in the language of shape derivatives whose formula is then computed for the Area and the Willmore functionals.

2. Preliminaries

2.1. **General concepts.** Our notation follows closely that of [8, Ch. 2, Sec. 3]. A *domain* is an open and bounded subset Ω of $\mathbb{R}^N$, and a *boundary* is the boundary of some domain, i.e., $\Gamma = \partial\Omega$. An $N-1$ *dimensional surface* in $\mathbb{R}^N$ is a reasonable subset of a boundary in $\mathbb{R}^N$. We will mainly consider $\Gamma = \partial\Omega$ as a surface and we will call it either surface or boundary, unless we clarify otherwise. If a boundary Γ is smooth, we denote the *normal vector field* by $\boldsymbol{n}$ and assume that it points outward of Ω. The *principal curvatures*, denoted by $\kappa_1, \dots, \kappa_{N-1}$, are the eigenvalues of the second fundamental form of Γ, which are all real. The *mean curvature* κ and

Gaussian curvature κ_g are

$$\kappa = \sum_{i=1}^{N-1} \kappa_i \qquad \text{and} \qquad \kappa_g = \prod_{i=1}^{N-1} \kappa_i. \tag{2.1}$$

These quantities can also be expressed in terms of the tangential derivatives of the normal; see Subection 2.3 for $N = 3$ and Section 8 for any dimension, where we introduce the geometric invariants of a surface, following Definition 3.46 of [21].

Given a Euclidean space $\mathbb{V}$ of finite dimension, a *tensor* S is an element of the set $\mathrm{Lin}(\mathbb{V})$ of linear operators from $\mathbb{V}$ into itself. The *tensor product* of two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ is the tensor $\boldsymbol{u} \otimes \boldsymbol{v}$ which satisfies $(\boldsymbol{u} \otimes \boldsymbol{v})\boldsymbol{w} = (\boldsymbol{v} \cdot \boldsymbol{w})\boldsymbol{u}$. The *trace* of a tensor S is $\mathrm{tr}(S) = \sum_i S\boldsymbol{e}_i \cdot \boldsymbol{e}_i$, with $\{\boldsymbol{e}_i\}$ any orthonormal basis of $\mathbb{V}$. The trace of a tensor $\boldsymbol{u} \otimes \boldsymbol{v}$ is $\mathrm{tr}(\boldsymbol{u} \otimes \boldsymbol{v}) = \boldsymbol{u} \cdot \boldsymbol{v}$.

The *scalar product of tensors* S and T is given by $S : T = \mathrm{tr}(S^T T)$, where S^T is the transpose of S, which satisfies $S\boldsymbol{u} \cdot \boldsymbol{v} = \boldsymbol{u} \cdot S^T\boldsymbol{v}$, and the *tensor norm* is $|S| = \sqrt{S : S}$. Given a basis of $\mathbb{V}$, S can be represented by a square matrix S_{ij}. We mainly consider $\mathbb{V} = \mathbb{R}^N$ with the canonical basis. We summarize some of their properties in the following lemma [14, Ch. I]:

Lemma 2.1 (Tensor Properties)**.** *For vectors* $\boldsymbol{u}$, $\boldsymbol{v}$, $\boldsymbol{a}$, $\boldsymbol{b} \in \mathbb{V}$, *and tensors* S, T, $P \in \mathrm{Lin}(\mathbb{V})$, *we have:*

- $S(\boldsymbol{u} \otimes \boldsymbol{v}) = S\boldsymbol{u} \otimes \boldsymbol{v}$ *and* $(\boldsymbol{u} \otimes \boldsymbol{v})S = \boldsymbol{u} \otimes S^T\boldsymbol{v}$,
- $I : S = \mathrm{tr}(S)$, *where* I *is the identity tensor,*
- $ST : P = S : PT^T = T : S^T P$,
- $S : \boldsymbol{u} \otimes \boldsymbol{v} = u \cdot S\boldsymbol{v}$,
- $(\boldsymbol{a} \otimes \boldsymbol{b}) : (\boldsymbol{u} \otimes \boldsymbol{v}) = (\boldsymbol{a} \cdot \boldsymbol{u})(\boldsymbol{b} \cdot \boldsymbol{v})$,
- $S : T = S : T^T = \frac{1}{2} S : (T + T^T)$ *if* S *is symmetric.*

2.2. **The oriented distance function.** The oriented distance function is a very useful tool for the study of geometric properties and smoothness of the boundary of a domain Ω. We see in Section 2.3 that it also provides a framework to deal with the tangential derivatives of functions defined on surfaces.

For a given domain $\Omega \subset \mathbb{R}^N$ with boundary Γ, the *oriented distance function* $b = b(\Omega) : \mathbb{R}^N \to \mathbb{R}$ is given by $b(x) = d(\Omega)(x) - d(\mathbb{R}^N \setminus \Omega)(x)$, where $d(\Omega)(x) = \inf_{y \in \Omega} |y - x|$. It is proved in [8, Sec. 7.8] that the smoothness of b in a neighborhood of Γ is equivalent to the local smoothness of Γ, and moreover, its gradient ∇b and its Hessian matrix $D^2 b$ coincide, respectively, with the outward unit normal $\boldsymbol{n}$ and the second fundamental form of the surface Γ when restricted to Γ. Furthermore, if Ω is a $\mathcal{C}^2$ domain with compact boundary Γ, then there exists a tubular neighborhood $S_h(\Gamma)$ such that $b \in \mathcal{C}^2(S_h(\Gamma))$, and Γ is a $\mathcal{C}^2$-manifold of dimension $N-1$ [8, Ch. 9, p. 492]. Therefore, ∇b is a $\mathcal{C}^1$ extension for the normal $\boldsymbol{n}$ which satisfies

$$|\nabla b|^2 \equiv 1 \quad \text{in } S_h(\Gamma). \tag{2.2}$$

From this eikonal equation we obtain some useful identities. First of all, (2.2) readily implies

$$D^2 b \, \nabla b \equiv 0. \tag{2.3}$$

Also, if Γ is $\mathcal{C}^3$, we can differentiate again to obtain

$$\operatorname{div}(D^2 b) \cdot \nabla b = -|D^2 b|^2, \tag{2.4}$$

where we have used that $\operatorname{div}(S^T \boldsymbol{v}) = S : \nabla \boldsymbol{v} + \boldsymbol{v} \cdot \operatorname{div} S$ for S and $\boldsymbol{v}$ tensor and vector valued differentiable functions, respectively [14, p. 30]. The divergence $\operatorname{div} S$ of a tensor valued function is a vector which satisfies $\operatorname{div} S \cdot \boldsymbol{e} = \operatorname{div}(S^T \boldsymbol{e})$ for any vector $\boldsymbol{e}$.

Applying the well known identity [14, p. 32]

$$\operatorname{div}(D\boldsymbol{v}^T) = \nabla(\operatorname{div} \boldsymbol{v}) \tag{2.5}$$

to $\boldsymbol{v} = \nabla b$, we can write (2.4) as follows:

$$\nabla \Delta b \cdot \nabla b = -|D^2 b|^2. \tag{2.6}$$

Since $\boldsymbol{n} = \nabla b|_\Gamma$, we can obtain from b additional geometric information about Γ. Indeed, the N eigenvalues of $D^2 b|_\Gamma$ are the principal curvatures $\kappa_1, \kappa_2, \ldots, \kappa_{N-1}$ of Γ and zero [8, Ch. 9, p. 500]. The mean curvature of Γ, given by (2.1), can also be obtained as $\kappa = \operatorname{tr} D^2 b = \Delta b$ (on Γ). Also, $|D^2 b|^2 = \operatorname{tr}(D^2 b)^2 = \sum \kappa_i^2$, the sum of the square of the principal curvatures, so that the Gaussian curvature is $\kappa_g = \frac{1}{2}\left[(\Delta b)^2 - |D^2 b|^2\right]$ (for $N = 3$); notice that the right-hand side of this last identity makes sense in $S_h(\Gamma)$ whereas the left-hand side is defined only on Γ, so that the equality holds on Γ. Moreover, from (2.6) and denoting $\partial_n := \boldsymbol{n} \cdot \nabla$, we obtain that

$$\partial_n \Delta b = -\sum \kappa_i^2 \quad \text{on } \Gamma. \tag{2.7}$$

The *projection* $p = p_\Gamma$ of a point $x \in \mathbb{R}^N$ onto Γ is $p(x) = \arg\min_{z\in\Gamma} |z - x|$. In the tubular neighborhood $S_h(\Gamma)$ it can be written in terms of the oriented distance function as follows [8, Ch. 9, p. 492]:

$$p(x) = x - b(x)\nabla b(x). \tag{2.8}$$

Note that $p \in \mathcal{C}^{k-1}(S_h(\Gamma))$ if $\Gamma \in \mathcal{C}^k$, $k \geq 1$. For any $x \in S_h(\Gamma)$, the *orthogonal projection operator* $P(x) = P_\Gamma(x)$ from $\mathbb{R}^N$ onto the tangent plane $T_{p(x)}(\Gamma)$ is given by $P(x) = I - \nabla b(x) \otimes \nabla b(x)$. Note that the tensor $P(x)$ is symmetric and

$$P = I - \boldsymbol{n} \otimes \boldsymbol{n} \quad \text{on } \Gamma. \tag{2.9}$$

The Jacobian of the projection vector field $p(x)$ is given, for $\Gamma \in \mathcal{C}^2$, by

$$Dp(x) = P(x) - b(x)D^2 b(x), \quad x \in S_h(\Gamma), \tag{2.10}$$

and satisfies $Dp|_\Gamma = P$ because $b = 0$ on Γ.

2.3. **Elements of tangential calculus.** We introduce some basic elements of differential calculus on a surface. We follow the approach of [8, Ch. 9, Sec. 5] that avoids local bases and coordinates by using intrinsic tangential derivatives. Other reference books are [13] and [16]. For a parametric approach in local coordinates, see [30], [7] and [5]. All proofs can be found in the cited books, except for Lemma 2.6, which is proved below. In what follows Γ denotes a sub-manifold of $\partial\Omega$ with the same regularity as Ω.

Definition 2.2 (Tangential derivatives)**.** Assume that $\Gamma \subset \partial\Omega$, for a domain Ω with a $\mathcal{C}^2$ boundary and a normal vector field $\boldsymbol{n}$. For a scalar field $f \in \mathcal{C}^1(\Gamma)$ and a vector field $\boldsymbol{w} \in \mathcal{C}^1(\Gamma, \mathbb{R}^N)$ the *tangential derivative operators* are defined as

$$\begin{aligned}\nabla_\Gamma f &:= \nabla F|_\Gamma - \partial_n F\, \boldsymbol{n},\\ D_\Gamma \boldsymbol{w} &:= D\boldsymbol{W}|_\Gamma - D\boldsymbol{W}|_\Gamma \boldsymbol{n} \otimes \boldsymbol{n},\\ \operatorname{div}_\Gamma \boldsymbol{w} &:= \operatorname{div} \boldsymbol{W}|_\Gamma - D\boldsymbol{W}|_\Gamma \boldsymbol{n} \cdot \boldsymbol{n},\end{aligned}$$

where F and $\boldsymbol{W}$ are $\mathcal{C}^1$-extensions to a neighborhood of Γ of the functions f and $\boldsymbol{w}$, respectively. If $\Gamma \in \mathcal{C}^2$ and $f \in \mathcal{C}^2(\Gamma)$, the second order tangential derivative of f is given by $D^2_\Gamma f = D_\Gamma(\nabla_\Gamma f)$, which is not a symmetric tensor, and the *Laplace–Beltrami operator* (or tangential Laplacian) is given by $\Delta_\Gamma f = \operatorname{div}_\Gamma \nabla_\Gamma f$. The tangential divergence of a tensor valued function S is defined to satisfy $\operatorname{div}_\Gamma S \cdot \boldsymbol{e} = \operatorname{div}_\Gamma(S^T \boldsymbol{e})$, for any vector $\boldsymbol{e}$. In particular, $(\operatorname{div}_\Gamma S)_i = \operatorname{div}_\Gamma(S_{i,\cdot})$, if S is a matrix. For a vector valued function $\boldsymbol{w}$, we define $\Delta_\Gamma \boldsymbol{w} = \operatorname{div}_\Gamma D_\Gamma \boldsymbol{w}$ in order to satisfy $(\Delta_\Gamma \boldsymbol{w})_i = \Delta_\Gamma w_i$.

As commented in [27, p. 85], tangential derivatives can also be defined for functions in Sobolev spaces, considering weak derivatives.

Note that $\nabla_\Gamma f \cdot \boldsymbol{n} = 0$ and $D_\Gamma \boldsymbol{w}\, \boldsymbol{n} = 0$, and using the orthogonal projection operator P given by (2.9), we can write the formulas in Definition 2.2 as

$$\nabla_\Gamma f = (P\, \nabla F)|_\Gamma, \qquad D_\Gamma \boldsymbol{w} = (D\boldsymbol{W}\, P)|_\Gamma, \qquad \operatorname{div}_\Gamma \boldsymbol{w} = (P : D\boldsymbol{W})|_\Gamma.$$

As it was proved in [8] these definitions are intrinsic, that is, they do not depend on the chosen extensions of f and $\boldsymbol{w}$ outside Γ. Among all extensions of f, there is one that simplifies the calculation of $\nabla_\Gamma f$. That extension is $f \circ p$, where p is the projection given by (2.8), and we call it the *canonical extension.* The following properties of the canonical extensions are proved in [8, Ch. 9, Sec. 5].

Lemma 2.3 (Canonical extension)**.** *For Γ, f and $\boldsymbol{w}$ satisfying the assumptions of Definition 2.2, consider $F = f \circ p$, and $\boldsymbol{W} = \boldsymbol{w} \circ p$, the canonical extensions of f and $\boldsymbol{w}$, respectively, where p is the projection given by* (2.8)*. Then, in a tubular neighborhood $S_h(\Gamma)$ where $b = b(\Omega) \in \mathcal{C}^2(S_h(\Gamma))$, we have*

$$\nabla(f \circ p) = [I - b\, D^2 b] \nabla_\Gamma f \circ p, \qquad D(\boldsymbol{w} \circ p) = D_\Gamma \boldsymbol{w} \circ p\, [I - b\, D^2 b],$$
$$\operatorname{div}(\boldsymbol{w} \circ p) = [I - b\, D^2 b] : D_\Gamma \boldsymbol{w} \circ p = \operatorname{div}_\Gamma \boldsymbol{w} \circ p - b D^2 b : D_\Gamma \boldsymbol{w} \circ p.$$

In particular,

$$\begin{aligned}\nabla_\Gamma f &= \nabla(f \circ p)|_\Gamma, & D_\Gamma \boldsymbol{w} &= D(\boldsymbol{w} \circ p)|_\Gamma,\\ \operatorname{div}_\Gamma \boldsymbol{w} &= \operatorname{div}(\boldsymbol{w} \circ p)|_\Gamma, & \Delta_\Gamma f &= \Delta(f \circ p)|_\Gamma.\end{aligned} \tag{2.11}$$

The product rule formulas for classical derivatives [14, p. 30] also hold for tangential differentiation. In the following lemma we gather those which will be needed later in this article. For a proof see, for instance, [16, Ch. 5.4.3], or note that they can be obtained from their classical counterparts using the expressions (2.11) given by canonical extensions.

