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A unified approach for high order sensitivity analysis

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Abstract

Many engineering problems require solving PDEs by means of numerical methods (type FEM/BEM) which sensitivity analysis entails taking derivatives of functions defined through integration. In sizing optimization problems, the integration domains are fixed, what enables the regular use of analytical sensitivity techniques. In shape optimization problems, the integration domains are nevertheless variable. This fact causes some cumbersome difficulties [1], that have traditionally been overcome by means of finite difference approximations [2]. Three kinds of analytical approaches have been proposed for computing sensitivity derivatives in shape optimization problems. The first is based on differentiation of the final discretized equations [1]. The second is based on variation of the continuum equations [1] and on the concept of material derivative. The third is based upon the existence of a mapping that links the material space with a fixed space of reference coordinates [3]. This is not restrictive, since such a transformation is inherent to FEM and BEM implementations.

In this paper, we present a generalization of the latter approach on the basis of a unified procedure for integration in manifolds. Our aim is to obtain a single, unified, compact procedure to compute arbitrarily high order directional derivatives of the objective function and the constraints in FEM/BEM shape optimization problems. Special care has been taken on heading for easy-to-compute recurrent expressions. The proposed scheme is basically independent from the specific form of the state equations, and can be applied to both, direct and adjoint state formulations. Thus, its numerical implementation in current engineering codes is straightforward.

An application example is finally presented.

1 Statement of the problem

The first step in the statement of a design optimization problem is the definition of the criteria that will allow to decide whether a candidate design is acceptable or not, as much as to select the preferable among the acceptable designs. The acceptability is normally expressed by means of equality ($h(\boldsymbol{\gamma}) = 0$) and inequality ($g(\boldsymbol{\gamma}) \leq 0$) constraints, while the preference is usually expressed by means of a suitable objective function $f(\boldsymbol{\gamma})$ that should take the lower values for the better designs. The magnitudes $\boldsymbol{\gamma}$, in terms of which the optimization problem is stated, are called control variables [4].

The second step is the definition of a design parametric model. In other words, the fundamental properties $\boldsymbol{\varphi}$ —that fully describe the object to be designed— must be expressed in terms of a reduced set of design parameters. Some of them will be design constants ($\boldsymbol{c}$), while the rest will be the so-called design variables $\boldsymbol{x}$ which optimal value must be found [4]. The set of all possible values of the design variables is called design space. The subset in which the constraints are verified is called feasible region.

Normally, most of control variables do not depend only on the properties of the design itself, but on the so-called state variables $\boldsymbol{\omega}$ that describe the performance of the design in construction, service or fail conditions. Hence, the third step is the definition of an analysis model to analyze the involved physical phenomena. Different analysis models could be proposed, each one requiring specific input data $\boldsymbol{\alpha}$ that must be well defined in terms of the properties $\boldsymbol{\varphi}$. We symbolically represent the analysis model by means of a system of n_ω implicit equations

$$\boldsymbol{\psi}(\boldsymbol{\alpha}, \boldsymbol{\omega}) = \mathbf{0}, \quad \boldsymbol{\psi}(\boldsymbol{\alpha}, \boldsymbol{\omega}) = \{\psi_i(\boldsymbol{\alpha}, \boldsymbol{\omega})\}, \qquad i = 1, \ldots, n_\omega, \tag{1}$$

with n_ω unknowns $\boldsymbol{\omega} = \{\omega_i\}$. This is the so-called state equation [4], which solution may involve severe difficulties in engineering problems.

Therefore, the optimum design problem takes the form of a general constrained minimization problem [4]

$$\begin{aligned}
&\text{GIVEN } \boldsymbol{c} \text{ OBTAIN } \boldsymbol{x} \text{ THAT} \\
&\quad \text{FOR } \boldsymbol{\varphi} = \boldsymbol{\varphi}(\boldsymbol{c}, \boldsymbol{x}), \quad \boldsymbol{\alpha} = \boldsymbol{\alpha}(\boldsymbol{\varphi}), \\
&\qquad \boldsymbol{\omega} \text{ SUCH THAT } \boxed{\boldsymbol{\psi}(\boldsymbol{\alpha}, \boldsymbol{\omega}) = \mathbf{0}}, \\
&\qquad \boldsymbol{\gamma} = \boldsymbol{\gamma}(\boldsymbol{\varphi}, \boldsymbol{\omega}), \\
&\quad \text{MINIMIZES } f(\boldsymbol{\gamma}) \\
&\quad \text{SUBJECT TO } g_j(\boldsymbol{\gamma}) \leq 0, \qquad j = 1, \ldots, m \\
&\qquad\qquad\quad\ h_\ell(\boldsymbol{\gamma}) = 0, \qquad \ell = 1, \ldots, p
\end{aligned} \tag{2}$$

