A SYSTEMATIC APPROACH TO SHAPE SENSITIVITY ANALYSIS†

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Abstract—A fully detailed development of the domain parameterization method is presented for shape sensitivity analysis. It is shown that equivalent results are obtained from the material derivative method. In fact, the material derivative method may be viewed as a special case of the domain parameterization method which occurs when the reference configuration coincides with the body configuration. The method is illustrated for the Laplace problem in which explicit shape sensitivities are derived by the adjoint and direct differentiation methods. Both finite element and boundary element applications are discussed. The similarities between this approach and the isoparametric finite/boundary element method are transparent. In the finite element approach, it is shown that the sensitivity integrals may be transformed to the boundary (as is commonly done in the material derivative method) for the adjoint method, however, this does not seem possible for the direct differentiation method. Finally, in the boundary element approach, the sensitivities do not require the differentiation of the fundamental solutions.

1. INTRODUCTION

In "conventional" design sensitivity analyses, derivatives of response measures are evaluated with respect to design parameters which describe the physical and material properties of the domain and the loads and boundary conditions. For example, the derivative of the temperature at a point is determined with respect to the thermal conductivity of an isotropic homogeneous body. To derive these sensitivities, the variational equations which govern the system are differentiated with respect to the design parameters. Similarly, in a "shape" sensitivity analysis, the response derivatives are evaluated with respect to shape parameters which describe the geometry of the domain. Difficulties are encountered here when the governing variational equations are differentiated with respect to the shape parameters. In effect, we are differentiating integrals with respect to their region of integration. The problem is analogous to that encountered in Eulerian (spatial) motion descriptions where a control volume is introduced.

In the following, a systematic approach for shape sensitivity analysis is presented. The foundation of the approach is domain parameterization in which a reference configuration is introduced. All quantities which are defined over the body configuration are transformed to field quantities defined on the fixed reference configuration. This approach is commonly employed in finite elasticity to transform the governing equations to the undeformed configuration and in the isoparametric finite/boundary element methods to transform the governing equations to the parent element. To obtain the sensitivities, the mapping which relates the reference and body configurations is varied. The adjoint and direct differentiation approaches for sensitivity analysis may then be applied to derive the explicit sensitivities. Both of these approaches are utilized to derive shape sensitivities of the Laplace problem. It is shown that the material derivative method for shape sensitivity analysis may be viewed as a special case of the domain parameterization method which arises when the reference and body configurations coincide. Both finite element and boundary element analysis applications are discussed; and in the finite element technique, it is shown that for the

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adjoint derivation, the domain integrals may be transformed to the boundary as is done in the so called "boundary" approach of the material derivative method. However, the ability to convert domain integrals to boundary integrals in the direct approach does not seem plausible. The boundary element sensitivity expressions are naturally derived and do not require the differentiation of the fundamental solutions.

Domain parameterizations, there referred to as the image of a fixed domain, were briefly discussed by Cea (1981) as early as 1981. However, the method did not receive much attention, as the material derivative (or speed method), was primarily used to derive shape sensitivities throughout the eighties [for example see Cea (1981a,b), Zolesio (1981), Choi and Huag (1983), Dems and Mroz (1984), Haug et al. (1986), Arora et al. (1991) and Petryk and Mroz (1986)]. In 1987 Haber (1987) used the domain parameterization method and a mixed form of the mutual energy principle to evaluate explicit adjoint shape sensitivities for a linear elastostatic continuum. Since then, numerous other applications of the domain parameterization method for shape sensitivity analysis have appeared [cf. Cardoso and Arora (1988), Phelan et al. (1989), Tortorelli and Haber (1989), Tortorelli et al. (1990), Tortorelli et al. (1990, 1991), Tortorelli et al. (1991), Arora et al. (1991) and Phelan and Haber (1989)]. Comparisons between these methods are denoted in Tortorelli et al. (1991) and Arora et al. (1991). All of these studies utilized the finite element method to evaluate the system performance and the sensitivities. Shape sensitivities have also been derived using the boundary element method, via both the adjoint variable approach (Meric, 1988; Park and Yoo, 1988; Choi and Kwak, 1988a,b; Aithal and Saigal, 1990; Mota Soares et al., 1984) and the direct differentiation method (Barone and Yang, 1988, 1989; Zhang and Mukherjee, 1991; Zhao, 1991). These boundary element analyses relied on either the material derivative technique or differentiation of the discretized equations to evaluate the sensitivities.

In the following, a detailed formulation of the domain parameterization method is presented. First, a review of some necessary continuum mechanics concepts and results are noted, e.g. the body and reference configurations, norm, transpose, tensor product, trace, derivative, gradient, divergence, Laplacian, divergence theorem, composite map, change of variable theorem, Jacobian and its derivatives, etc. Most of the material is self contained, although we do cite the texts by Gurtin (1981) and Ciarlet (1988) for derivations of some well known relations. At this point, we proceed to transform quantities from the body to the reference configuration and take their variations with respect to design changes. Next, we derive explicit shape sensitivities for the Laplace problem and discuss finite element and boundary element approaches for evaluating the sensitivities. The direct differentiation and adjoint methods are used to derive the sensitivities. Then we compare the results of the domain parameterization and the material derivative methods. Finally an example problem is provided.

2. CONTINUUM MECHANICS REVIEW

An attempt has been made to use consistent notation throughout this article. Direct notation is employed with uppercase bold faced Latin symbols denoting second-order tensor fields, lower case bold faced Latin symbols denoting vector fields, and lower case Greek symbols denoting scalar fields, with the exceptions of the design variation vector φ and reference map function χ. Lower case and upper case openface symbols denote points in the body configuration b and reference configuration B, respectively. Calligraphic letters represent sets. The inner product, trace, tensor product, transpose, inverse, inverse transpose, determinant, norm, gradient and divergence operators are denoted by $\cdot$, tr, $\otimes$, $^{\mathrm{T}}$, $^{-1}$, $^{-\mathrm{T}}$, det, $\| \ \|$, ∇ and div. The $\times$ delineates the set product and the caret $\hat{\ }$ denotes referential field quantities, defined through the composition $\circ$. Lin $(\mathscr{A}, \mathscr{B})$ denotes the space of linear operators from $\mathscr{A}$ to $\mathscr{B}$ and $\mathscr{C}^n(\mathscr{A}, \mathscr{B})$ denotes the space of n times continuously differentiable functions from $\mathscr{A}$ to $\mathscr{B}$. Upper and lower case sans serif symbols are used to denote vectors in the reference and body configurations, respectively. In our examples we use indicial notation where subscripts denote components with respect to a Cartesian coordinate

system with basis vectors **e** and **E** in b and B, respectively. Finally, D denotes differentiation with respect to the subscripted argument.

Where possible, the following results have been specialized to hasten the derivations in the following sections.

2.1. *The body and reference configurations and reference map*

In the ensuing analysis, we consider a body comprised of particles. We identify the particles by the places which they occupy in two configurations, the *body configuration* and the *reference configuration*.

The body configuration is denoted by $b \subset \mathscr{E}^n$ where $\mathscr{E}^n$ is an n-dimensional Euclidean point space with the associated vector space $\mathscr{V}^n$. The body configuration is assumed to be a regular region in $\mathscr{E}^n$ with outward unit normal vector $\mathbf{n} \in \mathscr{V}^n$ on the bounding surface ∂b. Points in the body configuration are denoted by $x \in b$ and are defined by their coordinates relative to the rectangular Cartesian coordinate system $\{o; \mathbf{e}_i\}$, $i = 1, n$. In general, lower case symbols are reserved for quantities associated with the body configuration.

The reference configuration is denoted by $B \subset \mathscr{E}^N$ where $\mathscr{E}^N$ is an N-dimensional Euclidean point space with the associated vector space $\mathscr{V}^N$. The reference configuration is also assumed to be a regular region with outward unit normal vector $\mathbf{N} \in \mathscr{V}^N$ on the bounding surface ∂B. Points in the reference configuration are denoted by $\mathbb{X} \in B$ and are defined by their components relative to the rectangular Cartesian coordinate system $\{\mathbb{O}; \mathbf{E}_i\}$, $i = 1, N$. Upper-case symbols are reserved for quantities associated with the reference configuration. We require that $1 \leqslant N \leqslant n \leqslant 3$.

We define a referential function $\chi: B \to \mathscr{E}^n$ which maps the reference configuration onto the body configuration. This mapping may be thought of as the deformation which takes the undeformed reference configuration into the deformed configuration in elasticity. The present approach is also consistent with isoparametric finite and boundary element formulations where the reference configuration is the parent element. We insist that the mapping χ have the properties of a proper deformation, i.e. it is invertible, differentiable, and orientation preserving.

The Laplace problem which we study in the sequel is defined over the body configuration. The body configuration, in turn, is defined on the reference configuration through the mapping χ. Thus, the results of our analysis clearly depend on the mapping χ. The objective of the shape sensitivity analysis is to evaluate this dependence. It is imperative, then, to quantify the referential map's dependence on the design, to wit we redefine the map as $\chi_\Phi: B \times \mathscr{D}^M \to \mathscr{E}^n$. This definition is analogous to that of a motion in elasticity where $\Phi \in \mathscr{D}^M$ replaces time. $\mathscr{D}^M$ is a subset of the M-dimensional real number space $\mathscr{R}^M$ (i.e. $\mathscr{D}^M \subset \mathscr{R}^M$), and its elements are the design vectors Φ which contain the parameters that define the geometry. Note that $\mathscr{D}^M$ could be replaced by an infinite dimensional function space, however, we have selected a finite dimensional set to be consistent with numerical discretization schemes such as the finite and boundary element methods. Now the body configuration is expressed $b_\Phi = \chi_\Phi(B)$ to note its dependence on the design Φ. Other quantities defined over b_Φ e.g. x and $\mathbf{n}$, are not subscripted with Φ, however we emphasize that they too are functions of the design Φ.

For notational convenience, we define $\chi(\mathbb{X}, \Phi) = \chi_\Phi(\mathbb{X})$ and write $x = \chi(\mathbb{X}, \Phi)$. Then $b_\Phi = \chi(B, \Phi)$ and we define the *design trajectory* as the set of pairs $\mathscr{T} = \{(x, \Phi): x \in b_\Phi, \Phi \in \mathscr{D}^M\}$. Again, analogies may be drawn between the definition of the design trajectory and the trajectory used in continuum mechanics. Here the design Φ replaces time. In essence, the design trajectory is the set of body configurations which is spanned by the design space.

Two examples of the mapping are illustrated in Figs 1 and 2. In the first example (Cea, 1981), $N = n = 2$ and the design Φ is an element of an infinite dimensional function space $\mathscr{D}$. The reference domain is the set of ordered pairs $B = \{(\mathbb{X}_1, \mathbb{X}_2) \in \mathscr{R}^2: 0 \leqslant \mathbb{X}_1 \leqslant 1$ and $0 \leqslant \mathbb{X}_2 \leqslant 1\}$; and the map $\chi: B \times \mathscr{D} \to \mathscr{E}^2$ is subsequently defined by the components

$$x_1 = \mathbb{X}_1,$$
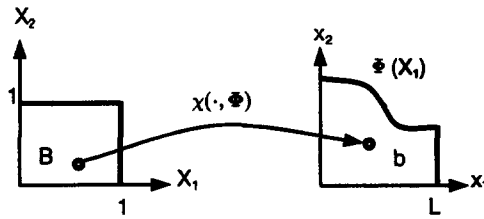
$$x_2 = \mathbb{X}_2 \Phi(\mathbb{X}_1), \tag{1}$$

Fig. 1. Mapping from 2-dimensions to 2-dimensions.

where the position vectors of x and $\mathbb{X}$ are given by $\Sigma_{i=1}^{2} x_i\mathbf{e}_i$ and $\Sigma_{i=1}^{2} \mathbb{X}_i\mathbf{E}_i$, respectively.

In the second example the isoparametric map of a three-dimensional continuum boundary element is used. The reference domain, or parent element, is the set of ordered pairs $B = \{(\mathbb{X}_1, \mathbb{X}_2) \in \mathscr{R}^2 : -1 \leqslant \mathbb{X}_1 \leqslant 1 \text{ and } -1 \leqslant \mathbb{X}_1 \leqslant 1\}$ and $\chi : B \times \mathscr{D}^{24} \to \mathscr{E}^3$ is locally defined by the components

$$x_1 = \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)x_1^I,$$

$$x_2 = \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)x_2^I,$$

$$x_3 = \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)x_3^I, \tag{2}$$

where the position vectors of x and $\mathbb{X}$ are given respectively by $x = \Sigma_{i=1}^{3} x_i\mathbf{e}_i$ and $\mathbb{X} = \Sigma_{i=1}^{2} \mathbb{X}_i\mathbf{E}_i$. In the above, x_i^J denotes the ith component of the Jth node and $\Psi^I : B \to \mathscr{R}$ is the Ith element shape (interpolation) function. Here $N = 2$ while $n = 3$ and the design parameter vector is the element node coordinate vector $\mathbf{\Phi} = (x_1^1, x_2^1, x_3^1, x_1^2, x_2^2, x_3^2, \dots, x_1^8, x_2^8, x_3^8) \in \mathscr{D}^{24}$. This latter finite dimensional example will be referenced occasionally throughout the article.

2.2. The norm, tensor product, transpose and trace

The norm, tensor product, transpose and trace yield unique quantities defined through their respective operations. The trace, transpose and inner product also possess several properties which we draw on for the ensuing sensitivity analyses. The definitions are given in direct notation. Where deemed appropriate complementary indicial notation definitions are supplied; we recall our restriction to orthonormal basis vectors.

Given the vector $\mathbf{a} \in \mathscr{V}^n$, then the *norm* $\|\mathbf{a}\| \in \mathscr{R}$ is defined as [cf. Gurtin (1981)]
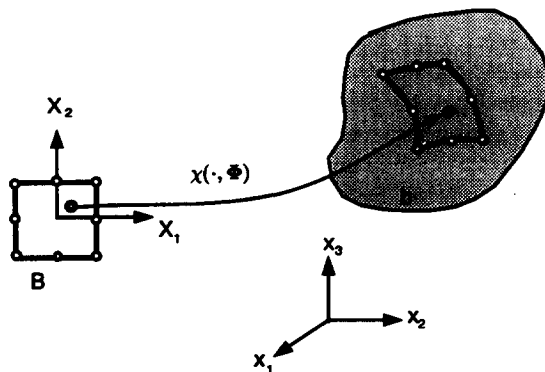

Fig. 2. Mapping from 2-dimensions to 3-dimensions.

$$\|\mathbf{a}\| = (\mathbf{a} \cdot \mathbf{a})^{1/2}, \quad \|\mathbf{a}\| = \left(\sum_{i=1}^{n} a_i a_i\right)^{1/2}, \tag{3}$$

where $\cdot$ denotes the vector inner product operator [cf. Gurtin (1981)].

The *tensor product* of the vectors $\mathbf{a}, \mathbf{b} \in \mathscr{V}^n$ defines the tensor $\mathbf{a} \otimes \mathbf{b} \in \text{Lin}(\mathscr{V}^n, \mathscr{V}^n)$ such that

$$(\mathbf{a} \otimes \mathbf{b})\mathbf{c} = (\mathbf{b} \cdot \mathbf{c})\mathbf{a}, \quad (\mathbf{a} \otimes \mathbf{b})_{ij} = a_i b_j, \tag{4}$$

for all $\mathbf{c} \in \mathscr{V}^n$ [cf. Gurtin (1981)].

Given the vectors $\mathbf{a}, \mathbf{b} \in \mathscr{V}^n$ and the second-order tensor $\mathbf{A} \in \text{Lin}(\mathscr{V}^n, \mathscr{V}^n)$, then the *transpose* $\mathbf{A}^T \in \text{Lin}(\mathscr{V}^n, \mathscr{V}^n)$ is defined via [cf. Gurtin (1981), p. 3]

$$\mathbf{a} \cdot \mathbf{A}\mathbf{b} = \mathbf{A}^T \mathbf{a} \cdot \mathbf{b}. \tag{5}$$

Given the tensor $\mathbf{A} \in \text{Lin}(\mathscr{V}^n, \mathscr{V}^n)$ and the vectors $\mathbf{a}, \mathbf{b} \in \mathscr{V}^n$, then the *trace* $\text{tr}(\mathbf{A}) \in \mathscr{R}$ is defined through the relation [cf. Gurtin (1981)]

$$\text{tr}(\mathbf{a} \otimes \mathbf{b}) = \mathbf{a} \cdot \mathbf{b}, \quad \text{tr}(\mathbf{A}) = \sum_{i=1}^{n} A_{ii}. \tag{6}$$

The inner product of the tensors $\mathbf{A}, \mathbf{B} \in \text{Lin}(\mathscr{V}^n, \mathscr{V}^n)$ is defined through

$$\mathbf{A} \cdot \mathbf{B} = \text{tr}(\mathbf{A}^T \mathbf{B}), \quad \mathbf{A} \cdot \mathbf{B} = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ij}, \tag{7}$$

[cf. Gurtin (1981)].

Given the tensors $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \text{Lin}(\mathscr{V}^n, \mathscr{V}^n)$, it may be shown that the transpose, trace and inner product yield the following relations which appear in Gurtin (1981):

$$\text{tr}(\mathbf{A}) = \mathbf{A} \cdot \mathbf{I},$$
$$\text{tr}(\mathbf{A}) = \text{tr}(\mathbf{A}^T),$$
$$\text{tr}(\mathbf{A}\mathbf{B}) = \text{tr}(\mathbf{B}\mathbf{A}),$$
$$\mathbf{A} \cdot (\mathbf{B}\mathbf{C}) = (\mathbf{B}^T \mathbf{A}) \cdot \mathbf{C} = (\mathbf{A}\mathbf{C}^T) \cdot \mathbf{B},$$
$$(\mathbf{A}\mathbf{B})^T = \mathbf{B}^T \mathbf{A}^T, \tag{8}$$

where $\mathbf{I}$ is the identity tensor [cf. Gurtin (1981)].

