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# A Formulation for Crack Shape Sensitivity Analysis Based on Galerkin BIE, Domain Differentiation and Adjoint Variable

## 1. Introduction and motivation

The consideration of sensitivity analysis of integral functionals with respect to shape parameters arises in many situations where a geometrical domain plays a primary role; shape optimization and inverse problems are the most obvious, as well as possibly the most important, of such instances. In addition to numerical differentiation, shape sensitivities can be evaluated using either a direct differentiation or the adjoint variable approach [10, 19], the present paper being focused on the latter. Besides, consideration of shape changes in otherwise linear problems makes it very attractive to use boundary integral equation (BIE) formulations, which constitute the minimal modelling as far as the geometrical support of unknown field variables is concerned.

In the BIE context, the direct differentiation approach rests upon an application of the material differentiation formula for surface integrals to the governing integral equations, in either singular form [1, 12] or regularized form [4, 11, 15] (the material differentiation formula is shown in [5] to remain valid for strongly singular or hypersingular surface integrals); the direct differentiation approach is thus in particular applicable in the presence of cracks. Sensitivity evaluation then rests upon solving as many new boundary-value problems as the number of shape parameters present. The fact that they all involve the original governing operator reduces the computational effort to building new right-hand sides and solving linear systems by backsubstitution.

The adjoint variable approach is even more attractive: it needs to solve only one new boundary-value problem (the so-called adjoint problem) per integral functional present (often only one), whatever the number of shape parameters. In connexion with BIE formulations alone, the adjoint variable approach has been successfully applied to many shape sensitivity problems [3, 9, 10, 13]. It relies critically upon the possibility of formulating the final, analytical expression of the shape sensitivity of a given integral functional as a *boundary* integral that involves the boundary traces of the primary and adjoint states. However, this step raises difficulties when cracks (elasticity) or screens (acoustics) are present: non-integrable quantities associated with crack front singularity of field variables arise in the process.

This paper purports to show that this difficulty is avoided by formulating, in the Lagrangian, the direct problem constraint as a symmetric Galerkin BIE. Explicit boundary-only expressions of sensitivities are obtained for shape perturbations of either voids or cracks, in linear acoustics and elastodynamics.

**The shape sensitivity problem.** Consider a domain  $B$  of  $\mathbb{R}^m$  ( $m = 2$  or  $3$ ) with external boundary  $S$ , containing an internal defect in the form of either a void  $V$  of boundary  $\Gamma$  (Fig. 1a) or a crack with crack surface  $\Gamma$  (Fig. 1b). Let  $\Omega$  denote the actual body (i.e. containing the defect):  $\Omega = B \setminus V$  or  $\Omega = B \setminus \Gamma$  and put  $A = \partial\Omega = S \cup \Gamma$ .

For ease of exposition, the main developments concentrate on scalar wave propagation in the frequency-domain, whereby some complex-valued field variable  $u$  (e.g.

the acoustic pressure) satisfies the Helmholtz equation  $(\Delta + k^2)u = 0$ , where  $k = \omega/c$  is the wave number ( $\omega$ : angular frequency,  $c$ : wave velocity). However, the treatment of shape sensitivity to follow is applicable to many other linear direct problems; its extension to steady-state elastodynamics is addressed in Sec 6.

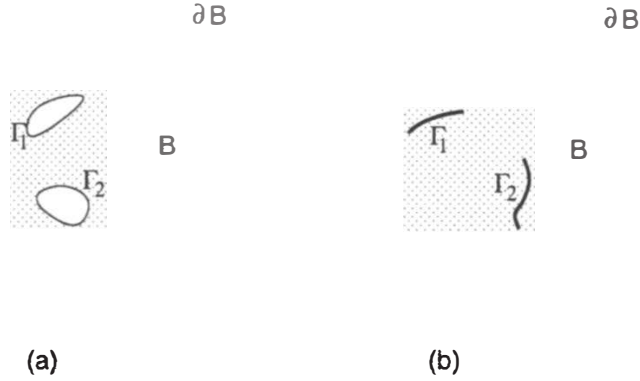


Figure 1: A body with an internal defect: (a) void, (b) crack.

The shape and position of the boundary  $\Gamma$  characterizing the defect are unknown. Suppose that a given flux  $\tilde{q}$  is imposed on  $B$ , while the defect surface is flux-free. The boundary value problem for given defect reads:

$$(\Delta + k^2)u = 0 \quad (\text{in } \Omega) \quad q(u) = \tilde{q} \quad (\text{on } S) \quad q(u) = 0 \quad (\text{on } \Gamma) \quad (1)$$

where  $q$  denotes the normal derivative of  $u$ :  $q = \partial u / \partial n$ . In the case of a crack, the variable  $u$  is allowed to jump across  $\Gamma$ ;  $\llbracket u \rrbracket \equiv u^+ - u^- \neq 0$ .

Let us thus introduce the generic objective function  $\mathcal{J}$ :

$$\mathcal{J}(\Gamma) = \int_S \varphi(u_\Gamma, \mathbf{x}) dS + \int_\Gamma \psi(\mathbf{x}) dS \quad (2)$$

where  $u_\Gamma$  denotes the solution of problem (1) for a given  $\Gamma$ . For instance, in the problem of determining the shape and position of the defect using experimental data for a physical quantity governed by problem (1), one may use  $2\varphi(u_\Gamma, \mathbf{x}) = \chi(S_m) |\hat{u} - u_\Gamma|^2$  where  $\hat{u}(\mathbf{x})$  is a measurement of  $u$  for  $\mathbf{x} \in S_m \subseteq S$  and  $\psi(\mathbf{x})$  serves to define a regularization term. Other kinds of sensitivity problems with different motivations (e.g. optimization) can be considered as well.

Evaluating the gradient of  $\mathcal{J}$  with respect to perturbations of  $\Gamma$  allows to use standard minimization algorithms, e.g. quasi-Newton. In view of the fact that  $\mathcal{J}$  defined by Eq. (2) depends only on boundary quantities and the problem (1) does not involve sources distributed over  $\Omega$ , it is natural to base the evaluation of  $\mathcal{J}$  and its gradient upon a boundary element treatment.

## 2. Shape sensitivity analysis

The shape of the body  $\Omega$  is now assumed to evolve with the values of a (small) time-like parameter  $p$ , according to a continuum kinematics-type Lagrangian description (with the “initial” configuration  $\Omega_0$  conventionally associated with  $p = 0$ ):

$$\mathbf{x} \in \Omega_0 \rightarrow \mathbf{x}^p = \Phi(\mathbf{x}, p) \in \Omega_p \quad \text{where} \quad (\forall \mathbf{x} \in \Omega_0), \Phi(\mathbf{x}, 0) = \mathbf{x} \quad (3)$$

The *geometrical transformation*  $\Phi(\mathbf{x}, p)$  must possess a strictly positive Jacobian.

