SHAPE DERIVATIVES FOR NONSMOOTH DOMAINS.*

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ABSTRACT. The object of this paper is to study the Shape gradient and the Shape Hessian by the Velocity (Speed) Method for arbitrary domains with or without constraints. It makes the connection between methods using a family of transformations such as first or second order Perturbations of the Identity Operator. New definitions for Shape derivatives are given. They naturally extend existing theories for C^k or Lipchitzian domains to arbitrary domains without any smoothness conditions on their geometric boundary. In this new framework extensions of the classical structure theorems are given for the Shape gradient and the Shape Hessian.

1. INTRODUCTION.

The object of this paper is to study the *Shape gradient* and the *Shape Hessian* by the *Velocity (Speed) Method* (cf. J. CÉA [1, 2] and J. P. ZOLÉSIO [1, 2]) for nonsmooth constrained and unconstrained domains and discuss their relationship to various methods based on perturbations of the identity operator. This extends basic results for C^k and Lipschitzian domains to non-smooth domains.

In section 2 we extend the Velocity (Speed) Method to nonsmooth domains Ω which are constrained to lie within a fixed domain D. This is done by a double use of the *Viability Theory* and the introduction of Bouligand contingent and Clarke tangent cones. We obtain natural extension of *Hadamard's structure theorem* for both the Shape gradient and the Shape Hessian (cf. DELFOUR-ZOLÉSIO [2, 3, 4] for a description of the smooth case) and recover known results in the smooth case. The *canonical structures* of the gradient and the Hessian are given for time-varying velocity fields. We show that Methods of Perturbation of the Identity Operator (first and second order) are special cases corresponding to a time varying velocity fields and indicate how to construct the associated velocity.

For the Shape gradient, the different methods yield expression which may look different but are all equal. However this is no longer true for the Shape Hessian. In fact we shall show in section 4 that different perturbations of the identity yield final expressions which are not equal. It turns out that we can introduce an infinity of definitions based on perturbations of the identity. However we shall show that they always contain a *canonical bilinear term* plus the Shape gradient of the functional acting in the direction of an *acceleration* field which is characteristic of the chosen perturbation. The canonical

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bilinear term exactly coincides with the second order Shape derivative obtained by the Velocity (Speed) Method for time-invariant velocity fields. Moreover each expression obtained by a method of perturbation of the identity can be strictly recovered by adding to the canonical term the Shape gradient acting in the direction of an appropriate acceleration field. In view of this we propose to refer to this canonical term as the *Shape Hessian.*

A few paper have dealt with the second variation of a Shape cost function for linear partial differential equations models. To our knowledge the first one by N. FUJII [1] used a second order perturbation of the identity along the normal to the boundary for second order linear elliptic problems. An extremely interesting paper by ARUMUGAN-PIRONNEAU [1, 2] used the Shape second variation to solve the *ribblet problem.* Finally J. SIMON [1] presented a computation of the second variation using a first order perturbation of the identity. The first general approach to the computation of Shape Hessians can be found in DELFOUR-ZOLÉSIO [2, 3, 4]. It uses the Velocity (Speed) Method and includes simple illustrative examples for the Neumann and Dirichlet problems.

In conclusion, we would like to reiterate that the Velocity method and methods using first and second order perturbations of the identity lead to three different second order Shape derivatives which are not equal. The Velocity method with constant velocity fields provides the canonical bilinear Shape Hessian and the expressions arising from the other method can be recovered by special choices of time-dependent velocity fields.

The proofs of the main theorems and lemmas are given in DELFOUR-ZOLÉSIO [5].

2. VELOCITY (SPEED) METHOD AND METHODS OF PERTURBATION OF THE IDENTITY.

In this section we review and extend the Velocity Method (cf. J.P. ZOLÉSIO [1, 2] and discuss its relationship to various methods based on perturbations of the identity. Under appropriate conditions we show how to construct a family of time-dependent transformations of $\mathbf{R}^N$ (or the closure of a subset D of $\mathbf{R}^N$) from a family of time dependent velocity fields. Conversely we show how to construct the family of time-dependent velocity fields from a family of time-dependent transformations of $\mathbf{R}^N$ (or the closure of a subset D of $\mathbf{R}^N$).

2.1. Unconstrained families of domains.

Let the real number $\tau > 0$ and the map $V : [0, \tau] \times \mathbf{R}^N \rightarrow \mathbf{R}^N$ be given. The map V can be viewed as a family $\{V(t) : 0 \le t \le \tau\}$ of time-dependent velocity fields on $\mathbf{R}^N$ defined by

$$x \mapsto V(t)(x) = V(t, x) : \mathbf{R}^N \mapsto \mathbf{R}^N. \tag{1}$$

Assume that

(V1) $\quad \forall x \in \mathbf{R}^N,\ V(\cdot, x) \in C^0([0, \tau]; \mathbf{R}^N),$

where $V(\cdot, x)$ is the function $t \mapsto V(t, x)$, and that

(V2) $\quad \exists c > 0, \forall x, y \in \mathbf{R}^N, \forall t \in [0, \tau], \quad |V(t, y) - V(t, x)| \le c|y - x|.$

Associate with V the solution $x(t;V)$ of the ordinary differential equation

$$\frac{dx}{dt}(t) = V(t, x(t)), \quad t \in [0,\tau], \quad x(0) = X \in \mathbf{R}^N \tag{2}$$

and introduce the homeomorphism

$$X \mapsto T_t(V)(X) = x(t;V) : \mathbf{R}^N \to \mathbf{R}^N. \tag{3}$$

and the maps

$$(t,X) \mapsto T_V(t,X) \stackrel{\text{def}}{=} T_t(V)(X) : [0,\tau] \times \mathbf{R}^N \to \mathbf{R}^N, \tag{4}$$

$$(t,x) \mapsto T_V^{-1}(t,x) \stackrel{\text{def}}{=} T_t^{-1}(V)(x) : [0,\tau] \times \mathbf{R}^N \to \mathbf{R}^N. \tag{5}$$

NOTATION 2.1. *In the sequel we shall drop the V in $T_V(t,X)$, $T_V^{-1}(t,x)$ and $T_t(V)$ whenever no confusion is possible.*

THEOREM 2.1.