2.3. *The derivative, gradient, variation, divergence, Laplacian and partial derivative*

In our derivations we require the derivative, second derivative, partial derivative, variation, gradient, divergence and Laplacian of scalar, vector and tensor fields. For completeness we choose to review these definitions. Throughout this section $\mathbf{A}$, $\mathbf{a}$ and α denote tensor, vector and scalar valued functions on $b_\oplus$; $\hat{\mathbf{A}}$, $\hat{\mathbf{a}}$ and $\hat{\alpha}$ denote tensor, vector and scalar valued functions on $B \times \mathscr{D}^M$; and the notation of the previous section is enforced. The following represent elements of their noted sets $\mathbf{u}, \mathbf{v} \in \mathscr{V}^n$, $\mathbf{U} \in \mathscr{V}^N$, and $\varphi \in \mathscr{D}^M$. In all cases we assume that the functions are sufficiently smooth to perform the indicated operations. The derivatives are defined on the open interiors of the sets, denoted by ($^\circ$); we assume that extensions to the set boundaries $\partial(\ )$ are possible.

Given the function $\alpha: b_\oplus^\circ \to \mathscr{R}$, the *derivative* at $\mathbf{x}$ is the linear operator $D\alpha(\mathbf{x}) \in \text{Lin}(\mathscr{V}^n, \mathscr{R})$ such that

$$D\alpha(x)u = \alpha(x+u) - \alpha(x) + o(u), \tag{9}$$

where $o(u)$ tends to zero faster than u. Thus, $D\alpha: b_{\Phi}^{\circ} \rightarrow \text{Lin}(\mathcal{V}^n, \mathcal{R})$. In essence, the derivative is a linear map which approximates the difference $\alpha(x+u) - \alpha(x)$ for small $\|u\|$. If the derivative exists and is continuous for all $x \in b_{\Phi}^{\circ}$ then we say that α belongs to the set of continuously differentiable functions, i.e. $\alpha \in \mathcal{C}^1(b_{\Phi}^{\circ}, \mathcal{R})$. [See Gurtin (1981) for additional discussion.] Similar definitions apply to vector and tensor fields.

If $\mathbf{a}$ maps into the vector space $\mathcal{V}^n$, i.e. if $\mathbf{a} \in \mathcal{C}^1(b_{\Phi}^{\circ}, \mathcal{V}^n)$, then the derivative defines a second-order tensor, i.e. $D\mathbf{a}(x) \in \text{Lin}(\mathcal{V}^n, \mathcal{V}^n)$. Where we recall that $\mathcal{V}^n$ is the vector field associated with b_{Φ}.

Considering the derivative $D\alpha: b_{\Phi}^{\circ} \rightarrow \text{Lin}(\mathcal{V}^n, \mathcal{R})$ as a function, we define the *second derivative* (Ciarlet, 1988) $D^2\alpha: b_{\Phi}^{\circ} \rightarrow \text{Lin}(\mathcal{V}^n, \text{Lin}(\mathcal{V}^n, \mathcal{R}))$ through

$$D^2\alpha(x) = DD\alpha(x). \tag{10}$$

If the second derivative exists and is continuous for all $x \in b_{\Phi}^{\circ}$ then we say that α belongs to the set of twice continuously differentiable functions, i.e. $\alpha \in \mathcal{C}^2(b_{\Phi}^{\circ}, \mathcal{R})$. It may be shown that $D^2\alpha(x): \mathcal{V}^n \times \mathcal{V}^n \rightarrow \mathcal{R}$ is a bilinear operator such that (Ciarlet, 1988)

$$D^2\alpha(x)(u, v) = (DD\alpha(x)u)v. \tag{11}$$

Similar definitions apply to vector and tensor fields. So the second derivative approximates the difference of the derivative, i.e. $D\alpha(x+v)u - D\alpha(x)u$ for small $\|u\|$ and $\|v\|$. We also note the symmetry of the second derivative (Ciarlet, 1988)

$$D^2\alpha(x)(u, v) = D^2\alpha(x)(v, u). \tag{12}$$

If $\alpha \in \mathcal{C}^1(b_{\Phi}^{\circ}, \mathcal{R})$ then α has the *variation* or *directional derivative* $\delta\alpha$ which is defined through (Ciarlet, 1988)

$$\delta\alpha(x; u) = D\alpha(x)u, \tag{13}$$

for all $u \in \mathcal{V}^n$. Thus, for the differentiable function α, the variation $\delta\alpha(x; u) \in \mathcal{R}$ equals the derivative acting on the increment u.†

For every linear scalar valued function, i.e. linear functional $\psi \in \text{Lin}(\mathcal{V}^n, \mathcal{R})$, the representation theorem for linear forms ensures the existence of a unique vector $\mathbf{a} \in \mathcal{V}^n$ such that $\psi(u) = \mathbf{a} \cdot u$ for any vector $u \in \mathcal{V}^n$ (Gurtin, 1981). Armed with this theorem and noting that $D\alpha(x) \in \text{Lin}(\mathcal{V}^n, \mathcal{R})$, we define the *gradient* $\nabla\alpha: b_{\Phi}^{\circ} \rightarrow \mathcal{V}^n$ through

$$\nabla\alpha(x) \cdot u = D\alpha(x)u \tag{14}$$

[see Gurtin (1981)]

The *divergence* div $\mathbf{a}: b_{\Phi}^{\circ} \rightarrow \mathcal{R}$ of the vector field $\mathbf{a} \in \mathcal{C}^1(b_{\Phi}^{\circ}, \mathcal{V}^n)$ is defined as (Gurtin, 1981)

$$\text{div } \mathbf{a}(x) = \text{tr } D\mathbf{a}(x). \tag{15}$$

The *divergence* div $\mathbf{A}: b_{\Phi}^{\circ} \rightarrow \mathcal{V}^n$ of a differentiable tensor field $\mathbf{A} \in \mathcal{C}^1(b_{\Phi}^{\circ}, \text{Lin}(\mathcal{V}^n, \mathcal{V}^n))$ is defined through (Gurtin, 1981)

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† We note that the variation is actually defined through the limit process, is not necessarily a linear operator, and may exist even if the derivative does not exist (Ciarlet, 1988). In the forthcoming analysis we limit ourselves to differentiable functions, so the above, over restrictive, definition suffices.

$$\text{div } A(x) \cdot u = \text{div } (A^T(x)u) \tag{16}$$

for all constant vectors $u \in \mathscr{V}^n$.

The *Laplacian* $\Delta\alpha: b_\Phi^\circ \to \mathscr{R}$ of a twice differentiable scalar field $\alpha \in \mathscr{C}^2(b_\Phi^\circ, \mathscr{R})$ is defined as (Gurtin, 1981)

$$\Delta\alpha(x) = \text{div } \nabla\alpha(x). \tag{17}$$

Next we define the partial derivative and its properties for the referential fields. As our referential functions are defined over the set product of the domain B and the design field $\mathscr{D}^M$, i.e. $B \times \mathscr{D}^M$, we require the use of the partial derivative. Formally, given the differentiable function $\hat{\alpha} \in \mathscr{C}^1(B^\circ \times \mathscr{D}^{\circ M}, \mathscr{R})$, we define the *partial derivatives* with respect to $\mathbb{X}$ and Φ (the first and second arguments) respectively, by (Ciarlet, 1988)

$$D_1\hat{\alpha}(\mathbb{X}, \Phi)U = D\hat{\alpha}(\mathbb{X}, \Phi)(U, 0),$$
$$D_2\hat{\alpha}(\mathbb{X}, \Phi)\varphi = D\hat{\alpha}(\mathbb{X}, \Phi)(0, \varphi), \tag{18}$$

hence, $D_1\hat{\alpha}: B^\circ \times \mathscr{D}^M \to \text{Lin } (\mathscr{V}^N, \mathscr{R})$ and $D_2\hat{\alpha}: B^\circ \times \mathscr{D}^M \to \text{Lin } (\mathscr{D}^M, \mathscr{R})$ (Ciarlet, 1988). The linearity of the derivative then yields (Ciarlet, 1988)

$$D\hat{\alpha}(\mathbb{X}, \Phi)(U, \varphi) = D_1\hat{\alpha}(\mathbb{X}, \Phi)U + D_2\hat{\alpha}(\mathbb{X}, \Phi)\varphi. \tag{19}$$

Similar definitions apply to vector and tensor valued functions.

We define the function $D_1D_2\hat{\alpha}: B^\circ \times \mathscr{D}^{\circ M} \to \text{Lin } (\mathscr{V}^N, \text{Lin } (\mathscr{D}^M, \mathscr{R}))$ in a similar fashion to the second derivative, and it has the property that

$$D_1D_2\hat{\alpha}(\mathbb{X}, \Phi)(U, \varphi) = (D_1D_2\hat{\alpha}(\mathbb{X}, \Phi)\varphi)U, \tag{20}$$

so that $D_1D_2\hat{\alpha}(\mathbb{X}, \Phi)$ approximates the difference $D_2\hat{\alpha}(\mathbb{X}+U, \Phi)\varphi - D_2\hat{\alpha}(\mathbb{X}, \Phi)\varphi$ for small $\|U\|$ and $\|\varphi\|$. Finally, like the second derivative, $D_1D_2\hat{\alpha}$ is bilinear and exhibits the symmetry

$$D_1D_2\hat{\alpha}(\mathbb{X}, \Phi)(U, \varphi) = D_2D_1\hat{\alpha}(\mathbb{X}, \Phi)(\varphi, U). \tag{21}$$

Again, similar definitions apply to vector and tensor valued functions.

The following *partial variation* and *partial gradient* are used in the sequel

$$\delta_2\hat{\alpha}(\mathbb{X}, \Phi; \varphi) = D_2\hat{\alpha}(\mathbb{X}, \Phi)\varphi,$$
$$\nabla_1\hat{\alpha}(X, \Phi) \cdot U = D_1\hat{\alpha}(\mathbb{X}, \Phi)U. \tag{22}$$

For the variation, similar definitions apply to vector and tensor valued functions. The *partial divergences* and *partial Laplacian* are defined through

$$\text{div}_1\hat{a}(X, \Phi) = \text{tr } D_1\hat{a}(X, \Phi),$$
$$\text{div}_1\hat{A}(X, \Phi) \cdot u = \text{div}_1(\hat{A}^T(X, \Phi)u),$$
$$\Delta_1\hat{\alpha}(X, \Phi) = \text{div}_1\nabla_1\hat{\alpha}(\mathbb{X}, \Phi), \tag{23}$$

where $\hat{\alpha} \in \mathscr{C}^1(B^\circ \times \mathscr{D}^{\circ M}, \mathscr{R})$, $\hat{a} \in \mathscr{C}^1(B^\circ \times \mathscr{D}^{\circ M}, \mathscr{V}^n)$, and $\hat{A} \in \mathscr{C}^1(B^\circ \times \mathscr{D}^{\circ M}, \text{Lin } (\mathscr{V}^N, \mathscr{V}^n))$.

2.4. *Elementary rules of differentiation*

In this section, we present some elementary rules of differentiation. All notational agreements of the previous sections remain in effect.
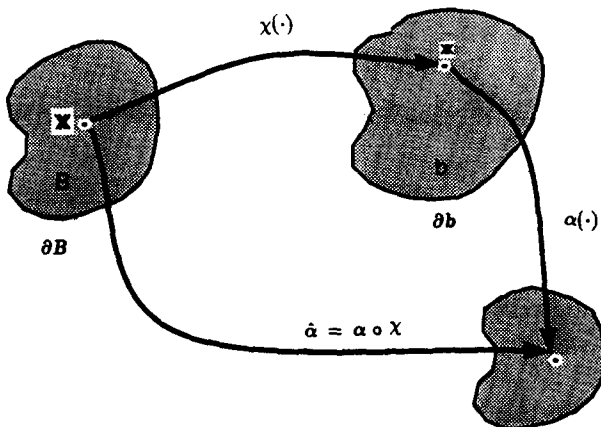
Fig. 3. Composite function.

Consider the differentiable maps $\alpha, \beta \in \mathscr{C}^1(b_\oplus^\circ, \mathscr{R})$, $\mathbf{a}, \mathbf{b} \in \mathscr{C}^1(b_\oplus^\circ, \mathscr{V}^n)$, and $\mathbf{A}, \mathbf{B} \in \mathscr{C}^1$ $(b_\oplus^\circ, \mathrm{Lin}\,(\mathscr{V}^n, \mathscr{V}^n))$ then it may be shown by the product rule of differentiation (Gurtin, 1981) that

$$D(\alpha(x)\mathbf{a}(x))\mathbf{u} = D\alpha(x)\mathbf{u}\mathbf{a}(x) + \alpha(x)D\mathbf{a}(x)\mathbf{u},$$

$$D(\alpha(x)\mathbf{A}(x))\mathbf{u} = D\alpha(x)\mathbf{u}\mathbf{A}(x) + \alpha(x)D\mathbf{A}(x)\mathbf{u},$$

$$D(\mathbf{A}(x)\mathbf{a}(x))\mathbf{u} = D\mathbf{A}(x)\mathbf{u}\mathbf{a}(x) + \mathbf{A}(x)D\mathbf{a}(x)\mathbf{u},$$

$$D(\mathbf{A}(x)\mathbf{B}(x))\mathbf{u} = D\mathbf{A}(x)\mathbf{u}\mathbf{B}(x) + \mathbf{A}(x)D\mathbf{B}(x)\mathbf{u}. \tag{24}$$

Using the above definitions for α, $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{A}$, the following relations may be verified (Gurtin, 1981):

$$\mathrm{div}\,(\alpha(x)\mathbf{a}(x)) = \alpha(x)\,\mathrm{div}\,\mathbf{a}(x) + \mathbf{a}(x) \cdot \nabla\alpha(x),$$

$$\mathrm{div}\,(\mathbf{A}^T(x)\mathbf{a}(x)) = \mathbf{A}(x) \cdot D\mathbf{a}(x) + \mathbf{a}(x) \cdot \mathrm{div}\,\mathbf{A}(x),$$

$$\mathrm{div}\,(\alpha(x)\mathbf{A}(x)) = \alpha(x)\,\mathrm{div}\,\mathbf{A}(x) + \mathbf{A}(x)\nabla\alpha(x),$$

$$\nabla(\mathbf{a}(x) \cdot \mathbf{b}(x)) = (D\mathbf{b}(x))^T\mathbf{a}(x) + (D\mathbf{a}(x))^T\mathbf{b}(x),$$

$$\nabla(\alpha(x)\beta(x)) = \beta(x)\nabla\alpha(x) + \alpha(x)\nabla\beta(x). \tag{25}$$

2.5. The composition, chain rule and Jacobian

To transform the governing equations from the body to the reference configuration we use composite functions.

Temporarily excluding the design from the domain, we consider the *composite* function (see Fig. 3) $\hat{\alpha}: B \to \mathscr{R}$ defined by $\hat{\alpha} = \alpha \circ \chi$ so that

$$\hat{\alpha}(X) = \alpha(\chi(X)), \tag{26}$$

where $\alpha \in \mathscr{C}^1(b_\oplus, \mathscr{R})$ and $\chi \in \mathscr{C}^1(B, \mathscr{E}^n)$ are both differentiable. Then by the *chain rule* of *differentiation* (Gurtin, 1981) for any $U \in \mathscr{V}^N$,

$$D\hat{\alpha}(X)U = D\alpha(\chi(X)) \circ D\chi(X)U$$

$$= D\alpha(\chi(X))(D\chi(X)U), \tag{27}$$

where $X \in B^\circ$. Similar results are obtained for vector and tensor valued functions on $b_\oplus$.
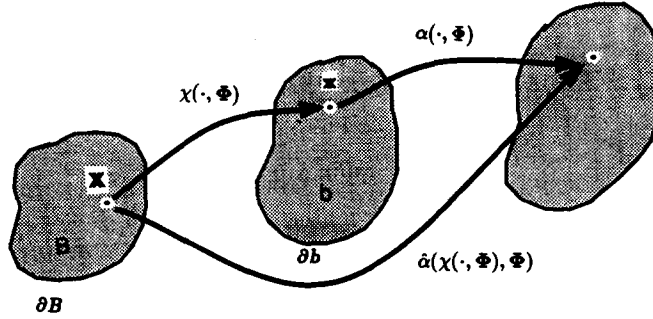
Fig. 4. Composite function.

Now we customize the result for our applications where we note the design's dependence on the functions $\alpha: \mathcal{T} \to \mathcal{R}$, $\hat{\alpha}: B \times \mathcal{D}^M \to \mathcal{R}$, and $\chi: B \times \mathcal{D}^M \to \mathcal{E}^n$. Then for $\mathbb{x} = \chi(\mathbb{X}, \Phi)$ the composite like function (see Fig. 4)

$$\hat{\alpha}(\mathbb{X}, \Phi) = \alpha(\chi(\mathbb{X}, \Phi), \Phi) \tag{28}$$

is differentiable. To evaluate the derivatives, we define the functions $g_1: B \to \mathcal{E}^n$, $g_2: \mathcal{D}^M \to \mathcal{E}^n$, $h_1: B \to \mathcal{E}^n$, and $h_2: \mathcal{D}^M \to \mathcal{E}^n$:

$$g_1(\mathbb{X}) = \chi(\mathbb{X}, \Phi),$$

$$g_2(\Phi) = \chi(\mathbb{X}, \Phi),$$

$$h_1(\mathbb{X}) = \Phi,$$

$$h_2(\Phi) = \Phi,$$

and their derivatives

$$Dg_1(\mathbb{X})\mathbf{U} = D_1\chi(\mathbb{X}, \Phi)\mathbf{U},$$

$$Dg_2(\Phi)\varphi = D_2\chi(\mathbb{X}, \Phi)\varphi,$$

$$Dh_1(\mathbb{X})\mathbf{U} = 0,$$

$$Dh_2(\Phi)\varphi = \varphi,$$

where we use eqn (19) and note the independence between $\mathbb{X}$ and Φ to derive the above. Using the above relations and eqns (19), (22) and (27) we obtain the following relations:

$$D_1\hat{\alpha}(\mathbb{X}, \Phi)\mathbf{U} = D_1\alpha(g_1(\mathbb{X}), h_1(\mathbb{X}))(Dg_1(\mathbb{X})\mathbf{U}) + D_2\alpha(g_1(\mathbb{X}), h_1(\mathbb{X}))(Dh_1(\mathbb{X})\mathbf{U})$$

$$= D_1\alpha(\chi(\mathbb{X}, \Phi), \Phi)(D_1\chi(\mathbb{X}, \Phi)\mathbf{U})$$

$$= \nabla_1\alpha(\chi(\mathbb{X}, \Phi), \Phi) \cdot D_1\chi(\mathbb{X}, \Phi)\mathbf{U},$$

$$D_2\hat{\alpha}(\mathbb{X}, \Phi)\varphi = D_1\alpha(g_2(\Phi), h_2(\Phi))(Dg_2(\Phi)\varphi) + D_2\alpha(g_2(\Phi), h_2(\Phi))(Dh_2(\Phi)\varphi)$$

$$= D_1\alpha(\chi(\mathbb{X}, \Phi), \Phi)(D_2\chi(\mathbb{X}, \Phi)\varphi) + D_2\alpha(\chi(\mathbb{X}, \Phi), \Phi)\varphi$$

$$= \nabla_1\alpha(\chi(\mathbb{X}, \Phi), \Phi) \cdot D_2\chi(\mathbb{X}, \Phi)\varphi + \nabla_2\alpha(\chi(\mathbb{X}, \Phi), \Phi) \cdot \varphi. \tag{29}$$

Again, drawing analogies from continuum mechanics, we note that $D_2\hat{\alpha}(\mathbb{X}, \Phi)\varphi$ resembles the material derivative for spatial fields, where time and Φ are interchanged (Gurtin, 1981). In the sequel, the caret ^ always indicates composite functions defined as above [eqn (28)].

