The shape derivative of the Gauss curvature∗

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Abstract

We introduce new results about the shape derivatives of scalar- and vector-valued functions. They extend the results from [8] to more general surface energies. In [8] 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 introduce a new scheme of Newton-type to approximate a minimizer of a shape functional. It is a mathematically sound generalization of the method presented in [5]. We finally find the particular formulas for the first and second order shape derivative of the area and the Willmore functional, which are necessary for the Newton-type method mentioned above.

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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

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energy occurs through surfaces include the minimal surface problem, the study of the shape of droplets (surface tension), image segmentation and shape of biomembranes, to name a few. In the language of the shape derivative theory [22, 7, 25], these energies are called shape functionals. This theory provides a solid mathematical framework to pose and solve minimization problems for such functionals.

For most of the problems of interest, the energy (shape functional) can be cast as \( \int_{\Gamma} F(\text{"geometrical quantities"}) \), where “geometrical quantities” stands for quantities such as the normal \( \mathbf{n} \), the mean curvature \( \kappa \), the Gauss curvature \( \kappa_g \), or in general any quantity that is well defined for a surface \( \Gamma \) as a geometric object, i.e., independent of the parametrization. For example, \( F = 1 \) in the case of minimal surface, \( F = F(x, \mathbf{n}) \) is used in the modeling of crystals [2, 1, 24, 23] in materials science. The Willmore functional corresponds to \( F = \frac{1}{2}\kappa^2 \) [27]—where \( \kappa \) 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 [13, 16, 15, 21]. The modified form of the Willmore functional, which corresponds to \( F = g(x)\kappa^2 \), is applied to model biomembranes 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 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 [7, 25] among other references. Particular cases of \( F = F(x, \mathbf{n}) \) are derived in [4, 18, 23]. The shape derivative of the mean curvature or particular cases of \( F = F(\kappa) \) can also be found in [26, 14, 20, 10, 9, 8, 25], where the shape derivative is computed from scratch; some using parametrizations, others in a more coordinate-free setting using the signed 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 [8], where Doğan and Nochetto propose a formula for the shape derivative of a functional of the form \( F = F(x, \mathbf{n}, \kappa) \), that relies on knowing the shape derivatives of \( \mathbf{n} \) and \( \kappa \). 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 is to find such a formula when \( F \) also depends on the Gauss curvature \( \kappa_g \) which, as far as we know, has not been provided elsewhere. In fact, we let \( F \) also depend on differential operators of basic geometric quantities such as \( \nabla\kappa \) or \( \Delta\kappa \). These are important when second order shape derivatives are necessary in Newton-type methods for minimizing functionals.

Our new results (Section 8) 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, provides a formula for the shape derivative of higher order tangential derivatives of geometrical quantities. In particular we give a nice formula for the shape derivative of the gaussian curvature and extend the results of [8] to more generals integrands.

These results are also instrumental to develop a relevant numerical method in applied
problems. More precisely, we introduce a new scheme of the Newton-type to find a minimizer of a surface shape functional. It is a mathematically sound generalization of the method used in [5].

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 through integrals over the domain. In Section 5 we motivate and introduce the concept of shape derivative of functions involved in the definition of shape functionals through integrals over the boundaries of domains. In Section 6 we explore the relationship between the shape derivative of domain functions and the classical derivative operators. In Section 7 we explore the relationship between the shape derivative of boundary functions and the tangential derivative operators. These last sections set the foundations for Section 8 where the shape derivatives of the tangential derivatives of geometric quantities are obtained. We end with Sections 9 and 10 where we apply the results to obtain 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 Willmore functional.

2 Preliminaries

2.1 General concepts

Our notation follows closely that of [7, 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 \( \mathbb{R}^N \) can be thought of as a reasonable subset of a boundary in \( \mathbb{R}^N \). If a boundary \( \Gamma \) is smooth, we denote the normal vector field by \( \mathbf{n} \) and assume that it points outward of \( \Omega \). The principal curvatures, denoted by \( \kappa_1, \ldots, \kappa_{N-1} \), are the eigenvalues of the second fundamental form of \( \Gamma \), which are all real. The mean curvature \( \kappa \) and Gaussian curvature \( \kappa_g \) are

\[
\kappa = \sum_{i=1}^{N-1} \kappa_i \quad \text{and} \quad \kappa_g = \prod_{i=1}^{N-1} \kappa_i. \tag{2.1}
\]

We will obtain analogous and more useful definitions of \( \kappa \) and \( \kappa_g \) using tangential derivatives of the normal; see (2.11) and (2.12) for \( N = 3 \), and Section 9 for any dimension, where we introduce the geometric invariants of a surface, following Definition 3.46 of [17].

In the scope of this work a tensor \( S \) is a bounded, linear operator from a normed vector space \( \mathbb{V} \) to itself. The set of tensors is denoted by \( \text{Lin}(\mathbb{V}) \). If \( \text{dim}(\mathbb{V}) = N \), \( S \) can be represented by an \( N \times N \) matrix \( S_{ij} \). We will mainly consider \( \mathbb{V} = \mathbb{R}^N \).

For a vector space with a scalar product, the tensor product of two vectors \( \mathbf{u} \) and \( \mathbf{v} \) is the tensor \( \mathbf{u} \otimes \mathbf{v} \) which satisfies \( (\mathbf{u} \otimes \mathbf{v}) \mathbf{w} = (\mathbf{v} \cdot \mathbf{w}) \mathbf{u} \). The trace of a tensor \( S \) is \( \text{tr}(S) = \sum_i S \mathbf{e}_i \cdot \mathbf{e}_i \), with \( \{ \mathbf{e}_i \} \) any orthonormal basis of \( \mathbb{V} \). The trace of a tensor \( \mathbf{u} \otimes \mathbf{v} \) is \( \text{tr}(\mathbf{u} \otimes \mathbf{v}) = \mathbf{u} \cdot \mathbf{v} \).

The scalar product of tensors \( S \) and \( T \) is given by \( S : T = \text{tr}(S^T T) \), where \( S^T \) is the
transpose of $S$, which satisfies $S\mathbf{u} \cdot \mathbf{v} = \mathbf{u} \cdot S^T \mathbf{v}$, and the tensor norm is $|S| = \sqrt{S : S}$. From [12, Ch. I] we have the following properties:

**Lemma 1** (Tensor Properties). For vectors $\mathbf{u}, \mathbf{v}, \mathbf{a}, \mathbf{b} \in \mathbb{V}$, and tensors $S, T, P \in \text{Lin}(\mathbb{V})$, we have:

- $S(\mathbf{u} \otimes \mathbf{v}) = S\mathbf{u} \otimes \mathbf{v}$ and $(\mathbf{u} \otimes \mathbf{v})S = \mathbf{u} \otimes S^T \mathbf{v}$,
- $I : S = \text{tr}(S)$,
- $ST : P = P : ST^T = T : S^TP$,
- $S : \mathbf{u} \otimes \mathbf{v} = \mathbf{u} \cdot Sv$,
- $(\mathbf{a} \otimes \mathbf{b}) : (\mathbf{u} \otimes \mathbf{v}) = (\mathbf{a} \cdot \mathbf{u})(\mathbf{b} \cdot \mathbf{v})$,
- $S : T = S : T^T = \frac{1}{2}S : (T + T^T)$ if $S$ is symmetric.

### 2.2 The signed distance function

For a given domain $\Omega \subset \mathbb{R}^N$, the signed distance function $b = b(\Omega) : \mathbb{R}^N \to \mathbb{R}$ is given by $b(\Omega)(x) = d_\Omega(x) - d_{\mathbb{R}^N \setminus \Omega}(x)$, where $d_\Omega(x) = \inf_{y \in \Omega} |y - x|$. If $\Omega$ is of class $C^{1,1}$ (see Definitions 3.1 and 3.2 in [7, Ch. 2]) then for each $x \in \Gamma = \partial \Omega$ there exists a neighborhood $W(x)$ such that $b \in C^{1,1}(W(x))$, $|\nabla b|^2 = 1$ in $W(x)$ and $\nabla b = \mathbf{n} \circ p$, where $\mathbf{n}$ is the unit normal vector field of $\Gamma$ and $p = p_r$ is the projection onto $\Gamma$ which is well defined for $y \in W(x)$ as $p(y) = \arg \min_{z \in \Gamma} |z - y|$ (see Theorem 8.5 of [7, Ch. 7]).

Moreover, if $\Omega$ is a $C^2$ domain with compact boundary $\Gamma$ then there exists a tubular neighborhood $S_h(\Gamma)$ such that $b \in C^2(S_h(\Gamma))$ ([7, Ch. 9, p. 492]), and $\Gamma$ is a $C^2$-manifold of dimension $N - 1$. Therefore, $\nabla b$ is a $C^1$ extension for $\mathbf{n}(\Gamma)$ which satisfies

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

This Eikonal equation readily implies

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

Also, if $\Omega$ is $C^3$, we can differentiate (2.3) to obtain

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

where we have used the product rule formula $\text{div}(S^T \mathbf{v}) = S : \nabla \mathbf{v} + \mathbf{v} \cdot \text{div} S$ where $S$ and $\mathbf{v}$ are tensor and vector valued differentiable functions, respectively, with $S = D^2 b$ and $\mathbf{v} = \nabla b$ (see [12], page 30). The divergence $\text{div} S$ of a tensor valued function is a vector which satisfies $\text{div} S \cdot \mathbf{e} = \text{div}(S^T \mathbf{e})$ for any vector $\mathbf{e}$.

Applying the well known identity [12, p. 32]

$$\text{div}(D\mathbf{v}^T) = \nabla(\text{div} \mathbf{v}), \tag{2.5}$$
to $\mathbf{v} = \nabla b$ we can write (2.4) as follows:
\[
\nabla \Delta b \cdot \nabla b = -|D^2b|^2. \tag{2.6}
\]

Since $\mathbf{n}(\Gamma) = \nabla b|_{\Gamma}$, we can obtain from $b$ more geometric information about $\Gamma$. Indeed, the $N$ eigenvalues of $D^2b|_{\Gamma}$ are the principal curvatures $\kappa_1, \kappa_2, \ldots, \kappa_{N-1}$ of $\Gamma$ and zero [7, Ch. 9, p. 500]. The mean curvature of $\Gamma$, given by (2.1), can also be obtained as $\kappa = \text{tr} D^2b = \Delta b$ (on $\Gamma$). Also, $|D^2b|^2 = \text{tr}(D^2b)^2 = \sum \kappa_i^2$, the sum of the square of the principal curvatures so that the Gaussian curvature is $\kappa_g = \frac{1}{2}[(\Delta b)^2 - |D^2b|^2]$; 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 $\Gamma$, so that the equality holds on $\Gamma$. Moreover, from (2.6) we obtain that
\[
\frac{\partial \Delta b}{\partial n} = -\sum \kappa_i^2,
\]
and with a slight abuse of notation we may say that $\frac{\partial b}{\partial n} = -\sum \kappa_i^2$.

The projection of a point $x \in S_h(\Gamma)$ onto $\Gamma$ is given by [7, Ch. 9, p. 492]
\[
p(x) = x - b(x) \nabla b(x), \tag{2.7}
\]
and also, for any $x \in S_h(\Gamma)$, the orthogonal projection operator of a vector of $\mathbb{R}^N$ onto the tangent plane $T_{p(x)}(\Gamma)$, for $\Gamma \in C^1$, is given by $P(x) = I - \nabla b(x) \otimes \nabla b(x)$. Note that the tensor $P(x)$ is symmetric and
\[
P = I - n \otimes n \quad \text{on } \Gamma. \tag{2.8}
\]

It will be useful to know that the Jacobian of the projection vector field $p(x)$ is given, for $\Gamma \in C^2$, by
\[
Dp(x) = P(x) - b(x)D^2b(x) \tag{2.9}
\]
and satisfies $Dp|_{\Gamma} = P$ because $b = 0$ on $\Gamma$.