(i) *Under hypotheses (V1) and (V2) the maps T and T^{-1} have the following properties*

$$(T1) \quad \begin{cases} \forall X \in \mathbf{R}^N, \quad T(\cdot, X) \in C^1([0,\tau]; \mathbf{R}^N) \\ \exists c > 0, \forall X, Y \in \mathbf{R}^N, \quad \|T(\cdot,Y) - T(\cdot,X)\|_{C^1([0,\tau];\mathbf{R}^N)} \le c|Y - X|, \end{cases}$$

$$(T2) \quad \forall t \in [0,\tau], \quad X \mapsto T_t(X) = T(t,X) : \mathbf{R}^N \to \mathbf{R}^N \quad \text{is bijective,}$$

$$(T3) \quad \begin{cases} \forall x \in \mathbf{R}^N; \quad T^{-1}(\cdot, x) \in C^0([0,\tau]; \mathbf{R}^N) \\ \exists c > 0, \forall x, y \in \mathbf{R}^N, \quad \|T^{-1}(\cdot,y) - T^{-1}(\cdot,x)\|_{C^0([0,\tau];\mathbf{R}^N)} \le c|y - x|. \end{cases}$$

(ii) *Given a real $\tau > 0$ and a map $T : [0,\tau] \times \mathbf{R}^N \to \mathbf{R}^N$ verifying hypotheses (T1), (T2) and (T3), then the map*

$$(t,x) \mapsto V(t,x) = \frac{\partial T}{\partial t}(t, T_t^{-1}(x)) : [0,\tau] \times \mathbf{R}^N \to \mathbf{R}^N, \tag{6}$$

verifies hypotheses (V1) and (V2), where T_t^{-1} is the inverse of $X \mapsto T_t(X) = T(t,X)$. □

This first theorem is an equivalence result which says that we can either start from a family of velocity fields $\{V(t)\}$ on $\mathbf{R}^N$ or a family of transformations $\{T_t\}$ of $\mathbf{R}^N$ provided that the map V, $V(t,x) = V(t)(x)$, verifies (V1) and (V2) or the map T, $T(t,X) = T_t(X)$, verifies (T1) to (T3). When we start from V, we obtain the velocity method. Given an initial domain Ω, the family of homeomorphisms $\{T_t(V)\}$ generates a family of transformed domains

$$\Omega_t = T_t(V)(\Omega) = \{T_t(V)(X) : X \in \Omega\}. \tag{7}$$

We shall see in sections 3 and 4 how this family of transformations of Ω can be used to define shape derivatives.

2.2. Perturbation of the identity operator.

In examples where we start from T, it is usually possible to verify hypotheses (T1) to (T3) and construct the corresponding velocity field V defined in (6). For instance perturbations of the identity to the first or second order fall in that category:

$$T_t(X) = X + tU(X) + \frac{t^2}{2}A(X) \quad (A = 0 \text{ for the first order }),\ t \geq 0, X \in \mathbf{R}^N, \tag{8}$$

where U and A are transformations of $\mathbf{R}^N$. It turns out that for Lipschitzian transformations U and A, hypotheses (T1) to (T3) are verified.

THEOREM 2.2. *Let U and A be two uniform Lipschitzian transformations of $\mathbf{R}^N$:*

$$\exists c > 0,\ \forall X,\ Y \in \mathbf{R}^N, \quad |U(Y) - U(X)| \leq c|Y - X|,\ |A(Y) - A(X)| \leq c|Y - X|.$$

For $\tau = \min\{1, 1/4c\}$ and T given by (8), the map T verifies hypotheses (T1) to (T3) on $[0,\tau]$. Moreover the associated velocity V is given by

$$(t,x) \mapsto V(t,x) = U(T_t^{-1}(x)) + tA(T_t^{-1}(x)) : [0,\tau] \times \mathbf{R}^N \to \mathbf{R}^N, \tag{9}$$

and it verifies hypotheses (V1) and (V2) on $[0,\tau]$. □

REMARK 2.1. Observe that from (8) and (9)

$$V(0) = U, \quad \overset{\bullet}{V}(0)(x) = \frac{\partial V}{\partial t}(t,x)|_{t=0} = A - [DU]U. \tag{10}$$

where DU is the Jacobian matrix of U. The term $\overset{\bullet}{V}(0)$ is an *acceleration* at $t = 0$ which will always be present even when $A = 0$. □

2.3. Constrained families of domains.

In many applications the family of admissible domains Ω is constrained to subsets of a fixed larger domain or *hold-all* D. To reflect that constraint we would like to consider transformations

$$T : [0,\tau] \times \bar{D} \to \mathbf{R}^N \tag{11}$$

with the following properties

$$(T1_D) \quad \begin{cases} \forall X \in \bar{D}, \quad T(\cdot,X) \in C^1([0,\tau];\mathbf{R}^N) \\ \exists c > 0, \forall X, Y \in \bar{D}, \quad \|T(\cdot,Y) - T(\cdot,X)\|_{C^1([0,\tau];\mathbf{R}^N)} \leq c|Y - X|, \end{cases}$$

$$(T2_D) \quad \forall t \in [0,\tau], \quad X \mapsto T_t(X) = T(t,X) : \bar{D} \to \bar{D} \quad \text{is bijective,}$$

$$(T3_D) \quad \begin{cases} \forall x \in \bar{D}, \quad T^{-1}(\cdot,x) \in C^0([0,\tau];\mathbf{R}^N) \\ \exists c > 0, \forall x, y \in \bar{D}, \quad \|T^{-1}(\cdot,y) - T^{-1}(\cdot,x)\|_{C^0([0,\tau];\mathbf{R}^N)} \leq c|y - x|. \end{cases}$$

where under hypothesis $(T2_D)$ T^{-1} is defined as

$$(t,x) \mapsto T^{-1}(t,x) = T_t^{-1}(x) : [0,\tau] \times \bar{D} \to \mathbf{R}^N. \tag{12}$$

Those three properties are the analogue for $\bar{D}$ of the same three properties obtained for $\mathbf{R}^N$. In fact Theorem 2.1 extends from $\mathbf{R}^N$ to $\bar{D}$ by adding one hypothesis to $(V1_D)$ and $(V2_D)$. Specifically we shall consider for $\tau > 0$ velocities

$$V : [0,\tau] \times \bar{D} \to \mathbf{R}^N \tag{13}$$

such that

$$\begin{array}{ll} (V1_D) & \forall x \in \bar{D}, \quad V(\cdot,x) \in C^0([0,\tau];\mathbf{R}^N) \\ (V2_D) & \exists n > 0, \forall x,y \in \bar{D}, \quad \|V(\cdot,y) - V(\cdot,x)\|_{C^0([0,\tau];\mathbf{R}^N)} \le n|y-x| \\ (V3_D) & \forall x \in \bar{D}, \forall t \in [0,\tau], \quad \pm V(t,x) \in T_D(x), \end{array}$$

where $T_D(x)$ is the Bouligand contingent cone to $\bar{D}$ at the point x in $\bar{D}$ (cf. AUBIN–CELLINA [1, p. 176]).

