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Distributed and boundary expressions of first and second order shape derivatives in nonsmooth domains

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ABSTRACT

We study distributed and boundary integral expressions of Eulerian and Fréchet shape derivatives for several classes of nonsmooth domains such as open sets, Lipschitz domains, polygons and curvilinear polygons, semiconvex and convex domains. For general shape functionals, we establish relations between distributed Eulerian and Fréchet shape derivatives in tensor form for Lipschitz domains, and infer two types of boundary expressions for Lipschitz and $\mathcal{C}^1$-domains. We then focus on the particular case of the Dirichlet energy, for which we compute first and second order distributed shape derivatives in tensor form. Depending on the type of nonsmooth domain, different boundary expressions can be derived from the distributed expressions. This requires a careful study of the regularity of the solution to the Dirichlet Laplacian in nonsmooth domains. These results are applied to obtain a matricial expression of the second order shape derivative for polygons.

RÉSUMÉ

Nous étudions les expressions intégrales distribuées et les expressions intégrales de bord des dérivées de forme eulériennes et de Fréchet pour plusieurs classes de domaines non réguliers tels que les domaines ouverts, Lipschitz, convexes et semi-convexes, ainsi que les polygones et les polygones curvilinéaires. Dans le cas de fonctionnelles de forme générales, nous montrons certaines relations entre les expressions tensorielles des dérivées de forme distribuées eulériennes et de Fréchet pour les domaines Lipschitz, et nous en déduisons deux types d'expressions intégrales de bord dans le cas des domaines Lipschitz et $\mathcal{C}^1$. Par la suite, nous nous concentrons sur le cas particulier de l'énergie de Dirichlet, pour laquelle nous calculons les expressions tensorielles des dérivées de forme distribuées de premier et de second ordre. En fonction du type de domaine non régulier, différentes expressions intégrales de bord peuvent être obtenues à partir des expressions distribuées, ce qui requiert une étude minutieuse de la régularité de la solution du laplacien avec conditions aux limites de Dirichlet dans les domaines non réguliers. Nous appliquons

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ensuite ces résultats pour obtenir une expression matricielle de la dérivée seconde de forme dans le cas particulier des polygones.

1. Introduction

The generic name "shape derivative", a key tool in shape optimization, may refer to different types of derivatives. It usually refers either to Eulerian semiderivatives, using the speed method to define domain perturbations; see [19,59], or to Fréchet derivatives, obtained using the method of perturbation of identity; see [19,35,57]. It is well-known that they yield the same expression for the first order derivative, but different expressions for second order derivatives. Both approaches are relevant for applications, and are usually treated independently in the literature. In this paper, they are investigated simultaneously in order to discuss their relations in the context of distributed expressions, and we refer to them as Eulerian and Fréchet shape derivatives.

In both cases, the question of the structure of first and second order shape derivatives has been studied in details for smooth domains. Zolésio's structure theorem [19] states that the first order shape derivative is a boundary distribution which depends only on normal perturbations of the boundary. Consequently, one usually strives to write shape derivatives in this canonical form. The structure of the second order Eulerian shape derivative has been studied by Delfour and Zolésio [17–19] as well as Bucur and Zolésio [7], and the structure of Fréchet derivatives by Novruzi and Pierre in [53].

Studies on the existence and structure of shape derivatives in nonsmooth domains have also been published. Their general structure in arbitrary nonsmooth domains has been studied in [18]. The structure of the Eulerian shape derivative in domains with cracks or with singularities due to mixed boundary conditions has been studied in [27–30], and the shape sensitivity analysis for the Laplace-Beltrami operator formulated on a two-dimensional manifold with a fracture in [26]. The structure of the second order Eulerian shape derivative in domains with cracks has been studied in [46]. Also, Lamboley and Pierre have shown that the standard structure of the Fréchet shape derivative can be extended to sets of finite perimeter; see [42,43]. Continuity properties of shape derivatives around nonsmooth domains have also been studied in [44,45], which are applied to obtain qualitative properties of optimal shapes for shape optimization problems under convexity constraints.

Shape functionals are usually defined as integrals on some manifold $\Omega \subset \mathbb{R}^d$ of dimension $q \leq d$, with or without boundary. In a first step, the shape derivative is obtained as an integral on Ω involving the perturbation field θ and its derivative $D\theta$. Since this expression of the shape derivative involves $D\theta$, the terminology *weak form* of the shape derivative is sometimes used. One can then apply an appropriate tangential divergence theorem on Ω which yields an expression involving integrals on Ω and on its boundary $\partial\Omega$, if $\partial\Omega$ is not empty, and where the integrands depend only on θ and not on $D\theta$. We then refer to such an expression as the *strong form* of the shape derivative. In shape optimization, Ω is usually either a d-dimensional open set, or the boundary of such a set, i.e. a manifold without boundary of dimension $d-1$. In the former case, the weak form of the shape derivative is an integral on Ω, and is commonly called *distributed shape derivative*, *domain expression* or *volumetric form* of the shape derivative, while the strong form is an integral on $\partial\Omega$, which is actually the structure theorem's canonical *boundary expression* of the shape derivative. The distributed expression is well-known, see for instance [16,20,26,34] and references therein, but is usually considered a less attractive option than the structure theorem's boundary expression, and is often a mere intermediate step towards the calculation of this boundary expression. However, the usefulness of volume expressions in the context of finite element analysis is known; see the discussions in [19, Chapter 1, Section 5] and [34, Section 3.3.7]. In particular, their utilization via a so-called *domain method* for finite elements has been pioneered in [34] and in [16] for optimization of triangular meshing.

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A revival of interest for numerical applications of domain integral expressions of shape derivatives has been observed recently, with applications in elasticity [24,47,52,61], electromagnetism [31,36], automatic differentiation [55], inverse problems [1–3,32,49], Steklov-Poincaré type metrics [56], reproducing kernel Hilbert spaces [22], and moving mesh methods [54]. This interest revival has been sparked by recent developments. In [4], it was shown that the discretization and the shape differentiation processes commute for the distributed expression but not for the boundary expression, meaning that the discretized boundary expression does not generally yield the same expression as the shape derivative computed in the discrete setting. In [34,37], the authors observe that distributed shape derivatives often offer better numerical accuracy than boundary representations. From a numerical point of view, the distributed expression is often easier to implement than the boundary expression; see for instance [47,49] where it is used for a compact implementation of the level set method.

In this paper, we study the existence and properties of distributed and boundary expressions of first and second order Fréchet and Eulerian shape derivatives around nonsmooth domains. Although their general structure in arbitrary nonsmooth domains has been studied in [18], a detailed analysis of the structure for specific classes of nonsmooth domains of interest is scarce. Also, we note that there are very few contributions dedicated to second order distributed shape derivatives around nonsmooth domains in the literature. Significant recent results on this topic include [55], where automatic differentiation for second order distributed shape derivatives is studied, and [45] where first and second order Fréchet shape derivatives around nonsmooth domains are studied for functionals depending on second order elliptic PDEs, with a particular emphasis on Lipschitz, convex and semiconvex domains. These specific classes of nonsmooth domains are also the focus of the present paper, along with the cases of curvilinear polygons and polygons which we investigate in details. We also rederive a few known formulae in $\mathcal{C}^k$ and $\mathcal{C}^{k,\alpha}$-domains for comparison purposes.

Our methodology relies on two key ideas from the literature that are used to study shape derivatives for nonsmooth domains and parameters. The first is to employ volume rather than boundary integrals as was done in [5,30,34,45,48,49,60]. The other crucial element is to avoid using the shape derivative of the state function, which can be done in several ways. In this paper we use the material derivative of the state function as in [29,35,45]; other approaches include Lagrangian-type methods such as the averaged adjoint method [48,49,60], a dual formulation of the shape functional as in [5], or using a variational approach as in [38,39].

Another key feature of the paper is the representation of shape derivatives using tensor expressions. This tensor form plays an important role in continuum mechanics, with the energy-momentum tensor introduced by Eshelby [23,52]; see also [5,6] for shape functionals defined as minima of integral functionals. The systematic study of properties of tensor representations for shape derivatives was initiated in [48,49,60], where it was shown that these tensor expressions are convenient for numerical and theoretical purposes, for instance to swiftly compute the corresponding boundary expressions. Here we continue this investigation and we analyse in particular these tensor representations for second order shape derivatives. We start by establishing general relations between Fréchet and Eulerian distributed first and second order shape derivatives written in tensor form. Then, we obtain two types of boundary expressions derived from the tensor expressions, for Lipschitz and $\mathcal{C}^1$-domains. We also show an extension result, which gives flexibility for choosing the tensors in the distributed shape derivatives.

The key ingredient to get the boundary expression from the distributed expression is the applicability of the divergence theorem in nonsmooth domains. For general shape functionals, one needs to assume some regularity for the tensors involved in the distributed shape derivatives in order to obtain boundary expressions. For shape functionals depending on a specific boundary value problem (BVP), the validation of these regularity assumptions ultimately depends on the regularity of the solution to the BVP. In this paper we study the specific case of the Dirichlet energy, for which sharp regularity results for Lipschitz, convex, semiconvex and polygonal domains are available. In the case of polygons for instance, we strongly rely on the

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theory of corner singularities; see [10,13]. In a similar way, sharp regularity results for Poisson-type equations were an essential element used in [45] to prove continuity results around nonsmooth domains for the first and second shape derivatives with respect to Sobolev norms of the boundary-traces of the displacements. For the Dirichlet energy, we establish a range of formulae for second order shape derivatives, depending on the domain regularity. First, distributed second order shape derivatives are given in the general setting of open sets. Then, several types of boundary expressions are provided, either based on the shape derivative of the solution to the BVP or on its material derivative, which requires lower domain regularity assumptions.

Beyond the case study of the Dirichlet Laplacian, the goal of this paper is to show a general methodology for calculating a range of boundary expressions derived from the distributed expression, depending on the available domain regularity. Another motivation is to provide a method for computing second order shape derivatives for polygons, which is useful for applications although it has seldom been discussed in the literature; see however [1–3], where the shape derivative in polygons is computed for the inverse conductivity problem and used for a numerical algorithm. We illustrate this method by providing a matricial expression for the second order Fréchet shape derivative for polygons.

The paper is organized as follows. In Section 2, we introduce some notations and recall various basic definitions and results about domain regularity and shape derivatives. In Section 3, several results about tensor representations of first and second order distributed shape derivatives are given. In Section 4, we illustrate the results of Section 3 with the help of the volume functional. In Section 5 we recall several useful regularity results for the Dirichlet Laplacian in nonsmooth domains. The first and second order distributed Eulerian and Fréchet shape derivatives for the Dirichlet energy are investigated in Sections 6 and 7; respectively. In Section 8, we present several possible boundary expressions for first and second order shape derivatives based on the material or shape derivatives of the solution to the Dirichlet problem. In Section 9, we obtain a matricial expression for the second order Fréchet shape derivative of the Dirichlet energy in the class of polygons.

2. Preliminaries

In this section we introduce notations, recall some definitions of domain regularity and function spaces, and give some useful formulae for tensor calculus. We also give tangential divergence theorems in smooth and polygonal domains that are key for computing boundary expressions of shape derivatives.

Definition 1 *(Lipschitz domains).* An open, bounded set $\Omega \subset \mathbb{R}^d$, $d \geq 2$, is called a bounded Lipschitz domain if for every $x_0 \in \partial\Omega$, there exists $\eta_x, \eta_t > 0$, a $(d-1)$-plane $P \subset \mathbb{R}^d$ passing through x_0, a choice ν of the unit normal to P, and an open set

$$C = C(x_0, P, \nu, \eta_x, \eta_t) := \{x' + t\nu \mid x' \in P, |x' - x_0| < \eta_x, |t| \leq \eta_t\},$$

called a local coordinate cylinder near x_0 (with axis along ν), such that

$$C \cap \Omega = C \cap \{x' + t\nu \mid x' \in P, t > \varphi(x')\},$$
$$C \cap \partial\Omega = C \cap \{x' + t\nu \mid x' \in P, t = \varphi(x')\},$$
$$C \cap (\overline{\Omega})^c = C \cap \{x' + t\nu \mid x' \in P, t < \varphi(x')\},$$

for some Lipschitz function $\varphi : P \to \mathbb{R}$ satisfying $\varphi(x_0) = 0$ and $|\varphi(x')| < \eta_t/2$ if $|x' - x_0| \leq \eta_x$.

In other words, a bounded domain is Lipschitz if it is locally representable as the graph of a Lipschitz function. It is well-known that the surface measure $d\sigma$ is well-defined on $\partial\Omega$ and there exists an outward pointing normal vector n at almost every point on $\partial\Omega$; see [25, Section 4.2, p. 127].

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In a similar way, domains of class $\mathcal{C}^k$ or $\mathcal{C}^{k,\alpha}$ are domains which are locally representable as the graph of a $\mathcal{C}^k$ or $\mathcal{C}^{k,\alpha}$ function, respectively. Let n be the outward unit normal vector to Ω, when it is well-defined. When Ω is of class $\mathcal{C}^2$, denote $\tilde{n}$ a $\mathcal{C}^1$ and unitary extension of n to a neighbourhood of $\partial\Omega$. When $\Omega \subset \mathbb{R}^2$, τ denotes the tangent vector (choosing an orientation for $\partial\Omega$).

Definition 2 *(Curvilinear polygons).* For $k \geq 2$, a bounded open subset $\Omega \subset \mathbb{R}^2$ is said to be a $\mathcal{C}^k$ *curvilinear polygon*, or more precisely a $\mathcal{C}^k$ *curvilinear m-gon*, if it is Lipschitz, simply connected, and has a piecewise $\mathcal{C}^k$ boundary $\partial\Omega = \bigcup_{i\in I} \overline{\Gamma_i}$, $I := \{1, 2, \ldots, m\}$, $m \geq 3$, where Γ_i is a $\mathcal{C}^k$ open arc. Denoting $\Gamma_{m+1} := \Gamma_1$, we define the vertex, or corner a_i as the common endpoint $a_i := \overline{\Gamma_i} \cap \overline{\Gamma_{i+1}}$, for $i \in I$. The corner angle α_i at a_i is the angle between the tangents to $\overline{\Gamma_i}$ and $\overline{\Gamma_{i+1}}$ at a_i, measured from the interior of Ω. We assume that $0 < \alpha_i < 2\pi$ and $\alpha_i \neq \pi$ for all $i \in I$. We also denote

$$\tau^-(a_i) := \lim_{x\to a_i, x\in\Gamma_i} \tau(x), \quad \text{and} \quad \tau^+(a_i) := \lim_{x\to a_i, x\in\Gamma_{i+1}} \tau(x),$$

where $\tau(x)$ is the tangent vector to $\partial\Omega$ at a point $x \in \partial\Omega \setminus \{a_i\}_{i\in I}$. In a similar way, we define $n^-(a_i)$ and $n^+(a_i)$. When Γ_i is a segment for all $i \in I$, then the curvilinear polygon Ω is called a polygon, or more precisely a m-gon.

Note that domains with cracks or with cusps are excluded in Definition 2 since Ω is assumed to be Lipschitz.

Definition 3 *(Semiconvex sets).* A bounded open subset $\Omega \subset \mathbb{R}^d$ is said to be *semiconvex* if it is Lipschitz and satisfies a uniform exterior ball condition in the following sense: there exists $r > 0$ such that for any $x \in \partial\Omega$, there exists $y \in \mathbb{R}^d$ with $\overline{B(y, r)} \cap \overline{\Omega} = \{x\}$.

A domain is semiconvex if it is locally representable as the graph of a semiconvex function, where a function $f : C \to \mathbb{R}$ is said semiconvex on a convex subset C of $\mathbb{R}^d$ if there exists $M \in \mathbb{R}$ such that $x \in C \mapsto f(x) + M|x|^2$ is convex.

Let Ω be an open bounded subset of $\mathbb{R}^d$, then $W^{s,p}(\Omega)$, $s \geq 0$, denotes the usual Sobolev-Slobodeckij spaces, and $H^s(\Omega)$, with $s \geq 0$, denotes Sobolev spaces of fractional order based on $L^2(\Omega)$. We will also need the Bessel potential spaces $H^{s,p}(\Omega)$, $s \geq 0$, $1 \leq p < \infty$, to describe known regularity results, in particular those of [40]. Note that in [40], the notation $L^p_s(\Omega)$ is used for Bessel potential spaces instead of $H^{s,p}(\Omega)$. When Ω is Lipschitz and bounded, we have $H^{s,2}(\Omega) = W^{s,2}(\Omega) = H^s(\Omega)$ for $s \geq 0$; see [8, Section 1.1.1]. We also have $H^{k,p}(\Omega) = W^{k,p}(\Omega)$ for $1 < p < \infty$ and $k \in \mathbb{N}$ for Ω Lipschitz and bounded; see [40, Section 2, (2.2)].

Let $\mathbb{P}(\mathcal{D})$ be the subset of open sets compactly contained in $\mathcal{D}$, where $\mathcal{D} \subset \mathbb{R}^d$ is assumed to be open and bounded.

Notations. *For sufficiently smooth $\Omega \subset \mathbb{R}^d$, vector-valued functions $a, b : \mathbb{R}^d \to \mathbb{R}^d$ and second order tensors $\mathbf{S} : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ and $\mathbf{T} : \mathbb{R}^d \to \mathbb{R}^{d\times d}$ whose entries are denoted by $\mathbf{S}_{ij}$ and $\mathbf{T}_{ij}$, the double dot product of $\mathbf{S}$ and $\mathbf{T}$ is defined as $\mathbf{S} : \mathbf{T} = \sum_{i,j=1}^d \mathbf{S}_{ij}\mathbf{T}_{ij}$, and the outer product $a \otimes b$ is defined as the second order tensor with entries $[a \otimes b]_{ij} = a_i b_j$. We use the following notations:*

- $\mathbf{I}_d$ *for the identity matrix in* $\mathbb{R}^{d\times d}$.
- $\mathrm{Id} : x \mapsto x$ *for the identity in* $\mathbb{R}^d$.
- $a \odot b := \frac{1}{2}(a \otimes b + b \otimes a)$ *for the symmetric outer product of a and b.*
- $D_\Gamma a := Da - (Da)n \otimes n$ *for the tangential derivative on* $\partial\Omega$.
- $\operatorname{div}_\Gamma a := \operatorname{div} a - (Da)n \cdot n$ *for the tangential divergence on* $\partial\Omega$.

- $\nabla_\Gamma a := \nabla a - (n \otimes n)\nabla a$ *for the tangential gradient on* $\partial\Omega$.
- $\operatorname{div}(\mathbf{S})$ *is defined as the vector of the divergence of the rows of* $\mathbf{S}$.
- $a_n := a \cdot n$ *and* $a_\tau := a - a_n n$.
- $\mathcal{H} := \frac{\operatorname{div}_\Gamma n}{d-1}$ *is the mean curvature of* $\partial\Omega$.
- $\mathcal{L}(U_0, U_1)$ *is the space of linear maps from vector space* U_0 *to vector space* U_1.

Remark 1. In the shape optimization literature, the notation $\mathcal{H}$ is sometimes used for the additive curvature $H := \operatorname{div}_\Gamma n = (d-1)\mathcal{H}$, which is the sum of the principal curvatures. Indeed, when integrating by parts on submanifolds of $\mathbb{R}^d$, the additive curvature appears naturally rather than the mean curvature. Note that the additive curvature is sometimes also called "mean curvature", therefore one should be careful about the precise definition of the curvature in shape derivative formulae. See [19, Chapter 2, Section 3.3] for a more detailed discussion.

Lemma 1 *(Tensor calculus). For sufficiently smooth* $f : \mathbb{R}^d \to \mathbb{R}$, *vector-valued functions* $a, b, c, d : \mathbb{R}^d \to \mathbb{R}^d$ *and second order tensor* $\mathbf{S} : \mathbb{R}^d \to \mathbb{R}^{d\times d}$, *we have*

1. $\operatorname{div}(\mathbf{S}^\mathsf{T} a) = \mathbf{S} : Da + a \cdot \operatorname{div}(\mathbf{S})$,
2. $\mathbf{S} : (a \otimes b) = a \cdot \mathbf{S}b = \mathbf{S}^\mathsf{T} a \cdot b = \mathbf{S}^\mathsf{T} : (b \otimes a)$,
3. $\mathbf{S}(a \otimes b) = \mathbf{S}a \otimes b$ *and* $(a \otimes b)\mathbf{S} = a \otimes \mathbf{S}^\mathsf{T} b$,
4. $(a \otimes b)c = (c \cdot b)a$,
5. $(a \otimes b) : (c \otimes d) = (a \cdot c)(b \cdot d) = (c \otimes b) : (a \otimes d) = c \cdot (a \otimes d)b$,
6. $\operatorname{div}(a \otimes b) = (\operatorname{div} b)a + (Da)b$ *and* $\operatorname{div}(f\mathbf{I}_d) = \nabla f$.

Lemma 2. *Assume* $\theta, \xi \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^d)$, $\Omega \in \mathbb{P}(\mathcal{D})$ *is* $\mathcal{C}^2$. *Then we have*

$$D_\Gamma\theta\xi_\tau \cdot n = D\theta\xi_\tau \cdot n = \nabla_\Gamma\theta_n \cdot \xi_\tau - D_\Gamma n\xi_\tau \cdot \theta_\tau \text{ on } \partial\Omega. \tag{1}$$

When $\Omega \subset \mathbb{R}^2$ *is a* $\mathcal{C}^2$ *curvilinear* m*-gon and* $\partial\Omega = \bigcup_{i\in I} \overline{\Gamma_i}$, *we obtain* (1) *on each* Γ_i *instead of* $\partial\Omega$.

Proof. We have $D\theta\xi \cdot n = D_\Gamma\theta\xi \cdot n + \xi_n D\theta n \cdot n$ and consequently

$$D\theta\xi_\tau \cdot n = D_\Gamma\theta\xi_\tau \cdot n. \tag{2}$$

Since $\Omega \subset \mathbb{R}^d$ is $\mathcal{C}^k$ for $k \geq 2$, $D_\Gamma n$ is well-defined and we have $\nabla_\Gamma(\theta \cdot n) \cdot \xi_\tau = D_\Gamma n\xi_\tau \cdot \theta + D_\Gamma\theta\xi_\tau \cdot n$, which yields, using (2),

$$D\theta\xi_\tau \cdot n = D_\Gamma\theta\xi_\tau \cdot n = \nabla_\Gamma\theta_n \cdot \xi_\tau - D_\Gamma n\xi_\tau \cdot \theta. \tag{3}$$

We also have

$$D_\Gamma n\xi_\tau \cdot \theta = D_\Gamma n\xi_\tau \cdot \theta_\tau + \theta_n D_\Gamma n\xi_\tau \cdot n. \tag{4}$$

Using the unitary and $\mathcal{C}^1$ extension $\tilde{n}$ of n, we have $\tilde{n} \cdot \tilde{n} = 1$ and $D\tilde{n}^\mathsf{T}\tilde{n} = 0$ in a neighbourhood of $\partial\Omega$. Thus, we get

$$D_\Gamma n\xi_\tau \cdot n = D\tilde{n}\xi_\tau \cdot n - (D\tilde{n}n \otimes n)\xi_\tau \cdot n = \xi_\tau \cdot D\tilde{n}^\mathsf{T} n - \xi_\tau \cdot (n \otimes D\tilde{n}n)n = -\xi_\tau \cdot (D\tilde{n}n \cdot n)n = 0 \text{ on } \partial\Omega,$$

which yields (1) using (3) and (4).

