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Shape derivatives in differential forms I: an intrinsic perspective

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Abstract We treat Zolésio's velocity method of shape calculus using the formalism of differential forms, in particular, the notion of Lie derivative. This provides a unified and elegant approach to computing even higher-order shape derivatives of domain and boundary integrals and avoids the tedious manipulations entailed by classical vector calculus. Hitherto unknown expressions for shape Hessians can be derived with little effort. The perspective of differential forms perfectly fits second-order boundary value problems (BVPs). We illustrate its power by deriving the shape derivatives of solutions to second-order elliptic BVPs with Dirichlet, Neumann and Robin boundary conditions. A new dual mixed variational approach is employed in the case of Dirichlet boundary conditions.

Keywords Differential forms · Lie derivative · shape derivative · Hadamard structure theorems · dual formulation

Mathematics Subject Classification (2000) 35B37 · 49J20 · 58A10

1 Introduction

Shape calculus, which is the differentiation of functionals and operators with respect to variations of a spatial domain, is one of the mathematical foundations of shape sensitivity analysis and shape optimization. Here, the control variable is no longer a set of parameters or functions but the shape or structure of a geometric object. For a comprehensive presentation, the reader is referred to the monograph [6]. In this work, shape calculus is approached via

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the *velocity method*, that is, shape perturbations are governed by flows generated by spatial vector fields. This paradigm of shape calculus will be adopted throughout the paper.

In this article, we derive shape derivatives using the calculus of differential forms as opposed to classical vector calculus. One might object that no new insights can be expected, because vector analysis offers a model "isomorphic" to the calculus of differential forms. Nevertheless, in our opinion, adopting differential forms brings a significant reward, for the following reasons:

– Differential forms facilitate the *unified treatment* of different spatial dimensions and different classes of boundary value problems (BVPs) and functionals corresponding to different orders of forms.
– The velocity method of shape calculus neatly fits the concept of *Lie derivative*, which is natural for differential forms.
– The calculus of differential forms can often use *simple formulas*, where vector calculus has to resort to complicated expressions.
– Differential forms offer a *coordinate independent* description of models, whereas vector calculus will depend on coordinates, whose choice is often arbitrary.
– Differential forms clearly separate terms that are invariant with respect to homeomorphic transformations and those that depend on metric.
– The exterior derivative of differential forms is the natural language for expressing conservation principles underlying many PDE-based models. It is the key differential operator occurring in second-order BVPs. Shape derivatives of their solutions play a central role in shape optimization.

The aim of this first paper is twofold. Firstly, we use the exterior calculus of differential forms and the Lie derivative to rederive the renowned Hadamard structure theorem [9], which essentially states that shape derivatives depend only on the normal component of the deformations on the boundary of the reference domain. We demonstrate how higher-order shape derivatives can be derived recursively by repeating the argument in the proof of first-order shape gradients.

Secondly, in the case of a second-order PDE with various boundary conditions, we illustrate how to determine the concrete shape derivatives of solutions of variational problems by applying our abstract structure theorems. In particular, we find that via a dual formulation, the boundary condition for the shape derivative of the solution of an elliptic PDE with Dirichlet boundary condition can be obtained rigorously in the weak sense. This is one of the several new results presented in this article.

The outline of the paper is as follows: Sect. 2 presents important notations and definitions connected with differential forms. Section 3 is devoted to the proof of structure theorems of shape derivatives by the exterior calculus of differential forms. In particular, the shape Hessians of domain and boundary integrals are further investigated, with emphasis on the asymmetry due to the Lie bracket of two velocity fields associated with the transformations. In Sect. 4, we reinterpret the abstract theory in Sect. 3 in terms of vector proxies, namely scalar functions and vector fields, with emphasis on the shape gradient and Hessian of domain and boundary integrals, bilinear forms, and normal derivatives. In Sect. 5, by a model problem, we illustrate the machinery for how to express the abstract structure theorems for second-order elliptic BVPs with natural (Neumann and Robin) boundary conditions. In Sect. 6, we derive, in particular via variational methods, the Dirichlet boundary conditions supplementing with the PDE for the shape derivative of the solution to the Dirichlet problem in the dual formulation.

2 Preliminaries

2.1 Notations

The interior and closure of a set $A \subset \mathbb{R}^n$ will be denoted, respectively, by $\operatorname{int} A$ and $\overline{A}$. Throughout the paper, the classical Euclidean space $\mathbb{R}^d$ ($d \in \mathbb{N}, d \geq 2$) of dimension d is equipped with the canonical orthonormal bases e_j's, $1 \leq j \leq d$, and norm $|\mathbf{x}| := \sqrt{x_1^2 + \cdots + x_d^2}$ for $\mathbf{x} = (x_1, \ldots, x_d)^T \in \mathbb{R}^d$, and inner product $\langle \mathbf{x}, \mathbf{y} \rangle$. The canonical orthonormal basis of $\mathbb{R}^d$ corresponds to a dual basis of $(\mathbb{R}^d)^*$, i.e., $\boldsymbol{d}x_1, \boldsymbol{d}x_2, \ldots, \boldsymbol{d}x_d$ with $\boldsymbol{d}x_i(e_j) = 1$ if $i = j$ and zero otherwise.

2.2 Differential forms

In this subsection, we briefly review some important notions and results about the exterior calculus of differential forms. Readers may refer to [4,8] for a detailed exposition of differential forms.[1]

A differential form $\boldsymbol{\omega}$ of degree l, $l \in \mathbb{N}_0 = \{0\} \cup \mathbb{N}$, and class C^m, $m \in \mathbb{N}_0$, in some domain $\Omega \subset \mathbb{R}^d$, is a mapping with values in the space of alternating l-multilinear forms $\bigwedge^l$ on $\mathbb{R}^d$:

$$\boldsymbol{\omega} = \sum_I \boldsymbol{\omega}_I \boldsymbol{d}\mathbf{x}_I : \mathbf{x} \in \Omega \subset \mathbb{R}^d \mapsto \boldsymbol{\omega}(\mathbf{x}) \in \bigwedge^l, \tag{1}$$

where all the components $\boldsymbol{\omega}_I(\mathbf{x}) \in C^m(\overline{\Omega})$, and summation is over all the increasing l-permutations $I = (i_1, \ldots, i_l)$, with $1 \leq i_1 < \cdots < i_l \leq d$, and we denote $\boldsymbol{d}\mathbf{x}_I = \boldsymbol{d}x_{i_1} \wedge \cdots \wedge \boldsymbol{d}x_{i_l}$. Hereafter, we write $\boldsymbol{\omega} \in \mathscr{DF}^{l,m}(\overline{\Omega})$. In an analogous way, we can define $\mathscr{DF}^{l,\infty}(\overline{\Omega})$ if all $\boldsymbol{\omega}_I(\mathbf{x}) \in C^\infty(\overline{\Omega})$, and $\mathscr{DF}_0^{l,\infty}(\Omega)$ if all $\boldsymbol{\omega}_I(\mathbf{x}) \in C_0^\infty(\Omega)$. Likewise, $\boldsymbol{H}^s\left(\Omega; \bigwedge^l(\mathbb{R}^d)\right)$ ($s \in \mathbb{R}_0^+$) denotes the space consisting of all differential forms with each component in $H^s(\Omega)$, which can be viewed as the Hilbert space obtained by means of the completion of $\mathscr{DF}^{l,\infty}(\overline{\Omega})$ with respect to the norm

$$\|\boldsymbol{\omega}\|^2_{\boldsymbol{H}^s\left(\Omega; \bigwedge^l(\mathbb{R}^d)\right)} := \sum_I \|\boldsymbol{\omega}_I\|^2_{H^s(\Omega)}. \tag{2}$$

In particular, we use $\boldsymbol{L}^2(\Omega; \bigwedge^l(\mathbb{R}^d))$ instead of $\boldsymbol{H}^0\left(\Omega; \bigwedge^l(\mathbb{R}^d)\right)$.

Differential forms can be represented by their coefficient functions, or *vector proxies*. Please see Table 1 (cf. [13, Section 2.1] and [2, Sect. 2.1]) for vector proxies of differential forms of different orders in three-dimensional Euclidean space and refer to Table 2 (cf. [8, Chapter 3]) for the interpretation of integrals of differential forms in terms of integrals of vector proxies.

The *exterior product* of differential forms $\boldsymbol{\omega} \in \mathscr{DF}^{l,m}(\overline{\Omega})$ and $\boldsymbol{\eta} \in \mathscr{DF}^{k,m}(\overline{\Omega})$ (cf. [4, p. 19]),and *contraction* of $\boldsymbol{\omega} \in \mathscr{DF}^{l,m}(\overline{\Omega})$ with a vector field $\mathbf{v} \in \mathbb{R}^d$ (cf. [8, Sect. 2.9.]) are denoted, respectively, as

$$\boldsymbol{\omega} \wedge \boldsymbol{\eta} \in \mathscr{DF}^{l+k,m}(\overline{\Omega}), \quad i_{\mathbf{v}}\boldsymbol{\omega} \in \mathscr{DF}^{l-1,m}(\overline{\Omega}). \tag{3}$$

[1] We adopt the convention that roman letters denote scalar quantities, functions, and their associated spaces etc., while boldface letters represent vector-valued quantities, functions, and their associated spaces etc. In particular, boldface Greek letters, $\boldsymbol{\omega}$, $\boldsymbol{\eta}$, $\boldsymbol{\nu}$ and $\boldsymbol{\rho}$ etc., are reserved for differential forms.