Since all of our composite functions use χ, for convenience, we define the *Jacobian* $\mathbf{J}: B \times \mathcal{D}^M \to \text{Lin}(\mathcal{V}^N, \mathcal{V}^n)$ as

$$\mathbf{J}(\mathbb{X}, \boldsymbol{\Phi}) = D_1 \chi(\mathbb{X}, \boldsymbol{\Phi}) \tag{30}$$

and the *determinant of the Jacobian* as

$$J(\mathbb{X}, \boldsymbol{\Phi}) = \det \mathbf{J}(\mathbb{X}, \boldsymbol{\Phi}), \tag{31}$$

where det denotes the determinant (Gurtin, 1981).

The determinant only makes sense if $N = n$. However, this does not present a problem as we may always redefine the map so that $N = n$ (DoCarmo, 1976). For our example problem [eqn (2)] one possible modification yields $\chi : (B \times \{\mathcal{R}\}) \times \mathcal{D}^{24} \to \mathcal{E}^n$:

$$\mathbb{x}_1 = \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_1',$$

$$\mathbb{x}_2 = \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_2',$$

$$\mathbb{x}_3 = \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_3' + \mathbb{X}_3, \tag{32}$$

where $\mathbb{X}_3$ is equated to zero and $(\mathbb{X}_1, \mathbb{X}_2) \in B \subset \mathcal{R}^2$. Likewise, any other functions defined on B, are redefined on $(B \times \{\mathcal{R}\})$, for the example illustrated in Fig. 2, $\hat{a}(\mathbb{X}_1, \mathbb{X}_2, \mathbb{X}_3) = \hat{a}(\mathbb{X}_1, \mathbb{X}_2)$. This modified example map χ will be used in the sequel. Note that problems for which $n \neq N$ may also be solved using manifold theory as described in Rousselet (1991).

For our example [eqn (32)],

$$[\mathbf{J}(\mathbb{X}, \boldsymbol{\Phi})] = \begin{bmatrix} \sum_{I=1}^{8} \nabla_1 \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_1' & \sum_{I=1}^{8} \nabla_2 \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_1' & 0 \\ \sum_{I=1}^{8} \nabla_1 \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_2' & \sum_{I=1}^{8} \nabla_2 \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_2' & 0 \\ \sum_{I=1}^{8} \nabla_1 \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_3' & \sum_{I=1}^{8} \nabla_2 \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\mathbb{x}_3' & 1 \end{bmatrix},$$

$$\{\delta_2 \chi(\mathbb{X}, \boldsymbol{\Phi}; \varphi)\} = \left\{ \begin{array}{c} \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\delta\mathbb{x}_1' \\ \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\delta\mathbb{x}_2' \\ \sum_{I=1}^{8} \Psi^I(\mathbb{X}_1, \mathbb{X}_2)\delta\mathbb{x}_3' \end{array} \right\}, \tag{33}$$

where $\varphi = (\delta\mathbb{x}_1^1, \delta\mathbb{x}_2^1, \delta\mathbb{x}_3^1, \delta\mathbb{x}_1^2, \delta\mathbb{x}_2^2, \delta\mathbb{x}_3^2, \ldots, \delta\mathbb{x}_1^8, \delta\mathbb{x}_2^8, \delta\mathbb{x}_3^8)$ for each element and represents perturbations of the node coordinates.

2.6. The divergence theorem and change of variable theorem

Here we review some integral theorems, namely the divergence theorem which is used in variational formulations and the change of variable theorem which is used to transform integrals from the body to the reference configuration.

Consider the differentiable functions $\alpha : \mathcal{T} \to \mathcal{R}$, $\mathbf{a} : \mathcal{T} \to \mathcal{V}^n$, and $\mathbf{A} : \mathcal{T} \to$ Lin $(\mathcal{V}^n, \mathcal{V}^n)$, then by the *divergence theorem* (Gurtin, 1981):

$$\int_{\partial b_\Phi} \alpha(\mathbf{x}, \Phi) \mathbf{n}(\mathbf{x}, \Phi) \, da_\mathbf{x} = \int_{b_\Phi} \nabla_1 \alpha(\mathbf{x}, \Phi) \, dv_\mathbf{x},$$

$$\int_{\partial b_\Phi} \mathbf{a}(\mathbf{x}, \Phi) \cdot \mathbf{n}(\mathbf{x}, \Phi) \, da_\mathbf{x} = \int_{b_\Phi} \mathrm{div}_1 \, \mathbf{a}(\mathbf{x}, \Phi) \, dv_\mathbf{x}, \quad \text{and}$$

$$\int_{\partial b_\Phi} \mathbf{A}(\mathbf{x}) \mathbf{n}(\mathbf{x}) \, da_\mathbf{x} = \int_{b_\Phi} \mathrm{div}_1 \, \mathbf{A}(\mathbf{x}) \, dv_\mathbf{x}, \tag{34}$$

where $\mathbf{n}(\mathbf{x}, \Phi)$ is the normal vector at the point $\mathbf{x}$ to the body surface ∂b_Φ; and $da_\mathbf{x}$ and $dv_\mathbf{x}$ represent differential elements in ∂b_Φ and b_Φ.

Given $\chi: B \times \mathcal{D}^M \to \mathcal{E}^n$ and the above definition for α, then by the *change of variable theorem* (Gurtin, 1981):

$$\int_{\chi(B,\Phi)} \alpha(\mathbf{x}, \Phi) \, dv_\mathbf{x} = \int_B \alpha(\chi(\mathbb{X}, \Phi), \Phi) J(\mathbb{X}, \Phi) \, dv_\mathbf{x} = \int_B \hat{\alpha}(\mathbb{X}, \Phi) J(\mathbb{X}, \Phi) \, dv_\mathbf{x}, \tag{35}$$

where $dv_\mathbf{x}$ is an elemental volume of B. Recall from Section 2.1 that $b_\Phi = \chi(B, \Phi)$ is the image of B under χ for the design Φ. Thus, this equation equates integrals in b_Φ to B. Similarly,

$$\int_{\partial \chi(B,\Phi)} \alpha(\mathbf{x}, \Phi) \, da_\mathbf{x} = \int_{\partial B} \alpha(\chi(\mathbb{X}, \Phi), \Phi) K(\mathbb{X}, \Phi) \, da_\mathbf{x} = \int_{\partial B} \hat{\alpha}(\mathbb{X}, \Phi) K(\mathbb{X}, \Phi) \, da_\mathbf{x}, \tag{36}$$

where $da_\mathbf{x}$ is an elemental volume of ∂B and $K(\mathbb{X}, \Phi) = J(\mathbb{X}, \Phi) \| \mathbf{J}^{-T}(\mathbb{X}, \Phi) \mathbf{N}(\mathbb{X}) \|$ (cf. Section 3.4). Finally note that the previous two relations are applicable to vector and tensor valued functions.

2.7. *Special derivatives*

Eventually, we require the design variations of the Jacobian $\mathbf{J}$, its inverse $\mathbf{J}^{-1}$, their transposes, and its determinant J. Some of these results require the condition that $N = n$, which we assume holds henceforth. However, this is not a restriction, as we may always modify the map so that $N = n$ as exemplified above [eqn (32)]. Of course, for the inverse $\mathbf{J}^{-1}$ to exist we assume that $\mathbf{J}$ is nonsingular, i.e. its determinant is nonzero and/or the columns of the matrix $\mathbf{J}$ are linearly independent, this condition is ensured if the mapping χ is invertible as previously discussed.

For $\mathbf{J}: B \times \mathcal{D}^M \to \mathrm{Lin}\,(\mathcal{V}^N, \mathcal{V}^n)$ we may readily verify that its design variation is given by the spatial gradient of the design variation of χ, i.e. $\delta_2 \mathbf{J} = D_1 \delta_2 \chi$. Indeed, by the symmetry of the partial derivative, the arbitrariness $\mathbf{U}$, and the definitions of the variation and Jacobian [cf. eqns (20), (22$_1$), (30)] we arrive at

$$(D_2 D_1 \chi(\mathbb{X}, \Phi) \mathbf{U}) \varphi = (D_1 D_2 \chi(\mathbb{X}, \Phi) \varphi) \mathbf{U},$$

$$D_2 (\mathbf{J}(\mathbb{X}, \Phi) \mathbf{U}) \varphi = D_1 \delta_2 \chi(\mathbb{X}, \Phi; \varphi) \mathbf{U},$$

$$\delta_2 \mathbf{J}(\mathbb{X}, \Phi; \varphi) \mathbf{U} = D_1 \delta_2 \chi(\mathbb{X}, \Phi; \varphi) \mathbf{U},$$

$$\delta_2 \mathbf{J}(\mathbb{X}, \Phi; \varphi) = D_1 \delta_2 \chi(\mathbb{X}, \Phi; \varphi). \tag{37}$$

For our example, a direct calculation on eqn (33) yields

$$\delta_2 J(\mathbb{X}, \mathbf{\Phi}; \varphi) = D_1 \delta_2 \chi(\mathbb{X}, \mathbf{\Phi}; \varphi)$$

$$= \begin{bmatrix} \sum_{l=1}^{8} \nabla_1 \Psi^l(\mathbb{X}_1, \mathbb{X}_2) \delta x_1^l & \sum_{l=1}^{8} \nabla_2 \Psi^l(\mathbb{X}_1, \mathbb{X}_2) \delta x_1^l & 0 \\ \sum_{l=1}^{8} \nabla_1 \Psi^l(\mathbb{X}_1, \mathbb{X}_2) \delta x_2^l & \sum_{l=1}^{8} \nabla_2 \Psi^l(\mathbb{X}_1, \mathbb{X}_2) \delta x_2^l & 0 \\ \sum_{l=1}^{8} \nabla_1 \Psi^l(\mathbb{X}_1, \mathbb{X}_2) \delta x_3^l & \sum_{l=1}^{8} \nabla_2 \Psi^l(\mathbb{X}_1, \mathbb{X}_2) \delta x_3^l & 0 \end{bmatrix}. \tag{38}$$

By invoking the chain rule [eqn (27)], the linearity of the trace, and the above result [eqn (37)], it is easily verified that

$$\delta_2 J^T(\mathbb{X}, \mathbf{\Phi}; \varphi) = D_1 \delta_2 \chi^T(\mathbb{X}, \mathbf{\Phi}; \varphi). \tag{39}$$

This result of differentiation of the transpose also appears in Gurtin (1981).

To determine the design variation of J^{-1} we use the relation $J^{-1}J = I$ where $^{-1}$ denotes the inverse operator (Gurtin, 1981). Differentiation of this relation by the product rule, the chain rule, the definition of the variation, the previous result [eqns (24_6), (27_2), (22_1) and (37)] the invertibility of J, and the fact that I is constant gives

$$J^{-1}(\mathbb{X}, \mathbf{\Phi})J(\mathbb{X}, \mathbf{\Phi}) = I,$$

$$D_2 J^{-1}(\mathbb{X}, \mathbf{\Phi})\varphi J(\mathbb{X}, \mathbf{\Phi}) + J^{-1}(\mathbb{X}, \mathbf{\Phi})D_2 J(\mathbb{X}, \mathbf{\Phi})\varphi = 0,$$

$$D_2 J^{-1}(\mathbb{X}, \mathbf{\Phi})\varphi = -J^{-1}(\mathbb{X}, \mathbf{\Phi})D_2 J(\mathbb{X}, \mathbf{\Phi})\varphi J^{-1}(\mathbb{X}, \mathbf{\Phi}),$$

which leads to

$$\delta_2 J^{-1}(\mathbb{X}, \mathbf{\Phi}; \varphi) = -J^{-1}(\mathbb{X}, \mathbf{\Phi})D_1 \delta_2 \chi(\mathbb{X}, \mathbf{\Phi}; \varphi)J^{-1}(\mathbb{X}, \mathbf{\Phi}). \tag{40}$$

A similar result appears in Gurtin (1981) for the differentiation of tensor inverses. Likewise, using the identity $J^{-T}J^T = I$ we obtain

$$\delta_2 J^{-T}(\mathbb{X}, \mathbf{\Phi}; \varphi) = -J^{-T}(\mathbb{X}, \mathbf{\Phi})D_1 \delta_2 \chi^T(\mathbb{X}, \mathbf{\Phi}; \varphi)J^{-T}(\mathbb{X}, \mathbf{\Phi}), \tag{41}$$

where the notation $J^{-T} = (J^{-1})^T$ is enforced (Gurtin, 1981).

To determine the design variation of J we first consider the map $\pi : \text{Lin}(\mathcal{V}^N, \mathcal{V}^N) \to \mathcal{R}$ such that

$$\pi_3 = \det \mathbf{A}. \tag{42}$$

Then, it may be shown [see Gurtin (1981) or see the alternative approach provided in the Appendix] that

$$D\pi_3(\mathbf{A})\mathbf{W} = \det \mathbf{A} \, \text{tr}(\mathbf{W}\mathbf{A}^{-1}), \tag{43}$$

where $\mathbf{A}, \mathbf{W} \in \text{Lin}(\mathcal{V}^N, \mathcal{V}^N)$. Using the chain rule [eqn (27_2)] where we equate $J(\mathbb{X}, \mathbf{\Phi}) = \pi_3 \circ J(\mathbb{X}, \mathbf{\Phi})$ so that $\mathbf{A} = J(\mathbb{X}, \mathbf{\Phi})$ and $\mathbf{W} = D_2 J(\mathbb{X}, \mathbf{\Phi})\varphi$ in the above, we obtain

$$D_2 J(\mathbb{X}, \mathbf{\Phi})\varphi = D\pi_3 \circ D_2 J(\mathbb{X}, \mathbf{\Phi})\varphi$$

$$= D\pi_3(D_2 J(\mathbb{X}, \mathbf{\Phi})\varphi)$$

$$= \det J(\mathbb{X}, \mathbf{\Phi}) \, \text{tr}(D_2 J(\mathbb{X}, \mathbf{\Phi})\varphi J^{-1}(\mathbb{X}, \mathbf{\Phi})), \tag{44}$$

which upon combining eqns (22_1), (8_1), (37) and (44), yields the result

$$\delta_2 J(\mathbb{X}, \Phi; \varphi) = J(\mathbb{X}, \Phi) \operatorname{tr} (D_1 \delta_2 \chi(\mathbb{X}, \Phi; \varphi) \mathbf{J}^{-1}(\mathbb{X}, \Phi))$$

$$= J(\mathbb{X}, \Phi) D_1 \delta_2 \chi(\mathbb{X}, \Phi; \varphi) \cdot \mathbf{J}^{-T}(\mathbb{X}, \Phi). \tag{45}$$

3. TRANSFORMATION TO THE REFERENCE CONFIGURATION

In order to transform our problem to the reference domain we must convert gradients, the divergence, the Laplacian, normal vectors, and elemental areas from the body configuration to the reference domain. To accomplish this, we repeatedly apply the chain rule and Piola's identity $\operatorname{div}_1(J\mathbf{J}^{-T}) = 0$ (Ciarlet, 1988). We also evaluate the design variation of some of these quantities.

3.1. *Transformation of gradients*

Consider the composite value scalar map $\hat{\alpha}: B \times \mathscr{D}^M \to \mathscr{R}$ defined by eqn (28) where $\alpha: \mathscr{T} \to \mathscr{R}$ and $\chi: B \times \mathscr{D}^M \to \mathscr{E}^n$ are defined in the usual manner. Then from the chain rule and the definitions of the gradient, Jacobian and transpose [eqns (29$_1$), (22$_2$), (30) and (5)]

$$\nabla_1 \hat{\alpha}(\mathbb{X}, \Phi) \cdot \mathbf{U} = \nabla_1 \alpha(\chi(\mathbb{X}, \Phi), \Phi) \cdot \mathbf{J}(\mathbb{X}, \Phi)\mathbf{U}$$

$$= \mathbf{J}^T(\mathbb{X}, \Phi)\nabla_1 \alpha(\chi(\mathbb{X}, \Phi), \Phi) \cdot \mathbf{U},$$

so that

$$\mathbf{J}^{-T}(\mathbb{X}, \Phi)\nabla_1 \hat{\alpha}(\mathbb{X}, \Phi) = \nabla_1 \alpha(\chi(\mathbb{X}, \Phi), \Phi), \tag{46}$$

where we used the invertibility of $\mathbf{J}$ and the arbitrariness of $\mathbf{U}$.

Next, we consider the vector value composite map $\hat{\mathbf{a}}: B \times \mathscr{D}^M \to \mathscr{V}^n$ defined in an analogous manner to $\hat{\alpha}$. Then by the chain rule, the definition of $\mathbf{J}$, invertibility of $\mathbf{J}$, and the arbitrariness of $\mathbf{U}$ [eqns (29$_1$), (30)] respectively, we obtain

$$D_1 \hat{\mathbf{a}}(\mathbb{X}, \Phi)\mathbf{U} = D_1 \mathbf{a}(\chi(\mathbb{X}, \Phi), \Phi)\mathbf{J}(\mathbb{X}, \Phi)\mathbf{U}$$

so that

$$D_1 \hat{\mathbf{a}}(\mathbb{X}, \Phi)\mathbf{J}^{-1}(\mathbb{X}, \Phi) = D_1 \mathbf{a}(\chi(\mathbb{X}, \Phi), \Phi). \tag{47}$$

3.2. *Transformation of the divergence*

Consider the equation

$$\operatorname{div}_1 \mathbf{a}(\mathbf{x}, \Phi) = 0 \quad \text{for} \quad (\mathbf{x}, \Phi) \in \mathscr{T}, \tag{48}$$

where $\mathbf{a}: \mathscr{T} \to \mathscr{V}^n$. For example, this represents the energy equation for a steady-state conduction system with no source where $\mathbf{a}$ is the heat flux vector and Φ represents the current design.