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When $\Omega \subset \mathbb{R}^2$ is a $\mathcal{C}^k$ curvilinear m-gon with $k \geq 2$, $D_\Gamma n$ is well-defined on each Γ_i. Considering a unitary and $\mathcal{C}^1$ extension $\tilde{n}$ of n in a tubular neighbourhood of Γ_i, we can follow the same reasoning and we obtain (1) on each Γ_i. □

Remark 2. The bilinear form $(\xi_\tau, \theta_\tau) \mapsto -D_\Gamma n \xi_\tau \cdot \theta_\tau$ appearing in Lemma 2, where $\xi_\tau(x), \theta_\tau(x)$ are vectors in the tangent space of $\partial\Omega$ at $x \in \partial\Omega$, is the second fundamental form of $\partial\Omega$, and is known to be symmetric.

Theorem 1 *(Tangential divergence theorem). Let $\Omega \subset \mathbb{R}^d$ be a domain of class $\mathcal{C}^k$, $k \geq 2$, and $F \in W^{1,1}(\partial\Omega, \mathbb{R}^d)$, then we get*

$$\int_{\partial\Omega} \operatorname{div}_\Gamma(F) = \int_{\partial\Omega} (d-1)\mathcal{H} F \cdot n.$$

Proof. See [19, Chapter 9, Section 5.5]. □

Theorem 2 *(Tangential divergence theorem for curvilinear polygons). Let $\Omega \subset \mathbb{R}^2$ be a $\mathcal{C}^k$ curvilinear m-gon, $k \geq 2$, with $\partial\Omega = \bigcup_{i\in I} \overline{\Gamma_i}$. Let $F \in W^{1,1}(\Gamma_i, \mathbb{R}^2) \cap \mathcal{C}^0(\overline{\Gamma_i}, \mathbb{R}^2)$, and denote $a_i := \overline{\Gamma_i} \cap \overline{\Gamma_{i+1}}$ and $a_0 := a_m$. Then for $i \in I$ we have*

$$\int_{\Gamma_i} \operatorname{div}_\Gamma(F) = \int_{\Gamma_i} \mathcal{H} F \cdot n + F(a_i) \cdot \tau^-(a_i) - F(a_{i-1}) \cdot \tau^+(a_{i-1}).$$

Proof. The result follows from [58, Section 7.2] and [19, Chapter 9, Section 5.5]. □

2.1. Eulerian shape derivatives

In this section, we recall basic notions about first and second order Eulerian shape derivatives. We define for $k \geq 0$ and $0 \leq \alpha \leq 1$,

$$\mathcal{C}_c^{k,\alpha}(\mathcal{D}, \mathbb{R}^d) := \{\theta \in \mathcal{C}^{k,\alpha}(\mathcal{D}, \mathbb{R}^d) \mid \theta \text{ has compact support in } \mathcal{D}\},$$

and $\mathcal{C}_c^k(\mathcal{D}, \mathbb{R}^d)$, $\mathcal{C}_c^\infty(\mathcal{D}, \mathbb{R}^d)$ in a similar way. Consider a vector field $\theta \in \mathcal{C}_c^{0,1}(\mathcal{D}, \mathbb{R}^d)$ and the associated flow $T_t^\theta : \mathcal{D} \to \mathcal{D}$, $t \in [0, t_0]$ defined for each $x_0 \in \mathcal{D}$ as $T_t^\theta(x_0) := x(t)$, where $x : [0, t_0] \to \mathbb{R}^d$ solves

$$\dot{x}(t) = \theta(x(t)) \quad \text{for } t \in [0, t_0], \quad x(0) = x_0. \tag{5}$$

For $\Omega \in \mathbb{P}(\mathcal{D})$, we consider the family of perturbed domains

$$\Omega_t := T_t^\theta(\Omega). \tag{6}$$

We are now ready to give the definition of the Eulerian shape derivative. In the literature, it is usually simply called *shape derivative*, but in this paper we add the prefix *Eulerian* in order to distinguish it from the Fréchet derivative.

Definition 4 *(Eulerian shape derivative).* Let $J : \mathbb{P}(\mathcal{D}) \to \mathbb{R}$ be a shape functional.

(i) The Eulerian semiderivative of J at Ω in direction $\theta \in \mathcal{C}_c^{0,1}(\mathcal{D}, \mathbb{R}^d)$ is defined by, when the limit exists,

$$D_E J(\Omega)(\theta) := \lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t}. \tag{7}$$

(ii) J is said to be *shape differentiable* at Ω if it has a Eulerian semiderivative at Ω for all $\theta \in \mathcal{C}_c^\infty(\mathcal{D}, \mathbb{R}^d)$ and the mapping

$$D_E J(\Omega) : \mathcal{C}_c^\infty(\mathcal{D}, \mathbb{R}^d) \to \mathbb{R},\ \theta \mapsto D_E J(\Omega)(\theta)$$

is linear and continuous, in which case $D_E J(\Omega)(\theta)$ is called the *Eulerian shape derivative* at Ω.

Definition 5 *(Second order Eulerian shape derivative).* Let $J : \mathbb{P}(\mathcal{D}) \to \mathbb{R}$ be a shape functional, and assume that for all $t \in [0, t_0]$, $D_E J(T_t^\xi(\Omega))(\theta)$ exists at $T_t^\xi(\Omega)$ in direction $\theta \in \mathcal{C}_c^{0,1}(\mathcal{D}, \mathbb{R}^d)$.

(i) The second order Eulerian semiderivative of J at Ω in direction $\theta \in \mathcal{C}_c^{0,1}(\mathcal{D}, \mathbb{R}^d)$ is defined by, when the limit exists,

$$D_E^2 J(\Omega)(\theta, \xi) := \lim_{t \searrow 0} \frac{D_E J(T_t^\xi(\Omega))(\theta) - D_E J(\Omega)(\theta)}{t}. \tag{8}$$

(ii) J is said to be *twice shape differentiable* at Ω if it has a second order Eulerian semiderivative at Ω for all $\theta, \xi \in \mathcal{C}_c^\infty(\mathcal{D}, \mathbb{R}^d)$ and the mapping

$$D_E^2 J(\Omega) : [\mathcal{C}_c^\infty(\mathcal{D}, \mathbb{R}^d)]^2 \to \mathbb{R},\ (\theta, \xi) \mapsto D_E^2 J(\Omega)(\theta, \xi)$$

is bilinear and continuous, in which case $D_E^2 J(\Omega)(\theta, \xi)$ is called the *second order Eulerian shape derivative* at Ω.

Remark 3. Alternatively, one can also view the second order Eulerian shape derivative as

$$D_E^2 J(\Omega)(\theta, \xi) = \frac{d}{dt}\left(\frac{d}{ds} J(T_s^\theta(T_t^\xi(\Omega)))_{|s=0}\right)_{|t=0}.$$

2.2. Fréchet shape derivatives

To define Fréchet derivatives, we use the notations of [53]. Let Θ_k be the space of vector fields from $\mathcal{C}^k(\mathcal{D}, \mathbb{R}^d)$, equipped with the usual $\mathcal{C}^k$-norm. Let

$$\Theta_k^1 := \{\theta \in \Theta_k \mid \|\theta\|_k < 1\}.$$

If $\theta \in \Theta_k^1$, then $\mathrm{Id} + \theta$ is a $\mathcal{C}^k$-diffeomorphism. For $\Omega \in \mathbb{P}(\mathcal{D})$, we define $\Omega_\theta := (\mathrm{Id} + \theta)(\Omega)$ and introduce the functional

$$\mathcal{J}(\theta) := J(\Omega_\theta), \qquad \forall \theta \in \Theta_k^1.$$

When it exists, we define the Fréchet shape derivative of order q of $J(\Omega)$ as the Fréchet derivative of order q of $\mathcal{J}$ at 0, and we denote it $D_F^q \mathcal{J}(0)$. We also introduce

$$\mathcal{O}_k := \{\Omega \in \mathbb{P}(\mathcal{D}) \mid \Omega \text{ of class } \mathcal{C}^k\}.$$

For $\Omega \in \mathcal{O}_k$ and $\theta \in \Theta_k^1$, Ω_θ is also of class $\mathcal{C}^k$.

2.3. Structure of shape derivatives

For the Eulerian shape derivative we have the following well-known structure proven by Zolésio.

Theorem 3 *(Structure theorem). Let Ω be open with $\partial\Omega$ compact and of class $\mathcal{C}^{k+1}$, $k \geq 0$. Assume J has a Eulerian shape derivative at Ω and $D_E J(\Omega)$ is continuous for the $\mathcal{C}^k(\mathcal{D}, \mathbb{R}^d)$-topology. Then, there exists a linear and continuous functional $l_E : \mathcal{C}^k(\partial\Omega) \to \mathbb{R}$ such that for all $\theta \in \mathcal{C}_c^k(\mathcal{D}, \mathbb{R}^d)$,*

$$D_E J(\Omega)(\theta) = l_E(\theta_{|\partial\Omega} \cdot n). \tag{9}$$

Proof. See [19, pp. 480-481]. □

For the first and second order Fréchet shape derivatives, we have the following result from [53].

Theorem 4. *Let $k \geq 1$.*

1. *Assume $\Omega \in \mathcal{O}_{k+1}$ and $\mathcal{J}$ is differentiable at 0 in Θ_k. Then there exists a continuous linear map $l_{F,1} : \mathcal{C}^k(\partial\Omega) \mapsto \mathbb{R}$ such that for any $\theta \in \Theta_k$:*

$$D_F \mathcal{J}(0)(\theta) = l_{F,1}(\theta_n). \tag{10}$$

2. *Assume $\Omega \in \mathcal{O}_{k+2}$ and $\mathcal{J}$ is twice differentiable at 0 in Θ_k. Then, there exists a continuous bilinear symmetric map $l_{F,2} : [\mathcal{C}^k(\partial\Omega)]^2 \mapsto \mathbb{R}$ such that for any $\theta, \xi \in \Theta_{k+1}$:*

$$D_F^2 \mathcal{J}(0)(\theta, \xi) = l_{F,2}(\theta_n, \xi_n) + l_{F,1}(-D_\Gamma n \xi_\tau \cdot \theta_\tau - D_\Gamma \theta \xi_\tau \cdot n - D_\Gamma \xi \theta_\tau \cdot n). \tag{11}$$

Alternatively, we can also write

$$D_F^2 \mathcal{J}(0)(\theta, \xi) = l_{F,2}(\theta_n, \xi_n) + l_{F,1}(D_\Gamma n \xi_\tau \cdot \theta_\tau - \nabla_\Gamma \theta_n \cdot \xi_\tau - \nabla_\Gamma \xi_n \cdot \theta_\tau). \tag{12}$$

Proof. The structures (10) and (11) are proven in [53, Theorem 2.1]. The structure (12) is given in [53, Remark 2.10], where (12) is obtained from (11) in the following way: using Lemma 2 and Remark 2, we have

$$\begin{aligned} D_\Gamma \theta \xi_\tau \cdot n &= \nabla_\Gamma \theta_n \cdot \xi_\tau - D_\Gamma n \xi_\tau \cdot \theta_\tau, \\ D_\Gamma \xi \theta_\tau \cdot n &= \nabla_\Gamma \xi_n \cdot \theta_\tau - D_\Gamma n \theta_\tau \cdot \xi_\tau = \nabla_\Gamma \xi_n \cdot \theta_\tau - \theta_\tau \cdot D_\Gamma n \xi_\tau, \end{aligned}$$

and (12) follows. □

On one hand, when both Eulerian and Fréchet first order shape derivatives exist, then one can verify that they have the same expressions, i.e.

$$D_F \mathcal{J}(0)(\theta) = D_E J(\Omega)(\theta), \tag{13}$$

and consequently $l_E = l_{F,1}$. On the other hand, it is well-known that the second order Eulerian and Fréchet shape derivatives are different and consequently do not have the same structure. In particular, the second order Fréchet shape derivative is a symmetric bilinear form whereas the Eulerian is not symmetric. In fact, it can be shown that they are related by:

$$D_E^2 J(\Omega)(\theta, \xi) = D_F^2 \mathcal{J}(0)(\theta, \xi) + D_F \mathcal{J}(0)(D\theta\xi), \tag{14}$$

see for instance [53] or [19, Chapter 9, Section 6.5], where the authors also observe that $D\theta\xi$ is the first half of the Lie bracket $[\theta,\xi] := D\theta\xi - D\xi\theta$. Combining (14) and the structure of the second order Fréchet shape derivative of Theorem 4, we can also write a structure theorem for the second order Eulerian shape derivative. The structures of these second order shape derivatives have been analysed in $\mathcal{C}^k$-domains, $k \geq 2$, in [7,17] and [53]. The structures of the first and second Eulerian shape derivatives for nonsmooth domains have also been studied in [18, Theorem 3.2] and in [18, Theorem 4.2], respectively; see also [19, Chapter 9, Section 6]. In [18,19], the nonautonomous case where θ also depends on t is investigated. In this paper we only consider the autonomous case for simplicity.

3. Tensor representations of shape derivatives

Although the structure theorems of Section 2.3 state that the shape derivatives are boundary distributions, it can be useful to express them as domain integrals for several reasons, as discussed in the introduction. One important property shown in [4] is that the discretization and shape differentiation processes commute for the distributed expression but not for the boundary expression, which makes the former convenient for numerical applications. Other useful properties are the improved numerical accuracy offered by distributed shape derivatives [37], and the simplified implementation of level set methods [47,49]. Also, it was shown in [48,49,60] that systematically expressing distributed shape derivatives using a tensor representation has several advantages for numerical and theoretical purposes. In particular it allows to swiftly compute the corresponding boundary expression when the domain is sufficiently regular. Although the systematic study of tensor representation of distributed shape derivatives was initiated in [48,49,60] in a general framework, a detailed analysis for specific classes of nonsmooth domains is still missing. In this paper we investigate this approach in more details and extend it to the study of second order distributed shape derivatives.

From a theoretical point of view, the main advantage of distributed expressions over boundary expressions is their availability for domains with lower regularity. More precisely, an important issue is to determine the minimal domain regularity for which boundary and distributed expressions exist. In this section, we first investigate this question for general shape functionals, and show that for Lipschitz domains, the existence of boundary expressions is determined by the regularity of the tensors appearing in the distributed shape derivative. In order to determine the minimal domain regularity required to obtain this tensor regularity, one needs to study the properties of the underlying BVP. Thus, in the next sections we investigate this issue for the specific case of the Dirichlet energy.

Our methodology consists in starting from the tensor representation as in [49], and then to prove the existence of boundary expressions by gradually increasing the domain regularity. In doing so, an important realization is that several types of "intermediary" boundary expressions may be obtained, which do not correspond to the structure theorem's canonical form, but can nevertheless be useful for certain applications thanks to their availability for low domain regularity. Note that in [49], the tensor representation is analysed for transmission problems, but in the present paper we chose not to treat this case in order to simplify the presentation. Nevertheless, we point out that the generalization to transmission problems is straightforward.

Definition 6 *(Tensor representation).* Let $\Omega \in \mathbb{P}(\mathcal{D})$ and assume $J : \mathbb{P}(\mathcal{D}) \mapsto \mathbb{R}$ has a Eulerian shape derivative at Ω. The Eulerian shape derivative of J admits a tensor representation of order 1 if there exist a first-order tensor $\mathbf{S}_0 \in L^1(\Omega,\mathbb{R}^d)$ and a second order tensor $\mathbf{S}_1 \in L^1(\Omega,\mathbb{R}^{d\times d})$ such that for all $\theta \in \mathcal{C}^1_c(\mathcal{D},\mathbb{R}^d)$,

$$D_E J(\Omega)(\theta) = \int\limits_{\Omega} \mathbf{S}_1 : D\theta + \mathbf{S}_0 \cdot \theta. \tag{15}$$

The following proposition is similar to [49, Proposition 4.3], but with weaker regularity assumptions.

Proposition 1. *Assume* $\Omega \in \mathbb{P}(\mathcal{D})$, $\theta \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^d)$, *and* J *has a Eulerian shape derivative at* Ω *with the tensor representation* (15). *If* $\mathbf{S}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, *then*

$$\operatorname{div}(\mathbf{S}_1) = \mathbf{S}_0 \quad \text{in } \Omega, \tag{16}$$

and

$$D_E J(\Omega)(\theta) = \int_\Omega \operatorname{div}(\mathbf{S}_1^\mathsf{T}\theta). \tag{17}$$

If in addition Ω *is Lipschitz, then we have the boundary expression*

$$D_E J(\Omega)(\theta) = \int_{\partial\Omega} (\mathbf{S}_1 n)\cdot\theta. \tag{18}$$

Moreover, if Ω *is of class* $\mathcal{C}^1$, *we obtain the boundary expression*

$$D_E J(\Omega)(\theta) = \int_{\partial\Omega} (\mathbf{S}_1 n\cdot n)\,\theta_n. \tag{19}$$

Proof. In view of [49, Theorem 2.2], if θ has compact support in Ω then the shape derivative vanishes. Thus, using Lemma 1(1) and $\mathbf{S}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, we get

$$D_E J(\Omega)(\theta) = \int_\Omega \mathbf{S}_1 : D\theta + \mathbf{S}_0\cdot\theta = \int_\Omega \operatorname{div}(\mathbf{S}_1^\mathsf{T}\theta) + \theta\cdot(\mathbf{S}_0 - \operatorname{div}\mathbf{S}_1) = 0 \quad \text{for all } \theta \in \mathcal{C}^1_c(\Omega, \mathbb{R}^d). \tag{20}$$

Since θ has compact support in Ω, we can extend $\mathbf{S}_1^\mathsf{T}\theta$ and $\theta\cdot(\mathbf{S}_0 - \operatorname{div}\mathbf{S}_1)$ by zero on $\mathcal{B}$, where $\mathcal{B}$ is a sufficiently large open ball which contains Ω. We keep the same notation for the extensions for simplicity. Since the extension satisfies $\mathbf{S}_1^\mathsf{T}\theta \in W^{1,1}(\mathcal{B}, \mathbb{R}^d)$, using the divergence theorem in $\mathcal{B}$ we get

$$\begin{aligned}\int_\Omega \operatorname{div}(\mathbf{S}_1^\mathsf{T}\theta) + \theta\cdot(\mathbf{S}_0 - \operatorname{div}\mathbf{S}_1) &= \int_\mathcal{B} \operatorname{div}(\mathbf{S}_1^\mathsf{T}\theta) + \theta\cdot(\mathbf{S}_0 - \operatorname{div}\mathbf{S}_1)\\ &= \int_{\partial\mathcal{B}} (\mathbf{S}_1^\mathsf{T}\theta)\cdot n + \int_\mathcal{B} \theta\cdot(\mathbf{S}_0 - \operatorname{div}\mathbf{S}_1)\\ &= \int_\Omega \theta\cdot(\mathbf{S}_0 - \operatorname{div}\mathbf{S}_1) = 0, \qquad \text{for all } \theta \in \mathcal{C}^1_c(\Omega, \mathbb{R}^d),\end{aligned}$$

which proves (16). Then, using (16) in (20) with $\theta \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^d)$ instead of $\theta \in \mathcal{C}^1_c(\Omega, \mathbb{R}^d)$, we get (17). Further, applying a divergence theorem in Lipschitz domains to (17), see for instance [25, Section 4.3, Theorem 1], we get (18).

Now, in view of (18) we have that $D_E J(\Omega)$ is continuous for the $\mathcal{C}^0(\mathcal{D}, \mathbb{R}^d)$-topology. Thus, if Ω is of class $\mathcal{C}^1$, we can apply Theorem 3 with $k = 0$. With Ω of class $\mathcal{C}^1$, we also have $n \in \mathcal{C}^0(\partial\Omega, \mathbb{R}^d)$ and $\theta_{|\partial\Omega}\cdot n \in \mathcal{C}^0(\partial\Omega)$. Let $\hat\theta \in \mathcal{C}^0(\mathcal{D}, \mathbb{R}^d)$ be an extension to $\mathcal{D}$ of $\theta_n n \in \mathcal{C}^0(\partial\Omega, \mathbb{R}^d)$, then using Theorem 3 we obtain

$$\begin{aligned}D_E J(\Omega)(\theta) &= l_E(\theta_{|\partial\Omega}\cdot n) = l_E(\hat\theta_{|\partial\Omega}\cdot n) = D_E J(\Omega)(\hat\theta)\\ &= \int_{\partial\Omega} (\mathbf{S}_1 n)\cdot\hat\theta = \int_{\partial\Omega} (\mathbf{S}_1 n)\cdot(\theta_n n) = \int_{\partial\Omega} (\mathbf{S}_1 n\cdot n)\theta_n,\end{aligned}$$

which yields expression (19). □

Even if Definition 6 and Proposition 1 are written for the Eulerian shape derivative for convenience, the results are also valid for the Fréchet shape derivative, if it exists, in view of (13).

The main difference between the boundary expressions (18) and (19) is that the shape derivative in (18) may depend on the tangential part θ_τ, whereas the shape derivative in (19) only depends on θ_n. In [43, Theorem 1.3], a general structure theorem is proven, which shows that the shape derivative can be written as $l_E(\theta_{|\Gamma} \cdot n)$ even when Ω is only a set of finite perimeter, which is in particular valid for Lipschitz sets. However, the linear form l_E is in general not a boundary integral if Ω is only Lipschitz. For instance, for piecewise smooth boundaries in two dimensions, the shape derivative of the perimeter contains Dirac measures at the vertices of $\partial\Omega$; see [43, Proposition 2.6]. However, since the perimeter is a boundary integral it leads to a shape derivative which can not be represented using the domain expression (15). Therefore, it is not excluded that expression (19) could also be valid for Lipschitz domains, in the case of shape derivatives which have a distributed expression of the form (15).

Also, expression (19) corresponds to the canonical structure $l_E(\theta_{|\Gamma} \cdot n)$ of Theorem 3 whereas (18) does not. In this respect, (18) can be considered an "intermediary" boundary expression, but may nevertheless be useful, for instance for piecewise smooth boundaries. Note that in [5, Theorem 3.7], a boundary expression of the type (18) is obtained for shape functionals defined as minima of integral functionals, for Lipschitz domains.

Now we discuss an extension result for the boundary expression of the shape derivative which is an immediate consequence of (18).

Proposition 2. *Assume $\Omega \in \mathbb{P}(\mathcal{D})$ is Lipschitz, $\theta \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^d)$, $D_E J(\Omega)(\theta)$ has the tensor representation (15) with $\mathbf{S}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, and let $\widehat{\mathbf{S}}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$. Then $\widehat{\mathbf{S}}_1$ satisfies*

$$\widehat{\mathbf{S}}_1 n = \mathbf{S}_1 n \quad \text{on } \partial\Omega \tag{21}$$

if and only if

$$D_E J(\Omega)(\theta) = \int_\Omega \widehat{\mathbf{S}}_1 : D\theta + \widehat{\mathbf{S}}_0 \cdot \theta \tag{22}$$

with $\widehat{\mathbf{S}}_0 := \operatorname{div}(\widehat{\mathbf{S}}_1)$.