which solution must be found by means of a suitable MP algorithm [5]. It is quite obvious that more efficient MP algorithms could be achieved if not just the values of the objective function and the constraints, but also their derivatives, are supplied [5]. The techniques that let us evaluate these derivatives receive the generic name of sensitivity analysis.

2 Sensitivity analysis

First we discuss how to obtain the directional derivative $D_{\mathrm{s}}z = (dz/d\boldsymbol{\gamma})\boldsymbol{s}$ of any given function $z(\boldsymbol{\gamma})$ of the control variables, for an arbitrary unit vector $\boldsymbol{s}$ in the design space. Direct differentiation of (2) leads to the first order direct scheme:

$$\begin{aligned}
&\text{GIVEN } \boldsymbol{s} \quad \text{OBTAIN } D_{\mathrm{s}}z = \frac{dz}{d\boldsymbol{\gamma}}\, D_{\mathrm{s}}\boldsymbol{\gamma} \\
&\qquad\qquad \text{FOR } D_{\mathrm{s}}\boldsymbol{\varphi} = \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}}\,\boldsymbol{s}, \quad D_{\mathrm{s}}\boldsymbol{\alpha} = \frac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{\varphi}}\, D_{\mathrm{s}}\boldsymbol{\varphi}, \\
&\qquad\qquad\qquad D_{\mathrm{s}}\boldsymbol{\omega} \quad \text{SUCH THAT } \boxed{\left[\frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{\omega}}\right] D_{\mathrm{s}}\boldsymbol{\omega} = -\frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{\alpha}}\, D_{\mathrm{s}}\boldsymbol{\alpha}}, \\
&\qquad\qquad\qquad D_{\mathrm{s}}\boldsymbol{\gamma} = \frac{\partial \boldsymbol{\gamma}}{\partial \boldsymbol{\varphi}}\, D_{\mathrm{s}}\boldsymbol{\varphi} + \frac{\partial \boldsymbol{\gamma}}{\partial \boldsymbol{\omega}}\, D_{\mathrm{s}}\boldsymbol{\omega},
\end{aligned} \tag{3}$$

where obtaining the directional derivatives of the state variables requires solving the boxed linear system of n_ω equations with n_ω unknowns.

It is easy to show how the direct differentiation computational scheme (3) can be reordered [6,4], giving the so-called adjoint state method

$$\begin{aligned}
&\text{GIVEN } \boldsymbol{s} \quad \text{OBTAIN } D_{\mathrm{s}}z = \frac{dz}{d\boldsymbol{\gamma}}\,\frac{\partial \boldsymbol{\gamma}}{\partial \boldsymbol{\varphi}}\, D_{\mathrm{s}}\boldsymbol{\varphi} + \boldsymbol{\mu}_z^T \frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{\alpha}}\, D_{\mathrm{s}}\boldsymbol{\alpha} \\
&\qquad\qquad \text{FOR } D_{\mathrm{s}}\boldsymbol{\varphi} = \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}}\,\boldsymbol{s}, \quad D_{\mathrm{s}}\boldsymbol{\alpha} = \frac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{\varphi}}\, D_{\mathrm{s}}\boldsymbol{\varphi}, \\
&\qquad\qquad\qquad \boldsymbol{\mu}_z \quad \text{SUCH THAT } \boxed{\left[\frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{\omega}}\right]^T \boldsymbol{\mu}_z = -\left(\frac{dz}{d\boldsymbol{\gamma}}\,\frac{\partial \boldsymbol{\gamma}}{\partial \boldsymbol{\omega}}\right)^T},
\end{aligned} \tag{4}$$