Differentiation of field variables and integrals in a domain perturbation is a well-documented subject [17, 19]; a few basic definitions and facts are recalled now, using notations introduced in [4]. The *initial transformation velocity* field  $\boldsymbol{\theta}(\mathbf{x})$ , defined by

$$\boldsymbol{\theta}(\mathbf{x}) = \Phi, p(\mathbf{x}, 0) \quad (4)$$

is the “initial” velocity of the “material” point which coincides with the geometrical point  $\mathbf{x}$  at “time”  $p = 0$ . The “Lagrangian” derivative at  $p = 0$  of a field quantity  $f(\mathbf{y}, p)$  in a geometrical transformation, denoted by  $f^*$ , is defined by:

$$f^* = \lim_{p \searrow 0} p^{-1} [f(\mathbf{x}^p, p) - f(\mathbf{x}, 0)] = f, p + \nabla f \cdot \boldsymbol{\theta} \quad (5)$$

The Lagrangian derivative of the gradient of a field quantity is then given by:

$$(\nabla f)^* = \nabla f - \nabla f \cdot \nabla \boldsymbol{\theta} \quad (6)$$

where the symbol “.” indicates the dot product of two vectors or tensors (e.g.  $\nabla f \cdot \nabla \boldsymbol{\theta} = f, i \theta, j \mathbf{e}_j$ ). Besides, the material derivatives of the unit normal  $\mathbf{n}$  to a “moving” surface  $S_p$  and the area differential element  $dS$  are given by:

$$dS^* = \text{div}_S \boldsymbol{\theta} dS = D_i \theta_i \mathbf{n}^* = -\mathbf{n} \cdot \nabla_S \boldsymbol{\theta} = -n_j D_i \theta_j \mathbf{e}_i \quad (7)$$

in terms of the surface gradient:  $\nabla_S f = \nabla f - (\nabla f \cdot \mathbf{n}) \mathbf{n} = (f, i - n_i f, n) \mathbf{e}_i \equiv (D_i f) \mathbf{e}_i$  and the surface divergence  $\text{div}_S \mathbf{u} = \text{div} \mathbf{u} - (\nabla \mathbf{u} \cdot \mathbf{n}) \cdot \mathbf{n} = D_i u_i$ . The material derivatives of domain and surface integrals are expressed by:

$$\frac{d}{dp} \int_{\Omega} f d\Omega = \int_{\Omega} (f^* + f \text{div} \boldsymbol{\theta}) d\Omega \quad \Omega: \text{any domain} \quad (8)$$

$$\frac{d}{dp} \int_S f dS = \int_S (f^* + f \text{div}_S \boldsymbol{\theta}) dS \quad S: \text{any surface} \quad (9)$$

From formula (9), the Lagrangian derivative of a double surface integral is given by:

$$\frac{d}{dp} \int_{\Gamma} \int_{\Gamma} f(\mathbf{x}, \mathbf{y}) dS_x dS_y = \int_{\Gamma} \int_{\Gamma} \{f^*(\mathbf{x}, \mathbf{y}) + f[\text{div}_S \boldsymbol{\theta}(\mathbf{x}) + \text{div}_S \boldsymbol{\theta}(\mathbf{y})]\} dS_x dS_y \quad (10)$$

**Remark 1.** The external boundary  $S$  and its neighbourhood are here assumed to be unaffected by the shape transformation, so  $\boldsymbol{\theta} = \mathbf{0}$  and  $\nabla \boldsymbol{\theta} = \mathbf{0}$  on  $S$ . However, if emerging cracks are considered,  $\boldsymbol{\theta}$  and  $\nabla \boldsymbol{\theta}$  do not vanish on some neighbourhood of the emerging edge (3-D problems) or point (2-D problems).

**Remark 2.** The pseudo-time  $p$  can be understood either as an abstract parameter, in the fashion of the calculus of variations (arbitrary shape perturbations being accommodated using  $\boldsymbol{\theta}$ ) or a geometrical parameter having a definite practical meaning (a radius, a major semiaxis, a centroid coordinate ...). As far as first-order derivatives are concerned, the analysis to follow considers for convenience a single shape parameter  $p$  but is in fact applicable to the case of finitely many shape parameters.

### 3. Adjoint problem for domain integral formulation

In this section, the classical way of defining an adjoint state, which rests upon a (weak) domain formulation of the direct problem (1), is recalled. The resulting sensitivity

expression involves a domain integral which, when the defect is a void, can be converted into a boundary integral (section 3.2). However, when the defect is a crack, the conversion into boundary integrals will be seen to break down (section 3.3).

**3.1. Definition of an adjoint state.** Introduce the following Lagrangian:

$$\mathcal{L}(u, v, \Gamma) = \mathcal{J}(\Gamma) + \int_{\Omega} (\nabla u \cdot \nabla \bar{v} - k^2 u \bar{v}) \, d\Omega - \int_S \bar{q} \bar{v} \, dS \quad (v \in H^1(\Omega)) \quad (11)$$

in which the weak formulation of the direct wave problem (1) appears as an equality constraint term, the test function  $v$  acting as the Lagrange multiplier. Taking into account Eqs. (5)–(9), the total material derivative of the Lagrangian with respect to a variation of the domain can be expressed as:

$$\begin{aligned} \dot{\mathcal{L}}(u, v, \Gamma) &= \int_S \varphi_{,u} \dot{u} \, dS + \int_{\Gamma} (\dot{\psi} \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS + \int_{\Omega} (\nabla \dot{u} \cdot \nabla \bar{v} - k^2 \dot{u} \bar{v}) \, d\Omega \\ &\quad - \int_{\Omega} \{ [\nabla u \cdot \nabla \bar{v} - k^2 u \bar{v}] \operatorname{div} \boldsymbol{\theta} - [\nabla u \otimes \nabla \bar{v} + \nabla \bar{v} \otimes \nabla u] \cdot \nabla \boldsymbol{\theta} \} \, d\Omega \end{aligned} \quad (12)$$

For cracks, the partial “time” derivative  $\nabla u_{,p}$  has generally a  $d^{-3/2}$  singularity along the crack edge  $\partial\Gamma$ , while  $\nabla(\dot{u})$  and  $\nabla u$  have the same  $d^{-1/2}$  singularity, where  $d$  is the distance to  $\partial\Gamma$ . For this reason, the Lagrangian derivative  $\dot{u}$  has been introduced instead of the partial derivative  $u_{,p}$ . The derivations made in this section are therefore valid for both void and crack problems. Note that the terms containing  $\dot{v}$  have been omitted in Eq. (12), because they merely repeat the equality constraint.