We may write for any $b'_\Phi \subset b_\Phi$

$$\int_{b'_\Phi} \operatorname{div}_1 \mathbf{a}(\mathbf{x}, \Phi) \, dv_{\mathbf{x}} = 0, \tag{49}$$

which after an application of the change of variable theorem [eqn (35)] becomes

$$\int_{B'} \text{div}_1 \, \mathbf{a}(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}) J(\mathbb{X}, \mathbf{\Phi}) \, dv_{\mathbf{x}} = \int_{\chi(B')} \text{div}_1 \, \mathbf{a}(\mathbf{x}, \mathbf{\Phi}) \, dv_{\mathbf{x}} = 0, \qquad (50)$$

where $\chi(B') = b'_{\mathbf{\Phi}}$. Then by the localization theorem (Gurtin, 1981)†

$$\text{div}_1 \, \mathbf{a}(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}) J(\mathbb{X}, \mathbf{\Phi}) = 0 \quad \text{for} \quad (\mathbb{X}, \mathbf{\Phi}) \in (B \times \mathscr{D}^M). \qquad (51)$$

Unfortunately, this equation is not expressed in terms of referential field quantities. To this end, we perform the following transformations:

$$\begin{aligned}
\text{div}_1 \, \mathbf{a}(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}) J(\mathbb{X}, \mathbf{\Phi}) &= \text{tr} \, (D_1 \mathbf{a}(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi})) J(\mathbb{X}, \mathbf{\Phi}) \\
&= D_1 \hat{\mathbf{a}}(\mathbb{X}, \mathbf{\Phi}) \cdot J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-T}(\mathbb{X}, \mathbf{\Phi}) \\
&= \text{div}_1 \, (J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-1}(\mathbb{X}, \mathbf{\Phi}) \hat{\mathbf{a}}(\mathbb{X}, \mathbf{\Phi})), \qquad (52)
\end{aligned}$$

where we use eqns (23_1), (47), (7), (25_2), and Piola's identity $\text{div}_1 \, (J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-T}(\mathbb{X}, \mathbf{\Phi})) = 0$ (see Appendix for details). Thus, we now have the equivalent equation defined solely by referential quantities

$$\text{div}_1 \, (J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-1}(\mathbb{X}, \mathbf{\Phi}) \hat{\mathbf{a}}(\mathbb{X}, \mathbf{\Phi})) = 0 \quad \text{for} \quad (\mathbb{X}, \mathbf{\Phi}) \in (B \times \mathscr{D}^M), \qquad (53)$$

where the fields are related through the composition $\mathbf{a}(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}) = \hat{\mathbf{a}}(\mathbb{X}, \mathbf{\Phi})$.

3.3. *Transformation of the Laplace equation*

Consider the Laplace equation

$$\Delta_1 \alpha(\mathbf{x}, \mathbf{\Phi}) = 0 \quad \text{for} \quad (\mathbf{x}, \mathbf{\Phi}) \in \mathscr{T}, \qquad (54)$$

where $\alpha : \mathscr{T} \to \mathscr{R}$. Proceeding as before and using the definition of the Laplacian [eqn (23_3)] we express for any $b'_{\mathbf{\Phi}} \subset b_{\mathbf{\Phi}}$

$$\int_{b'_{\mathbf{\Phi}}} \text{div}_1 \, \nabla_1 \alpha(\mathbf{x}, \mathbf{\Phi}) \, dv_{\mathbf{x}} = 0, \qquad (55)$$

which after an application of the change of variable theorem [eqn (35)] and localization theorem becomes

$$\text{div}_1 \, \nabla_1 \alpha(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}) J(\mathbb{X}, \mathbf{\Phi}) = 0 \quad \text{for} \quad (\mathbb{X}, \mathbf{\Phi}) \in (B \times \mathscr{D}^M). \qquad (56)$$

We now commence to transform this equation by sequentially applying eqns (23_1), (8_1), $\mathbf{J}^T \mathbf{J}^{-T} = \mathbf{I}$, (8_4), (47), (25_2), Piola's identity $\text{div}_1 (J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-T}(\mathbb{X}, \mathbf{\Phi})) = 0$, and (46):

$$\begin{aligned}
\text{div}_{\mathbf{x}} \, \nabla_{\mathbf{x}} \alpha(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}) J(\mathbb{X}, \mathbf{\Phi}) &= \text{tr} \, (D_{\mathbf{x}} \nabla_{\mathbf{x}} \alpha(\chi(\mathbb{X}, \mathbf{\Phi}))) J(\mathbb{X}, \mathbf{\Phi}) \\
&= \mathbf{J}^{-T}(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^T(\mathbb{X}, \mathbf{\Phi}) \cdot D_{\mathbf{x}} \nabla_{\mathbf{x}} \alpha(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}) J(\mathbb{X}, \mathbf{\Phi}) \\
&= J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-T}(\mathbb{X}, \mathbf{\Phi}) \cdot D_{\mathbf{x}} [\nabla_{\mathbf{x}} \alpha(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi})] \\
&= \text{div}_{\mathbf{x}} \, (J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-1}(\mathbb{X}, \mathbf{\Phi}) \nabla_{\mathbf{x}} \alpha(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi})) \\
&\quad - \text{div}_{\mathbf{x}} (J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-T}(\mathbb{X}, \mathbf{\Phi})) \cdot \nabla_{\mathbf{x}} \alpha(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}) \\
&= \text{div}_{\mathbf{x}} \, (J(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-1}(\mathbb{X}, \mathbf{\Phi}) \mathbf{J}^{-T}(\mathbb{X}, \mathbf{\Phi}) \nabla_{\mathbf{x}} \hat{\alpha}(\mathbb{X}, \mathbf{\Phi})). \qquad (57)
\end{aligned}$$

For clarity we used the subscripts $\mathbf{x}$ and $\mathbb{X}$ to denote partial differentiation with respect to

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†To use the localization theorem we require $\text{div}_1 \, \mathbf{a} J$ to be continuous and B' to be open.

the first argument for functions on $\mathcal{T}$ and $B \times \Phi$, respectively. Thus, we now express the equivalent expression for eqn (54) defined solely in terms of referential quantities:

$$\text{div}_1\left(J(\mathbb{X}, \Phi)\mathbf{J}^{-1}(\mathbb{X}, \Phi)\mathbf{J}^{-T}(\mathbb{X}, \Phi)\nabla_1\hat{\alpha}(\mathbb{X}, \Phi)\right) = 0 \quad \text{for} \quad (\mathbb{X}, \Phi) \in (B \times \mathscr{D}^M), \quad (58)$$

where the fields are again related through the composition $\alpha(\chi(\mathbb{X}, \Phi), \Phi) = \hat{\alpha}(\mathbb{X}, \Phi)$.

3.4. Nanson's relation

Combining the results of Section 3.2 [eqns (50) and (52)] yields

$$\int_{\chi(B')} \text{div}_1\, \mathbf{a}(\mathbf{x}, \Phi)\, dv_\mathbf{x} = \int_{B'} \text{div}_1\left(J(\mathbb{X}, \Phi)\mathbf{J}^{-1}(\mathbb{X}, \Phi)\hat{\mathbf{a}}(\mathbb{X}, \Phi)\right) dv_\mathbb{X} \quad (59)$$

which after an application of the divergence theorem [eqn (34_2)] becomes

$$\int_{\partial\chi(B')} \mathbf{a}(\mathbf{x}, \Phi) \cdot \mathbf{n}(\mathbf{x}, \Phi)\, da_\mathbf{x} = \int_{\partial B'} J(\mathbb{X}, \Phi)\mathbf{J}^{-1}(\mathbb{X}, \Phi)\hat{\mathbf{a}}(\mathbb{X}, \Phi) \cdot \mathbf{N}(\mathbb{X})\, da_\mathbb{X}. \quad (60)$$

Now by the arbitrariness of $\mathbf{a}(\chi(\mathbb{X}, \Phi)) = \hat{\mathbf{a}}(\mathbb{X}, \Phi)$ and the definition of the transpose [eqn (5)] we are led to *Nanson's relation*:

$$\mathbf{n}(\chi(\mathbb{X}, \Phi), \Phi)\, da_{\chi(\mathbb{X}, \Phi)} = J(\mathbb{X}, \Phi)\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})\, da_\mathbb{X}. \quad (61)$$

This relation appears in Gurtin (1981). Taking the norm of both sides and using the normalized normal vector $\mathbf{n}$, gives [cf. Ciarlet (1988)]

$$da_{\chi(\mathbb{X}, \Phi)} = J(\mathbb{X}, \Phi)\|\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})\|\, da_\mathbb{X}$$
$$= K(\mathbb{X}, \Phi)\, da_\mathbb{X}. \quad (62)$$

$K(\mathbb{X}, \Phi)$ then is a metric that relates surface differentials between the reference and body configurations [cf. eqn (36)]. Upon combining the previous two results we obtain

$$\mathbf{n}(\chi(\mathbb{X}, \Phi), \Phi) = \mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})/\|\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})\|$$
$$= J(\mathbb{X}, \Phi)\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})/K(\mathbb{X}, \Phi), \quad (63)$$

which is an expression relating normal vectors between the two configurations.

To derive the sensitivities we require the design variation of K. Multiple applications of eqns (3), (24), (27), (45), (41), symmetry of the inner product, and eqns (62) and (63) give

$$\delta_2 K(\mathbb{X}, \Phi; \varphi) = D_2 J(\mathbb{X}, \Phi)\varphi\|\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})\| + \tfrac{1}{2}J(\mathbb{X}, \Phi)\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})$$
$$\cdot D_2\mathbf{J}^{-T}(\mathbb{X}, \Phi)\varphi\mathbf{N}(\mathbb{X})/\|\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})\|$$
$$+ \tfrac{1}{2}J(\mathbb{X}, \Phi)D_2\mathbf{J}^{-T}(\mathbb{X}, \Phi)\varphi\mathbf{N}(\mathbb{X})$$
$$\cdot \mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})/\|\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})\|$$
$$= J(\mathbb{X}, \Phi)\, \text{tr}\,(D_1\delta_2\chi(\mathbb{X}, \Phi; \varphi)\mathbf{J}^{-1}(\mathbb{X}, \Phi))\|\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})\|$$
$$- J(\mathbb{X}, \Phi)\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X}) \cdot \mathbf{J}^{-T}(\mathbb{X}, \Phi)D_1\delta_2\chi^T(\mathbb{X}, \Phi; \varphi)\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})/$$
$$\|\mathbf{J}^{-T}(\mathbb{X}, \Phi)\mathbf{N}(\mathbb{X})\|$$
$$= K(\mathbb{X}, \Phi)[\text{tr}\,(D_1\delta_2\chi(\mathbb{X}, \Phi; \varphi)\mathbf{J}^{-1}(\mathbb{X}, \Phi)) - \mathbf{n}(\chi(\mathbb{X}, \Phi), \Phi)$$
$$\cdot \mathbf{J}^{-T}(\mathbb{X}, \Phi)D_1\delta_2\chi^T(\mathbb{X}, \Phi; \varphi)\mathbf{n}(\chi(\mathbb{X}, \Phi), \Phi)]. \quad (64)$$

4. SHAPE SENSITIVITIES FOR LAPLACE'S PROBLEM

In the following we transform Laplace's problem to the reference configuration and draw analogies to the isoparametric map used in the finite and boundary element methods. We also introduce the concept of a response functional and derive shape sensitivities via the direct and adjoint methods.

4.1. *Laplace's equation and the isoparametric formulations*

Consider the boundary-value problem governed by Laplace's equation

$$\Delta_1\alpha(x,\Phi) = 0 \qquad \text{for} \quad (x,\Phi)\in\mathcal{T},$$

$$\alpha(x,\Phi) = \alpha^p(x,\Phi) \quad \text{for} \quad (x,\Phi)\in\partial\mathcal{T}_1,$$

$$\nabla_1\alpha(x,\Phi)\cdot n(x,\Phi) = q^p(x,\Phi) \quad \text{for} \quad (x,\Phi)\in\partial\mathcal{T}_2, \tag{65}$$

where $\partial\mathcal{T}_2 = \{(x,\Phi)\,;\, x\in\partial b_{\Phi_1}, \Phi\in\mathscr{D}^M\}$, $\partial\mathcal{T}_2 = \{(x,\Phi)\,;\, x\in\partial b_{\Phi_2}, \Phi\in\mathscr{D}^M\}$. This could represent a steady-state conduction system with no source. Then, we have the prescribed temperature α^p on $\partial\mathcal{T}_1$ and the prescribed flux q^p on $\partial\mathcal{T}_2$.

As previously mentioned, to derive shape sensitivities we transform the above to the reference configuration, which from eqns (58), (46) and (63) becomes

$$\text{div}_1\,(J(X,\Phi)J^{-1}(X,\Phi)J^{-T}(X,\Phi)\nabla_1\hat{\alpha}(X,\Phi)) = 0 \qquad \text{for} \quad (X,\Phi)\in B\times\mathscr{D}^M$$

$$\hat{\alpha}(X,\Phi) = \hat{\alpha}^p(X,\Phi) \quad \text{for} \quad (X,\Phi)\in\partial\mathscr{B}_1\times\mathscr{D}^M$$

$$J^{-T}(X,\Phi)\nabla_1\hat{\alpha}(X,\Phi)\cdot J(X,\Phi)J^{-T}(X,\Phi)N(X)$$

$$= \hat{q}^p(X,\Phi)K(X,\Phi) \quad \text{for} \quad (X,\Phi)\in\partial B_2\times\mathscr{D}^M, \tag{66}$$

where $\hat{\alpha}^p(X,\Phi) = \alpha^p(\chi(X,\Phi),\Phi)$ and $\hat{q}^p(X,\Phi) = q^p(\chi(X,\Phi),\Phi)$ are composite functions. We now solve the above equations for the referential response $\hat{\alpha}$ and $\nabla_1\hat{\alpha}$. Once these quantities are determined α and $\nabla\alpha$ may be evaluated via eqns (28) and (46), i.e. $\alpha(\chi(X,\Phi),\Phi) = \hat{\alpha}(X,\Phi)$ and $\nabla_1\alpha(\chi(X,\Phi),\Phi) = J^{-T}(X,\Phi)\nabla_1\hat{\alpha}(X,\Phi)$.

A comment here, regarding the functions $\hat{\alpha}^p$ and $\hat{q}^p$ seems appropriate. These are functions of a reduced domain, as they are defined on the surface ∂B and not within the body B, and therefore have no normal derivatives. This has ramifications when we take the gradient of $\hat{\alpha}^p$ in later sections, e.g. eqn (76_2). Note that $\hat{\alpha}: B\to\mathscr{R}$ whereas $\hat{\alpha}^p: \partial B\to\mathscr{R}$, thus their spacial gradients which are defined on different domains are not equal, $\nabla_1\hat{\alpha}\neq\nabla_1\hat{\alpha}^p_1$. Similar remarks regarding $\hat{q}^p$ also apply.

The above equation may be solved by using the isoparametric finite and boundary element methods. Indeed, if we multiply eqn (66_1) by an arbitrary function $\hat{\lambda}: B\times\mathscr{D}^M\to\mathscr{R}$ and integrate over B we obtain

$$\int_B \hat{\lambda}\,\text{div}_1\,(JJ^{-1}J^{-T}\nabla_1\hat{\alpha})\,dv_X = 0, \tag{67}$$

where we suppressed the arguments for conciseness; a practice which we continue henceforth. Now application of eqns (25_1) and (34_2) to the above gives

$$\int_{\partial B} \hat{\lambda}JJ^{-1}J^{-T}\nabla_1\hat{\alpha}\cdot N\,da_X - \int_B \nabla_1\hat{\lambda}\cdot JJ^{-1}J^{-T}\nabla_1\hat{\alpha}\,dv_X = 0. \tag{68}$$

To derive the finite element equation, we restrict $\hat{\alpha}$ to the space of square integrable functions which satisfies eqn (66_2); and we restrict $\hat{\lambda}$ to the space of square integrable functions which equal zero on ∂B_1. Then we determine the $\hat{\alpha}$ from the admissable space of functions which satisfies

$$\int_{\partial B_2} \hat{\lambda}\hat{q}^p K \, da_{\mathbf{x}} = \int_B \mathbf{J}^{-T}\nabla_1\hat{\lambda}\cdot\mathbf{J}^{-T}\nabla_1\hat{\alpha}J \, dv_{\mathbf{x}} \tag{69}$$

for all admissible $\hat{\lambda}$. We derive the above from the definition of the transpose [eqn (5)], eqn (66₃), and the restriction that $\hat{\lambda} = 0$ on ∂B_1. The finite element method systematically develops the basis functions for the Galerkin method (Becker et al., 1981) which is used to obtain the approximate solution. We use the left- and right-hand sides of the above to form, in a piecewise manner, the load vector and symmetric stiffness matrix, respectively. In this piecewise approach, the map χ and Jacobian $\mathbf{J}$ are defined locally over elements (subregions) whose images collectively approximate b_Φ. In this way, the (typically numerical) integrations are performed individually over the elements and then summed. To be precise, in the isoparametric finite element method, we approximate $\hat{\alpha}$ and $\hat{\lambda}$ with the same interpolation functions which define χ. For our example [eqn (32)], $\hat{\alpha} = \Sigma_{I=1}^8 \Psi^I\hat{\alpha}^I$ and $\nabla_1\hat{\alpha} = \Sigma_{I=1}^8 \nabla_1\Psi^I\hat{\alpha}^I$ where the unknown (to be determined) parameter $\hat{\alpha}^I$ is the value of $\hat{\alpha}$ at the node with coordinates $\mathbf{x}^I$. These results are consistent with those appearing in Becker et al. (1981).