### 2.3 Elements of tangential calculus

Following [7, Ch. 9, Sec. 5] we will introduce some basic elements of differential calculus on a $C^1$-submanifold of codimension 1 denoted by $\Gamma$. This approach avoids local bases and coordinates by using intrinsic tangential derivatives. All proofs can be found in the cited book, except for Lemmas 4 and 6 which are proved below.

**Definition 2 (Tangential Derivatives).** Assume that $\Gamma \subset \partial \Omega$ and there exists a tubular neighborhood $S_h(\Gamma)$ such that $b = b(\Omega) \in C^1(S_h(\Gamma))$. For a scalar field $f \in C^1(\Gamma)$ and a vector field $\mathbf{w} \in C^1(\Gamma, \mathbb{R}^N)$ we define the **tangential derivative operators** as
\[
\nabla_T f := (I - n \otimes n) \nabla F; \quad D_T \mathbf{w} := DW - DW n \otimes n; \quad \text{div}_T \mathbf{w} := \text{div} W - DW n \cdot n,
\]
where $F$ and $W$ are $C^1$-extensions to a neighborhood of $\Gamma$ of the functions $f$ and $\mathbf{w}$, respectively.

For a scalar function $f \in C^2(\Gamma)$, the second order tangential derivative is given by $D^2_T f = D_T(\nabla_T f)$, which is not a symmetric tensor, and the **Laplace-Beltrami operator** (or tangential laplacian) is given by $\Delta_T f = \text{div}_T \nabla_T f$. 

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Using the orthogonal projection operator $P$ given by (2.8), we can write

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

As it was proved in the cited book [7], these definitions are intrinsic, that is, they do not depend on the chosen extensions of $f$ and $w$ outside $\Gamma$. Among all extensions of $f$, there is one, for $\Gamma \in C^2$, that simplifies the calculation of $\nabla_{\Gamma} f$. That extension is $f \circ p$, where $p$ is the projection given by (2.7), and we call it the canonical extension. The following properties of the canonical extensions are proved in [7, Ch. 9, Sec. 5.1]

Lemma 3 (Canonical extension). For $\Gamma$, $f$ and $w$ satisfying the assumptions of Definition 3, consider $F = f \circ p$, and $W = w \circ p$, the canonical extensions of $f$ and $w$, respectively, where $p$ is the projection given by (2.7). Then

$$\nabla (f \circ p) = [I - b D^2 b] \nabla_{\Gamma} f \circ p, \quad D (w \circ p) = D_{\Gamma} w \circ p [I - b D^2 b],$$  

$$\text{div} (w \circ p) = [I - b D^2 b] : D_{\Gamma} w \circ p = \text{div}_{\Gamma} w \circ p - b D^2 b : D_{\Gamma} w \circ p.$$  

In particular,

$$\nabla_{\Gamma} f = \nabla (f \circ p)|_{\Gamma}, \quad D_{\Gamma} w = D (w \circ p)|_{\Gamma}, \quad \text{div}_{\Gamma} w = \text{div} (w \circ p)|_{\Gamma}. \quad (2.10)$$  

The tangential divergence of a tensor valued function $S$ is defined as $\text{div}_{\Gamma} S \cdot e = \text{div}_{\Gamma} (S^T e)$, for any vector $e$. The expressions (2.10) of tangential derivatives given by canonical extensions allow us to prove directly the following product rule formulas, already known for classical derivatives [12, p. 30].

Lemma 4 (Product Rule for tangential derivatives). Let $\alpha$, $u$, $v$ and $S$ be smooth fields in $\Gamma$, with $\alpha$ scalar valued, $u$ and $v$ vector valued, and $S$ tensor valued. Then

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

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

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

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

(v) $\text{div}_{\Gamma} (S^T u) = S : D_{\Gamma} u + u \cdot \text{div}_{\Gamma} S.$  

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

It will be very useful for us to write the geometric invariants (see Section [11] of $\Gamma$ in terms of tangential derivatives of the normal vector field $n$. The tensor $-D_{\Gamma} n (x)$ (see [11, Ch. 1.3]) defined from the tangent plane $T_x(\Gamma)$ to itself, is called the Weingarten map and is associated to the second fundamental form of $\Gamma$. Since $n \circ p = \nabla b$, (2.10) implies $D_{\Gamma} n = D (n \circ p)|_{\Gamma} = D^2 b|_{\Gamma}$, so that

$$\kappa = \Delta b|_{\Gamma} = \text{tr} (D^2 b|_{\Gamma}) = \text{tr} (D_{\Gamma} n) = \text{div}_{\Gamma} n, \quad (2.11)$$

and $\sum \kappa_i^2 = |D^2 b|_{\Gamma}^2 = |D_{\Gamma} n|^2$ whence, for $N = 3$,

$$\kappa_g = \frac{1}{2} (\kappa^2 - |D_{\Gamma} n|^2). \quad (2.12)$$
In particular, as we will see in Section 9, any geometric invariant can be written in terms of \( I_p := \text{tr}(D_\Gamma n^p) \).

The Divergence Theorem for surfaces whose proof can be found in (Prop. 15 of [25]) is the following

**Lemma 5** (Tangential Divergence Theorem). If \( \Gamma = \partial \Omega \) is \( C^2 \) and \( w \in C^1(\Gamma, \mathbb{R}^N) \), then

\[
\int_\Gamma \text{div}_\Gamma w = \int_\Gamma \kappa \cdot n,
\]

(2.13)

where \( \kappa \) is the mean curvature of \( \Gamma \) and \( n \) its normal field. If \( \Gamma \subseteq \partial \Omega \), then

\[
\int_\Gamma \text{div}_\Gamma w = \int_\Gamma \kappa \cdot n + \int_{\partial \Gamma} w \cdot n_s,
\]

(2.14)

where \( n_s \) is the outward normal to \( \partial \Gamma \) which is also normal to \( n \).

The following Lemma is new and extends formula (2.5) for tangential derivatives.

**Lemma 6.** If \( \Gamma \) is \( C^3 \) and \( w \in C^3(\Gamma, \mathbb{R}^N) \), we have

\[
\nabla_\Gamma \text{div}_\Gamma w = P \text{div}_\Gamma D_\Gamma w^T - D_\Gamma n D_\Gamma w^T n,
\]

(2.15)

where \( P = I - n \otimes n \) is the orthogonal projection operator given by (2.8).

**Proof.** We use formula (2.10) to write tangential derivatives using the projection function \( p \):

\[
\nabla_\Gamma \text{div}_\Gamma w = \nabla \left( \text{div}_\Gamma (w \circ p) \right) |_\Gamma = \nabla \left( \text{div}(w \circ p) \circ p \right) |_\Gamma.
\]

Then we use successively the chain rule, the derivative of \( p \) given by (2.9) and the property of classical derivatives (2.5):

\[
\nabla_\Gamma \text{div}_\Gamma w = D_p^T |_\Gamma \nabla \text{div}(w \circ p) |_\Gamma = P \nabla \text{div}(w \circ p) |_\Gamma = P \text{div}(D(w \circ p)^T) |_\Gamma.
\]

Note that Lemma 3 implies \( D(w \circ p)^T = D_\Gamma w^T \circ p - b D^2 b (D_\Gamma w^T \circ p) \), and the product rule \( \text{div}(\alpha S) = \alpha \text{div} S + S \nabla \alpha \) implies

\[
\text{div}(D(w \circ p)^T) = \text{div}(D_\Gamma w^T \circ p) - b \text{div}(D^2 b D_\Gamma w^T \circ p) - D^2 b D_\Gamma w^T \circ p \nabla b.
\]

Then, after restricting to \( \Gamma \) we have \( \text{div}(D(w \circ p)^T) |_\Gamma = \text{div}_\Gamma(D_\Gamma w^T) - D_\Gamma n D_\Gamma w^T n \), which implies, from (2.15), the desired result.

Applying Lemma 6 to \( w = n \) we obtain for \( \kappa = \text{div}_\Gamma n \)

\[
\nabla_\Gamma \kappa = \nabla_\Gamma \text{div}_\Gamma n = P \text{div}_\Gamma \nabla_\Gamma n - D_\Gamma n D_\Gamma n^T n = P \Delta_\Gamma n
\]

(2.16)

because \( D_\Gamma n^T n = 0 \) and \( \Delta_\Gamma = \text{div}_\Gamma \nabla_\Gamma \).
3 Shape Functionals and Derivatives

A shape functional is a function \( J : A \to \mathbb{R} \) defined on a set \( A = \mathcal{A}(D) \) of admissible subsets of a hold-all domain \( D \subset \mathbb{R}^N \).

Let the elements of \( A \) be smooth domains and for each \( \Omega \in A \), let \( y(\Omega) \) be a function in \( W(\Omega) \) some Sobolev space over \( \Omega \). Then the shape functional given by \( J(\Omega) = \int_{\Omega} y(\Omega)(x) \, dx = \int_{\Omega} y(\Omega) \) 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 something more involved such as the solution of a PDE in \( \Omega \).

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

3.1 The velocity Method

On a hold-all domain \( D \) (not necessarily bounded), we call an autonomous velocity to a vector field \( v \in V^k(D) := \mathcal{C}_0^k(D, \mathbb{R}^N) \), the set of all \( \mathcal{C}^k \) functions \( f \) such that \( D^\alpha f \) has compact support contained in \( D \), for \( 0 \leq |\alpha| \leq k \); hereafter we assume that \( k \) is a fixed positive integer. A (nonautonomous) velocity field \( V \in C([0, \epsilon], V^k(D)) \), (Theorem 2.16 of [22]) induces a trajectory \( x = x_V \in C^1([0, \epsilon], V^k(D)) \), through the system of ODE

\[
\dot{x}(t) = V(t) \circ x(t), \quad t \in [0, \epsilon], \quad x(0) = \text{id}.
\]

where we use a point to denote derivative respect to the time variable \( t \).

Remark 7 (Initial velocity). We call \( v \) to the velocity field at \( t = 0 \), namely \( v = V(0) \). In the autonomous case, \( V(t) = v \) for any \( t \), with \( v \in V^k(D) \), and the trajectory \( x(t) \) is given by

\[
\dot{x}(t) = v \circ x(t), \quad t \in [0, \epsilon], \quad x(0) = \text{id}.
\]

3.2 Shape Differentiation

Given a velocity field \( V \) and a subset \( S \subset D \), the perturbed set at time \( t \) is given by \( S_t = x(t)(S) \), where \( x(t) \) is the trajectory given by (3.1). For a shape functional \( J : A \to \mathbb{R} \), where \( A \) is a family of admissible sets \( S \) (domains or boundaries), and a velocity field \( V \in C([0, T], V^k(D)) \), the Eulerian semiderivative of \( J \) at \( S \) in the direction \( V \) is given by

\[
dJ(S; V) = \lim_{t \searrow 0} \frac{J(S_t) - J(S)}{t},
\]

whenever the limit exist.
Definition 8 (Shape differentiable). We say that $J$ is shape differentiable at $S$ when the Eulerian semiderivative (3.3) exists for any $V$ in the vector space of velocities $\mathcal{C}([0, T], V^k(D))$, and the functional $V \to dJ(S; V)$ is linear and continuous.

Remark 9 (Hadamard differentiable). By Theorem 3.1 of [7, Ch. 9], if a functional $J$ is shape differentiable then $dJ(S, V)$ depends only on $v := V(0)$ (that is, $J$ is Hadamard differentiable at $S$ in the direction $v$).

Definition 10 (Shape derivative). If $J$ is shape differentiable we call $dJ$ its shape derivative.

Remark 11 (Taylor formula). Given $V \in \mathcal{C}([0, T], V^k(D))$ we can define $S + V$ to be $S_t$ for $t = 1$ provided it is admissible. Then if $J$ is shape differentiable (see [7, Ch. 9]) it follows that $J(S + V) = J(S) + dJ(S; V) + o(|V|)$.