THEOREM 2.3.

(i) *Let $\tau > 0$ and V be a family of velocity fields verifying hypotheses $(V1_D)$ to $(V3_D)$ and consider the family of transformations*

$$(t,X) \mapsto T(t,X) = x(t;X) : [0,\tau] \times \bar{D} \to \mathbf{R}^N \tag{14}$$

where $x(\cdot,X)$ is the solution of

$$\frac{dx}{dt}(t) = V(t,x(t)), \quad 0 \le t \le \tau,\ x(0) = X. \tag{15}$$

Then the family of transformations T verifies conditions $(T1_D)$ to $(T3_D)$.

(ii) *Conversely given a family of transformations T verifying hypotheses $(T1_D)$ to $(T3_D)$, the family of velocity fields*

$$(t,x) \mapsto V(t,x) = \frac{\partial T}{\partial t}\left(t, T_t^{-1}(x)\right) : [0,\tau] \times \bar{D} \to \mathbf{R}^N \tag{16}$$

verifies conditions $(V1_D)$ to $(V3_D)$ and the transformations constructed from this V coincide with T. □

REMARK 2.2. Under $(V1_D)$ to $(V3_D)$, $\{T_t : 0 \le t \le \tau\}$ is a family of homeomorphisms of $\bar{D}$ which map the interior $\overset{\circ}{D}$ (resp. the boundary ∂D) of D onto $\overset{\circ}{D}$ (resp. ∂D) (cf. J. DUGUNJI [1, p. 87–88]). □

REMARK 2.3. Assumption $(V3_D)$ is a double viability condition. M. NAGUMO [1]'s usual viability condition

$$V(t,x) \in T_D(x), \forall t \in [0,\tau], \forall x \in \bar{D} \tag{17}$$

is a necessary and sufficient condition for a *viable solution* to (15), that is

$$\forall t \in [0,\tau], \forall X \in \bar{D}, x(t;X) \in \bar{D} \text{ or } T_t(\bar{D}) \subset \bar{D} \tag{18}$$

(cf. AUBIN-CELLINA [1, p. 174 and p. 180]). Condition $(V3_D)$

$$\forall t \in [0,\tau], \forall x \in \bar{D}, \pm V(t,x) \in T_D(x) \tag{19}$$

is a *strict viability condition* which not only says that T_t maps $\bar{D}$ into $\bar{D}$ but also that

$$\forall t \in [0,\tau], \quad T_t : \bar{D} \to \bar{D} \quad \text{is a homeomorphism.} \tag{20}$$

In particular it keeps interior points in the interior and boundary points on the boundary. □

REMARK 2.4. Condition $(V3_D)$ is a generalization to arbitrary domains D of the following condition used by J.P. ZOLÉSIO [1] in 1979: for all x in ∂D

$$\begin{cases} V(t,x) \bullet n(x) = 0, & \text{if the outward normal } n(x) \text{ exists} \\ 0, & \text{otherwise . } \square \end{cases}$$

Theorem 2.2 is a generalization of Theorem 2.1 to arbitrary domains D. It shows that we can either start from a velocity V or a transformation T.

2.4. Transformation of condition $(V3_D)$ into a linear constraint.

Condition $(V3_D)$ is equivalent to

$$\forall t \in [0,\tau], \forall x \in \bar{D}, \; V(t,x) \in \{-T_D(x)\} \cap \{T_D(x)\} \tag{21}$$

since $T_{\bar{D}}(x) = T_D(x)$. If $T_D(x)$ was convex, then the above intersection would be a closed linear subspace of $\mathbf{R}^N$. This is true when D is convex. In that case $T_D(x) = C_D(x)$, where $C_D(x)$ is Clarke tangent cone and

$$L_D(x) = \{-C_D(x)\} \cap \{C_D(x)\} \tag{22}$$

is a closed linear subspace of $\mathbf{R}^N$. This means that $(V3_D)$ reduces to

$$\forall t \in [0,\tau], \forall x \in \bar{D}, \quad V(t,x) \in L_D(x). \tag{23}$$

It turns out that for continuous vector fields $V(t,\cdot)$ the equivalence of $(V3_D)$ and (23) extends to arbitrary domains D.

THEOREM 2.4. *Given a velocity field V verifying $(V1_D)$ and $(V2_D)$, then condition $(V3_D)$ is equivalent to*

$(V3_C)$ $\qquad \forall t \in [0,\tau], \forall x \in \bar{D},\ V(t,x) \in L_D(x) = \{-C_D(x)\} \cap C_D(x),$

where $C_D(x)$ is the (closed convex) Clarke tangent cone to $\bar{D}$ at x which is defined by

$$C_D(x) = \left\{ v \in \mathbf{R}^N : \lim_{\substack{h \to 0 \\ y \to_D x}} \quad d_D(y+hv)/h = 0 \right\}$$

$d_D(y)$ is the minimum distance from y to D, and $\to_D$ denotes the convergence in $\bar{D}$. Moreover $L_D(x)$ is a closed linear subspace of $\mathbf{R}^N$. □

The equivalence of (V3) and $(V3_C)$ is a direct consequence of the following lemma.