Proof. Assume $\widehat{\mathbf{S}}_1$ satisfies (21). Then, in view of assumption $\widehat{\mathbf{S}}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$ and Proposition 1, we have, using (21) and the divergence theorem,

$$D_E J(\Omega)(\theta) = \int_{\partial\Omega} (\mathbf{S}_1 n) \cdot \theta = \int_{\partial\Omega} (\widehat{\mathbf{S}}_1 n) \cdot \theta = \int_\Omega \operatorname{div}(\widehat{\mathbf{S}}_1^\mathsf{T} \theta) = \int_\Omega \widehat{\mathbf{S}}_1 : D\theta + \widehat{\mathbf{S}}_0 \cdot \theta,$$

which yields (22). The fact that $\widehat{\mathbf{S}}_0 := \operatorname{div}(\widehat{\mathbf{S}}_1)$ is a consequence of Proposition 1 using the tensor representation (22).

Reciprocally, assume $\widehat{\mathbf{S}}_1$ satisfies (22) and that $\widehat{\mathbf{S}}_0 := \operatorname{div}(\widehat{\mathbf{S}}_1)$. Then we have

$$D_E J(\Omega)(\theta) = \int_\Omega \mathbf{S}_1 : D\theta + \mathbf{S}_0 \cdot \theta = \int_\Omega \widehat{\mathbf{S}}_1 : D\theta + \widehat{\mathbf{S}}_0 \cdot \theta. \tag{23}$$

Using (23) and (18), we get for all $\theta \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^d)$ that

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$$\int_{\partial\Omega} ((\mathbf{S}_1 - \widehat{\mathbf{S}}_1)n) \cdot \theta = 0,$$

which yields (21). □

Proposition 2 essentially states that the tensor representation (15) is not unique, and that different choices of tensor representation must satisfy the boundary condition (21). Proposition 2 can also be seen as an extension result in the sense that $\mathbf{S}_1$ and $\widehat{\mathbf{S}}_1$ are two different extensions of the same boundary expression (21). From a practical perspective, Proposition 2 can be used to seek an alternative tensor $\widehat{\mathbf{S}}_1$ which is easier to implement than $\mathbf{S}_1$; see Sections 6.1 and 8.3 for concrete examples. Note that the second order distributed shape derivative can be calculated using $\widehat{\mathbf{S}}_1$ instead of $\mathbf{S}_1$, but in practice this does not seem to simplify the calculations; see the examples in Sections 6.1 and 8.3. We also observe in these examples that natural choices of alternative tensors $\widehat{\mathbf{S}}_1$ often require more regularity for the solution of the BVP.

Proposition 3 *(Second order Eulerian and Fréchet shape derivatives). Assume $\Omega \in \mathbb{P}(\mathcal{D})$ and $\theta, \xi \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$. Assume $J(\Omega)$ has a Eulerian shape derivative with the tensor representation (15) and $\mathbf{S}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, and $J(\Omega)$ has a second order Eulerian shape derivative with the tensor representation*

$$D^2_E J(\Omega)(\theta, \xi) = \int_{\Omega} \mathbf{S}^{2,E}_1(\theta) : D\xi + \mathbf{S}^{2,E}_0(\theta) \cdot \xi, \tag{24}$$

where $\mathbf{S}^{2,E}_1(\theta) \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$ and $\mathbf{S}^{2,E}_0(\theta) \in L^1(\Omega, \mathbb{R}^d)$. Assuming $J(\Omega)$ has a second order Fréchet shape derivative, then it admits the tensor representation

$$D^2_F \mathcal{J}(0)(\theta, \xi) = \int_{\Omega} \mathbf{S}^{2,F}_1(\theta) : D\xi + \mathbf{S}^{2,F}_0(\theta) \cdot \xi = \int_{\Omega} \mathbf{S}^{2,F}_1(\xi) : D\theta + \mathbf{S}^{2,F}_0(\xi) \cdot \theta, \tag{25}$$

with $\mathbf{S}^{2,F}_1(\theta) \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, $\mathbf{S}^{2,F}_0(\theta) = \operatorname{div}(\mathbf{S}^{2,F}_1(\theta)) \in L^1(\Omega, \mathbb{R}^d)$, and

$$\mathbf{S}^{2,F}_1(\theta) := \mathbf{S}^{2,E}_1(\theta) - D\theta^{\mathsf{T}} \mathbf{S}_1, \tag{26}$$

$$\mathbf{S}^{2,F}_0(\theta) := \mathbf{S}^{2,E}_0(\theta) - \operatorname{div}(D\theta^{\mathsf{T}} \mathbf{S}_1). \tag{27}$$

Now, we assume in addition that Ω is Lipschitz. Then, we have the boundary expression

$$D^2_E J(\Omega)(\theta, \xi) = \int_{\partial\Omega} (\mathbf{S}^{2,E}_1(\theta) n) \cdot \xi. \tag{28}$$

Moreover, the second order Fréchet shape derivative has the boundary expression

$$D^2_F \mathcal{J}(0)(\theta, \xi) = \int_{\partial\Omega} (\mathbf{S}^{2,F}_1(\theta) n) \cdot \xi = \int_{\partial\Omega} (\mathbf{S}^{2,F}_1(\xi) n) \cdot \theta. \tag{29}$$

If in addition Ω is of class $\mathcal{C}^1$, we get the boundary expression

$$D^2_E J(\Omega)(\theta, \xi) = \int_{\partial\Omega} (\mathbf{S}^{2,E}_1(\theta) n \cdot n) \xi_n. \tag{30}$$

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Proof. Assume $\Omega \in \mathbb{P}(\mathcal{D})$. In view of (14), using that $D_F\mathcal{J}(0) = D_E J(\Omega)$ and (17) we calculate

$$\begin{aligned} D_F^2\mathcal{J}(0)(\theta,\xi) &= D_E^2 J(\Omega)(\theta,\xi) - D_F\mathcal{J}(0)(D\theta\xi) \\ &= \int_\Omega \mathbf{S}_1^{2,E}(\theta) : D\xi + \mathbf{S}_0^{2,E}(\theta)\cdot\xi - \int_\Omega \operatorname{div}(\mathbf{S}_1^\mathsf{T} D\theta\xi). \end{aligned}$$

Then, using Lemma 1(1), we get

$$D_F^2\mathcal{J}(0)(\theta,\xi) = \int_\Omega \mathbf{S}_1^{2,E}(\theta) : D\xi + \mathbf{S}_0^{2,E}(\theta)\cdot\xi - \int_\Omega D\theta^\mathsf{T}\mathbf{S}_1 : D\xi + \xi\cdot\operatorname{div}(D\theta^\mathsf{T}\mathbf{S}_1),$$

which yields (25), also considering the regularity of $\mathbf{S}_1$ and the fact that $D_F^2\mathcal{J}(0)$ is a symmetric bilinear form.

Now, we assume in addition that Ω is Lipschitz. Expressions (28) and (30) follow immediately from the fact that $D_E^2 J(\Omega)(\theta,\xi)$ is the Eulerian shape derivative of $D_E J(\Omega)(\theta)$ according to Definition 5, so we can apply Proposition 1 to (24). To obtain (29), we write, using (25) and $\operatorname{div}(\mathbf{S}_1^{2,F}(\theta)) = \mathbf{S}_0^{2,F}(\theta)$,

$$D_F^2\mathcal{J}(0)(\theta,\xi) = \int_\Omega \mathbf{S}_1^{2,F}(\theta) : D\xi + \mathbf{S}_0^{2,F}(\theta)\cdot\xi = \int_\Omega \operatorname{div}(\mathbf{S}_1^{2,F}(\theta)^\mathsf{T}\xi),$$

and apply the divergence theorem [25, Section 4.3, Theorem 1], which gives the desired result. □

Remark 4. We may also write (27) as

$$\mathbf{S}_0^{2,F}(\theta) := \mathbf{S}_0^{2,E}(\theta) - D^2\theta\mathbf{S}_1 - D\theta^\mathsf{T}\mathbf{S}_0, \tag{31}$$

where the meaning of $D^2\theta\mathbf{S}_1$ needs to be clarified. Here, the second derivative $D^2\theta : \mathbb{R}^d \to \mathcal{L}(\mathbb{R}^d, \mathcal{L}(\mathbb{R}^d,\mathbb{R}^d))$ is a trilinear form and we use the notation $D^2\theta\xi$ for the bilinear form $D^2\theta\xi : x \mapsto D^2\theta(x)(\xi(x),\cdot,\cdot) \in \mathcal{L}(\mathbb{R}^d,\mathbb{R}^d)$. We also have

$$\mathbf{S}_1 : D^2\theta\xi = \sum_{i,j,k=1}^d \mathbf{S}_{1,ik}\frac{\partial^2\theta_i}{\partial x_k\partial x_j}\xi_j = \xi\cdot\left(\sum_{i=1}^d D^2\theta_i\mathbf{S}_{1,i}^\mathsf{T}\right),$$

where $\mathbf{S}_{1,i}^\mathsf{T}$ is the i-th column of $\mathbf{S}_1^\mathsf{T}$. For simplicity, let us adopt the notation

$$D^2\theta\mathbf{S}_1 := \sum_{i=1}^d D^2\theta_i\mathbf{S}_{1,i}^\mathsf{T}. \tag{32}$$

Using these notations, we have $D(D\theta\xi) = D^2\theta\xi + D\theta D\xi$. Then, a direct calculation shows that

$$\begin{aligned} \operatorname{div}(D\theta^\mathsf{T}\mathbf{S}_1)\cdot\xi &= \sum_{i,j,k=1}^d \mathbf{S}_{1,ik}\frac{\partial^2\theta_i}{\partial x_k\partial x_j}\xi_j + \sum_{i,j,k=1}^d \frac{\partial\theta_i}{\partial x_j}\frac{\partial\mathbf{S}_{1,ik}}{\partial x_k}\xi_j \\ &= D^2\theta\mathbf{S}_1\cdot\xi + \operatorname{div}(\mathbf{S}_1)\cdot D\theta\xi = D^2\theta\mathbf{S}_1\cdot\xi + D\theta^\mathsf{T}\mathbf{S}_0\cdot\xi, \end{aligned}$$

which yields (31).

We conclude this section by observing that expression (30) shows that $D_E^2 J(\Omega)(\theta,\xi)$ depends only on ξ_n and not on ξ_τ, which was expected since the second order Eulerian shape derivative is itself defined as a Eulerian semiderivative (see Definition 5), and hence should also satisfy the structure (9). In fact, (30) corresponds to a known structure of the second order Eulerian shape derivative; see [19, Chapter 9, Theorem 6.4] and [7]. On the other hand, the second order Fréchet shape derivative $D_F^2\mathcal{J}(0)(\theta,\xi)$ does not in general depend only on ξ_n but also on ξ_τ, as can be seen from the general structure (11).

In the next sections, we apply the results of Section 3 to the particular cases of the volume and the Dirichlet energy.

4. Shape derivatives of the volume

The case of the volume is relatively simple, since it does not involve the solution of a partial differential equation, but nevertheless instructive, as it exhibits the main mechanisms to compute the second order Eulerian and Fréchet shape derivatives for piecewise smooth domains. It is also useful for applications, since volume constraints are common in shape optimization, and the second order shape derivatives have an interesting structure due to Dirac measures appearing at the vertices. For $\Omega\in\mathbb{P}(\mathcal{D})$, denote by $V(\Omega)$ the volume of Ω and $\mathcal{V}(\theta) := V(\Omega_\theta)$ for $\theta\in\Theta_k^1$. We have the following result for Eulerian shape derivatives.

Proposition 4 *(Eulerian shape derivatives of the volume). Assume $\Omega\in\mathbb{P}(\mathcal{D})$, $\theta\in\mathcal{C}_c^2(\mathcal{D},\mathbb{R}^d)$ and $\xi\in\mathcal{C}_c^1(\mathcal{D},\mathbb{R}^d)$. Then*

$$D_E V(\Omega)(\theta) = \int_\Omega \mathbf{S}_1 : D\theta, \tag{33}$$

$$D_E^2 V(\Omega)(\theta,\xi) = \int_\Omega \mathbf{S}_1^{2,E}(\theta) : D\xi + \mathbf{S}_0^{2,E}(\theta)\cdot\xi, \tag{34}$$

where $\mathbf{S}_1 = \mathbf{I}_d$, $\mathbf{S}_1^{2,E}(\theta) = (\mathbf{S}_1 : D\theta)\mathbf{I}_d = \operatorname{div}(\theta)\mathbf{I}_d$ and $\mathbf{S}_0^{2,E}(\theta) = \nabla\operatorname{div}(\theta)$.

If in addition Ω is Lipschitz, we get

$$D_E V(\Omega)(\theta) = \int_{\partial\Omega} \theta_n, \tag{35}$$

$$D_E^2 V(\Omega)(\theta,\xi) = \int_{\partial\Omega} (\operatorname{div}\theta)\xi_n. \tag{36}$$

If in addition Ω is $\mathcal{C}^2$, we have

$$D_E^2 V(\Omega)(\theta,\xi) = \int_{\partial\Omega} (d-1)\mathcal{H}\xi_n\theta_n + D_E V(\Omega)([D\theta n\cdot n\xi_n - \nabla_\Gamma\xi_n\cdot\theta_\tau]n). \tag{37}$$

If $\Omega\subset\mathbb{R}^2$ is a $\mathcal{C}^2$ curvilinear m-gon, we have

$$\begin{aligned} D_E^2 V(\Omega)(\theta,\xi) = &\sum_{i=1}^m \int_{\Gamma_i} \mathcal{H}\xi_n\theta_n + D\theta n\cdot n\xi_n - \nabla_\Gamma\xi_n\cdot\theta_\tau \\ &+ \sum_{i=1}^m [(\xi\cdot n^-)(\theta\cdot\tau^-) - (\xi\cdot n^+)(\theta\cdot\tau^+)](a_i), \end{aligned} \tag{38}$$

where $a_i, i\in I$ are the vertices of Ω.

Proof. Using the change of variables $x \mapsto T_s^\theta(x)$ we get

$$V(\Omega_s) = \int\limits_{\Omega_s} 1 = \int\limits_{\Omega} \det DT_s^\theta.$$

Hence, we get $D_E V(\Omega)(\theta) = \int_\Omega \operatorname{div}(\theta)$ and then (33). Further, (35) follows from (18).

In view of Definition 5, the second order Eulerian shape derivative is given by

$$\begin{aligned}
D_E^2 V(\Omega)(\theta,\xi) &= \frac{d}{dt}\left(D_E V(T_t^\xi(\Omega))(\theta)\right)_{|t=0} = \frac{d}{dt}\left(\int\limits_{T_t^\xi(\Omega)} \mathbf{I}_d : D\theta\right)_{|t=0} \\
&= \frac{d}{dt}\left(\int\limits_{\Omega} \mathbf{I}_d : D\theta \circ T_t^\xi \det DT_t^\xi\right)_{|t=0} \\
&= \int\limits_{\Omega} \mathbf{I}_d : (D^2\theta\xi + \operatorname{div}\xi D\theta) = \int\limits_{\Omega} D^2\theta\mathbf{I}_d : \xi + (\mathbf{I}_d : D\theta)(\mathbf{I}_d : D\xi),
\end{aligned}$$

where $D^2\theta\mathbf{I}_d := \sum_{i=1}^d D^2\theta_i \mathbf{I}_{d,i}^\mathsf{T}$, using the notation (32). We compute

$$D^2\theta\mathbf{I}_d := \sum_{i=1}^d D^2\theta_i\mathbf{I}_{d,i} = \sum_{i=1}^d \nabla(\partial_i\theta_i) = \nabla\operatorname{div}(\theta),$$

which yields (34). Expression (36) follows immediately from (34) and (28).

Now assume that Ω is $\mathcal{C}^2$. From (36) we have, using the definition of $\operatorname{div}_\Gamma$,

$$D_E^2 V(\Omega)(\theta,\xi) = \int\limits_{\partial\Omega} (\operatorname{div}\theta)\xi_n = \int\limits_{\partial\Omega} \xi_n \operatorname{div}_\Gamma\theta + D\theta n\cdot n\xi_n.$$

Using $\operatorname{div}_\Gamma(\xi_n\theta) = \nabla_\Gamma\xi_n\cdot\theta_\tau + \xi_n\operatorname{div}_\Gamma\theta$, we get

$$D_E^2 V(\Omega)(\theta,\xi) = \int\limits_{\partial\Omega} \operatorname{div}_\Gamma(\xi_n\theta) - \nabla_\Gamma\xi_n\cdot\theta_\tau + D\theta n\cdot n\xi_n.$$

Since Ω is $\mathcal{C}^2$, and in view if (35), we obtain (37) using Theorem 1.

If $\Omega\subset\mathbb{R}^2$ is a $\mathcal{C}^2$ curvilinear m-gon, then we first write the boundary expression (35) as a sum of integrals on Γ_i, then we perform the same calculation as in the $\mathcal{C}^k$-case on each Γ_i. This yields the formula

$$D_E^2 V(\Omega)(\theta,\xi) = \sum_{i=1}^m \int\limits_{\Gamma_i} \operatorname{div}_\Gamma(\xi_n\theta) - \nabla_\Gamma\xi_n\cdot\theta_\tau + D\theta n\cdot n\xi_n.$$

Then, using Theorem 2 on each Γ_i and using the notation $a_0 := a_m$, we get

$$\sum_{i=1}^m \int\limits_{\Gamma_i} \operatorname{div}_\Gamma(\xi_n\theta) = \sum_{i=1}^m \int\limits_{\Gamma_i} \mathcal{H}\xi_n\theta_n + \sum_{i=1}^m [(\xi\cdot n^-)(\theta\cdot\tau^-)](a_i) - [(\xi\cdot n^+)(\theta\cdot\tau^+)](a_{i-1}),$$

which yields (38). □

Expression (36) can be found in [18, Example 4.1]. Expression (37) corresponds for instance to the first expression in [19, Chapter 9, Section 6.1 (6.3)]. In [59, Proposition 3.15], a formula similar to (38) is obtained for the first order Eulerian shape derivative of a boundary integral. The notable difference between formulae (37) and (38) is the appearance of the Dirac measures at the vertices a_i. Note also that formula (36), despite being valid for Lipschitz domains and therefore also for curvilinear polygons, does not involve Dirac measures.

Proposition 5 *(Fréchet shape derivatives of the volume). Assume* $\Omega \in \mathbb{P}(\mathcal{D})$, $\theta, \xi \in \mathcal{C}_c^2(\mathcal{D}, \mathbb{R}^d)$. *Then*

$$D_F^2\mathcal{V}(0)(\theta,\xi) = \int_\Omega \mathbf{S}_1^{2,F}(\theta) : D\xi = \int_\Omega \mathbf{S}_1^{2,F}(\xi) : D\theta, \tag{39}$$

with $\mathbf{S}_1^{2,F}(\theta) = (\mathbf{S}_1 : D\theta)\mathbf{I}_d - D\theta^\mathsf{T} = \operatorname{div}(\theta)\mathbf{I}_d - D\theta^\mathsf{T}$ *and* $\operatorname{div}(\mathbf{S}_1^{2,F}(\theta)) = 0$.

If in addition Ω *is Lipschitz we have*

$$D_F^2\mathcal{V}(0)(\theta,\xi) = \int_{\partial\Omega} ((\operatorname{div}\theta)n - D\theta^\mathsf{T} n)\cdot\xi. \tag{40}$$

If in addition Ω *is* $\mathcal{C}^2$, *we have*

$$D_F^2\mathcal{V}(0)(\theta,\xi) = \int_{\partial\Omega} (d-1)\mathcal{H}\xi_n\theta_n + D_F\mathcal{V}(0)([D_\Gamma n\xi_\tau\cdot\theta_\tau - \nabla_\Gamma\xi_n\cdot\theta_\tau - \nabla_\Gamma\theta_n\cdot\xi_\tau]n). \tag{41}$$

If $\Omega \subset \mathbb{R}^2$ *is a* $\mathcal{C}^2$ *curvilinear* m*-gon, we have*

$$D_F^2\mathcal{V}(0)(\theta,\xi) = \sum_{i=1}^m M_i\theta(a_i)\cdot\xi(a_i) + \sum_{i=1}^m \int_{\Gamma_i} \mathcal{H}\xi_n\theta_n + D_\Gamma n\xi_\tau\cdot\theta_\tau - \nabla_\Gamma\xi_n\cdot\theta_\tau - \nabla_\Gamma\theta_n\cdot\xi_\tau, \tag{42}$$

where $a_i, i \in I$ *are the vertices of* Ω, *and* $M_i := [n^- \otimes \tau^- - n^+ \otimes \tau^+](a_i)$ *is a symmetric matrix.*

Proof. The distributed expression (39) follows immediately from (34) and Proposition 3. We obtain using Proposition 3 and $\mathbf{S}_1 = \mathbf{I}_d$ that

$$\operatorname{div}(\mathbf{S}_1^{2,F}(\theta)) = \mathbf{S}_0^{2,F}(\theta) = \mathbf{S}_0^{2,E}(\theta) - \operatorname{div}(D\theta^\mathsf{T}\mathbf{S}_1) = \nabla\operatorname{div}(\theta) - \nabla\operatorname{div}(\theta) = 0.$$

If in addition Ω is Lipschitz, then boundary expression (40) follows from (29).

Now assume that Ω is $\mathcal{C}^2$. From (40) we have, using the definition of $\operatorname{div}_\Gamma$ and Lemma 2,

$$\begin{aligned} D_F^2\mathcal{V}(0)(\theta,\xi) &= \int_{\partial\Omega} ((\operatorname{div}\theta)n - D\theta^\mathsf{T} n)\cdot\xi = \int_{\partial\Omega} (\operatorname{div}\theta - D\theta^\mathsf{T} n\cdot n)\xi_n - \xi_\tau\cdot D\theta^\mathsf{T} n \\ &= \int_{\partial\Omega} \xi_n \operatorname{div}_\Gamma\theta - \nabla_\Gamma\theta_n\cdot\xi_\tau + D_\Gamma n\xi_\tau\cdot\theta_\tau. \end{aligned}$$

Using the property $\operatorname{div}_\Gamma(\xi_n\theta) = \nabla_\Gamma\xi_n\cdot\theta_\tau + \xi_n\operatorname{div}_\Gamma\theta$, we get

$$D_F^2\mathcal{V}(0)(\theta,\xi) = \int_{\partial\Omega} \operatorname{div}_\Gamma(\xi_n\theta) + D_\Gamma n\xi_\tau\cdot\theta_\tau - \nabla_\Gamma\xi_n\cdot\theta_\tau - \nabla_\Gamma\theta_n\cdot\xi_\tau.$$

Since Ω is $\mathcal{C}^2$, we obtain (41) using Theorem 1.