Lemma 2.4 (Product rule for tangential derivatives). *Let α, $\boldsymbol{u}$, $\boldsymbol{v}$ and S be smooth fields in Γ, with α scalar valued, $\boldsymbol{u}$ and $\boldsymbol{v}$ vector valued, and S tensor valued. Then*

(i) $D_\Gamma(\varphi\boldsymbol{u}) = \boldsymbol{u}\otimes\nabla_\Gamma\varphi + \varphi D_\Gamma\boldsymbol{u}$,

(ii) $\operatorname{div}_\Gamma(\varphi\boldsymbol{u}) = \varphi\operatorname{div}_\Gamma\boldsymbol{u} + \boldsymbol{u}\cdot\nabla_\Gamma\varphi$,

(iii) $\nabla_\Gamma(\boldsymbol{u}\cdot\boldsymbol{v}) = D_\Gamma\boldsymbol{u}^T\boldsymbol{v} + D_\Gamma\boldsymbol{v}^T\boldsymbol{u}$,

(iv) $\operatorname{div}_\Gamma(\boldsymbol{u}\otimes\boldsymbol{v}) = \boldsymbol{u}\operatorname{div}_\Gamma\boldsymbol{v} + D_\Gamma\boldsymbol{u}\,\boldsymbol{v}$,

(v) $\operatorname{div}_\Gamma(S^T\boldsymbol{u}) = S : D_\Gamma\boldsymbol{u} + \boldsymbol{u}\cdot\operatorname{div}_\Gamma S$,

(vi) $\operatorname{div}_\Gamma(\alpha S) = S\nabla_\Gamma\alpha + \alpha\operatorname{div}_\Gamma S$.

It is very useful to write the geometric invariants of Γ in terms of tangential derivatives of the normal vector field $\boldsymbol{n}$. From [8, Ch. 7, Theorem 8.5], we know that $\boldsymbol{n}\circ p = \nabla b$ in $S_h(\Gamma)$, that is, ∇b is the canonical extension of the normal $\boldsymbol{n}$. Then (2.11) implies $D_\Gamma\boldsymbol{n} = D(\boldsymbol{n}\circ p)|_\Gamma = D^2 b|_\Gamma$ and $\sum\kappa_i^2 = |D_\Gamma\boldsymbol{n}|^2$, and the mean and Gaussian curvatures can be written as $\kappa = \operatorname{div}_\Gamma\boldsymbol{n}$ (in any dimension N) and $\kappa_g = \frac{1}{2}\left(\kappa^2 - |D_\Gamma\boldsymbol{n}|^2\right)$ (for $N = 3$), respectively. In particular, as we will see in Section 8, any geometric invariant can be written in terms of $I_p := \operatorname{tr}(D_\Gamma\boldsymbol{n}^p)$, for $p = 1, \ldots, N-1$.

The Divergence Theorem for surfaces, whose proof can be found in [8, Ch. 9.5.5] (the first part) and in [30, Prop. 15] (the second), is the following.

Lemma 2.5 (Tangential Divergence Theorem). *If $\Gamma = \partial\Omega$ is $\mathcal{C}^2$ and $\boldsymbol{w}\in\mathcal{C}^1(\Gamma,\mathbb{R}^N)$, then*

$$\int_\Gamma \operatorname{div}_\Gamma\boldsymbol{w} = \int_\Gamma \kappa\,\boldsymbol{w}\cdot\boldsymbol{n}, \tag{2.12}$$

where κ is the mean curvature of Γ and $\boldsymbol{n}$ its normal field. If $N = 3$ and Γ is a smooth, oriented surface with boundary $\partial\Gamma$, then

$$\int_\Gamma \operatorname{div}_\Gamma\boldsymbol{w} = \int_\Gamma \kappa\,\boldsymbol{w}\cdot\boldsymbol{n} + \int_{\partial\Gamma}\boldsymbol{w}\cdot\boldsymbol{n}_s, \tag{2.13}$$

where $\boldsymbol{n}_s$ is the outward normal to $\partial\Gamma$ which is also orthogonal to $\boldsymbol{n}$.

The following lemma extends formula (2.5) for tangential derivatives. We must remark that we could not find it anywhere in the literature.

Lemma 2.6. *If Γ is $\mathcal{C}^3$ and $\boldsymbol{w}\in\mathcal{C}^2(\Gamma,\mathbb{R}^N)$, then $\nabla_\Gamma\operatorname{div}_\Gamma\boldsymbol{w} = P\operatorname{div}_\Gamma D_\Gamma\boldsymbol{w}^T - D_\Gamma\boldsymbol{n}D_\Gamma\boldsymbol{w}^T\boldsymbol{n}$, where $P = I - \boldsymbol{n}\otimes\boldsymbol{n}$ is the orthogonal projection operator given by (2.9).*

Proof. We resort to (2.11) to write tangential derivatives using the projection function p:

$$\nabla_\Gamma\operatorname{div}_\Gamma\boldsymbol{w} = \nabla(\operatorname{div}_\Gamma\boldsymbol{w}\circ p)|_\Gamma = \nabla(\operatorname{div}(\boldsymbol{w}\circ p)\circ p)|_\Gamma.$$

Then we use successively the chain rule, the derivative of p given by (2.10) and the property of classical derivatives (2.5):

$$\nabla_\Gamma\operatorname{div}_\Gamma\boldsymbol{w} = Dp^T|_\Gamma\nabla\operatorname{div}(\boldsymbol{w}\circ p)|_\Gamma = P\;\nabla\operatorname{div}(\boldsymbol{w}\circ p)|_\Gamma = P\;\operatorname{div}(D(\boldsymbol{w}\circ p)^T)|_\Gamma. \tag{2.14}$$

Note that Lemma 2.3 implies $D(\boldsymbol{w}\circ p)^T = D_\Gamma\boldsymbol{w}^T\circ p - b\,D^2 b\,(D_\Gamma\boldsymbol{w}^T\circ p)$, and the product rule $\operatorname{div}(\alpha S) = \alpha\operatorname{div}S + S\nabla\alpha$ implies

$$\operatorname{div}(D(\boldsymbol{w}\circ p)^T) = \operatorname{div}(D_\Gamma\boldsymbol{w}^T\circ p) - b\;\operatorname{div}(D^2 b\,D_\Gamma\boldsymbol{w}^T\circ p) - D^2 b\,D_\Gamma\boldsymbol{w}^T\circ p\,\nabla b.$$

Restricting to Γ we have $\operatorname{div}(D(\boldsymbol{w}\circ p)^T)|_\Gamma = \operatorname{div}_\Gamma(D_\Gamma \boldsymbol{w}^T) - D_\Gamma \boldsymbol{n} D_\Gamma \boldsymbol{w}^T \boldsymbol{n}$, which implies the assertion from (2.14), since $PD_\Gamma \boldsymbol{n} = D_\Gamma \boldsymbol{n}$. □

Applying Lemma 2.6 to $\boldsymbol{w} = \boldsymbol{n}$ we obtain for $\kappa = \operatorname{div}_\Gamma \boldsymbol{n}$

$$\nabla_\Gamma \kappa = \nabla_\Gamma \operatorname{div}_\Gamma \boldsymbol{n} = P \operatorname{div}_\Gamma D_\Gamma \boldsymbol{n} - D_\Gamma \boldsymbol{n} D_\Gamma \boldsymbol{n}\boldsymbol{n} = P\Delta_\Gamma \boldsymbol{n}. \tag{2.15}$$

From (2.11), $\Delta_\Gamma \boldsymbol{n} = \Delta(n\circ p)|_\Gamma = \operatorname{div}(D^2 b)|_\Gamma$, and (2.4) implies $\Delta_\Gamma \boldsymbol{n}\cdot\boldsymbol{n} = -|D_\Gamma \boldsymbol{n}|^2$, which yields

$$\nabla_\Gamma \kappa = \Delta_\Gamma \boldsymbol{n} + |D_\Gamma \boldsymbol{n}|^2 \boldsymbol{n},$$

for a $\mathcal{C}^3$-surface Γ.

3. Shape functionals and derivatives

A *shape functional* is a function $J : \mathcal{A} \to \mathbb{R}$ defined on a set $\mathcal{A} = \mathcal{A}(\mathbf{D})$ of admissible subsets of a hold-all domain $\mathbf{D} \subset \mathbb{R}^N$. Those subsets can be domains, boundaries or surfaces.

Let the elements of $\mathcal{A}$ be smooth domains and for each $\Omega \in \mathcal{A}$, let $y(\Omega) : \Omega \to \mathbb{R}$ be a function in $W(\Omega)$, some Sobolev space over Ω. Then the shape functional given by $J(\Omega) = \int_\Omega y(\Omega)$ is called a *domain functional*. For example the *volume functional* is obtained with $y(\Omega) \equiv 1$, but the *domain function* $y(\Omega)$ could be more involved, such as the solution of a PDE in Ω.

Our main interest in this work are the *boundary functionals* given by $J(\Gamma) = \int_\Gamma z(\Gamma)$, where z is a function that to each surface Γ in a family of admissible surfaces $\mathcal{A}$ it assigns a function $z(\Gamma) \in W(\Gamma)$, with $W(\Gamma)$ some Sobolev space on Γ. The area functional corresponds to $z(\Gamma) \equiv 1$, but more interesting functionals are obtained when the *boundary function* $z(\Gamma)$ depends on quantities such as the mean curvature κ of Γ or more generally on the geometric invariants $I_p(\Gamma) = \operatorname{tr}(D_\Gamma \boldsymbol{n}^p)$, with p a positive integer, or any real function which involves the normal field $\boldsymbol{n}$ or higher order tangential derivatives on Γ.

3.1. The velocity method.

On a hold-all domain $\mathbf{D}$ (not necessarily bounded), a *velocity field* is a vector field $\boldsymbol{v} \in V^k(\mathbf{D}) := \mathcal{C}^k_c(\mathbf{D}, \mathbb{R}^N)$, the set of all $\mathcal{C}^k$ vector value functions $\boldsymbol{f}$ such that $D^\alpha \boldsymbol{f}$ has compact support in $\mathbf{D}$, for $0 \le |\alpha| \le k$; hereafter we assume that k is a fixed positive integer. A velocity field $\boldsymbol{v}$ induces a *trajectory* $x = x_{\boldsymbol{v}} \in \mathcal{C}^1([0,\epsilon], V^k(\mathbf{D}))$, through the system of ODE [27, Theorem 2.16]

$$\dot{x}(t) = \boldsymbol{v}\circ x(t),\ t \in [0,\epsilon], \qquad x(0) = id, \tag{3.1}$$

where we use a dot to denote derivative with respect to the time variable t. More precisely, for every $p \in D$, $x(t)(p)$, $t \in [0,\epsilon]$ satisfies $\dot{x}(t)(p) = \boldsymbol{v}\big((x(t)(p)\big)$ and $x(0)(p) = p$.

3.2. Shape differentiation.

Given a velocity field $\boldsymbol{v}$ and a set $S \subset \mathbf{D}$, let $S_t = x(t)(S)$ be its perturbation by $\boldsymbol{v}$ at time t, where $x(t)$ is the trajectory given by (3.1). For a shape functional $J : \mathcal{A} \to \mathbb{R}$, where $\mathcal{A}$ is a family of admissible sets S (domains or boundaries), and a velocity field $\boldsymbol{v} \in V^k(\mathbf{D})$, the *Eulerian semi-derivative* of J at S in the direction $\boldsymbol{v}$ is given by

$$dJ(S;\boldsymbol{v}) = \lim_{t\searrow 0} \frac{J(S_t) - J(S)}{t}, \tag{3.2}$$

whenever the limit exists.

If the functional J is *shape differentiable* with respect to $V^k(\mathbf{D})$ (see [8] or [27] for the details on the definition) then the functional $\boldsymbol{v} \to dJ(S;\boldsymbol{v})$ is linear and continuous in $V^k(\mathbf{D})$.

Definition 3.1 (Shape derivative)**.** If J is shape differentiable, then dJ is called its shape derivative, and $dJ(S;\boldsymbol{v})$ is the shape derivative of J at S in the direction $\boldsymbol{v}$.

Remark 3.2 (Taylor formula)**.** Given $\boldsymbol{v} \in V^k(\mathbf{D})$ we define $S + \boldsymbol{v}$ to be S_t for $t = 1$ provided it is admissible. Then if J is shape differentiable (see [8, Ch. 9]) it follows that $J(S + \boldsymbol{v}) = J(S) + dJ(S;\boldsymbol{v}) + o(|\boldsymbol{v}|)$.

3.3. **The structure theorem.** One of the main results about shape derivatives is the (Hadamard–Zolesio) Structure Theorem (Theorem 3.6 of [8, Ch. 9]). It establishes that, if a shape functional J is shape differentiable at the domain Ω with boundary Γ, then the only relevant part of the velocity field $\boldsymbol{v}$ in $dJ(\Omega,\boldsymbol{v})$ is $v_n := \boldsymbol{v}\cdot\boldsymbol{n}|_\Gamma$. In other words, if $\boldsymbol{v}\cdot\boldsymbol{n} = 0$ in Γ, then $dJ(\Omega,\boldsymbol{v}) = 0$. More precisely:

Theorem 3.3 (Structure Theorem)**.** *Let $\Omega \in \mathcal{A}$ be a domain with $\mathcal{C}^{k+1}$-boundary Γ, $k \geq 0$ integer, and let $J : \mathcal{A} \to \mathbb{R}$ be a shape functional which is shape differentiable at Ω with respect to $V^k(\mathbf{D})$. Then there exists a functional $g(\Gamma) \in \left(\mathcal{C}^k(\Gamma)\right)'$ (called the shape gradient) such that $dJ(\Omega;\boldsymbol{v}) = \langle g(\Gamma), v_n\rangle_{\mathcal{C}^k(\Gamma)}$, where $v_n = \boldsymbol{v}\cdot\boldsymbol{n}$. Moreover, if the gradient $g(\Gamma) \in L^1(\Gamma)$, then $dJ(\Omega,\boldsymbol{v}) = \int_\Gamma g(\Gamma)\, v_n$.*

4. Shape differentiation of functions

Having defined the shape derivatives of functionals, we now turn to the definition of shape derivatives of *functions*. We consider, on the one hand, *domain functions* $y = y(\Omega)$ which assign a function $y(\Omega) : \Omega \to \mathbb{R}$ to each domain Ω in a class of admissible domains, and on the other hand, *boundary functions* $z = z(\Gamma)$ which assign a function $z(\Gamma) : \Gamma \to \mathbb{R}$ to each surface Γ in a set of admissible surfaces.