LEMMA 2.1. *Given a vector field $W \in C^0(\bar{D};\mathbf{R}^N)$, the following two conditions are equivalent:*

$$\forall x \in \bar{D}, \quad W(x) \in T_D(x); \tag{25}$$

$$\forall x \in \bar{D}, \quad W(x) \in C_D(x). \quad \square \tag{26}$$

REMARK 2.5. Lemma 2.1 essentially says that for continuous vector fields we can relax the condition of M. NAGUMO [1]'s theorem from $(V3_D)$ involving Bouligand contingent cone to $(V3_C)$ involving the smaller Clarke convex tangent cone. In dimension $N = 3, L_D(x)$ is $\{0\}$ a line, a plane or the whole space. □

NOTATION 2.1. In the sequel it will be convenient to introduce the following spaces and subspaces

$$\mathcal{L} = \{V : [0,\tau] \times \mathbf{R}^N \to \mathbf{R}^N : V \text{ verifies (V1) and (V2) on } \mathbf{R}^N\} \tag{27}$$

and for an arbitrary domain D in $\mathbf{R}^N$

$$\mathcal{L}_D = \{V : [0,\tau] \times \bar{D} \to \mathbf{R}^N : V \text{ verifies } (V1_D), (V2_D) \text{ and } (V3_C) \text{ on } \bar{D}\}. \tag{28}$$

For any integers $k \geq 0$ and $m \geq 0$ and any compact subset K of $\mathbf{R}^N$ define the following subspaces of $\mathcal{L}$

$$\begin{cases} \mathcal{V}_K^{m,0} = C^m\left([0,\tau], \mathcal{D}^0(K,\mathbf{R}^N)\right) \cap \mathcal{L}, & \text{if } k = 0 \\ \mathcal{V}_K^{m,k} = C^m\left([0,\tau], \mathcal{D}^k(K,\mathbf{R}^N)\right), & \text{if } k \geq 1, \end{cases} \tag{29}$$

where $\mathcal{D}^k(K,\mathbf{R}^N)$ is the space of k–times continuously differentiable transformations of $\mathbf{R}^N$ with compact support in K. In all cases $\mathcal{V}_K^{m,k} \subset \mathcal{L}_K$. As usual $\mathcal{D}^\infty(K,\mathbf{R}^N)$ will de written $\mathcal{D}(K,\mathbf{R}^N)$. □

3. SHAPE GRADIENT.

Consider the set $\mathcal{P}(D)$ of subsets Ω of a fixed domain D of $\mathbf{R}^N$ (possibly all of $\mathbf{R}^N$) which will play the role of a *hold-all*. Under the action of a velocity field V in $\mathcal{L}_D$, the domain Ω in $\mathcal{P}(D)$ is transformed into a new domain

$$\Omega_t(V) = T_t(V)(\Omega) = \{T_t(V)(X) : X \in \Omega\}. \tag{1}$$

This will now provide our first notion of derivative for a shape functional, that is a map

$$\Omega \mapsto J(\Omega) : \mathcal{P}(D) \to \mathbf{R}. \tag{2}$$

DEFINITION 3.1. *Given a velocity field V in $\mathcal{L}_D$, J is said to have an* Eulerian semiderivative *at Ω in the direction V if the following limit exists and is finite*

$$\lim_{t \searrow 0} [J(\Omega_t(V)) - J(\Omega)]/t. \tag{3}$$

Whenever it exists, the limit will be denoted $dJ(\Omega; V)$. □

This definition is quite general and may include situations where $dJ(\Omega; V)$ is not only a function of $V(0)$ but also of $V(t)$ in a neighbourhood of $t = 0$. This will not occur under some appropriate continuity hypothesis on the map $V \mapsto dJ(\Omega; V)$. This immediately raises the question of the choice of topology and eventually the choice of gradient when we specialize to time-invariant vector fields V. We choose to follow the classical philosophy of the Theory of Distributions (cf. L. SCHWARTZ [1]). Assume that D is an open domain in $\mathbf{R}^N$. Domains Ω in $\mathcal{P}(D)$ will be perturbed by velocity fields $V(t)$ with values in $\mathcal{D}^k(K,\mathbf{R}^N)$ for some compact subset K of D and integer $k \geq 0$. More precisely we shall consider velocity fields in

$$\vec{\mathcal{V}}_D^{m,k} = \varinjlim_{K} \left\{ \mathcal{V}_K^{m,k} : \forall K \text{ compact in } D \right\} \tag{4}$$

where $\varinjlim$ denotes the inductive limit set with respect to K endowed with its natural inductive limit topology. For time-invariant fields, the above construction reduce to

$$\mathcal{V}_D^k = \left\{ \begin{array}{ll} \mathcal{D}^0(D,\mathbf{R}^N) \cap \text{ Lip } (\mathbf{R}^N,\mathbf{R}^N), & k = 0 \\ \mathcal{D}^k(D,\mathbf{R}^N), & 1 \leq k \leq \infty \end{array} \right\} \tag{5}$$

where $\text{Lip}(\mathbf{R}^N,\mathbf{R}^N)$ denotes the space of uniformily Lipschitzian transformations of $\mathbf{R}^N$. In all cases hypotheses $(V1_D)$ to $(V3_D)$ are verified since for all $t \in [0,\tau], V(t,x) = 0$

for all x in ∂D. When $D = \mathbf{R}^N$ we drop the index D in the above definitions and simply write $\vec{\mathcal{V}}^{m,k}$ and $\mathcal{V}^k$.

THEOREM 3.1. *Let Ω be a domain in the fixed open hold-all D. Assume that there exist integers $m \geq 0$ and $k \geq 0$ such that*

$$\forall V \in \vec{\mathcal{V}}_D^{m,k}, \quad dJ(\Omega; V) \text{ exists,} \tag{6}$$

and that the map

$$V \mapsto dJ(\Omega; V) : \vec{\mathcal{V}}_D^{m,k} \to \mathbf{R} \tag{7}$$

is continuous. Then

$$\forall V \in \vec{\mathcal{V}}_D^{m,k}, \quad dJ(\Omega; V) = dJ(\Omega; V(0)), \tag{8}$$

where $dJ(\Omega; V(0))$ is the Eulerian semiderivative for the time-independent vector field equal to $V(0)$. □

By virtue of this theorem we can now specialize to time-invariant vector fields V to further study the properties and the structure of $dJ(\Omega; V)$.

DEFINITION 3.2. *Let Ω be a domain in the open hold-all D of $\mathbf{R}^N$.*

(i) The functional J is said to be shape differentiable *at Ω, if the Eulerian semiderivative $dJ(\Omega; V)$ exists for all V in $\mathcal{D}(D, \mathbf{R}^N)$ and the map*

$$V \mapsto dJ(\Omega; V) : \mathcal{D}(D, \mathbf{R}^N) \to \mathbf{R} \tag{9}$$

is linear and continuous.