If $\Omega \subset \mathbb{R}^2$ is a $\mathcal{C}^2$ curvilinear m-gon, then proceeding in the same way as in the proof of Proposition 4, we obtain

$$D_F^2\mathcal{V}(0)(\theta,\xi) = \sum_{i=1}^{m}\int_{\Gamma_i} \mathcal{H}\xi_n\theta_n + D_\Gamma n\xi_\tau\cdot\theta_\tau - \nabla_\Gamma\xi_n\cdot\theta_\tau - \nabla_\Gamma\theta_n\cdot\xi_\tau$$
$$+\sum_{i=1}^{m}[(\xi\cdot n^-)(\theta\cdot\tau^-) - (\xi\cdot n^+)(\theta\cdot\tau^+)](a_i).$$

Applying Lemma 1(5), we have

$$[(\xi\cdot n^-)(\theta\cdot\tau^-) - (\xi\cdot n^+)(\theta\cdot\tau^+)](a_i) = [\xi\cdot(n^-\otimes\tau^- - n^+\otimes\tau^+)\theta](a_i) = M_i\theta(a_i)\cdot\xi(a_i).$$

To show that M_i is symmetric, let $\{e_1, e_2\}$ be an orthonormal basis of $\mathbb{R}^2$, and denote $b_1\wedge b_2 := \frac{1}{2}(b_1\otimes b_2 - b_2\otimes b_1)$ the wedge product of two vectors b_1, b_2 of $\mathbb{R}^2$. Since $\{\tau^-, n^-\}$ are orthonormal, we have $\det[n^-,\tau^-] = -1$, and in the same way $\det[n^+,\tau^+] = -1$. Then we compute

$$M_i - M_i^\mathsf{T} = [(n^-\otimes\tau^- - \tau^-\otimes n^-) - (n^+\otimes\tau^+ - \tau^+\otimes n^+)](a_i) = 2[(n^-\wedge\tau^- - n^+\wedge\tau^+)](a_i)$$
$$= 2(\det[n^-,\tau^-] - \det[n^+,\tau^+])(a_i)e_1\wedge e_2 = 0,$$

showing that M_i is indeed symmetric. □

Expression (41) is the known formula encountered in the literature for the second order Fréchet derivative of the volume for $\mathcal{C}^2$-domains; see for instance [53, Proposition 5.1]. In (41), the structure (12) of the second order Fréchet shape derivative is apparent. We also observe that (42) shares similarities with the usual formula for the Fréchet derivative of the perimeter functional (in particular the curvature term $\mathcal{H}$), which was expected since the first order shape derivative of the volume can be written as a boundary integral; compare with the Fréchet derivative of the perimeter computed in [43, Example 2.5 and Proposition 2.6]. However, a notable difference with the derivative of the perimeter is the presence of the normal vectors $n^-(a_i)$ and $n^+(a_i)$ in M_i.

When Ω is $\mathcal{C}^2$, we can also directly compute (41) from (37) using the decomposition (14), which in this case reads

$$D_E^2V(\Omega)(\theta,\xi) = D_F^2\mathcal{V}(0)(\theta,\xi) + D_F\mathcal{V}(0)(D\theta\xi). \tag{43}$$

Indeed using (37), (43) and

$$D_F\mathcal{V}(0)(D\theta\xi) = \int_{\partial\Omega} D\theta\xi\cdot n = \int_{\partial\Omega}(D\theta n\cdot n)\xi_n + \nabla_\Gamma\theta_n\cdot\xi_\tau - D_\Gamma n\xi_\tau\cdot\theta_\tau$$

we get (41).

Propositions 4 and 5 show that a range of explicit boundary expressions for the second order shape derivative can be obtained, starting from the distributed shape derivative which is valid for open sets in the case of the volume functional. Observe that in the proofs of Propositions 4 and 5, the strategy to obtain the canonical structure of the boundary expressions for smooth domains consists in manipulating the intermediate boundary expression so that $\operatorname{div}_\Gamma(\xi_n\theta)$ appears, and then applying the tangential divergence theorem. In the case of curvilinear polygons, the strategy is the same, but the tangential divergence theorem is applied on each Γ_i, which yields the terms at the vertices a_i in (38) and (42). This general methodology can also be used for functionals depending on the solution of a BVP, as will be seen in Sections 6 and 7.

5. Regularity results for the Dirichlet problem in nonsmooth domains

In the next sections we will study shape derivatives when the functional depends on the solution of a BVP. We focus on the Laplacian with homogeneous Dirichlet conditions due in part to its simplicity, but mainly in view of the existence of many fine regularity results for domains Ω with low regularity, such as Lipschitz, convex, semiconvex and polygonal domains. In a similar fashion, sharp regularity results for second order elliptic PDEs were a key element used in [45] to prove continuity results for shape derivatives around these types of nonsmooth domains. Here, this allows us to explore several possible expressions of the shape derivatives for this problem, depending on the regularity of Ω. In this section we gather known regularity results for the Dirichlet problem in nonsmooth domains that will be useful to compute shape derivatives in the next sections.

For $\Omega \in \mathbb{P}(\mathcal{D})$ and $f \in H^1(\mathcal{D})$, let $u \in H_0^1(\Omega)$ be the solution of the Dirichlet problem

$$\int_\Omega \nabla u \cdot \nabla v = \int_\Omega f v, \qquad \forall v \in H_0^1(\Omega), \tag{44}$$

and define the shape functional

$$J(\Omega) := \frac{1}{2} \int_\Omega |\nabla u|^2.$$

Note that $J(\Omega)$ is the opposite of the Dirichlet energy associated with (44). It is well-known that if Ω is smooth, the regularity of the solution u of (44) depends only on the regularity of f, i.e. if $f \in H^s(\Omega)$, then we have $u \in H^{s+2}(\Omega)$. However, when Ω is not smooth, the regularity of u also depends on the regularity of Ω. There exists a vast literature on this topic for elliptic problems. In the present paper, we are interested in four particular classes of nonsmooth domains: (i) Ω Lipschitz, (ii) Ω semiconvex, (iii) Ω convex, (iv) Ω is a polygon or a curvilinear polygon. In the latter case, singularities depending on the interior angles appear at the vertices. These singularities have been studied extensively for elliptic operators; see [11,13–15,41,50]. In this section and for the rest of the paper, we will only consider the case of polygons with straight sides, for which regularity results in L^p are available; see Theorems 5 and 6. These regularity results in L^p will be useful to derive certain expressions of the shape derivatives further.

Following Definition 2, recall that the vertices of a m-gon $\Omega \subset \mathbb{R}^2$ are denoted a_i and the interior angles $0 < \alpha_i < 2\pi$, $\alpha_i \neq \pi$, for $i \in I$. Let (r_i, ϑ_i) be local polar coordinates with origin a_i and such that the internal angle α_i is spanned by the half-lines $\vartheta_i = 0$ and $\vartheta_i = \alpha_i$. We introduce the notations $\hat{\alpha} := \max_{i \in I} \alpha_i$ and also $\hat{p} := 2\hat{\alpha}/(2\hat{\alpha} - \pi)$ if $\hat{\alpha} > \pi/2$ and $\hat{p} = \infty$ if $\hat{\alpha} \leq \pi/2$. Let also $\chi_i(r_i)$ be a smooth cutoff function equal to 1 in a neighbourhood of the vertex a_i and 0 at all other vertices of Ω.

We start with a Theorem on $W^{2,p}$-regularity which is a particular case of [33, Theorem 4.4.3.7], where general boundary conditions are treated. Here, we restrict ourselves to the case of Dirichlet boundary conditions.

Theorem 5. *Let $\Omega \subset \mathbb{R}^2$ be a m-gon. Let $1 < p < \infty$ be such that $k_i := 2\alpha_i(p-1)/(p\pi)$ is non-integer for all $i \in I$. Let u be the solution of (44) with $f \in L^p(\Omega)$. Then, there exist coefficients $c_{i,k}$ such that*

$$u = u_r + \sum_{i \in I} w_i, \tag{45}$$

with $u_r \in W^{2,p}(\Omega)$ and

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$$w_i := \chi_i(r_i) \sum_{\substack{1 \le k < k_i, \\ k \in \mathbb{N}}} c_{i,k} r_i^{\frac{k\pi}{\alpha_i}} \sin\left(\frac{k\pi\vartheta_i}{\alpha_i}\right). \tag{46}$$

The relevance of Theorem 5 for our purposes is the following. If the sum in (46) is void, then we get $u = u_r \in W^{2,p}(\Omega)$. To get a void sum, we need $\max_{i \in I} k_i = 2\alpha_i(p-1)/(p\pi) < 1$, thus we deduce the range $p \in (1, \hat{p})$ for which we have $u \in W^{2,p}(\Omega)$. Note that within this range, the condition of Theorem 5 requesting k_i to be non-integer for all $i \in I$ is satisfied since $\max_{i \in I} k_i < 1$.

We have the following regularity results for the solution u of (44).

Theorem 6. *Assume $f \in H^1(\mathcal{D})$ and $\Omega \in \mathbb{P}(\mathcal{D})$.*

1. *We have $u \in H_0^1(\Omega)$.*
2. *If Ω is Lipschitz, we have $u \in H^{3/2}(\Omega)$.*
3. *If Ω is semiconvex, we have $u \in H^2(\Omega)$.*
4. *If Ω is a m-gon with corner angles $0 < \alpha_i < 2\pi$, $i \in I$, then $\hat{p} \in (4/3, \infty)$ and $u \in W^{2,p}(\Omega)$ for all $p \in (1, \hat{p})$. Moreover, $\hat{p} \in (4/3, 2)$ if Ω is a nonconvex m-gon.*

Proof. Item (1) is a standard result, see for instance [35, Proposition 3.1.20]. For (2), we refer to [40, Theorem B, p. 163]. For (3), we can apply [51, Theorem 5.5] since $f \in H^1(\mathcal{D})$. Regarding (4), $\hat{p} \in (4/3, \infty)$ is clear in view of the definition of $\hat{p}$, and we can apply Theorem 5 since $f \in H^1(\mathcal{D}) \subset L^p(\Omega)$ for all $p \in (1, \infty)$. Then, for $p \in (1, \hat{p})$ the sum in (46) is void and the regularity of u follows. When Ω is a nonconvex m-gon, we have $\hat{\alpha} > \pi$ which implies $\hat{p} \in (4/3, 2)$. □

We will also need the following result which can be found in [10, Theorem 2.3].

Theorem 7. *Let $\Omega \subset \mathbb{R}^2$ be a m-gon. Let u be the solution of (44) with $f \in H^{s-1}(\Omega)$, $s > 0$. Then, there exist coefficients $c_{i,\lambda}$ such that*

$$u = u_r + \sum_{i \in I} w_i, \tag{47}$$

with $u_r \in H^{1+s}(\Omega)$ and

$$w_i := \chi_i(r_i) \sum_{\substack{0 < \lambda < s, \\ \lambda \in \Lambda_i}} c_{i,\lambda} \Phi_{i,\lambda}(r_i, \vartheta_i), \tag{48}$$

where $\Lambda_i := \{\frac{k\pi}{\alpha_i}, k \in \mathbb{Z}^*\}$ and

$$\Phi_{i,\lambda}(r_i, \vartheta_i) := \begin{cases} r_i^\lambda \sin(\lambda\vartheta_i) & \text{if } \lambda \notin \mathbb{N}, \\ r_i^\lambda(\log(r_i)\sin(\lambda\vartheta_i) + \vartheta_i\cos(\lambda\vartheta_i)) - \frac{1}{\alpha_i}(-\frac{y_i}{\sin\alpha_i})^\lambda & \text{if } \lambda \in \mathbb{N}, \end{cases} \tag{49}$$

where $(x_i, y_i) = (r_i \cos\vartheta_i, r_i \sin\vartheta_i)$.

Note that Theorem 5 treats the case of L^p-regularity, whereas Theorem 7 deals with the case of higher L^2-regularity. The cases covered by the two theorems have a small intersection, indeed if we take $p = 2$ and Ω convex in Theorem 5, we get that the sum in (46) is empty and $u_r \in W^{2,2}(\Omega)$. In Theorem 7, we get the same result by choosing Ω convex and $s = 1$, indeed in this case it is easy to see that the sum in (48) is void since $\lambda \in \Lambda_i$ would have to be strictly greater than 1 but we also require $\lambda < s = 1$.

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We immediately deduce from Theorem 7 the following regularity result which will be convenient to describe the regularity of D^2u further.

Corollary 1. *Let $\Omega \subset \mathbb{R}^2$ be a m-gon and $f \in H^{s-1}(\Omega)$, $s > 0$. Then $u \in H^{1+s}(\Omega)$ for every $s < \pi/\hat{\alpha}$.*

Proof. Take $s < \pi/\hat{\alpha}$ in Theorem 7. Then, in the sum appearing in (48), we have for all $i \in I$ that $\lambda \in \Lambda_i$ implies $\lambda \geq \pi/\alpha_i \geq \pi/\hat{\alpha}$, but since we also require $\lambda < s < \pi/\hat{\alpha}$, the sum in (48) is void for all $i \in I$ and we get $u = u_r \in H^{1+s}(\Omega)$. □

Theorem 8. *Let $\Omega \subset \mathbb{R}^2$ be a convex m-gon. Let u be the solution of (44) with $f \in H^{s-1}(\Omega)$, $s = 3/2 + \delta$ and $0 < \delta < 1/2$, then $\nabla u \in \mathcal{C}^0(\overline{\Omega})$ and $D^2u|_{\partial\Omega} \in L^1(\partial\Omega)$.*

Proof. In view of Corollary 1 we have $u \in H^q(\Omega)$ with $q > 2$. Thus, $\nabla u \in H^{q-1}(\Omega) \subset \mathcal{C}^0(\overline{\Omega})$. Then, applying Theorem 7 we get $u_r \in H^{5/2+\delta}(\Omega)$. Since Ω is a convex m-gon, we have $\pi/\alpha_i > 1$ for all $i \in I$ and therefore for any $i \in I$ there is at most one term in the sum in (48), corresponding to $\lambda = \pi/\alpha_i$. If $\pi/\alpha_i > s = 3/2+\delta$, then the sum in (48) is empty, but the following reasoning is still valid by taking $c_{i,\lambda} = 0$. In view of (47) we have

$$D^2u = D^2u_r + \sum_{i \in I} D^2 w_i, \tag{50}$$

with $D^2u_r \in H^{s-1}(\Omega)$. Since $s - 1 = 1/2 + \delta > 1/2$, according to [21] we can take the trace of D^2u_r on $\partial\Omega$ and we have $D^2u_r|_{\partial\Omega} \in H^\delta(\partial\Omega)$. In view of (48) and (49), the singular terms in w_i are of the type $r^{\frac{\pi}{\alpha_i}}$. Indeed, the case $\lambda \in \mathbb{N}$ in (49) does not occur since we require $0 < \lambda < s < 2$ in (48), and the case $\lambda = 1$ would imply $\alpha_i = \pi$ or $\alpha_i = 2\pi$, which are excluded. Thus, the singular terms in D^2w_i are of the type $r^{\frac{\pi}{\alpha_i}-2}$. We have $\partial\Omega = \bigcup_{i\in I} \overline{\Gamma_i}$, where Γ_i are open segments, and $\frac{\pi}{\alpha_i} - 2 > -1$ since Ω is a convex m-gon. Thus, $D^2w_i|_{\Gamma_i} \in L^1(\Gamma_i)$ and $D^2w_i|_{\Gamma_{i+1}} \in L^1(\Gamma_{i+1})$. Finally, considering the regularity of D^2u_r and D^2w_i, in view of (50) we have shown that $D^2u|_{\partial\Omega} \in L^1(\partial\Omega)$. □

6. First order shape derivatives of the Dirichlet energy

For $\theta \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^d)$, consider the flow T^θ_s as defined in Section 2.1, the perturbed domain $\Omega_s := T^\theta_s(\Omega)$, and define u_s the solution of the perturbed problem

$$\int_{\Omega_s} \nabla u_s \cdot \nabla v_s = \int_{\Omega_s} f v_s, \qquad \forall v_s \in H^1_0(\Omega_s).$$

Using the change of variable $x \mapsto T^\theta_s(x)$, the shape functional evaluated on the perturbed domain is

$$J(\Omega_s) = \frac{1}{2} \int_{\Omega_s} |\nabla u_s|^2 = \frac{1}{2} \int_{\Omega} A(s) \nabla u^s \cdot \nabla u^s, \tag{51}$$

with $u^s := u_s \circ T^\theta_s$ and $A(s) := (\det DT^\theta_s)(DT^\theta_s)^{-1}(DT^\theta_s)^{-\mathsf{T}}$. After the change of variables $x \mapsto T^\theta_s(x)$ we obtain the variational equation

$$\int_{\Omega} A(s) \nabla u^s \cdot \nabla v = \int_{\Omega} F(s) v, \qquad \forall v \in H^1_0(\Omega), \tag{52}$$

with $F(s) := f \circ T^\theta_s \det DT^\theta_s$. Adapting the results from [19, Theorem 4.1, p. 482] and [60, Lemma 2.16], we can show that $s \mapsto A(s)$ belongs to $\mathcal{C}^1([0, t_0]; \mathcal{C}^0(\mathcal{D}, \mathbb{R}^{d\times d}))$ and $s \mapsto F(s)$ to $\mathcal{C}^1([0, t_0]; L^2(\mathcal{D}))$. When Ω is of

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class $\mathcal{C}^k$, $k \geq 1$, it is shown in [59, Proposition 2.82] that $s^{-1}(u^s - u)$ converges strongly to $\dot{u}(\theta)$ in $H_0^1(\Omega)$, where $\dot{u}(\theta)$ is the so-called *material derivative* of u^s solution of

$$\int_\Omega \nabla\dot{u}(\theta)\cdot\nabla v = -\int_\Omega A'(\theta)\nabla u\cdot\nabla v + \int_\Omega F'(\theta)v, \qquad \forall v \in H_0^1(\Omega), \tag{53}$$

with

$$A'(\theta) := \frac{dA}{ds}(0) = -D\theta - D\theta^\mathsf{T} + (\operatorname{div}\theta)\mathbf{I}_d, \tag{54}$$

$$F'(\theta) := \frac{dF}{ds}(0) = \operatorname{div}(f\theta). \tag{55}$$

Expression (53) is obtained by differentiating (52) with respect to s. The proof of [59, Proposition 2.82] extends straightforwardly to the case where Ω is open.

Proposition 6. *Assume $\Omega \in \mathbb{P}(\mathcal{D})$, $f \in H^1(\mathcal{D})$ and $\theta \in \mathcal{C}_c^1(\mathcal{D}, \mathbb{R}^d)$. The distributed expression of the shape derivative of $J(\Omega)$ is given by*

$$D_E J(\Omega)(\theta) = \int_\Omega \mathbf{S}_1 : D\theta + \mathbf{S}_0\cdot\theta, \tag{56}$$

with $\mathbf{S}_1 \in L^1(\Omega, \mathbb{R}^{d\times d})$, $\mathbf{S}_0 \in L^1(\Omega, \mathbb{R}^d)$ and

$$\mathbf{S}_1 = \left(-\frac{1}{2}|\nabla u|^2 + uf\right)\mathbf{I}_d + \nabla u\otimes\nabla u, \qquad \mathbf{S}_0 = \operatorname{div}(\mathbf{S}_1) = u\nabla f. \tag{57}$$

If, in addition, $\Omega \subset \mathbb{R}^d$ is semiconvex, or if $\Omega \in \mathbb{R}^2$ is a m-gon, then we obtain the boundary expression

$$D_E J(\Omega)(\theta) = \int_{\partial\Omega} \frac{|\partial_n u|^2}{2}\theta_n. \tag{58}$$

Proof. Taking the derivative with respect to s of expression (51) at $s = 0$ yields

$$D_E J(\Omega)(\theta) = \frac{1}{2}\int_\Omega A'(\theta)\nabla u\cdot\nabla u + \int_\Omega \nabla\dot{u}(\theta)\cdot\nabla u.$$

Then, using (53) with $v = u$ we get

$$D_E J(\Omega)(\theta) = -\frac{1}{2}\int_\Omega A'(\theta)\nabla u\cdot\nabla u + \int_\Omega F'(\theta)u.$$

Using (54)-(55) and rearranging the terms using $\operatorname{div}(\theta) = \mathbf{I}_d : D\theta$ and $D\theta : (\nabla u\otimes\nabla u) = D\theta\nabla u\cdot\nabla u$, we obtain (56). An explicit calculation using Lemma 1(6) shows that $\mathbf{S}_0 = \operatorname{div}(\mathbf{S}_1)$.

If Ω is semiconvex, then in view of Theorem 6(3) we have $u \in H^2(\Omega)$, since $f \in H^1(\mathcal{D})$. Thus, we have $D^2u \in L^2(\Omega, \mathbb{R}^{d\times d})$, $|\nabla u|^2 \in L^1(\Omega)$ and $\nabla|\nabla u|^2 = 2D^2u\nabla u \in L^1(\Omega, \mathbb{R}^d)$. Proceeding in a similar way for the other terms of $\mathbf{S}_1$, we get $\mathbf{S}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, and we can apply (18) from Proposition 1 to get

$$D_E J(\Omega)(\theta) = \int_{\partial\Omega} (\mathbf{S}_1 n)\cdot\theta. \tag{59}$$

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Using $u = 0$ on $\partial\Omega$ we have $\nabla u = (\partial_n u)n$ almost everywhere on $\partial\Omega$, which yields (58) after a simple calculation using (57).

When $\Omega \subset \mathbb{R}^2$ is a m-gon, we have in view of Theorem 5 and Theorem 6(4) that $u \in W^{2,p}(\Omega)$ for all $p \in (1, \hat{p})$, with $\hat{p} > 4/3$. Using Sobolev embeddings, we have that $\nabla u \in W^{1,p}(\Omega, \mathbb{R}^2) \subset L^4(\Omega, \mathbb{R}^2)$, thus $|\nabla u|^2 \in L^2(\Omega)$. Since $D^2 u \in L^p(\Omega, \mathbb{R}^{2\times 2})$ for all $p \in (1, \hat{p})$, we have in particular $D^2 u \in L^{4/3}(\Omega, \mathbb{R}^{2\times 2})$ and we get $\nabla |\nabla u|^2 = 2D^2 u \nabla u \in L^1(\Omega, \mathbb{R}^2)$. This yields $|\nabla u|^2 \in W^{1,1}(\Omega)$. Proceeding in a similar way for the other terms of $\mathbf{S}_1$, we obtain $\mathbf{S}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, and we can apply (18) from Proposition 1 to get (59) and then (58). □

Remark 5. In Proposition 6, we have obtained the boundary expression of the shape derivative for semiconvex and polygonal domains. When Ω is only Lipschitz, it is not clear whether or not the shape derivative can be written as a boundary integral. Indeed, in [9, Corollary 3.2] Costabel constructs a $\mathcal{C}^1$-domain for which the solution u of the Dirichlet Laplacian does not belong to $H^{3/2+\delta}(\Omega)$ for all $\delta > 0$, even for $f \in \mathcal{C}^\infty(\overline{\Omega})$. Thus, the regularity result $u \in H^{3/2}(\Omega)$ of Theorem 6(2) is sharp in the class of Lipschitz domains. Also, in [40, Proposition 3.2., pp. 176], Jerison and Kenig have built a $\mathcal{C}^1$-domain for which the trace of a function $g \in H^{3/2,2}(\mathbb{R}^2)$ on $\partial\Omega$ does not have a tangential derivative in $L^2(\partial\Omega)$. Thus, it is not clear if the trace of $|\nabla u|$ is in $L^2(\partial\Omega)$ for the solution u of (44), and we cannot conclude that $\mathbf{S}_1$ given by (57) has a trace in $L^1(\partial\Omega)$ when Ω is only Lipschitz.

