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Sensitivity analysis of 2D elastic structures in presence of stress singularities

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THE OBJECT OF THIS PAPER is the investigation of the influence of stress singularities on the sensitivity of two-dimensional linearized elastic fields and the corresponding functionals under a variation of the domain. This requires a detailed study of the local behaviour of the material and of the shape derivatives of the displacement field in the vicinity of boundary corner points. Using these regularity results, we apply the method of adjoint problems to express the shape derivatives of the functionals as boundary integrals and give precise conditions under which this approach can be justified. It turns out that in case of elastic structures with cracks, the sensitivity of the functionals depends also on the stress intensity factors of the solution of the adjoint problem.

Notations

$\langle \cdot, \cdot \rangle$	inner product in $\mathbb{R}^2$,
$\mathbf{s} : \mathbf{t}$	inner product of tensors $\mathbf{s}, \mathbf{t}$,
δ_{ij}	Kronecker's delta,
$\mathbf{D}v$	Jacobian of a vector function v,
$\mathbf{n}_\varepsilon$	perturbed unit normal vector,
u_ε	perturbed displacement field,
$e(u_\varepsilon)$	perturbed linearized strain tensor,
$\mathbf{C}$	$= \{c_{ijkl} : i, j, k, l = 1, 2\}$ Hooke's tensor,
$\sigma(u_\varepsilon)$	$= C : e(u_\varepsilon)$ perturbed linearized stress field,
$\dot{u}$	material derivative of u_ε,
u'	shape derivative of u_ε.

1. Introduction

THE INFLUENCE OF THE SHAPE of the domain on the elastic behaviour has been studied by many authors (see the monographs [6, 18] and the references therein). The corresponding sensitivity analysis is well developed for problems in smooth domains. In particular, the method of adjoint systems [2, 3] allows to express the shape derivatives of the functionals as boundary integrals if the underlying elastic fields are smooth enough. In practical situations the regularity of elastic fields is low because of stress singularities which appear at geometrical peculiarities like corners, cracks and notches and at points where the boundary conditions change. In this case the sensitivity analysis is much less developed and only few mathematically rigorous results are available. For example, in [13] the existence and the $H^1(\Omega)$-regularity of the material derivative is proved for the mixed boundary value problem for the Laplace equation in a smooth domain, using the implicit function theorem. Moreover, there exist a lot of papers on particular problems of fracture mechanics, where the sensitivity of the potential energy with respect to a variation of the crack tip is analyzed (see the classical paper by Rice [15] and the subsequent mathematical works [11, 4, 10, 12]).

In this paper we study the influence of stress singularities on the sensitivity of linearized elastic fields in general two-dimensional domains with corners, and of a class of corresponding functionals with respect to shape perturbation. To this end we apply the material derivative approach [5, 17, 6, 18], i.e. we introduce a fixed reference configuration and consider a class of small perturbations of the reference domain. The state equations as well as all fields which are defined over the actual configuration are transformed to the fixed reference configuration. Thus the investigation of the shape sensitivity can be reduced to the investigation of a regular perturbed boundary value problem for the transformed elastic fields. We expand the transformed quantities asymptotically with respect to the perturbation parameter ε and justify the asymptotics with the help of a-priori estimates in weighted Sobolev spaces. In this way we obtain the existence and precise regularity results for the material and the shape derivatives of the displacement fields. We apply the method of adjoint problems in order to express the derivatives of the functionals as boundary integrals and give conditions under which this approach can be justified. Then we show that in case of cracked structures, the sensitivity of functionals depends also on the stress intensity factors of the adjoint field, and the original version of the method of adjoint problems [2, 3] has to be modified. Finally, we apply these results to the sensitivity of several basic functionals.

2. Formulation of the problem

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain, whose boundary $\partial\Omega$ consists of two smooth open manifolds Γ^D, Γ^N and a set S of isolated points where stress singularities can occur, i.e. corner points and points where the boundary conditions change (see e.g. Fig. 1). We assume that $\Gamma^D \neq \emptyset$ and that the domain Ω is locally diffeomorphic in a neighbourhood of each singular point $P_i \in S$ to a wedge.