(ii) The map (9) defines a vector distribution $G(\Omega)$ which will be referred to as the shape gradient *of J at Ω.*

(iii) When there exists some finite $k \geq 0$ such that $G(\Omega)$ is continuous for the $\mathcal{D}^k(D, \mathbf{R}^N)$–topology, we say that the shape gradient $G(\Omega)$ is of order k. □

The next theorem gives additional properties of shape differentiable functionals.

NOTATION 3.1. Associate with a subset A of D and an integer $k \geq 0$ the set

$$L_A^k = \left\{ V \in \mathcal{D}^k(D, \mathbf{R}^N) : \forall x \in A, V(x) \in L_A(x) \right\}. \quad \square$$

THEOREM 3.2. *(Generalized Hadamard's structure theorem)*

Let Ω be a domain with boundary Γ in the open hold-all D of $\mathbf{R}^N$ and assume that J has a shape gradient $G(\Omega)$.

(i) *The support of the shape gradient $G(\Omega)$ is contained in $\Gamma_D \stackrel{\text{def}}{=} \Gamma \cap D$.*

(ii) *If Ω is open or closed in $\mathbf{R}^N$ and the shape gradient is of order k for some $k \geq 0$, then there exists $[G(\Omega)]$ in $(\mathcal{D}_D^k/L_\Omega^k)'$ such that for all V in $\mathcal{D}_D^k \overset{\text{def}}{=} \mathcal{D}^k(D, \mathbf{R}^N)$*

$$dJ(\Omega; V) = \langle [G(\Omega)], q_L V \rangle_{\mathcal{D}_D^k/L_\Omega^k} \tag{11}$$

where $q_L : \mathcal{D}_D^k \to \mathcal{D}_D^k/L_\Omega^k$ is the canonical quotient surjection. Moreover

$$G(\Omega) = {}^*(q_L)[G(\Omega)] \tag{12}$$

where ${}^*(q_L)$ denotes the transposed of the linear map q_L. □

REMARK 3.1. When the boundary Γ of Ω is compact and J is shape differentiable at Ω, the distribution $G(\Omega)$ is of finite order. Once this is known, the conclusions of Theorem 3.2(ii) apply with k equal to the order of $G(\Omega)$. □

The quotient space is very much related to a trace on the boundary Γ and when the boundary Γ is sufficiently smooth we can indeed make that identification.

COROLLARY. *Assume that the hypotheses of Theorem 3.2 are verified for an open domain Ω, that the order of $G(\Omega)$ is $k \geq 0$, and that the boundary Γ of Ω is C^{k+1}. Then for all x in Γ, $L_\Omega(x)$ is an $(N-1)$-dimensional hyperplane to Ω at x and there exists a unique outward unit normal $n(x)$ which belongs to $C^k(\Gamma; \mathbf{R}^N)$. As a result the kernel of the map*

$$V \to \gamma_\Gamma(V) \bullet n : \mathcal{D}^k(D, \mathbf{R}^N) \to \mathcal{D}^k(\Gamma \cap D) \tag{13}$$

coincides with L_Ω^k where $\gamma_\Gamma : \mathcal{D}^k(D, \mathbf{R}^N) \to \mathcal{D}^k(\Gamma \cap D, \mathbf{R}^N)$ is the trace of V on $\Gamma \cap D$. Moreover the map $p_L(V)$

$$q_L(V) \mapsto p_L(q_L(V)) = \gamma_\Gamma(V) \bullet n : \mathcal{D}_D^k/L_\Omega^k \to \mathcal{D}^k(\Gamma \cap D) \tag{14}$$

is a well-defined isomorphism. In particular there exists a scalar distribution $g(\Gamma)$ in $\mathcal{D}^k(\Gamma \cap D)'$ such that for all V in $\mathcal{D}^k(D, \mathbf{R}^N)$

$$dJ(\Omega; V) = \langle g(\Gamma), \gamma_\Gamma(V) \bullet n \rangle_{\mathcal{D}^k(\Gamma \cap D)} \tag{15}$$

and

$$G(\Omega) = {}^*(q_L)[G(\Omega)], \quad [G(\Omega)] = {}^*(p_L) g(\Gamma). \quad \square \tag{16}$$

REMARK 3.2. In 1907, J. HADAMARD [1] used velocity fields along the normal to the boundary Γ of a C^∞ domain to compute the derivative of the first eigenvalue of the plate. Theorem 3.2 and its corollary are generalizations to arbitrary shape functionals of that property to open or closed domains with an arbitrary boundary. The generalization to open domains with a C^{k+1} boundary was done by J.P. ZOLÉSIO [1] in 1979. □

REMARK 3.3. The space $\mathcal{D}^k(\Gamma \cap D)$ is not simple to characterize. However when Γ is compact and $D = \mathbf{R}^N$, it coincides with $C^k(\Gamma)$. □

EXAMPLE 3.1. For any measurable subset Ω of a measurable hold-all D of $\mathbf{R}^N$, consider the volume functional

$$J(\Omega) = \int_\Omega dx. \tag{17}$$

For Ω with finite volume and V in $\mathcal{D}^1(D, \mathbf{R}^N)$,

$$dJ(\Omega; V) = \int_\Omega \operatorname{div} V dx \tag{18}$$

but for a bounded open domain Ω with a C^1 boundary Γ

$$dJ(\Omega; V) = \int_\Gamma V \bullet n \quad d\Gamma \tag{19}$$

which is continuous on $\mathcal{D}^0(D, \mathbf{R}^N)$. Here the smoothness of the boundary decreases the order of the distribution $G(\Omega)$. This raises the following question: is it possible to characterize the family of all domains Ω of D for which the map

$$V \mapsto \int_\Omega \operatorname{div} V \, dx : \mathcal{D}^0(D, \mathbf{R}^N) \to \mathbf{R} \tag{20}$$

is continuous? The answer is yes. It is the family of *finite perimeter sets* with respect to D. It contains domains Ω whose characteristic function belongs to $BV(D)$, the space of L^1 functions on D with a distributional gradient in the space of (vectorial) bounded measures. Roughly speaking they are the sets with finite volume and perimeter. □