Table 1 Relationship between differential forms and vector proxies in three-dimensional Euclidean space $\mathbf{v}, \mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3 \in \mathbb{R}^3$

	Differential form	Related function u/vector field $\mathbf{u}$
$l=0$	$\mathbf{x} \mapsto \boldsymbol{\omega}(\mathbf{x})$	$u(\mathbf{x}) := \boldsymbol{\omega}(\mathbf{x})$
$l=1$	$\mathbf{x} \mapsto \{\mathbf{v} \mapsto \boldsymbol{\omega}(\mathbf{x})(\mathbf{v})\}$	$\langle \mathbf{u}(\mathbf{x}), \mathbf{v}\rangle := \boldsymbol{\omega}(\mathbf{x})(\mathbf{v})$
$l=2$	$\mathbf{x} \mapsto \{\mathbf{v}_1, \mathbf{v}_2 \mapsto \boldsymbol{\omega}(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2)\}$	$\langle \mathbf{u}(\mathbf{x}), \mathbf{v}_1 \times \mathbf{v}_2\rangle := \boldsymbol{\omega}(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2)$
$l=3$	$\mathbf{x} \mapsto \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3 \mapsto \boldsymbol{\omega}(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)\}$	$u(\mathbf{x}) \det(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) := \boldsymbol{\omega}(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$

Table 2 Relationship between integrals of differential forms and vector proxies in $\mathbb{R}^3$

	Integral of differential forms	Integral of related function u/vector field $\mathbf{u}$
$l=0$	$\int_P \boldsymbol{\omega}$	$\int_P u \,\mathrm{d}x := u(P)$
$l=1$	$\int_E \boldsymbol{\omega}$	$\int_E \mathbf{u} \cdot \mathrm{d}\overrightarrow{l} := \int_E \mathbf{u} \cdot \mathbf{t} \,\mathrm{d}l$
$l=2$	$\int_F \boldsymbol{\omega}$	$\int_F \mathbf{u} \cdot \mathrm{d}\overrightarrow{S} := \int_F \mathbf{u} \cdot \mathbf{n} \,\mathrm{d}S$
$l=3$	$\int_V \boldsymbol{\omega}$	$\int_V u \,\mathrm{d}V$

P, E, F, V denotes some point, oriented curve, oriented face and volume in $\mathbb{R}^3$ with $\mathbf{t}$ and $\mathbf{n}$ being the unit tangential vector along E and the unit normal vector on F, respectively, and $u(P)$ means point evaluation of u at P

Table 3 Relationship between contraction for differential forms and vector proxies in $\mathbb{R}^3$

	Contraction of differential forms	Contraction of related function u/vector field $\mathbf{u}$
$l=0$	$\mathbf{x} \mapsto i_{\mathbf{v}}\boldsymbol{\omega}$	$0 := i_{\mathbf{v}}\boldsymbol{\omega}(\mathbf{x})$
$l=1$	$\mathbf{x} \mapsto i_{\mathbf{v}}\boldsymbol{\omega}(\mathbf{x})$	$(\mathbf{u} \cdot \mathbf{v})\,(\mathbf{x}) := i_{\mathbf{v}}\boldsymbol{\omega}(\mathbf{x})$
$l=2$	$\mathbf{x} \mapsto \{\mathbf{v} \mapsto i_{\mathbf{v}}\boldsymbol{\omega}(\mathbf{x})(\mathbf{v})\}$	$(\mathbf{u} \times \mathbf{v})\,(\mathbf{x}) := i_{\mathbf{v}}\boldsymbol{\omega}(\mathbf{x})(\mathbf{v})$
$l=3$	$\mathbf{x} \mapsto \{\mathbf{v}_1, \mathbf{v}_2 \mapsto i_{\mathbf{v}}\boldsymbol{\omega}(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2)\}$	$\det(u(\mathbf{x})\mathbf{v}, \mathbf{v}_1, \mathbf{v}_2) := i_{\mathbf{v}}\boldsymbol{\omega}(\mathbf{x})(\mathbf{v}_1, \mathbf{v}_2)$

Table 3 gives the operation of contraction for vector proxies in three-dimensional Euclidean space.

If $\mathscr{T} : \widehat{\Omega} \mapsto \Omega$ is a diffeomorphism between two smooth manifolds in $\mathbb{R}^d$, then the *pullback* $\mathscr{T}^* : \mathscr{DF}^{l,\infty}(\overline{\Omega}) \mapsto \mathscr{DF}^{l,\infty}(\widehat{\Omega})$ [4, p. 28] is given by

$$((\mathscr{T}^*\boldsymbol{\omega})(\widehat{\mathbf{x}}))(\mathbf{v}_1, \ldots, \mathbf{v}_l) = (\boldsymbol{\omega}(\mathscr{T}(\widehat{\mathbf{x}})))(D\mathscr{T}(\widehat{\mathbf{x}})\mathbf{v}_1, \ldots, D\mathscr{T}(\widehat{\mathbf{x}})\mathbf{v}_l), \tag{4}$$

where $\mathbf{v}_1, \ldots, \mathbf{v}_l \in \mathbb{R}^d$ and the linear map $D\mathscr{T}(\widehat{\mathbf{x}}) : \mathbb{R}^d \mapsto \mathbb{R}^d$ is the derivative (Jacobian) of $\mathscr{T}$ at $\widehat{\mathbf{x}}$. The pullbacks satisfy the transformation rule

$$\int_{\mathscr{T}(\widehat{\Omega})} \boldsymbol{\omega} = \int_{\widehat{\Omega}} \mathscr{T}^*\boldsymbol{\omega}. \tag{5}$$

For a differential l-form $\boldsymbol{\omega} = \sum_I \boldsymbol{\omega}_I \boldsymbol{d}\mathbf{x}_I \in \mathscr{DF}^{l,\infty}(\overline{\Omega})$, its *exterior derivative* $\boldsymbol{d\omega}$ through the *exterior differential operator* $\boldsymbol{d}$ [4, p. 20] is defined by

$$\boldsymbol{d\omega} := \sum_{i=1}^{d} \sum_{I} \frac{\partial \omega_I}{\partial x_i} \boldsymbol{d}x_i \wedge \boldsymbol{d}\mathbf{x}_I \in \mathscr{DF}^{l+1,\infty}(\overline{\Omega}), \tag{6}$$

and if $l \geq d$, $\boldsymbol{d\omega} = 0$ by definition. In terms of vector proxies, the incarnation of $\boldsymbol{d}$ is **grad**, **curl** and div when $l = 0$, 1 and 2, respectively, in $\mathbb{R}^3$. We also recall Stokes' theorem

$$\int_{\partial\Omega} \boldsymbol{\omega} = \int_{\Omega} \boldsymbol{d\omega}, \tag{7}$$

and the first Poincaré Lemma, namely

$$\boldsymbol{dd\omega} = 0, \tag{8}$$

for all $\boldsymbol{\omega}$ (cf. [4]). We remind of the fact that the pullback commutes with the exterior derivative, i.e.,

$$\mathscr{T}^*(\boldsymbol{d\omega}) = \boldsymbol{d}(\mathscr{T}^*\boldsymbol{\omega}), \quad \forall\, \boldsymbol{\omega} \in \mathscr{DF}^{l,\infty}(\overline{\Omega}), \tag{9}$$

and with the exterior product

$$\mathscr{T}^*(\boldsymbol{\omega} \wedge \boldsymbol{\eta}) = \mathscr{T}^*\boldsymbol{\omega} \wedge \mathscr{T}^*\boldsymbol{\eta}, \quad \forall\, \boldsymbol{\omega} \in \mathscr{DF}^{l,\infty}(\overline{\Omega}),\ \boldsymbol{\eta} \in \mathscr{DF}^{k,\infty}(\overline{\Omega}). \tag{10}$$

Important Hilbert spaces of differential forms are [2, Sect. 2.2]

$$\boldsymbol{H}^k\left(\boldsymbol{d}, \Omega, \bigwedge^l(\mathbb{R}^d)\right) := \left\{\boldsymbol{\omega} \in \boldsymbol{H}^k\left(\Omega; \bigwedge^l(\mathbb{R}^d)\right) \mid \boldsymbol{d\omega} \in \boldsymbol{H}^k\left(\Omega; \bigwedge^{l+1}(\mathbb{R}^d)\right)\right\}$$

for $k \in \mathbb{N}_0$, with the natural graph norm

$$\|\boldsymbol{\omega}\|^2_{\boldsymbol{H}^k\left(\boldsymbol{d},\Omega,\bigwedge^l(\mathbb{R}^d)\right)} := \|\boldsymbol{\omega}\|^2_{\boldsymbol{H}^k(\Omega,\bigwedge^l(\mathbb{R}^d))} + \|\boldsymbol{d\omega}\|^2_{\boldsymbol{H}^k(\Omega,\bigwedge^{l+1}(\mathbb{R}^d))}. \tag{11}$$

Specifically, we simply put $\boldsymbol{H}(\boldsymbol{d}, \Omega, \bigwedge^l(\mathbb{R}^d))$ when $k = 0$.

2.3 Lie derivatives of differential forms

Our approach to shape calculus will be based on the velocity method (cf. [6,18]). We start from a given bounded domain Ω of class C^m (cf. [1]), (with m sufficiently large and to be specified in different contexts, say, e.g., $m \geq 2$ in the sequel) and with boundary $\Gamma = \partial\Omega$. We fix $D \subset \mathbb{R}^d$ with sufficiently smooth boundary such that $\Omega \Subset D$. This D is known as *hold-all domain*, and we may, without loss of generality, take D either as a ball with sufficiently large radius containing Ω, or the whole space $\mathbb{R}^d$.

Given a Lipschitz continuous velocity field

$$\mathbf{v} : D \to \mathbb{R}^d$$

and an initial configuration $\mathbf{x}(0, X) = X \in \mathbb{R}^d$, the associated flow $\mathbf{x}(t, X)$ can be defined through the differential equation

$$\frac{\partial \mathbf{x}}{\partial t}(t, X) = \mathbf{v}(X), \tag{12}$$

$$\mathbf{x}(0, X) = X, \quad X \in D. \tag{13}$$

A unique solution of the problem (12), (13) exists when $\mathbf{v} \in C^m(D, \mathbb{R}^d)$ and $\mathbf{v} \cdot \mathbf{n} = 0$ on ∂D. The flow spawns a family of C^m-diffeomorphism

$$T_t(\mathbf{v})X := \mathbf{x}(t, X) \quad t \geq 0,\ X \in D. \tag{14}$$

Thus, we can define a family of deformed domains

$$\Omega_t(\mathbf{v}) := T_t(\mathbf{v})(\Omega) = \{T_t(\mathbf{v})(X) : \forall\, X \in \Omega\}. \tag{15}$$

Table 4 Lie derivatives for Euclidean vector proxies in $\mathbb{R}^3$

	Vector proxy in $\mathbb{R}^3$	Vector proxy for Lie derivative
$l=0$	$\omega \leftrightarrow u$	$\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega} \leftrightarrow \mathbf{grad}\, u$
$l=1$	$\omega \leftrightarrow \mathbf{u}$	$\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega} \leftrightarrow \mathbf{curl}\,\mathbf{u} \times \mathbf{v} + \mathbf{grad}(\mathbf{v}\cdot\mathbf{u})$
$l=2$	$\omega \leftrightarrow \mathbf{u}$	$\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega} \leftrightarrow \mathbf{v}(\operatorname{div}\mathbf{u}) + \mathbf{curl}(\mathbf{u}\times\mathbf{v})$
$l=3$	$\omega \leftrightarrow u$	$\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega} \leftrightarrow \operatorname{div}(\mathbf{v}u)(\mathbf{x})$

The association of vector proxies with differential forms indicated by $\leftrightarrow$ follows the rules laid out in Table 1

parametrized by the *pseudo-time* t. Since $T_t(\mathbf{v})$ is a diffeomorphism of class C^m, we see that the normal field $\mathbf{n}_t(\mathbf{v})$ on the boundary $\Gamma_t(\mathbf{v}) := \partial\,(\Omega_t(\mathbf{v}))$ belongs to $C^{m-1}(\Gamma_t, \mathbb{R}^d)$ [18, p. 16].