where the unknown vector $\boldsymbol{\mu}_z$ is known as the *adjoint state* corresponding to the function $z(\boldsymbol{\gamma})$. While in (3) it is necessary to compute the derivatives of the state variables ($D_{\mathrm{s}}\boldsymbol{\omega}$) as an intermediate result for each direction $\boldsymbol{s}$, in (4) it is necessary to compute $\boldsymbol{\mu}_z$ for each function $z(\boldsymbol{\gamma})$. Therefore, (4) will be preferred rather than (3) when the number of functions to be derived is significantly smaller than the number of directions in which derivatives must be computed [6]. Normally, the adjoint state scheme in design optimization does not offer significant advantages over the direct differentiation scheme. Consider that in practical optimization problems, the number of constraints is often much larger than the number of design variables. In any case, a wide purpose optimum design system must include the possibility of using any of both schemes, depending on the problem statement.

A scheme for high order directional sensitivity analysis can be easily derived following the same principles outlined before [4]. Conceptually, a high order scheme is just slightly more complex than the first order one, although the computational requirements increase with the order of differentiation due to the number of derivatives to be computed [4,5].

3 The FEM/BEM discretized state equation

In engineering practice, equation (1) is frequently a discretized form of a certain boundary-value problem. Let the exact solution to this problem be:

$$u(\boldsymbol{r},\boldsymbol{\varphi}), \qquad \boldsymbol{r} \in \bar{\Omega}(\boldsymbol{\varphi}) \subset \mathbb{R}^{n_r=\dim(\Omega)} \tag{5}$$

where Ω is an open bounded domain with lipschitzian boundary $\partial\Omega$ and closure $\bar{\Omega}$ and $\boldsymbol{r}$ is the material coordinates vector of an arbitrary point in $\bar{\Omega}$. Let $\bar{\Gamma}$ be the subset of $\bar{\Omega}$ in which (boundary) conditions are prescribed. Since this exact solution is generally unknown, engineers pursue to approximate $u(\boldsymbol{r},\boldsymbol{\varphi})$ by means of numerical techniques in a finite-dimensional context. Thus, for a certain set of so-called trial functions $(\{\nu_i(\boldsymbol{r},\boldsymbol{\alpha})\},\ i=1,\ldots,n_\omega)$, one considers discretized approximations type

$$\widehat{u}(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega}) = \sum_{i=1}^{n_\omega} \omega_i \nu_i(\boldsymbol{r},\boldsymbol{\alpha}). \tag{6}$$

Namely, for given values of the fundamental properties $\boldsymbol{\varphi}$, the input variables $\boldsymbol{\alpha}$ are known, while the unknown values of the state variables $\boldsymbol{\omega}$ must be determined in such a way that the corresponding discretized approximation (6) is as close as possible to the exact solution (5). Thus, each numerical technique involves solving a corresponding state equation (1), that is just the specific way of choosing the desired approximation.

In integral methods —such as FEM and BEM— the strong form of the problem is first reduced to an equivalent weak (or variational) form on the basis of a weighted residual approach, while domains $\bar{\Omega}$ and $\bar{\Gamma}$ are discretized in subdomains [7] (also called elements) due to practical reasons. Thus, these approaches yield state equations type

$$\boldsymbol{\psi}(\boldsymbol{\alpha},\boldsymbol{\omega}) = \sum_{e=1}^{n_e} \boldsymbol{\psi}_e^E(\boldsymbol{\alpha},\boldsymbol{\omega}) = 0, \tag{7}$$

which require computing and assembling the so-called element contributions

$$\boldsymbol{\psi}^E(\boldsymbol{\alpha},\boldsymbol{\omega}) = \int_{\boldsymbol{r}\in E(\boldsymbol{\alpha})} \boldsymbol{\phi}^E(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega})\ dE, \tag{8}$$

where $\bar{E}(\boldsymbol{\alpha})$ is an element (that is, a closed subdomain with nonempty interior $E(\boldsymbol{\alpha})$ and lipschitzian boundary $\partial E(\boldsymbol{\alpha})$) of dimension $\dim(E) = n_\xi \leq n_r = \dim(\Omega)$ within domain $\bar{\Omega}$.

Most of the available wide purpose FEM or BEM codes do not provide the derivatives of the state function ($[\partial\boldsymbol{\psi}/\partial\boldsymbol{\omega}]$ and $\partial\boldsymbol{\psi}/\partial\boldsymbol{\alpha}$) required by (3). It is obvious that one can always use finite difference approximations, but this produces a significative loss of accuracy in the information supplied to the MP algorithm and a high computational cost [1,2]. On the other hand, to implement the additional computations required by (3) may involve some unexpected conceptual and practical difficulties, specially in shape optimization problems.