4. SHAPE HESSIAN.

We first study the second order Eulerian semiderivative $d^2J(\Omega; V; W)$ of a functional $J(\Omega)$ for two time-dependent vector fields V and W. A first theorem shows that under some natural continuity hypotheses, $d^2J(\Omega; V; W)$ is the sum of two terms: the *canonical term* $d^2J(\Omega; V(0); W(0))$ plus the first order Eulerian semiderivative $dJ(\Omega; \dot{V}(0))$ at Ω in the direction $\dot{V}(0)$ of the time-partial derivative $\partial_t V(t,x)$ at $t = 0$. As in the study of first order Eulerian semiderivatives, this first theorem reduces the study of second order Eulerian semiderivatives to the time-invariant case. So we shall specialize to fields V and W in $\mathcal{D}^k(D, \mathbf{R}^N)$ and give the equivalent of Hadamard's structure theorem for the canonical term.

4.1. Time-dependent case.

The basic framework introduced in sections 2 and 3 has reduced the computation of the Eulerian semiderivative of $J(\Omega)$ to the computation of the derivative

$$j'(0) = dJ(\Omega; V(0)) \tag{1}$$

of the function

$$j(t) = J(\Omega_t(V)). \tag{2}$$

For $t \geq 0$, we naturally obtain

$$j'(t) = dJ(\Omega_t(V); V(t)). \tag{3}$$

This suggests the following definition.

DEFINITION 4.1. *Let V and W belong to $\mathcal{L}_D$ and assume that for all $t \in [0,\tau], dJ(\Omega_t(W); V(t))$ exists for $\Omega_t(W) = T_t(W)(\Omega)$. The functional J is said to have a second order Eulerian semiderivative at Ω in the directions (V, W) if the following limit exists*

$$\lim_{t \searrow 0} [dJ(\Omega_t(W); V(t)) - dJ(\Omega; V(0))]/t. \tag{4}$$

When it exists, it is denoted $d^2 J(\Omega; V; W)$. □

REMARK 4.1. This last definition is compatible with the second order expansion of $j(t)$ with respect to t around $t = 0$:

$$j(t) \cong j(0) + tj'(0) + \frac{t^2}{2} j''(0), \tag{5}$$

where

$$j''(0) = d^2 J(\Omega; V; V). \quad \square \tag{6}$$

REMARK 4.2. It is easy to construct simple examples (see Example 4.2) with time-invariant fields V and W showing that $d^2 J(\Omega; V; W) \neq d^2 J(\Omega; W; V)$ (cf. DELFOUR-ZOLÉSIO [2]).□

The next theorem is the analogue of Theorem 3.1 and provides the canonical structure of the second order Eulerian semiderivative.

THEOREM 4.1. *Let Ω be a domain in the fixed open hold-all D of $\mathbf{R}^N$ and let $m \geq 0$ and $\ell \geq 0$ be integers. Assume that*

(i) $\forall V \in \overrightarrow{\mathcal{V}}_D^{m+1,\ell}$, $\forall W \in \overrightarrow{\mathcal{V}}_D^{m,\ell}$, *$d^2 J(\Omega; V; W)$ exists,*

(ii) $\forall W \in \overrightarrow{\mathcal{V}}_D^{m,\ell}$, $\forall t \in [0,\tau]$, J has a shape gradient at $\Omega_t(W)$ of order ℓ,

(iii) $\forall\, U \in \mathcal{V}_D^{\ell}$, the map

$$W \mapsto d^2 J(\Omega; U; W) : \overrightarrow{\mathcal{V}}_D^{m,\ell} \to \mathbf{R} \tag{7}$$

is continuous.

Then for all V in $\vec{\mathcal{V}}_D^{m+1,\ell}$ and all W in $\vec{\mathcal{V}}_D^{m,\ell}$

$$d^2 J(\Omega; V; W) = d^2 J(\Omega; V(0); W(0)) + dJ(\Omega; \dot{V}(0)), \tag{8}$$

where

$$\dot{V}(0)(x) = \lim_{t \searrow 0} [V(t,x) - V(0,x)]/t. \quad \Box \tag{9}$$

This important theorem gives the canonical structure of the second order Eulerian semiderivative: a first term which depends on $V(0)$ and $W(0)$ and a second term which is equal to $dJ(\Omega; \dot{V}(0))$. When V is time-invariant the second term disappears and the semiderivative coincides with $d^2 J(\Omega; V; W(0))$ which can be separately studied for time-invariant vector fields in $\mathcal{V}_D^\ell$.

4.2. Time-invariant Case.

DEFINITION 4.2. *Let Ω be a domain in the open hold-all D of $\mathbf{R}^N$.*

(i) *The functional $J(\Omega)$ is said to be* twice shape differentiable *at Ω if*

$$\forall\, V,\ \forall\, W \text{ in } \mathcal{D}(D, \mathbf{R}^N), \quad d^2 J\ (\Omega; V; W) \text{ exists} \tag{11}$$

and the map

$$(V, W) \mapsto d^2 J(\Omega; V; W) : \mathcal{D}(D, \mathbf{R}^N) \times \mathcal{D}(D, \mathbf{R}^N) \to \mathbf{R} \tag{12}$$

is bilinear and continuous. We denote by h the map (12).

(ii) *Denote by $H(\Omega)$ the vector distribution in $(\mathcal{D}(D, \mathbf{R}^N) \otimes \mathcal{D}(D, \mathbf{R}^N))'$ associated with h:*

$$d^2 J(\Omega; V; W) = \langle H(\Omega), V \otimes W \rangle = h(V, W), \tag{13}$$

where $V \otimes W$ is the tensor product of V and W defined as

$$(V \otimes W)_{ij}(x, y) = V_i(x) W_j(y), \quad 1 \le i,\ j \le N, \tag{14}$$

and $V_i(x)$ (resp. $W_j(y)$) is the i-th (resp. j-th) component of the vector V (resp. W) (cf. L. SCHWARTZ *[2]'s kernel theorem and* GELFAND-VILENKIN *[1]). $H(\Omega)$ will be called the* Shape Hessian *of J at Ω.*