### 3.3 The Structure Theorem

One of the main results about shape derivatives is the (Hadamard-Zolesio) Structure Theorem (Theorem 3.6 of [7, Ch. 9]). It establishes that, if a shape functional $J$ is shape differentiable at the domain $\Omega$ with boundary $\Gamma$, then the only relevant part of the velocity field $V$ in $dJ(\Omega, V)$ is $v_n := V(0) \cdot n|\Gamma$. In other words, if $V(0) \cdot n = 0$ in $\Gamma$, then $dJ(\Omega, V) = 0$. More precisely,

**Theorem 12** (Structure Theorem). Let $\Omega \in \mathcal{A}$ be a domain with $C^{k+1}$-boundary $\Gamma$, $k \geq 0$ integer, and let $J : \mathcal{A} \to \mathbb{R}$ be a shape functional which is shape differentiable at $\Omega$ with respect to $V^k(D)$. Then there exists a functional $g(\Gamma) \in (C^k(\Gamma))^\prime$ (called the shape gradient) such that $dJ(\Omega, V) = \langle g(\Gamma), v_n \rangle_{C^k(\Gamma)}$, where $v_n = V(0) \cdot n$. Moreover, if the gradient $g(\Gamma) \in L^1(\Gamma)$, then $dJ(\Omega, V) = \int_{\Gamma} g(\Gamma) v_n$.

### 4 Shape Derivatives of Domain Functions

In this section and the following, we find specialized formulas for the shape derivatives of domain and boundary functionals. These, in turn, will induce definitions for the shape derivatives of domain and boundary functions.

#### 4.1 Shape differentiation of a domain functional

Consider a velocity field $V \in \mathcal{C}([0, \epsilon], V^k(D))$, $k \geq 1$, with trajectories $x \in \mathcal{C}^1([0, \epsilon], V^k(D))$ satisfying (3.1), and note that the Eulerian semiderivative (3.3) can be written as $dJ(\Omega; V) = \frac{d}{dt} J(\Omega_t)|_{t=0}$, where $\Omega_t = x(t)(\Omega)$ and $\Omega_0 = \Omega$. Then, from a well known change of variables formula [7, Ch. 9, Sec. 4.1], we have

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

where $\gamma(t) := \det Dx(t)$, with $Dx(t)$ denoting derivative with respect to the spatial variable $X$. Note that if $y(\Omega_t) \in W^{r,p}(\Omega_t)$ for each $t$ then $y(\Omega_t) \circ x(t) \in W^{r,p}(\Omega)$ (if $0 \leq r \leq k$). The
following Lemma (Theorem 4.1 in Ch. 9, p. 482 of [7]) provides some insight on the nature of $\dot{\gamma}$.

**Lemma 13** (Time derivative of $\gamma$). If $V \in C([0, \epsilon], V^1(D))$ then $\gamma \in C^1([0, \epsilon], V^1(D))$, and its (time) derivative is given by $\dot{\gamma}(t) = \gamma(t) [\text{div} \, V(t) \circ x(t)]$. In particular, $\dot{\gamma}(0) = \text{div} \, v$, where $v = V(0)$.

In order to motivate the definition of material and shape derivative, consider the following situation. Let $y$ be a domain function which assigns a function $y(\Omega) \in W(\Omega)$ to each domain $\Omega$ in a class $A$ of admissible smooth domains. Suppose that the function $f : [0, \epsilon] \to L^1(\Omega)$ given by $f(t) = y(\Omega_t) \circ x(t)$ is differentiable at $t = 0$ in $L^1(\Omega)$, that is, there exists $\dot{f}(0) \in L^1(\Omega)$ such that $\lim_{t \to 0} \|\frac{f(t) - f(0)}{t} - \dot{f}(0)\|_{L^1(\Omega)} = 0$. Then we can differentiate inside the integral (4.1) to obtain

$$\frac{d}{dt} J(\Omega_t)|_{t=0} = \int_\Omega \dot{f}(0) y(0) + f(0) \dot{y}(0).$$

(4.2)

Finally, using Lemma 13 and that $\gamma(0) = 1$ and $f(0) = y(\Omega)$, we obtain

$$dJ(\Omega, V) = \int_\Omega \dot{y}(0) + y(\Omega) \text{div} \, v,$$

where $v = V(0)$.

### 4.2 Material and shape derivatives

**Definition 14** (Material Derivative (Def. 2.71, p. 98 of [22])). Consider a velocity vector field $V \in C([0, \epsilon], V^k(D))$, with $k \geq 1$, an admissible set $S \subset D$ (domain or boundary) of class $C^k$, and a function $y(S) \in W^{r,p}(S)$, with $r \in (0, k] \cap \mathbb{Z}$. Suppose there exists $y(S_t) \in W^{r,p}(S_t)$ for all $0 < t < \epsilon$, where $S_t = x(t)(S)$ is the perturbation set of $S$ by the trajectories $x(t)$ given by $V$. The **material derivative** of $y(S)$ at $S$ in the direction $V$ is the function $\dot{y}(S, V) \in W^{r-1,p}(S)$, given by

$$\dot{y}(S, V) = \left. \frac{d}{dt} [y(S_t) \circ x(t)] \right|_{t=0} = \lim_{t \to 0} \frac{y(S_t) \circ x(t) - y(S)}{t},$$

(4.4)

whenever the limit exists in the sense of $W^{r-1,p}(S)$. In this case we say that the material derivative of $y(S)$ exists at $S$ in $W^{r-1,p}(S)$ in the direction $V$. We can replace the space $W^{r-p}(S)$ by $C^r(\Omega)$, $1 \leq r \leq k$, obtaining $\dot{y}(S, V) \in C^{r-1}(\Omega)$.

With this definition, the existence of material derivative of $y(\Omega) \in W^{1,1}(\Omega)$ implies the differentiability of $f(t)$ at $t = 0$ in $L^1(\Omega)$, which was the assumption needed for equation (4.2) to hold. Then, for $J(\Omega) = \int_\Omega y(\Omega)$, we have

$$dJ(\Omega, V) = \int_\Omega \dot{y}(\Omega, V) + y(\Omega) \text{div} \, v.$$

(4.5)
Remark 15 (Autonomous dependence). If \( J(\Omega) = \int_{\Omega} y(\Omega) \) is shape differentiable at \( \Omega \) and \( \dot{y}(\Omega, V) \) exists for any velocity \( V \), we obtain from Remark 9 and equation (4.5) that \( \dot{y}(\Omega, V) = \dot{y}(\Omega, v) \), where \( v = V(0) \).

As a particular case, suppose that \( y(\Omega) \) is independent of the geometry, namely: \( y(\Omega) = \phi|_{\Omega} \), with \( \phi \in W^{1,1}(D) \). Then, by the chain rule, \( \dot{y}(\Omega, V) = \nabla \phi \cdot v \), and we have \( dJ(\Omega, V) = \int_{\Omega} \nabla \phi \cdot v + \phi \text{ div } v = \int_{\Omega} \text{div } (\phi v) \). If the boundary \( \Gamma = \partial \Omega \in C^1 \) then, the Divergence Theorem yields \( dJ(\Omega; V) = \int_{\Gamma} \phi \nu_n \, d\Gamma \). This dependence of \( dJ(\Omega, V) \) on \( V \) only through the normal component of \( v \) in \( \Gamma \) was expected by the Structure Theorem.

In the general case, when \( y(\Omega) \in W^{1,1}(\Omega) \) depends on the geometry of \( \Omega \), from (4.5) we can write

\[
dJ(\Omega, V) = \int_{\Omega} [\dot{y}(\Omega, V) - \nabla y(\Omega) \cdot v] + \text{div } (y(\Omega)v) .
\]

Which leads to the following definition of \textit{shape derivative of a domain function}.

Definition 16 (Shape derivative of a domain function). Given a velocity field \( V \in C([0,\epsilon], V^k(D)) \), if there exists the material derivative of \( y(\Omega) \in W^{r,p}(\Omega) \), with \( 1 \leq r \leq k \), then the \textit{domain shape derivative} \( y'(\Omega, V) \in W^{r-1,p}(\Omega) \) is given by

\[
y'(\Omega, V) = \dot{y}(\Omega, V) - \nabla y(\Omega) \cdot v ,
\]

where \( v = V(0) \).

If \( y'(\Omega, V) \in W^{r-1,p}(\Omega) \) exists, then we have

\[
dJ(\Omega; V) = \int_{\Omega} y'(\Omega, V) + \text{div } (y(\Omega)V(0)) = \int_{\Omega} y'(\Omega, V) = \int_{\Gamma} y(\Omega) \nu_n ,
\]

whenever \( \Gamma \) is \( C^1 \).

5 \hspace{0.5cm} \text{Shape derivative of boundary functions}

Consider now a boundary functional of the form \( J(\Gamma) = \int_{\Gamma} z(\Gamma) \, d\Gamma \), where \( \Gamma = \partial \Omega \) is a boundary which is also a \( C^k \)-manifold, and for each admissible \( \Gamma, z(\Gamma) \in W^{r,p}(\Gamma) \), with \( 1 \leq r \leq k \). Below we derive a formula for the shape derivative \( dJ(\Gamma, V) \) analogous to (4.7) which uses the concepts from tangential calculus given in Section 2.3.

5.1 \hspace{0.5cm} \text{Shape differentiation of a boundary functional}

For \( \Gamma_t := x(t)(\Gamma) \), we have that

\[
J(\Gamma_t) = \int_{\Gamma_t} z(\Gamma) \, d\Gamma_t = \int_{\Gamma} [z(\Gamma) \circ x(t)] \omega(t) \, d\Gamma ,
\]

where \( \omega(t) = ||M(Dx(t))n|| = \gamma(t)||Dx(t)^-T n|| \), with \( \gamma(t) = \det Dx(t) \) and \( M(Dx(t)) = \gamma(t)Dx(t)^-T \) is the cofactor matrix of the Jacobian \( Dx(t) \). This well known change of variable formula can be found in Proposition 2.47 of [22, p. 78]. We can also find there a formula for the derivative of \( \omega(t) \) at \( t = 0 \), which we now cite using the notation of tangential divergence.
Lemma 17 (Derivative of \( \omega \) (Lemma 2.49, p. 80, of [22])). The mapping \( t \to \omega(t) \) is differentiable from \([0, \varepsilon]\) into \( C^{k-1}(\Gamma) \), and the derivative at \( t = 0 \) is given by

\[
\dot{\omega}(0) = \text{div}_\Gamma v,
\]

where \( \text{div}_\Gamma v = \text{div} v - Dv n \cdot n \) is the tangential divergence of \( v = V(0) \).

Assuming that the material derivative \( \dot{z}(\Gamma, V) \), given by Definition 14, exists in \( L^1(\Gamma) \), we can differentiate inside the integral in (5.1) and then obtain

\[
dJ(\Gamma, V) = \int_\Gamma \dot{z}(\Gamma, V) + z(\Gamma) \text{div}_\Gamma v.
\]

Using the product rule formula \( \text{div}_\Gamma (zv) = z \text{div}_\Gamma v + v \cdot \nabla_\Gamma z \) (Lemma 4) we can write

\[
dJ(\Gamma, V) = \int_\Gamma [\dot{z}(\Gamma, V) - \nabla_\Gamma z(\Gamma) \cdot v] + \text{div}_\Gamma (z(\Gamma)v).
\]

We are now in position to introduce the concept of shape derivative of a boundary function.

Definition 18 (Shape Derivative of a boundary function). Let \( z \) be a boundary function which satisfies \( z(\Gamma) \in W^{r,p}(\Gamma) \) for all \( \Gamma \) in an admissible set \( A \) of boundaries of class \( C^k \). If the material derivative \( \dot{z}(\Gamma, V) \) exists in \( W^{r-1,p}(\Gamma) \) (Definition 14) for a velocity \( V \in C([0, \varepsilon], V^k(D)) \), then the shape derivative \( z'(\Gamma, V) \in W^{r-1,p}(\Gamma) \) is given by \( z'(\Gamma, V) = \dot{z}(\Gamma, V) - \nabla_\Gamma z(\Gamma) \cdot v \), where \( v = V(0) \).