4 A unified procedure for integration

It is obvious that trying to calculate the element contributions (8) in terms of the material coordinates $\boldsymbol{r}$ would be awkward [7]. However, in most of the cases it is relatively easy to introduce an invertible differentiable mapping

$$\begin{array}{ll} \boldsymbol{\rho}: \bar{\Xi} \times A & \longrightarrow \bar{\Omega} \\ (\boldsymbol{\xi}, \boldsymbol{\alpha}) & \boldsymbol{r} = \boldsymbol{\rho}(\boldsymbol{\xi}, \boldsymbol{\alpha}) \end{array} \tag{9}$$

such that the element $\bar{E}(\boldsymbol{\alpha}) = \boldsymbol{\rho}(\bar{\Xi}, \boldsymbol{\alpha})$ is the image of a convenient fixed reference domain $\bar{\Xi}$ (also called master element or parent domain) by the coordinate transformation $\boldsymbol{\rho}$ (see Figure 1).

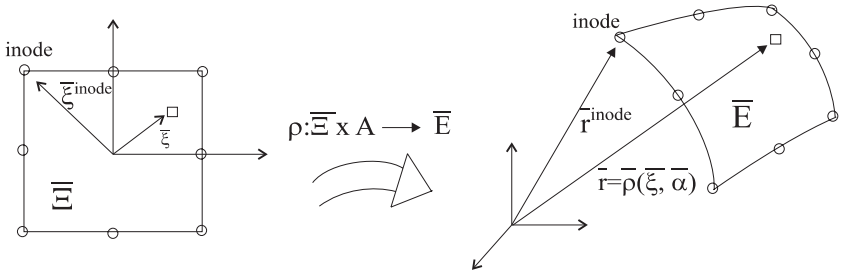

Fig. 1.– Standard FEM Mapping

Thus, every point in element $\bar{E}$, given by its material (global) coordinates

$$\boldsymbol{r} = \{r_i\}, \qquad i = 1, \ldots, n_r = \dim(\Omega) \tag{10}$$

is the image by the mapping $\boldsymbol{\rho}$ of a unique corresponding point in the reference domain $\bar{\Xi}$, given by its reference (or local) coordinates

$$\boldsymbol{\xi} = \{\xi_i\}, \qquad i = 1, \ldots, n_\xi = \dim(E). \tag{11}$$

In a FEM context such a transformation is normally written as

$$\boldsymbol{\rho}(\boldsymbol{\xi}, \boldsymbol{\alpha}) = \sum_{inode=1}^{nnode} \boldsymbol{r}^{inode}(\boldsymbol{\alpha})\, N^{inode}(\boldsymbol{\xi}), \tag{12}$$

where the master element $\bar{\Xi}$ is defined by the reference coordinates $\{\boldsymbol{\xi}^{inode}\}$ of the "*nnode*" so-called nodal points (or nodes) of the element [7]. Therefore, each element $\bar{E}$ is defined by the corresponding material coordinates of its nodal points $\{\boldsymbol{r}^{inode}(\boldsymbol{\alpha})\}$, and its so-called shape functions $\{N^{inode}(\boldsymbol{\xi})\}$ that must verify the standard interpolation conditions

$$N^{inode}(\boldsymbol{\xi}^{jnode}) = \begin{cases} 0, & \text{if } inode \neq jnode; \\ 1, & \text{otherwise.} \end{cases} \tag{13}$$

In these terms, the jacobian matrix of the mapping (9) can be written as

$$\boldsymbol{J}(\boldsymbol{\xi}, \boldsymbol{\alpha}) = \frac{\partial \boldsymbol{\rho}(\boldsymbol{\xi}, \boldsymbol{\alpha})}{\partial \boldsymbol{\xi}} = \sum_{inode=1}^{nnode} \boldsymbol{r}^{inode}(\boldsymbol{\alpha})\, \frac{\partial}{\partial \boldsymbol{\xi}}\, N^{inode}(\boldsymbol{\xi}). \tag{14}$$