We start with the first kind, and to motivate the definition, consider a shape functional of the form $J(\Omega) = \int_\Omega y(\Omega) d\Omega$, where $y(\Omega) \in W^{r,p}(\Omega)$ $(1 \leq r \leq k)$ for any admissible C^k domain Ω, and a velocity field $\boldsymbol{v} \in V^k(\mathbf{D})$, $k \geq 1$, with trajectories $x \in \mathcal{C}^1([0,\epsilon], V^k(\mathbf{D}))$ satisfying (3.1). Note that the Eulerian semi-derivative (3.2) can be written as $dJ(\Omega;\boldsymbol{v}) = \frac{d}{dt^+} J(\Omega_t)|_{t=0}$, where $\Omega_t = x(t)(\Omega)$ and $\Omega_0 = \Omega$. Then,

$$J(\Omega_t) = \int_{\Omega_t} y(\Omega_t) = \int_\Omega [y(\Omega_t)\circ x(t)]\,\gamma(t), \tag{4.1}$$

where $\gamma(t) := \det Dx(t)$, with $Dx(t)$ denoting derivative of $x(t)$ with respect to the spatial variable. From Theorem 4.1 of [8, Ch. 9] we know that $\gamma \in \mathcal{C}^1([0,\epsilon], V^1(\mathbf{D}))$, and its (time) derivative at $t = 0$ is given by $\dot{\gamma}(0) := \frac{d\gamma(t)}{dt}|_{t=0} = \operatorname{div}\boldsymbol{v}$.

If we suppose that the function $t \to y(\Omega_t) \circ x(t)$ from $[0, \epsilon]$ to $W^{r,p}(\Omega)$ is differentiable at $t = 0$ in the sense of $L^1(\Omega)$, and denote its time derivative at $t = 0$ with $\dot{y}(\Omega, \boldsymbol{v})$, then we can differentiate inside the integral (4.1) to obtain

$$\begin{aligned} dJ(\Omega; \boldsymbol{v}) &= \int_\Omega \dot{y}(\Omega, \boldsymbol{v})\gamma(0) + y(\Omega)\dot{\gamma}(0) \\ &= \int_\Omega [\dot{y}(\Omega, \boldsymbol{v}) - \nabla y(\Omega) \cdot \boldsymbol{v}] + \operatorname{div}(y(\Omega)\boldsymbol{v}) . \end{aligned} \tag{4.2}$$

As a particular case, suppose that $y(\Omega)$ is independent of the geometry, namely: $y(\Omega) = \phi|_\Omega$, with $\phi \in W^{1,1}(\mathbf{D})$. The chain rule yields $\dot{y}(\Omega, \boldsymbol{v}) - \nabla y(\Omega) \cdot \boldsymbol{v} = 0$ in Ω, which suggests the following definition [27, Sec. 2.30].

Definition 4.1 (Shape derivative of a domain function)**.** Consider a velocity vector field $\boldsymbol{v} \in V^k(\mathbf{D})$, with $k \geq 1$, an admissible domain $\Omega \subset \mathbf{D}$ of class $\mathcal{C}^k$, and a function $y(\Omega) \in W^{r,p}(\Omega)$, with $r \in [1, k] \cap \mathbb{Z}$. Suppose there exists $y(\Omega_t) \in W^{r,p}(\Omega_t)$ for all $0 < t < \epsilon$, where $\Omega_t = x(t)(\Omega)$ is the perturbation of Ω by the trajectory $x(t)$ induced by $\boldsymbol{v}$. If the limit $\dot{y}(\Omega, \boldsymbol{v}) := \frac{d}{dt^+}[y(\Omega_t) \circ x(t)]_{t=0}$ exists in $W^{r-1,p}(\Omega)$, then the (domain) shape derivative of $y(\Omega)$ at Ω in the direction $\boldsymbol{v}$ is given by

$$y'(\Omega, \boldsymbol{v}) := \dot{y}(\Omega, \boldsymbol{v}) - \nabla y(\Omega) \cdot \boldsymbol{v}.$$

We can replace the space $W^{r,p}(\Omega)$ by $\mathcal{C}^r(\Omega)$, $1 \leq r \leq k$, obtaining $y'(\Omega, \boldsymbol{v}) \in \mathcal{C}^{r-1}(\Omega)$.

With this definition, the existence of $y'(\Omega, \boldsymbol{v}) \in W^{r-1,p}(\Omega)$ gives us

$$dJ(\Omega; \boldsymbol{v}) = \int_\Omega y'(\Omega, \boldsymbol{v}) + \operatorname{div}(y(\Omega)\boldsymbol{v}) .$$

If $\partial\Omega \in \mathcal{C}^1$, the Divergence Theorem leads to

$$dJ(\Omega; \boldsymbol{v}) = \int_\Omega y'(\Omega, \boldsymbol{v}) + \int_{\partial\Omega} y(\Omega)\, v_n, \quad \text{with } v_n = \boldsymbol{v} \cdot \boldsymbol{n}.$$

In the particular case of $y(\Omega) = \phi|_\Omega$ for $\phi \in W^{1,1}(D)$, we have $y'(\Omega, \boldsymbol{v}) = 0$.

Remark 4.2 (Extension for vector and tensor valued functions)**.** For a general finite dimensional space $\mathbb{V}$, the shape derivative of a vector valued function $\boldsymbol{w}(\Omega) \in W^{r,p}(\Omega, \mathbb{V})$ is given component-wise by the shape derivative of each component of $\boldsymbol{w}(\Omega)$ on some basis, whenever they exist. In particular, if $\mathbb{V} = \mathbb{R}^N$, then $\boldsymbol{w}'(\Omega, \boldsymbol{v}) \in W^{r-1,p}(\Omega, \mathbb{R}^N)$ is given by

$$\boldsymbol{w}'(\Omega, \boldsymbol{v}) = \dot{\boldsymbol{w}}(\Omega, \boldsymbol{v}) - D\boldsymbol{w}\boldsymbol{v}. \tag{4.3}$$

For a tensor valued function $A(\Omega) : \Omega \to \operatorname{Lin}(\mathbb{V})$, the shape derivative $A'(\Omega, \boldsymbol{v})$ is the tensor valued function which satisfies

$$A'(\Omega, \boldsymbol{v})\boldsymbol{e} = (A\boldsymbol{e})'(\Omega, \boldsymbol{v}) \quad \text{for any } \boldsymbol{e} \in \mathbb{V}.$$

Remark 4.3 (Material derivatives)**.** For S domain or boundary, the limit

$$\dot{y}(S, \boldsymbol{v}) := \frac{d}{dt^+}[y(S_t) \circ x(t)]_{t=0}$$

is called *material derivative* of y at S in the direction $\boldsymbol{v}$ (see [27] for a proper definition).

Consider now a boundary integral functional of the form $J(\Gamma) = \int_\Gamma z(\Gamma)$ where $z(\Gamma) \in W^{r,p}(\Gamma)$ for each admissible $\mathcal{C}^k$-boundary Γ, $1 \le r \le k$. Omitting the details, that can be found in [27, Sec. 2.33], we obtain a formula for $dJ(\Gamma;\boldsymbol{v})$ analogous to (4.2):

$$dJ(\Gamma;\boldsymbol{v}) = \int_\Gamma [\dot z(\Gamma,\boldsymbol{v}) - \nabla_\Gamma z(\Gamma)\cdot\boldsymbol{v}] + \mathrm{div}_\Gamma(z(\Gamma)\boldsymbol{v}),$$

where we assume that the time derivative $\dot z(\Gamma,\boldsymbol{v}) := \frac{d}{dt}[z(\Gamma_t)\circ x(t)]_{t=0}$ exists in $L^1(\Gamma)$. By analogy with the previous case of domain functions, we arrive at the following definition.

Definition 4.4 (Shape derivative of a boundary function)**.** Let z be a boundary function which satisfies $z(\Gamma) \in W^{r,p}(\Gamma)$ for all Γ in an admissible set $\mathcal{A}$ of boundaries of class $\mathcal{C}^{k+1}$, with $1 \le r \le k$. If, for a velocity field $\boldsymbol{v} \in V^k(\mathbf{D})$, $\Gamma_t \in \mathcal{A}$ for all small $t > 0$ and the limit $\dot z(\Gamma,\boldsymbol{v}) := \frac{d}{dt^+}[z(\Gamma_t)\circ x(t)]_{t=0}$ exists in $W^{r-1,p}(\Gamma)$, then the *(boundary) shape derivative of* $z(\Gamma)$ *at* Γ *in the direction* $\boldsymbol{v}$ is given by

$$z'(\Gamma,\boldsymbol{v}) = \dot z(\Gamma,\boldsymbol{v}) - \nabla_\Gamma z(\Gamma)\cdot\boldsymbol{v},$$

and it belongs to $W^{r-1,p}(\Gamma)$. We can replace the space $W^{r,p}(\Gamma)$ by $\mathcal{C}^r(\Gamma)$, $1 \le r \le k$, obtaining $z'(\Gamma,\boldsymbol{v}) \in \mathcal{C}^{r-1}(\Gamma)$. This definition extends for vector and tensor valued functions analogously to Remark 4.2 for domain functions.

With this definition we obtain

$$dJ(\Gamma;\boldsymbol{v}) = \int_\Gamma z'(\Gamma,\boldsymbol{v}) + \mathrm{div}_\Gamma(z(\Gamma)\boldsymbol{v}) = \int_\Gamma z'(\Gamma,\boldsymbol{v}) + \kappa z(\Gamma) v_n, \tag{4.4}$$

where the last equality arises, for $\Gamma \in \mathcal{C}^2$, from the tangential divergence formula (2.12) of Lemma 2.5.

It is worth noticing that in the particular case of $z(\Gamma) = \phi|_\Gamma$ for $\phi \in W^{r+1,p}(D)$ (which gives $z(\Gamma) \in W^{r,p}(\Gamma)$), it is *not true* in general that $z'(\Gamma;\boldsymbol{v}) = 0$. Instead, $z'(\Gamma,\boldsymbol{v}) = \partial_n\phi\, v_n$, with $v_n = \boldsymbol{v}\cdot\boldsymbol{n}$.

Remark 4.5 (Boundary conditions on Γ)**.** For a surface $\Gamma \subsetneq \partial\Omega$, we can consider the space of velocity fields $V_\Gamma^k(\mathbf{D}) = V^k(\mathbf{D}) \bigcap \{\boldsymbol{v} : \boldsymbol{v}|_{\partial\Gamma} = 0\}$, in order to obtain (4.4) by applying formula (2.13) of Lemma 2.5.

4.1. **Warning: shape derivatives are different for domain and boundary functions.** If a boundary function $z(\Gamma)$ is the restriction to Γ of a domain function $y(\Omega)$, *it is not true*, in general, that its shape derivative $z'(\Gamma,\boldsymbol{v})$ is $y'(\Omega,\boldsymbol{v})|_\Gamma$. Even though practitioners know this, they (we) sometimes get confused.

In order to clarify this issue, let us first consider a function $\Phi \in \mathcal{C}_c^2(\mathbf{D})$ and, for any domain $\Omega \subset \mathbf{D}$ with boundary Γ, define $y(\Omega) := \Phi|_\Omega$ and $z(\Gamma) := \Phi|_\Gamma$. It is easy to check, for any velocity field $\boldsymbol{v}$, that $\dot y(\Omega,\boldsymbol{v}) = \nabla\Phi\cdot\boldsymbol{v}$ in Ω, and also $\dot z(\Gamma,\boldsymbol{v}) = \nabla\Phi\cdot\boldsymbol{v}$ on Γ (the material derivatives *do* coincide). Then, Definitions 4.1 and 4.4 yield $y'(\Omega,\boldsymbol{v}) = 0$ and $z'(\Gamma,\boldsymbol{v}) = (\nabla\Phi|_\Gamma - \nabla_\Gamma\Phi)\cdot\boldsymbol{v} = \partial_n\Phi\, v_n$, respectively, with $v_n = \boldsymbol{v} \cdot \boldsymbol{n}$. That is, the shape derivative of a domain function $y(\Omega)$ and a boundary function $z(\Gamma)$ are different, even if they are restrictions of the same global function Φ. The relationship that holds in general is summarized in the following lemma, whose proof is immediate from Definitions 4.1 and 4.4.

Lemma 4.6. *Consider a domain Ω with $\mathcal{C}^2$-boundary Γ, and functions defined on Γ: $z(\Gamma)$ and $\boldsymbol{z}(\Gamma)$, scalar and vector valued, respectively, such that $z(\Gamma) = y(\Omega)|_\Gamma$ and $\boldsymbol{z}(\Gamma) = \boldsymbol{y}(\Omega)|_\Gamma$, for some $y(\Omega) \in \mathcal{C}^2(\Omega)$ and $\boldsymbol{y}(\Omega) \in \mathcal{C}^2(\Omega, \mathbb{R}^N)$. If $y(\Omega)$ and $\boldsymbol{y}(\Omega)$ are (domain) shape differentiable at Ω in the direction $\boldsymbol{v} \in V^k(\mathbf{D})$, then $z(\Gamma)$ and $\boldsymbol{z}(\Gamma)$ are (boundary) shape differentiable at Γ in the direction $\boldsymbol{v}$, and*

$$z'(\Gamma, \boldsymbol{v}) = y'(\Omega, \boldsymbol{v})|_\Gamma + \partial_n y \, v_n, \qquad \boldsymbol{z}'(\Gamma, \boldsymbol{v}) = \boldsymbol{y}'(\Omega, \boldsymbol{v})|_\Gamma + D\boldsymbol{y}|_\Gamma \boldsymbol{n} \, v_n,$$

with $\partial_n = \boldsymbol{n} \cdot \nabla$ and $v_n = \boldsymbol{v} \cdot \boldsymbol{n}$.

The identities in the previous lemma hold for any extension $y(\Omega)$ of $z(\Gamma)$. In the particular case when $y(\Omega)$ coincides with the canonical extension of $z(\Gamma)$ in a tubular neighborhood $S_h(\Gamma)$ (see Lemma 2.3) we get $z'(\Gamma, \boldsymbol{v}) = y'(\Omega, \boldsymbol{v})|_\Gamma$ because $\partial_n y(\Omega)|_\Gamma = 0$. The existence of such an extension $y(\Omega)$ from $z(\Gamma)$ is justified (for low regularity) in the following lemma.