Note that \( \dot{z}(\Gamma, V) \) and \( z'(\Gamma, V) \) are intrinsic to \( \Gamma \), because they do not depend on any extension of \( z(\Gamma) \) to an open set containing \( \Gamma \). With this notation, for \( J(\Gamma) = \int_\Gamma z(\Gamma) d\Gamma \) we have \( dJ(\Gamma; V) = \int_\Gamma z'(\Gamma, V) + \text{div}_\Gamma (z(\Gamma)v) \).

If \( \Gamma \in C^2 \), then the tangential divergence formula (2.13) of Lemma 5 gives us the expression

\[
dJ(\Gamma; V) = \int_\Gamma z'(\Gamma, V) + \kappa z(\Gamma) v_n, \tag{5.2}
\]

where \( \kappa = \kappa(\Gamma) \) is the mean curvature function on \( \Gamma \), and \( v_n = v \cdot n \).

Remark 19. For a surface \( \Gamma \subset \partial \Omega \), we can consider the space of velocity fields \( V^k(\Omega) = V^k(\Omega) \cap \{ v : v|_{\partial \Omega} = 0 \} \), in order to obtain (5.2) by applying formula (2.13) of Lemma 5.

5.2 Relation between domain and boundary function

Suppose that \( z(\Gamma) \) is the restriction of a domain function \( y(\Omega) \) to its boundary, that is: \( z(\Gamma) = y(\Omega)|_{\Gamma} \), where \( \partial \Omega = \Gamma \) and suppose that \( y(\Omega) \) is shape differentiable at \( \Omega \) in the direction \( V \). The material derivatives of both \( z(\Gamma) \) and \( y(\Omega) \) are the same, as is established in the following Lemma.
Lemma 20 (Proposition 2.75 of [22]). Assume that the material derivative of a domain function \( y(\Omega) \in W^{r,p}(\Omega) \) exists at the domain \( \Omega \) of class \( C^k \) in the direction of a velocity field \( V \in C([0, \varepsilon], V^k(D)) \), and that \( y(\Omega, V) \in W^{r-1,p}(\Omega) \). Then for \( r > \frac{1}{p} + 1 \), there exists the material derivative of \( z(\Gamma) = y(\Omega)|_\Gamma \) at \( \Gamma \) in the direction \( V \), and

\[
\dot{z}(\Gamma, V) = \dot{y}(\Omega, V)|_\Gamma \in W^{r-1,\frac{1}{p}p}(\Omega)
\]

However, the shape derivatives of domain and boundary functions are not generally equal for the same function, as is shown in the next lemma.

Lemma 21 (Domain and boundary function). Consider a domain \( \Omega \) with boundary \( \Gamma \), and functions \( z(\Gamma) \) and \( y(\Omega) \) such that \( z(\Gamma) = y(\Omega)|_\Gamma \). Then, \( z(\Gamma) \) is shape differentiable in \( \Gamma \) at direction \( V \in C([0, \varepsilon], V^k(D)) \) if \( y(\Omega) \) is shape differentiable in \( \Omega \) at direction \( V \), and

\[
z'(\Gamma, V) = y'(\Omega, V)|_\Gamma + \frac{\partial y(\Omega)}{\partial n} v_n, \quad \text{where } v_n = v \cdot n.
\]

Proof. Since \( y(\Omega) \) is an extension to \( \Omega \) of \( z(\Gamma) \), we have \( \nabla_\Gamma z = \nabla y|_\Gamma - \frac{\partial y}{\partial n} n \). Then, using Lemma 20 and comparing Definitions 16 and 18, we obtain the desired result. \( \square \)

Going back to formula (5.2), if \( z(\Gamma) \) admits an extension \( y(\Omega) \), Lemma 21 gives us

\[
dJ(\Gamma; V) = \int_\Gamma y'(\Omega, V)|_\Gamma + \left( \frac{\partial y(\Omega)}{\partial n} + \kappa z(\Gamma) \right) v_n.
\]

6 Properties of shape derivatives of domain functions

We first extend the Definition 16 of domain shape derivative to vector and tensor valued functions.

Definition 22 (Vector and tensor valued domain functions). Consider a vector field \( w(\Omega) \in W^{r,p}(\Omega, \mathbb{R}^N) \) which exists for all admissible domains \( \Omega \in A(D) \). For a given velocity field \( V \), we say that \( w(\Omega) \) is shape differentiable at \( \Omega \) in the direction of \( V \) if there exists the material derivative \( \dot{w}(\Omega, V) = \frac{d}{dt}[w(\Omega_t) \circ x(t)]_{t=0} \in W^{r-1,p}(\Omega, \mathbb{R}^N) \). In that case the (domain) shape derivative belongs to \( W^{r-1,p}(\Omega, \mathbb{R}^N) \) and is given by

\[
w'(\Omega, V) = \dot{w}(\Omega, V) - Dw(\Omega)v,
\]

where \( v = V(0) \). If \( N = 1 \), we consider \( Dw = (\nabla w)^T \).

For a tensor valued function \( A(\Omega) : \Omega \to \text{Lin}(V) \), we say that \( A \) is shape differentiable at \( \Omega \) in the direction of \( V \) if so is the vector valued function \( Ae \), for any vector \( e \in V \). The shape derivative \( A'(\Omega, V) \) is the tensor valued function which satisfies

\[
A'(\Omega, V)e = (Ae)'(\Omega, V) \quad \text{for any } e \in V.
\]

(6.1)

Throughout this paper we consider \( V = \mathbb{R}^N \).
Lemma 23. For a given admissible domain $\Omega \subset \mathbf{D}$ with boundary $\mathcal{C}^k$, $k \geq 2$, a velocity field $V \in C([0, \epsilon], V^k(\mathbf{D}))$ and a shape differentiable function $y(\Omega) \in W^{r,p}(\Omega)$, $1 \leq r \leq k$, $1 \leq p < \infty$, we have the following properties:

1. If the mapping $V \rightarrow y'(\Omega, V)$ is continuous from $C([0, \epsilon], V^k(\mathbf{D}))$ into $W^{r-1,p}(\Omega)$, then $y'(\Omega, V) = y'(\Omega, v)$, where $v = V(0)$ (Proposition 2.86 of [22]).

2. Suppose that $V \rightarrow y'(\Omega, V)$ is continuous from $C([0, \epsilon], V^k(\mathbf{D}))$ into $W^{r-1,p}(\Omega)$. If the velocity fields $V_1$ and $V_2$ are such that $V_1(0) \cdot n = V_2(0) \cdot n$ on $\Gamma = \partial \Omega$, then $y'(\Omega, V_1) = y'(\Omega, V_2)$ (Proposition 2.87 of [22]).

3. If $y(\Omega) = \phi|_{\Omega}$, for $\phi \in W^{r,p}(\mathbf{D})$, then $y$ is shape differentiable in $\Omega$ for any direction $V$, and $y'(\Omega, V) = 0$ (Proposition 2.72 of [22]).

Lemma 24 (Lemma 4 from [14]). Suppose that $y(\Omega) \in H^{\frac{1}{2}+\epsilon}(\Omega)$ satisfies $y(\Omega)|_{\Gamma} = 0$ for all domains $\Omega \in \mathcal{A}$ and that the shape derivative $y'(\Omega; V)$ exists in $H^{\frac{1}{2}+\epsilon}(\Omega)$ for some $\epsilon > 0$. Then, we have

$$y'(\Omega, V)|_{\Gamma} = -\frac{\partial y}{\partial n} v_n$$

(6.2)

where $v_n = v \cdot n$ and $v = V(0)$.

**Proof.** This Lemma is proved in [14]. However, it can be also demonstrated 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 $\dot{z}(\Gamma, V) = 0$ and $\nabla_{\Gamma} z(\Gamma) = 0$, so that $z'(\Gamma, V) = 0$. The claim thus follows from Lemma [21].

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 25. Let $F \in \text{Lin}(V_1, V_2)$, with $V_1$ and $V_2$ two finite dimensional vector or tensor spaces, and let $w(S) \in C^k(S, V_1)$ for any admissible domain or boundary $S \subset \mathbf{D}$ and $k \geq 1$. If $w(S)$ is shape differentiable at $S$ in the direction $V$, then $F \circ w(S) \in C^k(S, V_2)$ is also shape differentiable at $S$ in the direction $V$, and its shape derivative is given by

$$(F \circ w)'(S, V) = F \circ w'(S, V).$$

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

Lemma 26 (Chain rule). Consider two finite dimensional vector or tensor spaces $V_1$ and $V_2$, a function $F \in C^1(V_1, V_2)$ and a domain (or boundary) function $y(S) \in C^1(S, V_1)$, where $S$ is an admissible domain (boundary) in $\mathbf{D} \subset \mathbb{R}^N$ with a $C^1$ boundary. If $y(\Omega)$ is shape differentiable at $\Omega$ in the direction $V$, then the function $F \circ y(\Omega) \in C^1(\Omega, V_2)$ is also shape differentiable at $\Omega$ in the direction $V$, and its shape derivative is given by

$$(F \circ y)'(\Omega, V) = DF \circ y(\Omega) [y'(S, V)].$$
Proof. Since $F$ is differentiable, for every $X \in \mathbb{V}_1$ there exists a linear operator $DF(X) \in \text{Lin}(\mathbb{V}_1, \mathbb{V}_2)$ 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 $DF(X) \in \text{Lin}(\mathbb{V}_1, \mathbb{V}_2)$ to $u \in \mathbb{V}_1$. With this notation, the chain rule applied to $F \circ y$ reads $D(F \circ y)[v] = DF \circ y[Du[v]]$ ($\forall v \in \mathbb{R}^N$), so that from Definition 22.

$(F \circ y)'(\Omega, V) = (F \circ y)'(\Omega, V) - D(F \circ y)[V] = (F \circ y)'(\Omega, V) - DF \circ y[Du[V]]$, in $\Omega$,
with $(F \circ y)'(\Omega, V)$ denoting the material derivative of $F \circ y$. Then we only need to prove the chain rule for the material derivative of $y(\Omega) \in C^1(\Omega, \mathbb{V}_1)$ in the direction $V$, i.e.,

$$(F \circ y)'(\Omega, V) = DF \circ y[y(\Omega, V)].$$

If we recall that $(F \circ y)'(\Omega, V) = \frac{d}{dt}[F \circ y(\Omega_t) \circ x(t)]_{t=0}$, the proof of this last equality is straightforward from usual chain rule applied to the mapping $t \to F \circ (y(\Omega_t) \circ x(t))$. The details are left to the reader.

Remark 27 (Product rule for shape derivatives). The product rules for domain shape derivatives follow directly from Definitions 16 and 22.

The following Lemma allows us to swap shape derivatives with classical derivatives of domain functions. It is worth noting that this is not true for boundary functions and tangential derivatives. This will be discussed in Section 8 where the main results of this article are presented.

Lemma 28 (Mixed shape and classical derivatives). The following results about interchanging classical and shape derivatives are satisfied.

1. If $y(\Omega) \in C^2(\Omega)$ is shape differentiable at $\Omega$ in the direction $V \in C([0, \epsilon], V^k(D))$, $k \geq 2$, then $\nabla y(\Omega) \in C^1(\Omega, \mathbb{R}^N)$ is also shape differentiable at $\Omega$ and

$$(\nabla y)'(\Omega, V) = \nabla y'(\Omega, V).$$

2. If $w(\Omega) \in C^2(\Omega, \mathbb{R}^N)$ is shape differentiable at $\Omega$ in the direction $V \in C([0, \epsilon], V^k(D))$, $k \geq 2$, then $Dw(\Omega) \in C^1(\Omega, \mathbb{R}^{N \times N})$ and $\text{div } w(\Omega) \in C^1(\Omega)$ is also shape differentiable and

$$(Dw)'(\Omega, V) = Dw'(\Omega, V), \quad (\text{div } w)'(\Omega, V) = \text{div } w'(\Omega, V).$$

3. If $y(\Omega) \in C^3(\Omega)$ is shape differentiable at $\Omega$ in the direction $V \in C([0, \epsilon], V^k(D))$, $k \geq 3$, then $\Delta y(\Omega) \in C^1(\Omega)$ is also shape differentiable at $\Omega$ and

$$(\Delta y)'(\Omega, V) = \Delta y'(\Omega, V).$$
Proof. We will prove the first assertion. The other ones are analogous.