Now, it seems clear that contributions (8) should be computed by integration in the reference system. Thus (8) must be reduced to the form

$$\boldsymbol{\psi}^E(\boldsymbol{\alpha},\boldsymbol{\omega}) = \int_{\boldsymbol{\xi}\in\Xi} \boldsymbol{\phi}^{\Xi}(\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\omega}) \left|\frac{dE}{d\Xi}\right| d\Xi, \qquad d\Xi = \prod_{i=1}^{n_\xi} d\xi_i, \tag{15}$$

where it is obvious that

$$\boldsymbol{\phi}^{\Xi}(\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\omega}) = \boldsymbol{\phi}^{E}(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega})\Big|_{\boldsymbol{r}=\boldsymbol{\rho}(\boldsymbol{\xi},\boldsymbol{\alpha})}. \tag{16}$$

On the other hand, it is widely known [8] that for $n_\xi = n_r$ the integration jacobian $|dE/d\Xi|$ is the determinant of the jacobian matrix (14). Otherwise, it is generally computed by means of a specific expression that depends on the dimensions n_r and n_ξ. In engineering practice $n_r \leq 3$. Thus, when $n_\xi = 1$, E is a curve and $|dE/d\Xi|$ is computed as the modulus of the tangent vector; on the other hand, when $n_\xi = 2$, E is a surface and $|dE/d\Xi|$ is computed as the modulus of the normal vector.

It seems to be not so widely known that the integration jacobian $|dE/d\Xi|$ in (15) admits the following unified expression

$$\left|\frac{dE}{d\Xi}\right| = \sqrt{\det\left[\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha})\right]}, \qquad \text{where} \qquad \boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha}) = \boldsymbol{J}^T(\boldsymbol{\xi},\boldsymbol{\alpha})\boldsymbol{J}(\boldsymbol{\xi},\boldsymbol{\alpha}) \tag{17}$$

is the so-called metric tensor [9] of the riemannian manifold $E(\boldsymbol{\alpha})$. Obviously, the metric tensor is required to be positive-definite, for the mapping (12) to be acceptable [9]. Therefore, $\det\left[\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha})\right] > 0$ and the integration jacobian in (18) is always well defined. It is interesting to notice that this expression for the integration jacobian is intrinsic to the riemannian n_ξ–dimensional manifold, and indeed equivalent to the usual expressions for the arc length, surface and volume differential elements when $n_r \leq 3$.

Hence, contributions (8) can be computed as

$$\boldsymbol{\psi}^E(\boldsymbol{\alpha},\boldsymbol{\omega}) = \int_{\boldsymbol{\xi}\in\Xi} \boldsymbol{\phi}^{\Xi}(\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\omega}) \sqrt{\det\left[\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha})\right]}\, d\Xi, \tag{18}$$

being this expression valid for all cases $n_\xi \leq n_r$. An original, comprehensive and straightforward proof of (17) is given in [Navarrina et al.] [9]. A classical, more involved proof can be found in [Courant and John] [8].

Finally, a numerical quadrature (very often a Gauss type formula) could be implemented, resulting in

$$\boldsymbol{\psi}^E(\boldsymbol{\alpha},\boldsymbol{\omega}) \approx \sum_{igaue=1}^{ngaue} \boldsymbol{\phi}^{\Xi}(\boldsymbol{\xi}^{igaue},\boldsymbol{\alpha},\boldsymbol{\omega}) \sqrt{\det\left[\boldsymbol{G}(\boldsymbol{\xi}^{igaue},\boldsymbol{\alpha})\right]}\, W^{igaue}. \tag{19}$$

for the selected sets of integration points $\{\boldsymbol{\xi}^{igaue}\}$ and weights $\{W^{igaue}\}$.

The above stated numerical integration procedure does not depend on the dimensions n_r and n_ξ. Thus, a general purpose subroutine should be able to compute contributions (8) independently from the dimension of the problem (1D, 2D or 3D) and from the dimension of the elements being used.