Definition 1 (cf. [8]) If the following limit exists, the *Lie derivative* $\mathscr{L}_{\mathbf{v}}$ of a l-form ω in the direction of the vector field $\mathbf{v}$ is defined as:

$$\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega} := \lim_{t\to 0} \frac{T_t(\mathbf{v})^*\boldsymbol{\omega} - \boldsymbol{\omega}}{t}. \tag{16}$$

By Cartan's formula [8, Theorem 4.23], we can represent the Lie derivative as

$$\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega} = (i_{\mathbf{v}}\,\boldsymbol{d} + \boldsymbol{d}\,i_{\mathbf{v}})\,\boldsymbol{\omega}, \tag{17}$$

from which it is immediate that the Lie derivative and exterior derivative commute

$$\boldsymbol{d}\mathscr{L}_{\mathbf{v}} = \mathscr{L}_{\mathbf{v}}\boldsymbol{d}. \tag{18}$$

Expressions for the Lie derivative in 3D Euclidean vector proxies can be found in Table 4.

3 Shape calculus in forms

In this section, we will investigate abstract shape calculus in differential forms and prove Hadamard-style fundamental structure theorems from the perspective of differential forms for shape derivatives of domain and boundary integrals. Our results can be applied for the characterization of shape derivatives associated with a wide range of PDEs, in particular via variational methods. New proofs in coordinate-free setting become available. Thanks to Stokes' theorem, the treatment of the shape derivatives of boundary integrals can be reduced to the case of domain integrals. Moreover, higher-order shape derivatives can be derived in a recursive way within the new framework.

Let us briefly review shape calculus, see [6,18] for more details. Consider the set $\mathscr{P}(D) = \{\Omega \text{ is of class } C^m : \Omega \Subset D\}$ of the subsets of D. A shape functional is a map

$$J\, :\, \mathscr{A}(D) \to \mathbb{K}, \tag{19}$$

where $\mathscr{A}(D)$ is some admissible family of domains in $\mathscr{P}(D)$ and $\mathbb{K}$ stands for $\mathbb{R}$ or $\mathbb{C}$. For a domain Ω of class C^m transformed by any velocity field $\mathbf{v} \in C^m(D, \mathbb{R}^d)$, $\mathscr{A}(D)$ can be chosen as the set of all possible transformed domain $\Omega_t(\mathbf{v})$ when t is small enough. For ease of exposition, we set D to be $\mathbb{R}^d$ in the sequel.

Definition 2 (*Shape derivative of shape functionals*) (cf. [6,18]) Let $\mathbf{v}$ be a vector field $\mathbf{v} \in C^m(\mathbb{R}^d, \mathbb{R}^d)$. The shape functional J is said to have a shape derivative at Ω in the direction $\mathbf{v}$ if the following limit exists and it is finite

$$\lim_{t\to 0}\frac{J(T_t(\mathbf{v})(\Omega))-J(\Omega)}{t}. \tag{20}$$

It is written as $\mathrm{d}J(\Omega;\mathbf{v})$, if it exists.

Next, we will elaborate on the shape derivatives of two special functionals: domain and boundary integrals, which commonly occur as output functionals for solutions of BVPs for PDEs.

Let $\Omega\subset\mathbb{R}^d$ be a bounded d-dimensional manifold of class C^m. The domain functional of a density form $\boldsymbol{\omega}\in\mathscr{D}\mathscr{F}^{d,m}(\mathbb{R}^d)$ defined globally is

$$J(\Omega)=\int\limits_{\Omega}\boldsymbol{\omega}. \tag{21}$$

To define higher-order shape derivatives of domain and boundary integrals, we introduce velocity fields $\mathbf{v}_1,\ldots,\mathbf{v}_k\in C^m(\mathbb{R}^d,\mathbb{R}^d)$. Then, the multiply transformed domain is

$$\Omega_{t_1,\ldots,t_k}(\mathbf{v}_1,\ldots,\mathbf{v}_k)=T_{t_1}(\mathbf{v}_1)\left(\ldots\left(T_{t_k}(\mathbf{v}_k)(\Omega)\right)\right). \tag{22}$$

Thus, the deformed domain integral of the corresponding density form $\boldsymbol{\omega}$ is

$$J_{\mathbf{v}_1,\ldots,\mathbf{v}_k}(t_1,\ldots,t_k)=\int\limits_{\Omega_{t_1,\ldots,t_k}(\mathbf{v}_1,\ldots,\mathbf{v}_k)}\boldsymbol{\omega}. \tag{23}$$

Definition 3 [6, p. 371] The *shape derivatives of domain integrals* of different orders are under suitable smoothness conditions on the domain and velocity fields $\mathbf{v},\mathbf{w},\mathbf{v}_1,\ldots,\mathbf{v}_k$, defined as follows:

$$\begin{aligned}
\langle\mathrm{d}J(\Omega),\mathbf{v}\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}J_{\mathbf{v}}(t)\Big|_{t=0},\\
\left\langle\mathrm{d}^2J(\Omega);\mathbf{v},\mathbf{w}\right\rangle &= \frac{\partial}{\partial s}\left\{\frac{\partial}{\partial t}J_{\mathbf{v},\mathbf{w}}(t,s)\Big|_{t=0}\right\}\Big|_{s=0},\\
\left\langle\mathrm{d}^kJ(\Omega);\mathbf{v}_1,\ldots,\mathbf{v}_k\right\rangle &= \frac{\partial}{\partial t_k}\left\{\ldots\frac{\partial}{\partial t_1}J_{\mathbf{v}_{t_1},\ldots,\mathbf{v}_k}(t_1,\ldots,t_k)\Big|_{t_1=0}\ldots\right\}\Big|_{t_k=0}.
\end{aligned}$$

3.1 Domain integral

We are now in a position to present the first main result on the shape derivatives of domain integrals.

Theorem 1 (First fundamental structure theorem) *The domain functional $J(\Omega)$ from (21) is shape differentiable, with shape gradient*

$$\langle\mathrm{d}J(\Omega),\mathbf{v}\rangle=\int\limits_{\Omega}\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega}=\int\limits_{\Omega}\boldsymbol{d}i_{\mathbf{v}}\boldsymbol{\omega}=\int\limits_{\partial\Omega}i_{\mathbf{v}}\boldsymbol{\omega}, \tag{24}$$

and shape Hessian

$$\left\langle\mathrm{d}^2J(\Omega);\mathbf{v},\mathbf{w}\right\rangle=\int\limits_{\Omega}\mathscr{L}_{\mathbf{w}}\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega}=\int\limits_{\Omega}\boldsymbol{d}\,i_{\mathbf{w}}\left(\boldsymbol{d}\,i_{\mathbf{v}}\boldsymbol{\omega}\right)=\int\limits_{\partial\Omega}i_{\mathbf{w}}\left(\boldsymbol{d}\,i_{\mathbf{v}}\boldsymbol{\omega}\right), \tag{25}$$

and kth order shape derivatives ($k > 2$)

$$\left\langle \mathrm{d}^k J(\Omega); \mathbf{v}_1, \ldots, \mathbf{v}_k \right\rangle = \int_\Omega \left(\mathscr{L}_{\mathbf{v}_k} \ldots \mathscr{L}_{\mathbf{v}_1} \right) \boldsymbol{\omega} = \int_\Omega \boldsymbol{d}\, i_{\mathbf{v}_k} \left(\boldsymbol{d}\, i_{\mathbf{v}_{k-1}} \left(\cdots \left(\boldsymbol{d}\, i_{\mathbf{v}_1} \boldsymbol{\omega} \right)\right)\right)$$
$$= \int_{\partial\Omega} i_{\mathbf{v}_k} \left(\boldsymbol{d}\, i_{\mathbf{v}_{k-1}} \cdots \left(\boldsymbol{d}\, i_{\mathbf{v}_1} \boldsymbol{\omega} \right)\right). \tag{26}$$

Proof We first use the pullback to transform from Ω_t to Ω and make use of the definition of the Lie derivative of a density form $\boldsymbol{\omega}$. Then, we obtain

$$\begin{aligned}
\langle \mathrm{d}J(\Omega), \mathbf{v}\rangle &= \frac{\mathrm{d}}{\mathrm{d}t} J_{\mathbf{v}}(t)\Big|_{t=0} = \left(\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_t(\mathbf{v})} \boldsymbol{\omega} \right)\Bigg|_{t=0} = \left(\frac{\mathrm{d}}{\mathrm{d}t} \int_{T_t(\mathbf{v})(\Omega)} \boldsymbol{\omega} \right)\Bigg|_{t=0} \\
&= \left(\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega T_t(\mathbf{v})^* \boldsymbol{\omega} \right)\Bigg|_{t=0} \overset{\langle * \rangle}{=} \int_\Omega \mathscr{L}_{\mathbf{v}} \boldsymbol{\omega} \overset{(17)}{=} \int_\Omega (\boldsymbol{d}\, i_{\mathbf{v}} + i_{\mathbf{v}} \boldsymbol{d}) \boldsymbol{\omega} \\
&\overset{(8)}{=} \int_\Omega \boldsymbol{d}\, i_{\mathbf{v}} \boldsymbol{\omega} \overset{(7)}{=} \int_{\partial\Omega} i_{\mathbf{v}} \boldsymbol{\omega},
\end{aligned}$$

where the definition of the Lie derivative is used in step $\langle * \rangle$. We have also used the fact $\boldsymbol{d\omega} = 0$ since $\boldsymbol{d\omega}$ is a $(d+1)$-form on a d-dimensional manifold.

Similar manipulations yield the shape Hessian,

$$\begin{aligned}
\left\langle \mathrm{d}^2 J(\Omega), \mathbf{v}, \mathbf{w} \right\rangle &= \frac{\partial}{\partial s} \left\{ \frac{\partial}{\partial t} J_{\mathbf{v},\mathbf{w}}(t,s) \Big|_{t=0} \right\}\Bigg|_{s=0} \\
&= \frac{\partial}{\partial s} \left(\left(\frac{\partial}{\partial t} \int_{\Omega_{t,s}(\mathbf{v},\mathbf{w})} \boldsymbol{\omega} \right)\Bigg|_{t=0} \right)\Bigg|_{s=0} \\
&= \frac{\partial}{\partial s} \left(\left(\frac{\partial}{\partial t} \int_\Omega T_s(\mathbf{w})^* T_t(\mathbf{v})^* \boldsymbol{\omega} \right)\Bigg|_{t=0} \right)\Bigg|_{s=0} \\
&\overset{\langle * \rangle}{=} \int_\Omega \mathscr{L}_{\mathbf{w}} \left(\mathscr{L}_{\mathbf{v}} \boldsymbol{\omega} \right) \overset{(17)}{=} \int_\Omega (\boldsymbol{d}\, i_{\mathbf{w}} + i_{\mathbf{w}} \boldsymbol{d})(\boldsymbol{d}\, i_{\mathbf{v}} + i_{\mathbf{v}} \boldsymbol{d}) \boldsymbol{\omega} \\
&\overset{(8)}{=} \int_\Omega \boldsymbol{d}\, i_{\mathbf{w}} \left(\boldsymbol{d}\, i_{\mathbf{v}} \boldsymbol{\omega} \right) \overset{(7)}{=} \int_{\partial\Omega} i_{\mathbf{w}} \left(\boldsymbol{d}\, i_{\mathbf{v}} \boldsymbol{\omega} \right).
\end{aligned}$$