First note that

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

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

$$\frac{\partial}{\partial t} \nabla (y(\Omega_t) \circ x(t)) \big|_{t=0} = \frac{\partial}{\partial t} Dx(t)^T \big|_{t=0} \nabla y(\Omega) + \dot{\nabla} y(\Omega, V) \quad (6.3)$$

where we have used that $x(0) = id$, $Dx(0) = I$ and Definition 14, denoting with $\dot{\nabla} y(\Omega, V)$ the material derivative of $\nabla y(\Omega)$.

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

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

so that

$$\frac{\partial}{\partial t} Dx(t)|_{t=0} = Dv \quad \text{pointwise in } D. \quad (6.4)$$

Analogously, the existence of the material derivative $\dot{y}(\Omega, V)$ in $C^1(\Omega)$ 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, V), \quad \text{for } 1 \leq i \leq N,$n

and then

$$\frac{\partial}{\partial t} \nabla (y(\Omega_t) \circ x(t)) \big|_{t=0} = \nabla \dot{y}(\Omega, V) \quad \text{pointwise in } \Omega. \quad (6.5)$$

Replacing with (6.4) and (6.5) in (6.3), we obtain

$$\nabla \dot{y}(\Omega, V) = Dv^T \nabla y(\Omega) + \dot{\nabla} y(\Omega, V).$$

By Definition 16 of shape derivative we have

$$\nabla y'(\Omega, V) = \nabla \dot{y}(\Omega, V) - \nabla (\nabla y(\Omega) \cdot v) = \nabla \dot{y}(\Omega, V) - Dv^T \nabla y(\Omega) - D^2 y(\Omega)^T v$$

$$= \dot{\nabla} y(\Omega, V) - D^2 y(\Omega)^T v = (\nabla y)'(\Omega, V),$$

where we have used Definition 22 and the fact that $D^2 y(\Omega)^T$ is symmetric because $y(\Omega) \in C^2(\Omega)$.

Shape derivative of the signed distance function

Concerning the shape derivative of the signed distance function $b = b(\Omega)$, we cite [7] and [14]. Since $b|_\Gamma = 0$, we can use Lemma 24 to obtain

$$b'(\Omega, V)|_\Gamma = -v \cdot n = -v_n, \quad (6.6)$$

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where we have used that \( \frac{\partial b}{\partial n} = \nabla b \cdot \nabla b |_\Gamma = 1 \). Note that this is the shape derivative of \( b(\Omega) \) only on \( \Gamma \).

In order to find the shape derivative of \( w(\Omega) := \nabla b(\Omega) \), we derive the Eikonal Equation (2.2) to obtain \( (\nabla b)'(\Omega, V) \cdot \nabla b = 0 \). This means that, when restricted to \( \Gamma \), \((\nabla b)'(\Omega, V)\) is orthogonal to the normal vector field \( n \). But also from Lemma 28 \( (\nabla b)'(\Omega, V) = \nabla b'(\Omega, V) \) so that \((\nabla b)'(\Omega, V)|_\Gamma = \nabla \Gamma(b'(\Omega, V)) = \nabla \Gamma b'(\Omega, V) \).

Finally, using formula (6.6), we obtain \( (\nabla b)'(\Omega, V)|_\Gamma = -\nabla \Gamma v_n \), where \( v_n = v \cdot n \). (6.7)

This identity will be used later to obtain the shape derivative of the boundary (vector valued) function \( n \).

7 Properties of the shape derivative of boundary functions

We first extend Definition 18 to vector and tensor valued functions defined on a boundary \( \Gamma = \partial \Omega \). To consider shape derivatives in a fixed surface \( \Gamma \subseteq \partial \Omega \), we consider the space of velocities \( V_\Gamma(D) \) instead of \( V(D) \) as it was done in Remark 19.

Definition 29 (Vector Boundary Functions). Consider a vector field \( w(\Gamma) \in W^{r,p}(\Gamma, \mathbb{R}^N) \) which exists for all admissible domains \( \Omega \subset D \) with boundary \( \Gamma \in C^k \), with \( 1 \leq r \leq k \). For a given velocity field \( V \in C([0, \varepsilon], V^k(D)) \), we say that \( w(\Gamma) \) is shape differentiable in \( \Gamma \) in the direction of \( V \) if there exists the material derivative \( \dot{w}(\Gamma, V) = \frac{d}{dt}[w(\Gamma_t) \circ x(t)]|_{t=0} \) in \( W^{r-1,p}(\Gamma, \mathbb{R}^N) \). In that case the (boundary) shape derivative belongs to \( W^{r-1,p}(\Gamma, \mathbb{R}^N) \) and is given by

\[
\dot{w}(\Gamma, V) = \frac{d}{dt}[w(\Gamma_t) \circ x(t)]|_{t=0} = \nabla \dot{w} = \frac{d}{dt}[w(\Gamma_t) \circ x(t)]|_{t=0}.
\]

where \( v = V(0) \).

Analogously to tensor valued domain functions, for a tensor valued boundary function \( A(\Gamma) : \Gamma \to \mathbb{R}^{N \times N} \) the shape derivative \( A'(\Gamma, V) \) is the tensor valued function which satisfies (6.1), with \( \Omega \) replaced by \( \Gamma \).

We now extend Lemma 21 to vector valued functions. The proof is straightforward from the fact that \( w(\Omega, V) \cdot e = (w \cdot e)'(\Omega, V) \) for any fixed vector \( e \), because \( w \to w \cdot e \) is a linear transformation.

Lemma 30 (Extension). Let \( \Omega \) be a domain with a \( C^1 \) boundary \( \Gamma \). If the boundary function \( w(\Gamma) \in C^1(\Gamma, \mathbb{R}^N) \) admits an extension \( W(\Omega) \) which is shape differentiable at \( \Omega \) in the direction \( V \in C([0, \varepsilon], V^k(D)) \), \( k \geq 1 \), then the shape derivative of \( w(\Gamma) \) in \( \Gamma \) at \( V \) is given by

\[
w'(\Gamma, V) = W'(\Omega, V)|_{\Gamma} + DW n v_n.
\]

Remark 31 (Comparison with Lemma 23). The first two assertions of Lemma 23 are also valid for boundary functions (the proofs can be found in [22]). Instead of the third assertion, we have the following one, which is an immediate consequence of Lemma 21.

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Lemma 32 (Shape derivative of \( \phi|_\Gamma \)). If \( z(\Gamma) = \phi|_\Gamma \), for \( \phi \in W^{r,p}(D) \), \( r - \frac{1}{p} \geq 1 \), then \( z \) is shape differentiable in \( \Gamma \) for any direction \( V \), and \( y'(\Gamma, V) = \frac{\partial \phi}{\partial n}v_n \).

The shape derivatives of \( n \) and \( \kappa \)

Since the normal vector field \( n \) at \( \Gamma \) has the gradient of the signed distance function \( b(\Omega) \) as an extension, we can use the results of Section 7.1 to obtain the shape derivative of \( n \).

Lemma 33 (Shape derivative of \( n \)). Let \( \Gamma \) be the boundary of a \( C^2 \)-domain \( \Omega \) and let \( n(\Gamma) \) be the unit normal vector field of \( \Gamma \). Then \( n \) is shape differentiable and \( n'(\Gamma, V) = -\nabla_{\Gamma}v_n \), where \( v_n = V(0) \cdot n \), for all \( V \in C([0, \epsilon], V^1(D)) \).

Proof. Since \( n(\Gamma) = \nabla b|_\Gamma \), where \( b \) is the signed distance function of \( \Omega \), we use Lemma 30 to obtain

\[
n'(\Gamma, V) = (\nabla b)'(\Omega, V)|_\Gamma + D^2b|_\Gamma n \cdot v_n.
\]

Since by equation (2.3) \( D^2b \nabla b = 0 \) everywhere, the second term vanishes and (6.7) yields the desired result. \( \square \)

Concerning the mean curvature \( \kappa = \kappa(\Gamma) \) given by (2.1), we recall that \( \Delta b(\Omega) = \text{tr}(D^2b) \) is an extension of \( \kappa \) to a tubular neighborhood of \( \Gamma \) (see Section 2.2). Then, on the one hand, the shape derivative of \( \kappa \) can be obtained using Lemma 21, as we will do in the proof of the next Lemma. On the other hand, since \( D^2b|_\Gamma = D_{\Gamma}n \), we can also express the mean curvature using tangential derivatives, as \( \kappa = \text{div}_{\Gamma}n \). Then, Corollary 36 gives us quickly the same formula for the shape derivative of \( \kappa \).

Lemma 34 (Shape derivative of \( \kappa \)). If \( \kappa \) is the mean curvature of \( \Gamma \), the boundary of a \( C^3 \) domain \( \Omega \), then \( \kappa \) is shape differentiable in \( \Gamma \) and

\[
\kappa'(\Gamma, V) = -\Delta_{\Gamma}v_n - |D_{\Gamma}n|^2v_n,
\]

where \( v_n = V(0) \cdot n \), \( |D_{\Gamma}n|^2 = D_{\Gamma}n : D_{\Gamma}n = \text{tr}(D^2n^2) \) and \( \Delta_{\Gamma}f = \text{div}_{\Gamma}\nabla_{\Gamma}f \) is the Laplace-Beltrami operator of \( f \).

Proof. Since \( \kappa = \Delta b|_\Gamma \), by Lemma 21

\[
\kappa'(\Gamma, V) = (\Delta b)'(\Omega, V)|_\Gamma + (\nabla \Delta b \cdot \nabla b)|_\Gamma v_n.
\]

The second term is equal to \(-|D_{\Gamma}n|^2v_n\) using equation (2.6), and the fact that \( D_{\Gamma}n = D^2b|_\Gamma \). For the first term, we use Lemma 28 and the definition of tangential divergence (2.10) to obtain

\[
(\Delta b)'(\Omega, V) = \text{div}(\nabla b)'(\Omega, V) = \text{div}_{\Gamma}(\nabla b)'(\Omega, V) + D^2b|_\Gamma n \cdot n
\]

\[
= -\text{div}_{\Gamma}(\nabla_{\Gamma}v_n) = -\Delta_{\Gamma}v_n,
\]

where we have used (6.7) and the fact that \( D^2b|_\Gamma n = D^2b|_\Gamma \nabla b|_\Gamma = (D^2b \nabla b)|_\Gamma = 0 \). \( \square \)
8 The 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 will find the shape derivatives of boundary functions of the form $\nabla_\Gamma z$, $D_\Gamma w$, $\text{div}_\Gamma w$ and $\Delta_\Gamma z$, when $z(\Gamma)$ and $w(\Gamma)$ are shape differentiable boundary functions, scalar and vector valued, respectively. Examples of important applications will be presented in the two subsequent sections.

It is worth noting the difference with Lemma 28 where we established that standard differential operators commute with the shape derivative of domain functions.

**Theorem 35** (Shape derivative of surface derivatives). For any admissible boundary $\Gamma = \partial \Omega$, where $\Omega$ is a $C^2$ domain in $D \subset \mathbb{R}^N$, consider a real function $z(\Gamma) \in C^2(\Gamma)$. If $z$ is shape differentiable at $\Gamma$ in the direction $\mathbf{V} \in C([0, \epsilon], V^2(D))$, then $\nabla_\Gamma z$ is shape differentiable at $\Gamma$ in the direction $\mathbf{V}$, and

$$
(\nabla_\Gamma z)'(\Gamma, \mathbf{V}) = \nabla_\Gamma z'(\Gamma, \mathbf{V}) + (n \otimes \nabla_\Gamma v_n - v_n D_\Gamma n) \nabla_\Gamma z,
$$

where $v_n = \mathbf{V}(0) \cdot n$.