In equation (12), the test function  $v$  is now chosen so that the terms which contain  $\dot{u}$  combine to zero for any  $\dot{u}$ , i.e. solves the *adjoint problem*:

$$\int_{\Omega} (\nabla \bar{v} \cdot \nabla \dot{u} - k^2 \bar{v} \dot{u}) \, d\Omega + \int_S \varphi_{,u} \dot{u} \, dS = 0 \quad (\forall \dot{u} \in H^1(\Omega)) \quad (13)$$

whose strong formulation is:

$$(\Delta + k^2)v = 0 \quad (\text{in } \Omega) \quad q(v) = -\bar{\varphi}_{,u} \quad (\text{on } S) \quad q(v) = 0 \quad (\text{on } \Gamma) \quad (14)$$

Finally,  $J$  is expressed from Eq. (12) in terms of the direct and adjoint states  $(u_{\Gamma}, v_{\Gamma})$ :

$$\begin{aligned} \dot{\mathcal{J}}(\Gamma) &= \dot{\mathcal{L}}(u_{\Gamma}, \bar{v}_{\Gamma}, \Gamma) = \int_{\Gamma} (\dot{\psi} \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS \\ &\quad + \int_{\Omega} \{ [\nabla u_{\Gamma} \cdot \nabla \bar{v}_{\Gamma} - k^2 u_{\Gamma} \bar{v}_{\Gamma}] \operatorname{div} \boldsymbol{\theta} - (\nabla u_{\Gamma} \cdot \nabla \boldsymbol{\theta}) \cdot \nabla \bar{v}_{\Gamma} - (\nabla \bar{v}_{\Gamma} \cdot \nabla \boldsymbol{\theta}) \cdot \nabla u_{\Gamma} \} \, d\Omega \end{aligned} \quad (15)$$

**3.2. Conversion into boundary integrals (void problem).** The formula (16) for the sensitivity of  $\mathcal{J}$ , expressed by a domain integral, is not suitable for BEM-based computations. However, for void defects, it can be recast in boundary-only form. In order to do so, one first notices that  $u_{\Gamma}$  and  $v_{\Gamma}$  verify:

$$\begin{aligned} &[\nabla u \otimes \nabla \bar{v} + \nabla \bar{v} \otimes \nabla u] \cdot \nabla \boldsymbol{\theta} \\ &= \operatorname{div}[(\nabla u_{\Gamma} \cdot \boldsymbol{\theta}) \nabla \bar{v}_{\Gamma} + (\nabla \bar{v}_{\Gamma} \cdot \boldsymbol{\theta}) \nabla u_{\Gamma}] + k^2 \nabla(u_{\Gamma} \bar{v}_{\Gamma}) \cdot \boldsymbol{\theta} - \nabla(\nabla u_{\Gamma} \cdot \nabla \bar{v}_{\Gamma}) \cdot \boldsymbol{\theta} \end{aligned} \quad (16)$$

Then, using this identity and after some additional manipulation, one obtains:

$$\begin{aligned} & (\nabla u_\Gamma \cdot \nabla \bar{v}_\Gamma - k^2 u_\Gamma \bar{v}_\Gamma) \operatorname{div} \boldsymbol{\theta} - (\nabla u_\Gamma \cdot \nabla \boldsymbol{\theta}) \cdot \nabla \bar{v}_\Gamma - (\nabla \bar{v}_\Gamma \cdot \nabla \boldsymbol{\theta}) \cdot \nabla u_\Gamma \\ & = \operatorname{div} [(\nabla u_\Gamma \cdot \nabla \bar{v}_\Gamma - k^2 u_\Gamma \bar{v}_\Gamma) \boldsymbol{\theta} - (\nabla u_\Gamma \cdot \boldsymbol{\theta}) \nabla \bar{v}_\Gamma - (\nabla \bar{v}_\Gamma \cdot \boldsymbol{\theta}) \nabla u_\Gamma] \end{aligned} \quad (17)$$

which allows us to recast Eq. (16) into a boundary integral by means of the divergence formula. One obtains (using the fact that  $S$  is unperturbed, i.e.  $\boldsymbol{\theta} = \mathbf{0}$  on  $S$ ):

$$\begin{aligned} \star \mathcal{J}(\Gamma) &= \int_\Gamma [\nabla u_\Gamma \cdot \nabla \bar{v}_\Gamma - k^2 u_\Gamma \bar{v}_\Gamma] \theta_n \, dS \\ &\quad - \int_\Gamma \{ (\nabla u_\Gamma \cdot \boldsymbol{\theta}) q(\bar{v}_\Gamma) + (\nabla \bar{v}_\Gamma \cdot \boldsymbol{\theta}) q(u_\Gamma) \} \, dS + \int_\Gamma (\psi^\star \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS \end{aligned} \quad (18)$$

(where  $\theta_n \equiv \boldsymbol{\theta} \cdot \mathbf{n}$ ). Further, splitting gradients into tangential and normal parts and using the boundary conditions  $q(u) = q(v) = 0$  on the void surface  $\Gamma$ , Eq. (18) becomes:

$$\star \mathcal{J}(\Gamma) = \int_\Gamma [\nabla_S u_\Gamma \cdot \nabla_S \bar{v}_\Gamma - k^2 u_\Gamma \bar{v}_\Gamma] \theta_n \, dS + \int_\Gamma (\psi^\star \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS \quad (19)$$

Formula (19) allows the computation of the derivatives of any objective functional  $\mathcal{J}$  of the type (2) with respect to shape parameters. In particular, since  $\nabla_S u_\Gamma$ ,  $\nabla_S v_\Gamma$  depend only on the boundary traces of  $u_\Gamma$  and  $v_\Gamma$ , the sensitivity (19) is computable directly from the BEM solution of the primary and adjoint problems.

**3.3. Inapplicability to crack problems.** Consider the case where the unknown defect is a crack, i.e. the limiting case of a void bounded by two surfaces  $\Gamma^+$  and  $\Gamma^-$  identical and of opposite orientations (Fig. 2).

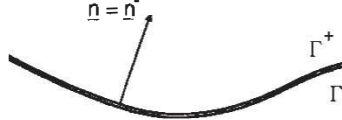


Figure 2: A crack bounded by two almost identical surfaces  $\Gamma^+$  and  $\Gamma^-$ .