6.1. Alternative expressions of the distributed shape derivative

In this section we investigate alternative tensor representations for (57) in the spirit of Proposition 2. Assume $\Omega \in \mathbb{P}(\mathcal{D})$ is semiconvex, then $u \in H^2(\Omega)$ in view of Theorem 6(3). In view of (58), a natural choice for $\widehat{\mathbf{S}}_1$ is

$$\widehat{\mathbf{S}}_1 = \frac{|\nabla u|^2}{2}\mathbf{I}_d,$$

which yields, using Lemma 1(6),

$$\widehat{\mathbf{S}}_0 = \mathrm{div}(\widehat{\mathbf{S}}_1) = \frac{1}{2}\,\mathrm{div}(|\nabla u|^2 \mathbf{I}_d) = \frac{1}{2}\nabla(|\nabla u|^2) = D^2 u \nabla u.$$

We have indeed

$$\widehat{\mathbf{S}}_1 n = \frac{|\partial_n u|^2}{2} n = \mathbf{S}_1 n \quad \text{ on } \partial\Omega,$$

therefore $\widehat{\mathbf{S}}_1$ satisfies condition (21) of Proposition 2. Using $u \in H^2(\Omega)$, we get $\widehat{\mathbf{S}}_0 \in L^1(\Omega, \mathbb{R}^d)$ and $\widehat{\mathbf{S}}_1 \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$. Thus, we obtain the following alternative expression of the distributed shape derivative (56):

$$D_E J(\Omega)(\theta) = \int_\Omega \widehat{\mathbf{S}}_1 : D\theta + \widehat{\mathbf{S}}_0 \cdot \theta = \int_\Omega \mathrm{div}(\widehat{\mathbf{S}}_1^\mathsf{T} \theta) = \frac{1}{2}\int_\Omega \mathrm{div}(|\nabla u|^2 \theta). \tag{60}$$

We observe that expression (60) is simpler than (56) but requires more regularity for Ω, due to the presence of $D^2 u$ in $\widehat{\mathbf{S}}_0$.

Another admissible $\widehat{\mathbf{S}}_1$ would be

$$\widehat{\mathbf{S}}_1 = \frac{\nabla u \otimes \nabla u}{2},$$

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which also satisfies the conditions of Proposition 2. This choice yields, using Lemma 1(6) and assuming Ω semiconvex,

$$\widehat{\mathbf{S}}_0 = \operatorname{div}(\widehat{\mathbf{S}}_1) = \frac{1}{2}\operatorname{div}(\nabla u \otimes \nabla u) = \frac{\Delta u \nabla u + D^2 u \nabla u}{2} = \frac{-f\nabla u + D^2 u \nabla u}{2} \in L^1(\Omega, \mathbb{R}^d).$$

Note that this also requires more regularity for Ω than (57) due to the presence of $D^2 u$.

Another interesting choice which combines the two alternatives given above is

$$\widehat{\mathbf{S}}_1 = -\frac{1}{2}|\nabla u|^2 \mathbf{I}_d + \nabla u \otimes \nabla u, \qquad \widehat{\mathbf{S}}_0 = \operatorname{div}(\widehat{\mathbf{S}}_1) = -f\nabla u.$$

Indeed, this alternative is quite similar to (57), but is slightly simpler, and does not involve $D^2 u$ as in the other alternatives.

7. Second order distributed shape derivatives of the Dirichlet energy

The *shape derivative* $u'(\theta)$ of u is defined as (see [59])

$$u'(\theta) := \dot{u}(\theta) - \nabla u \cdot \theta. \tag{61}$$

We have the following regularity results for the material and shape derivatives of u.

Theorem 9. *Assume $\Omega \in \mathbb{P}(\mathcal{D})$, $\theta \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$ and $f \in H^1(\mathcal{D})$.*

1. *We have $\dot{u}(\theta) \in H^1_0(\Omega)$.*
2. *If Ω is semiconvex, we have $\dot{u}(\theta) \in H^2(\Omega)$ and $u'(\theta) \in H^1(\Omega)$.*
3. *If Ω is a m-gon with corner angles $0 < \alpha_i < 2\pi$, $i \in I$, then $\hat{p} \in (4/3, \infty)$ and $\dot{u}(\theta) \in W^{2,p}(\Omega)$ for all $p \in (1, \hat{p})$ if $\hat{p} \le 2$ and for all $p \in (1, 2]$ if $\hat{p} > 2$.*

Proof. (1) For Ω open we have $u \in H^1_0(\Omega)$ due to Theorem 6(1). Thus, in view of (53) we have

$$\int_\Omega \nabla \dot{u}(\theta) \cdot \nabla v = \langle \operatorname{div}(A'(\theta)\nabla u)), v\rangle_{H^{-1}(\Omega), H^1_0(\Omega)} + \int_\Omega \operatorname{div}(f\theta) v, \qquad \forall v \in H^1_0(\Omega). \tag{62}$$

Using [35, Proposition 3.1.20] we obtain $\dot{u}(\theta) \in H^1_0(\Omega)$.

(2) If Ω is semiconvex, then Theorem 6(3) yields $u \in H^2(\Omega)$. Thus, for $v \in H^1_0(\Omega)$ we have $(A'(\theta)\nabla u)v \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, and we can apply the divergence theorem (see [25, Section 4.3, Theorem 1]) on the right-hand side of (53), which yields

$$\int_\Omega \nabla \dot{u}(\theta) \cdot \nabla v = \int_\Omega (\operatorname{div}(f\theta) + \operatorname{div}(A'(\theta)\nabla u))v, \qquad \forall v \in H^1_0(\Omega). \tag{63}$$

Since $\theta \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$, we get $A'(\theta) \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^{d\times d})$. Thus, $\operatorname{div}(f\theta) + \operatorname{div}(A'(\theta)\nabla u) \in L^2(\Omega)$ and in view of (63) and [51, Theorem 5.5] we get $\dot{u}(\theta) \in H^2(\Omega)$. The regularity of the shape derivative $u'(\theta)$ is then an immediate consequence of definition (61) and the regularity of u and $\dot{u}(\theta)$.

(3) Since $f \in H^1(\mathcal{D}) \subset L^p(\mathcal{D})$ for all $p \in (1, \infty)$, applying Theorem 5 the solution u of (44) belongs to $W^{2,p}(\Omega)$ for all $p \in (1, \hat{p})$. Thus $\operatorname{div}(f\theta) + \operatorname{div}(A'(\theta)\nabla u) \in L^p(\Omega)$ for all $p \in (1, \hat{p})$ if $\hat{p} \le 2$ and for all $p \in (1, 2]$ if $\hat{p} > 2$. Applying Theorem 5 again, this proves item (3). □

7.1. Second order distributed Eulerian shape derivative

Assume $\Omega \in \mathbb{P}(\mathcal{D})$, $f \in H^2(\mathcal{D})$, $\theta \in \mathcal{C}_c^2(\mathcal{D}, \mathbb{R}^d)$ and $\xi \in \mathcal{C}_c^1(\mathcal{D}, \mathbb{R}^d)$. In view of definition (8) we have, using the notation $\Omega_t := T_t^\xi(\Omega)$,

$$D_E^2 J(\Omega)(\theta, \xi) = \left(\frac{d}{dt} D_E J(T_t^\xi(\Omega))(\theta)\right)_{|t=0} = \left(\frac{d}{dt}\int_{\Omega_t} \mathbf{S}_1(\Omega_t) : D\theta + \mathbf{S}_0(\Omega_t)\cdot\theta\right)_{|t=0}.$$

Using the change of variables $x \mapsto T_t^\xi(x)$, we get

$$\begin{aligned}
&D_E J(T_t^\xi(\Omega))(\theta)\\
&= \int_\Omega [\mathbf{S}_1(\Omega_t)\circ T_t^\xi : D\theta\circ T_t^\xi + \mathbf{S}_0(\Omega_t)\circ T_t^\xi\cdot\theta\circ T_t^\xi]\det DT_t^\xi\\
&= \int_\Omega \left[\left(-\frac{1}{2}B(t)\nabla u^t\cdot\nabla u^t + u^t f\circ T_t^\xi\right)\mathbf{I}_d + (DT_t^\xi)^{-\mathsf{T}}\nabla u^t \otimes (DT_t^\xi)^{-\mathsf{T}}\nabla u^t\right] : D\theta\circ T_t^\xi \det DT_t^\xi\\
&\quad + \int_\Omega [u^t\nabla f\circ T_t^\xi]\cdot\theta\circ T_t^\xi\det DT_t^\xi,
\end{aligned}$$

where $B(t) := (DT_t^\xi)^{-1}(DT_t^\xi)^{-\mathsf{T}}$ and $\mathbf{S}_0, \mathbf{S}_1$ are defined in (57). In a similar way as we proceeded for the function $s \mapsto A(s)$ in the proof of Proposition 6, we can show that the function $t \mapsto B(t)$ belongs to $\mathcal{C}^1([0, t_0]; \mathcal{C}^0(\mathcal{D}, \mathbb{R}^{d\times d}))$. We have also seen that $t \mapsto f\circ T_t^\xi \det DT_t^\xi$ belongs to $\mathcal{C}^1([0, t_0]; L^2(\mathcal{D}))$, and in a similar way we have that $t \mapsto \nabla f\circ T_t^\xi\det DT_t^\xi$ belongs to $\mathcal{C}^1([0, t_0]; L^2(\mathcal{D}, \mathbb{R}^d))$, as $\nabla f \in H^1(\mathcal{D}, \mathbb{R}^d)$. Since $t \mapsto u^t$ has the derivative $\dot{u}(\xi)$ in $H_0^1(\Omega)$, then $t \mapsto \nabla u^t$ has the derivative $\nabla\dot{u}(\xi)$ in $L^2(\Omega, \mathbb{R}^d)$. Gathering these results and taking the derivative of $D_E J(T_t^\xi(\Omega))(\theta)$ with respect to t, we obtain

$$\begin{aligned}
D_E^2 J(\Omega)(\theta, \xi) = &\int_\Omega \left(-2D\xi^{\mathsf{T}}\nabla u\odot\nabla u + \nabla u\otimes\nabla u\operatorname{div}\xi + 2\nabla\dot{u}(\xi)\odot\nabla u\right) : D\theta\\
&+ \int_\Omega \mathbf{S}_1 : D^2\theta\xi + [\dot{u}(\xi)\nabla f + uD^2 f\xi + u\operatorname{div}\xi\nabla f]\cdot\theta + \mathbf{S}_0\cdot D\theta\xi\\
&+ \int_\Omega \left(-\frac{1}{2}B'(\xi)\nabla u\cdot\nabla u - \frac{1}{2}\operatorname{div}(\xi)|\nabla u|^2 - \nabla\dot{u}(\xi)\cdot\nabla u\right)\operatorname{div}(\theta)\\
&+ \int_\Omega (\dot{u}(\xi)f + u\nabla f\cdot\xi + uf\operatorname{div}(\xi))\operatorname{div}(\theta),
\end{aligned}$$

where

$$B'(\xi) := \frac{dB}{dt}(0) = -D\xi - D\xi^{\mathsf{T}}. \tag{64}$$

Using Lemma 1(2), we compute

$$\begin{aligned}
2(\nabla\dot{u}(\xi)\odot\nabla u) : D\theta - \nabla\dot{u}(\xi)\cdot\nabla u\operatorname{div}\theta &= D\theta\nabla u\cdot\nabla\dot{u}(\xi) + \nabla u\cdot D\theta\nabla\dot{u}(\xi) - \nabla\dot{u}(\xi)\cdot\nabla u\operatorname{div}\theta\\
&= -A'(\theta)\nabla u\cdot\nabla\dot{u}(\xi).
\end{aligned}\tag{65}$$

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Using $\dot{u}(\xi) f \operatorname{div}(\theta) + \dot{u}(\xi)\nabla f \cdot \theta = \operatorname{div}(f\theta)\dot{u}(\xi)$ and (65), and gathering the terms involving $\operatorname{div}(\xi)$ in $D^2_E J(\Omega)(\theta, \xi)$, we obtain

$$D^2_E J(\Omega)(\theta,\xi) = \int_\Omega \left(-\frac{1}{2}B'(\xi)\nabla u \cdot \nabla u + u\nabla f \cdot \xi\right)\operatorname{div}(\theta) + \int_\Omega -(2D\xi^\mathsf{T}\nabla u \odot \nabla u) : D\theta - A'(\theta)\nabla u \cdot \nabla \dot{u}(\xi) + \operatorname{div}(f\theta)\dot{u}(\xi) + \int_\Omega \mathbf{S}_1 : D^2\theta\xi + uD^2 f\xi\cdot\theta + \mathbf{S}_0 \cdot D\theta\xi + (\mathbf{S}_1 : D\theta + \mathbf{S}_0\cdot\theta)\operatorname{div}(\xi).$$

Note that $D^2_E J(\Omega)(\theta, \xi)$ is also a first-order shape derivative with respect to ξ, so we can apply Proposition 1, but we need first to write $D^2_E J(\Omega)(\theta, \xi)$ in the tensor form (15) with θ replaced by ξ. In particular, we need to transform the terms depending on $\dot{u}(\xi)$ in $D^2_E J(\Omega)(\theta, \xi)$ as they do not depend explicitly on ξ. Choosing the test function $v = \dot{u}(\xi)$ in (53) we get

$$\int_\Omega \nabla\dot{u}(\theta)\cdot\nabla\dot{u}(\xi) = -\int_\Omega A'(\theta)\nabla u\cdot\nabla\dot{u}(\xi) + \int_\Omega \operatorname{div}(f\theta)\dot{u}(\xi).$$

In a similar way, we also have the equation

$$\int_\Omega \nabla\dot{u}(\xi)\cdot\nabla\dot{u}(\theta) = -\int_\Omega A'(\xi)\nabla u\cdot\nabla\dot{u}(\theta) + \int_\Omega \operatorname{div}(f\xi)\dot{u}(\theta). \tag{66}$$

Using these formulae allows us to replace $\dot{u}(\xi)$ with $\dot{u}(\theta)$ in $D^2_E J(\Omega)(\theta, \xi)$. Using (64), we obtain

$$D^2_E J(\Omega)(\theta,\xi) = \int_\Omega (D\xi\nabla u \cdot \nabla u + u\nabla f\cdot\xi)\operatorname{div}(\theta) + \int_\Omega -(2D\xi^\mathsf{T}\nabla u \odot \nabla u) : D\theta - A'(\xi)\nabla u \cdot \nabla \dot{u}(\theta) + \operatorname{div}(f\xi)\dot{u}(\theta) + \int_\Omega \mathbf{S}_1 : D^2\theta\xi + uD^2 f\xi\cdot\theta + \mathbf{S}_0 \cdot D\theta\xi + (\mathbf{S}_1 : D\theta + \mathbf{S}_0\cdot\theta)\operatorname{div}(\xi).$$

Using Lemma 1(2), we also have

$$-A'(\xi)\nabla u\cdot\nabla\dot{u}(\theta) = (2\nabla\dot{u}(\theta)\odot\nabla u) : D\xi - \nabla\dot{u}(\theta)\cdot\nabla u\operatorname{div}(\xi)$$

and

$$\begin{aligned}
-(2D\xi^\mathsf{T}\nabla u\odot\nabla u) : D\theta &= -(D\xi^\mathsf{T}\nabla u\otimes\nabla u + \nabla u\otimes D\xi^\mathsf{T}\nabla u) : D\theta \\
&= -D\xi^\mathsf{T}\nabla u\cdot D\theta\nabla u - \nabla u : D\theta D\xi^\mathsf{T}\nabla u \\
&= -\nabla u\cdot D\xi D\theta\nabla u - \nabla u\cdot D\xi D\theta^\mathsf{T}\nabla u \\
&= -(\nabla u\otimes D\theta\nabla u + \nabla u\otimes D\theta^\mathsf{T}\nabla u) : D\xi \\
&= -[(\nabla u\otimes\nabla u)(D\theta + D\theta^\mathsf{T})] : D\xi.
\end{aligned}$$

Then, using $D\xi\nabla u\cdot\nabla u(\operatorname{div}\theta) = (\nabla u\otimes\nabla u)((\operatorname{div}\theta)\mathbf{I}_d) : D\xi$ we get

$$D\xi\nabla u\cdot\nabla u\operatorname{div}(\theta)-(2D\xi^{\mathsf T}\nabla u\odot\nabla u):D\theta=(\nabla u\otimes\nabla u)A'(\theta):D\xi.$$

Gathering the previous results, we can now write the tensor expression for $D^2_E J(\Omega)(\theta,\xi)$.

Proposition 7 *(Second order distributed Eulerian shape derivative). Assume $\Omega\in\mathbb{P}(\mathcal{D})$, $f\in H^2(\mathcal{D})$, $\theta\in\mathcal{C}^2_c(\mathcal{D},\mathbb{R}^d)$ and $\xi\in\mathcal{C}^1_c(\mathcal{D},\mathbb{R}^d)$. The second order distributed Eulerian shape derivative is given by*

$$D^2_E J(\Omega)(\theta,\xi)=\int_\Omega \mathbf{S}^{2,E}_1(\theta):D\xi+\mathbf{S}^{2,E}_0(\theta)\cdot\xi,\tag{67}$$

where

$$\mathbf{S}^{2,E}_1(\theta)=[-\nabla\dot u(\theta)\cdot\nabla u+\dot u(\theta)f+\mathbf{S}_1:D\theta+\mathbf{S}_0\cdot\theta]\mathbf{I}_d+2\nabla\dot u(\theta)\odot\nabla u+(\nabla u\otimes\nabla u)A'(\theta),\tag{68}$$

$$\mathbf{S}^{2,E}_0(\theta)=(\dot u(\theta)+u\operatorname{div}\theta)\nabla f+uD^2f\theta+D^2\theta\mathbf{S}_1+D\theta^{\mathsf T}\mathbf{S}_0,\tag{69}$$

with $D^2\theta\mathbf{S}_1$ defined in (32), $\mathbf{S}^{2,E}_1(\theta)\in L^1(\Omega,\mathbb{R}^{d\times d})$ and $\mathbf{S}^{2,E}_0(\theta)\in L^1(\Omega,\mathbb{R}^d)$. If, in addition, $\Omega\subset\mathbb{R}^d$ is semiconvex or if $\Omega\subset\mathbb{R}^2$ is a polygon, we get the additional regularity $\mathbf{S}^{2,E}_1(\theta)\in W^{1,1}(\Omega,\mathbb{R}^{d\times d})$.

Proof. The regularity of $\mathbf{S}^{2,E}_1(\theta)$ and $\mathbf{S}^{2,E}_0(\theta)$ when Ω is open follows from the regularity of u and $\dot u(\theta)$ in Theorems 6 and 9, respectively, and from the expressions (68)-(69).

When Ω is semiconvex, we have in view of Theorems 6 and 9 that both $\nabla\dot u(\theta)$ and ∇u belong to $H^1(\Omega)$, which yields $\nabla\dot u(\theta)\cdot\nabla u\in W^{1,1}(\Omega)$. Proceeding in a similar way for the other terms of $\mathbf{S}^{2,E}_1(\theta)$, we obtain the desired result.

When $\Omega\subset\mathbb{R}^2$ is a polygon, we can take $p=4/3$ in Theorem 6(4) and Theorem 9(3) which yields $u\in W^{2,4/3}(\Omega)$ and $\dot u(\theta)\in W^{2,4/3}(\Omega)$. Using Sobolev embeddings we have that $\nabla\dot u(\theta),\nabla u\in W^{1,4/3}(\Omega,\mathbb{R}^d)\subset L^4(\Omega,\mathbb{R}^d)$, thus $\nabla u\cdot\nabla\dot u(\theta)\in L^2(\Omega)$. Since $D^2\dot u(\theta),D^2u\in L^{4/3}(\Omega,\mathbb{R}^{d\times d})$, we get $D^2u\nabla\dot u(\theta)\in L^1(\Omega,\mathbb{R}^d)$ and $D^2\dot u(\theta)\nabla u\in L^1(\Omega,\mathbb{R}^d)$. This yields $\nabla(\nabla u\cdot\nabla\dot u(\theta))=D^2u\nabla\dot u(\theta)+D^2\dot u(\theta)\nabla u\in L^1(\Omega,\mathbb{R}^d)$, and in turn $\nabla\dot u(\theta)\cdot\nabla u\in W^{1,1}(\Omega)$. Proceeding in a similar way for the other terms of $\mathbf{S}^{2,E}_1(\theta)$, we obtain the desired regularity. □

7.2. Second order distributed Fréchet shape derivative

Using Proposition 7, we obtain the following result.

Proposition 8 *(Second order distributed Fréchet shape derivative). Assume $\Omega\in\mathbb{P}(\mathcal{D})$, $f\in H^2(\mathcal{D})$ and $\theta,\xi\in\mathcal{C}^2_c(\mathcal{D},\mathbb{R}^d)$. The second order distributed Fréchet shape derivative is given by*

$$D^2_F\mathcal{J}(0)(\theta,\xi)=\int_\Omega \mathbf{S}^{2,F}_1(\theta):D\xi+\mathbf{S}^{2,F}_0(\theta)\cdot\xi=\int_\Omega \mathbf{S}^{2,F}_1(\xi):D\theta+\mathbf{S}^{2,F}_0(\xi)\cdot\theta,\tag{70}$$

where

$$\mathbf{S}^{2,F}_1(\theta)=[-\nabla\dot u(\theta)\cdot\nabla u+\dot u(\theta)f+\mathbf{S}_1:D\theta+\mathbf{S}_0\cdot\theta]\mathbf{I}_d+2\nabla\dot u(\theta)\odot\nabla u+(\nabla u\otimes\nabla u)A'(\theta)-D\theta^{\mathsf T}\mathbf{S}_1,$$

$$\mathbf{S}^{2,F}_0(\theta)=(\dot u(\theta)+u\operatorname{div}\theta)\nabla f+uD^2f\theta,$$

with $\mathbf{S}^{2,F}_1(\theta)\in L^1(\Omega,\mathbb{R}^{d\times d})$ and $\mathbf{S}^{2,F}_0(\theta)\in L^1(\Omega,\mathbb{R}^d)$. If, in addition, $\Omega\subset\mathbb{R}^d$ is semiconvex or if $\Omega\subset\mathbb{R}^2$ is a polygon, we get the additional regularity $\mathbf{S}^{2,F}_1(\theta)\in W^{1,1}(\Omega,\mathbb{R}^{d\times d})$.