Furthermore, for higher-order shape derivatives, we arrive at the last conclusion (26) by recursively repeating the previous arguments. □

In particular, regarding the structure of the shape Hessian, due to the composition of consecutive transformations of Ω along velocity fields $\mathbf{v}$ and $\mathbf{w}$, the Lie bracket comes into play. Observing (25), we have

$$\left\langle \mathrm{d}^2 J(\Omega), \mathbf{v}, \mathbf{w} \right\rangle = \int_\Omega \mathscr{L}_{\mathbf{w}} \mathscr{L}_{\mathbf{v}} \boldsymbol{\omega} \quad \text{and} \quad \left\langle \mathrm{d}^2 J(\Omega), \mathbf{w}, \mathbf{v} \right\rangle = \int_\Omega \mathscr{L}_{\mathbf{v}} \mathscr{L}_{\mathbf{w}} \boldsymbol{\omega}, \tag{27}$$

and in light of the Lie derivative identity [4,7,15]

$$\mathscr{L}_{\mathbf{w}}\mathscr{L}_{\mathbf{v}}\boldsymbol{\omega} - \mathscr{L}_{\mathbf{v}}\mathscr{L}_{\mathbf{w}}\boldsymbol{\omega} = \mathscr{L}_{[\mathbf{w},\mathbf{v}]}\boldsymbol{\omega}, \tag{28}$$

where for two differentiable velocity fields, the Lie bracket is defined by [8, Sect. 4]

$$[\mathbf{w}, \mathbf{v}] = (D\mathbf{v})\,\mathbf{w} - (D\mathbf{w})\,\mathbf{v}, \tag{29}$$

with $D\mathbf{v}$, $D\mathbf{w}$ being the Jacobians of the vector fields $\mathbf{v}$ and $\mathbf{w}$, respectively. Thus, we arrive at the following symmetry condition, which was also found in [3,5,6] via vector calculus.

Corollary 1 *A sufficient condition for the symmetry of the shape Hessian of the domain integral* (21)*, namely*

$$\left\langle \mathrm{d}^2 J(\Omega), \mathbf{v}, \mathbf{w} \right\rangle = \left\langle \mathrm{d}^2 J(\Omega), \mathbf{w}, \mathbf{v} \right\rangle, \tag{30}$$

is

$$\int_{\Omega} \mathscr{L}_{[\mathbf{w},\mathbf{v}]}\boldsymbol{\omega} = 0. \tag{31}$$

3.2 Boundary integrals

The boundary functional of a surface density form $\boldsymbol{\eta} \in \mathscr{D}\mathscr{F}^{d-1,m}(D)$ (initially globally defined on D) is

$$I(\Gamma) = \int_{\partial\Omega} \boldsymbol{\eta}. \tag{32}$$

Thanks to the Stokes theorem, we see that $I(\Gamma) = \int_{\Omega} \boldsymbol{d}\boldsymbol{\eta}$. Thus, the structure theorem for boundary integrals immediately follows from Theorem 1 via the Stokes theorem and the fact that the exterior derivative and Lie derivative commute.

Corollary 2 (Second fundamental structure theorem) *The boundary functional $I(\Gamma)$ is shape differentiable under suitable smoothness conditions on the domain and the velocity fields $\mathbf{v}_1, \ldots, \mathbf{v}_k$, with shape derivatives for $k \geq 1$*

$$\left\langle \mathrm{d}^k I(\Gamma), \mathbf{v}_1, \ldots, \mathbf{v}_k \right\rangle = \int_{\Gamma} i_{\mathbf{v}_k}\boldsymbol{d}\,\left(i_{\mathbf{v}_{k-1}}\boldsymbol{d}\ldots\left(i_{\mathbf{v}_1}\boldsymbol{d}\,(\boldsymbol{\eta})\right)\right). \tag{33}$$

Obviously, only the values of $\boldsymbol{\eta}$ on Γ matter for the shape derivatives. As regards the structure of the shape Hessian of the boundary integral (32), a result similar to Corollary 1 involving the Lie bracket holds. Observe

$$\left\langle \mathrm{d}^2 I(\Gamma), \mathbf{v}, \mathbf{w} \right\rangle = \int_{\Omega} \mathscr{L}_{\mathbf{w}}\mathscr{L}_{\mathbf{v}}\boldsymbol{d}\boldsymbol{\eta} \quad \text{and} \quad \left\langle \mathrm{d}^2 I(\Gamma), \mathbf{w}, \mathbf{v} \right\rangle = \int_{\Omega} \mathscr{L}_{\mathbf{v}}\mathscr{L}_{\mathbf{w}}\boldsymbol{d}\boldsymbol{\eta}. \tag{34}$$

Therefore, the symmetry condition for the shape Hessian of boundary integrals is

$$\int_{\Gamma} \mathscr{L}_{[\mathbf{w},\mathbf{v}]}\boldsymbol{\eta} = 0, \tag{35}$$

which is the same as in Corollary 1 except for the domain of integration Γ.

3.3 Shape derivative for bilinear forms

For PDE-constrained shape optimization problems, bilinear forms often arise in the variational formulation of the PDE constraints, which have to be differentiated with respect to small domain variations. This is the reason why we single out this particular functional.

Lemma 1 *For two l-forms, $\boldsymbol{\omega}, \boldsymbol{\eta} \in \mathcal{DF}^{l,m}(\overline{\Omega})$ $(0 \leq l \leq d-1)$, the bilinear form given by*

$$J(\Omega) = \int_{\Omega} *\boldsymbol{d\omega} \wedge \boldsymbol{d\eta}, \tag{36}$$

where $*$ is the Hodge star operator (cf. [4,7,8]*), has the following shape derivative:*

$$\langle \mathrm{d}J(\Omega), \mathbf{v} \rangle = \int_{\Omega} \mathscr{L}_{\mathbf{v}} (*\boldsymbol{d\omega} \wedge \boldsymbol{d\eta}) = \int_{\Gamma} i_{\mathbf{v}} (*\boldsymbol{d\omega} \wedge \boldsymbol{d\eta}). \tag{37}$$

Proof Understanding $*\boldsymbol{d\omega} \wedge \boldsymbol{d\eta}$ as a density form, the assertion follows directly from Theorem 1. □

4 Shape calculus in vector proxies

In this section, we will express the abstract theory in Sect. 3 in terms of vector proxies in d-dimensional Euclidean space (cf. Table 1).

For later use, we introduce surface differential operators as follows: Let $\widetilde{u}$ (resp. $\widetilde{\mathbf{v}}$) be the classical extension of some scalar function u (resp. vector fields $\mathbf{v}$) on the surface Γ to the whole space $\mathbb{R}^d$ by means of the signed smooth distance function within some neighborhood of Γ [6,16,19]. Then, two key surface differential operators can be defined,

$$\begin{aligned} \text{Surface gradient}: \quad & \mathbf{grad}_{\Gamma}\, u = \mathbf{grad}\, \widetilde{u}|_{\Gamma} - (\mathbf{grad}\, \widetilde{u} \cdot \mathbf{n})\, \mathbf{n}|_{\Gamma}, \\ \text{Surface divergence}: \quad & \mathrm{div}_{\Gamma} \mathbf{v} = \mathrm{div}\, \widetilde{\mathbf{v}} - D\widetilde{\mathbf{v}}\mathbf{n} \cdot \mathbf{n}, \end{aligned}$$

with $\mathbf{n}$ being the outward unit normal vector on Γ. They are linked by the tangential Stokes and Green Formulae on the hypersurface Γ of codimension one without boundary in $\mathbb{R}^d$ [6, Eqs. (5.26) and (5.27) on p. 367]: For a function $f \in C^1(\Gamma)$ and a vector $\mathbf{v} \in \left(C^1(\Gamma)\right)^d$, we have the tangential Stokes formula

$$\int_{\Gamma} \mathrm{div}_{\Gamma} \mathbf{v}\, \mathrm{d}s = \int_{\Gamma} \mathfrak{H} \mathbf{v} \cdot \mathbf{n}\, \mathrm{d}s, \tag{38}$$

and the tangential Green formula

$$\int_{\Gamma} f\, \mathrm{div}_{\Gamma} \mathbf{v} + \mathbf{grad}_{\Gamma} f \cdot \mathbf{v}\, \mathrm{d}s = \int_{\Gamma} \mathfrak{H} f \mathbf{v} \cdot \mathbf{n}\, \mathrm{d}s, \tag{39}$$

where

$$\mathfrak{H} := (d-1)\overline{\mathfrak{H}} \tag{40}$$

is the additive curvature and $\overline{\mathfrak{H}}$ is the mean curvature of the surface Γ (cf. [6]).

4.1 Domain integrals

Given a sufficiently smooth function f and a smooth domain Ω of class C^m with boundary Γ, the domain integral functional is

$$J(\Omega) = \int_\Omega f \,\mathrm{d}x. \tag{41}$$

In terms of vector proxies in Euclidean space, see Table 1, and understanding f as vector proxy for a d-dimensional volume form $\boldsymbol{\omega} \in \mathscr{DF}^{d,m}(\overline{\Omega})$, the formulae in Theorem 1 can be recast as follows:

Lemma 2 *Under suitable smoothness conditions on f, Ω and the velocity fields $\mathbf{v}$ and $\mathbf{w}$, the shape gradient of J from (41) exists and can be written as:*

$$\langle \mathrm{d}J(\Omega), \mathbf{v}\rangle = \int_\Gamma (f\,\mathbf{v}) \cdot \mathbf{n}\,\mathrm{d}s.$$

The shape Hessian is

$$\begin{aligned}
\left\langle \mathrm{d}^2 J(\Omega), \mathbf{v}, \mathbf{w}\right\rangle = &\int_\Gamma \left(\frac{\partial f}{\partial \mathbf{n}} + \kappa f\right)(\mathbf{v}\cdot\mathbf{n})\,(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}s \\
&- \int_\Gamma f\,\big(\langle S\mathbf{v}_\Gamma, \mathbf{w}_\Gamma\rangle - \mathbf{w}_\Gamma \cdot \mathbf{grad}_\Gamma\,(\mathbf{v}\cdot\mathbf{n}) - \mathbf{v}_\Gamma\cdot\mathbf{grad}_\Gamma\,(\mathbf{w}\cdot\mathbf{n})\big)\,\mathrm{d}s \\
&+ \int_\Gamma f\,(D\mathbf{v}\mathbf{w})\cdot\mathbf{n}\,\mathrm{d}s,
\end{aligned} \tag{42}$$

where $S = D\mathbf{n}$ is the second fundamental form (or Weingarten map or shape operator [8,17]) of the surface Γ and $\mathbf{n}$ is the outward unit normal field on Γ.