(iii) *When there exists a finite integer $\ell \ge 0$ such that $H(\Omega)$ is continuous for the $\mathcal{D}^\ell(D, \mathbf{R}^N) \otimes \mathcal{D}^\ell(D, \mathbf{R}^N)$-topology, we say that $H(\Omega)$ is of* order ℓ. $\Box$

THEOREM 4.2. *Let Ω be a domain with boundary Γ in the open hold-all D of $\mathbf{R}^N$ and assume that J is twice shape differentiable.*

(i) *The vector distribution $H(\Omega)$ has support in*

$$(\Gamma \cap D) \times (\Gamma \cap D).$$

(ii) *If Ω is an open or closed domain in D and $H(\Omega)$ is of order $\ell \geq 0$, then there exists a continuous bilinear form*

$$[h] : (\mathcal{D}_D^\ell / D_\Gamma^\ell) \times (\mathcal{D}_D^\ell / L_\Omega^\ell) \to \mathbf{R} \tag{15}$$

such that for all $[V]$ in $\mathcal{D}_D^\ell / D_\Gamma^\ell$ and $[W]$ in $\mathcal{D}_D^\ell / L_\Omega^\ell$

$$d^2 J(\Omega; V; W) = [h](q_D(V), q_L(W)) \tag{16}$$

where $q_D : \mathcal{D}_D^\ell \to \mathcal{D}_D^\ell / D_\Gamma^\ell$ and $q_L : \mathcal{D}_D^\ell \to \mathcal{D}_D^\ell / L_\Omega^\ell$ are the canonical quotient surjections and

$$D_\Gamma^\ell = \left\{ V \in \mathcal{D}^\ell(D, \mathbf{R}^N) : \partial^\alpha V = 0 \text{ on } \Gamma \cap D, \forall |\alpha| \leq \ell \right\}. \quad \Box \tag{17}$$

The next and last result is the extension of Hadamard's structure theorem to second order Eulerian semiderivatives. We need the result established in the Corollary to Theorem 3.2. For a domain Ω with a boundary Γ which is $C^{\ell+1}, \ell \geq 0$, the map

$$q_L(W) \mapsto p_L(q_L(W)) = \gamma_\Gamma(W) \bullet n : \mathcal{D}_\Omega^\ell / L_\Omega^\ell \to \mathcal{D}^\ell(\Gamma \cap D) \tag{18}$$

is a well-defined isomorphism. This will be used for the V-component. For the W-component we need the following lemma.

LEMMA 4.1. *Assume that the boundary Γ of Ω is $C^{\ell+1}, \ell \geq 0$. Then the map*

$$q_D(V) \mapsto p_D(q_D(V)) = \gamma_\Gamma(V) : \mathcal{D}_D^\ell / D_\Gamma^\ell \to \mathcal{D}^\ell(\Gamma \cap D, \mathbf{R}^N) \tag{19}$$

is a well-defined isomorphism where

$$p_D : \mathcal{D}_D^\ell \to \mathcal{D}_D^\ell / D_\Gamma^\ell \tag{20}$$

is the canonical surjection. $\Box$

REMARK 4.3. When $D = \mathbf{R}^N$ and Γ is compact, $\mathcal{D}^\ell(\Gamma \cap D, \mathbf{R}^N) = \mathcal{D}^\ell(\Gamma, \mathbf{R}^N)$ coincides with the space of ℓ-times continuously differentiables maps from Γ to $\mathbf{R}^N$. $\Box$

THEOREM 4.3. *Assume that the hypotheses of Theorem 4.2(ii) hold and that the boundary Γ of the open domain Ω is $C^{\ell+1}$ for $\ell \geq 0$.*

(i) *The map*

$$\begin{cases} (v,w) \mapsto h_{D\times L}(v,w) = [h](p_D^{-1}v, p_L^{-1}w) \\ : \mathcal{D}^\ell(\Gamma_D, \mathbf{R}^N) \times \mathcal{D}^\ell(\Gamma_D) \to \mathbf{R} \end{cases} \tag{21}$$

is bilinear and continuous and for all V and W in $\mathcal{D}^\ell(D, \mathbf{R}^N)$

$$d^2J(\Omega; V; W) = h_{D\times L}(\gamma_\Gamma V, ((\gamma_\Gamma W) \bullet n)), \tag{22}$$

where $\Gamma_D = \Gamma \cap D$.

(ii) *This induces a vector distribution $h(\Gamma_D \otimes \Gamma_D)$ on $\mathcal{D}^\ell(\Gamma_D, \mathbf{R}^N) \otimes \mathcal{D}^\ell(\Gamma_D)$ of order ℓ*

$$h(\Gamma_D \otimes \Gamma_D) : \mathcal{D}^\ell(\Gamma_D, \mathbf{R}^N) \otimes \mathcal{D}^\ell(\Gamma_D) \to \mathbf{R} \tag{23}$$

such that for all V and W in $\mathcal{D}^\ell(D, \mathbf{R}^N)$

$$\langle h(\Gamma_D \otimes \Gamma_D), (\gamma_\Gamma V) \otimes ((\gamma_\Gamma W) \bullet n)\rangle = d^2J(\Omega; V; W), \tag{24}$$

where $(\gamma_\Gamma V) \otimes ((\gamma_\Gamma W) \bullet n)$ is defined as the tensor product

$$((\gamma_\Gamma V) \otimes ((\gamma_\Gamma W) \bullet n))_i(x,y) = (\gamma_\Gamma V_i)(x)((\gamma_\Gamma W) \bullet n)(y), \quad x, y \in \Gamma_D \tag{25}$$

$V_i(x)$ is the i-th component of $V(x)$ and

$$(\gamma_\Gamma(W) \bullet n)(y) = (\gamma_\Gamma W)(y) \bullet n(y), \quad \forall y \in \Gamma_D. \quad \square \tag{26}$$