5 Sensitivity analysis of the state equation

At this point we recall equations (3). For a given arbitrary unit vector $\boldsymbol{s}$ in the design space one should easily compute the directional derivative of the input variables ($D_{\rm s}\boldsymbol{\alpha}$). Then, taking into account equations (7), one concludes that the terms which computation must be discussed are

$$\left[\frac{\partial \boldsymbol{\psi}}{\partial \boldsymbol{\omega}}\right] = \sum_{e=1}^{n_e} \left[\frac{\partial}{\partial \boldsymbol{\omega}} \boldsymbol{\psi}_e^E(\boldsymbol{\alpha},\boldsymbol{\omega})\right] \qquad \text{and} \qquad D_{\rm s}^{\boldsymbol{\alpha}} \boldsymbol{\psi} = \sum_{e=1}^{n_e} D_{\rm s}^{\boldsymbol{\alpha}} \boldsymbol{\psi}_e^E(\boldsymbol{\alpha},\boldsymbol{\omega}), \quad (20)$$

where we introduce the symbolic operator

$$D_{\rm s}^{\boldsymbol{\alpha}} \square = \frac{\partial \square}{\partial \boldsymbol{\alpha}}\, D_{\rm s}\boldsymbol{\alpha}. \quad (21)$$

Hence, the desired derivatives of the state function should be obtained by computing and assembling derivatives of the element contributions (8) type

$$\left[\frac{\partial}{\partial \boldsymbol{\omega}} \boldsymbol{\psi}^E(\boldsymbol{\alpha},\boldsymbol{\omega})\right] = \left[\frac{\partial}{\partial \boldsymbol{\omega}} \left(\int_{\boldsymbol{r}\in E(\boldsymbol{\alpha})} \boldsymbol{\phi}^E(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega})\; dE \right)\right], \quad (22)$$

and

$$D_{\rm s}^{\boldsymbol{\alpha}} \boldsymbol{\psi}^E(\boldsymbol{\alpha},\boldsymbol{\omega}) = D_{\rm s}^{\boldsymbol{\alpha}} \left(\int_{\boldsymbol{r}\in E(\boldsymbol{\alpha})} \boldsymbol{\phi}^E(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega})\; dE \right). \quad (23)$$

Normally, the element shape will not depend on the state variables. Thus, computing terms (22) is considered trivial since the integration domains are fixed. Thus

$$\left[\frac{\partial}{\partial \boldsymbol{\omega}} \boldsymbol{\psi}^E(\boldsymbol{\alpha},\boldsymbol{\omega})\right] = \left[\int_{\boldsymbol{r}\in E(\boldsymbol{\alpha})} \frac{\partial}{\partial \boldsymbol{\omega}} \boldsymbol{\phi}^E(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega})\; dE\right], \quad (24)$$

which can be computed by integration in reference coordinates as

$$\left[\frac{\partial}{\partial \boldsymbol{\omega}} \boldsymbol{\psi}^E(\boldsymbol{\alpha},\boldsymbol{\omega})\right] = \left[\int_{\boldsymbol{\xi}\in\Xi} \frac{\partial}{\partial \boldsymbol{\omega}} \boldsymbol{\phi}^{\Xi}(\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\omega}) \sqrt{\det\left[\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha})\right]}\; d\Xi\right]. \quad (25)$$

The shape of the elements should be defined by part of the input variables $\boldsymbol{\alpha}$. For this reason, computing the remaining terms (23) may be much more difficult, since the integration domains could be variable.

In optimum structural design, explicit distinctions are made between *sizing optimization* (fixed-geometry) and *shape optimization* [1,4]. In the former, the difficulties involved in the differentiation of the state equation are significantly reduced, provided that the input variables that define the structural shape do not depend on the design variables, but only on the design constants. Thus, the integration domains are fixed, and terms (23) can be easily obtained. In the latter, the input variables that define the structural shape depend on the design variables. Thus, some non obvious aspects —related to the differentiation of functions defined by integration in variable domains— interfere in the sensitivity analysis.

6 High order shape sensitivity

Using equation (18) we can write terms (23) as

$$D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{\psi}^{E}(\boldsymbol{\alpha},\boldsymbol{\omega}) = \int_{\boldsymbol{\xi}\in\Xi} D_{\mathrm{s}}^{\boldsymbol{\alpha}}\left(\boldsymbol{\phi}^{\Xi}(\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\omega})\,\sqrt{\det\left[\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha})\right]}\right)\,d\Xi. \tag{26}$$