Proof The scalar smooth function f can be viewed as a vector proxy of a density form. Since the contraction with a velocity field amounts to a simple product of a scalar function f and a vector field (see Table 3), and the exterior derivative $\boldsymbol{d}$ is nothing but the div operator in this case, following (24) in Theorem 1, the shape gradient of (41) reads:

$$\langle \mathrm{d}J(\Omega), \mathbf{v}\rangle = \int_\Omega \mathrm{div}(f\mathbf{v})\,\mathrm{d}x = \int_\Gamma (f\,\mathbf{v})\cdot\mathbf{n}\,\mathrm{d}s.$$

This formula agrees with [18, Proposition 2.4.6 on p. 77] or [6, Theorem 4.2, p. 353].

The shape Hessian can be derived from (25) in a similar way, we obtain

$$\begin{aligned}
\left\langle \mathrm{d}^2 J(\Omega), \mathbf{v}, \mathbf{w}\right\rangle &= \int_\Omega \mathrm{div}\,(\mathbf{w}\,\mathrm{div}(f\mathbf{v}))\,\mathrm{d}x = \int_\Gamma \mathrm{div}(f\mathbf{v})\,(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}x \\
&= \int_\Gamma (\mathbf{grad}\,f\cdot\mathbf{v} + f\,\mathrm{div}\,\mathbf{v})\,(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}s \\
&\overset{(4)}{=} \int_\Gamma \left(\mathbf{grad}_\Gamma\,f\cdot\mathbf{v}_\Gamma + \frac{\partial f}{\partial\mathbf{n}}\mathbf{v}\cdot\mathbf{n} + f\,(D\mathbf{v}\mathbf{n}\cdot\mathbf{n} + \mathrm{div}_\Gamma\mathbf{v})\right)(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}s
\end{aligned}$$

$$\overset{\langle 5\rangle}{=} \int\limits_{\Gamma} \left(\mathbf{grad}_\Gamma\, f \cdot \mathbf{v}_\Gamma + \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right) \mathbf{v}\cdot\mathbf{n} + f\, D\mathbf{v}\mathbf{n}\cdot\mathbf{n} + f\, \mathrm{div}_\Gamma\, \mathbf{v}_\Gamma\right)$$
$$\times\, (\mathbf{w}\cdot\mathbf{n})\ \mathrm{d}s$$
$$\overset{\langle 6\rangle}{=} \int\limits_{\Gamma} \left(\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right) \mathbf{v}\cdot\mathbf{n} + f\, D\mathbf{v}\mathbf{n}\cdot\mathbf{n}\right)(\mathbf{w}\cdot\mathbf{n}) - f\,\mathbf{v}_\Gamma\cdot \mathbf{grad}_\Gamma\, (\mathbf{w}\cdot\mathbf{n})\ \mathrm{d}s \tag{43}$$

Note that $\mathfrak{H}$ is the additive mean curvature defined in (40). Here we have used the decomposition

$$\mathbf{v} = (\mathbf{v}\cdot\mathbf{n})\mathbf{n} + \mathbf{v}_\Gamma, \tag{44}$$

where $(\cdot)_\Gamma$ denotes the tangential component of a vector field on Γ, and the definition of surface divergence

$$\mathrm{div}\, \mathbf{v} = D\mathbf{v}\mathbf{n}\cdot\mathbf{n} + \mathrm{div}_\Gamma \mathbf{v}, \tag{45}$$

cf. [18, Def. 2.52, p. 82] or [6, Eq. (5.19), p. 366], in the fourth equality $\langle 4\rangle$. The fifth equality $\langle 5\rangle$ follows from the identity

$$\mathrm{div}_\Gamma \mathbf{v} = \mathrm{div}_\Gamma \mathbf{v}_\Gamma + \mathfrak{H}\mathbf{v}\cdot\mathbf{n}, \tag{46}$$

(cf. [18, Prop. 2.57, p. 86] or [6, Eq. (5.22), p. 366]). And the last equality $\langle 6\rangle$ is a consequence of the tangential Green formula (39) applied to $\mathbf{v}_\Gamma$ and $(\mathbf{w}\cdot\mathbf{n})\, f$:

$$\int\limits_{\Gamma} \mathbf{grad}_\Gamma\, ((\mathbf{w}\cdot\mathbf{n})\, f)\cdot \mathbf{v}_\Gamma + (\mathbf{w}\cdot\mathbf{n})\, f\, \mathrm{div}_\Gamma\, \mathbf{v}_\Gamma\, \mathrm{d}s = 0. \tag{47}$$

Note that the formula (43) is exactly the same as [6, Eq.(6.3) on p. 373]. However, we avoid a lot of complicated intermediate steps and need not introduce some auxiliary distance functions and surface calculus. Moreover, in light of [6, Eq. (5.23) on p. 366], one may further symmetrize the shape Hessian in (43) as [6, Eq. (6.4) on p. 373] to derive a symmetric principal part plus the first half of the Lie bracket of two velocity fields to obtain (42). This completes the proof. □

In terms of a vector proxy f of a density form, the sufficient condition from Corollary 1 for the symmetry of the shape Hessian is equivalent to

$$\int\limits_{\Omega} \mathrm{div}\, (f\, [\mathbf{w},\mathbf{v}])\ \mathrm{d}x = \int\limits_{\partial\Omega} (f\, [\mathbf{w},\mathbf{v}])\cdot\mathbf{n}\, \mathrm{d}s = \int\limits_{\partial\Omega} f\, ((D\mathbf{v})\,\mathbf{w} - (D\mathbf{w})\,\mathbf{v})\cdot\mathbf{n}\, \mathrm{d}s = 0,$$

which agrees with the observation in [6, Eq. (6.5) on p. 373]. Related investigations of the structure of the shape Hessian of domain integrals can be found in [3,5].

Remark 1 In particular for shape optimization problems, only normal variations (still perturbations of infinite dimension) are taken into account, namely $\mathbf{v}$ and $\mathbf{w}$ are chosen to be along the normal direction of the surface Γ. In such a case, the symmetry of the shape Hessian is still not guaranteed from the velocity method, which is quite opposite to our intuition of finite dimensional calculus. So one should be very cautious about assuming the symmetry of the shape Hessian in shape optimization problems.

Remark 2 A detailed theoretical analysis of higher-order shape derivatives for domain integrals ($k > 2$) is still possible but extremely tedious. Structure of higher-order shape derivatives can be derived from Theorem 1. Yet, they are seldom used in theoretical analysis and numerical methods due to their rather low regularity. One can formally derive higher-order shape derivatives given the necessary regularity of the functions and domain, but the interpretation of the resulting expressions is very difficult and their numerical approximation is even harder.

4.2 Boundary integrals

Given a scalar smooth function f globally defined in $\mathbb{R}^d$, the boundary integral on $\Gamma := \partial\Omega$ is

$$I(\Gamma) = \int_\Gamma f \, \mathrm{d}s. \tag{48}$$

Observe that

$$I(\Gamma) = \int_\Gamma f \, \mathrm{d}s = \int_\Gamma f \mathbf{n} \cdot \mathbf{n} \, \mathrm{d}s \tag{49}$$

where $f\mathbf{n}$ can be understood as $i_\mathbf{n}\boldsymbol{\omega}$, with f being the vector proxy of some volume density form $\boldsymbol{\omega} \in \mathscr{DF}^{d,m}(\overline{\Omega})$. It must be pointed out that once Γ is given, we can extend the outward unit normal $\mathbf{n}$ to be a globally defined velocity field such that $i_\mathbf{n}\boldsymbol{\omega}$ is a $(d-1)$-form which does not depend on Ω_t.

Lemma 3 *Under suitable smoothness conditions on f, Ω and the velocity fields $\mathbf{v}$ and $\mathbf{w}$, the shape gradient of the boundary integral* (48) *reads:*

$$\langle \mathrm{d}I(\Gamma), \mathbf{v} \rangle = \int_\Gamma (\mathbf{v} \cdot \mathbf{n}) \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f \right) \mathrm{d}s.$$

The shape Hessian is

$$\begin{aligned}\left\langle \mathrm{d}^2 I(\Gamma), \mathbf{v}, \mathbf{w} \right\rangle = \int_\Gamma \Bigg(&\left(D^2 f \mathbf{n} \cdot \mathbf{n} + 2\mathfrak{H} \frac{\partial f}{\partial \mathbf{n}} + \left(\mathfrak{H}^2 - \frac{1}{2}\mathrm{trace}(S^2) \right) f \right) (\mathbf{v} \cdot \mathbf{n})\, (\mathbf{w} \cdot \mathbf{n}) \\ &+ \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f \right) \left(S(\mathbf{v}_\Gamma, \mathbf{w}_\Gamma) - \mathbf{w}_\Gamma \cdot \mathbf{grad}_\Gamma\, (\mathbf{v} \cdot \mathbf{n}) - \mathbf{v}_\Gamma \cdot \mathbf{grad}_\Gamma\, (\mathbf{w} \cdot \mathbf{n}) \right) \\ &+ \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f \right) ((D\mathbf{v})\, \mathbf{w}) \cdot \mathbf{n} \Bigg) \mathrm{d}s.\end{aligned}$$

Proof In light of the observation (49), the integrand $f\mathbf{n}_t(\mathbf{v})$ after deformation can be understood as a surface density form depending on the boundary since $\mathbf{n}_t(\mathbf{v})$, being the normal field on $\partial\Omega_t(\mathbf{v})$ transformed along the velocity field $\mathbf{v}$, depends on the pseudo-time t.

Now interpreting $\boldsymbol{d}$ as div and contraction as simple multiplication, we have

$$\begin{aligned}\langle \mathrm{d}I(\Gamma), \mathbf{v}\rangle &= \underbrace{\int_\Gamma \operatorname{div}(f\mathbf{n})(\mathbf{v}\cdot\mathbf{n})\,\mathrm{d}s}_{I} + \underbrace{2\int_\Gamma f(\mathbf{n}_t^{'}(\mathbf{v})|_{t=0})\cdot\mathbf{n}\,\mathrm{d}s}_{II} \\ &= \int_\Gamma (\mathbf{grad}\, f\cdot\mathbf{n} + f\operatorname{div}(\mathbf{n}))\,(\mathbf{v}\cdot\mathbf{n})\,\mathrm{d}s \\ &= \int_\Gamma (\mathbf{v}\cdot\mathbf{n})\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)\mathrm{d}s. \end{aligned} \tag{50}$$

where we have to apply the product rule of differentiation to the boundary integral (49). The first term (I) follows from Corollary 2 through freezing $\mathbf{n} = \mathbf{n}_t(\mathbf{v})|_{t=0}$ and extending it unitarily to the global domain by the signed distance technique, while the second one (II) is a temporal derivative of the integrand $f\mathbf{n}_t(\mathbf{v})\cdot\mathbf{n}_t(\mathbf{v})$ evaluating at $t=0$. Notice that

$$\mathbf{n}_t^{'}(\mathbf{v})|_{t=0} = -\,\mathbf{grad}_\Gamma(\mathbf{v}\cdot\mathbf{n}), \tag{51}$$

which is a tangential vector on the surface Γ (please refer to details in [6, Eq. (4.38) on p. 360 and p. 370]. Therefore, we see immediately that (II) vanishes.