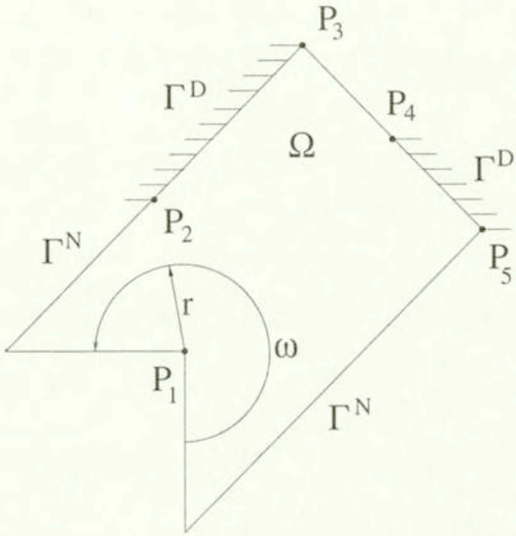

FIG. 1. A plate with singular points $P_1, \ldots, P_5$.

We introduce a family of mappings

$$\{\Phi_\varepsilon \in [C^3(\overline{\Omega})]^2;\ \varepsilon \in [0, \varepsilon_0]\} \tag{2.1}$$

which admit Taylor expansions

$$\Phi_\varepsilon(x) = x + \varepsilon\Phi(x) + \varepsilon^2\Phi_R(\varepsilon, x) \tag{2.2}$$

with $\Phi, \Phi_R \in [C^3(\overline{\Omega})]^2$. The function $\Phi_R(\varepsilon, x)$ is bounded with respect to ε for every $x \in \Omega$. The perturbations $(\Omega_\varepsilon, \Gamma_\varepsilon^D, \Gamma_\varepsilon^N)$ of the reference configuration $(\Omega, \Gamma^D, \Gamma^N)$ are defined by

$$\Omega_\varepsilon = \Phi_\varepsilon(\Omega), \quad \Gamma_\varepsilon^D = \Phi_\varepsilon(\Gamma^D), \quad \Gamma_\varepsilon^N = \Phi_\varepsilon(\Gamma^N). \tag{2.3}$$

Since $\Phi_\varepsilon \in [C^3(\overline{\Omega})]^2$, the number of singular points in Ω_ε is constant for every ε.

We consider the following mixed boundary value problem for the displacement field u_ε in an anisotropic linear elastic body occupying the perturbed configuration

$$\begin{aligned} Lu_\varepsilon(x_\varepsilon) := -\mathrm{div}\sigma(u_\varepsilon)(x_\varepsilon) &= f_\varepsilon(x_\varepsilon) \qquad \text{in} \quad \Omega_\varepsilon, \\ u_\varepsilon(x_\varepsilon) &= 0 \qquad \text{on} \quad \Gamma_\varepsilon^D, \\ \sigma(u_\varepsilon)\mathbf{n}_\varepsilon(x_\varepsilon) &= h_\varepsilon(x_\varepsilon) \qquad \text{on} \quad \Gamma_\varepsilon^N, \end{aligned} \tag{2.4}$$

where $\sigma(u_\varepsilon) = C : e(u_\varepsilon)$ is the linearized stress tensor with the components $\sigma_{ij} = c_{ijkl}e_{ij}$, $e_{ij} = (\partial_i u_j + \partial_j u_i)/2$ is the linearized strain tensor,

$\mathbf{C} = \{c_{ijkl}, i,j,k,l = 1,2\}$ is the Hooke's tensor and $\mathbf{n}_\varepsilon$ is the outer unit normal vector on $\partial\Omega_\varepsilon$. Moreover, we consider functionals associated with the elastic fields u_ε and $\sigma(u_\varepsilon)$

$$J(\Omega_\varepsilon) = \int_{\Omega_\varepsilon} F(u_\varepsilon, \sigma(u_\varepsilon))dx_\varepsilon. \tag{2.5}$$