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Alternatively, we can also write the second order distributed Fréchet shape derivative using the following symmetric expression:

$$D_F^2\mathcal{J}(0)(\theta,\xi) = \int_\Omega \mathcal{K}(\theta,\xi), \tag{71}$$

with

$$\begin{aligned}\mathcal{K}(\theta,\xi) &:= \nabla\dot{u}(\theta)\cdot\nabla\dot{u}(\xi) + \mathbf{S}_0\cdot(\theta\operatorname{div}\xi + \xi\operatorname{div}\theta) + \mathbf{S}_1 : (D\theta\operatorname{div}\xi + D\xi\operatorname{div}\theta)\\ &\quad + \left(\frac{1}{2}|\nabla u|^2 - uf\right)(\operatorname{div}\xi\operatorname{div}\theta + D\theta^{\mathsf{T}} : D\xi)\\ &\quad - (D\theta D\xi + D\xi D\theta + D\xi D\theta^{\mathsf{T}})\nabla u\cdot\nabla u + uD^2f\theta\cdot\xi.\end{aligned}$$

Proof. For the proof of existence of the second order Fréchet derivative, we refer to [35, Section 5.3.5]. The proof of (70) is a direct consequence of Proposition 7, Proposition 3, (57), and of the fact that $D_F^2\mathcal{J}(0)$ is a symmetric bilinear form.

To prove (71), we compute

$$\begin{aligned}(\nabla u\otimes\nabla u)A'(\theta) : D\xi &= (\nabla u\otimes\nabla u) : D\xi\operatorname{div}\theta - (\nabla u\otimes\nabla u)(D\theta + D\theta^{\mathsf{T}}) : D\xi\\ &= \mathbf{S}_1 : D\xi\operatorname{div}\theta + \left(\frac{1}{2}|\nabla u|^2 - uf\right)\operatorname{div}\xi\operatorname{div}\theta - (\nabla u\otimes(D\theta^{\mathsf{T}}\nabla u + D\theta\nabla u)) : D\xi\\ &= \mathbf{S}_1 : D\xi\operatorname{div}\theta + \left(\frac{1}{2}|\nabla u|^2 - uf\right)\operatorname{div}\xi\operatorname{div}\theta - D\xi D\theta^{\mathsf{T}}\nabla u\cdot\nabla u - D\xi D\theta\nabla u\cdot\nabla u,\end{aligned} \tag{72}$$

and also

$$\begin{aligned}-D\theta^{\mathsf{T}}\mathbf{S}_1 : D\xi &= \left(\frac{1}{2}|\nabla u|^2 - uf\right)D\theta^{\mathsf{T}} : D\xi - D\theta^{\mathsf{T}}(\nabla u\otimes\nabla u) : D\xi\\ &= \left(\frac{1}{2}|\nabla u|^2 - uf\right)D\theta^{\mathsf{T}} : D\xi - D\theta D\xi\nabla u\cdot\nabla u.\end{aligned} \tag{73}$$

Then, observing that $u\operatorname{div}\theta\nabla f\cdot\xi = \mathbf{S}_0\cdot\xi\operatorname{div}\theta$, and using (66), (72) and (73) in (70), we obtain

$$\begin{aligned}D_F^2\mathcal{J}(0)(\theta,\xi) &= \int_\Omega \nabla\dot{u}(\theta)\cdot\nabla\dot{u}(\xi) + (\mathbf{S}_1 : D\theta + \mathbf{S}_0\cdot\theta)\operatorname{div}\xi\\ &\quad + \int_\Omega \mathbf{S}_1 : D\xi\operatorname{div}\theta + \left(\frac{1}{2}|\nabla u|^2 - uf\right)\operatorname{div}\xi\operatorname{div}\theta - D\xi D\theta^{\mathsf{T}}\nabla u\cdot\nabla u - D\xi D\theta\nabla u\cdot\nabla u\\ &\quad + \int_\Omega \left(\frac{1}{2}|\nabla u|^2 - uf\right)D\theta^{\mathsf{T}} : D\xi - D\theta D\xi\nabla u\cdot\nabla u + \mathbf{S}_0\cdot\xi\operatorname{div}\theta + uD^2f\theta\cdot\xi,\end{aligned}$$

which yields (71). □

The purpose of (71) is to provide a formula which is clearly symmetric. We will use this formula for the calculation of the second order shape derivative for polygons.

Remark 6. One could legitimately wonder if the tensors $\mathbf{S}_0^{2,E}(\theta), \mathbf{S}_1^{2,E}(\theta)$ of Proposition 7 and $\mathbf{S}_0^{2,F}(\theta), \mathbf{S}_1^{2,F}(\theta)$ of Proposition 8 could be written using the shape derivative $u'(\theta)$ defined in (61) instead of the material

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derivative $\dot{u}(\theta)$. Formally, this can be done by substituting $\dot{u}(\theta)$ by $u'(\theta) + \nabla u \cdot \theta$ in the tensors expressions. However, we have $\dot{u}(\theta) = u'(\theta) + \nabla u \cdot \theta \in H^1(\Omega)$ when Ω is only open, whereas $u'(\theta)$ and $\nabla u \cdot \theta$ are both only in $L^2(\Omega)$. Thus, by doing so one would work with more singular functions, even if these singularities are artificial since they cancel each other, so this defeats the purpose of the distributed expressions. In fact, the main purpose of writing $D^2_E J(\Omega)(\theta, \xi)$ using $u'(\theta)$ is to find the canonical boundary structure (9) or (10), (11) in the case of the Fréchet shape derivatives, so the substitution is unnecessary if we aim at a distributed expression. This artificial singularity is a standard problem when working with the shape derivative $u'(\theta)$; see for instance [45, Section 3.1] where the same issue is discussed in the context of shape derivative estimates with respect to Sobolev norms of boundary displacements.

8. Boundary expressions of second order shape derivatives

In Section 7, we have obtained second order distributed shape derivatives for open sets. Assuming more regularity, we obtain in this section several types of boundary expressions for second order shape derivatives. In particular, we obtain boundary expressions based on the material derivative $\dot{u}(\theta)$, which require less domain regularity than the usual expressions based on the shape derivative $u'(\theta)$.

8.1. Boundary expressions for the second order Eulerian shape derivative

Proposition 9. *Assume $f \in H^2(\mathcal{D})$, $\theta \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$, $\xi \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^d)$ and $\Omega \subset \mathbb{R}^d$ is semiconvex or $\Omega \subset \mathbb{R}^2$ is a polygon. The second order Eulerian shape derivative has the following boundary expression based on the material derivative $\dot{u}(\theta)$:*

$$D^2_E J(\Omega)(\theta, \xi) = \int_{\partial\Omega} \left(\partial_n u \partial_n \dot{u}(\theta) - |\partial_n u|^2 D\theta n \cdot n + \frac{1}{2} |\partial_n u|^2 \operatorname{div} \theta \right) \xi_n. \tag{74}$$

Proof. If $\Omega \subset \mathbb{R}^d$ is semiconvex or $\Omega \subset \mathbb{R}^2$ is a polygon, we get in view of Proposition 7 that $\mathbf{S}^{2,E}_1(\theta) \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$. Thus, we can apply (18) from Proposition 1 and we get

$$D^2_E J(\Omega)(\theta, \xi) = \int_{\partial\Omega} (\mathbf{S}^{2,E}_1(\theta) n) \cdot \xi. \tag{75}$$

Using $u = 0$, $\dot{u}(\theta) = 0$, and $\nabla u = \partial_n u\, n$, $\nabla \dot{u}(\theta) = \partial_n \dot{u}(\theta) n$ on $\partial\Omega$, we have in view of (68)

$$\begin{aligned}
\mathbf{S}^{2,E}_1(\theta) n &= \left(-\partial_n \dot{u}(\theta) \partial_n u + |\nabla u|^2 D\theta n \cdot n - \frac{1}{2} |\partial_n u|^2 \operatorname{div}(\theta) \right) n \\
&\quad + 2\partial_n \dot{u}(\theta) \partial_n u (n \odot n) n + |\partial_n u|^2 (n \otimes n) A'(\theta) n \\
&= \left(-\partial_n \dot{u}(\theta) \partial_n u + \frac{1}{2} |\partial_n u|^2 \operatorname{div}(\theta) + 2\partial_n \dot{u}(\theta) \partial_n u - |\partial_n u|^2 D\theta n \cdot n \right) n \quad \text{on } \partial\Omega,
\end{aligned}$$

and using (75) this yields (74). □

Proposition 10. *Assume $f \in H^2(\mathcal{D})$, $\theta \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$, $\xi \in \mathcal{C}^1_c(\mathcal{D}, \mathbb{R}^d)$, and $\Omega \subset \mathbb{R}^2$ is a convex polygon. The second order Eulerian shape derivative has the following boundary expression based on the shape derivative $u'(\theta)$:*

$$D^2_E J(\Omega)(\theta, \xi) = \int_{\partial\Omega} \left((\partial_n u'(\theta) + D^2 u n \cdot \theta) \partial_n u + \frac{1}{2} |\partial_n u|^2 \operatorname{div} \theta \right) \xi_n. \tag{76}$$

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Proof. By definition we have $u'(\theta) = \dot{u}(\theta) - \nabla u \cdot \theta$, thus

$$\nabla u'(\theta) = \nabla \dot{u}(\theta) - \nabla(\nabla u \cdot \theta) = \nabla \dot{u}(\theta) - D^2 u\theta - D\theta^\mathsf{T} \nabla u. \tag{77}$$

Since Ω is convex, Theorem 9 and Theorem 8 yield $\nabla \dot{u}(\theta) \in H^1(\Omega)$, $\nabla u \in \mathcal{C}^0(\overline{\Omega})$ and $D^2 u|_{\partial\Omega} \in L^1(\partial\Omega)$. Thus, we can take the trace of (77) on $\partial\Omega$ and we get

$$\nabla u'(\theta) = \nabla \dot{u}(\theta) - D^2 u\theta - D\theta^\mathsf{T} \nabla u \in L^1(\partial\Omega).$$

Using $\nabla u = \partial_n u\, n$ on $\partial\Omega$, we get

$$\partial_n u'(\theta) = \partial_n \dot{u}(\theta) - D^2 un \cdot \theta - D\theta n \cdot n \partial_n u \in L^1(\partial\Omega).$$

Considering that $\partial_n u \in L^\infty(\partial\Omega)$, we can substitute $\partial_n \dot{u}(\theta)$ with $\partial_n u'(\theta) + D^2 un \cdot \theta + D\theta n \cdot n\partial_n u$ in (74), which yields (76). □

Roughly speaking, Propositions 9 and 10 indicate that $D^2_E J(\Omega)(\theta, \xi)$ can be written in boundary form for any polygon using the material derivative $\dot{u}(\theta)$, but only for convex polygons using the shape derivative. Indeed, the regularity of $u'(\theta)$ is determined by ∇u, and the singularity of u becomes too strong as soon as the domain Ω has a re-entrant corner. However, this lack of regularity of $u'(\theta)$ is rather artificial, since the singularities of $\partial_n u'(\theta)$ and $D^2 un \cdot \theta$ in (76) actually cancel each other and their sum is more regular, as can be seen from (77); see Remark 6.

Note that in view of the definition (8), $D^2_E J(\Omega)(\theta, \xi)$ can also be seen as the first order Eulerian shape derivative of $D_E J(\Omega)(\theta)$ in direction ξ. Then, it is interesting to observe that when considered as first order shape derivatives in direction ξ, expressions (74) and (76) have a structure of the type $l_E(\xi_{|\partial\Omega} \cdot n)$ as in (9), even though Ω does not have the regularity required in Theorem 3.

8.2. Boundary expressions for the second order Fréchet shape derivative

Proposition 11. *Assume $f \in H^2(\mathcal{D})$, $\theta, \xi \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$, and $\Omega \subset \mathbb{R}^d$ is semiconvex or $\Omega \subset \mathbb{R}^2$ is a m-gon. The second order Fréchet shape derivative has the following boundary expression based on the material derivative $\dot{u}(\theta)$:*

$$D^2_F \mathcal{J}(0)(\theta, \xi) = \int_{\partial\Omega} \left(\partial_n u \partial_n \dot{u}(\theta) + \frac{1}{2}|\partial_n u|^2 \operatorname{div}(\theta) - \frac{3}{2}|\partial_n u|^2 D\theta n \cdot n \right) \xi_n - \frac{|\partial_n u|^2}{2}(D\theta^\mathsf{T} n) \cdot \xi_\tau. \tag{78}$$

If in addition $\Omega \subset \mathbb{R}^2$ is a convex m-gon with $\partial\Omega = \bigcup_{i=1}^m \overline{\Gamma_i}$, then we have the following boundary expression based on the shape derivative $u'(\theta)$:

$$D^2_F \mathcal{J}(0)(\theta, \xi) = \int_{\partial\Omega} \left(\partial_n u'(\theta) \partial_n u + D^2 un \cdot n \partial_n u\, \theta_n \right) \xi_n - \sum_{i=1}^m \int_{\Gamma_i} \frac{|\partial_n u|^2}{2} (\nabla_\Gamma \xi_n \cdot \theta_\tau + \nabla_\Gamma \theta_n \cdot \xi_\tau). \tag{79}$$

Proof. When $\Omega \subset \mathbb{R}^d$ is semiconvex or $\Omega \subset \mathbb{R}^2$ is a m-gon, we have due to Proposition 3 the following boundary expression for the second order Fréchet shape derivative:

$$\begin{aligned} D^2_F \mathcal{J}(0)(\theta, \xi) &= \int_{\partial\Omega} (\mathbf{S}_1^{2,F}(\theta) n) \cdot \xi = \int_{\partial\Omega} (\mathbf{S}_1^{2,E}(\theta) n) \cdot \xi - (D\theta^\mathsf{T} \mathbf{S}_1 n) \cdot \xi \\ &= D^2_E J(\Omega)(\theta, \xi) - \int_{\partial\Omega} (D\theta^\mathsf{T} \mathbf{S}_1 n) \cdot \xi. \end{aligned} \tag{80}$$

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In view of (57) and $\nabla u = \partial_n u\, n$ on $\partial\Omega$, we have $D\theta^\mathsf{T}\mathbf{S}_1 n = \frac{1}{2}|\partial_n u|^2 D\theta^\mathsf{T} n$ a.e. on $\partial\Omega$. Using (74) and $\xi = \xi_\tau + \xi_n n$ in (80), we get (78).

Now, assume that $\Omega \subset \mathbb{R}^2$ is a convex m-gon. Using (76), (80), splitting the integral containing $\operatorname{div}\theta$ as a sum of integrals on Γ_i and then using $\operatorname{div}\theta = \operatorname{div}_\Gamma \theta + D\theta n \cdot n$, we get

$$D^2_F \mathcal{J}(0)(\theta,\xi) = \int_{\partial\Omega} \left((\partial_n u'(\theta) + D^2 un\cdot\theta)\partial_n u\right)\xi_n + \sum_{i=1}^m \int_{\Gamma_i} \frac{1}{2}|\partial_n u|^2 \operatorname{div}_\Gamma(\theta)\xi_n - \frac{1}{2}|\partial_n u|^2 (D\theta^\mathsf{T} n)\cdot\xi_\tau. \quad (81)$$

Using Theorem 8, we have on Γ_i, for all $i \in I$:

$$\begin{aligned} \frac{1}{2}\operatorname{div}_\Gamma(|\nabla u|^2\xi_n\theta) &= \frac{|\nabla u|^2}{2}\xi_n \operatorname{div}_\Gamma\theta + \xi_n \frac{1}{2}\nabla_\Gamma(|\nabla u|^2)\cdot\theta + \frac{|\nabla u|^2}{2}\nabla_\Gamma\xi_n\cdot\theta \\ &= \frac{|\partial_n u|^2}{2}\xi_n \operatorname{div}_\Gamma\theta + \partial_n u\xi_n(D^2un\cdot\theta - D^2un\cdot n\theta_n) + \frac{|\partial_n u|^2}{2}\nabla_\Gamma\xi_n\cdot\theta \quad \text{in } L^1(\Gamma_i), \end{aligned} \quad (82)$$

where we have used $\nabla u = (\partial_n u)n$ and

$$\nabla_\Gamma(|\nabla u|^2) = (\mathbf{I}_d - n\otimes n)\nabla(|\nabla u|^2) = 2D^2u\nabla u - 2(D^2u\nabla u\cdot n)n.$$

Now, we use (82) in (81) and we get

$$\begin{aligned} D^2_F \mathcal{J}(0)(\theta,\xi) = &\int_{\partial\Omega} \partial_n u'(\theta)\partial_n u\xi_n + D^2un\cdot n\partial_n u\theta_n\xi_n \\ &+ \sum_{i=1}^m \int_{\Gamma_i} \frac{1}{2}\operatorname{div}_\Gamma(|\nabla u|^2\xi_n\theta) - \frac{|\partial_n u|^2}{2}\nabla_\Gamma\xi_n\cdot\theta - \frac{|\partial_n u|^2}{2}(D\theta^\mathsf{T} n)\cdot\xi_\tau. \end{aligned} \quad (83)$$

Using Lemma 2 and the expression of the first-order shape derivative (58), and also using that $D_\Gamma n = 0$ on Γ_i since Ω is a m-gon, we obtain

$$\begin{aligned} D^2_F \mathcal{J}(0)(\theta,\xi) = &\int_{\partial\Omega} \left(\partial_n u'(\theta)\partial_n u + D^2un\cdot n\partial_n u\,\theta_n\right)\xi_n \\ &+ \sum_{i=1}^m \int_{\Gamma_i} \frac{1}{2}\operatorname{div}_\Gamma(|\nabla u|^2\xi_n\theta) - \frac{|\partial_n u|^2}{2}(\nabla_\Gamma\xi_n\cdot\theta_\tau + \nabla_\Gamma\theta_n\cdot\xi_\tau). \end{aligned} \quad (84)$$

To get (79), we use Theorem 2 which yields

$$\int_{\Gamma_i} \operatorname{div}_\Gamma(|\nabla u|^2\xi_n\theta) = \left[|\nabla u|^2(\xi\cdot n^-)(\theta\cdot\tau^-)\right](a_i) - \left[|\nabla u|^2(\xi\cdot n^+)(\theta\cdot\tau^+)\right](a_{i-1}) + \int_{\Gamma_i} \mathcal{H}|\nabla u|^2\theta_n\xi_n.$$

In view of Theorem 8, we have $\nabla u \in \mathcal{C}^0(\overline{\Omega})$. We have $\nabla u(a_i)\cdot\tau^+(a_i) = 0$ and $\nabla u(a_i)\cdot\tau^-(a_i) = 0$ due to the Dirichlet boundary conditions. Since $\tau^+(a_i)$ and $\tau^-(a_i)$ are not colinear, we get $\nabla u(a_i) = 0$ for $1 \le i \le m$. Considering also that the curvature $\mathcal{H}$ is zero on each Γ_i since Ω is a m-gon, this leads to

$$\int_{\Gamma_i} \operatorname{div}_\Gamma(|\nabla u|^2\xi_n\theta) = 0,$$

which proves the result. □

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Remark 7. In [42, Theorem 0.2], the structure of the second order shape derivative when Ω is an optimal shape (i.e. when the first-order shape derivative vanishes) is given when Ω is a set of finite perimeter. The author observes that when the shape is not optimal, it is difficult to know what the structure of the second order shape derivative is, since in the smooth case it includes terms requiring more regularity such as $D_\Gamma n$; see (11)-(12).

In the smooth case, the term $D^2un \cdot n$ appearing in (79) is further transformed using the formula $D^2un \cdot n = -f - (d-1)\mathcal{H}\partial_n u$ in order to remove the second derivative of u. For convex polygons, this substitution is still possible as will be seen in Corollary 2, but one needs to be cautious due to the low regularity of u and Ω.

Corollary 2. *Assume $f \in H^2(\mathcal{D})$, $\theta, \xi \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$, and $\Omega \subset \mathbb{R}^2$ is a convex m-gon. Then, the second order Fréchet shape derivative is given by*

$$D^2_F \mathcal{J}(0)(\theta, \xi) = \int_{\partial\Omega} (\partial_n u'(\theta)\partial_n u - f\partial_n u\,\theta_n)\,\xi_n - \sum_{i=1}^m \int_{\Gamma_i} \frac{|\partial_n u|^2}{2}(\nabla_\Gamma \xi_n \cdot \theta_\tau + \nabla_\Gamma \theta_n \cdot \xi_\tau). \tag{85}$$

Proof. For $\varepsilon > 0$ sufficiently small, define the open rectangle $\Gamma_i^\varepsilon := \{x + \delta n \mid x \in \Gamma_i, |\delta| < \varepsilon\}$. Note that n is constant on Γ_i. In view of Corollary 1, we have $u \in H^{2+\delta}(\Omega)$, with $0 < \delta < \pi/\hat{\alpha} - 1$, and consequently $D^2u \in H^\delta(\Omega)$. Then, we observe that the unitary extension $\tilde{n}$ of n in $\Gamma_i^\varepsilon \cap \Omega$ is actually constant, thus $D\tilde{n} = 0$ and $\operatorname{div}(\tilde{n}) = 0$ in $\Gamma_i^\varepsilon \cap \Omega$. Thus, we compute

$$\begin{aligned}
&\operatorname{div}(\nabla u - (\tilde{n} \otimes \tilde{n})\nabla u) - D(\nabla u - (\tilde{n} \otimes \tilde{n})\nabla u)\tilde{n} \cdot \tilde{n} \\
&\quad = \Delta u - D^2u(\tilde{n} \otimes \tilde{n}) - D^2u\tilde{n} \cdot \tilde{n} + D((\nabla u \cdot \tilde{n})\tilde{n})\tilde{n} \cdot \tilde{n} \\
&\quad = \Delta u - 2D^2u\tilde{n} \cdot \tilde{n} + (\tilde{n} \otimes \nabla(\nabla u \cdot \tilde{n}))\tilde{n} \cdot \tilde{n} = \Delta u - D^2u\tilde{n} \cdot \tilde{n} \quad \text{in } H^\delta(\Gamma_i^\varepsilon \cap \Omega).
\end{aligned}$$

Taking the trace on Γ_i using Theorem 8, and using the fact that $u = 0$ on $\partial\Omega$ we get

$$\begin{aligned}
0 &= \Delta_\Gamma u = \operatorname{div}_\Gamma(\nabla_\Gamma u) \\
&= \operatorname{div}(\nabla u - (\tilde{n} \otimes \tilde{n})\nabla u) - D(\nabla u - (\tilde{n} \otimes \tilde{n})\nabla u)\tilde{n} \cdot \tilde{n} = \Delta u - D^2un \cdot n \quad \text{in } L^1(\Gamma_i).
\end{aligned}$$

Thus, we have obtained $D^2un \cdot n = \Delta u = -f$ in $L^1(\partial\Omega)$. Substituting in (79), we obtain (85). □

Note that with the assumptions of Corollary 2, since $f \in H^2(\mathcal{D})$ we have $f \in \mathcal{C}^0(\overline{\mathcal{D}})$ by Sobolev embedding, and this yields the higher regularity $D^2un \cdot n = -f$ in $\mathcal{C}^0(\partial\Omega)$.

Now we compute the Fréchet derivative in the smooth case, written in the canonical form (12) of the structure theorem.