In the derivation of the previous formula (50), we have used the identities

$$\operatorname{div}(f\mathbf{n}) = \mathbf{grad}(f)\cdot\mathbf{n} + f\operatorname{div}(\mathbf{n})$$

and $\operatorname{div}(\mathbf{n}) = \operatorname{Trace}(D\mathbf{n}) = \mathfrak{H}$. This formula agrees with [6, Theorem 4.3 on p. 355], but we could arrive at it much more easily.

As for the shape Hessian, we may repeat the argument in the derivation of the shape gradient recursively and thus obtain from Corollary 2

$$\begin{aligned}\left\langle \mathrm{d}^2 I(\Gamma), \mathbf{v}, \mathbf{w}\right\rangle &= \int_\Gamma \operatorname{div}(\mathbf{v}\operatorname{div}(f\mathbf{n}))\,(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}s \\ &= \int_\Gamma \operatorname{div}(\mathbf{v}\,(\mathbf{grad}(f)\cdot\mathbf{n} + f\operatorname{div}(\mathbf{n})))\,(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}s \\ &= \int_\Gamma \Big(\operatorname{div}\mathbf{v}\,(\mathbf{grad}(f)\cdot\mathbf{n} + f\operatorname{div}(\mathbf{n})) \\ &\qquad + \mathbf{grad}\,(\mathbf{grad}(f)\cdot\mathbf{n} + \mathfrak{H} f)\cdot\mathbf{v}\Big)(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}s. \end{aligned}$$

We point out that we have used the product rule of differentiation and the orthogonality (51) twice in pseudo-time s and t consecutively in deriving the shape Hessian for boundary integrals. To the best knowledge of the authors, this is a new result.

We can further symmetrize the formula into a symmetric principal part plus the first half of the Lie bracket:

$$
\begin{aligned}
\left\langle \mathrm{d}^2 I(\Gamma), \mathbf{v}, \mathbf{w}\right\rangle &= \int_\Gamma \left(\operatorname{div}\mathbf{v}\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right) + \mathbf{v}\cdot\mathbf{grad}\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)\right)(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}s \\
&\overset{\langle 2\rangle}{=} \int_\Gamma \Bigg((\operatorname{div}_\Gamma \mathbf{v}_\Gamma + \mathfrak{H}\mathbf{v}\cdot\mathbf{n} + D\mathbf{v}\mathbf{n}\cdot\mathbf{n})\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right) \\
&\quad + \mathbf{v}_\Gamma\cdot\mathbf{grad}_\Gamma\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right) + (\mathbf{v}\cdot\mathbf{n})\cdot\frac{\partial}{\partial \mathbf{n}}\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)\Bigg)(\mathbf{w}\cdot\mathbf{n})\,\mathrm{d}s \\
&\overset{\langle 3\rangle}{=} \int_\Gamma \Bigg(\left(D^2 f\mathbf{n}\cdot\mathbf{n} + 2\mathfrak{H}\frac{\partial f}{\partial \mathbf{n}} + \left(\mathfrak{H}^2 - \frac{1}{2}\operatorname{trace}(S^2)\right)f\right)(\mathbf{v}\cdot\mathbf{n})(\mathbf{w}\cdot\mathbf{n}) \\
&\quad + (\operatorname{div}_\Gamma \mathbf{v}_\Gamma + D\mathbf{v}\mathbf{n}\cdot\mathbf{n})\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)(\mathbf{w}\cdot\mathbf{n}) \\
&\quad + \mathbf{v}_\Gamma\cdot\mathbf{grad}_\Gamma\left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)(\mathbf{w}\cdot\mathbf{n})\Bigg)\,\mathrm{d}s \\
&\overset{\langle 4\rangle}{=} \int_\Gamma \Bigg(\left(D^2 f\mathbf{n}\cdot\mathbf{n} + 2\mathfrak{H}\frac{\partial f}{\partial \mathbf{n}} + \left(\mathfrak{H}^2 - \frac{1}{2}\operatorname{trace}(S^2)\right)f\right)(\mathbf{v}\cdot\mathbf{n})(\mathbf{w}\cdot\mathbf{n}) \\
&\quad + \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)(D\mathbf{v}\mathbf{n}\cdot\mathbf{n})(\mathbf{w}\cdot\mathbf{n}) \\
&\quad - \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)\mathbf{v}_\Gamma\cdot\mathbf{grad}_\Gamma(\mathbf{w}\cdot\mathbf{n})\Bigg)\,\mathrm{d}s \\
&\overset{\langle 5\rangle}{=} \int_\Gamma \Bigg(\left(D^2 f\mathbf{n}\cdot\mathbf{n} + 2\mathfrak{H}\frac{\partial f}{\partial \mathbf{n}} + \left(\mathfrak{H}^2 - \frac{1}{2}\operatorname{trace}(S^2)\right)f\right)(\mathbf{v}\cdot\mathbf{n})(\mathbf{w}\cdot\mathbf{n}) \\
&\quad + \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)\left(S(\mathbf{v}_\Gamma, \mathbf{w}_\Gamma) - \mathbf{w}_\Gamma\cdot\mathbf{grad}_\Gamma(\mathbf{v}\cdot\mathbf{n}) - \mathbf{v}_\Gamma\cdot\mathbf{grad}_\Gamma(\mathbf{w}\cdot\mathbf{n})\right) \\
&\quad + \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)(D\mathbf{v}\mathbf{w})\cdot\mathbf{n}\Bigg)\,\mathrm{d}s
\end{aligned}
$$

Here we have used the decomposition identities [6, Eqs. (5.19) and (5.22), p. 366] in the second equality $\langle 2\rangle$, [16, Eq. (2.5.155)] in the third equality $\langle 3\rangle$, the surface Green formula in the fourth equality $\langle 4\rangle$. In the last equality $\langle 5\rangle$, we decompose $((D\mathbf{v})\,\mathbf{n}\cdot\mathbf{n})\,(\mathbf{w}\cdot\mathbf{n})$ as in the discussion of the shape Hessian of the domain integral by using [6, Eqs. (5.23) p. 366 and (6.3) on p. 373]. Apparently, this formula is new. □

In terms of a scalar function f, the sufficient condition for the symmetry of the shape Hessian of the boundary integral is equivalent to

$$
\int_\Gamma \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)[\mathbf{w}, \mathbf{v}]\cdot\mathbf{n}\,\mathrm{d}s = \int_\Gamma \left(\frac{\partial f}{\partial \mathbf{n}} + \mathfrak{H} f\right)((D\mathbf{v})\,\mathbf{w} - (D\mathbf{w})\,\mathbf{v})\cdot\mathbf{n}\,\mathrm{d}s = 0.
$$

Again, in terms of normal variations, this term will not necessarily drop out. This sufficient condition is also new to the shape optimization community.

4.3 Shape derivative for bilinear forms

The formula in (37) holds true for **grad**, **curl** and div, respectively, in three dimensions. These special cases can be summarized in the following version of Lemma 1.

Lemma 4 *Under suitable smoothness conditions on* Ω *and the velocity field* $\mathbf{v}$*, the shape derivatives of the bilinear form on* $H(\mathscr{D}, \Omega)$

$$J(\Omega) = \int_{\Omega} \kappa \mathscr{D}u \cdot \mathscr{D}v \, \mathrm{d}x, \tag{52}$$

is

$$\langle \mathrm{d}J(\Omega), \mathbf{v}\rangle = \int_{\Gamma} (\kappa \mathscr{D}u \cdot \mathscr{D}v)\, \mathbf{v} \cdot \mathbf{n} \, \mathrm{d}s, \tag{53}$$

with $\mathscr{D}$ *being replaced with* **grad**, **curl** *and* div*, respectively,* u *and* v *vector fields for the latter two cases, and* κ *some coefficient, which could be any constant, smooth function or tensor field.*

Note that those formulae for **curl** and div operators are new and of particular importance in deriving shape derivatives for Maxwell solutions arising in electromagnetics, and for the Stokes system arising in fluid dynamics, respectively.

4.4 Normal derivative

Since normal derivatives are often encountered, we would like to discuss this special case with an auxiliary lemma. Let Γ be the boundary of a bounded domain Ω of class C^m and $f \in H^2_{\mathrm{loc}}(\mathbb{R}^m)$ be given. Consider the shape functional

$$I(\Gamma) = \int_{\Gamma} \frac{\partial f}{\partial \mathbf{n}} \, \mathrm{d}s = \int_{\Gamma} \mathbf{grad}\, f \cdot \mathbf{n} \, \mathrm{d}s. \tag{54}$$

In this case, f is understood as a 0-form $\boldsymbol{\omega}$ and **grad** is the incarnation of $\boldsymbol{d} : \mathscr{D}\mathscr{F}^{0,m}(\overline{\Omega}) \mapsto \mathscr{D}\mathscr{F}^{1,m}(\overline{\Omega})$, thus $\int_{\Gamma} \mathbf{grad}\, f \cdot \mathbf{n}\, \mathrm{d}s$ may be expressed by $\int_{\Gamma} *\boldsymbol{d\omega}$, where $\boldsymbol{d\omega}$ is a 1-form, which is mapped by the Euclidean Hodge to $*\boldsymbol{d\omega}$, a $(d-1)$-form (or **grad** f in the vector proxy). Now Corollary 2 is applicable for this case.

Lemma 5 *Under suitable smoothness conditions on* Ω *and the velocity fields* $\mathbf{v}$*, the shape derivative of* (54) *exists and it holds that*

$$\left\langle \mathrm{d}\int_{\Gamma} \mathbf{grad}\, f \cdot \mathbf{n}, \mathbf{v} \right\rangle \tag{55}$$

$$= \int_{\Gamma} \left(\mathrm{div}_{\Gamma}\, \mathbf{grad}_{\Gamma}\, f + D^2 f \mathbf{n} \cdot \mathbf{n} + \mathfrak{H}\, \mathbf{grad}\, f \cdot \mathbf{n}\right) (\mathbf{v} \cdot \mathbf{n}) \, \mathrm{d}s. \tag{56}$$

Proof By Corollary 2, we have

$$\left\langle \mathrm{d} \int_\Gamma \mathbf{grad}\, f \cdot \mathbf{n}, \mathbf{v} \right\rangle = \int_\Gamma \mathrm{div}(\mathbf{grad}\, f)\,(\mathbf{v}\cdot\mathbf{n})\;\mathrm{d}s$$
$$= \int_\Gamma \left(\mathrm{div}_\Gamma\, \mathbf{grad}_\Gamma\, f + D^2 f \mathbf{n}\cdot\mathbf{n} + \mathfrak{H}\,\mathbf{grad}\, f\cdot\mathbf{n}\right)(\mathbf{v}\cdot\mathbf{n})\;\mathrm{d}s.$$

where we have used the decomposition of the div operator as in (45) and (46) in the second equality. □

5 Application: shape derivative of solutions of second-order BVPs

In this section, we will study a model elliptic BVP and express the shape derivatives of weak solutions of BVPs via shape calculus of domain and boundary integrals.