The function F satisfies for a positive constant c the growth conditions

$$F(p,q) \leqslant a(p)(c + |q|^2),\ \partial_q F(p,q) \leqslant a(p)(c + |q|) \tag{2.6}$$

for some $a \in C(\mathbb{R}^2)$ and all $p \in \mathbb{R}^2$, $q \in \mathbb{R}^4$. This guarantees that the functional (2.5) is well defined for all displacements $u_\varepsilon \in [W^1_{2+\delta}(\Omega_\varepsilon)]^2$ and all stresses $\sigma(u_\varepsilon) \in [L_{2+\delta}(\Omega_\varepsilon)]^4$ with a small $\delta > 0$ [1, Lemma 9.5]. Examples of such functionals will be given in Sec. 7.

Our goal is to derive formulae for the sensitivity of the functional J with respect to the perturbation mapping Φ_ε, i.e. we want to calculate the shape derivative

$$dJ(\Omega, \Phi_\varepsilon) = \lim_{\varepsilon \to 0} \frac{J(\Phi_\varepsilon(\Omega)) - J(\Omega)}{\varepsilon} \tag{2.7}$$

and to express $dJ(\Omega, \Phi_\varepsilon)$ as an integral over $\partial\Omega$.

3. Regularity of elastic fields in 2D non-smooth domains

In this section we omit the index ε.
The behaviour of solutions of elliptic boundary value problems like (2.4) in the neighbourhood of singular points $P_i \in S$ was mathematically analyzed by KONDRAT'EV [8] (see also the monograph [9], whose general theory was applied to problems of the theory of isotropic linearized elasticity in [16]. Stress singularities were investigated earlier by many engineers using formal methods (see e.g. [7]). According to Kondrat'ev's results, the weak solution $\theta u - u_\varepsilon$ of the boundary value problem (2.4) admits a decomposition into a linear combination of singular functions S_j which have (in polar coordinates (r, ω) centred on P_i) the form

$$S_j = r^{\alpha_j} \varphi_j(\log r, \omega), \tag{3.1}$$

and a more regular remainder $\tilde{u}$

$$u = \sum_j c_j S_j + \tilde{u} \tag{3.2}$$

provided that the given forces satisfy appropriate regularity assumptions. The singular functions S_j are solutions of the problem (2.4) with vanishing body and boundary forces in the infinite wedge $W(P_i)$ which coincides with Ω in some neighbourhood of P_i. The exponents α_j and the functions φ_j can be interpreted as eigenvalues and (generalized) eigenfunctions of a certain operator pencil $\mathcal{A}(P_i)$ (see [8, 9] for details). The exponents α_j in (3.1) are complex roots of special transcendent equations [7, 16] and have to be calculated numerically. For the functions φ_j of S_j many explicit formulae are available (see [7, 16] for isotropic elasticity). In this paper we are interested mainly in the eigenvalue with the smallest positive real part which determines the regularity of the weak solution. To this end we define $a_0 = \min\{\mathrm{Re}\alpha_j\}$, where the minimum is taken over all eigenvalues α_j of $\mathcal{A}(P_i)$ with a positive real part $\mathrm{Re}\alpha_j$ for every singular point $P_i \in S$. Note that $a_0 \geqslant 1/2$ in case of a pure Dirichlet or a pure Neumann problem, whereas for mixed boundary value problems we have only $a_0 \geqslant 1/4$ [16]. In case of a pure Dirichlet or a pure Neumann problem in a domain with reentrant corners we have $a_0 < 1$, i.e. the stresses are unbounded. At points where the boundary conditions change, stress singularities can occur even if the boundary is smooth.

For the formulation of the regularity results we use weighted Sobolev spaces which describe not only the regularity of functions in the interior of Ω but also their behaviour near singular points.