Proposition 12. *Assume $\Omega \subset \mathbb{R}^d$ is of class $\mathcal{C}^{2,1}$, $f \in H^2(\mathcal{D})$ and $\theta, \xi \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$. Then, the second order Fréchet shape derivative is given by*

$$\begin{aligned}
D^2_F \mathcal{J}(0)(\theta, \xi) = &\int_{\partial\Omega} \left(\partial_n u'(\theta)\partial_n u - f\partial_n u\,\theta_n - \frac{1}{2}|\partial_n u|^2(d-1)\mathcal{H}\theta_n\right)\xi_n \\
&+ D_F\mathcal{J}(0)([D_\Gamma n\xi_\tau \cdot \theta_\tau - \nabla_\Gamma \xi_n \cdot \theta_\tau - \nabla_\Gamma \theta_n \cdot \xi_\tau]n).
\end{aligned} \tag{86}$$

Proof. In view of [33, Theorem 2.5.1.1], we have $u \in H^3(\Omega)$. This yields $D^2u|_{\partial\Omega} \in H^{1/2}(\partial\Omega)$ and $\partial_n u'(\theta)|_{\partial\Omega} \in H^{1/2}(\partial\Omega)$. Since $\theta, \xi \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$ and Ω is of class $\mathcal{C}^{2,1}$, we have n of class $\mathcal{C}^{1,1}$, and combining these results we get $|\nabla u|^2\xi_n\theta \in W^{1,1}(\partial\Omega, \mathbb{R}^d)$. Applying Theorem 1 we obtain

$$\int_{\partial\Omega} \mathrm{div}_\Gamma(|\nabla u|^2 \xi_n \theta) = \int_{\partial\Omega} (d-1)\mathcal{H}|\nabla u|^2 \theta_n \xi_n. \tag{87}$$

Now, using that n is of class $\mathcal{C}^{1,1}$, the sum of the integrals on Γ_i in (84) can be written as an integral on $\partial\Omega$. Also, compared to (84) we have an additional term $D_\Gamma n\xi_\tau \cdot \theta_\tau$ which was vanishing in (84) since Ω was a polygon. Thus, from (87) and (84) we obtain

$$\begin{aligned} D^2_\theta \mathcal{J}(0)(\theta,\xi) = &\int_{\partial\Omega} \left(\partial_n u'(\theta)\partial_n u + \frac{1}{2}|\partial_n u|^2(d-1)\mathcal{H}\theta_n + D^2 un\cdot n\partial_n u\theta_n\right)\xi_n \\ &+ D_F\mathcal{J}(0)([D_\Gamma n\xi_\tau\cdot\theta_\tau - \nabla_\Gamma\xi_n\cdot\theta_\tau - \nabla_\Gamma\theta_n\cdot\xi_\tau]n). \end{aligned} \tag{88}$$

Since Ω is $\mathcal{C}^{2,1}$ and $u \in H^3(\Omega)$, using [35, Proposition 5.4.12], and $u = 0$ on $\partial\Omega$ we get

$$D^2 un\cdot n = \Delta u - \Delta_\Gamma u - (d-1)\mathcal{H}\partial_n u = -f - (d-1)\mathcal{H}\partial_n u. \tag{89}$$

Using (89) in (88) we get (86). □

Apart from the curvature and the $D_\Gamma n$ terms which both vanish when Ω is a polygon, expression (85) is similar to (86). However, the proof of Proposition 11 shows that additional terms actually appear at the vertices of the polygon, but for this particular functional they vanish due to $|\nabla u|^2(a_i) = 0$. Thus, in general one can expect second shape derivatives for polygons to have additional terms at the vertices a_i, as in the case of the volume; see (42).

Expression (86) corresponds to the structure (12), even though Ω is only assumed to be $\mathcal{C}^{2,1}$, while Theorem 4 requires $\mathcal{C}^3$-regularity. Although written in a different way, (86) is equal to well-known formulae in the literature, see for instance [53, (5.21)] or [12, Lemma 2.2]. It is not difficult to see that the first integral on the right-hand side of (88) coincides with the formula [53, (5.21)], considering first that one needs to divide [53, (5.21)] by a factor 2 to get the same functional, and then that in (88), we have

$$\begin{aligned} \int_{\partial\Omega} \partial_n u'(\theta)\partial_n u\,\xi_n &= \int_{\partial\Omega} -\partial_n u'(\theta)u'(\xi) = \int_\Omega -\Delta u'(\theta)u'(\xi) - \nabla u'(\xi)\cdot\nabla u'(\theta) \\ &= \int_\Omega -\nabla u'(\xi)\cdot\nabla u'(\theta) = \int_{\partial\Omega} -\partial_n u'(\xi)u'(\theta), \end{aligned}$$

where we have used the fact that the shape derivative $u'(\theta)$ satisfies $-\Delta u'(\theta) = 0$ in Ω and $u'(\theta) = -\partial_n u\,\theta_n$ on $\partial\Omega$, see for instance [59, Section 3.1].

8.3. Alternative second order distributed Eulerian shape derivative

The search for a simpler alternative to $\mathbf{S}_1^{2,E}(\theta)$ in (68) is guided by the boundary expression (74), which suggests the following natural alternative tensor form.

Proposition 13. *Assume $\Omega \in \mathbb{P}(\mathcal{D})$ is semiconvex and $\theta, \xi \in \mathcal{C}^2_c(\mathcal{D}, \mathbb{R}^d)$, Then, the second order distributed Eulerian shape derivative has the alternative form*

$$D^2_E J(\Omega)(\theta,\xi) = \int_\Omega \widehat{\mathbf{S}_1^{2,E}}(\theta) : D\xi + \widehat{\mathbf{S}_0^{2,E}}(\theta)\cdot\xi, \tag{90}$$

with

$$\widehat{\mathbf{S}_1^{2,E}}(\theta) = \left(\nabla \dot{u}(\theta) \cdot \nabla u + \frac{|\nabla u|^2}{2} \operatorname{div} \theta\right) \mathbf{I}_d - \nabla u \otimes D\theta \nabla u,$$

$$\widehat{\mathbf{S}_0^{2,E}}(\theta) = \operatorname{div}(\widehat{\mathbf{S}_1^{2,E}}(\theta)) = D^2 u \nabla \dot{u}(\theta) + D^2 \dot{u}(\theta) \nabla u + D^2 u \nabla u \operatorname{div}(\theta) + \frac{|\nabla u|^2}{2} \nabla \operatorname{div} \theta - \operatorname{div}(D\theta \nabla u) \nabla u - D^2 u D\theta \nabla u,$$

and $\widehat{\mathbf{S}_1^{2,E}}(\theta) \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$.

Proof. We compute, using $\nabla \dot{u}(\theta) = \partial_n \dot{u}(\theta)\, n$ and $\nabla u = \partial_n u\, n$ on $\partial\Omega$, and in view of (74),

$$\begin{aligned}\widehat{\mathbf{S}_1^{2,E}}(\theta) n &= \left(\nabla \dot{u}(\theta) \cdot \nabla u + \frac{|\nabla u|^2}{2} \operatorname{div} \theta\right) n - (\nabla u \otimes D\theta \nabla u) n \\ &= \left(\partial_n u \partial_n \dot{u}(\theta) - |\partial_n u|^2 D\theta n \cdot n + \frac{1}{2} |\partial_n u|^2 \operatorname{div} \theta\right) n = \mathbf{S}_1^{2,E}(\theta) n \quad \text{ on } \partial\Omega,\end{aligned}$$

so that (21) is satisfied. Since Ω is semiconvex, we have $u, \dot{u}(\theta) \in H^2(\Omega)$ in view of Theorem 6(3) and Theorem 9(2), therefore $\widehat{\mathbf{S}_1^{2,E}}(\theta) \in W^{1,1}(\Omega, \mathbb{R}^{d\times d})$, also using that $\theta \in \mathcal{C}_c^2(\mathcal{D}, \mathbb{R}^d)$. Thus, we can apply Proposition 2 and we get (90). Finally, using Lemma 1(6), it is straightforward to compute $\widehat{\mathbf{S}_0^{2,E}}(\theta) = \operatorname{div}(\widehat{\mathbf{S}_1^{2,E}}(\theta))$. □

In the same way as for the first order shape derivative, we observe that the tensor $\widehat{\mathbf{S}_1^{2,E}}(\theta)$ has a simpler expression than $\mathbf{S}_1^{2,E}(\theta)$ given in (68), but requires more regularity for Ω due to the presence of $D^2 u$ and $D^2 \dot{u}(\theta)$ in $\widehat{\mathbf{S}_0^{2,E}}(\theta)$, so there is a trade-off between simplicity and regularity with this alternative.

9. Second order shape derivative in matricial form for polygons

9.1. Second order distributed Fréchet shape derivatives for Lipschitz perturbations

In the previous sections we have shown how the expression of the second order Fréchet shape derivative can be deduced from the expression of the second order Eulerian shape derivative using Proposition 3. However, a limitation of this approach is that the second order Eulerian shape derivative requires more regularity for one of the perturbation fields than the second order Fréchet shape derivative. This difference is apparent for instance in (69), where $\mathbf{S}_0^{2,E}(\theta)$ depends on $D^2\theta$, whereas its Fréchet counterpart $\mathbf{S}_0^{2,F}(\theta)$ only depends on $D\theta$, see (70). This is also apparent in the case of the volume functional, compare the results of Propositions 4 and 5. This difference corresponds in fact to the term $D_F \mathcal{J}(0)(D\theta\xi)$ in (14) which generates the terms depending on $D^2\theta$.

Therefore, this approach is not appropriate in the case of perturbation fields in $W^{1,\infty}$, i.e. for Lipschitz vector fields. However, domain perturbations using Lipschitz vector fields are necessary when working in the class of polygons. In this case, employing only the Fréchet shape derivative seems preferable. In the case of the Dirichlet energy, it is known that $W^{1,\infty}(\mathcal{D}, \mathbb{R}^2) \ni \theta \mapsto \mathcal{J}(\theta)$ is of class $\mathcal{C}^k$ in a neighbourhood of 0 for Ω open and $f \in H^k(\mathcal{D})$; see [35, Corollary 5.3.8] and also [45, Theorem 3.13] in the case $f \in W^{m,\infty}(\mathcal{D})$ and for a general elliptic PDE. In order to directly compute the distributed expression of the second order Fréchet shape derivative in this case, we can use the following expression

$$\mathcal{J}(\theta) := J(\Omega_\theta) = \frac{1}{2} \int_{\Omega_\theta} |\nabla u_\theta|^2 = \frac{1}{2} \int_\Omega \mathcal{A}(\theta) \nabla u^\theta \cdot \nabla u^\theta, \tag{91}$$

with $u^\theta := u_\theta \circ (\mathrm{Id} + \theta)$ and $\mathcal{A}(\theta) := (\det(\mathrm{Id} + \theta))(\mathrm{Id} + D\theta)^{-1}(\mathrm{Id} + D\theta)^{-\mathsf{T}}$. We also have the following variational formulation for u^θ:

$$\int_\Omega \mathcal{A}(\theta)\nabla u^\theta \cdot \nabla v = \int_\Omega \mathcal{F}(\theta)v, \qquad \forall v \in H_0^1(\Omega), \tag{92}$$

with $\mathcal{F}(\theta) := f \circ (\mathrm{Id} + \theta) \det(\mathrm{Id} + \theta)$. Differentiating (91) twice with respect to $\theta \in W^{1,\infty}(\mathcal{D}, \mathbb{R}^2)$ and using (92), we obtain the same expression (70) for the second order Fréchet shape derivative. Note that the calculations for differentiating (91) twice with respect to θ are similar to the calculations in Section 7.1. Eventually, this shows that (70) is also valid for $\theta, \xi \in W^{1,\infty}(\mathcal{D}, \mathbb{R}^2)$. A similar calculation based on volume integrals and the material derivative of u has actually been used in [45] to prove estimates for Fréchet shape derivatives of functionals depending on the solution of a general linear elliptic PDE, see in particular [45, Section 3.1] for the case of the Dirichlet energy. We also observe that some of the regularity results of Theorem 9(2) and Theorem 9(3) are not valid anymore for $\theta \in W^{1,\infty}(\mathcal{D}, \mathbb{R}^2)$. In this case we can only say that $\dot{u}(\theta) \in H_0^1(\Omega)$. Therefore we only have $\mathbf{S}_1^{2,F}(\theta) \in L^1(\Omega, \mathbb{R}^{d\times d})$ and $\mathbf{S}_0^{2,F}(\theta) \in L^1(\Omega, \mathbb{R}^d)$ in (70) for $\theta, \xi \in W^{1,\infty}(\mathcal{D}, \mathbb{R}^2)$ even when Ω is a polygon.

9.2. Lipschitz perturbations for polygonal domains

Let $\Omega \in \mathbb{P}(\mathcal{D})$ be a m-gon with $m \geq 3$ vertices; see Definition 2. Let $\mathcal{T}$ be a triangulation of Ω, then it is known that $\mathcal{T}$ consists of $m-2$ triangles. For all $i \in I$, there exists a piecewise linear *hat function* $\varphi_i \in W^{1,\infty}(\mathcal{D})$ with compact support in $\mathcal{D}$, satisfying $\varphi_i(a_i) = 1$ and $\varphi_i(a_j) = 0$ for all $j \neq i$, and linear on each Γ_i, $i \in I$. Such a function φ_i can be obtained in the following way. Let $\mathcal{T}_i$ be the subset of triangles of $\mathcal{T}$ which contains the vertex a_i. Then on each $\mathscr{T} \in \mathcal{T}_i$, $\varphi_{i|\mathscr{T}}$ is chosen as a linear function satisfying $\varphi_i(a_i) = 1$ and $\varphi_i = 0$ at the other vertices of $\mathscr{T}$. Then for $\mathscr{T} \in \mathcal{T} \setminus \mathcal{T}_i$, we take $\varphi_i(x) = 0$ for all $x \in \mathscr{T}$. Finally, choosing an appropriate polygon $\hat{\Omega}$ such that $\Omega \subset \widehat{\Omega}$ and $\hat{\Omega}$ has compact support in $\mathcal{D}$ and taking $\varphi_i \equiv 0$ on $\mathcal{D} \setminus \widehat{\Omega}$, we can find a piecewise linear $\varphi_{i|\widehat{\Omega}}$, using a similar construction, so that $\varphi_i \in W^{1,\infty}(\mathcal{D})$ and φ_i has compact support in $\mathcal{D}$. In this way, φ_i satisfies the desired conditions.

Let $\theta_i \in \mathbb{R}^2$, $i \in I$, be given vectors which represent the perturbations of the vertices $a_i \in \mathbb{R}^2$, and let us choose a specific vector field

$$\theta := \sum_{i=1}^m \theta_i \varphi_i \in W^{1,\infty}(\mathcal{D}, \mathbb{R}^2), \tag{93}$$

then θ satisfies $\theta(a_i) = \theta_i$ for all $i \in I$, and since φ_i is linear on Γ_i for all $i \in I$, we have that $(\mathrm{Id} + \theta)(\Omega)$ is also a m-gon if $\max_{i\in I} \|\theta_i\|_\infty$ is sufficiently small. In a similar way, we also define

$$\xi := \sum_{j=1}^m \xi_j \varphi_j \in W^{1,\infty}(\mathcal{D}, \mathbb{R}^2). \tag{94}$$

Using the transformations $\mathrm{Id} + \theta$ and $\mathrm{Id} + \xi$, we are able to compute the second order Fréchet shape derivative in matricial form.

9.3. Material derivative-based second order Fréchet shape derivative in matricial form

In this section, we compute the second order Fréchet shape derivative in matricial form using the distributed expression (70), which is based on the material derivative. In this way, we obtain a formula which is valid for all m-gons. We defer the rather tedious calculations to the Appendix. Although Proposition 8 requires that $\theta, \xi \in \mathcal{C}_c^2(\mathcal{D}, \mathbb{R}^2)$, the result is also valid for $\theta, \xi \in W^{1,\infty}(\mathcal{D}, \mathbb{R}^2)$ in view of the discussion in Section 9.1. Thus, we can substitute expressions (93) and (94) in (70), and we obtain

$$D_F^2 \mathcal{J}(0)(\theta, \xi) = \sum_{i,j=1}^{m} \mathbb{M}_{ij} \theta_i \cdot \xi_j, \tag{95}$$

with $\mathbb{M}_{ij} \in \mathbb{R}^{2\times 2}$ given by

$$\begin{aligned}\mathbb{M}_{ij} := & \int_\Omega DU_j DU_i^\mathsf{T} + \varphi_i(\nabla\varphi_j \otimes \mathbf{S}_0) + \varphi_j(\mathbf{S}_0 \otimes \nabla\varphi_i) + \nabla\varphi_j \otimes \mathbf{S}_1 \nabla\varphi_i + \mathbf{S}_1 \nabla\varphi_j \otimes \nabla\varphi_i \\ & + \int_\Omega \left(\frac{1}{2}|\nabla u|^2 - uf\right)(2\nabla\varphi_i \odot \nabla\varphi_j) + u\varphi_i\varphi_j D^2 f \\ & + \int_\Omega -(\nabla\varphi_j \cdot \nabla u)(\nabla\varphi_i \otimes \nabla u) - (\nabla\varphi_i \cdot \nabla u)(\nabla u \otimes \nabla\varphi_j) - (\nabla\varphi_i \cdot \nabla\varphi_j)(\nabla u \otimes \nabla u),\end{aligned}$$

where $U_i \in H_0^1(\Omega, \mathbb{R}^2)$ is the solution of, for $i \in I$,

$$\int_\Omega DU_i \nabla v = \int_\Omega -(\nabla\varphi_i \otimes \nabla u)\nabla v + 2(\nabla u \odot \nabla v)\nabla\varphi_i + \int_\Omega v\nabla(\varphi_i f), \qquad \forall v \in H_0^1(\Omega).$$

Note that we have the property $\dot{u}(\theta) = \sum_{i=1}^m \theta_i \cdot U_i$.

Definition 7. Let $\mathcal{M} \in \mathbb{R}^{2m\times 2m}$ be a block matrix whose blocks are, for $1 \le i, j \le m$,

$$\begin{bmatrix} \mathcal{M}_{(2j-1)(2i-1)} & \mathcal{M}_{(2j-1)(2i)} \\ \mathcal{M}_{(2j)(2i-1)} & \mathcal{M}_{(2j)(2i)} \end{bmatrix} = \mathbb{M}_{ij},$$

and let $\Theta \in \mathbb{R}^{2m}$ and $\Xi \in \mathbb{R}^{2m}$ be block vectors such that for $1 \le i, j \le m$, we have

$$\begin{bmatrix} \Theta_{2i-1} \\ \Theta_{2i} \end{bmatrix} = \theta_i, \qquad \begin{bmatrix} \Xi_{2j-1} \\ \Xi_{2j} \end{bmatrix} = \xi_j.$$

Then, we can show the following result.

Lemma 3. *Let $\mathcal{M}, \Theta, \Xi$ be given in Definition 7, and $\mathbb{M}_{ij}$ defined in (95), then $\mathcal{M}$ is symmetric and*

$$\mathcal{M}\Theta \cdot \Xi = \sum_{i,j=1}^{m} \mathbb{M}_{ij} \theta_i \cdot \xi_j.$$

Proof. Indeed, we have

$$\mathcal{M}\Theta \cdot \Xi = \sum_{p=1}^{2m} \sum_{q=1}^{2m} \mathcal{M}_{pq} \Theta_q \Xi_p.$$

The sum over p is divided into two sums using the indices $p = 2j - 1$ and $p = 2j$, for $j \in I$, and the sum over q using the indices $q = 2i - 1$ and $q = 2i$, for $i \in I$. This yields

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$$\mathcal{M}\Theta \cdot \Xi = \sum_{i,j=1}^{m} \mathcal{M}_{(2j-1)(2i-1)}\Theta_{2i-1}\Xi_{2j-1} + \mathcal{M}_{(2j-1)(2i)}\Theta_{2i}\Xi_{2j-1}$$
$$+ \sum_{i,j=1}^{m} \mathcal{M}_{(2j)(2i-1)}\Theta_{2i-1}\Xi_{2j} + \mathcal{M}_{(2j)(2i)}\Theta_{2i}\Xi_{2j} = \sum_{i,j=1}^{m} \mathbb{M}_{ij}\theta_i \cdot \xi_j.$$

In view of the definition of $\mathbb{M}_{ij}$, it is straightforward to verify that $\mathbb{M}_{ij} = (\mathbb{M}_{ji})^\mathsf{T}$ for all $1 \le i, j \le m$. Since $\mathcal{M}$ is a block matrix whose blocks are the $\mathbb{M}_{ij}$, this proves the symmetry of $\mathcal{M}$. □

Thus, we have obtained the following result.

Proposition 14. *Let $\Omega \subset \mathbb{R}^2$ be a m-gon, $\mathcal{M}, \Theta, \Xi$ be given in Definition 7, and θ, ξ be defined in (93), (94). Then, the second order Fréchet shape derivative is given in matricial form by*

$$D_F^2\mathcal{J}(0)(\theta, \xi) = \mathcal{M}\Theta \cdot \Xi.$$

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Appendix A

In this section we compute the matrix $\mathbb{M}_{ij}$ appearing in (95) of Section 9.3. We start with a few useful formulae.

Lemma 4. *Let $A \in \mathbb{R}^{d\times d}$ and θ defined in (93), then we have*

$$D\theta = \sum_{i=1}^{m} \theta_i \otimes \nabla\varphi_i, \quad D\theta^\mathsf{T} = \sum_{i=1}^{m} \nabla\varphi_i \otimes \theta_i$$
$$A : D\theta = \sum_{i=1}^{m} \theta_i \cdot A\nabla\varphi_i, \quad \operatorname{div}\theta = \sum_{i=1}^{m} \theta_i \cdot \nabla\varphi_i,$$
$$\operatorname{div}(f\theta) = \nabla f \cdot \theta + f \operatorname{div}\theta = \sum_{i=1}^{m} \theta_i \cdot (\varphi_i\nabla f + f\nabla\varphi_i) = \sum_{i=1}^{m} \theta_i \cdot \nabla(\varphi_i f),$$
$$D\theta\nabla u \cdot \nabla v = \sum_{i=1}^{m} [(\theta_i \otimes \nabla\varphi_i)\nabla u] \cdot \nabla v = \sum_{i=1}^{m} (\theta_i \cdot \nabla v)(\nabla\varphi_i \cdot \nabla u),$$
$$D\theta^\mathsf{T}\nabla u \cdot \nabla v = \sum_{i=1}^{m} (\theta_i \cdot \nabla u)(\nabla\varphi_i \cdot \nabla v).$$

In view of (53) we have using Lemma 4 and Lemma 1(4),

$$\int_\Omega \nabla\dot{u}(\theta) \cdot \nabla v = -\int_\Omega A'(\theta)\nabla u \cdot \nabla v + \int_\Omega \operatorname{div}(f\theta)v$$

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$$= \sum_{i=1}^m \theta_i \cdot \left(\int_\Omega -(\nabla u \cdot \nabla v)\nabla\varphi_i + (\nabla\varphi_i \cdot \nabla u)\nabla v + (\nabla\varphi_i \cdot \nabla v)\nabla u + \int_\Omega v\nabla(\varphi_i f) \right)$$

$$= \sum_{i=1}^m \theta_i \cdot \left(\int_\Omega -(\nabla\varphi_i \otimes \nabla u)\nabla v + 2(\nabla u \odot \nabla v)\nabla\varphi_i + \int_\Omega v\nabla(\varphi_i f) \right), \qquad \forall v \in H_0^1(\Omega).$$

Introduce functions $U_i \in H_0^1(\Omega, \mathbb{R}^2)$, $i \in I$, such that $\dot{u}(\theta) = \sum_{i=1}^m \theta_i \cdot U_i$. Since $\nabla\dot{u}(\theta)\cdot\nabla v = \sum_{i=1}^m \theta_i \cdot DU_i \nabla v$, the equations for U_i, $i \in I$, are

$$\int_\Omega DU_i \nabla v = \int_\Omega -(\nabla\varphi_i \otimes \nabla u)\nabla v + 2(\nabla u \odot \nabla v)\nabla\varphi_i + \int_\Omega v\nabla(\varphi_i f), \qquad \forall v \in H_0^1(\Omega). \tag{96}$$

Note that (96) can also be written as two independent BVPs.