Lemma 4.7 (Canonical extension)**.** *If $1 \le k \le 2$, $\Gamma = \partial\Omega \in \mathcal{C}^{k+1}$ and $z(\Gamma) \in W^{k,p}(\Gamma)$, $1 \le p \le \infty$, then there exists $y(\Omega) \in W^{k,p}(\Omega)$ such that $y(\Omega)|_\Gamma = z(\Gamma)$ a.e. and $\partial_n y(\Omega)|_\Gamma = 0$.*

Proof. Since $\Gamma \in \mathcal{C}^{k+1}$, the orthogonal projection p is a $\mathcal{C}^k$-function in $S_h(\Gamma)$ and then the canonical extension $f = z(\Gamma) \circ p \in W^{k,p}(S_h(\Gamma))$. Then we obtain from f an extension $F \in W^{k,p}(\mathbb{R}^N)$ (see [12, Ch. 5.4]) and finally we define $y(\Omega) := F|_\Omega$, which satisfies the desired properties. □

The difference between the definitions of shape derivatives for domain and boundary functions, which coincide when using the canonical extension, has led to confusion in the literature. For instance, in Lemma 6.2 we show that the shape derivative of the mean curvature $\kappa(\Gamma)$, which is a boundary function, is $\kappa'(\Gamma, \boldsymbol{v}) = -\Delta_\Gamma v_n - |D_\Gamma n|^2 v_n$. However, the expression $\kappa'(\Gamma, \boldsymbol{v}) = -\Delta_\Gamma v_n$ can be found in [9] and [30], where they obtained not the (boundary) shape derivative of $\kappa(\Gamma)$ but the domain shape derivative of its extension Δb, which satisfies $(\Delta b)'(\Omega, \boldsymbol{v})|_\Gamma = -\Delta_\Gamma v_n$, which can be found in [17, p. 451]. Note also that Δb is not the canonical extension of κ, as can be deduced from (2.7). On the other hand, ∇b is the canonical extension of the normal $\boldsymbol{n}$, giving $\boldsymbol{n}'(\Gamma, \boldsymbol{v}) = (\nabla b)'(\Omega, \boldsymbol{v})|_\Gamma = -\nabla_\Gamma v_n$ (cf. Section 6).

In this paper, the type of shape derivative we use is established from the kind of function considered (domain or boundary).

5. Properties of shape derivatives of functions

The following lemma establishes the dependence of $y'(\Omega, \boldsymbol{v})$ and $z'(\Gamma, \boldsymbol{v})$ on $\boldsymbol{v}$ only through $v_n = \boldsymbol{v} \cdot \boldsymbol{n}$ restricted to Γ. This was expected by the Structure Theorem 3.3 applied to the integral functionals $\int_\Omega y(\Omega)$ and $\int_\Gamma z(\Gamma)$, respectively.

Lemma 5.1 ([27, Propositions 2.86, 2.87 and 2.90])**.** *Consider an admissible set $S \subset \mathbf{D}$ (domain or boundary) such that S is $\mathcal{C}^{k+1}$, $k \geq 1$, a velocity field $\boldsymbol{v} \in V^k(\mathbf{D})$ and a shape differentiable function $w(S) \in W^{r,p}(S)$, $1 \leq r \leq k$, $1 \leq p < \infty$. Suppose that $\boldsymbol{v} \to w'(S, \boldsymbol{v})$ is linear and continuous from $V^k(\mathbf{D})$ into $W^{r-1,p}(S)$. If the velocity fields $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are such that $\boldsymbol{v}_1 \cdot \boldsymbol{n} = \boldsymbol{v}_2 \cdot \boldsymbol{n}$ on Γ ($\Gamma = \partial S$ for S domain, $\Gamma = S$ for S boundary), then $w'(S, \boldsymbol{V_1}) = w'(S, \boldsymbol{V_2})$.*

The following lemma states that shape derivatives commute with linear transformations, both for domain and boundary functions. The proof is straightforward from the definitions.

Lemma 5.2. *Let $F \in \operatorname{Lin}(\mathbb{V}_1, \mathbb{V}_2)$, with $\mathbb{V}_1$ and $\mathbb{V}_2$ two finite dimensional vector or tensor spaces, and let $w(S) \in \mathcal{C}^k(S, \mathbb{V}_1)$ for any admissible domain or boundary $S \subset \mathbf{D}$ which is $\mathcal{C}^{k+1}$, $k \geq 1$. If $w(S)$ is shape differentiable at S in the direction $\boldsymbol{v}$, then $F \circ w(S) \in \mathcal{C}^k(S, \mathbb{V}_2)$ is also shape differentiable at S in the direction $\boldsymbol{v}$, and its shape derivative is given by*

$$(F \circ w)'(S, \boldsymbol{v}) = F \circ w'(S, \boldsymbol{v}).$$

The next lemma states a chain rule combining usual derivatives with shape derivatives.

Lemma 5.3 (Chain rule)**.** *Consider two finite dimensional vector or tensor spaces $\mathbb{V}_1$ and $\mathbb{V}_2$, a function $F \in \mathcal{C}^1(\mathbb{V}_1, \mathbb{V}_2)$ and a domain (or boundary) function $y(S) \in \mathcal{C}^1(S, \mathbb{V}_1)$, where S is an admissible domain (boundary) in $\mathbf{D} \subset \mathbb{R}^N$ with a $\mathcal{C}^2$ boundary. If $y(S)$ is shape differentiable at S in the direction $\boldsymbol{v}$, then the function $F \circ y(S) \in \mathcal{C}^1(S, \mathbb{V}_2)$ is also shape differentiable at S in the direction $\boldsymbol{v}$, and its shape derivative is given by*

$$(F \circ y)'(S, \boldsymbol{v}) = DF \circ y(S)\,[y'(S, \boldsymbol{v})]. \tag{5.1}$$

Proof. First suppose that S is a domain, then $Dy(x) \in \operatorname{Lin}(\mathbb{R}^N, \mathbb{V}_1)$ for any $x \in S$. Since F is differentiable, for every $X \in \mathbb{V}_1$ there exists a linear operator $DF(X) \in \operatorname{Lin}(\mathbb{V}_1, \mathbb{V}_2)$ such that

$$\lim_{\|u\|_{\mathbb{V}_1} \to 0} \frac{\|F(X+u) - F(X) - DF(X)[u]\|_{\mathbb{V}_2}}{\|u\|_{\mathbb{V}_1}} = 0,$$

where $DF(X)[u]$ denotes the application of the linear operator $DF(X) \in \operatorname{Lin}(\mathbb{V}_1, \mathbb{V}_2)$ to $u \in \mathbb{V}_1$. With this notation, the chain rule applied to $F \circ y$ reads $D(F \circ y)[\boldsymbol{v}] = DF \circ y[Dy[\boldsymbol{v}]]$ ($\forall \boldsymbol{v} \in \mathbb{R}^N$), so that from (4.3),

$$(F \circ y)'(S, \boldsymbol{v}) = (F \circ y)^{\cdot}(S, \boldsymbol{v}) - D(F \circ y)[\boldsymbol{v}] = (F \circ y)^{\cdot}(S, \boldsymbol{v}) - DF \circ y[Dy[\boldsymbol{v}]] \quad \text{in } S,$$

with $(F \circ y)^{\cdot}(S, \boldsymbol{v}) = \frac{d}{dt^+}\left[F \circ y(S_t) \circ x(t)\right]_{t=0}$ denoting the material derivative of $F \circ y$. Then we only need to prove the chain rule for the material derivative of $y(S) \in \mathcal{C}^1(S, \mathbb{V}_1)$ in the direction $\boldsymbol{v}$, i.e.,

$$(F \circ y)^{\cdot}(S, \boldsymbol{v}) = DF \circ y[\dot{y}(S, \boldsymbol{v})],$$

which is straightforward from the usual chain rule applied to the mapping $t \to F \circ (y(S_t) \circ x(t))$. The remaining details are left to the reader.

Suppose now that $S = \Gamma = \partial\Omega$ and $y(\Gamma)$ is a boundary function, and consider the canonical extension $\hat{y}(\Omega)$ that satisfies $y'(\Gamma, \boldsymbol{v}) = \hat{y}'(\Omega, \boldsymbol{v})|_\Gamma$. Then $F \circ \hat{y}$ is the canonical extension of $F \circ y$ and (5.1) applied to the domain function $\hat{y}(\Omega)$ yields the desired result for $y(\Gamma)$. □

Remark 5.4 (Product rule for shape derivatives)**.** The product rules for domain shape derivatives follow directly from Definition 4.1.

The following lemma allows us to swap shape derivatives with classical derivatives of domain functions. This is a known result, which we decided to include here to make the article more self-contained. It is worth noting that this is not true for boundary functions and tangential derivatives. This issue is discussed in Section 7, where the main results of this article are presented.

Lemma 5.5 (Mixed shape and classical derivatives)**.** *The following results about interchanging classical and shape derivatives hold:*

(1) If $y(\Omega) \in \mathcal{C}^2(\Omega)$ is shape differentiable at Ω in the direction $\boldsymbol{v} \in V^k(\mathbf{D})$, $k \geq 2$, then $\nabla y(\Omega) \in \mathcal{C}^1(\Omega, \mathbb{R}^N)$ is also shape differentiable at Ω and

$$(\nabla y)'(\Omega, \boldsymbol{v}) = \nabla y'(\Omega, \boldsymbol{v}).$$

(2) If $\boldsymbol{w}(\Omega) \in \mathcal{C}^2(\Omega, \mathbb{R}^N)$ is shape differentiable at Ω in the direction $\boldsymbol{v} \in V^k(\mathbf{D})$, $k \geq 2$, then $D\boldsymbol{w}(\Omega) \in \mathcal{C}^1(\Omega, \mathbb{R}^{N\times N})$ and $\operatorname{div} \boldsymbol{w}(\Omega) \in \mathcal{C}^1(\Omega)$ is also shape differentiable and

$$(D\boldsymbol{w})'(\Omega, \boldsymbol{v}) = D\boldsymbol{w}'(\Omega, \boldsymbol{v}), \qquad (\operatorname{div} \boldsymbol{w})'(\Omega, \boldsymbol{v}) = \operatorname{div} \boldsymbol{w}'(\Omega, \boldsymbol{v}).$$

(3) If $y(\Omega) \in \mathcal{C}^3(\Omega)$ is shape differentiable at Ω in the direction $\boldsymbol{v} \in V^k(\mathbf{D})$, $k \geq 3$, then $\Delta y(\Omega) \in \mathcal{C}^1(\Omega)$ is also shape differentiable at Ω and

$$(\Delta y)'(\Omega, \boldsymbol{v}) = \Delta y'(\Omega, \boldsymbol{v}).$$

Proof. We will prove the first assertion. The other ones are analogous.

First note that

$$\nabla \left(y(\Omega_t) \circ x(t)\right) = Dx(t)^T\, \nabla y(\Omega_t) \circ x(t) \quad \text{in } \Omega.$$

Differentiating with respect to t and evaluating at $t = 0$ we have

$$\frac{\partial}{\partial t} \nabla \left(y(\Omega_t) \circ x(t)\right)|_{t=0} = \frac{\partial}{\partial t} Dx(t)^T|_{t=0} \nabla y(\Omega) + \dot{\nabla} y(\Omega, \boldsymbol{v}), \tag{5.2}$$

where we denote with $\dot{\nabla} y(\Omega, \boldsymbol{v}) := \frac{d}{dt^+}[\nabla y(\Omega_t) \circ x(t)]_{t=0}$ the material derivative of $\nabla y(\Omega)$.

Since $x \in \mathcal{C}^1([0,\epsilon], V^k(\mathbf{D}))$, $k \geq 1$, and recalling that $\dot{x}(0) = \frac{\partial}{\partial t} x(t, \cdot)|_{t=0} = \boldsymbol{v}$, we have that, uniformly,

$$\lim_{t \searrow 0} D^\alpha \left(\frac{x(t) - x(0)}{t} \right) = D^\alpha \boldsymbol{v} \quad \text{for any } 0 \leq |\alpha| \leq k,$$

so that

$$\frac{\partial}{\partial t} Dx(t)|_{t=0} = D\boldsymbol{v} \quad \text{pointwise in } \mathbf{D}. \tag{5.3}$$

Analogously, the existence of the material derivative $\dot{y}(\Omega, \boldsymbol{v})$ in $\mathcal{C}^1(\Omega)$ implies that, uniformly,

$$\lim_{t \searrow 0} \frac{\partial}{\partial X_i} \left(\frac{y(\Omega_t) \circ x(t) - y(\Omega)}{t} \right) = \frac{\partial}{\partial X_i} \dot{y}(\Omega, \boldsymbol{v}) \quad \text{for } 1 \leq i \leq N,$$

and then

$$\frac{\partial}{\partial t} \nabla \left(y(\Omega_t) \circ x(t) \right) |_{t=0} = \nabla \dot{y}(\Omega, \boldsymbol{v}) \quad \text{pointwise in } \Omega. \tag{5.4}$$

Replacing (5.3) and (5.4) in (5.2), we obtain

$$\nabla \dot{y}(\Omega, \boldsymbol{v}) = D\boldsymbol{v}^T \nabla y(\Omega) + \dot{\nabla} y(\Omega, \boldsymbol{v}).$$

By Definition 4.1 of shape derivative we have

$$\begin{aligned} \nabla y'(\Omega, \boldsymbol{v}) &= \nabla \dot{y}(\Omega, \boldsymbol{v}) - \nabla \left(\nabla y(\Omega) \cdot \boldsymbol{v} \right) = \nabla \dot{y}(\Omega, \boldsymbol{v}) - D\boldsymbol{v}^T \nabla y(\Omega) - D^2 y(\Omega)^T \boldsymbol{v} \\ &= \dot{\nabla} y(\Omega, \boldsymbol{v}) - D^2 y(\Omega)^T \boldsymbol{v} = \left(\nabla y \right)' (\Omega, \boldsymbol{v}), \end{aligned}$$

where we have used that $D^2 y(\Omega)^T$ is symmetric because $y(\Omega) \in \mathcal{C}^2(\Omega)$. ☐

6. The shape derivative of b, $\boldsymbol{n}$ and κ

Although some of these results can be found in [8] and [17], we present here a derivation for the sake of completeness. In the following, we consider a domain $\Omega \subset \mathbf{D}$ with a $\mathcal{C}^2$-boundary Γ and a velocity field $\boldsymbol{v} \in V^1(\mathbf{D})$. The next lemma gives the connection to obtain the shape derivatives of the geometric quantities from the shape derivative of the oriented distance function.

Lemma 6.1 ([17, Lemma 4]). *Suppose that $y(\Omega) \in H^{\frac{3}{2}+\epsilon}(\Omega)$ satisfies $y(\Omega)|_\Gamma = 0$ for all domains $\Omega \in \mathcal{A}$ and that the shape derivative $y'(\Omega; \boldsymbol{v})$ exists in $H^{\frac{1}{2}+\epsilon}(\Omega)$ for some $\epsilon > 0$. Then, we have*

$$y'(\Omega, \boldsymbol{v})|_\Gamma = -\partial_n y \, v_n, \quad \textit{with } v_n = \boldsymbol{v} \cdot \boldsymbol{n}.$$

Proof. This lemma is proved in [17]. However, it can be more directly obtained if we consider the boundary function $z(\Gamma) := y(\Omega)|_\Gamma$. In fact, by hypothesis, $z(\Gamma_t) \equiv 0$ for all small $t \geq 0$. This gives us $\dot{z}(\Gamma, \boldsymbol{v}) = 0$ and $\nabla_\Gamma z(\Gamma) = 0$, so that $z'(\Gamma, \boldsymbol{v}) = 0$. The claim thus follows from Lemma 4.6. ☐

This lemma allows us to obtain the shape derivative of an extension to Ω of the oriented distance function $b = b_\Gamma$, and thus for ∇b and Δb. Since $b|_\Gamma = 0$, Lemma 6.1 leads to

$$b'(\Omega, \boldsymbol{v})|_\Gamma = -v_n, \tag{6.1}$$

where we have used that $\partial_n b = \nabla b \cdot \nabla b|_\Gamma = 1$. Note that this is the shape derivative of the *domain function* b, but restricted to Γ.