For the sake of compacity we define the symbolic operator

$$\mathcal{D}_{\mathrm{s}}^{\Xi}\square = D_{\mathrm{s}}^{\boldsymbol{\alpha}}\square + \square\,\frac{1}{2}\,D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\ln\Big(\det\left[\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha})\right]\Big), \tag{27}$$

which reduces (26) to the compact form

$$D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{\psi}^{E}(\boldsymbol{\alpha},\boldsymbol{\omega}) = \int_{\boldsymbol{\xi}\in\Xi} \mathcal{D}_{\mathrm{s}}^{\Xi}\left(\boldsymbol{\phi}^{\Xi}(\boldsymbol{\xi},\boldsymbol{\alpha},\boldsymbol{\omega})\right)\,\sqrt{\det\left[\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha})\right]}\,d\Xi. \tag{28}$$

Finally, by means of some additional analytical work [9] we obtain the explicit ready-for-computation expression

$$\mathcal{D}_{\mathrm{s}}^{\Xi}\square = D_{\mathrm{s}}^{\boldsymbol{\alpha}}\square + \square\,\frac{1}{2}\,\mathrm{Tr}\Big[\boldsymbol{G}^{-1}(\boldsymbol{\xi},\boldsymbol{\alpha})\,D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha})\Big], \tag{29}$$

where direct differentiation of (17) and (14) give

$$D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{G}(\boldsymbol{\xi},\boldsymbol{\alpha}) = \left[\boldsymbol{J}^{T}(\boldsymbol{\xi},\boldsymbol{\alpha})D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{J}(\boldsymbol{\xi},\boldsymbol{\alpha})\right] + \left[\boldsymbol{J}^{T}(\boldsymbol{\xi},\boldsymbol{\alpha})D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{J}(\boldsymbol{\xi},\boldsymbol{\alpha})\right]^{T}, \tag{30}$$

$$D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{J}(\boldsymbol{\xi},\boldsymbol{\alpha}) = \sum_{inode=1}^{nnode} D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{r}^{inode}(\boldsymbol{\alpha})\,\frac{\partial}{\partial\boldsymbol{\xi}}\,N^{inode}(\boldsymbol{\xi}). \tag{31}$$

On the other hand, (28) can be written in terms of material coordinates as

$$D_{\mathrm{s}}^{\boldsymbol{\alpha}}\,\boldsymbol{\psi}^{E}(\boldsymbol{\alpha},\boldsymbol{\omega}) = \int_{\boldsymbol{r}\in E(\boldsymbol{\alpha})} \mathcal{D}_{\mathrm{s}}^{E}\,\boldsymbol{\phi}^{E}(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega})\,dE, \tag{32}$$

by means of the corresponding symbolic operator

$$\mathcal{D}_{\mathrm{s}}^{E}\square = \mathcal{D}_{\mathrm{s}}^{\Xi}\left(\square\Big|_{\boldsymbol{r}=\boldsymbol{\rho}(\boldsymbol{\xi},\boldsymbol{\alpha})}\right)\Big|_{\boldsymbol{\xi}=\boldsymbol{\rho}^{-1}(\boldsymbol{r},\boldsymbol{\alpha})}. \tag{33}$$

Expressions (28) and (32) are equivalent. So are operators (29) and (33). Since integration is performed in reference coordinates, the expression (28) and the operator (29) will be preferred in practice. However, equation (32) shows that the derivative of an integral with respect to a parameter that modifies the integration domain can be easily calculated as the integral of the operator (33) applied to the subintegrand function, that is

$$D_{\mathrm{s}}^{\boldsymbol{\alpha}}\left(\int_{\boldsymbol{r}\in E(\boldsymbol{\alpha})}\boldsymbol{\phi}^{E}(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega})\,dE\right) = \int_{\boldsymbol{r}\in E(\boldsymbol{\alpha})}\mathcal{D}_{\mathrm{s}}^{E}\,\boldsymbol{\phi}^{E}(\boldsymbol{r},\boldsymbol{\alpha},\boldsymbol{\omega})\,dE, \tag{34}$$

which explains why recurrency is allowed. Thus, high order shape sensitivity expressions can be immediately obtained [9] by reiterative application of operators (29) or (33). Notice that the shape variation is entirely introduced in the sensitivity analysis by means of the sequential directional derivatives of the jacobian matrix (14) of the transformation, that is, through the sequential directional derivatives of the nodal coordinates $\boldsymbol{r}^{inode}(\boldsymbol{\alpha})$, that must be known in advance up to the desired order.