It is tempting to still apply Eq. (19) to compute sensitivities with respect to crack perturbations. However, Eq. (19) is not applicable to crack defects. For instance, considering a domain shape transformation such that  $\theta_n = 0$  on the crack surface  $\Gamma$  (i.e. allowing crack perturbations along the tangent plane at the crack front, i.e. crack extensions), Eq. (19) gives  $d\mathcal{J}/dp = 0$ , which is certainly not true in general. In contrast, when  $\Gamma$  is the piecewise smooth boundary of a void,  $\theta_n = 0$  means that the void is unperturbed. This apparent paradox may be explained as follows: identity (16), which plays a key role in establishing the boundary-only expression (19), involves the field quantity  $\nabla(\nabla u \cdot \nabla v)$ . For cracks,  $u$  and  $v$  behave like  $d^{1/2}$  in the vicinity of the crack front ( $d$ : distance to  $\partial\Gamma$ ). Then,  $\nabla(\nabla u \cdot \nabla v)$  behaves like  $d^{-2}$  and the domain integral  $\int_\Omega \nabla(\nabla u \cdot \nabla v) \cdot \boldsymbol{\theta} \, d\Omega$  is divergent.

Hence, the adjoint state defined by Eqs. (13) or (14) leads to boundary-only sensitivity expressions for functionals of the form (2) only when the defect is a void. To retain the boundary-only character of sensitivity expressions when the defect is a crack, a suitable and different definition of the adjoint problem approach is called for. In what follows, this objective is shown to be fulfilled by enforcing the direct problem constraint as a symmetric Galerkin boundary integral equation (SGBIE).

#### 4. Symmetric Galerkin BIE formulation

The direct problem (1) admits, if the defect is a void, the following regularized SGBIE formulation, obtained from a weighted residual statement of the (initially hypersingular) flux boundary integral equation:

$$\mathcal{B}_{AA}(u, w) = \mathcal{F}(w) \quad \forall w \in H^{1/2}(A) \quad (20)$$

where

$$\mathcal{B}_{XY}(u, w) = \int_X \int_Y G(\mathbf{x}-\mathbf{y}) \{ R_i u(\mathbf{y}) R_i \bar{w}(\mathbf{x}) - k^2 n_i(\mathbf{y}) n_i(\mathbf{x}) u(\mathbf{y}) \bar{w}(\mathbf{x}) \} dS_y dS_x \quad (21)$$

$$\begin{aligned} \mathcal{F}(w) = & \int_S \int_S [H(\mathbf{y}, \mathbf{x}) \bar{w}(\mathbf{x}) - H^0(\mathbf{y}, \mathbf{x}) \bar{w}(\mathbf{y})] \tilde{q}(\mathbf{y}) dS_y dS_x \\ & + \int_\Gamma \int_S H(\mathbf{y}, \mathbf{x}) \bar{w}(\mathbf{x}) \tilde{q}(\mathbf{y}) dS_y dS_x - \int_S \tilde{q}(\mathbf{y}) \bar{w}(\mathbf{y}) dS_y \end{aligned} \quad (22)$$

In these expressions,  $R_i u$  denotes the  $i$ -th component of the *surface curl* of the scalar function  $u$ :  $R_i u = e_{ijk} n_j u_{,k}$ , which is a tangential differential operator [14] associated to a variant of the Stokes formula:

$$\int_C R_i f dS = 0 \quad C: \text{any piecewise smooth closed surface} \quad (23)$$

$G(\mathbf{x}-\mathbf{y}) = e^{ikr}/(4\pi r)$  is the infinite-space fundamental solution of the Helmholtz equation ( $r = |\mathbf{y} - \mathbf{x}|$ ), and  $H(\mathbf{y}, \mathbf{x}) = G_{,j}(\mathbf{x}-\mathbf{y}) n_j(\mathbf{x})$ ,  $H^0(\mathbf{y}, \mathbf{x}) = -(x_j - y_j) n_j(\mathbf{x})/(4\pi r^3)$ . The expression (21) of  $\mathcal{B}(u, w)$  stems in fact from the following identity verified by  $G$ :

$$-n_i(\mathbf{y}) n_j(\mathbf{x}) G_{,ij}(\mathbf{x}-\mathbf{y}) = k^2 G(\mathbf{x}-\mathbf{y}) - R_i^y R_i^x G(\mathbf{x}-\mathbf{y}) \quad (24)$$

When the defect is a crack, the corresponding SGBIE formulation is obtained by taking the limiting form of Eqs. (20–21–22) when the cavity becomes infinitely thin. For example, one can consider a cavity of boundary  $\Gamma^+ \cup \Gamma^-$ , where  $\Gamma^+, \Gamma^-$  (the crack faces) are identical open surfaces with opposite orientations. Let  $\Gamma \equiv \Gamma^-$  and  $\mathbf{n} \equiv \mathbf{n}^-$ . Using test functions  $w$  which are continuous over  $\Gamma^+ \cup \Gamma^-$  and vanish on  $\Gamma^+$  (in particular, such  $w$  vanish on the edge  $\partial\Gamma$ ), the SGBIE formulation turns out to be:

$$\mathcal{B}_{AS}(u, w) + \mathcal{B}_{A\Gamma}(\phi, w) \mathcal{F}(w) \quad (25)$$

where  $\phi(\mathbf{y}) = \llbracket u \rrbracket(\mathbf{y}) \equiv u^+(\mathbf{y}) - u^-(\mathbf{y})$  is the discontinuity of  $u$  across the crack.

When there is no external boundary (void or crack embedded in an infinite medium, known incident wave  $u^I$ ), the SGBIE formulation reads ( $u$ : total field):

$$\mathcal{B}_{\Gamma\Gamma}(u, w) = \int_\Gamma q^I \bar{w} dS \quad (\text{void}) \quad \mathcal{B}_{\Gamma\Gamma}(\phi, w) = - \int_\Gamma q^I \bar{w} dS \quad (\text{crack}) \quad \forall w \in H^{1/2}$$

## 5. Adjoint problem formulation for crack defects

In order to define a suitable adjoint problem, the constraint corresponding to the direct wave problem is now introduced in its SGBIE form (20) in a Lagrangian  $\mathcal{L}_B$ :

$$\mathcal{L}_B(u, w, \Gamma) = \mathcal{J}(\Gamma) + \mathcal{B}(u, w) - \mathcal{F}(w) \quad (26)$$

where  $\mathcal{B}_{AA}(u, w)$  (noted  $\mathcal{B}(u, w)$  for brevity) and  $\mathcal{F}(w)$  are given by Eqs. (21) and (22), respectively. Since the latter are respectively bilinear and linear, the material derivative of  $\mathcal{L}_B$  is expected to take the form:

$$\begin{aligned} \mathcal{L}_B^*(u, w, \Gamma) = & \int_S \varphi_{,u} \dot{u} \, dS + \int_\Gamma (\dot{\psi} \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS \\ & + \mathcal{B}(\dot{u}, w) + \mathcal{B}^1(u, w; \boldsymbol{\theta}) - \mathcal{F}^1(w; \boldsymbol{\theta}) \end{aligned} \quad (27)$$

having, again, omitted the terms containing  $\dot{w}$  for the same reasons as in Sec. 3.1. The new terms  $\mathcal{B}^1(u, w; \boldsymbol{\theta})$  and  $\mathcal{F}^1(w; \boldsymbol{\theta})$ , respectively bilinear in  $(u, w)$  and linear in  $w$ , are both linear in  $\boldsymbol{\theta}$ ; they result from application of the differentiation formulas (9) and (10) to Eqs. (21) and (22) and will be detailed later.