Consider now the canonical extension $\hat{\boldsymbol{n}} \in \mathcal{C}^1(\mathbf{D})$ of $\boldsymbol{n} \in \mathcal{C}^1(\Gamma)$ given by $\hat{\boldsymbol{n}}|_{S_h(\Gamma)} = \nabla b$. Computing the shape derivative of $\hat{\boldsymbol{n}}(\Omega) \cdot \hat{\boldsymbol{n}}(\Omega)$ which equals 1 in $S_h(\Gamma)$ we obtain $\hat{\boldsymbol{n}}'(\Omega, \boldsymbol{v}) \cdot \boldsymbol{n}(\Omega) = 0$ in $S_h(\Gamma)$, so that, if $x \in \Gamma$, $\hat{\boldsymbol{n}}'(\Omega, \boldsymbol{v})(x)$ belongs to the tangent plane $T_x(\Gamma)$. Also, from Lemma 5.5, $\hat{\boldsymbol{n}}'(\Omega, \boldsymbol{v}) = (\nabla b)'(\Omega, \boldsymbol{v}) = \nabla b'(\Omega, \boldsymbol{v})$

in $S_h(\Gamma)$, so that $\hat{\boldsymbol{n}}'(\Omega,\boldsymbol{v})|_\Gamma = \nabla_\Gamma b'(\Omega,\boldsymbol{v}) = -\nabla_\Gamma v_n$ from (6.1). We have thus obtained

$$\hat{\boldsymbol{n}}'(\Omega,\boldsymbol{v})|_\Gamma = -\nabla_\Gamma v_n, \quad \text{where } \hat{\boldsymbol{n}}|_{S_h(\Gamma)} = \nabla b. \tag{6.2}$$

Since $\hat{\boldsymbol{n}}$ is the canonical extension of the outward normal $\boldsymbol{n} = \boldsymbol{n}(\Gamma)$, we conclude, from Lemma 4.6 and the fact that $D\hat{\boldsymbol{n}}\hat{\boldsymbol{n}} = D^2 b \nabla b = 0$ from (2.3), the known result

$$\boldsymbol{n}'(\Gamma,\boldsymbol{v}) = -\nabla_\Gamma v_n. \tag{6.3}$$

Consider now $\Gamma \in \mathcal{C}^3$. To obtain the domain shape derivative of an extension of Δb (restricted to the boundary Γ), we commute derivatives and use the definition of tangential divergence (Definition 2.2) to obtain

$$(\Delta b)'(\Omega,\boldsymbol{v})|_\Gamma = \operatorname{div}(\nabla b)'(\Omega,\boldsymbol{v})|_\Gamma = \operatorname{div}_\Gamma(\hat{\boldsymbol{n}}'(\Omega,\boldsymbol{v})|_\Gamma) + D\hat{\boldsymbol{n}}'(\Omega,\boldsymbol{v})|_\Gamma \boldsymbol{n}\cdot\boldsymbol{n}.$$

Computing the shape derivative with respect to Ω of $D\hat{\boldsymbol{n}}\hat{\boldsymbol{n}} = 0$ we obtain

$$D\hat{\boldsymbol{n}}'(\Omega,\boldsymbol{v})\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}} = -D\hat{\boldsymbol{n}}\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}}'(\Omega,\boldsymbol{v}) = 0 \quad \text{in } S_h(\Gamma)$$

and then (6.2) implies

$$(\Delta b)'(\Omega,\boldsymbol{v})|_\Gamma = -\Delta_\Gamma v_n.$$

Since the mean curvature of Γ satisfies $\kappa(\Gamma) = \Delta b|_\Gamma$, by Lemma 4.6 we have $\kappa'(\Gamma,\boldsymbol{v}) = (\Delta b)'(\Omega,\boldsymbol{v})|_\Gamma + (\nabla\Delta b\cdot\nabla b)|_\Gamma v_n$. The second term is equal to $-|D_\Gamma\boldsymbol{n}|^2 v_n$ due to (2.6), and the fact that $D_\Gamma\boldsymbol{n} = D^2 b|_\Gamma$. We have thus obtained the following formula for the shape derivative of the mean curvature (boundary function).

Lemma 6.2 (Shape derivative of κ)**.** *If κ is the mean curvature of Γ, the boundary of a $\mathcal{C}^3$ domain Ω, then κ is shape differentiable in Γ and*

$$\kappa'(\Gamma,\boldsymbol{v}) = -\Delta_\Gamma v_n - |D_\Gamma\boldsymbol{n}|^2 v_n, \tag{6.4}$$

where $v_n = \boldsymbol{v}\cdot\boldsymbol{n}$, $|D_\Gamma\boldsymbol{n}|^2 = D_\Gamma\boldsymbol{n} : D_\Gamma\boldsymbol{n} = \operatorname{tr}(D_\Gamma\boldsymbol{n}^2)$ and $\Delta_\Gamma f = \operatorname{div}_\Gamma\nabla_\Gamma f$ is the Laplace–Beltrami operator of f.

As a consistency check, note that, since $\kappa = \operatorname{div}_\Gamma\boldsymbol{n}$, the same result about the shape derivative of κ can be obtained without considering the extension Δb, using only Corollary 7.2 of the next section and formula (6.3) for $\boldsymbol{n}'(\Gamma,\boldsymbol{v})$.

7. Shape derivatives of tangential operators

We are now in position to present the main results of this paper, namely, formulas for the shape derivatives of boundary functions that are tangential derivatives of boundary functions. More precisely, we find the shape derivatives of boundary functions of the form $\nabla_\Gamma z$, $D_\Gamma\boldsymbol{w}$, $\operatorname{div}_\Gamma\boldsymbol{w}$ and $\Delta_\Gamma z$, when $z(\Gamma)$ and $\boldsymbol{w}(\Gamma)$ are shape differentiable boundary functions, scalar and vector valued, respectively. Examples of important applications are presented in the two subsequent sections.

It is worth noting the difference with Lemma 5.5 where we established that standard differential operators commute with the shape derivative of domain functions.

Theorem 7.1 (Shape derivative of surface derivatives)**.** *For any admissible boundary $\Gamma = \partial\Omega$, where Ω is a $\mathcal{C}^2$ domain in $\mathbf{D}\subset\mathbb{R}^N$, consider a real function $z(\Gamma)\in\mathcal{C}^2(\Gamma)$ such that there exists an extension y to Ω, i.e., $z(\Gamma) = y(\Omega)|_\Gamma$,* *which is shape differentiable at* Ω *in the direction* $\boldsymbol{v} \in V^2(\mathbf{D})$*. Then* $z(\Gamma)$ *and* $\nabla_\Gamma z$ *are shape differentiable at* Γ *in the direction* $\boldsymbol{v}$*, and*

$$(\nabla_\Gamma z)'(\Gamma, \boldsymbol{v}) = \nabla_\Gamma z'(\Gamma, \boldsymbol{v}) + (\boldsymbol{n} \otimes \nabla_\Gamma v_n - v_n D_\Gamma \boldsymbol{n}) \nabla_\Gamma z(\Gamma), \tag{7.1}$$

where $v_n = \boldsymbol{v} \cdot \boldsymbol{n}$*.*

Proof. Let $y = y(\Omega)$ be an extension of $z(\Gamma)$ to Ω, i.e., $z(\Gamma) = y(\Omega)|_\Gamma$; then by definition

$$\nabla_\Gamma z(\Gamma) = \nabla y|_\Gamma - \partial_n y \boldsymbol{n} = (\nabla y - (\nabla y \cdot \nabla b)\nabla b)\,|_\Gamma.$$

Then $\boldsymbol{\Phi}(\Omega) := \nabla y - (\nabla y \cdot \nabla b)\nabla b$ is an extension to Ω of $\nabla_\Gamma z(\Gamma)$. Due to Lemma 4.6 these shape derivatives satisfy

$$(\nabla_\Gamma z)'(\Gamma, \boldsymbol{v}) = \boldsymbol{\Phi}'(\Omega, \boldsymbol{v})|_\Gamma + D\boldsymbol{\Phi}(\Omega)|_\Gamma \boldsymbol{n}\, v_n. \tag{7.2}$$

We now compute the domain shape derivative of $\boldsymbol{\Phi}(\Omega)$. Using the product rule we have

$$\begin{aligned}\boldsymbol{\Phi}'(\Omega, \boldsymbol{v}) &= (\nabla y)'(\Omega, \boldsymbol{v}) - (\nabla y)'(\Omega, \boldsymbol{v}) \cdot \nabla b\ \nabla b \\ &\quad - \nabla y \cdot (\nabla b)'(\Omega, \boldsymbol{v})\ \nabla b - \nabla y \cdot \nabla b\ (\nabla b)'(\Omega, \boldsymbol{v}) \\ &= (I - \nabla b \otimes \nabla b)\, \nabla y'(\Omega, \boldsymbol{v}) - \nabla y \cdot (\nabla b)'(\Omega, \boldsymbol{v})\ \nabla b - \nabla y \cdot \nabla b\ (\nabla b)'(\Omega, \boldsymbol{v}),\end{aligned}$$

where we have used Lemma 5.5 to commute the shape derivative and the gradient of y. Restricting to Γ, using the definition of tangential gradient and formula (6.2) for $(\nabla b)'(\Omega, \boldsymbol{v})|_\Gamma$, we obtain

$$\boldsymbol{\Phi}'(\Omega, \boldsymbol{v})|_\Gamma = \nabla_\Gamma y'(\Omega, \boldsymbol{v}) + (\boldsymbol{n} \otimes \nabla_\Gamma v_n)\nabla_\Gamma z(\Gamma) + \partial_n y \nabla_\Gamma v_n,$$

where we have used $\nabla y(\Omega)|_\Gamma \cdot \nabla_\Gamma v_n\ \boldsymbol{n} = \nabla_\Gamma z(\Gamma) \cdot \nabla_\Gamma v_n\ \boldsymbol{n} = (\boldsymbol{n} \otimes \nabla_\Gamma v_n)\nabla_\Gamma z(\Gamma)$. From Lemma 4.6 $y'(\Omega, \boldsymbol{v})|_\Gamma = z'(\Gamma, \boldsymbol{v}) - \partial_n y\, v_n$ and the product rule for tangential derivative yields

$$\begin{aligned}\boldsymbol{\Phi}'(\Omega, \boldsymbol{v})|_\Gamma &= \nabla_\Gamma z'(\Gamma, \boldsymbol{v}) - \nabla_\Gamma(\partial_n y\, v_n) + (\boldsymbol{n} \otimes \nabla_\Gamma v_n)\nabla_\Gamma z(\Gamma) + \partial_n y \nabla_\Gamma v_n \\ &= \nabla_\Gamma z'(\Gamma, \boldsymbol{v}) + (\boldsymbol{n} \otimes \nabla_\Gamma v_n)\nabla_\Gamma z(\Gamma) - v_n \nabla_\Gamma(\partial_n y).\end{aligned}$$

Then, from (7.2), to complete the proof of (7.1) we need to show that

$$D\boldsymbol{\Phi}(\Omega)|_\Gamma \boldsymbol{n} - \nabla_\Gamma(\partial_n y) = -D_\Gamma \boldsymbol{n} \nabla_\Gamma z(\Gamma). \tag{7.3}$$

Applying the product rule of classical derivatives to $\boldsymbol{\Phi}(\Omega) = \nabla y - (\nabla y \cdot \nabla b)\nabla b$, we obtain, using $\boldsymbol{n} = \nabla b|_\Gamma$,

$$\begin{aligned}D\boldsymbol{\Phi}(\Omega)|_\Gamma \boldsymbol{n} &= D^2 y|_\Gamma \boldsymbol{n} - (\boldsymbol{n} \otimes \nabla(\nabla y \cdot \nabla b)|_\Gamma)\, \boldsymbol{n} - \partial_n y D^2 b \nabla b|_\Gamma \\ &= D^2 y|_\Gamma \boldsymbol{n} - \partial_n(\nabla y \cdot \nabla b)\boldsymbol{n},\end{aligned}$$

because $D^2 b \nabla b = 0$. Besides,

$$\begin{aligned}\nabla_\Gamma(\partial_n y) &= \nabla(\nabla y \cdot \nabla b)|_\Gamma - \partial_n(\nabla y \cdot \nabla b)\boldsymbol{n} \\ &= D^2 y|_\Gamma \boldsymbol{n} - D^2 b \nabla y|_\Gamma - \partial_n(\nabla y \cdot \nabla b)\boldsymbol{n} \\ &= D\boldsymbol{\Phi}(\Omega)|_\Gamma \boldsymbol{n} - D_\Gamma \boldsymbol{n} \nabla_\Gamma z(\Gamma),\end{aligned}$$

where we have used that $D^2 b \nabla y|_\Gamma = D_\Gamma \boldsymbol{n} \nabla_\Gamma y = D_\Gamma \boldsymbol{n} \nabla_\Gamma z(\Gamma)$. From this equation we obtain (7.3) and the assertion follows. ☐

Corollary 7.2 (For vector fields). *If the function $\boldsymbol{w}(\Gamma) \in \mathcal{C}^2(\Gamma, \mathbb{R}^N)$ has an extension $\boldsymbol{W}(\Omega)$ to Ω, with $\Gamma = \partial\Omega \in \mathcal{C}^2$, and if $\boldsymbol{W}(\Omega)$ is shape differentiable at Ω in the direction $\boldsymbol{v} \in V^2(\mathbf{D})$, then $\boldsymbol{w}(\Gamma)$, $D_\Gamma \boldsymbol{w}$ and $\operatorname{div}_\Gamma \boldsymbol{w}$ are shape differentiable at Γ in the direction $\boldsymbol{v}$ and*

$$(D_\Gamma \boldsymbol{w})'(\Gamma, \boldsymbol{v}) = D_\Gamma \boldsymbol{w}'(\Gamma, \boldsymbol{v}) + D_\Gamma \boldsymbol{w}(\Gamma)[\nabla_\Gamma v_n \otimes \boldsymbol{n} - v_n D_\Gamma \boldsymbol{n}], \tag{7.4}$$

$$(\operatorname{div}_\Gamma \boldsymbol{w})'(\Gamma, \boldsymbol{v}) = \operatorname{div}_\Gamma \boldsymbol{w}'(\Gamma, \boldsymbol{v}) + [\boldsymbol{n} \otimes \nabla_\Gamma v_n - v_n D_\Gamma \boldsymbol{n}] : D_\Gamma \boldsymbol{w}(\Gamma), \tag{7.5}$$

where $S : T = \operatorname{tr}(S^T T)$ denotes the scalar product of tensors.