Before proceeding to the proof it is worth noticing the differences with Lemma 28 where we have shown that the shape derivative of domain integrands commutes with the space derivatives.

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

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

because $\partial_n y = \frac{\partial y}{\partial n} = \nabla y \cdot n$. Then $\Phi(\Omega) := \nabla y - (\nabla y \cdot \nabla b) \nabla b$ is an extension to $\Omega$ of $\nabla_\Gamma z(\Gamma)$. Due to Lemma 30 these shape derivatives satisfy

$$
(\nabla_\Gamma z)'(\Gamma, \mathbf{V}) = \Phi'(\Omega, \mathbf{V})|_\Gamma + D\Phi(\Omega)|_\Gamma n v_n.
$$

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

$$
\Phi'(\Omega, \mathbf{V}) = (\nabla y)'(\Omega, \mathbf{V}) - (\nabla y)'(\Omega, \mathbf{V}) \cdot \nabla b \nabla b - \nabla y \cdot (\nabla b)'(\Omega, \mathbf{V}) \nabla b - \nabla y \cdot \nabla b (\nabla b)'(\Omega, \mathbf{V})
$$

$$
= (I - \nabla b \otimes \nabla b) \nabla y'(\Omega, \mathbf{V}) - \nabla y \cdot (\nabla b)'(\Omega, \mathbf{V}) \nabla b - \nabla y \cdot \nabla b (\nabla b)'(\Omega, \mathbf{V}),
$$

where we have used Lemma 28 to commute the shape derivative and the gradient of $y$. Repeating the same argument we obtain

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

where we have used $\nabla y(\Omega)|_\Gamma \cdot \nabla_\Gamma v_n = \nabla_\Gamma z \cdot \nabla_\Gamma v_n = (n \otimes \nabla_\Gamma v_n) \nabla_\Gamma z$. From Lemma 21 $y'(\Omega, \mathbf{V})|_\Gamma = z'(\Gamma, \mathbf{V}) - \partial_n y v_n$ and the product rule for tangential derivative gives

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

$$
= \nabla_\Gamma z'(\Gamma, \mathbf{V}) + (n \otimes \nabla_\Gamma v_n) \nabla_\Gamma z - v_n \nabla_\Gamma (\partial_n y).
$$
Then, from (8.2), to complete the proof of (8.1), we need to show that
\[ D\Phi(\Omega)|_\Gamma n - \nabla_\Gamma(\partial_n y) = -D_\Gamma n \nabla_\Gamma z. \] (8.3)

Applying the product rule of classical derivatives to \( \Phi(\Omega) = \nabla y - (\nabla y \cdot \nabla b) \nabla b \), we obtain, using \( n = \nabla b|_\Gamma \),
\[ D\Phi(\Omega)|_\Gamma n = D^2_y|_\Gamma n - (n \otimes \nabla(\nabla y \cdot \nabla b)|_\Gamma) n - \partial_n y D^2 b \nabla b|_\Gamma \]
\[ = D^2_y|_\Gamma n - \partial_n(\nabla y \cdot \nabla b) n, \]
because \( D^2 b \nabla b = 0 \). Besides,
\[ \nabla_\Gamma(\partial_n y) = \nabla(\nabla y \cdot \nabla b)|_\Gamma - \partial_n(\nabla y \cdot \nabla b) n \]
\[ = D^2_y|_\Gamma n - D^2 b \nabla y|_\Gamma - \partial_n(\nabla y \cdot \nabla b) n \]
\[ = D\Phi(\Omega)|_\Gamma n - D_\Gamma n \nabla_\Gamma z, \]
where we have used that \( D^2 b \nabla y|_\Gamma = D_\Gamma n \nabla_\Gamma y = D_\Gamma n \nabla_\Gamma z \). From this equation we obtain (8.3) and the claim follows. \( \square \)

**Corollary 36** (For vector fields). *If the functions \( z(\Gamma) \in C^2(\Gamma) \) and \( w(\Gamma) \in C^2(\Gamma, \mathbb{R}^N) \) are shape differentiable at \( \Gamma \in C^2 \) in the direction \( V \in C([0,\varepsilon], V^2(\mathcal{D})) \), then \( D_\Gamma w \) and \( \text{div}_\Gamma w \) are also shape differentiable at \( \Gamma \) in the direction \( V \) and
\[ (D_\Gamma w)'(\Gamma, V) = D_\Gamma w'(\Gamma, V) + D_\Gamma w'[\nabla_\Gamma v_n \otimes n - v_n D_\Gamma n], \] (8.4)
\[ (\text{div}_\Gamma w)'(\Gamma, V) = \text{div}_\Gamma w'(\Gamma, V) + [n \otimes \nabla_\Gamma v_n - v_n D_\Gamma n] : D_\Gamma w, \] (8.5)
where \( S : T = \text{tr}(S^T T) \) denote the scalar product of tensors.*

*Proof.* In order to obtain (8.4), note that \( D_\Gamma w^T e_i = \nabla_\Gamma w_i \), where \( w_i = w \cdot e_i \), with \( \{e_1, \ldots, e_N\} \) being the canonical basis of \( \mathbb{R}^N \). By definition, the shape derivative of the tensor \( D_\Gamma w^T \) must satisfy
\[ (D_\Gamma w^T)'(\Gamma, V)e_i = (D_\Gamma w^T e_i)'(\Gamma, V) = (\nabla_\Gamma w_i)'(\Gamma, V). \]
Applying (8.1) to \( z(\Gamma) = w_i = w \cdot e_i \), we obtain
\[ (D_\Gamma w^T)'(\Gamma, V)e_i = (\nabla_\Gamma w_i)'(\Gamma, V) \]
\[ = \nabla_\Gamma w_i'(\Gamma, V) + [n \otimes \nabla_\Gamma v_n - v_n D_\Gamma n] \nabla_\Gamma w_i \]
\[ = (D_\Gamma w'(\Gamma, V)^T + [n \otimes \nabla_\Gamma v_n - v_n D_\Gamma n] D_\Gamma w^T)e_i. \]
The linearity of the transpose operator and Lemma 25 yield the desired result.

Finally, we recall that \( (\text{div}_\Gamma w)'(\Gamma, V) = \text{tr}(D_\Gamma w)'(\Gamma, V) \) and \( (a \otimes b) : S = a \cdot S b \). Therefore (8.4) implies
\[ (\text{div}_\Gamma w)'(\Gamma, V) = \text{div}_\Gamma w'(\Gamma, V) + D_\Gamma w \nabla_\Gamma v_n \cdot n - v_n D_\Gamma n : D_\Gamma w, \]
and (8.5) follows. \( \square \)
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 37** (Shape derivative of Laplace-Beltrami). If \( z = z(\Gamma) \in C^3(\Gamma) \) is shape differentiable at a \( C^3 \)-boundary \( \Gamma \) in the direction \( V \in C([0, \varepsilon], V^3(D)) \), then \( \Delta_\Gamma z := \text{div}_\Gamma \nabla_\Gamma z \) is also shape differentiable at \( \Gamma \) in the direction \( V \), and its shape derivative is given by

\[
(\Delta_\Gamma z)'(\Gamma, V) = \Delta_\Gamma z'(\Gamma, V) - 2v_n D_\Gamma n : D_\Gamma^2 z + (\kappa \nabla_\Gamma v_n - 2D_\Gamma n \nabla_\Gamma v_n - v_n \nabla_\Gamma \kappa) \cdot \nabla_\Gamma z
\]

\[
= \Delta_\Gamma z'(\Gamma, V) - v_n (2D_\Gamma n : D_\Gamma^2 z + \nabla_\Gamma \kappa \cdot \nabla_\Gamma z) + \nabla_\Gamma v_n \cdot (\kappa \nabla_\Gamma z - 2D_\Gamma n \nabla_\Gamma z).
\] (8.6)

**Proof.** In order to simplify the calculation, we denote \( M = n \otimes \nabla_\Gamma v_n - v_n D_\Gamma n \). Using successively the formulas for the shape derivative of a tangential divergence (Corollary 36) and for a tangential gradient (Theorem 35), we have

\[
(\Delta_\Gamma z)'(\Gamma, V) = (\text{div}_\Gamma \nabla_\Gamma z)'(\Gamma, V)
= \text{div}_\Gamma ((\nabla_\Gamma z)'(\Gamma, V)) + M : D_\Gamma \nabla_\Gamma z
= \text{div}_\Gamma [\nabla_\Gamma z'(\Gamma, V) + M \nabla_\Gamma z] + M : D_\Gamma^2 z
= \Delta_\Gamma z'(\Gamma, V) + \text{div}_\Gamma (M \nabla_\Gamma z) + M : D_\Gamma^2 z.
\]

Using the product rule (v) of Lemma 4 we obtain

\[
(\Delta_\Gamma z)'(\Gamma, V) = \Delta_\Gamma z'(\Gamma, V) + M^T : D_\Gamma^2 z + \text{div}_\Gamma M^T : \nabla_\Gamma z + M : D_\Gamma^2 z
= \Delta_\Gamma z'(\Gamma, V) + (M + M^T) : D_\Gamma^2 z + \text{div}_\Gamma M^T : \nabla_\Gamma z.
\] (8.7)

Since \( D_\Gamma n^T = D_\Gamma n \), the second term of the right-hand side reads

\[
M + M^T = n \otimes \nabla_\Gamma v_n + \nabla_\Gamma v_n \otimes n - 2v_n D_\Gamma n.
\]

Using the tensor property \((a \otimes b) : S = a \cdot Sb\) and that \( D_\Gamma^2 z n = 0 \), we obtain

\[
(M + M^T) : D_\Gamma^2 z = n \cdot D_\Gamma^2 z \nabla_\Gamma v_n - 2v_n D_\Gamma n : D_\Gamma^2 z.
\]

Observe that differentiating \( n \cdot \nabla_\Gamma z = 0 \) leads to \( D_\Gamma n^T = -D_\Gamma^2 z \nabla_\Gamma v_n = -D_\Gamma n \nabla_\Gamma v_n \cdot \nabla_\Gamma z \) which implies \( n \cdot D_\Gamma^2 z \nabla_\Gamma v_n = -D_\Gamma n \nabla_\Gamma v_n \cdot \nabla_\Gamma z \). Then

\[
(M + M^T) : D_\Gamma^2 z = -D_\Gamma n \nabla_\Gamma v_n \cdot \nabla_\Gamma z - 2v_n D_\Gamma n : D_\Gamma^2 z.
\] (8.8)

The third term of (8.7) contains \( \text{div}_\Gamma M^T \) which can be computed with the product rules of Lemma 4 to obtain

\[
\text{div}_\Gamma M^T = \text{div}_\Gamma (\nabla_\Gamma v_n \otimes n) - \text{div}_\Gamma (v_n D_\Gamma n)
= \nabla_\Gamma v_n \cdot \text{div}_\Gamma n + D_\Gamma \nabla_\Gamma v_n n - D_\Gamma n \nabla_\Gamma v_n - v_n \text{div}_\Gamma (D_\Gamma n)
= \kappa \nabla_\Gamma v_n - D_\Gamma n \nabla_\Gamma v_n - v_n \Delta_\Gamma n,
\]
where we have used that \( \kappa = \text{div}_\Gamma \mathbf{n} \) and \( D_T \nabla v_n \mathbf{n} = D^2 v_n \mathbf{n} = 0 \). Since \( \Delta_\Gamma \mathbf{n} \cdot \nabla \Gamma z = (P \Delta_\Gamma \mathbf{n}) \cdot \nabla \Gamma z \), where \( P \) is the orthogonal projection to the tangent plane, equation (2.16) yields \((P \Delta_\Gamma \mathbf{n}) = \nabla \kappa \) whence

\[
\text{div}_\Gamma M^T \cdot \nabla \Gamma z = \kappa \nabla \Gamma v_n \cdot \nabla \Gamma z - D_T \mathbf{n} \nabla \Gamma v_n \cdot \nabla \Gamma z - v_n \nabla \kappa \cdot \nabla \Gamma z. \tag{8.9}
\]