Again, the adjoint state  $w_\Gamma$  is defined by imposing that all terms containing  $\dot{u}$  vanish in Eq. (27). Therefore,  $w_\Gamma$  is the solution to the adjoint SGBIE formulation:

$$\mathcal{B}(w, \dot{u}) = - \int_S \bar{\varphi}_{,u} \dot{u} \, dS \quad \forall \dot{u} \in H^{1/2}(A) \quad (28)$$

where of course the symmetric character of the bilinear form  $\mathcal{B}(u, w)$  has been used.

**Remark 3.** The adjoint problem Eq. (28) is the SGBIE formulation of problem (13), but in *indirect* form. Therefore, the solution  $w_\Gamma$  to Eq. (28) is a double-layer density, and is *not* equal to the boundary trace of the solution  $v_\Gamma$  to Eq. (13), except in the special case of cracks in infinite media.

The material derivative of the functional  $\mathcal{J}$  is then expressed as:

$$\mathcal{J}^*(\Gamma) = \mathcal{L}_B^*(u_\Gamma, w_\Gamma, \Gamma) = \int_\Gamma (\dot{\psi} \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS + \mathcal{B}^1(u_\Gamma, w_\Gamma; \boldsymbol{\theta}) - \mathcal{F}^1(w_\Gamma; \boldsymbol{\theta}) \quad (29)$$

The remaining task is to establish explicit expressions for the terms  $\mathcal{B}^1(u, w; \boldsymbol{\theta})$  and  $\mathcal{F}^1(w; \boldsymbol{\theta})$ . This is achieved in quite straightforward fashion, by applying the differentiation formulas (9) and (10) to the simple and double integrals involved in Eqs. (21) and (22) which define  $\mathcal{B}(u, w)$  and  $\mathcal{F}(w)$ . It is important to note at this point that all double integrations in Eqs. (21) and (22) consist in a weakly singular inner integral followed by a nonsingular outer integral.

In order to perform this calculation, let us first collect some useful formulas. First, for any kernel function of the form  $K(\mathbf{y} - \mathbf{x})$ , one has:

$$\dot{K}(\mathbf{y} - \mathbf{x}) = [\theta_i(\mathbf{x}) - \theta_i(\mathbf{y})] K_{,i}(\mathbf{y} - \mathbf{x}) \quad (30)$$



Then, from Eqs. (7), it is easy to show that

$$(n_i dS)^* = (n_i D_j \theta_j - n_j D_i \theta_j) dS = e_{ijk} R_k \theta_j dS \quad (31)$$

In addition, using Eqs. (6), (7) and (31), one has:

$$\begin{aligned} (R_i u dS)^* &= e_{ijk} (e_{jab} R_b \theta_a u_{,k} - n_j u_a \theta_{a,k}) dS = (R_k \theta_i - R_i \theta_k) u_{,k} - R_i \theta_a u_{,a} \\ &= -R_a \theta_i u_{,a} = R_a u D_i \theta_a \end{aligned} \quad (32)$$

The last equality results from invoking again the definition of the surface curl and its consequence  $n_a R_a u = 0$ . Using Eqs. (10), (30), (31) and (32), it is then a simple matter to show (again assuming that  $\dot{w} = 0$ ) that:

$$\dot{\mathcal{B}}(u, w) = \mathcal{B}(\dot{u}, w) + \mathcal{B}^1(u, w; \boldsymbol{\theta}) \quad (33)$$

where  $\mathcal{B}^1(u, w; \boldsymbol{\theta})$  is given by:

$$\mathcal{B}^1(u, w; \boldsymbol{\theta}) = \int_A \int_A \{ R_i u(\mathbf{y}) R_j \bar{w}(\mathbf{x}) B_{ij}^1(\mathbf{y}, \mathbf{x}; \boldsymbol{\theta}) - k^2 u(\mathbf{y}) \bar{w}(\mathbf{x}) A^1(\mathbf{y}, \mathbf{x}; \boldsymbol{\theta}) \} dS_y dS_x \quad (34)$$

with the new kernel functions:

$$B_{ij}^1(\mathbf{y}, \mathbf{x}; \boldsymbol{\theta}) = [\theta_k(\mathbf{x}) - \theta_k(\mathbf{y})] G_{,k}(\mathbf{x} - \mathbf{y}) \delta_{ij} + [\theta_{i,j}(\mathbf{x}) + \theta_{i,j}(\mathbf{y})] G(\mathbf{x} - \mathbf{y}) \quad (35)$$

$$\begin{aligned} A^1(\mathbf{y}, \mathbf{x}; \boldsymbol{\theta}) &= n_i(\mathbf{y}) n_i(\mathbf{x}) [\theta_j(\mathbf{x}) - \theta_j(\mathbf{y})] G_{,j}(\mathbf{x} - \mathbf{y}) \\ &\quad + e_{ijk} [n_i(\mathbf{y}) R_k \theta_j(\mathbf{x}) + n_i(\mathbf{x}) R_k \theta_j(\mathbf{y})] G(\mathbf{x} - \mathbf{y}) \end{aligned} \quad (36)$$

Under the conditions of the present study,  $\boldsymbol{\theta} = \mathbf{0}$  on  $S$  should be enforced in Eq. (34).