Considering expression (71) of $D_F^2\mathcal{J}(0)(\theta,\xi)$, we compute first

$$F(\theta,\xi) = L_1 + L_2 + L_3 + L_4 + L_5 + L_6,$$

with

$$L_1 := \nabla\dot{u}(\theta)\cdot\nabla\dot{u}(\xi), \qquad L_2 := \mathbf{S}_0 \cdot (\theta \operatorname{div}\xi + \xi \operatorname{div}\theta)$$

$$L_3 := \mathbf{S}_1 : (D\theta \operatorname{div}\xi + D\xi \operatorname{div}\theta), \qquad L_4 := \left(\frac{1}{2}|\nabla u|^2 - uf\right)(\operatorname{div}\xi \operatorname{div}\theta + D\theta^\mathsf{T} : D\xi)$$

$$L_5 := -(D\theta D\xi + D\xi D\theta + D\xi D\theta^\mathsf{T})\nabla u \cdot \nabla u, \qquad L_6 := uD^2 f\theta \cdot \xi.$$

First of all we have

$$L_1 = \sum_{i=1}^m M_{1,ij}\theta_i \cdot \xi_j, \tag{97}$$

with $M_{1,ij} := DU_j DU_i^\mathsf{T}$. Using Lemma 1(5) and Lemma 4 we get

$$\mathbf{S}_0 \cdot \theta \operatorname{div}\xi = \sum_{i,j=1}^m \varphi_i(\mathbf{S}_0 \cdot \theta_i)(\xi_j \cdot \nabla\varphi_j) = \sum_{i,j=1}^m \xi_j \cdot \varphi_i(\nabla\varphi_j \otimes \mathbf{S}_0)\theta_i.$$

Thus, using the symmetry of the terms in L_2 we get

$$L_2 = \sum_{i,j=1}^m M_{2,ij}\theta_i \cdot \xi_j,$$

with $M_{2,ij} := \varphi_i(\nabla\varphi_j \otimes \mathbf{S}_0) + \varphi_j(\mathbf{S}_0 \otimes \nabla\varphi_i)$. Then, using Lemma 1(5) and Lemma 4, we get

$$\mathbf{S}_1 : D\theta \operatorname{div}\xi = \sum_{i,j=1}^m (\theta_i \cdot \mathbf{S}_1\nabla\varphi_i)(\xi_j \cdot \nabla\varphi_j) = \sum_{i,j=1}^m \xi_j \cdot (\nabla\varphi_j \otimes \mathbf{S}_1\nabla\varphi_i)\theta_i.$$

Thus, using the symmetry of the terms in L_3 we get

$$L_3 = \sum_{i,j=1}^m M_{3,ij}\theta_i \cdot \xi_j$$

with $M_{3,ij} := \nabla\varphi_j \otimes \mathbf{S}_1\nabla\varphi_i + \mathbf{S}_1\nabla\varphi_j \otimes \nabla\varphi_i$. Then, using Lemma 1(5) and Lemma 4 we compute

$$\operatorname{div}\xi \operatorname{div}\theta = \sum_{i,j=1}^{m}(\theta_i\cdot\nabla\varphi_i)(\xi_j\cdot\nabla\varphi_j) = \sum_{i,j=1}^{m}\xi_j\cdot(\nabla\varphi_j\otimes\nabla\varphi_i)\theta_i,$$

$$D\theta^{\mathsf{T}} : D\xi = \sum_{i,j=1}^{m}(\nabla\varphi_i\otimes\theta_i):(\xi_j\otimes\nabla\varphi_j) = \sum_{i,j=1}^{m}\xi_j\cdot(\nabla\varphi_i\otimes\nabla\varphi_j)\theta_i.$$

This yields $L_4 = \sum_{i,j=1}^{m} M_{4,ij}\theta_i\cdot\xi_j$, with $M_{4,ij} := \left(\frac{1}{2}|\nabla u|^2 - uf\right)(\nabla\varphi_i\otimes\nabla\varphi_j + \nabla\varphi_j\otimes\nabla\varphi_i)$. Then, we compute

$$D\xi\nabla u\cdot D\theta^{\mathsf{T}}\nabla u = \sum_{i=1}^{m}(\theta_i\cdot\nabla u)(\nabla\varphi_i\cdot D\xi\nabla u) = \sum_{i,j=1}^{m}(\theta_i\cdot\nabla u)(\xi_j\cdot\nabla\varphi_i)(\nabla\varphi_j\cdot\nabla u)$$
$$= \sum_{i,j=1}^{m}\xi_j\cdot[(\nabla\varphi_j\cdot\nabla u)(\nabla\varphi_i\otimes\nabla u)\theta_i].$$

In a similar way we have

$$D\theta\nabla u\cdot D\xi^{\mathsf{T}}\nabla u = \sum_{i,j=1}^{m}\xi_j\cdot[(\nabla\varphi_i\cdot\nabla u)(\nabla u\otimes\nabla\varphi_j)\theta_i],$$

$$D\theta^{\mathsf{T}}\nabla u\cdot D\xi^{\mathsf{T}}\nabla u = \sum_{i,j=1}^{m}\xi_j\cdot[(\nabla\varphi_i\cdot\nabla\varphi_j)(\nabla u\otimes\nabla u)\theta_i].$$

This yields $L_5 = \sum_{i,j=1}^{m} M_{5,ij}\theta_i\cdot\xi_j$, with

$$M_{5,ij} := -(\nabla\varphi_j\cdot\nabla u)(\nabla\varphi_i\otimes\nabla u) - (\nabla\varphi_i\cdot\nabla u)(\nabla u\otimes\nabla\varphi_j) - (\nabla\varphi_i\cdot\nabla\varphi_j)(\nabla u\otimes\nabla u).$$

Then, we compute $L_6 = \sum_{i,j=1}^{m} M_{6,ij}\theta_i\cdot\xi_j$, where $M_{6,ij} := u\varphi_i\varphi_j D^2 f$. Thus, we have obtained

$$D_F^2\mathcal{J}(0)(\theta,\xi) = L_1 + L_2 + L_3 + L_4 + L_5 + L_6 = \sum_{i,j=1}^{m}\mathbb{M}_{ij}\theta_i\cdot\xi_j,$$

with

$$\mathbb{M}_{ij} := \sum_{k=1}^{6}\int_\Omega M_{k,ij} \in \mathbb{R}^{2\times 2}. \tag{98}$$

References

[1] E. Beretta, E. Francini, S. Vessella, Differentiability of the Dirichlet to Neumann map under movements of polygonal inclusions with an application to shape optimization, SIAM J. Math. Anal. (ISSN 0036-1410) 49 (2) (2017) 756–776, https://doi.org/10.1137/16M1082160.

[2] E. Beretta, E. Francini, S. Vessella, A transmission problem on a polygonal partition: regularity and shape differentiability, Appl. Anal. 98 (2018) 1862–1874, https://doi.org/10.1080/00036811.2018.1469012.

[3] E. Beretta, S. Micheletti, S. Perotto, M. Santacesaria, Reconstruction of a piecewise constant conductivity on a polygonal partition via shape optimization in EIT, J. Comput. Phys. (ISSN 0021-9991) 353 (2018) 264–280, https://doi.org/10.1016/j.jcp.2017.10.017.

[4] M. Berggren, A unified discrete-continuous sensitivity analysis method for shape optimization, in: Applied and Numerical Partial Differential Equations, in: Comput. Methods Appl. Sci., vol. 15, Springer, New York, 2010, pp. 25–39.

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[5] G. Bouchitté, I. Fragalà, I. Lucardesi, Shape derivatives for minima of integral functionals, Math. Program. (ISSN 0025-5610) 148 (1–2, Ser. B) (2014) 111–142, https://doi.org/10.1007/s10107-013-0712-6.
[6] G. Bouchitté, I. Fragalà, I. Lucardesi, A variational method for second order shape derivatives, SIAM J. Control Optim. (ISSN 0363-0129) 54 (2) (2016) 1056–1084, https://doi.org/10.1137/15100494X.
[7] D. Bucur, J.-P. Zolésio, Anatomy of the shape Hessian via Lie brackets, Ann. Mat. Pura Appl. (4) (ISSN 0003-4622) 173 (1997) 127–143, https://doi.org/10.1007/BF01783465.
[8] S.N. Chandler-Wilde, D.P. Hewett, A. Moiola, Sobolev spaces on non-Lipschitz subsets of $\mathbb{R}^n$ with application to boundary integral equations on fractal screens, Integral Equ. Oper. Theory (ISSN 0378-620X) 87 (2) (2017) 179–224, https://doi.org/10.1007/s00020-017-2342-5.
[9] M. Costabel, On the limit Sobolev regularity for Dirichlet and Neumann problems on Lipschitz domains. ArXiv e-prints, Nov. 2017.
[10] M. Costabel, M. Dauge, Singularities of electromagnetic fields in polyhedral domains, Arch. Ration. Mech. Anal. (ISSN 0003-9527) 151 (3) (2000) 221–276, https://doi.org/10.1007/s002050050197.
[11] M. Costabel, M. Dauge, S. Nicaise, Analytic regularity for linear elliptic systems in polygons and polyhedra, Math. Models Methods Appl. Sci. (ISSN 0218-2025) 22 (8) (2012) 1250015, https://doi.org/10.1142/S0218202512500157.
[12] M. Dambrine, J. Lamboley, Stability in shape optimization with second variation. ArXiv e-prints, Oct. 2014.
[13] M. Dauge, Elliptic Boundary Value Problems on Corner Domains: Smoothness and Asymptotics Of Solutions, Lecture Notes in Mathematics, vol. 1341, Springer-Verlag, Berlin, ISBN 3-540-50169-X, 1988.
[14] M. Dauge, S. Nicaise, M. Bourlard, J.M.-S. Lubuma, Coefficients des singularités pour des problèmes aux limites elliptiques sur un domaine à points coniques. I. Résultats généraux pour le problème de Dirichlet, Modél. Math. Anal. Numér. (ISSN 0764-583X) 24 (1) (1990) 27–52, https://doi.org/10.1051/m2an/1990240100271.
[15] M. Dauge, S. Nicaise, M. Bourlard, J.M.-S. Lubuma, Coefficients des singularités pour des problèmes aux limites elliptiques sur un domaine à points coniques. II. Quelques opérateurs particuliers, Modél. Math. Anal. Numér. (ISSN 0764-583X) 24 (3) (1990) 343–367, https://doi.org/10.1051/m2an/1990240303431.
[16] M. Delfour, G. Payre, J.-P. Zolésio, An optimal triangulation for second-order elliptic problems, Comput. Methods Appl. Mech. Eng. (ISSN 0045-7825) 50 (3) (1985) 231–261, https://doi.org/10.1016/0045-7825(85)90095-7.
[17] M.C. Delfour, J.-P. Zolésio, Anatomy of the shape Hessian, Ann. Mat. Pura Appl. (4) (ISSN 0003-4622) 159 (1991) 315–339, https://doi.org/10.1007/BF01766307.
[18] M.C. Delfour, J.-P. Zolésio, Structure of shape derivatives for nonsmooth domains, J. Funct. Anal. (ISSN 0022-1236) 104 (1) (1992) 1–33, https://doi.org/10.1016/0022-1236(92)90087-Y.
[19] M.C. Delfour, J.-P. Zolésio, Shapes and Geometries: Metrics, Analysis, Differential Calculus, and Optimization, second edition, Advances in Design and Control, vol. 22, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, ISBN 978-0-898719-36-9, 2011.
[20] M.C. Delfour, Z. Mghazli, J.-P. Zolésio, Computation of shape gradients for mixed finite element formulation, in: Partial Differential Equation Methods in Control and Shape Analysis (Pisa), in: Lecture Notes in Pure and Appl. Math., vol. 188, Dekker, New York, 1997, pp. 77–93.
[21] Z. Ding, A proof of the trace theorem of Sobolev spaces on Lipschitz domains, Proc. Am. Math. Soc. (ISSN 0002-9939) 124 (2) (1996) 591–600, https://doi.org/10.1090/S0002-9939-96-03132-2.
[22] M. Eigel, K. Sturm, Reproducing kernel Hilbert spaces and variable metric algorithms in PDE-constrained shape optimization, Optim. Methods Softw. (ISSN 1055-6788) 33 (2) (2018) 268–296, https://doi.org/10.1080/10556788.2017.1314471.
[23] J.D. Eshelby, The elastic energy-momentum tensor, J. Elast. (ISSN 0374-3535) 5 (3–4) (1975) 321–335, https://doi.org/10.1007/BF00126994, special issue dedicated to A.E. Green.
[24] T. Etling, R. Herzog, Optimum experimental design by shape optimization of specimens in linear elasticity, SIAM J. Appl. Math. (ISSN 0036-1399) 78 (3) (2018) 1553–1576, https://doi.org/10.1137/17M1147743.
[25] L.C. Evans, R.F. Gariepy, Measure Theory and Fine Properties of Functions, Studies in Advanced Mathematics, CRC Press, Boca Raton, FL, ISBN 0-8493-7157-0, 1992.
[26] J. Ferchichi, J.-P. Zolésio, Shape sensitivity for the Laplace-Beltrami operator with singularities, J. Differ. Equ. (ISSN 0022-0396) 196 (2) (2004) 340–384, https://doi.org/10.1016/j.jde.2003.07.008.
[27] G. Fremiot, Eulerian semiderivatives of the eigenvalues for Laplacian in domains with cracks, Adv. Math. Sci. Appl. (ISSN 1343-4373) 12 (1) (2002) 115–134.
[28] G. Fremiot, J. Sokolowski, Shape sensitivity analysis of problems with singularities, in: Shape Optimization and Optimal Design, Cambridge, 1999, in: Lecture Notes in Pure and Appl. Math., vol. 216, Dekker, New York, 2001, pp. 255–276.
[29] G. Fremiot, J. Sokolowski, Hadamard formula in nonsmooth domains and applications, in: Partial Differential Equations on Multistructures, Luminy, 1999, in: Lecture Notes in Pure and Appl. Math., vol. 219, Dekker, New York, 2001, pp. 99–120.
[30] G. Frémiot, W. Horn, A. Laurain, M. Rao, J. Sokołowski, On the analysis of boundary value problems in nonsmooth domains, Diss. Math. (ISSN 0012-3862) 462 (2009) 149.
[31] P. Gangl, U. Langer, A. Laurain, H. Meftahi, K. Sturm, Shape optimization of an electric motor subject to nonlinear magnetostatics, SIAM J. Sci. Comput. (ISSN 1064-8275) 37 (6) (2015) B1002–B1025, https://doi.org/10.1137/15100477X.
[32] M. Giacomini, O. Pantz, K. Trabelsi, Certified descent algorithm for shape optimization driven by fully-computable a posteriori error estimators, ESAIM Control Optim. Calc. Var. (ISSN 1292-8119) 23 (3) (2017) 977–1001, https://doi.org/10.1051/cocv/2016021.
[33] P. Grisvard, Elliptic Problems in Nonsmooth Domains, Monographs and Studies in Mathematics, vol. 24, Pitman (Advanced Publishing Program), Boston, MA, ISBN 0-273-08647-2, 1985.
[34] E.J. Haug, K.K. Choi, V. Komkov, Design Sensitivity Analysis of Structural Systems, Mathematics in Science and Engineering, vol. 177, Academic Press, Inc., Orlando, FL, ISBN 0-12-332920-5, 1986.
[35] A. Henrot, M. Pierre, Shape Variation and Optimization: A Geometrical Analysis, EMS Tracts in Mathematics, vol. 28, European Mathematical Society (EMS), Zürich, ISBN 978-3-03719-178-1, 2018, English version of the French publication [MR2512810] with additions and updates.

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[36] M. Hintermüller, A. Laurain, I. Yousept, Shape sensitivities for an inverse problem in magnetic induction tomography based on the eddy current model, Inverse Probl. (ISSN 0266-5611) 31 (6) (2015) 065006, https://doi.org/10.1088/0266-5611/31/6/065006.
[37] R. Hiptmair, A. Paganini, S. Sargheini, Comparison of approximate shape gradients, BIT Numer. Math. (ISSN 0006-3835) 55 (2) (2015) 459–485, https://doi.org/10.1007/s10543-014-0515-z.
[38] K. Ito, K. Kunisch, G.H. Peichl, Variational approach to shape derivatives for a class of Bernoulli problems, J. Math. Anal. Appl. (ISSN 0022-247X) 314 (1) (2006) 126–149, https://doi.org/10.1016/j.jmaa.2005.03.100.
[39] K. Ito, K. Kunisch, G.H. Peichl, Variational approach to shape derivatives, ESAIM Control Optim. Calc. Var. (ISSN 1292-8119) 14 (3) (2008) 517–539, https://doi.org/10.1051/cocv:2008002.
[40] D. Jerison, C.E. Kenig, The inhomogeneous Dirichlet problem in Lipschitz domains, J. Funct. Anal. (ISSN 0022-1236) 130 (1) (1995) 161–219, https://doi.org/10.1006/jfan.1995.1067.
[41] V.A. Kozlov, V.G. Maz'ya, J. Rossmann, Elliptic Boundary Value Problems in Domains with Point Singularities, Mathematical Surveys and Monographs, vol. 52, American Mathematical Society, Providence, RI, ISBN 0-8218-0754-4, 1997.
[42] J. Lamboley, Variations around irregular and optimal shapes, Theses, École normale supérieure de Cachan - ENS Cachan, https://tel.archives-ouvertes.fr/tel-00346316, Dec. 2008.
[43] J. Lamboley, M. Pierre, Structure of shape derivatives around irregular domains and applications, J. Convex Anal. (ISSN 0944-6532) 14 (4) (2007) 807–822.
[44] J. Lamboley, A. Novruzi, M. Pierre, Regularity and singularities of optimal convex shapes in the plane, Arch. Ration. Mech. Anal. (ISSN 0003-9527) 205 (1) (2012) 311–343, https://doi.org/10.1007/s00205-012-0514-7.
[45] J. Lamboley, A. Novruzi, M. Pierre, Estimates of first and second order shape derivatives in nonsmooth multidimensional domains and applications, J. Funct. Anal. (ISSN 0022-1236) 270 (7) (2016) 2616–2652, https://doi.org/10.1016/j.jfa.2016.02.013.
[46] A. Laurain, Structure of shape derivatives in nonsmooth domains and applications, Adv. Math. Sci. Appl. (ISSN 1343-4373) 15 (1) (2005) 199–226.
[47] A. Laurain, A level set-based structural optimization code using FEniCS, Struct. Multidiscip. Optim. (ISSN 1615-147X) 58 (3) (2018) 1311–1334, https://doi.org/10.1007/s00158-018-1950-2.
[48] A. Laurain, K. Sturm, Domain expression of the shape derivative and application to electrical impedance tomography, Preprint, Weierstraß-Institut für Angewandte Analysis und Stochastik (1863), 2013, ISSN 0946-8633.
[49] A. Laurain, K. Sturm, Distributed shape derivative via averaged adjoint method and applications, Math. Model. Numer. Anal. (ISSN 0764-583X) 50 (4) (2016) 1241–1267, https://doi.org/10.1051/m2an/2015075.
[50] V. Maz'ya, S. Nazarov, B. Plamenevskij, Asymptotic Theory of Elliptic Boundary Value Problems in Singularly Perturbed Domains, vol. I, Operator Theory: Advances and Applications, vol. 111, Birkhäuser Verlag, Basel, ISBN 3-7643-6397-5, 2000, translated from the German by Georg Heinig and Christian Posthoff.
[51] D. Mitrea, M. Mitrea, L. Yan, Boundary value problems for the Laplacian in convex and semiconvex domains, J. Funct. Anal. (ISSN 0022-1236) 258 (8) (2010) 2507–2585, https://doi.org/10.1016/j.jfa.2010.01.012.
[52] A.A. Novotny, J. Sokołowski, Topological Derivatives in Shape Optimization, Interaction of Mechanics and Mathematics, Springer, Heidelberg, ISBN 978-3-642-35244-7, 2013.
[53] A. Novruzi, M. Pierre, Structure of shape derivatives, J. Evol. Equ. (ISSN 1424-3199) 2 (3) (2002) 365–382, https://doi.org/10.1007/s00028-002-8093-y.
[54] A. Paganini, F. Wechsung, P.E. Farrell, Higher-order moving mesh methods for PDE-constrained shape optimization, SIAM J. Sci. Comput. (ISSN 1064-8275) 40 (4) (2018) A2356–A2382, https://doi.org/10.1137/17M1133956.
[55] S. Schmidt, Weak and strong form shape Hessians and their automatic generation, SIAM J. Sci. Comput. (ISSN 1064-8275) 40 (2) (2018) C210–C233, https://doi.org/10.1137/16M1099972.
[56] V.H. Schulz, M. Siebenborn, K. Welker, Efficient PDE constrained shape optimization based on Steklov-Poincaré-type metrics, SIAM J. Optim. (ISSN 1052-6234) 26 (4) (2016) 2800–2819, https://doi.org/10.1137/15M1029369.
[57] J. Simon, Differentiation with respect to the domain in boundary value problems, Numer. Funct. Anal. Optim. (ISSN 0163-0563) 2 (7–8) (1980) 649–687, https://doi.org/10.1080/01630563.1980.10120631.
[58] L. Simon, Lectures on geometric measure theory, in: Proceedings of the Centre for Mathematical Analysis, Australian National University, vol. 3, Australian National University, Centre for Mathematical Analysis, Canberra, ISBN 0-86784-429-9, 1983.
[59] J. Sokołowski, J.-P. Zolésio, Introduction to Shape Optimization: Shape Sensitivity Analysis, Springer Series in Computational Mathematics, vol. 16, Springer-Verlag, Berlin, ISBN 3-540-54177-2, 1992.
[60] K. Sturm, On Shape Optimization with Non-linear Partial Differential Equations, PhD thesis, Technische Universität Berlin, October 2014.
[61] K. Sturm, M. Hintermüller, D. Hömberg, Distortion compensation as a shape optimisation problem for a sharp interface model, Comput. Optim. Appl. (ISSN 0926-6003) 64 (2) (2016) 557–588, https://doi.org/10.1007/s10589-015-9816-7.

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