To derive the boundary element equation we start with eqn (68) and again use eqns (25₁), (34₂), (5), (66₂) and (66₃) to obtain

$$-\int_{\partial B_1} \hat{\alpha}^p \mathbf{J}^{-T}\nabla_1\hat{\lambda}\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N} \, da_{\mathbf{x}} + \int_{\partial B_2} \hat{\lambda}\hat{q}^p K \, da_{\mathbf{x}} = -\int_{\partial B_1} \hat{\lambda}\mathbf{J}^{-T}\nabla_1\hat{\alpha}\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N} \, da_{\mathbf{x}}$$

$$+\int_{\partial B_2} \hat{\alpha}\mathbf{J}^{-T}\nabla_1\hat{\lambda}\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N} \, da_{\mathbf{x}} - \int_B \hat{\alpha}\,\mathrm{div}_1\,(J\mathbf{J}^{-1}\mathbf{J}^{-T}\nabla_1\hat{\lambda}) \, dv_{\mathbf{x}}. \tag{70}$$

Next we choose $\hat{\lambda}(\mathbb{X}, \Phi) = \lambda(\chi(\mathbb{X}, \Phi))$ where $\lambda: b_\Phi \to \mathcal{R}$ is the design independent fundamental solution [cf. Carey and Oden (1983)] so that the volume integral becomes $\frac{1}{2}\hat{\alpha}(\mathbb{Y}, \Phi)$ for $\mathbb{Y} \in \partial B$. Hence, the above reduces to

$$-\int_{\partial B_1} \hat{\alpha}^p \mathbf{J}^{-T}\nabla_1\hat{\lambda}\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N} \, da_{\mathbf{x}} + \int_{\partial B_2} \hat{\lambda}\hat{q}^p K \, da_{\mathbf{x}} =$$

$$-\int_{\partial B_1} \hat{\lambda}\mathbf{J}^{-T}\nabla_1\hat{\alpha}\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N} \, da_{\mathbf{x}} + \int_{\partial B_2} \hat{\alpha}\mathbf{J}^{-T}\nabla_1\hat{\lambda}\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N} \, da_{\mathbf{x}}$$

$$-\frac{1}{2}\hat{\alpha}(\mathbb{Y}, \Phi) \quad \text{for} \quad \mathbb{Y} \in \partial B. \tag{71}$$

The left- and right-hand sides of the above are used to form the load vector and non-symmetric stiffness matrix, respectively. These results are consistent with those appearing in Carey and Oden (1983). Again, as in the finite element method, the map χ and Jacobian $\mathbf{J}$ are defined piecewise over the elements (sub-surfaces).

4.2. The response functional

To gage the performance of a system we may evaluate a general response functional of the form

$$G(\Phi) = \int_{\partial b_\Phi} g(\alpha, \nabla_1\alpha\cdot\mathbf{n}, \mathbf{x}) \, da_{\mathbf{x}}. \tag{72}$$

Clearly, we expect $G(\Phi)$ to vary as Φ is varied. The effect is two fold, the region of integration ∂b_Φ varies with Φ and the solution $(\alpha, \nabla_1\alpha)$ to the boundary value problem varies with b_Φ. For the heat transfer problem $G(\Phi)$ might be used to evaluate the mean temperature or surface flux over the boundary. Localized quantities may also be obtained by incorporating the appropriate weighting functions in g. For example, to evaluate α at the point $\mathbf{x}'$ we equate $g = \alpha\delta(\mathbf{x} - \mathbf{x}')$ where $\delta(\ )$ is the Dirac delta function.

The above functional is defined in terms of the body's response quantities. However, we are not directly evaluating α and $\nabla_1\alpha$ during our analysis (so that we may derive the shape sensitivities and be consistent with the isoparametric formulations). Instead, we invoke eqns (28), (36), (46) and (63) and the definition of χ to write the equivalent functional over the reference configuration

$$G(\boldsymbol{\Phi}) = \int_{\partial B} \hat{g}(\hat{\alpha}, \mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha} \cdot \ \mathbf{J}\mathbf{J}^{-\mathrm{T}}\mathbf{N}/K, \chi)K\,da_{\mathbb{X}}, \tag{73}$$

where $\hat{g}$ is defined on the set product of the $\mathscr{C}^1$ continuously differentiable functions. Specifically, $\hat{g}: \mathscr{C}^1(B\times\mathscr{D}^M,\mathscr{R})\times\mathscr{C}^1(B\times\mathscr{D}^M,\mathscr{R})\times\mathscr{C}^1(B\times\mathscr{D}^M,\mathscr{E}^n)\to\mathscr{R}$.

The objective of a sensitivity analysis is to determine the design variation of G, i.e. we wish to evaluate $\delta G(\boldsymbol{\Phi}; \varphi)$ which upon noting the independence of $\mathbb{X}$ from $\boldsymbol{\Phi}$ and applying eqns (13), (19), (20), (22$_1$), (22$_2$), (24), (27$_2$) and (5) becomes

$$\delta G = \int_{\partial B} [\nabla_1\hat{g}\delta_2\hat{\alpha}K + \nabla_2\hat{g}(\nabla_1\delta_2\hat{\alpha}\cdot\mathbf{J}^*\mathbf{N} + \nabla_1\hat{\alpha}\cdot\delta_2\mathbf{J}^*\mathbf{N}$$

$$-\nabla_1\hat{\alpha}\cdot\mathbf{J}^*\mathbf{N}\delta_2K/K) + \nabla_3\hat{g}\cdot\delta_2\chi K + \hat{g}\delta_2K]\,da_{\mathbb{X}}, \tag{74}$$

where the identities $\mathbf{J}^* = \mathbf{J}^{*\mathrm{T}} \equiv J\mathbf{J}^{-1}\mathbf{J}^{-\mathrm{T}}$ and $\delta_2\mathbf{J}^* = \delta_2\mathbf{J}^{*\mathrm{T}} = \delta_2J\mathbf{J}^{-1}\mathbf{J}^{-\mathrm{T}} + J\delta_2\mathbf{J}^{-1}\mathbf{J}^{-\mathrm{T}} + J\mathbf{J}^{-1}\delta_2\mathbf{J}^{-\mathrm{T}}$ are defined for convenience. Note that since χ, its derivatives, and $\hat{g}$ are explicitly defined, then all of the terms in eqn (74) are readily evaluated with the exception of $\delta_2\hat{\alpha}$ and $\nabla_1\delta_2\hat{\alpha}$. These terms are implicitly defined by the design $\boldsymbol{\Phi}$ through the boundary value problem [eqn (66)]. In the following sensitivity analyses, we will show that it is possible to explicitly evaluate δG.

4.3. Direct differentiation

In the direct differentiation method we *evaluate* $\delta_2\hat{\alpha}$ and $\nabla_1\delta_2\hat{\alpha}$. Once these quantities are determined, we may determine δG directly from eqn (74) or the response variation via eqn (76). We compute the referential response variations by differentiating eqn (66) with respect to the design, whereupon [using eqns (20), (24) and (27.2)]

$$\mathrm{div}_1\,(\delta_2\mathbf{J}^*\nabla_1\hat{\alpha} + \mathbf{J}^*\nabla_1\delta_2\hat{\alpha}) = 0 \qquad \text{for} \quad (\mathbb{X},\boldsymbol{\Phi})\in B\times\mathscr{D}^M,$$

$$\delta_2\hat{\alpha} = \mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}^p\cdot\delta_2\chi + \delta_2\alpha^p \qquad \text{for} \quad (\mathbb{X},\boldsymbol{\Phi})\in\partial B_1\times\mathscr{D}^M,$$

$$\nabla_1\delta_2\hat{\alpha}\cdot\mathbf{J}^*\mathbf{N} + \nabla_1\hat{\alpha}\cdot\delta_2\mathbf{J}^*\mathbf{N} = \mathbf{J}^{-\mathrm{T}}\nabla_1\hat{q}^p\cdot\delta_2\chi K + \delta_2q^pK + \hat{q}^p\delta_2K \quad \text{for} \quad (\mathbb{X},\boldsymbol{\Phi})\in\partial B_2\times\mathscr{D}^M,$$

$$\tag{75}$$

where it is henceforth understood that all occurrences of α^p and q^p are evaluated at $(\mathbf{x},\boldsymbol{\Phi}) = (\chi(\mathbb{X},\boldsymbol{\Phi}),\boldsymbol{\Phi})$. Now we solve the above for $\delta_2\hat{\alpha}$ and $\nabla_1\delta_2\hat{\alpha}$ and substitute these quantities into eqn (74) to obtain the explicit sensitivity. To solve this equation we may use either the finite or boundary element methods.

Once we know $\delta_2\hat{\alpha}$, we may evaluate $\delta_2\alpha$. Indeed by using the chain rule [eqn (29$_2$)] we obtain the relation

$$\delta_2\hat{\alpha}(\mathbb{X},\boldsymbol{\Phi}; \varphi) = \nabla_1\alpha(\chi(\mathbb{X},\boldsymbol{\Phi}),\boldsymbol{\Phi})\cdot\delta_2\chi(\mathbb{X},\boldsymbol{\Phi}; \varphi) + \delta_2\alpha(\chi(\mathbb{X},\boldsymbol{\Phi}),\boldsymbol{\Phi}; \varphi)$$

$$= \mathbf{J}^{-\mathrm{T}}(\mathbb{X},\boldsymbol{\Phi})\nabla_1\hat{\alpha}(\mathbb{X},\boldsymbol{\Phi})\cdot\delta_2\chi(\mathbb{X},\boldsymbol{\Phi}; \varphi) + \delta_2\alpha(\chi(\mathbb{X},\boldsymbol{\Phi}),\boldsymbol{\Phi}; \varphi)$$

so that

$$\delta_2\alpha(\chi(\mathbb{X},\boldsymbol{\Phi}),\boldsymbol{\Phi}; \varphi) = \delta_2\hat{\alpha}(\mathbb{X},\boldsymbol{\Phi}; \varphi) - \mathbf{J}^{-\mathrm{T}}(\mathbb{X},\boldsymbol{\Phi})\nabla_1\hat{\alpha}(\mathbb{X},\boldsymbol{\Phi})\cdot\delta_2\chi(\mathbb{X},\boldsymbol{\Phi}; \varphi), \tag{76}$$

where we used eqns (22$_1$), (22$_2$) and (46). The above represents the design variation of α

at fixed position x in the body configuration. A similar relation for $\nabla_1 \delta_2 \alpha$ may also be developed.

To obtain the finite and boundary element equations, we proceed as before. First we multiply eqn (75$_1$) by $\hat{\lambda}$, integrate over B, and apply eqns (25$_1$) and (34$_2$)

$$\int_{\partial B} \hat{\lambda} \delta_2 \mathbf{J}^* \nabla_1 \hat{\alpha} \cdot \mathbf{N}\, da_{\mathrm{x}} - \int_B \nabla_1 \hat{\lambda} \cdot \delta_2 \mathbf{J}^* \nabla_1 \hat{\alpha}\, dv_{\mathrm{x}} =$$

$$- \int_{\partial B} \hat{\lambda} \mathbf{J}^* \nabla_1 \delta_2 \hat{\alpha} \cdot \mathbf{N}\, da_{\mathrm{x}} + \int_B \nabla_1 \hat{\lambda} \cdot \mathbf{J}^* \nabla_1 \delta_2 \hat{\alpha}\, dv_{\mathrm{x}}, \quad (77)$$

where the explicit and implicit quantities appear on the left- and right-hand sides, respectively.

Now, for the finite element equation, we restrict $\delta_2 \hat{\alpha}$ to the space of square integrable functions which satisfy eqn (75$_2$); and we restrict $\hat{\lambda}$ to the space of square integrable functions which equal zero on ∂B_1. Then, we are to determine the $\delta_2 \hat{\alpha}$ from the space of admissible functions which satisfies

$$\int_{\partial B_2} \hat{\lambda} (\mathbf{J}^{-\mathrm{T}} \nabla \hat{q}^p \cdot \delta_2 \chi K + \delta_2 q^p K + \hat{q}^p \delta_2 K)\, da_{\mathrm{x}}$$

$$- \int_B \nabla_1 \hat{\lambda} \cdot \delta_2 \mathbf{J}^* \nabla_1 \hat{\alpha}\, dv_{\mathrm{x}} = \int_B \mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{\lambda} \cdot \mathbf{J}^{-\mathrm{T}} \nabla_1 \delta_2 \hat{\alpha} J\, dv_{\mathrm{x}} \quad (78)$$

for all admissible $\hat{\lambda}$. We derived the above from eqn (77) by using eqns (5) and (75$_3$), the symmetry of $\mathbf{J}^*$, and the restriction that $\hat{\lambda} = 0$ on ∂B_1. We could have also derived this by direct differentiation of eqn (69). Note that this equation resembles eqn (69) in that the known terms are on the left-hand side and the unknown quantities are on the right-hand side. In the finite element analysis, the left-hand side forms the load vector while the right-hand side forms the stiffness matrix. Further, note that the right-hand sides of eqns (69) and (78) are similar. In fact, they both define the same finite element stiffness matrix. This implies that the decomposed stiffness matrix which is used to evaluate the *primal* response $\hat{\alpha}$ can also be used to evaluate the *pseudo* response $\delta_2 \hat{\alpha}$. Thus, the pseudo response is efficiently computed by merely performing a pseudo load vector assembly corresponding to the left-hand side of eqn (78) and a back substitution into the existing decomposed stiffness matrix. Of course, we compute $\nabla_1 \delta_2 \hat{\alpha}$ from $\delta_2 \hat{\alpha}$ in the usual finite element manner. Once we have determined these quantities we may evaluate δG via eqn (74).

For the boundary element approach, we begin with eqn (77), apply eqns (25$_1$) and (34$_2$) to the right-hand side and use eqns (75$_2$) and (75$_3$) to obtain (after isolating the implicit and explicit variations)

$$\int_{\partial B_1} \hat{\lambda} \delta_2 \mathbf{J}^* \nabla_1 \hat{\alpha} \cdot \mathbf{N}\, da_{\mathrm{x}} - \int_B \nabla_1 \hat{\lambda} \cdot \delta_2 \mathbf{J}^* \nabla_1 \hat{\alpha}\, dv_{\mathrm{x}} + \int_{\partial B_2} \hat{\lambda} (\mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{q}^p \cdot \delta_2 \chi K$$

$$+ \delta_2 q^p K + q^p \delta_2 K)\, da_{\mathrm{x}} - \int_{\partial B_1} (\mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{\alpha}^p \cdot \delta_2 \chi + \delta_2 \alpha^p) \mathbf{J}^* \nabla_1 \hat{\lambda} \cdot \mathbf{N}\, da_{\mathrm{x}}$$

$$= - \int_{\partial B_1} \hat{\lambda} \mathbf{J}^* \nabla_1 \delta_2 \hat{\alpha} \cdot \mathbf{N}\, da_{\mathrm{x}} + \int_{\partial B_2} \delta_2 \hat{\alpha} \mathbf{J}^* \nabla_1 \hat{\lambda} \cdot \mathbf{N}\, da_{\mathrm{x}}$$

$$- \int_B \delta_2 \hat{\alpha} \operatorname{div}_1 (\mathbf{J}^* \nabla_1 \hat{\lambda})\, dv_{\mathrm{x}}. \quad (79)$$

This equation may be solved via the boundary element, however we now have a load term which is defined in the domain, to which the following transformations are applied:

$$\int_B \nabla_1\hat{\lambda}\cdot\delta_2\mathbf{J}^*\nabla_1\hat{\alpha}\,dv_\mathbf{x}$$

$$= \int_B \nabla_1\hat{\lambda}\cdot(JD_1\delta_2\chi\cdot\mathbf{J}^{-\mathrm{T}}\mathbf{J}^{-1}\mathbf{J}^{-\mathrm{T}}-JJ^{-1}D_1\delta_2\chi\mathbf{J}^{-1}\mathbf{J}^{-\mathrm{T}}$$

$$-JJ^{-1}\mathbf{J}^{-\mathrm{T}}D_1\delta_2\chi^\mathrm{T}\mathbf{J}^{-\mathrm{T}})\nabla_1\hat{\alpha}\,dv_\mathbf{x}$$

$$= \int_B [JJ^{-\mathrm{T}}\nabla_1\hat{\alpha}\cdot\mathbf{J}^{-\mathrm{T}}(D_1(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}))^\mathrm{T}\delta_2\chi+JJ^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\mathbf{J}^{-\mathrm{T}}(D_1(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}))^\mathrm{T}\delta_2\chi$$

$$+\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}D_1\delta_2\chi\cdot JJ^{-\mathrm{T}}-(D_1(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}))^\mathrm{T}\delta_2\chi\cdot JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}$$

$$-(D_1(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}))^\mathrm{T}\delta_2\chi\cdot JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}-D_1\delta_2\chi^\mathrm{T}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\cdot JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}$$

$$-D_1\delta_2\chi^\mathrm{T}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}]\,dv_\mathbf{x}$$

$$= \int_B [D_1(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha})\cdot JJ^{-1}\delta_2\chi+\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\,\mathrm{div}_1\,(JJ^{-1}\delta_2\chi)$$

$$-\mathrm{div}_1(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\delta_2\chi JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha})-\mathrm{div}_1(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\cdot\delta_2\chi JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda})$$

$$+\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\delta_2\chi\,\mathrm{div}_1\,(JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha})+\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\cdot\delta_2\chi\,\mathrm{div}_1(JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda})]\,dv_\mathbf{x}$$

$$= \int_{\partial B} [\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\delta_2\chi-\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\cdot\delta_2\chi\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}-\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\delta_2\chi\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}]$$

$$\cdot JJ^{-\mathrm{T}}\mathbf{N}\,da_\mathbf{x}+\int_B [\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\cdot\delta_2\chi\,\mathrm{div}_1\,(JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda})+\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}$$

$$\cdot\delta_2\chi\,\mathrm{div}_1\,(JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha})]\,dv_\mathbf{x}, \tag{80}$$

where we systematically applied the definition of $\delta_2\mathbf{J}^*$ and eqns (45$_2$), (40), (41), (5), (8$_4$), (25$_2$), (25$_4$), Piola's identity $\mathrm{div}_1\,(JJ^{-\mathrm{T}}) = 0$, (25$_1$) and (34$_2$). The above proof also requires the symmetry of $\mathbf{J}^{-\mathrm{T}}(D_1(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}))^\mathrm{T}$, indeed, eqn (8$_5$) and repeated use of eqn (47) yields $(\mathbf{J}^{-\mathrm{T}}(D_\mathbf{x}(\mathbf{J}^{-\mathrm{T}}\nabla_\mathbf{x}\hat{\lambda}))^\mathrm{T})^\mathrm{T} = D_\mathbf{x}(\mathbf{J}^{-\mathrm{T}}\nabla_\mathbf{x}\hat{\lambda})\mathbf{J}^{-1} = D_\mathbf{x}(\nabla_\mathbf{x}\lambda)$. So symmetry is proved as $D_\mathbf{x}(\nabla_\mathbf{x}\lambda)$ is symmetric by eqn (12). Again, for clarity, the subscripts $\mathbf{X}$ and $\mathbf{x}$ denote differentiation of fields on $\mathscr{T}$ and $B\times\mathscr{D}^M$ with respect to the first argument.