Next, one has, from the definition of  $H(\mathbf{y}, \mathbf{x})$  and using again Eqs. (30) and (31):

$$\begin{aligned} (H(\mathbf{y}, \mathbf{x}) dS_x)^* &= (G_{,i}(\mathbf{x} - \mathbf{y}) n_i(\mathbf{x}) dS_x)^* \\ &= (\theta_i(\mathbf{x}) G_{,ij}(\mathbf{x} - \mathbf{y}) n_i(\mathbf{x}) + G_{,i}(\mathbf{x} - \mathbf{y}) e_{ijk} R_k \theta_j(\mathbf{x})) dS_x \end{aligned}$$

where  $\mathbf{x}$  and  $\mathbf{y}$  are assumed to lie on  $\Gamma$  and  $S$ , respectively, so that  $\boldsymbol{\theta}(\mathbf{y}) = \mathbf{0}$ . In addition, one has (since here  $\mathbf{x} \neq \mathbf{y}$ ):

$$\begin{aligned} G_{,ij}(\mathbf{x} - \mathbf{y}) n_i(\mathbf{x}) &= e_{ijk} R_k^x G_{,i}(\mathbf{x} - \mathbf{y}) + n_j(\mathbf{x}) G_{,ii}(\mathbf{x} - \mathbf{y}) \\ &= e_{ijk} R_k^x G_{,i}(\mathbf{x} - \mathbf{y}) - k^2 n_j(\mathbf{x}) G(\mathbf{x} - \mathbf{y}) \end{aligned}$$

and hence, combining these relations:

$$(H(\mathbf{y}, \mathbf{x}) dS_x)^* = e_{ijk} R_k^x (G_{,i}(\mathbf{x} - \mathbf{y}) \theta_i(\mathbf{x})) - k^2 \theta_n(\mathbf{x}) G(\mathbf{x} - \mathbf{y}) \quad (37)$$

One is now in a position to calculate the material derivative of  $\mathcal{F}(w)$ . The differentiation of Eq. (22) is performed under the assumption that the surface  $S$  is left

unperturbed by the domain transformation  $\boldsymbol{\theta} = \mathbf{0}$  and hence affects only *single* integrals. By virtue of the identity (37) and using the Stokes identity (23), one finds:

$$\begin{aligned} \mathcal{F}^*(w) &= \mathcal{F}^1(w; \boldsymbol{\theta}) \\ &= \int_{\Gamma} \int_S \{ e_{ijk} R_k^x (G_{,i}(\mathbf{x}-\mathbf{y}) \theta_i(\mathbf{x})) - k^2 \theta_n(\mathbf{x}) G(\mathbf{x}-\mathbf{y}) \} \bar{w}(\mathbf{x}) \tilde{q}(\mathbf{y}) \, dS_y \, dS_x \\ &= - \int_{\Gamma} \int_S \{ G_{,i}(\mathbf{x}-\mathbf{y}) \theta_i(\mathbf{x}) e_{ijk} R_k \bar{w}(\mathbf{x}) + k^2 \theta_n(\mathbf{x}) G(\mathbf{x}-\mathbf{y}) \bar{w}(\mathbf{x}) \} \tilde{q}(\mathbf{y}) \, dS_y \, dS_x \quad (38) \end{aligned}$$

Equations (33) to (36) and (38) provide the sought-for explicit expressions of  $\mathcal{B}^1(u, w; \boldsymbol{\theta})$  and  $\mathcal{F}^1(w; \boldsymbol{\theta})$ . The sensitivity formula (29) is then completely determined.

**Remark 4.** Equations (33) to (36) and (38), and hence the sensitivity formula (29), are applicable for both voids and cracks. The derivation of  $\mathcal{B}^1(u, w; \boldsymbol{\theta})$ , presented for Eq. (21) (void), is essentially repeated when applied to Eq. (25) (crack).

**Remark 5.** When dealing with void defects, two alternative sensitivity expressions, Eqs. (19) and (29), are thus available.

**Remark 6.** The inner integrals in Eqs. (33) to (36) and (38) are weakly singular if  $\boldsymbol{\theta} \in C^{0,1}(\Gamma)$ , while the outer ones are regular. Moreover, due to the double surface integration, the integrals in Eqs. (25), (29) are convergent even in the presence of a  $d^{-1/2}$  crack front singularity of  $R_i \phi_{\Gamma}$  and  $R_i \bar{w}_{\Gamma}$ .

**Remark 7.** The approach developed in Sections 5 and 6 for the first-order material derivative can be carried out one step further for the evaluation of second-order derivatives. Indeed this has been done in [6] to formulate and compute first- and second-order material derivatives of the elastic potential energy at equilibrium, as part of a numerical scheme to study the stability of quasi-static crack extension. Recall, however, that the second-order material derivative (assuming a finite number of geometrical parameters) and domain derivative do not coincide in general [18].

## 6. Frequency-domain elastodynamics

This section presents the generalization of the previous formulations to linear isotropic elastodynamics. The displacement vector  $\mathbf{u}$ , strain tensor  $\boldsymbol{\varepsilon}$  and stress tensor  $\boldsymbol{\sigma}$  are related through the equilibrium, constitutive and compatibility field equations:

$$\operatorname{div} \boldsymbol{\sigma} + \rho \omega^2 \mathbf{u} = \mathbf{0} \quad \boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} \quad \boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + \nabla^T \mathbf{u}) \quad \text{in } \Omega \quad (39)$$

where  $\mathbf{C}$  is the fourth-order Hooke tensor of elastic moduli, whose components possess the symmetry properties  $C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}$ . For isotropic elasticity, one has  $C_{ijkl} = \mu(\kappa \delta_{ij} \delta_{kl} + \delta_{jl} \delta_{ik} + \delta_{il} \delta_{jk})$  ( $\mu$ : shear Lamé modulus,  $\nu$ : Poisson ratio,  $\kappa = 2\nu/(1 - 2\nu)$ ). Equations (39) are supplemented by boundary conditions:

$$\mathbf{t}(\mathbf{u}) = \tilde{\mathbf{t}} \quad (\text{on } S) \quad \mathbf{t}(\mathbf{u}) = \mathbf{0} \quad (\text{on } \Gamma) \quad (40)$$

where  $\mathbf{t}(\mathbf{u}) = \boldsymbol{\sigma}(\mathbf{u}) \cdot \mathbf{n}$  is the elastic traction vector.

**6.1. Adjoint formulation for the void defect.** Considering objective functions similar to Eq. (2), the Lagrangian incorporating the problem (39–40) in weak form is:

$$\mathcal{L}(\mathbf{u}, \mathbf{v}, \Gamma) = \mathcal{J}(\Gamma) + \int_{\Omega} (\boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}}) - \rho\omega^2 \mathbf{u} \cdot \bar{\mathbf{v}}) \, d\Omega - \int_S \tilde{\mathbf{t}} \cdot \bar{\mathbf{v}} \, dS \quad (\mathbf{v} \in [H^1(\Omega)]^3) \quad (41)$$