7 Application example

Following, we show some results for a simply supported concrete shell (see Figure 2). A detailed description of this shape optimization problem can be found in [3,9]. The shape optimization was performed by the **DAO^2** system [4] using second order directional sensitivity analysis [5].

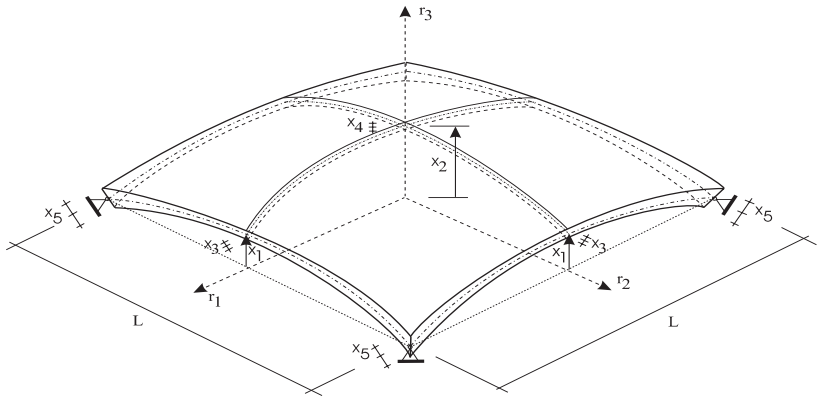

Fig. 2.– Design Model

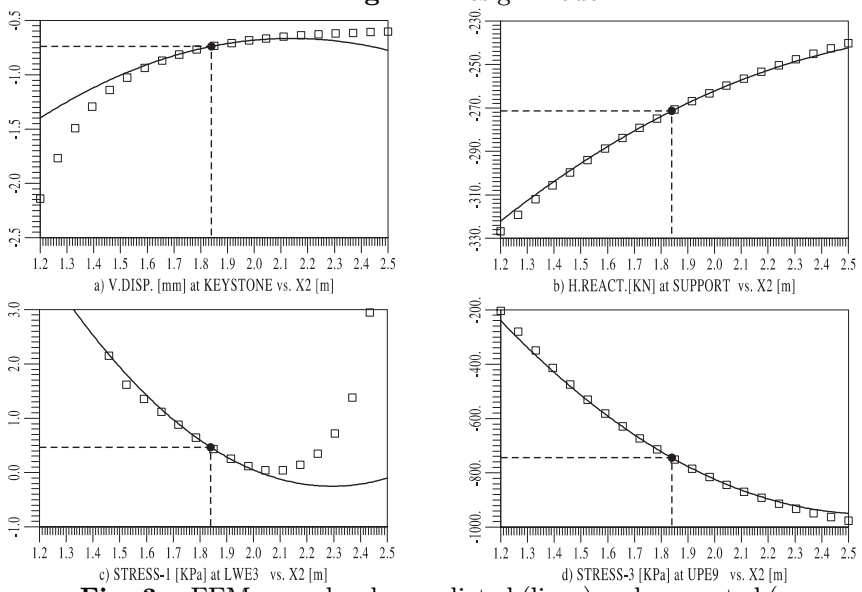

Fig. 3.– FEM second order predicted (lines) and computed (squares) values of: a) vertical displacement at the keystone, b) horizontal reaction at the support, c) σ_I at GP-LWE3 and d) σ_{III} at GP-UPE9, versus x_2. [$x_2^{opt} = 1.83992\ m$ (circles)]

Figure 3 compares some predicted values (obtained from the second order sensitivity analysis at the optimal solution) with the corresponding FEM computed results for different values of the design variable x_2. (Note:

GP-LWE# and GP-UPE# respectively stand for the central lower and central upper Gauss points of element number #; being element 9 the closest to the support, and element 3 the closest to the center of the free border.)

Conclusions

A unified approach for high order shape design sensitivity analysis has been presented in this paper. The proposed approach is based on a generic procedure for integration in manifolds which implementation in standard FEM and BEM engineering codes is straightforward. Special care has been taken on giving the final results in terms of easy-to-compute compact expressions that could be applied to any kind of elements, and special emphasis has been made in holding recurrence and simplicity of intermediate operations. The proposed scheme does not depend on any particular form of the state equations, and can be used in both, direct and adjoint state formulations.

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