Substituting eqn (80) into eqn (79) gives

$$\int_{\partial B_1}\hat{\lambda}\delta_2\mathbf{J}^*\nabla_1\hat{\alpha}\cdot\mathbf{N}\,da_\mathbf{x}-\int_{\partial B}[\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\delta_2\chi-\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\cdot\delta_2\chi\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}$$

$$-\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\delta_2\chi\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}]\cdot JJ^{-\mathrm{T}}\mathbf{N}\,da_\mathbf{x}-\int_B [\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}\cdot\delta_2\chi\,\mathrm{div}_1\,(JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda})$$

$$+\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\lambda}\cdot\delta_2\chi\,\mathrm{div}_1\,(JJ^{-1}\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha})]\,dv_\mathbf{x}+\int_{\partial B_2}\hat{\lambda}(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{q}^p\cdot\delta_2\chi K$$

$$+\delta_2 q^p K+\hat{q}^p\delta_2 K)\,da_\mathbf{x}-\int_{\partial B_1}(\mathbf{J}^{-\mathrm{T}}\nabla_1\hat{\alpha}^p\cdot\delta_2\chi+\delta_2\alpha^p)\mathbf{J}^*\nabla_1\hat{\lambda}\cdot\mathbf{N}\,da_\mathbf{x}=$$

$$-\int_{\partial B_1}\hat{\lambda}\mathbf{J}^*\nabla_1\delta_2\hat{\alpha}\cdot\mathbf{N}\,da_\mathbf{x}+\int_{\partial B_2}\delta_2\hat{\alpha}\mathbf{J}^*\nabla_1\hat{\lambda}\cdot\mathbf{N}\,da_\mathbf{x}$$

$$-\int_B \delta_2\hat{\alpha}\,\mathrm{div}_1\,(\mathbf{J}^*\nabla_1\hat{\lambda})\,dv_\mathbf{x}. \tag{81}$$

Now, we use eqn (66₁) and the property of the fundamental solution to eliminate the remaining domain integrals, whereby

$$\int_{\partial B_1} \hat{\lambda}\delta_2 \mathbf{J}^*\nabla_1\hat{\alpha}\cdot\mathbf{N}\,da_x - \int_{\partial B} [\mathbf{J}^{-T}\nabla_1\hat{\lambda}\cdot\mathbf{J}^{-T}\nabla_1\hat{\alpha}\delta_2\chi - \mathbf{J}^{-T}\nabla_1\hat{\alpha}\cdot\delta_2\chi\mathbf{J}^{-T}\nabla_1\hat{\lambda}$$

$$-\mathbf{J}^{-T}\nabla_1\hat{\lambda}\cdot\delta_2\chi\mathbf{J}^{-T}\nabla_1\hat{\alpha}]\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N}\,da_x - \tfrac{1}{2}\mathbf{J}^{-T}\nabla_1\hat{\alpha}(\mathbb{Y},\boldsymbol{\Phi})\cdot\delta_2\chi(\mathbb{Y},\boldsymbol{\Phi};\varphi)$$

$$+\int_{\partial B_2} \hat{\lambda}(\mathbf{J}^{-T}\nabla_1\hat{q}^p\cdot\delta_2\chi K + \delta_2 q^p K + \hat{q}^p\delta_2 K)\,da_x - \int_{\partial B_1}(\mathbf{J}^{-T}\nabla_1\hat{\alpha}^p\cdot\delta_2\chi$$

$$+\delta_2\alpha^p)\mathbf{J}^*\nabla_1\hat{\lambda}\cdot\mathbf{N}\,da_x = -\int_{\partial B_1}\hat{\lambda}\mathbf{J}^*\nabla_1\delta_2\hat{\alpha}\cdot\mathbf{N}\,da_x + \int_{\partial B_2}\delta_2\hat{\alpha}\mathbf{J}^*\nabla_1\hat{\lambda}\cdot\mathbf{N}\,da_x$$

$$-\tfrac{1}{2}\delta_2\hat{\alpha}(\mathbb{Y},\boldsymbol{\Phi}) \quad \text{for} \quad \mathbb{Y}\in\partial B. \tag{82}$$

When incorporating the boundary element method, this equation may be solved in the same manner as eqn (70) so that no additional stiffness matrix assemblies or decompositions are required. As in the finite element case, we only require the pseudo load vector formation and back substitution to evaluate the pseudo response. Note that we could have derived this equation directly from eqn (70) with the use of eqn (80). Had we instead differentiated eqn (71) we would require the design derivatives of the fundamental solution $\hat{\lambda}$, as $\hat{\lambda}$ is design dependent even though λ is not. In essence the difference between differentiating eqn (70) and (71) has to do with the fact that in eqn (70), $\hat{\lambda}$ is any admissible function, therefore we can use $\delta_2\hat{\lambda}$ as it too will be admissible. Thus, when we differentiate eqn (70), the coefficients of the $\delta_2\hat{\lambda}$ terms cancel by virtue of eqn (70). On the other hand, if we differentiate eqn (71), the $\delta_2\hat{\lambda}$ terms do not cancel, and therefore must be included.

The above analyses are valid for a specific design variation φ. However, we may compute each of the response gradient components $(\nabla_2\hat{\alpha})_i$ by appropriately defining the components of φ as $\varphi_j = \delta_{ij}$ where δ_{ij} is the Kronecker delta. Upon obtaining all of the $(\nabla_2\hat{\alpha})_i$ we may compute ∇G and subsequently $\delta G = \nabla G\cdot\varphi$ for any design perturbation. Note that the evaluation of $\nabla\hat{\alpha}$ requires M pseudo analyses, M being the dimension of the design space $\mathscr{D}^M$.

4.4. Adjoint method

In the adjoint method we *eliminate* the response variations $\delta_2\hat{\alpha}$ and $\nabla_1\delta_2\hat{\alpha}$. This is accomplished via the standard Lagrange multiplier method where we impose a subsidiary condition on G. In this case, the subsidiary condition is the governing integral equation (67) and we define the augmented functional G^+ as

$$G^+(\boldsymbol{\Phi}) = \int_{\partial B}\hat{g}(\hat{\alpha},\mathbf{J}^{-T}\nabla_1\hat{\alpha}\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N}/K,\chi)K\,da_x - \int_B\hat{\lambda}\,\mathrm{div}_1\,(\mathbf{J}\mathbf{J}^{-1}\mathbf{J}^{-T}\nabla_1\hat{\alpha})\,dv_x, \tag{83}$$

where $\hat{\lambda}$ plays the role of the Lagrange multiplier. Note that $G = G^+$ since the augmented term is identically zero.

Next, we proceed to take the design variation of G^+ and note that $\delta G = \delta G^+$ since the design variation of the augmented term is zero. Using eqns (74) and (79) [the latter is derived from the design variation of eqn (67)], and (67) (where $\delta_2\hat{\lambda}$ replaces $\hat{\lambda}$) we arrive at the following expression for δG^+:

$$\delta G^+ = \int_{\partial B}[\nabla_1\hat{g}\delta_2\hat{\alpha}K + \nabla_2\hat{g}(\nabla_1\delta_2\hat{\alpha}\cdot\mathbf{J}^*\mathbf{N} + \nabla_1\hat{\alpha}\cdot\delta_2\mathbf{J}^*\mathbf{N} - \nabla_1\hat{\alpha}\cdot\mathbf{J}^*\mathbf{N}\delta_2 K/K)$$

$$+\nabla_3\hat{g}\cdot\delta_2\chi K + \hat{g}\delta_2 K]\,da_x - \int_{\partial B_1}\hat{\lambda}\delta_2\mathbf{J}^*\nabla_1\hat{\alpha}\cdot\mathbf{N}\,da_x + \int_B\nabla_1\hat{\lambda}\cdot\delta_2\mathbf{J}^*\nabla_1\hat{\alpha}\,dv_x$$

$$-\int_{\partial B_2} \hat{\lambda}(\mathbf{J}^{-T}\nabla_1\hat{q}^p \cdot \delta_2\chi K + \delta_2 q^p K + \hat{q}^p\delta_2 K)\,da_{\mathbf{x}} + \int_{\partial B_1}(\mathbf{J}^{-T}\nabla_1\hat{\alpha}^p \cdot \delta_2\chi$$

$$+ \delta_2\alpha^p)\mathbf{J}^*\nabla_1\hat{\lambda}\cdot\mathbf{N}\,da_{\mathbf{x}} - \int_{\partial B_1}\hat{\lambda}\mathbf{J}^*\nabla_1\delta_2\hat{\alpha}\cdot\mathbf{N}\,da_{\mathbf{x}} + \int_{\partial B_2}\delta_2\hat{\alpha}\mathbf{J}^*\nabla_1\hat{\lambda}\cdot\mathbf{N}\,da_{\mathbf{x}}$$

$$-\int_B \delta_2\hat{\alpha}\,\mathrm{div}_1\,(\mathbf{J}^*\nabla_1\hat{\lambda})\,dv_{\mathbf{x}}. \tag{84}$$

Rearranging the above to isolate the explicit δG_E^+, and implicit δG_I^+, variations gives

$$\delta G^+ = \delta G_E^+ + \delta G_I^+, \tag{85}$$

where

$$\delta G_E^+ = \int_{\partial B}[\nabla_3\hat{g}\cdot\delta_2\chi K + \hat{g}\delta_2 K]\,da_{\mathbf{x}} + \int_{\partial B_1}[\nabla_2\hat{g}(\nabla_1\hat{\alpha}\cdot\delta_2\mathbf{J}^*\mathbf{N}$$

$$-\nabla_1\hat{\alpha}\cdot\mathbf{J}^*\mathbf{N}\delta_2 K/K)]\,da_{\mathbf{x}} + \int_{\partial B_2}\nabla_2\hat{g}(\mathbf{J}^{-T}\nabla_1\hat{q}^p \cdot \delta_2\chi K + \delta_2 q^p K)\,da_{\mathbf{x}}$$

$$-\int_{\partial B_1}\hat{\lambda}\delta_2\mathbf{J}^*\nabla_1\hat{\alpha}\cdot\mathbf{N}\,da_{\mathbf{x}} + \int_B \nabla_1\hat{\lambda}\cdot\delta_2\mathbf{J}^*\nabla_1\hat{\alpha}\,dv_{\mathbf{x}}$$

$$-\int_{\partial B_2}\hat{\lambda}(\mathbf{J}^{-T}\nabla_1\hat{q}^p \cdot \delta_2\chi K + \delta_2 q^p K + \hat{q}^p\delta_2 K)\,da_{\mathbf{x}}$$

$$+\int_{\partial B_1}(\mathbf{J}^{-T}\nabla_1\hat{\alpha}^p \cdot \delta_2\chi + \delta_2\alpha^p)(\mathbf{J}^*\nabla_1\hat{\lambda}\cdot\mathbf{N} + \nabla_1\hat{g}K)\,da_{\mathbf{x}}, \tag{86}$$

and using the symmetry of $\mathbf{J}^*$

$$\delta G_I^+ = \int_{\partial B_1}(\nabla_2\hat{g} - \hat{\lambda})\nabla_1\delta_2\hat{\alpha}\cdot\mathbf{J}^*\mathbf{N}\,da_{\mathbf{x}} + \int_{\partial B_2}(\nabla_1\hat{g}K + \mathbf{J}^*\nabla_1\hat{\lambda}\cdot\mathbf{N})\delta_2\hat{\alpha}\,da_{\mathbf{x}}$$

$$-\int_B \delta_2\hat{\alpha}\,\mathrm{div}_1\,(\mathbf{J}^*\nabla_1\hat{\lambda})\,dv_{\mathbf{x}}. \tag{87}$$

The objective now is to determine the *adjoint* response $\hat{\lambda}$ which drives δG_I^+ to zero. Then we can substitute this $\hat{\lambda}$ into eqn (84) so that $\delta G = \delta G^+ = \delta G_E^+$ can be explicitly computed. Upon examination of the above, we see that to annihilate δG_I^+ the following conditions must be attained:

$$\mathrm{div}_1\,(JJ^{-1}J^{-T}\nabla_1\hat{\lambda}) = 0 \qquad \text{for} \quad (\mathbb{X},\mathbf{\Phi})\in B\times\mathscr{D}^M,$$

$$\hat{\lambda} = \nabla_2\hat{g} \qquad \text{for} \quad (\mathbb{X},\mathbf{\Phi})\in\partial B_1\times\mathscr{D}^M,$$

$$J^{-T}\nabla_1\hat{\lambda}\cdot JJ^{-T}\mathbf{N} = -\nabla_1\hat{g}K \qquad \text{for} \quad (\mathbb{X},\mathbf{\Phi})\in\partial B_2\times\mathscr{D}^M, \tag{88}$$

where we use the definition of $\mathbf{J}^*$. Note that with the exception of the data, this adjoint problem is identical to the primal problem [cf. eqn (66)] and hence, we may evaluate the adjoint response via either the finite or boundary element methods. So when these methods are used to evaluate the primal response, then the decomposed stiffness matrix may be used to compute the adjoint response. We merely form the adjoint load vector where we replace $\hat{\alpha}^p$ and $\hat{q}^p$ with $\nabla_2\hat{g}$ and $-\nabla_1\hat{g}$, respectively; and perform the back substitution.

Substituting eqn (88_2) into (86), gives

$$\delta G_E^+ = \int_{\partial B} [\nabla_3 \hat{g} \cdot \delta_2 \chi K + \hat{g} \delta_2 K] \, da_x + \int_{\partial B_1} [\nabla_2 \hat{g}(-\nabla_2 \hat{\alpha} \cdot \mathbf{J^*N} \delta_2 K/K)] \, da_x$$

$$+ \int_{\partial B_2} \nabla_2 \hat{g}(\mathbf{J^{-T}} \nabla_1 \hat{q}^p \cdot \delta_2 \chi K + \delta_2 q^p K) \, da_x + \int_B \nabla_1 \hat{\lambda} \cdot \delta_2 \mathbf{J^*} \nabla_1 \hat{\alpha} \, dv_x$$

$$- \int_{\partial B_2} \hat{\lambda}(\mathbf{J^{-T}} \nabla_1 \hat{q}^p \cdot \delta_2 \chi K + \delta_2 q^p K + \hat{q}^p \delta_2 K) \, da_x$$

$$+ \int_{\partial B_1} (\mathbf{J^{-T}} \nabla_1 \hat{\alpha}^p \cdot \delta_2 \chi + \delta_2 \alpha^p)(\mathbf{J^*} \nabla_1 \hat{\lambda} \cdot \mathbf{N} + \nabla_1 \hat{g} K) \, da_x. \qquad (89)$$

This equation is best suited for finite element applications where all of the information is accurately extracted within the domain. If the boundary element method is used to evaluate the sensitivities it is advantageous to use eqn (80) to express

$$\delta G_E^+ = \int_{\partial B} [\nabla_3 \hat{g} \cdot \delta_2 \chi K + \hat{g} \delta_2 K] \, da_x + \int_{\partial B_1} [\nabla_2 \hat{g}(-\nabla_1 \hat{\alpha} \cdot \mathbf{J^*N} \delta_2 K/K)] \, da_x$$

$$+ \int_{\partial B_2} \nabla_2 \hat{g}(\mathbf{J^{-T}} \nabla_1 \hat{q}^p \cdot \delta_2 \chi K + \delta_2 q^p K) \, da_x + \int_{\partial B} [\mathbf{J^{-T}} \nabla_1 \hat{\lambda} \cdot \mathbf{J^{-T}} \nabla_1 \hat{\alpha} \delta_2 \chi$$

$$- \mathbf{J^{-T}} \nabla_1 \hat{\lambda} \cdot \delta_2 \chi \mathbf{J^{-T}} \nabla_1 \hat{\alpha} - \mathbf{J^{-T}} \nabla_1 \hat{\alpha} \cdot \delta_2 \chi \mathbf{J^{-T}} \nabla_1 \hat{\lambda}] \cdot \mathbf{JJ^{-T}N} \, da_x$$

$$- \int_B [\mathbf{J^{-T}} \nabla_1 \hat{\alpha} \cdot \delta_2 \chi \, \text{div}_1 \, (JJ^{-1} \mathbf{J^{-T}} \nabla_1 \hat{\lambda}) + \mathbf{J^{-T}} \nabla_1 \hat{\lambda} \cdot \delta_2 \chi \, \text{div}_1 \, (JJ^{-1} \mathbf{J^{-T}} \nabla_1 \hat{\alpha})] \, dv_x$$

$$- \int_{\partial B_2} \hat{\lambda}(\mathbf{J^{-T}} \nabla_1 \hat{q}^p \cdot \delta_2 \chi K + \delta_2 q^p K + \hat{q}^p \delta_2 K) \, da_x$$

$$+ \int_{\partial B_1} [(\mathbf{J^{-T}} \nabla_1 \hat{\alpha}^p \cdot \delta_2 \chi + \delta_2 \alpha^p)(\nabla_1 \hat{g} K + \mathbf{J^*} \nabla_1 \hat{\lambda} \cdot \mathbf{N})] \, da_x. \qquad (90)$$

We use eqns (66_1) and (88_1) to eliminate the domain integral, thus

$$\delta G_E^+ = \int_{\partial B} [\nabla_3 \hat{g} \cdot \delta_2 \chi K + \hat{g} \delta_2 K] \, da_x + \int_{\partial B_1} [\nabla_2 \hat{g}(-\nabla_1 \hat{\alpha} \cdot \mathbf{J^*N} \delta_2 K/K)] \, da_x$$

$$+ \int_{\partial B_2} \nabla_2 \hat{g}(\mathbf{J^{-T}} \nabla_1 \hat{q}^p \cdot \delta_2 \chi K + \delta_2 q^p K) \, da_x + \int_{\partial B} [\mathbf{J^{-T}} \nabla_1 \hat{\lambda} \cdot \mathbf{J^{-T}} \nabla_1 \hat{\alpha} \delta_2 \chi$$

$$- \mathbf{J^{-T}} \nabla_1 \hat{\lambda} \cdot \delta_2 \chi \mathbf{J^{-T}} \nabla_1 \hat{\alpha} - \mathbf{J^{-T}} \nabla_1 \hat{\alpha} \cdot \delta_2 \chi \mathbf{J^{-T}} \nabla_1 \hat{\lambda}] \cdot \mathbf{JJ^{-T}N} \, da_x$$

$$- \int_{\partial B_2} \hat{\lambda}(\mathbf{J^{-T}} \nabla_1 \hat{q}^p \cdot \delta_2 \chi K + \delta_2 q^p K + \hat{q}^p \delta_2 K) \, da_x$$

$$+ \int_{\partial B_1} [(\mathbf{J^{-T}} \nabla_1 \hat{\alpha}^p \cdot \delta_2 \chi + \delta_2 \alpha^p)(\nabla_1 \hat{g} K + \mathbf{J^*} \nabla_1 \hat{\lambda} \cdot \mathbf{N})] \, da_x. \qquad (91)$$

This equation is best suited for boundary element applications in which accurate gradients are readily extracted over the surface [however, it may also be evaluated via a finite element analysis, although it has been shown to be less accurate than eqn (86) (Haug *et al.*, 1986)]. Finally, note that for the boundary element adjoint sensitivity analysis, we again require no differentiation of the fundamental equation.