Finally we add equations (8.8) and (8.9) and replace in (8.7) to obtain

\[
(\Delta_\Gamma z)'(\Gamma, \mathbf{V}) = \Delta_\Gamma z'(\Gamma, \mathbf{V}) - 2D_T \mathbf{n} \nabla \Gamma v_n \cdot \nabla \Gamma z - 2v_n D_T : D^2 \Gamma z + \kappa \nabla \Gamma v_n \cdot \nabla \Gamma z - v_n \nabla \kappa \cdot \nabla \Gamma z,
\]

which completes the proof.

\[\square\]

**Corollary 38** (Shape derivative of the first fundamental form). For a \( C^3 \) surface \( \Gamma \) and a smooth velocity field \( \mathbf{V} \), the shape derivatives of the mean curvature \( \kappa = \text{div}_\Gamma \mathbf{n} \) and the tensor \( D_T \mathbf{n} \) at \( \mathbf{V} \) are given by

\[
\kappa'(\Gamma, \mathbf{V}) = -\Delta_\Gamma v_n - |D_T \mathbf{n}|^2 v_n, \tag{8.10}
\]

and

\[
(D_T \mathbf{n})'(\Gamma, \mathbf{V}) = -D^2_\Gamma v_n + D_T \mathbf{n} \nabla \Gamma v_n \otimes \mathbf{n} - v_n D_T \mathbf{n}^2. \tag{8.11}
\]

**Proof.** Since, by Lemma 33 \( \mathbf{n}'(\Gamma, \mathbf{V}) = -\nabla \Gamma v_n \), we will use corollary 36 to obtain the shape derivatives of \( D_T \mathbf{n} \) and \( \kappa = \text{div}_\Gamma \mathbf{n} \). From (8.4) we have

\[
(D_T \mathbf{n})'(\Gamma, \mathbf{V}) = D_T \mathbf{n}'(\Gamma, \mathbf{V}) + D_T \mathbf{n}[\nabla \Gamma v_n \otimes \mathbf{n} - v_n D_T \mathbf{n}]
= -D^2_\Gamma v_n + D_T \mathbf{n} \nabla \Gamma v_n \otimes \mathbf{n} - v_n D_T \mathbf{n}^2,
\]

whence (8.11) holds. To obtain the shape derivative of \( \kappa = \text{div}_\Gamma \mathbf{n} \) we can use equation (8.5) or observe that \( (\text{div}_\Gamma \mathbf{n})'(\Gamma, \mathbf{V}) = \text{tr}(D_T \mathbf{n})'(\Gamma, \mathbf{V}) \) and use (8.11). In both cases, note that \( \text{div}_\Gamma \nabla \Gamma v_n = \text{tr}(D^2_\Gamma v_n) = \Delta_\Gamma v_n \) and \( D_T \mathbf{n} : D_T \mathbf{n} = \text{tr}(D_T \mathbf{n}^2) = |D_T \mathbf{n}|^2 \). Also, since \( D_T \mathbf{n} \mathbf{n} = 0 \), we have

\[
\text{tr}(D_T \mathbf{n} \nabla \Gamma v_n \otimes \mathbf{n}) = \mathbf{n} \otimes \nabla \Gamma v_n : D_T \mathbf{n} = D_T \mathbf{n} \nabla \Gamma v_n \cdot \mathbf{n} = 0.
\]

We have thus obtained \( (\text{div}_\Gamma \mathbf{n})'(\Gamma, \mathbf{V}) = \kappa'(\Gamma, \mathbf{V}) = -\Delta_\Gamma v_n - |D_T \mathbf{n}|^2 v_n. \)

\[\square\]

## 9 Geometric invariants and Gaussian curvature

The geometric invariants of a \( C^2 \)-surface \( \Gamma \) allow us to define its intrinsic properties. They are defined as the geometric invariants of the tensor \( D_T \mathbf{n} \), which, in turn, are the coefficients of its characteristic polynomial \( p(\lambda) \) (see [19]). The geometric invariants of \( \Gamma \), \( i_j(\Gamma) : \Gamma \to \mathbb{R}, j = 1, \ldots, N \), thus satisfy

\[
p(\lambda) = \det(D_T \mathbf{n}(X) - \lambda I) = \lambda^N + i_1 \lambda^{N-1} + i_2 \lambda^{N-2} + \ldots + i_{N-1} \lambda + i_N,
\]

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and can also be expressed using the eigenvalues of the tensor $D_{\Gamma} n$, which are zero and the principal curvatures $\kappa_1, \ldots, \kappa_{N-1}$, namely

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

We can observe from definitions (2.1) that the first invariant $i_1(\Gamma)$ is the mean curvature $\kappa$ and the last nonzero invariant $i_{N-1}(\Gamma)$ is the Gaussian curvature $\kappa_g$. The invariant $i_k(\Gamma)$, for $2 \leq k \leq N-2$, is the so-called $k$-th mean curvature [17, Ch. 3F].

The geometric invariants of $\Gamma$ can also be defined through the functions $I_p(\Gamma) : \Gamma \to \mathbb{R}$, given by

$$I_p(\Gamma) = \text{tr}(D_{\Gamma} n^p), \quad p = 1, \ldots, N-1.$$  

In particular, the first 4 invariants are

$$i_1 = I_1 = \text{div}_{\Gamma} n,$$

$$i_2 = \frac{1}{2!} (I_1^2 - I_2) = \frac{1}{2} (\kappa^2 - |D_{\Gamma} n|^2),$$

$$i_3 = \frac{1}{3!} (I_1^3 - 3I_1 I_2 + 2I_3),$$

$$i_4 = \frac{1}{4!} (I_1^4 - 6I_1^2 I_2 + 3I_2^2 + 8I_1 I_3 - 6I_4).$$

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

**Proposition 39** (Shape derivatives of the invariants). Let $\Gamma$ be a $C^2$-boundary in $\mathbb{R}^N$ and $p$ a positive integer. The shape derivative of the scalar valued boundary function $I_p(\Gamma) := \text{tr}(D_{\Gamma} n^p)$ at $\Gamma$ in the direction $V \in C([0, \epsilon], V^2(D))$ is given by

$$(I_p)'(\Gamma, V) = -p (D_{\Gamma}^2 v_n : D_{\Gamma} n^{p-1} + v_n I_{p+1}),$$

where $v_n = V(0) \cdot n$.

For the proof of this proposition we will need the following Lemma.

**Lemma 40.** Let $A(\Gamma) : \Gamma \to \text{Lin}(V)$ be a symmetric tensor valued function and let $p$ be a positive integer. If $A(\Gamma)$ is shape differentiable at $\Gamma$ in the direction $V$, then the shape derivative of $A^p(\Gamma)$ satisfies

$$(A^p)'(\Gamma, V) : A^j = p \left( A'(\Gamma, V) : A^{j+p-1} \right), \quad (9.1)$$

for any integer $j \geq 0$. 

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Proof. We will proceed by induction. It is trivial to see that equation (9.1) holds for \( p = 1 \) and any integer \( j \geq 0 \).

Assuming that equation (9.1) holds for \( p \geq 1 \) and any \( j \geq 0 \), we want to prove

\[
(A^{p+1})'(\Gamma, V) : A^j = (p + 1) \left( A'(\Gamma, V) : A^{j+p} \right), \quad \text{for any integer } j \geq 0.
\]  

(9.2)

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

\[
(A^{p+1})'(\Gamma, V) : A^j = (A^p)'(\Gamma, V) \cdot A^j + A^p A'(\Gamma, V) : A^j.
\]

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

\[
(A^{p+1})'(\Gamma, V) : A^j = (A^p)'(\Gamma, V) : A^{j+1} + A'(\Gamma, V) : A^{j+p}.
\]

(9.3)

The inductive assumption for \( p \) and \( j + 1 \) implies \( (A^p)'(\Gamma, V) : A^{j+1} = p \left( A'(\Gamma, V) : A^{j+p} \right) \). Using this in equation (9.3), we obtain the desired result (9.2).

Proof of Proposition 39. First note that

\[
I'_p(\Gamma, V) = \text{tr}(D_{\Gamma} n^p)'(\Gamma, V) = (D_{\Gamma} n^p)'(\Gamma, V) : D_{\Gamma} n^0.
\]

Then Lemma 40 with \( j = 0 \) and \( A = D_{\Gamma} n \), which is a symmetric tensor, lead to

\[
I'_p(\Gamma, V) = p \left( D_{\Gamma} n'(\Gamma, V) : D_{\Gamma} n^{p-1} \right).
\]

From formula (8.11) we have that \( (D_{\Gamma} n)'(\Gamma, n) : D_{\Gamma} n^{p-1} = -D_{\Gamma}^2 v_n : D_{\Gamma} n^{p-1} - v_n I_{p+1}(\Gamma) \), where we have used that \( D_{\Gamma} n \nabla_v n \otimes n : D_{\Gamma} n^{p-1} = 0 \) for any integer \( p \geq 1 \). This completes the proof.

We now obtain the shape derivatives of the geometric invariants, which will give 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 \( i_1 = \kappa \):

\[
i'_{1}(\Gamma, v) = I'_1(\Gamma, v) = -D_{\Gamma}^2 v_n : D_{\Gamma} n^0 - v_n I_2 = -\Delta_{\Gamma} v_n - v_n I_2,
\]

which is consistent with the previous result (8.10). Since \( I_2 = i_1^2 - 2i_2 \),

\[
i'_1(\Gamma, v) = -\Delta_{\Gamma} v_n - v_n i_1^2(\Gamma) + 2v_n i_2(\Gamma).
\]

(9.4)

For the second invariant, note that \( I'_2(\Gamma, v) = -2 \left( D_{\Gamma}^2 v_n : D_{\Gamma} n + v_n I_3 \right) \). Since \( i_2 = \frac{1}{2}(I_1^2 - I_2) \), we have

\[
i'_2(\Gamma, V) = I_1 I'_1(\Gamma, V) - \frac{1}{2} I'_2(\Gamma, V) = -I_1 \Delta_{\Gamma} v_n - v_n I_1 I_2 + D_{\Gamma}^2 v_n : D_{\Gamma} n + v_n I_3
\]

\[
= -I_1 \Delta_{\Gamma} v_n + D_{\Gamma}^2 v_n : D_{\Gamma} n + v_n (I_3 - I_1 I_2).
\]

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To obtain a formula only involving the invariants $i_k$, observe that
\[ i_3 := \frac{1}{3!}(I_3 - I_1 I_2 + 2I_3) = \frac{1}{3}(I_3 - I_1 I_2 + i_1 i_2), \]
as can be checked by replacing $i_1$ by $I_1$ and $i_2$ by $\frac{1}{2}(J^2 - I_2)$ in the right-hand side, whence
\[ i_2'(\Gamma, V) = -i_1 \Delta_\Gamma v_n + D^2_\Gamma v_n : D_\Gamma n + v_n(3i_3 - i_1 i_2). \quad (9.5) \]

If $N = 3$, the Gaussian curvature $\kappa_g$ is the second invariant $i_2(\Gamma)$. Then, on the one hand, from (9.4), we have the following expression for the shape derivative of the mean curvature $\kappa$ in terms of $\kappa_g$:
\[ \kappa'(\Gamma, v) = -\Delta_\Gamma v_n - v_n \kappa^2 + 2v_n \kappa \kappa_g. \quad (9.6) \]

On the other hand, since $i_3 = 0$ for $N = 3$, we obtain from (9.5) the following formula for the shape derivative of the Gaussian curvature.