Given a bounded domain $\Omega \subset \mathbb{R}^d$ of class C^m, consider an elliptic BVP for an l-form $\boldsymbol{\omega}$, see [12, Sect. 2],

$$(-1)^{d-l}\boldsymbol{d} *_\alpha \boldsymbol{d\omega} + *_\gamma \boldsymbol{\omega} = \boldsymbol{\psi} \qquad \text{in } \Omega, \tag{57}$$
$$\mathrm{Tr}\,(*_\alpha \boldsymbol{d\omega}) = (-1)^{d-l}\mathrm{Tr}\left(*_\beta \boldsymbol{\omega} + \boldsymbol{\phi}\right) \qquad \text{on } \Gamma, \tag{58}$$

where $*_\alpha$, $*_\gamma$ and $*_\beta$ are fixed Hodge operators in Ω and on Γ, respectively, Tr is the trace operator on the boundary [2], and $\boldsymbol{\psi}$ ($(d-l)$-form) and $\boldsymbol{\phi}$ ($(d-l-1)$-form) are two smooth differential forms defined globally. Equation (58) corresponds to the Robin boundary condition, which reduces to the Neumann case when $*_\beta = 0$.

The weak form of (57), (58) is obtained through the integration by parts formula [13, Eq. (2.23)] and reads: Seek $\boldsymbol{\omega} \in \{\boldsymbol{\eta} \in \boldsymbol{H}(\boldsymbol{d}, \Omega, \bigwedge^l(\mathbb{R}^d)),\ \mathrm{Tr}(\boldsymbol{\eta}) \in L^2(\Gamma, \bigwedge^l(\mathbb{R}^d))\}$ such that for all smooth test forms $\boldsymbol{\eta}$

$$\int_\Omega \left(*_\alpha \boldsymbol{d\omega}\wedge\boldsymbol{d\eta} + *_\gamma\boldsymbol{\omega}\wedge\boldsymbol{\eta}\right) + \int_\Gamma \mathrm{Tr}\left(*_\beta\boldsymbol{\omega}\wedge\boldsymbol{\eta}\right) = \int_\Omega \boldsymbol{\psi}\wedge\boldsymbol{\eta} - \int_\Gamma \mathrm{Tr}\,(\boldsymbol{\phi}\wedge\boldsymbol{\eta})\,. \tag{59}$$

Definition 4 (*Shape derivatives of forms*) Given a velocity field $\mathbf{v} \in C^m(\mathbb{R}^d, \mathbb{R}^d)$ and the corresponding perturbed domains $\Omega_t := T_t(\mathbf{v})(\Omega)$, the shape derivatives of a solution $\boldsymbol{\omega}$ of (57), (58), which depends on the domain Ω_t, in the direction of $\mathbf{v}$, denoted by $\delta\boldsymbol{\omega}$, is defined by (cf. [6,18])

$$\delta\boldsymbol{\omega} := \frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\omega}(\Omega_t)\Big|_{t=0}. \tag{60}$$

In an abstract way, we can characterize the corresponding shape derivative of the solution to (57), (58) by differentiating (59) with respect to t, but with Ω and $\boldsymbol{\omega}(\Omega)$ replaced by Ω_t and $\boldsymbol{\omega}(\Omega_t)$ in (59), respectively. Straightforward application of Theorem 1, Corollary 2 and Definition 4 yields:

Lemma 6 *The shape derivative,* $\delta\boldsymbol{\omega} \in \{\boldsymbol{\eta} \in \boldsymbol{H}(\boldsymbol{d}, \Omega, \bigwedge^l(\mathbb{R}^d)) :\ \mathrm{Tr}(\boldsymbol{\eta}) \in L^2(\Gamma, \bigwedge^l(\mathbb{R}^d))\}$, *of the solution* $\boldsymbol{\omega} \in \boldsymbol{H}^1\left(\boldsymbol{d}, \Omega, \bigwedge^l(\mathbb{R}^d)\right)$ *of* (59) *is the unique solution to the following variational problem:*

$$\int_{\Omega} \left(*_\alpha \boldsymbol{d}(\delta\boldsymbol{\omega}) \wedge \boldsymbol{d}\boldsymbol{\eta} + *_\gamma \delta\boldsymbol{\omega} \wedge \boldsymbol{\eta}\right) + \int_{\Gamma} \mathrm{Tr}\left(*_\beta \delta\boldsymbol{\omega}\right) \wedge \boldsymbol{\eta}.$$
$$= \int_{\Gamma} i_{\mathbf{v}}\left(\boldsymbol{\psi} \wedge \boldsymbol{\eta}\right) - \int_{\Gamma} i_{\mathbf{v}}\left(*_\alpha \boldsymbol{d}\boldsymbol{\omega} \wedge \boldsymbol{d}\boldsymbol{\eta} + *_\gamma \boldsymbol{\omega} \wedge \boldsymbol{\eta}\right)$$
$$- \int_{\Gamma} i_{\mathbf{v}} \boldsymbol{d}\mathrm{Tr}\left(\left(*_\beta \boldsymbol{\omega} + \boldsymbol{\phi}\right) \wedge \boldsymbol{\eta}\right), \tag{61}$$

for all smooth test forms $\boldsymbol{\eta} \in \mathscr{D}\mathscr{F}^{l,\infty}(\mathbb{R}^d)$.

The weak form (59) corresponds to $H^1(\Omega)$-, $\boldsymbol{H}(\mathbf{curl};\Omega)$- and $\boldsymbol{H}(\mathrm{div};\Omega)$-elliptic variational problems when $d = 3$, $l = 0$, 1 and 2, respectively. In terms of vector proxies, we can incarnate the Hodge operators as multiplication with coefficient functions denoted by α, β and γ.

We give details for 0-forms ($l = 0$, for $l > 0$, please refer to [14]), and use scalar functions $f \in L^2(\Omega)$ and $g \in H^2(\Omega)$ as vector proxies of the forms $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$ in (59). Related studies have been conducted in [10,11,18].

Corollary 3 *The shape derivative,* $\delta u \in \left\{w \in H^1(\Omega) : w|_{\partial\Omega} \in H^1(\Gamma)\right\}$, *of the solution* $u \in H^2(\Omega)$ *of* (59) *for* $l = 0$ *is the unique solution of the following variational problem:*

$$\int_{\Omega} (\alpha\, \mathbf{grad}\, \delta u \cdot \mathbf{grad}\, v + \gamma \delta u v) + \int_{\Gamma} \beta \delta u$$
$$= \int_{\Gamma} f v \mathbf{v} \cdot \mathbf{n} - \int_{\Gamma} \left(\alpha\, \mathbf{grad}_\Gamma\, u \cdot \mathbf{grad}_\Gamma\, v + \gamma u v\right) \mathbf{v} \cdot \mathbf{n}$$
$$- \int_{\Gamma} \mathbf{v} \cdot \mathbf{n} \left(\frac{\partial}{\partial \mathbf{n}}(\beta u + g) + \mathfrak{H}(\beta u + g)\right) v, \tag{62}$$

for all $v \in C^\infty(\mathbb{R}^d)$.

Proof A simple translation from differential forms to scalar functions (0-forms) with Lemmas 2 and 3 yields the right-hand side of (61) in terms of vector proxies

$$\int_{\Gamma} f v \mathbf{v} \cdot \mathbf{n} - \int_{\Gamma} (\alpha\, \mathbf{grad}\, u \cdot \mathbf{grad}\, v + \gamma u v)\, \mathbf{v} \cdot \mathbf{n} - \int_{\Gamma} \mathbf{v} \cdot \mathbf{n} \left(\frac{\partial}{\partial \mathbf{n}}((\beta u + g) v) + \mathfrak{H}(\beta u + g) v\right).$$

Notice that

$$\frac{\partial}{\partial \mathbf{n}}((\beta u + g)v) = \frac{\partial}{\partial \mathbf{n}}(\beta u + g)\, v + (\beta u + g)\frac{\partial v}{\partial \mathbf{n}},$$

and

$$\alpha\, \mathbf{grad}\, u \cdot \mathbf{grad}\, v = \alpha\, \mathbf{grad}_\Gamma\, u \cdot \mathbf{grad}_\Gamma\, v + \alpha \frac{\partial u}{\partial \mathbf{n}} \cdot \frac{\partial v}{\partial \mathbf{n}}.$$

In view of the Robin boundary condition $\alpha \frac{\partial u}{\partial \mathbf{n}} + (\beta u + g) = 0$, the last terms in the previous two equations cancel each other and the proof is done. □

Once we arrive at the variational characterization of the shape derivative, we can reformulate the strong form of the PDE for the shape derivative δu under suitable regularity conditions by testing (62) first with smooth functions v with vanishing trace, and, subsequently, with smooth functions v with non-zero trace. The strong form of (62) follows from (39):

$$-\operatorname{div}(\alpha\,\mathbf{grad}\,\delta u)+\gamma\delta u=0\quad\text{in }\Omega, \tag{63}$$

$$\begin{aligned}\alpha\frac{\partial(\delta u)}{\partial\mathbf{n}}+\beta\delta u=&\operatorname{div}_\Gamma\big((\mathbf{v}\cdot\mathbf{n})\alpha\,\mathbf{grad}_\Gamma u\big)\\ &-\mathbf{v}\cdot\mathbf{n}\left(\frac{\partial(\beta u+g)}{\partial\mathbf{n}}+\mathfrak{H}(\beta u+g)\right)+(f-\gamma u)\mathbf{v}\cdot\mathbf{n}\quad\text{on }\Gamma.\end{aligned} \tag{64}$$

Thus, we obtain the elliptic BVP for the shape derivative δu and its associated Robin boundary condition (or its Neumann counterpart when $\beta=0$).