In the adjoint approach, we are able to compute ∇G directly after the solution of one adjoint problem, whereas in the direct method we require the solution of M pseudo

problems. However, the adjoint approach requires the solution of one problem for each functional G, so if the functions out number the dimension of the design space, then the direct approach is preferred, and vice versa.

5. MATERIAL DERIVATIVE METHOD

We may derive the material derivative method solutions directly from the domain parameterization method. In material derivative formulations $\phi \in \mathscr{D} \subset \mathscr{R}$ and the scalar $\boldsymbol{\Phi}$ is analogous to time [cf. Haug *et al.* (1986), eqn (3.2.1)]. The reference configuration coincides with the body configuration so that $x = \mathbb{X} = \chi(\mathbb{X}, \boldsymbol{\Phi})$.

The *design velocity* $\mathbf{v} \colon B \times \mathscr{D}^M \to \text{Lin} (\mathscr{D}^M, \mathscr{V}^n)$ is defined as

$$\mathbf{v}(\mathbb{X}, \boldsymbol{\Phi}; \varphi) = \delta_2 \chi(\mathbb{X}, \boldsymbol{\Phi}; \varphi). \tag{92}$$

This definition merely equates the design velocity to the design variation of χ in the direction φ.

For this choice of χ, $D_1\chi(\mathbb{X}, \boldsymbol{\Phi})[\mathbf{U}] = \mathbf{U}$ so that $J(\mathbb{X}, \boldsymbol{\Phi}) = 1$, $K(\mathbb{X}, \boldsymbol{\Phi}) = 1$, $\mathbf{J}(\mathbb{X}, \boldsymbol{\Phi}) = \mathbf{I}$ and $\mathbf{n}(\chi(\mathbb{X}, \boldsymbol{\Phi}), \boldsymbol{\Phi}) = \mathbf{N}(\mathbb{X}, \boldsymbol{\Phi})$. Substitution of these values into eqns (37), (39), (40), (41) and (45) allows us to obtain eqns (3.2.15)–(3.2.18) in Haug *et al.* (1986), respectively, i.e.

$$D_2 J = D_1 \mathbf{v}; \; D_2 \mathbf{J}^{\mathrm{T}} = D_1 \mathbf{v}^{\mathrm{T}}; \; D_2 \mathbf{J}^{-1} = -D_1 \mathbf{v}; \; D_2 \mathbf{J}^{-\mathrm{T}} = -D_1 \mathbf{v}^{\mathrm{T}}; \; D_2 J = \text{div} \, \mathbf{v}. \tag{93}$$

The simplified equations (61), (63) and (62) are identical to eqns (3.2.29)–(3.2.31) in Haug *et al.* (1986). For this choice of the reference configuration, eqn (64) becomes

$$\delta_2 K = \text{div} \, \mathbf{v} - \mathbf{n} \cdot D_1 \mathbf{v}^{\mathrm{T}} \mathbf{n} = \mathbf{v} \cdot \mathbf{n} H, \tag{94}$$

which is consistent with eqns (3.2.34) and (3.2.95) in Haug *et al.* (1986), where the restriction $\mathbf{v}(\mathbb{X}, \boldsymbol{\Phi}; \varphi) = V(\mathbb{X}, \boldsymbol{\Phi}; \varphi) \mathbf{N}(\mathbb{X})$, i.e. $\mathbf{v}$ is a normal velocity with magnitude $V(\mathbb{X}, \boldsymbol{\Phi}, \varphi)$, and $H = \text{div} \, \mathbf{n}$ is the surface curvature which is applied to the rightmost equality.

Equation (89) for $\delta \hat{G}_{\mathrm{E}}^+$ is consistent with the equation derived via the "domain" approach of the material derivative method which appears in Haug *et al.* (1986). To reduce this equation, we let $\nabla_3 \hat{g} = \nabla_2 \hat{g} = 0$, recall that $J = 1$, $K = 1$, $\mathbf{J} = I$, $\mathbf{v} = V\mathbf{n}$, $\delta_2 K = H\mathbf{v} \cdot \mathbf{n}$, and use the identity (resulting from an application of the divergence theroem on the $(\delta_2 J) \mathbf{J}^{-1} \mathbf{J}^{-\mathrm{T}}$ term)

$$\int_B \nabla_1 \hat{\lambda} \cdot \delta_2 (J \mathbf{J}^{-1} \mathbf{J}^{-\mathrm{T}}) \nabla_1 \hat{\alpha} \, dv_{\mathbb{X}} = \int_{\partial B} \mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{\lambda} \cdot \mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{\alpha} \mathbf{v} \cdot J \mathbf{J} \mathbf{J}^{-\mathrm{T}} \mathbf{N} \, da_{\mathbb{X}}$$

$$- \int_B [\mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{\lambda} \cdot \mathbf{J}^{-\mathrm{T}} \nabla_1 (\mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{\alpha} \cdot \mathbf{v}) + \mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{\alpha} \cdot \mathbf{J}^{-\mathrm{T}} \nabla_1 (\mathbf{J}^{-\mathrm{T}} \nabla_1 \hat{\lambda} \cdot \mathbf{v})] J \, dv_{\mathbb{X}}$$

to obtain

$$\delta G_{\mathrm{E}}^+ = \int_{\partial B} \hat{g} H \mathbf{v} \cdot \mathbf{n} \, da_{\mathbb{X}} + \int_{\partial B} \nabla_1 \lambda \cdot \nabla_1 \alpha \mathbf{v} \cdot \mathbf{n} \, da_{\mathbb{X}}$$

$$- \int_B [\nabla_1 \lambda \cdot \nabla_1 (\nabla_1 \alpha \cdot \mathbf{v}) + \nabla_1 \alpha \cdot \nabla_1 (\nabla_1 \lambda \cdot \mathbf{v})] \, dv_{\mathbb{X}}. \tag{95}$$

This is identical to eqn (24) in Park and Yoo (1988) after the appropriate simplifications have been made to their analysis.

Equation (91) is consistent with the "boundary" version of the sensitivity equation which appears in Haug *et al.* (1986). To arrive at the material derivative version of this
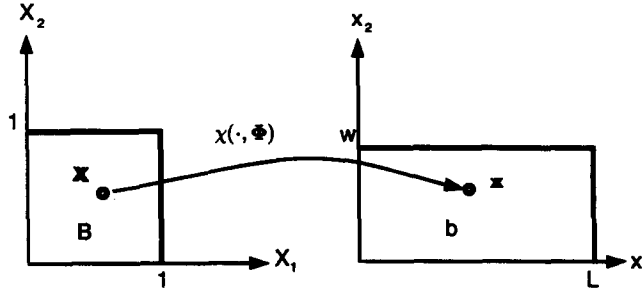
Fig. 5. Referential map.

equation, we set $\nabla_3 \hat{g} = 0$, use $J = 1$, $K = 1$ and $\mathbf{J} = \mathbf{I}$, $\mathbf{n} = \mathbf{N}$; and require that $\mathbf{v} = V\mathbf{n}$, so that $\delta_2 K = H\mathbf{v} \cdot \mathbf{n}$. In light of these equalities, eqn (91) reduces to

$$\delta G_E^+ = \int_{\partial B} \hat{g} H\mathbf{v} \cdot \mathbf{n} \, da_{\mathbf{x}} - \int_{\partial B_1} \nabla_2 \hat{g} (\nabla_1 \alpha \cdot \mathbf{n} H\mathbf{v} \cdot \mathbf{n}) \, da_{\mathbf{x}} + \int_{\partial B_2} \nabla_2 \hat{g} (\nabla_1 q^p \cdot \mathbf{v} + \delta_2 q^p) \, da_{\mathbf{x}}$$

$$- \int_{\partial B} \nabla_1 \alpha \cdot \mathbf{v} \nabla_1 \lambda \cdot \mathbf{n} \, da_{\mathbf{x}} + \int_{\partial B} [\nabla_1 \lambda \cdot \nabla_1 \alpha \mathbf{v} - \nabla_1 \lambda \cdot \mathbf{v} \nabla_1 \alpha] \cdot \mathbf{n} \, da_{\mathbf{x}}$$

$$- \int_{\partial B_2} \lambda (\nabla_1 q^p \cdot \mathbf{v} + \delta_2 q^p + q^p H\mathbf{v} \cdot \mathbf{n}) \, da_{\mathbf{x}} + \int_{\partial B_1} (\nabla_1 \alpha^p \cdot \mathbf{v} + \delta_2 \alpha^p)(\nabla_1 \hat{g} + \nabla_1 \lambda \cdot \mathbf{n}) \, da_{\mathbf{x}}.$$

(96)

This equation is identical to eqn (23) in Meric (1988) after the appropriate simplifications are made to their analysis.

6. EXAMPLE

In the following example, we present a simple problem with an analytical solution to validate the previous methodologies. It is henceforth understood that vectors and tensors will be identified by their matrices of components.

6.1. *Mapping*

Consider the reference configuration via the map (see Fig. 5)

$$\chi_1(\mathbb{X}, \mathbf{\Phi}) = x_1 = L\mathbb{X}_1,$$

$$\chi_2(\mathbb{X}, \mathbf{\Phi}) = x_2 = w\mathbb{X}_2,$$

(97)

where $(\mathbb{X}_1, \mathbb{X}_2)$, (x_1, x_2) and (w, L) are respectively the components of $\mathbb{X} \in \mathscr{E}^2$, $x \in \mathscr{E}^2$ and $\mathbf{\Phi} \in \mathscr{R}^2$. This mapping transforms the reference configuration $\{(\mathbb{X}_1, \mathbb{X}_2); 0 \leqslant \mathbb{X}_1 \leqslant 1, 0 \leqslant \mathbb{X}_2 \leqslant 1\}$ into the body configuration $\{(x_1, x_2); 0 \leqslant x_1 \leqslant L, 0 \leqslant x_2 \leqslant w\}$.

For this mapping [eqn (97)], we obtain the Jacobian from eqn (30):

$$\mathbf{J}(\mathbb{X}, \mathbf{\Phi}) = \nabla_1 \chi(\mathbb{X}, \mathbf{\Phi}) = \begin{pmatrix} L & 0 \\ 0 & w \end{pmatrix}.$$

(98)

The above results yield

$$J = \det \mathbf{J}(\mathbb{X}, \mathbf{\Phi}) = Lw, \tag{99}$$

$$\mathbf{J}^{-1} = \mathbf{J}^{-T} = \begin{bmatrix} \dfrac{1}{L} & 0 \\ 0 & \dfrac{1}{w} \end{bmatrix} \tag{100}$$

and

$$\mathbf{J}^* = J\mathbf{J}^{-1}\mathbf{J}^{-T} = Lw \begin{bmatrix} \dfrac{1}{L} & 0 \\ 0 & \dfrac{1}{w} \end{bmatrix} \begin{bmatrix} \dfrac{1}{L} & 0 \\ 0 & \dfrac{1}{w} \end{bmatrix} = \begin{bmatrix} \dfrac{w}{L} & 0 \\ 0 & \dfrac{L}{w} \end{bmatrix}. \tag{101}$$

We evaluate K from eqn (62). On the boundaries $\mathbb{X}_2 = 0$ and $\mathbb{X}_2 = 1$, $\mathbf{N}(\mathbb{X}) = (0, -1)^T$ and $\mathbf{N}(\mathbb{X}) = (0, 1)^T$, hence

$$K(\mathbb{X}, \mathbf{\Phi}) = Lw \left\| \begin{bmatrix} \dfrac{1}{L} & 0 \\ 0 & \dfrac{1}{w} \end{bmatrix} \begin{pmatrix} 0 \\ \pm 1 \end{pmatrix} \right\| = L. \tag{102}$$

Similarly on the boundaries $\mathbb{X}_1 = 0$ and $\mathbb{X}_1 = 1$, $\mathbf{N}(\mathbb{X}) = (-1, 0)^T$ and $\mathbf{N}(\mathbb{X}) = (1, 0)^T$

$$K(\mathbb{X}, \mathbf{\Phi}) = Lw \left\| \begin{bmatrix} \dfrac{1}{L} & 0 \\ 0 & \dfrac{1}{w} \end{bmatrix} \begin{pmatrix} \pm 1 \\ 0 \end{pmatrix} \right\| = w. \tag{103}$$

For a design variation of $\varphi = (\delta w, \delta L)$, we obtain $\delta_2 \chi$ from eqns (22_1)

$$\delta_2 \chi(\mathbb{X}, \mathbf{\Phi}; \varphi) = \begin{pmatrix} \mathbb{X}_1 \delta L \\ \mathbb{X}_2 \delta w \end{pmatrix}. \tag{104}$$

We may verify eqn (37) from (104)

$$\nabla_1 \delta_2 \chi(\mathbb{X}, \mathbf{\Phi}; \varphi) = \begin{pmatrix} \delta L & 0 \\ 0 & \delta w \end{pmatrix} \tag{105}$$

and verify eqn (40) from (100)

$$\delta_2 \mathbf{J}^{-1}(\mathbb{X}, \mathbf{\Phi}; \varphi) = \begin{bmatrix} \dfrac{-\delta L}{L^2} & 0 \\ 0 & \dfrac{-\delta w}{w^2} \end{bmatrix}. \tag{106}$$

Similarly we may verify eqn (45) from (99)

$$\delta_2 J(\mathbb{X}, \mathbf{\Phi}, \varphi) = L\delta w + w\delta L \tag{107}$$
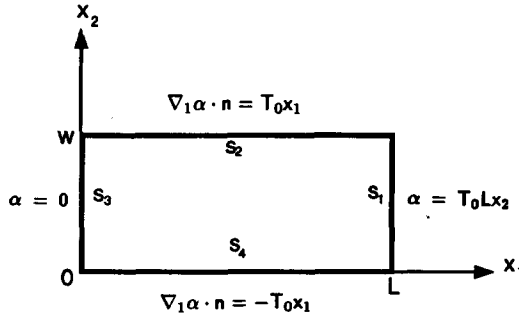
and from eqn (101), we may verify the chain rule

Fig. 6. Rectangular domain with boundary conditions.

$$\delta_2 \mathbf{J}^* = \delta_2 J \mathbf{J}^{-1}\mathbf{J}^{-T} + J\delta_2 \mathbf{J}^{-1}\mathbf{J}^{-T} + J\mathbf{J}^{-1}\delta_2 \mathbf{J}^{-T},$$

$$\delta_2 \mathbf{J}^*(\mathbb{X}, \mathbf{\Phi}\,;\,\varphi) = \begin{bmatrix} \dfrac{\delta w}{L} & 0 \\[2mm] 0 & \dfrac{-L\delta w}{w^2} \end{bmatrix} + \begin{bmatrix} -\dfrac{w\delta L}{L^2} & 0 \\[2mm] 0 & \dfrac{\delta L}{w} \end{bmatrix}. \tag{108}$$

On the boundaries $\mathbb{X}_2 = 0$, $\mathbb{X}_2 = 1$, we verify eqn (64) from (102)

$$\delta_2 K(\mathbb{X}, \mathbf{\Phi}\,;\,\varphi) = \delta L \tag{109}$$

and on the boundaries $\mathbb{X}_1 = 0$, $\mathbb{X}_1 = 1$, we verify eqn (64) from (103)

$$\delta_2 K(\mathbb{X}, \mathbf{\Phi}\,;\,\varphi) = \delta w. \tag{110}$$

6.2. Laplace problem

Consider the following boundary value problem defined over the previously described rectangular domain and with nonhomogeneous boundary conditions (see Fig. 6) :

$$\begin{aligned}
\Delta_1 \alpha(\mathbf{x}, \mathbf{\Phi}) &= 0 && \text{for} \quad 0 \leqslant \mathbf{x}_1 \leqslant L \quad \text{and} \quad 0 \leqslant \mathbf{x}_2 \leqslant w, \\
\alpha(\mathbf{x}, \mathbf{\Phi}) &= 0 && \text{for} \quad \mathbf{x}_1 = 0, \\
\alpha(\mathbf{x}, \mathbf{\Phi}) &= T_0 L \mathbf{x}_2 && \text{for} \quad \mathbf{x}_1 = L, \\
\nabla_1 \alpha(\mathbf{x}, \mathbf{\Phi}) \cdot \mathbf{n}(\mathbf{x}, \mathbf{\Phi}) &= -T_0 \mathbf{x}_1 && \text{for} \quad \mathbf{x}_2 = 0, \\
\nabla_1 \alpha(\mathbf{x}, \mathbf{\Phi}) \cdot \mathbf{n}(\mathbf{x}, \mathbf{\Phi}) &= T_0 \mathbf{x}_1 && \text{for} \quad \mathbf{x}_2 = w.
\end{aligned} \tag{111}$$

Using separation of variables (Boyce and Diprima, 1986), the solution is readily determined

$$\alpha(\mathbf{x}, \mathbf{\Phi}) = T_0 \mathbf{x}_1 \mathbf{x}_2. \tag{112}$$

The referential response may be evaluated from eqns (28) and (112) :

$$\hat{\alpha}(\mathbb{X}, \mathbf{\Phi}) = \alpha(\chi(\mathbb{X}), \mathbf{\Phi}) = T_0 L w \mathbb{X}_1 \mathbb{X}_2. \tag{113}$$

We may also verify eqn (66), using the above result for $\hat{\alpha}$ [i.e. eqn (113)]

$$\operatorname{div}(\mathbf{J}^* \nabla \hat{\alpha}) = \frac{w}{L} \frac{\partial^2 \hat{\alpha}}{\partial \mathbb{X}_1^2} + \frac{L}{w} \frac{\partial^2 \hat{\alpha}}{\partial \mathbb{X}_2^2} = 0 \qquad \text{for} \quad 0 \leqslant \mathbb{X}_1 \leqslant 1 \quad \text{and} \quad 0 \leqslant \mathbb{X}_2 \leqslant 1,$$

$$\hat{\alpha}(\mathbb{X}, \mathbf{\Phi}) = 0 \qquad \text{for} \quad \mathbb{X}_1 = 0,$$

$$\hat{\alpha}(\mathbb{X}, \mathbf{\Phi}) = T_0 Lw\mathbb{X}_2 \quad \text{for} \quad \mathbb{X}_1 = 1,$$

$$\frac{\partial \hat{\alpha}}{\partial \mathbb{X}_2}(\mathbb{X}, \mathbf{\Phi}) = T_0 Lw\mathbb{X}_1 \quad \text{for} \quad \mathbb{X}_2 = 0,$$

$$\frac{\partial \hat{\alpha}}{\partial \mathbb{X}_2}(\mathbb{X}, \mathbf{\Phi}) = T_0 Lw\mathbb{X}_1 \quad \text{for} \quad \mathbb{X}_2 = 1. \tag{114}$$

Here $\partial\hat{\alpha}/\partial\mathbb{X}_i = D_1\hat{\alpha}\cdot\mathbf{E}_i$, i.e. the partial derivative of $\hat{\alpha}$ with respect to $\mathbb{X}_i$ of the $\{\mathbb{O}; \mathbf{E}_i\}$ coordinate system.