Proof. In order to obtain (7.4), note that $D_\Gamma \boldsymbol{w}^T \boldsymbol{e}_i = \nabla_\Gamma w_i$, where $w_i = \boldsymbol{w} \cdot \boldsymbol{e}_i$, with $\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_N\}$ being the canonical basis of $\mathbb{R}^N$. By definition, the shape derivative of the tensor $D_\Gamma \boldsymbol{w}^T$ must satisfy

$$(D_\Gamma \boldsymbol{w}^T)'(\Gamma, \boldsymbol{v})\boldsymbol{e}_i = (D_\Gamma \boldsymbol{w}^T \boldsymbol{e}_i)'(\Gamma, \boldsymbol{v}) = (\nabla_\Gamma w_i)'(\Gamma, \boldsymbol{v}).$$

Applying (7.1) to $z(\Gamma) = w_i = \boldsymbol{w} \cdot \boldsymbol{e}_i$, we obtain

$$\begin{aligned}
(D_\Gamma \boldsymbol{w}^T)'(\Gamma, \boldsymbol{v})\boldsymbol{e}_i &= (\nabla_\Gamma w_i)'(\Gamma, \boldsymbol{v}) \\
&= \nabla_\Gamma w_i'(\Gamma, \boldsymbol{v}) + [\boldsymbol{n} \otimes \nabla_\Gamma v_n - v_n D_\Gamma \boldsymbol{n}] \nabla_\Gamma w_i(\Gamma) \\
&= \big(D_\Gamma \boldsymbol{w}'(\Gamma, \boldsymbol{v})^T + [\boldsymbol{n} \otimes \nabla_\Gamma v_n - v_n D_\Gamma \boldsymbol{n}] D_\Gamma \boldsymbol{w}^T(\Gamma) \big) \boldsymbol{e}_i.
\end{aligned}$$

The linearity of the transpose operator and Lemma 5.2 yield the desired result.

Finally, we recall that $(\operatorname{div}_\Gamma \boldsymbol{w})'(\Gamma, \boldsymbol{v}) = \operatorname{tr}(D_\Gamma \boldsymbol{w})'(\Gamma, \boldsymbol{v})$ and $(\boldsymbol{a} \otimes \boldsymbol{b}) : S = \boldsymbol{a} \cdot S\boldsymbol{b}$. Therefore (7.4) implies

$$(\operatorname{div}_\Gamma \boldsymbol{w})'(\Gamma, \boldsymbol{v}) = \operatorname{div}_\Gamma \boldsymbol{w}'(\Gamma, \boldsymbol{v}) + D_\Gamma \boldsymbol{w} \nabla_\Gamma v_n \cdot \boldsymbol{n} - v_n D_\Gamma \boldsymbol{n} : D_\Gamma \boldsymbol{w},$$

and (7.5) follows. □

As an immediate consequence of this corollary we can compute the shape derivative of the second fundamental form.

Corollary 7.3 (Shape derivative of the second fundamental form). *For a $\mathcal{C}^3$ surface Γ and a smooth velocity field $\boldsymbol{v}$, the shape derivative of the tensor $D_\Gamma \boldsymbol{n}$ at Γ in the direction $\boldsymbol{v}$ is given by*

$$(D_\Gamma \boldsymbol{n})'(\Gamma, \boldsymbol{v}) = -D_\Gamma^2 v_n + D_\Gamma \boldsymbol{n} \nabla_\Gamma v_n \otimes \boldsymbol{n} - v_n D_\Gamma \boldsymbol{n}^2. \tag{7.6}$$

We end this section establishing the shape derivative of the Laplace–Beltrami operator of a boundary function, which is more involved because it is of second order.

Theorem 7.4 (Shape derivative of the surface Laplacian). *If $\Gamma = \partial\Omega$ is a $\mathcal{C}^3$-boundary contained in $\mathbf{D}$, $z = z(\Gamma) \in \mathcal{C}^3(\Gamma)$, and if there exists an extension $y(\Omega)$ of $z(\Gamma)$ which is shape differentiable at Ω in the direction $\boldsymbol{v} \in V^3(\mathbf{D})$, then $z(\Gamma)$ and $\Delta_\Gamma z := \operatorname{div}_\Gamma \nabla_\Gamma z$ are shape differentiable at Γ in the direction $\boldsymbol{v}$, and the shape* *derivative of* $\Delta_\Gamma z$ *is given by*

$$\begin{aligned}(\Delta_\Gamma z)'(\Gamma,\boldsymbol{v}) &= \Delta_\Gamma z'(\Gamma,\boldsymbol{v}) - 2v_n D_\Gamma \boldsymbol{n} : D^2_\Gamma z \\ &\quad + (\kappa\nabla_\Gamma v_n - 2D_\Gamma\boldsymbol{n}\nabla_\Gamma v_n - v_n\nabla_\Gamma\kappa)\cdot\nabla_\Gamma z \\ &= \Delta_\Gamma z'(\Gamma,\boldsymbol{v}) - v_n\big(2D_\Gamma\boldsymbol{n} : D^2_\Gamma z + \nabla_\Gamma\kappa\cdot\nabla_\Gamma z\big) \\ &\quad + \nabla_\Gamma v_n\cdot(\kappa\nabla_\Gamma z - 2D_\Gamma\boldsymbol{n}\nabla_\Gamma z)\,.\end{aligned}$$

Proof. In order to simplify the calculation, we denote $M = \boldsymbol{n}\otimes\nabla_\Gamma v_n - v_n D_\Gamma\boldsymbol{n}$. Using successively the formulas for the shape derivative of a tangential divergence (Corollary 7.2) and for a tangential gradient (Theorem 7.1), we have

$$\begin{aligned}(\Delta_\Gamma z)'(\Gamma,\boldsymbol{v}) &= (\operatorname{div}_\Gamma\nabla_\Gamma z)'(\Gamma,\boldsymbol{v}) \\ &= \operatorname{div}_\Gamma((\nabla_\Gamma z)'(\Gamma,\boldsymbol{v})) + M : D_\Gamma\nabla_\Gamma z \\ &= \operatorname{div}_\Gamma[\nabla_\Gamma z'(\Gamma,\boldsymbol{v}) + M\nabla_\Gamma z] + M : D^2_\Gamma z \\ &= \Delta_\Gamma z'(\Gamma,\boldsymbol{v}) + \operatorname{div}_\Gamma(M\nabla_\Gamma z) + M : D^2_\Gamma z.\end{aligned}$$

Using the product rule (v) of Lemma 2.4 we obtain

$$\begin{aligned}(\Delta_\Gamma z)'(\Gamma,\boldsymbol{v}) &= \Delta_\Gamma z'(\Gamma,\boldsymbol{v}) + M^T : D^2_\Gamma z + \operatorname{div}_\Gamma M^T\cdot\nabla_\Gamma z + M : D^2_\Gamma z \\ &= \Delta_\Gamma z'(\Gamma,\boldsymbol{v}) + (M+M^T) : D^2_\Gamma z + \operatorname{div}_\Gamma M^T\cdot\nabla_\Gamma z.\end{aligned} \tag{7.7}$$

Since $D_\Gamma\boldsymbol{n}^T = D_\Gamma\boldsymbol{n}$, the second term in the right-hand side reads

$$M + M^T = \boldsymbol{n}\otimes\nabla_\Gamma v_n + \nabla_\Gamma v_n\otimes\boldsymbol{n} - 2v_n D_\Gamma\boldsymbol{n}.$$

Using the tensor property $(\boldsymbol{a}\otimes\boldsymbol{b}) : S = \boldsymbol{a}\cdot S\boldsymbol{b}$ and that $D^2_\Gamma z\,\boldsymbol{n} = 0$, we obtain

$$(M+M^T) : D^2_\Gamma z = \boldsymbol{n}\cdot D^2_\Gamma z\nabla_\Gamma v_n - 2v_n D_\Gamma\boldsymbol{n} : D^2_\Gamma z.$$

Observe that differentiating $\boldsymbol{n}\cdot\nabla_\Gamma z = 0$ leads to $D^2_\Gamma z^T\boldsymbol{n} = -D_\Gamma\boldsymbol{n}\nabla_\Gamma z$, which implies $\boldsymbol{n}\cdot D^2_\Gamma z\nabla_\Gamma v_n = -D_\Gamma\boldsymbol{n}\nabla_\Gamma v_n\cdot\nabla_\Gamma z$. Then

$$(M+M^T) : D^2_\Gamma z = -D_\Gamma\boldsymbol{n}\nabla_\Gamma v_n\cdot\nabla_\Gamma z - 2v_n D_\Gamma\boldsymbol{n} : D^2_\Gamma z. \tag{7.8}$$

The last term in the second line of (7.7) contains $\operatorname{div}_\Gamma M^T$, which can be computed with the product rules of Lemma 2.4 to obtain

$$\begin{aligned}\operatorname{div}_\Gamma M^T &= \operatorname{div}_\Gamma(\nabla_\Gamma v_n\otimes\boldsymbol{n}) - \operatorname{div}_\Gamma(v_n D_\Gamma\boldsymbol{n}) \\ &= \nabla_\Gamma v_n\cdot\operatorname{div}_\Gamma\boldsymbol{n} + D_\Gamma\nabla_\Gamma v_n\boldsymbol{n} - D_\Gamma\boldsymbol{n}\nabla_\Gamma v_n - v_n\operatorname{div}_\Gamma(D_\Gamma\boldsymbol{n}) \\ &= \kappa\nabla_\Gamma v_n - D_\Gamma\boldsymbol{n}\nabla_\Gamma v_n - v_n\Delta_\Gamma\boldsymbol{n},\end{aligned}$$

where we have used that $\kappa = \operatorname{div}_\Gamma\boldsymbol{n}$ and $D_\Gamma\nabla_\Gamma v_n\boldsymbol{n} = D^2_\Gamma v_n\boldsymbol{n} = 0$. Since $\Delta_\Gamma\boldsymbol{n}\cdot\nabla_\Gamma z = (P\Delta_\Gamma\boldsymbol{n})\cdot\nabla_\Gamma z$, where P is the orthogonal projection to the tangent plane, equation (2.15) yields $P\Delta_\Gamma\boldsymbol{n} = \nabla_\Gamma\kappa$, whence

$$\operatorname{div}_\Gamma M^T\cdot\nabla_\Gamma z = \kappa\nabla_\Gamma v_n\cdot\nabla_\Gamma z - D_\Gamma\boldsymbol{n}\nabla_\Gamma v_n\cdot\nabla_\Gamma z - v_n\nabla_\Gamma\kappa\cdot\nabla_\Gamma z. \tag{7.9}$$

Finally we add equations (7.8) and (7.9) and replace in (7.7) to obtain

$$\begin{aligned}(\Delta_\Gamma z)'(\Gamma,\boldsymbol{v}) &= \Delta_\Gamma z'(\Gamma,\boldsymbol{v}) - 2D_\Gamma\boldsymbol{n}\nabla_\Gamma v_n\cdot\nabla_\Gamma z \\ &\quad - 2v_n D_\Gamma\boldsymbol{n} : D^2_\Gamma z + \kappa\nabla_\Gamma v_n\cdot\nabla_\Gamma z - v_n\nabla_\Gamma\kappa\cdot\nabla_\Gamma z,\end{aligned}$$

which completes the proof. □

8. Geometric invariants and Gaussian curvature

The *geometric invariants* of a $\mathcal{C}^2$-surface Γ determine its intrinsic properties. They are defined as the invariants of the tensor $D_\Gamma \boldsymbol{n}$, which, in turn, are the coefficients of its characteristic polynomial $p(\lambda)$ (see [23]). The geometric invariants of Γ, $i_j(\Gamma) : \Gamma \to \mathbb{R}$, $j = 1, \ldots, N$, thus satisfy

$$p(\lambda) = \det(D_\Gamma \boldsymbol{n}(X) - \lambda I) = \lambda^N + i_1\lambda^{N-1} + i_2\lambda^{N-2} + \cdots + i_{N-1}\lambda + i_N,$$

and can also be expressed using the eigenvalues of the tensor $D_\Gamma \boldsymbol{n}$, one of which is always zero and the others are the principal curvatures $\kappa_1, \ldots, \kappa_{N-1}$. Indeed,

$$i_1(\Gamma) = \sum_{j=1}^{N-1} \kappa_j, \quad i_2(\Gamma) = \sum_{j_1 \neq j_2} \kappa_{j_1}\kappa_{j_2}, \ \ldots, \ i_{N-1}(\Gamma) = \kappa_1 \ldots \kappa_{N-1}, \quad i_N(\Gamma) = 0.$$

We can observe from definitions (2.1) that the first invariant $i_1(\Gamma)$ is the *mean curvature* κ and the last nonzero invariant $i_{N-1}(\Gamma)$ is the *Gaussian curvature* κ_g. The invariant $i_k(\Gamma)$, for $2 \leq k \leq N-2$, is the so-called *k-th mean curvature* [21, Ch. 3F].

The geometric invariants of Γ can also be defined recursively through the functions $I_p(\Gamma) : \Gamma \to \mathbb{R}$, given by $I_p(\Gamma) = \operatorname{tr}(D_\Gamma \boldsymbol{n}^p) = (D_\Gamma \boldsymbol{n})^{p-1} : D_\Gamma \boldsymbol{n}$, $p = 1, \ldots, N-1$. More exactly, from [18, Ch. 4.5] we have:

$$\begin{aligned}
i_1 &= I_1, \\
i_2 &= \tfrac{1}{2}\left(i_1 I_1 - I_2\right), \\
i_3 &= \tfrac{1}{3}\left(i_2 I_1 - i_1 I_2 + I_3\right), \\
&\ \vdots \\
i_p &= \tfrac{1}{p}\left(i_{p-1} I_1 - i_{p-2} I_2 + \cdots + (-1)^{p-1} I_p\right) \\
&= \tfrac{1}{p}\sum_{i=1}^{p} (-1)^{i-1} i_{p-i} I_i.
\end{aligned}$$

Note that $I_1 = \operatorname{div}_\Gamma \boldsymbol{n}$ and $I_2 = |D_\Gamma \boldsymbol{n}|^2$, which leads to $i_1 = \kappa$ and (for $N = 3$) $i_2 = \kappa_g$.

We now establish the shape derivatives of the functions $I_p(\Gamma) = \operatorname{tr}(D_\Gamma \boldsymbol{n}^p)$, which are also intrinsic to the surface Γ and will lead to the shape derivatives of the geometric invariants $i_p(\Gamma)$.

Proposition 8.1 (Shape derivatives of the invariants)**.** *Let Γ be a $\mathcal{C}^3$-boundary in $\mathbb{R}^N$ and p a positive integer. For any integer $p \geq 1$, the shape derivative of the scalar valued boundary function $I_p(\Gamma) := \operatorname{tr}(D_\Gamma \boldsymbol{n}^p)$ at Γ in the direction $\boldsymbol{v} \in V^2(\mathbf{D})$ is given by*

$$(I_p)'(\Gamma, \boldsymbol{v}) = -p\big(D^2_\Gamma v_n : D_\Gamma \boldsymbol{n}^{p-1} + v_n I_{p+1}\big),$$

where $v_n = \boldsymbol{v} \cdot \boldsymbol{n}$ and $D_\Gamma \boldsymbol{n}^0 = \mathrm{I}$, the identity tensor in $\mathbb{V}$.

For the proof of this proposition we need the following lemma.