6 Dual formulation

For PDEs with Neumann or Robin boundary conditions, it is natural to derive the corresponding Neumann or Robin boundary conditions of the shape gradient of solutions to the PDEs from its primal variational formulation. In this section, we will rigorously derive the shape derivative for BVPs with Dirichlet boundary condition from the dual variational formulation. The aforementioned elliptic BVP (57) for general l-forms will be further discussed from the dual perspective, but equipped with some Dirichlet boundary condition

$$\boldsymbol{\omega}=\boldsymbol{\phi}\quad\text{on }\Gamma. \tag{65}$$

To derive the dual formulation, we introduce a $(d-l-1)$-form

$$\boldsymbol{\rho}=*_\alpha\boldsymbol{d}\boldsymbol{\omega}, \tag{66}$$

or

$$*_{\alpha^{-1}}\boldsymbol{\rho}=(-1)^{(l+1)(d-l-1)}\boldsymbol{d}\boldsymbol{\omega}. \tag{67}$$

where $*_{\alpha^{-1}}$, up to sign, is the inverse of the Hodge operator $*_\alpha$ with $*_{\alpha^{-1}}\circ *_\alpha = (-1)^{(l+1)(d-l-1)}\,Id$. Then, the PDE (57) can be rewritten as (67) plus

$$(-1)^{d-l}\boldsymbol{d}\boldsymbol{\rho}+*_\gamma\boldsymbol{\omega}=\boldsymbol{\psi}\quad\text{in }\Omega. \tag{68}$$

Now the dual mixed formulation of (67) and (68) is as follows:

$$\int_\Omega *_{\alpha^{-1}}\boldsymbol{\rho}\wedge\boldsymbol{\tau}+(-1)^{(l+1)(d-l)}\boldsymbol{\omega}\wedge\boldsymbol{d}\boldsymbol{\tau}+(-1)^{(l+1)(d-l-1)}\int_\Gamma \mathrm{Tr}\boldsymbol{\phi}\wedge\mathrm{Tr}\boldsymbol{\tau}=0, \tag{69}$$

$$\int_\Omega(-1)^{(d-l)}\boldsymbol{d}\boldsymbol{\rho}\wedge\boldsymbol{\nu}+\int_\Omega *_\gamma\boldsymbol{\omega}\wedge\boldsymbol{\nu}=\int_\Omega\boldsymbol{\psi}\wedge\boldsymbol{\nu}, \tag{70}$$

for all smooth $\boldsymbol{\tau}\in\mathscr{D}\mathscr{F}^{d-l-1,\infty}(\mathbb{R}^d)$ and $\boldsymbol{\nu}\in\mathscr{D}\mathscr{F}^{d-l,\infty}(\mathbb{R}^d)$. Taking the shape derivative of the mixed formulation, namely differentiating the above formulation in the perturbed domain Ω_t with respect to the pseudo-time t, we conclude from Theorem 1 and Corollary 2,

$$\int_\Omega *_{\alpha^{-1}}\delta\boldsymbol{\rho}\wedge\boldsymbol{\tau}+(-1)^{(l+1)(d-l)}\delta\boldsymbol{\omega}\wedge\boldsymbol{d\tau}$$
$$+(-1)^{(l+1)(d-l-1)}\int_\Gamma i_{\mathbf{v}}\boldsymbol{d}\left(\mathrm{Tr}\boldsymbol{\phi}\wedge\mathrm{Tr}\boldsymbol{\tau}\right)$$
$$\int_\Gamma i_{\mathbf{v}}\mathrm{Tr}\left(*_{\alpha^{-1}}\boldsymbol{\rho}\wedge\boldsymbol{\tau}+(-1)^{(l+1)(d-l)}\boldsymbol{\omega}\wedge\boldsymbol{d\tau}\right)=0, \tag{71}$$
$$\int_\Omega(-1)^{(d-l)}\boldsymbol{d}\delta\boldsymbol{\rho}\wedge\boldsymbol{\nu}+\int_\Omega *_\gamma\delta\boldsymbol{\omega}\wedge\boldsymbol{\nu}$$
$$+\int_\Gamma i_{\mathbf{v}}\mathrm{Tr}\left((-1)^{(d-l)}\boldsymbol{d\rho}\wedge\boldsymbol{\nu}+*_\gamma\boldsymbol{\omega}\wedge\boldsymbol{\nu}-\boldsymbol{\psi}\wedge\boldsymbol{\nu}\right)=0. \tag{72}$$

Up to here, we have characterized the shape derivatives $\delta\boldsymbol{\omega}$ and $\delta\boldsymbol{\rho}$ of the primal form $\boldsymbol{\omega}$ and dual form $\boldsymbol{\rho}$ in the variational sense, which is now amenable to further investigation for concrete settings.

Here, we discuss the special case $l=0$ and, for the sake of simplicity, assume $\alpha=1$ and $*_\gamma=0$. The scalar functions $f\in L^2(\mathbb{R}^d)$ and $g\in H^2(\mathbb{R}^d)$ will serve as vector proxies for the differential forms $\boldsymbol{\psi}$ and $\boldsymbol{\phi}$ (57) and (59). Thus, we arrive at the Dirichlet problem

$$-\Delta u=f\quad\text{on}\,\Omega,\quad u=g\quad\text{in}\,\Gamma, \tag{73}$$

whose dual weak form emerges from setting

$$\mathbf{q}=\mathbf{grad}\,u, \tag{74}$$

and reads: Seek $u\in L^2(\Omega)$ and $\mathbf{q}\in\boldsymbol{H}(\mathrm{div};\Omega)$ such that

$$\begin{cases}\int_\Omega\mathbf{q}\cdot\mathbf{p}\,\mathrm{d}x+\int_\Omega u\,\mathrm{div}\,\mathbf{p}\,\mathrm{d}x=\int_\Gamma g\mathbf{p}\cdot\mathbf{n}, & \forall\,\mathbf{p}\in\boldsymbol{H}(\mathrm{div};\Omega),\\ \int_\Omega\mathrm{div}\,\mathbf{q}v\,\mathrm{d}x=\int_\Omega fv\,\mathrm{d}x, & \forall\,v\in L^2(\Omega).\end{cases} \tag{75}$$

For smooth domains and data, we can expect $u\in H^2(\Omega)$ and $\mathbf{q}\in\boldsymbol{H}^1(\mathrm{div};\Omega)$. Write $\delta\mathbf{q}$ and δu as the shape derivatives of $\mathbf{q}$ and u, respectively, in the direction of some given velocity field $\mathbf{v}$. Understanding $\mathbf{q}$ and u as a $(d-1)$-form and a 0-form, respectively, in $\mathbb{R}^d$, and reinterpreting (71) and (72) in terms of vector proxies, we have the variational equation for shape derivatives:

Seek $\delta\mathbf{q}\in\boldsymbol{H}(\mathrm{div};\Omega)$ and $\delta u\in L^2(\Omega)$ such that for all $\mathbf{p}\in(C^\infty(\Omega))^d$ and $v\in C^\infty(\Omega)$

$$\begin{cases}\int_\Omega\delta\mathbf{q}\cdot\mathbf{p}\,\mathrm{d}x+\int_\Omega\delta u\,\mathrm{div}\,\mathbf{p}\,\mathrm{d}x\\ \quad+\int_\Gamma\mathbf{v}\cdot\mathbf{n}\,(\mathbf{q}\cdot\mathbf{p}+u\,\mathrm{div}\,\mathbf{p})\,\mathrm{d}s=\int_\Gamma\mathbf{v}\cdot\mathbf{n}\left(\frac{\partial(g\mathbf{p}\cdot\mathbf{n})}{\partial\mathbf{n}}+\mathfrak{H}g\mathbf{p}\cdot\mathbf{n}\right)\mathrm{d}s,\\ \int_\Omega\mathrm{div}\,\delta\mathbf{q}v\,\mathrm{d}x+\int_\Gamma\mathbf{v}\cdot\mathbf{n}\,(\mathrm{div}\,\mathbf{q}-f)\,v\,\mathrm{d}x=0.\end{cases} \tag{76}$$

The loss of regularity in $\delta\mathbf{q}$ and δu compared with $\mathbf{q}$ and u follows from differentiation with respect to the domain, in particular due to the weaker regularity of the boundary data.

To determine the boundary condition satisfied by the shape derivative δu, we first test the first equation of (76) with $\mathbf{p}\in\left(C_0^\infty(\Omega)\right)^d$ and $v\in C_0^\infty(\Omega)$ and learn

$$\delta\mathbf{q}=\mathbf{grad}\,\delta u. \tag{77}$$

Therefore, $\delta u \in L^2(\Omega)$ and $\delta \mathbf{q} \in \boldsymbol{L}^2(\Omega)$ implies $\delta u \in H^1(\Omega)$. Next, testing the first equation of (76) with $\mathbf{p} \in \left(C^\infty(\overline{\Omega})\right)^d$ and splitting the third term there in normal and tangential directions, we see, in light of [6, Eqs. (5.19) and (5.22), p. 366], that

$$\begin{aligned}\mathbf{q}\cdot\mathbf{p} + u\,\mathrm{div}\,\mathbf{p} = {} & (\mathbf{q}\cdot\mathbf{n})\,(\mathbf{p}\cdot\mathbf{n}) + \mathbf{q}_\Gamma\cdot\mathbf{p}_\Gamma \\ & + u(D\mathbf{p})\mathbf{n}\cdot\mathbf{n} + u\mathrm{div}_\Gamma\mathbf{p}_\Gamma + \mathfrak{H}u\mathbf{p}\cdot\mathbf{n}.\end{aligned} \tag{78}$$

Noticing by the chain rule that

$$\frac{\partial(g\mathbf{p}\cdot\mathbf{n})}{\partial\mathbf{n}} = \frac{\partial g}{\partial\mathbf{n}}\mathbf{p}\cdot\mathbf{n} + g(D\mathbf{p})\mathbf{n}\cdot\mathbf{n} + g(D\mathbf{n})\mathbf{p}\cdot\mathbf{n}. \tag{79}$$

The last term in (79) vanishes since $D\mathbf{n}\mathbf{p} = S\mathbf{p}$ is a tangential vector due to orthogonality of the Weingarten map S (cf. [17]). Now straightforward calculation combined with $u = g$ on Γ, (74) and (39) for $\mathbf{q}_\Gamma\cdot\mathbf{p}_\Gamma$ and $u\mathrm{div}_\Gamma\mathbf{p}_\Gamma$ yields

$$\int_\Gamma \left(\delta u + \mathbf{v}\cdot\mathbf{n}\left(\frac{\partial u}{\partial\mathbf{n}} - \frac{\partial g}{\partial\mathbf{n}}\right)\right)\mathbf{p}\cdot\mathbf{n}\,\mathrm{d}s = 0. \tag{80}$$

As $\mathbf{p}$ is arbitrary, we immediately have

$$\delta u = -\left(\frac{\partial u}{\partial\mathbf{n}} - \frac{\partial g}{\partial\mathbf{n}}\right)\mathbf{v}\cdot\mathbf{n} \quad \text{on } \Gamma \tag{81}$$

in the trace space $H^{\frac{1}{2}}(\Omega)$, since u and $g \in H^2(\Omega)$.

7 Conclusion

In the present paper, we have presented shape derivatives from the perspective of differential forms and shape calculus via exterior calculus of differential forms. This approach is in particular convenient for deriving shape derivatives of solutions of second-order BVPs in both primal and dual variational formulation. It reveals the essential structure of shape derivatives in terms of recursive composition of Lie derivatives. Moreover, a sufficient condition for the symmetry of the second-order shape Hessian is stated in terms of a vanishing Lie bracket. We have demonstrated the power of our approach by illustrating some typical examples like boundary and domain integrals, bilinear forms and normal derivatives, etc. We have also treated a concrete example, a model second-order BVP that covers all kinds of boundary conditions. For the first time, we show how to derive the boundary condition to the shape derivative of the solution to the PDE with a non-homogeneous Dirichlet boundary condition via the dual mixed formulation.

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