6.3. Response function

We choose to evaluate the net flux over surface S_1 (see Fig. 6), therefore the following response functional is defined

$$G(\mathbf{\Phi}) = \int_{S_1} \nabla\alpha\cdot\mathbf{n}\, da_\mathbf{x}, \tag{115}$$

where $g = \nabla\alpha\cdot\mathbf{n}$ in eqn (72).

In the reference domain, this functional is expressed as [see eqn (73)]

$$G(\mathbf{\Phi}) = \int_{S_1} \nabla\hat{\alpha}\cdot\mathbf{J^*N}\, da_\mathbf{x}, \tag{116}$$

where $\hat{g} = \mathbf{J}^{-T}\nabla\hat{\alpha}\cdot\mathbf{J}\mathbf{J}^{-T}\mathbf{N}/K = \nabla\hat{\alpha}\cdot\mathbf{J^*N}/K$. Using eqns (112), (113) and (101) we confirm that eqns (115) and (116) yield identical results:

$$G(\mathbf{\Phi}) = \int_{S_1} \frac{\partial\alpha}{\partial\mathbf{x}_1}\, da_\mathbf{x} = \frac{T_0 w^2}{2} = \int_{S_1} \frac{w}{L}\frac{\partial\hat{\alpha}}{\partial\mathbb{X}_1}\, da_\mathbf{x}. \tag{117}$$

Here $\partial\alpha/\partial\mathbf{x}_i = D_1\alpha\cdot\mathbf{e}_i$, i.e. the partial derivative of α with respect to $\mathbf{x}_i$ of the $\{\mathbb{o}; \mathbf{e}_i\}$ coordinate system.

Next we consider the shape variation $w \to w + \delta w$ and $L \to L + \delta L$ and from eqn (112), we obtain

$$\delta_2\alpha(\mathbf{x}, \mathbf{\Phi}; \varphi) = 0. \tag{118}$$

We may also determine this result from eqn (76)

$$\delta_2\alpha(\chi(\mathbb{X}, \mathbf{\Phi}), \mathbf{\Phi}; \varphi) = \delta_2\hat{\alpha}(\mathbb{X}, \mathbf{\Phi}; \varphi) - \mathbf{J}^{-T}(\mathbb{X}, \mathbf{\Phi}, \varphi)\nabla_1\hat{\alpha}(\mathbb{X}, \mathbf{\Phi})\cdot\delta_2\chi,$$

$$0 = \delta_2\hat{\alpha}(\mathbb{X}, \mathbf{\Phi}; \varphi) - \begin{pmatrix} T_0 w\mathbb{X}_2 \\ T_0 L\mathbb{X}_1 \end{pmatrix}\cdot\begin{pmatrix} \mathbb{X}_1\delta L \\ \mathbb{X}_2\delta w \end{pmatrix},$$

where, a direct calculation for eqn (113) gives

$$\delta_2\hat{\alpha}(\mathbb{X}, \mathbf{\Phi}; \varphi) = T_0 L\mathbb{X}_1\mathbb{X}_2\delta w + T_0 w\mathbb{X}_1\mathbb{X}_2\delta L. \tag{119}$$

6.4. Direct differentiation and adjoint method

We may verify the solution $\delta_2\hat{\alpha}$ in (119) by the direct differentiation method, where $\delta_2\hat{\alpha}$ satisfies eqn (75). For our example, eqn (75) becomes

$$\frac{w}{L}\frac{\partial^2 \delta_2 \hat{\alpha}}{\partial X_1^2} + \frac{L}{w}\frac{\partial^2 \delta_2 \hat{\alpha}}{\partial X_2^2} = \left(-\frac{\delta w}{L} + \frac{w\delta L}{L^2}\right)\frac{\partial^2 \hat{\alpha}}{\partial X_1^2} + \left(\frac{L\delta w}{w^2} - \frac{\delta L}{w}\right)\frac{\partial^2 \hat{\alpha}}{\partial X_2^2}$$

$$\text{for} \quad 0 \leqslant X_1 \leqslant 1 \quad \text{and} \quad 0 \leqslant X_2 \leqslant 1,$$

$$\delta_2 \hat{\alpha}(\mathbb{X}, \boldsymbol{\Phi}) = 0 \qquad\qquad\qquad \text{for} \quad X_1 = 0,$$

$$\delta_2 \hat{\alpha}(\mathbb{X}, \boldsymbol{\Phi}) = T_0 L X_2 \delta w + T_0 w X_2 \delta L \quad \text{for} \quad X_1 = 1,$$

$$\nabla_1 \delta_2 \hat{\alpha} \cdot \mathbf{J^*N} + \nabla_1 \hat{\alpha} \cdot \delta_2 \mathbf{J^*N} = -2T_0 L X_1 \delta L \qquad \text{for} \quad X_2 = 0,$$

$$\nabla_1 \delta_2 \hat{\alpha} \cdot \mathbf{J^*N} + \nabla_1 \hat{\alpha} \cdot \delta_2 \mathbf{J^*N} = 2T_0 L x_1 \delta L \qquad \text{for} \quad X_2 = 1. \tag{120}$$

Where $\delta_2 \mathbf{J^*}$ is given in eqn (108). A straightforward calculation may be used to validate eqn (119) as the solution to the above problem.

From eqn (74), we obtain (with $\nabla_1 g = \nabla_3 g = 0$)

$$\delta G = \int_{S_1} [\nabla_2 \hat{g}(\nabla_1 \delta_2 \hat{\alpha} \cdot \mathbf{J^*N} + \nabla_1 \hat{\alpha} \cdot \delta_2 \mathbf{J^*N} - \nabla_1 \hat{\alpha} \cdot \mathbf{J^*N}\delta_2 K/K) + \hat{g}\delta_2 K]\, da_{\mathbb{X}}. \tag{121}$$

The variation of G is also determined directly from eqn (117)

$$\delta_2 G(\boldsymbol{\Phi}; \varphi) = T_0 w \delta w.$$

To verify the direct differentiation method, we substitute eqns (108), (110) and (119) into eqn (121), and obtain the identical result, i.e. $\delta G = T_0 w \delta w$.

We may also obtain the same result by the adjoint method. In this technique, we first evaluate the adjoint response $\hat{\lambda}$, which from eqns (88) and (117), must satisfy

$$\text{div}_1 (JJ^{-1}J^{-T}\nabla_1 \hat{\lambda}) = 0 \quad \text{for} \quad 0 \leqslant X_1 \leqslant 1 \quad \text{and} \quad 0 \leqslant X_2 \leqslant 1,$$

$$\hat{\lambda} = 0 \quad \text{for} \quad X_1 = 0,$$

$$\hat{\lambda} = 1 \quad \text{for} \quad X_1 = 1,$$

$$\mathbf{J^{-T}}\nabla_1 \hat{\lambda} \cdot JJ^{-T}\mathbf{N} = 0 \quad \text{for} \quad X_2 = 0 \quad \text{and} \quad X_2 = 1. \tag{122}$$

The solution is determined by separation of variables as

$$\hat{\lambda} = X_1. \tag{123}$$

Using the above result, and eqns (99), (100), (101), (102), (103), (106), (107), (108), (110) and (113), we may evaluate the adjoint sensitivity via either eqn (89) or (91)

$$\delta G_E^+ = \int_{S_1} \hat{g}\delta_2 K \, da_{\mathbb{X}} + \int_{S_1} \nabla_2 \hat{g}(-\nabla_1 \hat{\alpha} \cdot \mathbf{J^*N}\delta_2 K/K)\, da_{\mathbb{X}} + \int_{\partial B} (\mathbf{J^{-T}}\nabla_1 \hat{\lambda} \cdot \mathbf{J^{-T}}\nabla_1 \hat{\alpha}\delta_2 \chi$$

$$- \mathbf{J^{-T}}\nabla_1 \hat{\lambda} \cdot \delta_2 \chi \mathbf{J^{-T}}\nabla_1 \hat{\alpha} - \mathbf{J^{-T}}\nabla_1 \hat{\alpha} \cdot \delta_2 \chi \mathbf{J^{-T}}\nabla_1 \hat{\lambda}) \cdot JJ^{-T}\mathbf{N}\, da_{\mathbb{X}}$$

$$- \int_{\partial B_2} \hat{\lambda}(\mathbf{J^{-T}}\nabla_1 \hat{q}^p \cdot \delta_2 \chi K + \delta_2 q^p K + \hat{q}^p \delta_2 K)\, da_{\mathbb{X}}$$

$$+ \int_{S_1} (\mathbf{J^{-T}}\nabla_1 \hat{\alpha}^p \cdot \delta_2 \chi + \delta_2 \alpha^p)\mathbf{J^*}\nabla_1 \hat{\lambda} \cdot \mathbf{N}\, da_{\mathbb{X}}$$

$$= T_0 w \delta w. \tag{124}$$

7. CONCLUSION

Shape sensitivities have been derived for the Laplace problem via the direct and adjoint approaches. The formulation is developed from the domain parameterization methodology, of which the material derivative method may be viewed as a special case. A generic derivation is developed and is readily adopted for both finite and boundary element applications. In the case of the boundary element approach, the need to differentiate the fundamental solution is circumvented; and in the finite element method it is shown that the sensitivities may be expressed over the boundary for the adjoint approach, but not for the direct method.

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APPENDIX

A.1. *Alternative proof of eqn (42)*

This proof is due to Carlson and Hodger (1986) and relies on the Cayley–Hamilton theorem (Gurtin, 1981) which states that the second order tensor $\mathbf{A}$ satisfies its characteristic equation, i.e.

$$\mathbf{A}^3 - \pi_1(\mathbf{A})\mathbf{A}^2 + \pi_2(\mathbf{A})\mathbf{A} - \pi_3(\mathbf{A})\mathbf{I} = 0, \tag{A1}$$

where π_1, π_2 and π_3 are the principal invariants

$$\begin{aligned}
\pi_1(\mathbf{A}) &= \operatorname{tr}(\mathbf{A}), \\
\pi_2(\mathbf{A}) &= \tfrac{1}{2}((\operatorname{tr}(\mathbf{A}))^2 - \operatorname{tr}(\mathbf{A}^2)) = \tfrac{1}{2}(\pi_1^2(\mathbf{A}) - \pi_1(\mathbf{A}^2)), \\
\pi_3(\mathbf{A}) &= \det(\mathbf{A}).
\end{aligned} \tag{A2}$$

Taking the trace of eqn (A1) and substitution of eqn (A2), after some rearranging, gives

$$\pi_3(\mathbf{A}) = \tfrac{1}{3}[\pi_1(\mathbf{A}^3) - \pi_1(\mathbf{A})\pi_1(\mathbf{A}^2) + \tfrac{1}{2}(\pi_1^2(\mathbf{A}) - \pi_1(\mathbf{A}^2))\pi_1(\mathbf{A})]. \tag{A3}$$

Using eqns (24), (27) and (8₃) we may readily verify

$$D\pi_1(\mathbf{A})\mathbf{U} = \pi_1(\mathbf{U}),$$

$$D\pi_1(\mathbf{A}^2)\mathbf{U} = 2\pi_1(\mathbf{A}\mathbf{U}), \tag{A4}$$

$$D\pi_1(\mathbf{A}^3)\mathbf{U} = 3\pi_1(\mathbf{A}^2\mathbf{U}). \tag{A5}$$

Taking the derivative of eqn (A3) via the product rule [eqn (24)] and substituting eqn (A4) we obtain

$$\begin{aligned}
D\pi_3(\mathbf{A})\mathbf{U} &= \tfrac{1}{3}[3\pi_1(\mathbf{A}^2\mathbf{U}) - \pi_1(\mathbf{U})\pi_1(\mathbf{A}^2) - 2\pi_1(\mathbf{A})\pi_1(\mathbf{A}\mathbf{U}) \\
&\quad + \tfrac{1}{2}(2\pi_1(\mathbf{A})\pi_1(\mathbf{U}) - 2\pi_1(\mathbf{A}\mathbf{U})\pi_1(\mathbf{A}) - \pi_1(\mathbf{A}^2)\pi_1(\mathbf{U}))] \\
&= [\mathbf{A}^2 - \pi_1(\mathbf{A})\mathbf{A} + \pi_2(\mathbf{A})\mathbf{I}]^{\mathrm{T}} \cdot \mathbf{U} \\
&= [\mathbf{A}^{-1}\pi_3(\mathbf{A})]^{\mathrm{T}} \cdot \mathbf{U}, \tag{A6}
\end{aligned}$$

where we used eqns (5) and (A1) to obtain the second and third equalities, respectively. Equation (43) follows immediately from the above and eqn (5).

A.2. *Alternative proof of Piola's identity*

This proof of Piola's identity is supplied by Carlson (1991) and is a component-free alternative to the proof presented in Chadwick (1976) and Ciarlet (1988). Here the previous notation remains in effect and $\mathbf{a}$, $\mathbf{u}$, $\mathbf{v} \in \mathscr{V}^N$ are constants.

The following relations are required

$$\nabla_1 J(\mathbb{X}, \boldsymbol{\Phi}) \cdot \mathbf{u} = J(\mathbb{X}, \boldsymbol{\Phi}) \operatorname{tr}(\mathbf{J}^{-1}(\mathbb{X}, \boldsymbol{\Phi}) D_1 \mathbf{J}(\mathbb{X}, \boldsymbol{\Phi})\mathbf{u}), \tag{A7}$$

which follows from eqns (14) and (45). Also required is

$$\begin{aligned}
D_1^2 \chi(\mathbb{X}, \boldsymbol{\Phi})(\mathbf{u}, \mathbf{v}) &= (D_1 \mathbf{J}(\mathbb{X}, \boldsymbol{\Phi})\mathbf{v})\mathbf{u} \\
&= (D_1 \mathbf{J}(\mathbb{X}, \boldsymbol{\Phi})\mathbf{u})\mathbf{v}, \tag{A8}
\end{aligned}$$

which is obtained from eqns (30) and (12). The last preliminary argument is

$$D_1(\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a})\mathbf{u} = -\mathbf{J}^{-1}(\mathbb{X},\Phi)D_1\mathbf{J}(\mathbb{X},\Phi)\mathbf{u}\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}$$
$$= -\mathbf{J}^{-1}(\mathbb{X},\Phi)D_1\mathbf{J}(\mathbb{X},\Phi)(\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a})\mathbf{u}, \tag{A9}$$

which follows from eqns (40) and (A8) where $\mathbf{v} = \mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}$.

The proof is now presented:

$$\begin{aligned}
\mathrm{div}_1\,(J(\mathbb{X},\Phi)\mathbf{J}^{-T}(\mathbb{X},\Phi))\cdot\mathbf{a} &= \mathrm{div}_1\,(J(\mathbb{X},\Phi)\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}) \\
&= D_1 J(\mathbb{X},\Phi)\cdot\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a} + J(\mathbb{X},\Phi)\,\mathrm{div}_1(\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}) \\
&= J(\mathbb{X},\Phi)\,\mathrm{tr}\,(\mathbf{J}^{-1}(\mathbb{X},\Phi)D_1\mathbf{J}(\mathbb{X},\Phi)[\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}]) \\
&\quad + J(\mathbb{X},\Phi)\,\mathrm{tr}\,(D_1\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}) \\
&= J(\mathbb{X},\Phi)\,\mathrm{tr}\,(\mathbf{J}^{-1}(\mathbb{X},\Phi)D_1\mathbf{J}(\mathbb{X},\Phi)[\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}]) \\
&\quad - J(\mathbb{X},\Phi)\,\mathrm{tr}\,(\mathbf{J}^{-1}(\mathbb{X},\Phi)D_1\mathbf{J}(\mathbb{X},\Phi)[\mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}]) \\
&= 0, \tag{A10}
\end{aligned}$$

where eqns (23_2), (25_2), (131) (with $\mathbf{u} = \mathbf{J}^{-1}(\mathbb{X},\Phi)\mathbf{a}$), and (133) (with the arbitrariness of $\mathbf{u}$) are systematically applied.