Its material derivative is given by:

$$\begin{aligned} \dot{\mathcal{L}}(\mathbf{u}, \mathbf{v}, \Gamma) &= \int_S \varphi_{,u} \cdot \dot{\mathbf{u}} \, dS + \int_{\Omega} (\boldsymbol{\sigma}(\dot{\mathbf{u}}) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}}) - \rho\omega^2 \dot{\mathbf{u}} \cdot \bar{\mathbf{v}}) \, d\Omega + \int_{\Gamma} (\dot{\psi} \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS \\ &+ \int_{\Omega} \{ [\boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}}) - \rho\omega^2 \mathbf{u} \cdot \bar{\mathbf{v}}] \operatorname{div} \boldsymbol{\theta} - \boldsymbol{\sigma}(\mathbf{u}) : (\nabla \bar{\mathbf{v}} \cdot \nabla \boldsymbol{\theta}) - \boldsymbol{\sigma}(\bar{\mathbf{v}}) : (\nabla \mathbf{u} \cdot \nabla \boldsymbol{\theta}) \} \, d\Omega \end{aligned} \quad (42)$$

(note that the terms containing  $\dot{\bar{\mathbf{v}}}$  have been, again, dropped). The adjoint field  $\mathbf{v}$  is thus found to solve the field equations (39) together with the boundary conditions:

$$\mathbf{t}(\mathbf{v}) = -\bar{\varphi}_{,u} \quad (\text{on } S) \quad \mathbf{t}(\mathbf{v}) = \mathbf{0} \quad (\text{on } \Gamma) \quad (43)$$

Besides, the solutions  $\mathbf{u}_{\Gamma}$  and  $\mathbf{v}_{\Gamma}$  to the direct and adjoint problems (and, indeed, any pair  $(\mathbf{u}, \mathbf{v})$  solving the field equations (39) as well) are found to verify:

$$\begin{aligned} &[\boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}}) - \rho\omega^2 \mathbf{u} \cdot \bar{\mathbf{v}}] \operatorname{div} \boldsymbol{\theta} - \boldsymbol{\sigma}(\mathbf{u}) : (\nabla \bar{\mathbf{v}} \cdot \nabla \boldsymbol{\theta}) - \boldsymbol{\sigma}(\bar{\mathbf{v}}) : (\nabla \mathbf{u} \cdot \nabla \boldsymbol{\theta}) \\ &= \operatorname{div} ([\boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}}) - \rho\omega^2 \mathbf{u} \cdot \bar{\mathbf{v}}] \boldsymbol{\theta} - \boldsymbol{\sigma}(\mathbf{u}) (\nabla \bar{\mathbf{v}} \cdot \boldsymbol{\theta}) - \boldsymbol{\sigma}(\bar{\mathbf{v}}) (\nabla \mathbf{u} \cdot \boldsymbol{\theta})) \end{aligned}$$

so that, for void defects, the sensitivity of  $\mathcal{J}$  is expressed in boundary-only form as:

$$\dot{\mathcal{J}} = \int_{\Gamma} [\boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}}) - \rho\omega^2 \mathbf{u} \cdot \bar{\mathbf{v}}] \theta_n \, dS + \int_{\Gamma} (\dot{\psi} \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS \quad (44)$$

having taken into account the homogeneous boundary conditions on  $\Gamma$ . Further, the strain energy density  $\boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}})$  can be expressed in terms of the tangential derivatives  $\nabla_S \mathbf{u}$ ,  $\nabla_S \bar{\mathbf{v}}$  and of the tractions  $\mathbf{t}(\mathbf{u})$ ,  $\mathbf{t}(\bar{\mathbf{v}})$ . Since the latter vanish on  $\Gamma$ , one obtains:

$$\boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\bar{\mathbf{v}}) = \mu \left\{ \frac{2\nu}{1-\nu} \operatorname{div}_S \mathbf{u} \operatorname{div}_S \bar{\mathbf{v}} + (\nabla_S \mathbf{u} + \nabla_S^T \mathbf{u}) : \nabla_S \bar{\mathbf{v}} - (\mathbf{n} \cdot \nabla_S \mathbf{u}) \cdot (\mathbf{n} \cdot \nabla_S \bar{\mathbf{v}}) \right\} \quad (45)$$

**6.2. Adjoint formulation for the crack defect.** The direct problem (39) admits, if the defect is a void, the following regularized SCBIE formulation, obtained from a weighted residual statement of the traction boundary integral equation:

$$\mathcal{B}_{AA}(\mathbf{u}, \mathbf{w}) = \mathcal{F}(\mathbf{w}) \quad \forall \mathbf{w} \in [H^{1/2}(A)]^3 \quad (46)$$

where

$$\mathcal{B}_{XY}(\mathbf{u}, \mathbf{v}) = \int_X \int_Y \left\{ R_q u_i(\mathbf{y}) R_s \bar{w}_k(\mathbf{x}) B_{ikqs}(\mathbf{x} - \mathbf{y}) + k_T^2 n_j(\mathbf{y}) n_\ell(\mathbf{x}) u_i(\mathbf{y}) \bar{w}_k(\mathbf{x}) A_{ijkl}(\mathbf{x} - \mathbf{y}) \right\} dS_y dS_x \quad (47)$$

$$\begin{aligned} \mathcal{F}(\mathbf{w}) &= \int_S \int_S [T_i^k(\mathbf{y}, \mathbf{x}) \bar{w}_k(\mathbf{x}) - T_i^{(0)k}(\mathbf{y}, \mathbf{x}) \bar{w}_k(\mathbf{y})] \tilde{t}_a(\mathbf{y}) dS_y dS_x \\ &+ \int_\Gamma \int_S T_i^k(\mathbf{y}, \mathbf{x}) \bar{w}_k(\mathbf{x}) \bar{w}_k(\mathbf{x}) \tilde{t}_a(\mathbf{y}) dS_y dS_x - \int_S \tilde{t}_a(\mathbf{y}) \bar{w}_k(\mathbf{y}) dS_y \end{aligned} \quad (48)$$

In Eq. (48),  $T_i^k(\mathbf{y}, \mathbf{x})$  (resp.  $T_i^{(0)k}(\mathbf{y}, \mathbf{x})$ ) denotes the traction vector associated with the dynamical (resp. static) infinite-space fundamental solution  $U_i^k(\mathbf{x} - \mathbf{y})$  (resp.  $U_i^{(0)k}(\mathbf{x} - \mathbf{y})$ ) of (39):

$$\begin{aligned} U_i^k &= 2(1 - \nu) [\Delta F + k_L^2 F] \delta_{ik} - F_{,ik} & U_i^{(0)k} &= 2(1 - \nu) \Delta F^0 \delta_{ik} - F_{,ik}^0 \\ \Sigma_{ij}^k &= \lambda \delta_{ij} U_{i,i}^k + \mu (U_{i,j}^k + U_{j,i}^k) & \Sigma_{ij}^{(0)k} &= \lambda \delta_{ij} U_{i,i}^{(0)k} + \mu (U_{i,j}^{(0)k} + U_{j,i}^{(0)k}) \\ T_i^k &= \Sigma_{ij}^k n_j & T_i^{(0)k} &= \Sigma_{ij}^{(0)k} n_j \end{aligned}$$