Lemma 8.2. *Let $A(\Gamma) : \Gamma \to \mathrm{Lin}(\mathbb{V})$ be a symmetric tensor valued function and let p be a positive integer. If $A(\Gamma)$ is shape differentiable at Γ in the direction $\boldsymbol{v}$, then the shape derivative of $A^p(\Gamma)$ satisfies*

$$(A^p)'(\Gamma, \boldsymbol{v}) : A^j = p\big(A'(\Gamma, \boldsymbol{v}) : A^{j+p-1}\big), \tag{8.1}$$

for any integer $j \geq 0$.

Proof. We proceed by induction. It is trivial to see that equation (8.1) holds for $p = 1$ and any integer $j \geq 0$.

Assuming that equation (8.1) holds for $p \geq 1$ and any $j \geq 0$, we want to prove that

$$(A^{p+1})'(\Gamma, \boldsymbol{v}) : A^j = (p+1)\big(A'(\Gamma, \boldsymbol{v}) : A^{j+p}\big), \quad \text{for any integer } j \geq 0. \tag{8.2}$$

Applying the product rule for the shape derivative to $A^{p+1} = A^p A$, we have

$$(A^{p+1})'(\Gamma, \boldsymbol{v}) : A^j = (A^p)'(\Gamma, \boldsymbol{v})A : A^j + A^p A'(\Gamma, \boldsymbol{v}) : A^j.$$

The tensor product property $BC : D = B : DC^T = C : B^T D$ and the fact that the tensor A is symmetric, yield

$$(A^{p+1})'(\Gamma, \boldsymbol{v}) : A^j = (A^p)'(\Gamma, \boldsymbol{v}) : A^{j+1} + A'(\Gamma, \boldsymbol{v}) : A^{j+p}. \tag{8.3}$$

The inductive assumption for p and $j+1$ implies

$$(A^p)'(\Gamma, \boldsymbol{v}) : A^{j+1} = p\big(A'(\Gamma, \boldsymbol{v}) : A^{j+p}\big).$$

Using this in equation (8.3), we obtain the desired result (8.2). □

Proof of Proposition 8.1. Note that $I_p'(\Gamma, \boldsymbol{v}) = \mathrm{tr}(D_\Gamma \boldsymbol{n}^p)'(\Gamma, \boldsymbol{v}) = (D_\Gamma \boldsymbol{n}^p)'(\Gamma, \boldsymbol{v}) : D_\Gamma \boldsymbol{n}^0$. Then Lemma 8.2 with $j = 0$ and $A = D_\Gamma \boldsymbol{n}$, which is a symmetric tensor, leads to

$$I_p'(\Gamma, \boldsymbol{v}) = p\big(D_\Gamma \boldsymbol{n}'(\Gamma, \boldsymbol{v}) : D_\Gamma \boldsymbol{n}^{p-1}\big).$$

From formula (7.6) we have that $(D_\Gamma \boldsymbol{n})'(\Gamma, \boldsymbol{n}) : D_\Gamma \boldsymbol{n}^{p-1} = -D_\Gamma^2 v_n : D_\Gamma \boldsymbol{n}^{p-1} - v_n I_{p+1}(\Gamma)$, where we have used that $D_\Gamma \boldsymbol{n} \nabla_\Gamma v_n \otimes \boldsymbol{n} : D_\Gamma \boldsymbol{n}^{p-1} = 0$ for any integer $p \geq 1$. This completes the proof. □

We now obtain the shape derivatives of the geometric invariants, which gives us, as particular cases, the shape derivatives of the Gaussian and mean curvatures. The goal is to obtain them in terms of the geometric invariants.

We start with $i_1 = \kappa$:

$$i_1'(\Gamma, \boldsymbol{v}) = I_1'(\Gamma, \boldsymbol{v}) = -D_\Gamma^2 v_n : D_\Gamma \boldsymbol{n}^0 - v_n I_2 = -\Delta_\Gamma v_n - v_n I_2,$$

which is consistent with the previous result (6.4). Since $I_2 = i_1^2 - 2i_2$, we can also write $i_1'(\Gamma, \boldsymbol{v})$ in terms of i_p as follows:

$$i_1'(\Gamma, \boldsymbol{v}) = -\Delta_\Gamma v_n - v_n i_1^2(\Gamma) + 2v_n i_2(\Gamma). \tag{8.4}$$

For the second invariant, note that $I_2'(\Gamma, \boldsymbol{v}) = -2\left(D^2_\Gamma v_n : D_\Gamma \boldsymbol{n} + v_n I_3\right)$. Since $i_2 = \frac{1}{2}(I_1^2 - I_2)$, we have

$$\begin{aligned} i_2'(\Gamma, \boldsymbol{v}) &= I_1 I_1'(\Gamma, \boldsymbol{v}) - \frac{1}{2} I_2'(\Gamma, \boldsymbol{v}) = -I_1 \Delta_\Gamma v_n - v_n I_1 I_2 + D^2_\Gamma v_n : D_\Gamma \boldsymbol{n} + v_n I_3 \\ &= -I_1 \Delta_\Gamma v_n + D^2_\Gamma v_n : D_\Gamma \boldsymbol{n} + v_n (I_3 - I_1 I_2). \end{aligned}$$

To obtain a formula only involving the invariants i_p, observe that $i_3 = \frac{1}{3}(I_3 - I_1 I_2 + i_1 i_2)$, whence

$$i_2'(\Gamma, \boldsymbol{v}) = -i_1 \Delta_\Gamma v_n + D^2_\Gamma v_n : D_\Gamma \boldsymbol{n} + v_n (3 i_3 - i_1 i_2). \tag{8.5}$$

Remember that, for $N = 3$, the Gaussian curvature κ_g is the second invariant $i_2(\Gamma)$. Then, on the one hand, from (8.4), we have the following expression for the shape derivative of the mean curvature κ in terms of κ_g:

$$\kappa'(\Gamma, \boldsymbol{v}) = -\Delta_\Gamma v_n - v_n \kappa^2 + 2 v_n \kappa_g. \tag{8.6}$$

On the other hand, since $i_3 = 0$, we obtain from (8.5) the following formula for the shape derivative of the Gaussian curvature.

Theorem 8.3 (Shape derivative of the Gauss curvature)**.** *For a $\mathcal{C}^3$-surface Γ in $\mathbb{R}^3$, the shape derivative of the Gaussian curvature κ_g is given by*

$$\kappa_g'(\Gamma, \boldsymbol{v}) = -\kappa \Delta_\Gamma v_n + D^2_\Gamma v_n : D_\Gamma \boldsymbol{n} - v_n \kappa \kappa_g,$$

where κ is the mean or additive curvature, $\boldsymbol{n}$ the normal vector field and $v_n = \boldsymbol{v} \cdot \boldsymbol{n}$.

9. Application: A Newton-type method

Most of shape optimization problems consist in finding a minimum of some functional restricted to a family of admissible sets (domains or surfaces), e.g.,

$$\Gamma_* = \arg\min_{\Gamma \in \mathcal{A}} J(\Gamma). \tag{9.1}$$

If J is shape differentiable in $\mathcal{A}$ and Γ_* is a minimizer, then $dJ(\Gamma_*, \boldsymbol{v}) = 0$ for all $\boldsymbol{v} \in \boldsymbol{\mathcal{V}}$, where $\boldsymbol{\mathcal{V}}$ is a vector space of admissible velocity fields, for example $\boldsymbol{\mathcal{V}} = \boldsymbol{V}^k(\mathbf{D}) := \mathcal{C}^k_c(\mathbf{D}, \mathbb{R}^N)$, or a proper subset to account for boundary restrictions of the admissible shapes $\mathcal{A}$. We thus focus our attention in the following alternative problem:

$$\text{Find } \Gamma_* \in \mathcal{A}: \quad dJ(\Gamma_*, \boldsymbol{v}) = 0, \quad \text{for all} \boldsymbol{v} \in \boldsymbol{\mathcal{V}}. \tag{9.2}$$

A scheme to approximate the solutions of (9.2) for surfaces of prescribed constant mean curvature was presented in [5], where numerical experiments document its performance and fast convergence. The scheme was a variation of the Newton algorithm, which requires the computation of second derivatives of the shape functional. There, the computations were tailored to the specific problem of prescribed mean curvature, and based on variational calculus using parametrizations, rather than using shape calculus. Similar schemes for specific problems can be found in [17, 24].

Observe that, due to the Structure Theorem (Theorem 3.3), Problem (9.2) is equivalent to the following:

$$\text{Find } \Gamma_* \in \mathcal{A}: \quad dJ(\Gamma_*, v\hat{\boldsymbol{n}}_*) = 0, \quad \text{for all } v \in \mathcal{V}_* := \{w \in \mathcal{V} : \partial_n w = 0 \text{ in } \Gamma_*\}, \tag{9.3}$$

where $\mathcal{V} = \mathcal{C}_c^k(\mathbf{D})$ and $\hat{\boldsymbol{n}}_* \in \boldsymbol{\mathcal{V}}$ is an extension of $\boldsymbol{n}_*$ the normal vector of Γ_* (this equivalence arises if, for each $\boldsymbol{v} \in \boldsymbol{\mathcal{V}}$, we let $v \in \mathcal{V}_*$ be the canonical extension of $\boldsymbol{v} \cdot \boldsymbol{n}_*$, as it was done in Lemma 4.7).

We now present a Newton-type method to approximate the solution of (9.3) that generalizes the previous works. It uses the language of shape derivatives and it has the potential to work for a large class of shape functionals, not just the area or other specific function.

Furthermore it allows us to apply the computational power of the results previously obtained in this work. Namely, to give computable expressions for interesting examples.

We start by defining, for each $\Gamma \in \mathcal{A}$ and $v \in \mathcal{V}$, the functional $J_v(\Gamma) := dJ(\Gamma, v\hat{\boldsymbol{n}})$ (with $\hat{\boldsymbol{n}} \in \boldsymbol{\mathcal{V}}$ denoting an extension of the normal $\boldsymbol{n}$ of Γ), so that the solution Γ_* satisfies $J_v(\Gamma_*) = 0$ for all $v \in \mathcal{V}_*$. Assume now that $\Gamma_0 \in \mathcal{A}$ is sufficiently close to the solution Γ_* so that there exists $\boldsymbol{u} \in \boldsymbol{\mathcal{V}}$ (small, in some sense) such that $\Gamma_* := \Gamma_0 + \boldsymbol{u}$, in the sense of Remark 3.2; this Remark also implies that

$$J_v(\Gamma_*) = J_v(\Gamma_0 + \boldsymbol{u}) = J_v(\Gamma_0) + dJ_v(\Gamma_0, \boldsymbol{u}) + o(|\boldsymbol{u}|). \tag{9.4}$$

The goal of finding $\Gamma_* = \Gamma_0 + \boldsymbol{u}$ such that $J_v(\Gamma_0 + \boldsymbol{u}) = 0$ is now switched to a simplified problem of finding $\boldsymbol{u}_0$ such that the linear approximation of J_v around Γ_0 vanishes at $\Gamma_1 := \Gamma_0 + \boldsymbol{u_0}$, i.e., $J_v(\Gamma_0) + dJ_v(\Gamma_0, \boldsymbol{u}_0) = 0$. Another simplification arises when asking this equality to hold for all $v \in \mathcal{V}_0 := \{w \in \mathcal{V} : \partial_n w = 0 \text{ in } \Gamma_0\}$ (instead of $\mathcal{V}_*$). Moreover, we simplify it further by considering only $v \in V(\Gamma_0) := C^k(\Gamma_0)$ and defining $J_v(\Gamma_0) := dJ(\Gamma_0, \hat{v}\hat{\boldsymbol{n}}_0)$, where $\hat{v} \in \mathcal{V}_0$ coincides, in some tubular neighborhood of Γ_0, with the canonical extension $v \circ p_{\Gamma_0}$. Since $dJ_v(\Gamma_0, \boldsymbol{u}_0)$ only depends on the normal component of $\boldsymbol{u}_0$ on Γ_0, this last problem has multiple solutions, so we restrict it by considering normal velocities of the form $\boldsymbol{u}_0 = \hat{u}_0 \hat{\boldsymbol{n}}_0$ with $u_0 \in V(\Gamma_0)$, and arrive at the following problem:

$$\text{Find } u_0 \in V(\Gamma_0): \quad J_v(\Gamma_0) + dJ_v(\Gamma_0, u_0 \boldsymbol{n}_0) = 0 \quad \forall v \in V(\Gamma_0). \tag{9.5}$$

Hereafter, we usually identify scalar/velocity fields defined on Γ with their canonical extensions, and we slightly abuse the notation writing $dJ_v(\Gamma_0, u_0\boldsymbol{n}_0)$ to denote $dJ_v(\Gamma_0, \hat{u}_0\hat{\boldsymbol{n}}_0)$, owing to the Structure Theorem. Finally, define $\Gamma_1 = \Gamma_0 + P(u_0\boldsymbol{n}_0)$, with P some projection from C^{k-1} to C^k. This sets the basis for an iterative method that will be implemented and further investigated in forthcoming articles.

9.1. **Examples.** Using the results of Section 8, we provide computable expressions for the functional $dJ_v(\Gamma, u\boldsymbol{n})$ of (9.5) for the cases when $J(\Gamma)$ is a boundary integral operator. Later we will apply those formulas to the area and the Willmore functional.

Lemma 9.1. *Let $\mathcal{A}$ be a family of admissible $\mathcal{C}^{k+1}$ surfaces contained in $\mathbf{D}$, with $k \geq 2$, $z = z(\Gamma) \in \mathcal{C}^2(\Gamma)$ and $J(\Gamma) = \int_\Gamma z$ a shape differentiable functional on $\mathcal{A}$ with respect to $\boldsymbol{V}^k(\mathbf{D})$. Let $\Gamma_0 \in \mathcal{A}$ and $u, v \in C^k(\Gamma_0)$; then*

$$dJ_v(\Gamma_0, u\boldsymbol{n}_0) = \int_{\Gamma_0} z'_v(\Gamma_0, u\boldsymbol{n}_0) + 2zuv\, i_2 - zv\Delta_\Gamma u + \kappa(vz_u + uz_v), \tag{9.6}$$

where $z_w := z'(\Gamma; w\boldsymbol{n})$, for each Γ with normal $\boldsymbol{n}$ and each $w \in C^k(\Gamma_0)$, and i_2 is the second geometric invariant of Γ.