REMARK 4.4. Finally under the hypotheses of Theorem 4.1 and 4.3

$$\begin{aligned} d^2J(\Omega; V; W) = {} & \langle h(\Gamma_D \otimes \Gamma_D), (\gamma_\Gamma V(0)) \otimes ((\gamma_\Gamma W(0)) \bullet n)\rangle \\ & + \langle (g(\Gamma_D), (\gamma_\Gamma \overset{\bullet}{V}(0)) \bullet n\rangle \end{aligned} \tag{27}$$

for all V in $\vec{V}_D^{m+1,\ell}$ and W in $\vec{V}_D^{m,\ell}$. $\square$

EXAMPLE 4.1. Consider Example 3.1. Recall that for V in $\mathcal{D}^1(D, \mathbf{R}^N)$

$$dJ(\Omega; V) = \int_\Omega \operatorname{div} V \, dx. \tag{28}$$

Now for V in $\mathcal{D}^2(D, \mathbf{R}^N)$ and W in $\mathcal{D}^1(D, \mathbf{R}^N)$

$$d^2J(\Omega; V; W) = \int_\Omega \operatorname{div}[(\operatorname{div} V)W] \, dx \tag{29}$$

and if Γ is C^1

$$d^2J(\Omega;V;W) = \int_\Gamma \operatorname{div} V \; W \bullet n \quad d\Gamma \tag{30}$$

which is continuous for pairs $(V;W) \in \mathcal{D}^1(D,\mathbf{R}^N)\times\mathcal{D}^0(D,\mathbf{R}^N)$ or $\mathcal{D}^1(\Gamma,\mathbf{R}^N)\times\mathcal{D}^0(\Gamma,\mathbf{R}^N)$. □

Another interesting observation is that the shape Hessian is, in general, not symmetrical as can be seen from the following example in DELFOUR-ZOLÉSIO [2].

EXAMPLE 4.2. We use the functional (28) and expression (30) in Example 4.1. Choose the following two vector fields

$$V(x,y) = (1,0) \quad \text{and} \quad W(x,y) = (x^2/2, 0).$$

Then

$$\operatorname{div} V = 0, \quad \text{and} \quad W|_\Gamma = x = \cos\theta$$

and

$$V \bullet n = n_x = \cos\theta \text{ on } \Gamma.$$

As a result $d^2J(\Omega;V;W) = 0$ and

$$d^2J(\Omega;W;V) = \int_\Gamma \operatorname{div}\, W \; (V \bullet n) d\Gamma = \int_0^{2\pi} \cos^2\theta d\theta > 0. \quad \square$$

4.3. Comparison with methods of perturbation of the identity.

At this juncture it is instructive to compare first and second order Eulerian semiderivatives obtained by the Velocity (Speed) Method with those obtained by first and second order perturbations of the identity: that is, when the transformations T_t are specified a priori by

$$T_t(X) = X + tU(X) + \frac{t^2}{2}A(X), \; X \in \mathbf{R}^N, \tag{31}$$

where U and A are transformations of $\mathbf{R}^N$ verifying the hypotheses of Theorem 2.2. The transformation T_t in (31) is a *second order* perturbation when $A \neq 0$ and a *first order* perturbation when $A = 0$. According to Theorem 2.2, first and second order Eulerian semiderivatives associated with (31) can be equivalently obtained by applying the Velocity (Speed) Method to the time-varying velocity fields V_{UA} given by (2.9) and

$$dJ(\Omega;V_{UA}) = dJ(\Omega;V_{UA}(0)) = dJ(\Omega;U) \tag{32}$$

where we have used Remark 2.1 which says that

$$V_{UA}(0) = U \text{ and } \dot{V}_{UA}(0) = A - [DU]U. \tag{33}$$

Similarly if V_{WB} is another velocity field corresponding to

$$T_t(X) = X + tW(X) + \frac{t^2}{2}B(X), \; X \in \mathbf{R}^N, \tag{34}$$

where W and B verify the hypotheses of Theorem 2.2, then

$$d^2J(\Omega; V_{UA}; V_{WB}) = d^2J(\Omega; V_{UA}(0); V_{WB}(0)) + dJ(\Omega; \dot{V}_{UA}(0)) \tag{35}$$

and

$$d^2J(\Omega; V_{UA}; V_{WB}) = d^2J(\Omega; U; W) + dJ(\Omega; A - [DU]U). \tag{36}$$

Expressions (32) and (35) are to be compared with the following expressions obtained by the Velocity (Speed) Method for two time-invariant vector fields U and W

$$dJ(\Omega; U) \text{ and } d^2J(\Omega; U; W). \tag{37}$$

For the Shape gradient the two expressions coincide; for the Shape Hessian we recognize the bilinear term in (36) and (37) but the two expressions differ by the term

$$dJ(\Omega; A - [DU]U). \tag{38}$$

Even for a first order perturbation ($A = 0$), we have a quadratic term in U. This situation is analogous to the classical problem of defining second order derivatives on a manifold. The term (38) would correspond to the connexion while the bilinear term $d^2J(\Omega; V; W)$ would be the candidate for the *canonical* second order shape derivative. In this context we shall refer to the corresponding distribution $H(\Omega)$ as the *canonical Shape Hessian*. All other second order shape derivatives will be obtained from $H(\Omega)$ by adding the gradient term $G(\Omega)$ acting as the appropriate acceleration field (connexion).

REMARK 4.5. The method of perturbation of the identity can be made *more canonical* by using the following family of transformations

$$T_t(X) = X + tU(X) + \frac{t^2}{2}(A + [DU]U) \tag{39}$$

which yields

$$dJ(\Omega; U) \text{ for the gradient} \tag{40}$$

and

$$d^2J(\Omega; U; W) + dJ(\Omega; A) \text{ for the Hessian,} \tag{41}$$

where for a first order perturbation ($A = 0$) the second term disappears.□

REMARK 4.6. When Ω^* is an appropriately smooth domain which minimizes a twice shape differentiable functional $J(\Omega)$ without constraints on Ω, the classical necessary conditions would be (at least formally)

$$dJ(\Omega^*; V) = 0, \;\; \forall V, \tag{42}$$

$$d^2J(\Omega^*; W; W) \geq 0, \;\; \forall W, \tag{43}$$

or equivalently for "smooth velocity fields V and W"

$$dJ(\Omega^*; V(0)) = 0, \;\; \forall V \tag{44}$$

$$d^2J(\Omega^*; W(0); W(0)) + dJ(\Omega^*; \dot{V}(0)) \geq 0, \;\; \forall W. \tag{45}$$

But in view of (44), condition (45) reduces to the following condition on the canonical Shape Hessian

$$d^2J(\Omega^*; W(0); W(0)) \geq 0, \;\; \forall W.\square \tag{46}$$

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