with

$$F(\mathbf{x} - \mathbf{y}) = \frac{1}{4\pi\mu k_T^2} (e^{ik_L r} - e^{ik_T r}) \frac{1}{r} F^0(\mathbf{x} - \mathbf{y}) = \frac{1}{16\pi\mu(1 - \nu)} r \quad (49)$$

with  $k_L^2 = \rho\omega^2/(\lambda + 2\mu)$ ,  $k_T^2 = \rho\omega^2/\mu$ . The latter functions verify:

$$\Delta^2 F = \frac{1}{4\pi\mu k_T^2} (k_L^4 e^{ik_L r} - k_T^4 e^{ik_T r}) \frac{1}{r} \quad \Delta^2 F^0 = 0 \quad (\mathbf{x} \neq \mathbf{y}) \quad (50)$$

Besides, Eq. (47) stems from the following identity (given in [16] and generalized to anisotropic elasticity in [2]):

$$-C_{ijab} C_{klcd} U_{a,bd}^c(\mathbf{x} - \mathbf{y}) n_j(\mathbf{x}) n_\ell(\mathbf{y}) = R_q^x R_s^y B_{ikqs}(\mathbf{x} - \mathbf{y}) + k_T^2 A_{ijkl}(\mathbf{x} - \mathbf{y}) n_j(\mathbf{x}) n_\ell(\mathbf{y})$$

where the kernel functions  $B_{ikqs}(\mathbf{x} - \mathbf{y})$  and  $A_{ijkl}(\mathbf{x} - \mathbf{y})$  are given by:

$$B_{ikqs}(\mathbf{x} - \mathbf{y}) = -e_{iep} e_{kgr} \mu^2 [4\nu \delta_{pq} \delta_{rs} + 2(1 - \nu)(\delta_{pr} \delta_{qs} + \delta_{ps} \delta_{qr})] F_{,eg} \quad (51)$$

$$\begin{aligned} A_{ijkl}(\mathbf{x} - \mathbf{y}) &= (1 - 2\nu) k_T^2 C_{ijab} C_{klcd} \delta_{ac} F_{,bd} \\ &+ [2(1 - \nu)(\delta_{ik} \delta_{jl} + \delta_{jk} \delta_{il}) + 4\nu \delta_{ij} \delta_{kl}] \Delta^2 F \end{aligned} \quad (52)$$

and are both weakly singular in view of Eqs. (49a) and (50).

Introducing the Lagrangian  $\mathcal{L}_B(\mathbf{u}, \mathbf{w}, \Gamma) = \mathcal{J}(\Gamma) + \mathcal{B}(\mathbf{u}, \mathbf{w}) - \mathcal{F}(\mathbf{w})$ , the analysis of Sec. 5 is essentially repeated: the adjoint state  $\mathbf{w}_\Gamma$  is the solution to the adjoint SGBIE formulation:

$$\mathcal{B}(\mathbf{w}, \hat{\mathbf{u}}) = - \int_S \hat{\varphi}_{,u} \cdot \hat{\mathbf{u}} dS \quad \forall \hat{\mathbf{u}} \in [H^{1/2}(A)]^3 \quad (53)$$

The material derivative of the functional  $\mathcal{J}$  is then expressed as:

$$\dot{\mathcal{J}}(\Gamma) = \int_{\Gamma} (\dot{\psi} \cdot \boldsymbol{\theta} + \psi \operatorname{div}_S \boldsymbol{\theta}) \, dS + \mathcal{B}^1(\mathbf{u}_{\Gamma}, \mathbf{w}_{\Gamma}; \boldsymbol{\theta}) - \mathcal{F}^1(\mathbf{w}_{\Gamma}; \boldsymbol{\theta}) \quad (54)$$

A calculation similar to that performed in Sec. 5. then gives:

$$\begin{aligned} \mathcal{B}^1(\mathbf{u}, \mathbf{w}) = \int_A \int_A \{ & R_{\mathbf{q}} u_i(\mathbf{y}) R_s \bar{w}_k(\mathbf{x}) B_{ikqs}^1(\mathbf{y}, \mathbf{x}; \boldsymbol{\theta}) \\ & + k_T^2 n_j(\mathbf{y}) n_{\ell}(\mathbf{x}) u_i(\mathbf{y}) \bar{w}_k(\mathbf{x}) A_{ij\ell k}^1(\mathbf{y}, \mathbf{x}; \boldsymbol{\theta}) \} \, dS_y \, dS_x \quad (55) \end{aligned}$$

with

$$\begin{aligned} B_{ikqs}^1(\mathbf{y}, \mathbf{x}; \boldsymbol{\theta}) = & \theta_{q,m}(\mathbf{x}) B_{ikms}(\mathbf{x} - \mathbf{y}) + \theta_{s,m}(\mathbf{y}) B_{ikqm}(\mathbf{x} - \mathbf{y}) \\ & + [\theta_m(\mathbf{x}) - \theta_m(\mathbf{y})] B_{ikqs,m}(\mathbf{x} - \mathbf{y}) \quad (56) \end{aligned}$$

$$\begin{aligned} A_{ij\ell k}^1(\mathbf{y}, \mathbf{x}; \boldsymbol{\theta}) = & [\theta_m(\mathbf{x}) - \theta_m(\mathbf{y})] B_{ikqs,m}(\mathbf{x} - \mathbf{y}) + [D_m \theta_m(\mathbf{x}) + D_m \theta_m(\mathbf{y})] A_{ijk\ell}(\mathbf{x} - \mathbf{y}) \\ & - D_m \theta_j(\mathbf{x}) A_{imk\ell}(\mathbf{x} - \mathbf{y}) - D_m \theta_{\ell}(\mathbf{y}) A_{ijkm}(\mathbf{x} - \mathbf{y}) \quad (57) \end{aligned}$$

and

$$\begin{aligned} \mathcal{F}^1(\mathbf{w}; \boldsymbol{\theta}) = - \int_{\Gamma} \int_S \{ & e_{jma} \theta_m(\mathbf{x}) \Sigma_{ij}^k(\mathbf{x} - \mathbf{y}) R_a^x \bar{w}_k(\mathbf{y}) \\ & + \mu k_T^2 \theta_n(\mathbf{x}) U_i^k(\mathbf{x} - \mathbf{y}) \bar{w}_k(\mathbf{x}) \} \tilde{t}_a(\mathbf{y}) \, dS_y \, dS_x \quad (58) \end{aligned}$$

which completes our result for the elastodynamic case.

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