**Theorem 41** (Shape derivative of the Gauss curvature). For a $C^2$-surface $\Gamma$ in $\mathbb{R}^3$, the shape derivative of the Gaussian curvature $\kappa_g$ is given by
\[ \kappa'_g(\Gamma, V) = -\kappa \Delta_\Gamma v_n + D^2_\Gamma v_n : D_\Gamma n - v_n \kappa \kappa_g, \]
where $\kappa$ is the mean or additive curvature, $n$ the normal vector field and $v_n = V(0) \cdot n$.

## 10 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.,
\[ \Gamma_* = \arg \min_{\Gamma \in \mathcal{A}} J(\Gamma) \quad (10.1) \]

For example, given a regular curve $\gamma$ in $\mathbb{R}^3$, a minimal surface $\Gamma$ with boundary $\gamma$ is a solution of (10.1) with $J(\Gamma) = \int_{\Gamma} d\Gamma$, the area functional, and the admissible family $\mathcal{A} = \mathcal{A}(\gamma)$ consisting of all regular 2 dimensional surfaces in $\mathbb{R}^3$ with boundary $\gamma$.

If $J$ is shape differentiable in $\mathcal{A}$, and $\Gamma_*$ is a minimizer, then $dJ(\Gamma_*, v) = 0$ for all $v \in \mathcal{V}$, where $\mathcal{V}$ is a vector space of admissible autonomous velocities, for example $\mathcal{V} = C^k_c(\mathcal{D}, \mathbb{R}^N)$.

We thus focus our attention in the following alternative problem:
\[ \text{Find } \Gamma_* \in \mathcal{A} : \quad dJ(\Gamma_*, v) = 0, \text{ for all } v \in \mathcal{V} := C^k_c(\mathcal{D}, \mathbb{R}^N). \quad (10.2) \]

An interesting scheme to approximate the solutions of (10.2) for surfaces of prescribed constant mean curvature was presented in [5]. There, results from numerical experiments document its performance and fast convergence. The scheme was a variation of the Newton algorithm, which needs the computation of second derivatives of the shape functional. The computations there were tailored to the specific problem of prescribed mean curvature, and based on variational calculus using parametrizations, rather than using shape calculus.
We first observe that, due to the structure Theorem (Theorem 12), Problem (10.2) is equivalent to the following:

Find $\Gamma_\ast \in \mathcal{A}$: $dJ(\Gamma_\ast, v\nabla b_{\Gamma_\ast}) = 0$, for all $v \in \mathcal{V} := \left\{ w \in \mathcal{V} : \frac{\partial w}{\partial n_{\Gamma_\ast}} = 0 \right\}$, (10.3)

where $b_{\Gamma_\ast} := b(\Omega_\ast)$ is the signed distance function corresponding to the domain $\Omega_\ast$ whose boundary is $\Gamma_\ast$, $\mathcal{V} = C_0^k(D)$ and $n_{\ast} = \nabla b_{\Gamma_\ast}$ is the normal vector to $\Gamma_\ast$.

We now present a scheme to approximate the solution of (10.3) using a Newton-type method that generalizes the idea of [5] in at least two ways. First, it uses the language of shape derivatives and secondly, it has the potential to work for a large class of shape functionals, not just the area functional.

We start by defining, for each $\Gamma \in \mathcal{A}$ and $v \in \mathcal{V}$, the functional $J_v(\Gamma) = dJ(\Gamma, v\nabla b_{\Gamma})$, so that the solution $\Gamma_\ast$ satisfies $J_v(\Gamma_\ast) = 0$ for all $v \in \mathcal{V}_\ast$. Assume now that $\Gamma_0 \in \mathcal{A}$ is sufficiently close to the solution $\Gamma_\ast$ so that there exists $u \in \mathcal{V}$ (small, in some sense) such that $\Gamma_\ast := \Gamma_0 + u$, in the sense of Remark 11; this Remark also implies that

$$J_v(\Gamma_\ast) = J_v(\Gamma_0 + u) = J_v(\Gamma_0) + dJ_v(\Gamma_0, u) + o(|u|).$$

(10.4)

The goal of finding $\Gamma_\ast = \Gamma_0 + u$ such that $J_v(\Gamma_0 + u) = 0$ is now switched to a simplified problem of finding $u_0$ such that the linear approximation of $J_v$ around $\Gamma_0$ vanishes at $\Gamma_1 := \Gamma_0 + u_0$, i.e., $J_v(\Gamma_0) + dJ_v(\Gamma_0, u_0) = 0$. Another simplification arises when asking this equality to hold for all $v \in \mathcal{V}_0 := \left\{ w \in \mathcal{V} : \frac{\partial w}{\partial n_{\Gamma_0}} = 0 \right\}$ (instead of $\mathcal{V}_\ast$ or $\mathcal{V}_1$).

Since $dJ_v(\Gamma_0, u_0)$ only depends on the normal component of $u_0$ on $\Gamma_0$, this last problem has multiple solutions, so we restrict it by considering normal velocities of the form $u_0 = u_0n_0$ with $u_0 \in V(\Gamma_0) = C^k(\Gamma_0)$ and $n_0$ the normal vector to $\Gamma_0$, and arrive at the following problem:

Find $u_0 \in V(\Gamma_0)$: $J_v(\Gamma_0) + dJ_v(\Gamma_0, u_0n_0) = 0 \ \forall v \in \mathcal{V}_0$. (10.5)

Finally, define $\Gamma_1 = \Gamma_0 + u_0n_0$. This sets the basis for an iterative method that will be implemented and further investigated in forthcoming articles.

### 10.1 Area and Willmore functionals

We end this paper with the precise form of the second order shape derivatives of two important functionals: the area functional and the Willmore functional.

For a shape differentiable boundary functional $J(\Gamma) = \int_\Gamma z(\Gamma)$, and a function $v \in C^k_b(D)$, the functional $J_v(\Gamma) := dJ(\Gamma, v\nabla b_\Gamma)$ is given by $J_v(\Gamma) = \int_\Gamma z_v(\Gamma) + \kappa z(\Gamma)v$, where $z_v(\Gamma) = z'(\Gamma; v\nabla b_\Gamma)$. Hence [5.2] yields

$$dJ_v(\Gamma, u) = \int_\Gamma z_v'(\Gamma, u)(\kappa'(\Gamma, u)(\kappa(\Gamma)z'(\Gamma, u)) + v + \kappa(\Gamma)z(\Gamma)v' + z_v(\Gamma) + \kappa(\Gamma)z(\Gamma)v)\kappa(\Gamma)u,$$

where $u = u \cdot \nabla b_\Gamma$. 

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Since $v$ does not depend on $\Gamma$, Definitions 14 and 18 yield $v'(\Gamma, u) = \hat{v}(\Gamma, u) - \nabla v \cdot u = \nabla v \cdot u - \nabla u \cdot v = \frac{\partial v}{\partial n} u$. Recall from (8.10) that $\kappa'(\Gamma, u) = -\Delta u - |D_{\Gamma} n|^2$. Using the second invariant $i_2(\Gamma) = \frac{1}{2}(\kappa^2 - |D_{\Gamma} n|^2)$, we can write

$$dJ_v(\Gamma, u) = \int_{\Gamma} 2i_2(\Gamma) z(\Gamma) uv + v(z_u(\Gamma) \kappa(\Gamma) - \Delta u z(\Gamma)) + u \kappa(\Gamma) \left( \frac{\partial v}{\partial n} z(\Gamma) + z_v(\Gamma) \right) + z'_v(\Gamma, u).$$

10.1.2 Willmore functional

For the Willmore functional $J_v(\Gamma) = \int_{\Gamma} d\Gamma$, we have $z(\Gamma) \equiv 1$, $z_v(\Gamma) \equiv 0$ and $z'_v(\Gamma, u) \equiv 0$. Then $J_v(\Gamma) = \int_{\Gamma} \kappa(\Gamma) v$ and by (10.6)

$$dJ_v(\Gamma, u) = \int_{\Gamma} 2i_2(\Gamma) uv + \nabla v \cdot \nabla u + u \frac{\partial v}{\partial n} \kappa(\Gamma),$$

where we have used an integration by parts formula, to replace $\int_{\Gamma} \Delta u v$ by $\int_{\Gamma} \nabla \cdot \nabla u v$.

10.1.1 Area Functional

For the area functional $J(\Gamma) = \int_{\Gamma} d\Gamma$, we have $z(\Gamma) \equiv 1$, $z_v(\Gamma) \equiv 0$ and $z'_v(\Gamma, u) \equiv 0$. Then $J_v(\Gamma) = \int_{\Gamma} \kappa(\Gamma) v$ and by (10.6)

$$dJ_v(\Gamma, u) = \int_{\Gamma} 2i_2(\Gamma) uv + \nabla v \cdot \nabla u + u \frac{\partial v}{\partial n} \kappa(\Gamma),$$

where we have used an integration by parts formula, to replace $\int_{\Gamma} \Delta u v$ by $\int_{\Gamma} \nabla \cdot \nabla u v$.

10.1.2 Willmore functional

For the Willmore functional $J(\Gamma) = \int_{\Gamma} \frac{1}{2} \kappa(\Gamma)^2$ we have $z(\Gamma) = \frac{1}{2} \kappa(\Gamma)^2$ and by the product rule for shape derivatives (Remark 27) $z_v(\Gamma) = z'(\Gamma, v \nabla b) = \kappa(\Gamma) \kappa'(\Gamma, v \nabla b) = -\kappa(\Gamma)(\Delta v + v I_2(\Gamma))$. In order to apply formula (10.6) we need to compute

$$z'(\Gamma, u) = -\kappa'(\Gamma, u)(\Delta v + v I_2(\Gamma)) - \kappa(\Gamma)((\Delta_v)^2(\Gamma, u) + v'(\Gamma, u) I_2(\Gamma) + v I_2(\Gamma, u)).$$

Recall that $\kappa'(\Gamma, u) = -\Delta u - u |D_{\Gamma} n|^2$, $I_2(\Gamma, u) = -2 \left(D^2 u : D_{\Gamma} n + u I_3(\Gamma) \right)$ by Proposition 39, $v'(\Gamma, u) = u \frac{\partial v}{\partial n}$, and that the shape derivative of $\Delta v$ is, by Theorem 37

$$(\Delta v)'(\Gamma, u) = \Delta (u \frac{\partial v}{\partial n}) - u \left(2D_{\Gamma} n : D^2_v v + \nabla \kappa \cdot \nabla v \right) + \nabla u \cdot (\kappa \nabla v - 2D_{\Gamma} n \nabla v).$$

Putting all these ingredients together we obtain

$$dJ_v(\Gamma, u) = \int_{\Gamma} i_2(\Gamma) \kappa(\Gamma)^2 v - \kappa(\Gamma)^2 \Delta u v - 2 \kappa(\Gamma)^2 |D_{\Gamma} n|^2 u v - \frac{\kappa(\Gamma)^2}{2} \Delta u v$$

$$+ \frac{\kappa(\Gamma)^3}{2} u \frac{\partial v}{\partial n} - \kappa(\Gamma)^2 u \Delta v + \left(\Delta u + |D_{\Gamma} n|^2 u \right)(\Delta v + |D_{\Gamma} n|^2 v)$$

$$- \kappa(\Gamma) \Delta u \frac{\partial v}{\partial n} + 2 \kappa(\Gamma) u D^2_{\Gamma} v : D_{\Gamma} n + \kappa(\Gamma) u \nabla \kappa v \cdot \nabla v - \kappa(\Gamma)^2 \nabla v$$

$$+ 2 \kappa(\Gamma) \nabla u \cdot D_{\Gamma} n \nabla v - \kappa(\Gamma) |D_{\Gamma} n|^2 u \frac{\partial v}{\partial n} + 2 \kappa(\Gamma) v D^2_{\Gamma} u : D_{\Gamma} n + 2 \kappa(\Gamma) I_3(\Gamma) u v.$$
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