Proof. Consider functions $v, u \in \mathcal{V} = C^k_c(\mathbf{D})$ and $\boldsymbol{n}$ the normal vector of Γ. Then, from (4.4) the functional $J_v(\Gamma) := dJ(\Gamma, v\boldsymbol{n})$ is given by $J_v(\Gamma) = \int_\Gamma z_v + \kappa z v$. Hence (4.4) again yields

$$dJ_v(\Gamma, u\boldsymbol{n}) = \int_\Gamma z'_v(\Gamma, u\boldsymbol{n}) + \kappa'(\Gamma, u\boldsymbol{n})zv + \kappa z'(\Gamma, u\boldsymbol{n})v + \kappa z v'(\Gamma, u\boldsymbol{n}) + z_v \kappa u + \kappa^2 zvu.$$

Recall from (8.4) that $\kappa'(\Gamma, u\boldsymbol{n}) = -\Delta_\Gamma u - u\kappa^2 + 2ui_2$. Then

$$dJ_v(\Gamma, u\boldsymbol{n}) = \int_\Gamma z'_v(\Gamma, u\boldsymbol{n}) - zv\Delta_\Gamma u + 2i_2 zvu + \kappa\,(vz_u + uz_v) + \kappa z\, v'(\Gamma, u\boldsymbol{n})$$

for any $u, v \in \mathcal{V}$. Since v does not depend on Γ, we have obtained at the beginning of Subsection 4.1 that $v'(\Gamma, u\boldsymbol{n}) = u\partial_n v$. If we fix $\Gamma_0 \in \mathcal{A}$, we have $v'(\Gamma_0, u\boldsymbol{n}) = 0$ for any $v \in \mathcal{V}$ such that $\partial_n v = 0$ in Γ_0. Then we have obtained (9.6) for any $u \in \mathcal{V}$ and $v \in \mathcal{V}_0 := \{w \in \mathcal{V} : \partial_n w = 0 \text{ in } \Gamma_0\}$. In particular, for any $u, v \in C^k(\Gamma_0)$, we have (9.6) for their canonical extensions. ☐

Area functional. Given a regular surface Γ_0 in $\mathbb{R}^N$ with boundary γ, a minimal surface Γ^* with boundary γ is a solution of the minimization problem (9.1) with $J(\Gamma) = \int_\Gamma d\Gamma$, the area functional, and the admissible family $\mathcal{A} = \mathcal{A}(\gamma)$ consists of all regular $N-1$ dimensional surfaces in $\mathbb{R}^N$ with boundary γ. For a fixed $\Gamma_0 \in \mathcal{A}$, the set of scalar velocity fields we need to consider is $V^k(\Gamma_0) = \{w \in C^k(\Gamma_0) : w|_{\partial\Gamma_0} = 0\}$.

For the area functional we have $z(\Gamma) \equiv 1$, $z_v(\Gamma) \equiv 0$ and $z'_v(\Gamma, u\boldsymbol{n}) \equiv 0$. Then $J_v(\Gamma) = \int_\Gamma \kappa(\Gamma)v$ and, for a fixed Γ_0, formula (9.6) gives us

$$dJ_v(\Gamma_0, u\boldsymbol{n}_0) = \int_{\Gamma_0} 2i_2 uv + \nabla_\Gamma u \cdot \nabla_\Gamma v,$$

for any $u \in \mathcal{V}$ and $v \in V(\Gamma_0)$, where we have used formula (2.13) of Lemma 2.5 to obtain $\int_{\Gamma_0} -\Delta_\Gamma u\, v = \int_{\Gamma_0} \nabla_\Gamma u \cdot \nabla_\Gamma v$.

If $N = 3$, the second invariant i_2 coincides with the Gaussian curvature κ_g. Then, solving (9.5) for a $\mathcal{C}^2$-surface $\Gamma_0 \in \mathcal{A}(\gamma)$ is equivalent to finding $u_0 \in V^1(\Gamma_0)$ such that

$$\int_{\Gamma_0} \nabla_\Gamma u_0 \cdot \nabla_\Gamma v + 2\kappa_g u_0 v = -\int_{\Gamma_0} \kappa v, \quad \forall v \in V^1(\Gamma_0).$$

Willmore functional. Consider now the Willmore functional $J(\Gamma) = \int_\Gamma z(\Gamma)$ with $z(\Gamma) = \frac{1}{2}\kappa^2$, and the scalar velocities $u, v \in \mathcal{V}$. By the product rule for shape derivatives (Remark 5.4), we have $z_v = z'(\Gamma, v\boldsymbol{n}) = \kappa\kappa'(\Gamma, v\boldsymbol{n}) = -\kappa\big(\Delta_\Gamma v + vI_2\big)$, where $I_2 = |D_\Gamma \boldsymbol{n}|^2$. In order to apply formula (9.6) we need to compute, for $\boldsymbol{u} = u\boldsymbol{n}$,

$$z_v'(\Gamma, \boldsymbol{u}) = -\kappa'(\Gamma, \boldsymbol{u})\big(\Delta_\Gamma v + vI_2\big) - \kappa\big((\Delta_\Gamma v)'(\Gamma, \boldsymbol{u}) + v'(\Gamma, \boldsymbol{u})I_2 + vI_2'(\Gamma, \boldsymbol{u})\big).$$

Recall that $\kappa'(\Gamma, \boldsymbol{u}) = -\Delta_\Gamma u - uI_2$, $I_2'(\Gamma, \boldsymbol{u}) = -2\left(D_\Gamma^2 u : D_\Gamma \boldsymbol{n} + uI_3\right)$ by Proposition 8.1, $v'(\Gamma, \boldsymbol{u}) = u\partial_n v$, and the shape derivative of $\Delta_\Gamma v$ is, by Theorem 7.4,

$$\begin{aligned}(\Delta_\Gamma v)'(\Gamma, \boldsymbol{u}) = \Delta_\Gamma(u\partial_n v) &- u\left(2D_\Gamma \boldsymbol{n} : D_\Gamma^2 v + \nabla_\Gamma \kappa \cdot \nabla_\Gamma v\right) \\ &+ \nabla_\Gamma u \cdot (\kappa \nabla_\Gamma v - 2D_\Gamma \boldsymbol{n} \nabla_\Gamma v).\end{aligned}$$

For a fixed Γ_0, consider any $u \in \mathcal{V}$ and $v \in \mathcal{V}_0$ in order to have $\partial_n v = 0$ in Γ_0. Putting all these ingredients together in (9.6), we obtain

$$\begin{aligned}dJ_v(\Gamma_0, u\boldsymbol{n}_0) = \int_{\Gamma_0} &\big(\Delta_\Gamma u + uI_2\big)\big(\Delta_\Gamma v + vI_2\big) + 2\kappa v\big(D_\Gamma^2 u : D_\Gamma \boldsymbol{n}_0 + uI_3\big) \\ &+ \kappa u\big(2D_\Gamma \boldsymbol{n}_0 : D_\Gamma^2 v + \nabla_\Gamma \kappa \cdot \nabla_\Gamma v\big) - \kappa^2 \nabla_\Gamma u \cdot \nabla_\Gamma v \\ &+ 2\kappa \nabla_\Gamma u \cdot D_\Gamma \boldsymbol{n}_0 \nabla_\Gamma v + \kappa^2 uv\, i_2 - \frac{1}{2}\kappa^2 v \Delta_\Gamma u \\ &- \kappa^2\big(v\Delta_\Gamma u + u\Delta_\Gamma v + 2uv\, I_2\big).\end{aligned}$$

Considering the canonical extension of functions $u, v \in V^2(\Gamma_0) := \{w \in \mathcal{C}^2(\Gamma_0) : w|_{\Gamma_0} = 0\}$, we obtain (omitting technical details) the following simplification of the Newton problem (9.5) for a $\mathcal{C}^3$-surface $\Gamma_0 \subset \mathbb{R}^N$:

$$\text{Find } u \in V^2(\Gamma_0): \quad b_{\Gamma_0}(u, v) = l_{\Gamma_0}(v) \quad \forall v \in V^2(\Gamma_0), \tag{9.7}$$

with

$$l_\Gamma(v) = \int_\Gamma \nabla_\Gamma v \cdot \nabla_\Gamma \kappa + v(\frac{k^3}{2} - \kappa I_2)$$

and

$$b_\Gamma(u, v) = \int_\Gamma \Delta_\Gamma u\, \Delta_\Gamma v + \nabla_\Gamma u \cdot A_\Gamma \nabla_\Gamma v + uv\, c_\Gamma,$$

where A_Γ is a tensor-valued function defined on Γ by

$$A_\Gamma := \left(\frac{3}{2}\kappa^2 - 2I_2\right)\mathrm{I} - 2\kappa D_\Gamma \boldsymbol{n},$$

with I being the identity matrix, and c_Γ is a scalar function on Γ given by

$$c_\Gamma := \frac{\kappa^4}{2} - \frac{5}{2}\kappa^2 I_2 + I_2^2 + 2\kappa I_3 + |\nabla_\Gamma \kappa|^2 - \kappa\Delta_\Gamma \kappa + \Delta_\Gamma I_2 + 2D_\Gamma \boldsymbol{n} : D_\Gamma^2 \kappa.$$

References

[1] Almgren, F., and Taylor, J. E. Optimal geometry in equilibrium and growth. In: Symposium in Honor of Benoit Mandelbrot (Curaçao, 1995). *Fractals* 3 (1995), no. 4, 713–723. MR 1410290.

[2] Almgren, F., Taylor, J. E., and Wang, L. Curvature-driven flows: a variational approach. *SIAM J. Control Optim.* 31 (1993), no. 2, 387–438. MR 1205983.

[3] Baumgart, T., Das, S., Webb, W. W., and Jenkins, J. T. Membrane elasticity in giant vesicles with fluid phase coexistence. *Biophys. J.* 89 (2005), no. 2, 1067–1080.

[4] Bellettini, G., and Paolini, M. Anisotropic motion by mean curvature in the context of Finsler geometry. *Hokkaido Math. J.* 25 (1996), no. 3, 537–566. MR 1416006.

[5] Chicco-Ruiz, A., Morin, P., and Pauletti, M. S. An algorithm for prescribed mean curvature using isogeometric methods. *J. Comput. Phys.* 317 (2016), 185–203. MR 3498811.

[6] Cicuta, P., Keller, S., and Veatch, S. Diffusion of liquid domains in lipid bilayer membranes. *J. Phys. Chem. B* 111 (2007), no. 13, 3328–3331.

[7] Deckelnick, K., Dziuk, G., and Elliott, C. M. Computation of geometric partial differential equations and mean curvature flow. *Acta Numer.* 14 (2005), 139–232. MR 2168343.

[8] Delfour, M., and Zolésio, J.-P. *Shapes and geometries: Metrics, analysis, differential calculus, and optimization.* Second edition. Society for Industrial and Applied Mathematics, 2011. MR 2731611.

[9] Doğan, G., and Nochetto, R. H. First variation of the general curvature-dependent surface energy. *ESAIM Math. Model. Numer. Anal.* 46 (2012), no. 1, 59–79. MR 2846367.

[10] Droske, M., and Bertozzi, A. Higher-order feature-preserving geometric regularization. *SIAM J. Imaging Sci.* 3 (2010), no. 1, 21–51. MR 2609457.

[11] Dziuk, G. Computational parametric Willmore flow. *Numer. Math.* 111 (2008), no. 1, 55–80. MR 2448203.

[12] Evans, L. C. Partial differential equations. Second edition. Graduate Studies in Mathematics, vol. 19. American Mathematical Society, Providence, RI, 2010. MR 2597943.

[13] Giga, Y. Surface evolution equations. Monographs in Mathematics, vol. 99. Birkhäuser Verlag, Basel, 2006. MR 2238463.

[14] Gurtin, M. E. An introduction to continuum mechanics. Mathematics in Science and Engineering, vol. 158. Academic Press, New York-London, 1981. MR 0636255.

[15] Helfrich, W. Elastic properties of lipid bilayers: theory and possible experiments. *Z. Naturforsch. C* 28 (1973), 693–703.

[16] Henrot, A., and Pierre, M. Variation et optimisation de formes: une analyse géométrique. Mathématiques & Applications, vol. 48. Springer, Berlin, 2005. MR 2512810.

[17] Hintermüller, M., and Ring, W. A second order shape optimization approach for image segmentation. *SIAM J. Appl. Math.* 64 (2003/04), no. 2, 442–467. MR 2049659.

[18] Itskov, M. Tensor algebra and tensor analysis for engineers. Fourth edition. Springer, Cham, 2015. MR 3309924.

[19] Jenkins, J. The equations of mechanical equilibrium of a model membrane. *SIAM J. Appl. Math.* 32 (1977), no. 4, 755–764. MR 0441076.

[20] Jenkins, J. Static equilibrium configurations of a model red blood cell. *J. Math. Biol.* 4 (1977), no. 2, 149–169.

[21] Kühnel, W. *Differential geometry: Curves—surfaces—manifolds.* Third edition. Student Mathematical Library, vol. 77. American Mathematical Society, Providence, RI, 2015. MR 3443721.

[22] McFadden, G. B., Wheeler, A. A., Braun, R. J., Coriell, S. R., and Sekerka, R. F. Phase-field models for anisotropic interfaces. *Phys. Rev. E (3)* 48 (1993), no. 3, 2016–2024. MR 1377920.

[23] Qi, L. Eigenvalues and invariants of tensors. *J. Math. Anal. Appl.* 325 (2007), no. 2, 1363–1377. MR 2270090.

[24] Roche, J. R., and Sokołowski, J. Numerical methods for shape identification problems. In: Shape optimization and scientific computations (Warsaw, 1995). *Control Cybernet.* 25 (1996), no. 5, 867–894. MR 1464028.

[25] Rusu, R. E. An algorithm for the elastic flow of surfaces. *Interfaces Free Bound.* 7 (2005), no. 3, 229–239. MR 2171130.
[26] Seifert, U., Berndl, K., and Lipowsky, R. Shape transformations of vesicles: Phase diagram for spontaneous- curvature and bilayer-coupling models. *Phys. Rev. A* 44 (1991), no. 2, 1182–1202.
[27] Sokołowski, J., and Zolésio, J.-P. Introduction to shape optimization: Shape sensitivity analysis. Springer Series in Computational Mathematics, vol. 16. Springer-Verlag, Berlin, 1992. MR 1215733.
[28] Taylor, J. E. II—Mean curvature and weighted mean curvature. *Acta Metall. Mater.* 40 (1992), no. 7, 1475–1485.
[29] Taylor, J. E. Crystalline variational problems. *Bull. Amer. Math. Soc.* 84 (1978), no. 4, 568–588. MR 0493671.
[30] Walker, S. The shapes of things: A practical guide to differential geometry and the shape derivative. Society for Industrial and Applied Mathematics, Philadelphia, 2015. MR 3486164.
[31] Willmore, T. J. *Total curvature in Riemannian geometry.* Ellis Horwood Series in Mathematics and its Applications. Ellis Horwood, Chichester; Halsted Press, New York, 1982. MR 0686105.
[32] Willmore, T. J. *Riemannian geometry.* Oxford Science Publications. The Clarendon Press, Oxford University Press, New York, 1993. MR 1261641.

A. Chicco-Ruiz
Facultad de Ingeniería Química, UNL, CONICET, Santiago del Estero 2829, S3000AOM, Santa Fe, Argentina
`achicco@santafe-conicet.gov.ar`

P. Morin ✉
Facultad de Ingeniería Química, UNL, CONICET, Santiago del Estero 2829, S3000AOM, Santa Fe, Argentina
`pmorin@santafe-conicet.gov.ar`

M. S. Pauletti
Facultad de Ingeniería Química, UNL, CONICET, Santiago del Estero 2829, S3000AOM, Santa Fe, Argentina
`pauletti@santafe-conicet.gov.ar`

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