DEFINITION 3.1. [8, 9] *For $d = 0, 1, 2, \ldots$ we define the weighted Sobolev space $V^d_\beta(\Omega)$ as the closure of $C^\infty_0(\overline{\Omega} \setminus S)$ with respect to the norm*

$$\|u\|_{V^d_\beta(\Omega)} := \left(\sum_{|\gamma| \leqslant d} \|\tilde{r}^{\beta - d + |\gamma|} D^\gamma_x u\|^2_{L_2(\Omega)} \right)^{1/2}, \tag{3.3}$$

where $\tilde{r} = \mathrm{dist}(x, S)$. The trace spaces $V^{d+1/2}_\beta(\partial\Omega)$, $V^{d+1/2}_\beta(\Gamma^D)$, $V^{d+1/2}_\beta(\Gamma^N)$ are defined in the usual way.

Roughly speaking, a function u belongs to $V^d_\beta(\Omega)$ if it belongs to $H^d(\tilde{\Omega})$ for every open subset $\tilde{\Omega} \subset \Omega$ and $u(x) \leqslant c|x - P_i|^{d-\beta-1}$ in the neighbourhood of every singular point $P_i \in S$ with some positive constant c.

THEOREM 3.2. [8, 16, 9] *Let $d = 0, 1, 2, \ldots$, $\beta := d + 1 - a_0 + \delta$ with a small positive δ and $f \in [V^d_\beta(\Omega)]^2$, $h \in [V^{d+1/2}_\beta(\Gamma^N)]^2$. Then the unique weak solution $u \in [H^1(\Omega)]^2$ of (2.4) belongs to $[V^{d+2}_\beta(\Omega)]^2$ and the following a priori estimate is valid:*

$$\|u\|_{[V^{d+2}_\beta(\Omega)]^2} \leqslant c \left\{ \|f\|_{[V^d_\beta(\Omega)]^2} + \|h\|_{[V^{d+1/2}_\beta(\Gamma^N)]^2} \right\} \tag{3.4}$$

with a positive real constant c.

4. Existence and regularity of the material and the shape derivative

Let us investigate the existence and the regularity of the material derivative

$$\dot{u} := \left.\frac{d(u_\varepsilon \circ \Phi_\varepsilon)}{d\varepsilon}\right|_{\varepsilon=0} \tag{4.1}$$

and the shape derivative

$$u' := \left.\frac{du_\varepsilon}{d\varepsilon}\right|_{\varepsilon=0} \tag{4.2}$$

of the perturbed displacement field u_ε. To this end we transform the problem (2.4) onto the reference configuration by means of a change of variables $x_\varepsilon = \Phi_\varepsilon(x)$ and obtain in this way a boundary value problem for the transformed field $u_\varepsilon \circ \Phi_\varepsilon$

$$\begin{aligned} L^\varepsilon(u_\varepsilon \circ \Phi_\varepsilon)(x) &= f_\varepsilon \circ \Phi_\varepsilon(x) && \text{in} \quad \Omega, \\ u_\varepsilon \circ \Phi_\varepsilon(x) &= 0 && \text{on} \quad \Gamma^D, \\ \sigma^\varepsilon(u_\varepsilon \circ \Phi_\varepsilon)(\mathbf{n}_\varepsilon \circ \Phi_\varepsilon)(x) &= h_\varepsilon \circ \Phi_\varepsilon(x) && \text{on} \quad \Gamma^N. \end{aligned} \tag{4.3}$$

Here, L^ε and σ^ε are differential operators whose coefficients depend smoothly on ε and admit expansions in Taylor series

$$L^\varepsilon := L + \varepsilon L_1 + \varepsilon^2 L_R(\varepsilon), \tag{4.4}$$

$$\sigma^\varepsilon := \sigma + \varepsilon \sigma_1 + \varepsilon^2 \sigma_R(\varepsilon), \tag{4.5}$$

where $L = -\mathrm{div}\sigma$ and the coefficients of L_R and σ_R are bounded with respect to $\varepsilon \in [0, \varepsilon_0]$. Note that the Theorem 3.2 can be applied also to boundary value problems with the operators $L^\varepsilon, \sigma^\varepsilon$ instead of L, σ provided that ε is small enough.

Let us assume that the transformed forces $f_\varepsilon \circ \Phi_\varepsilon$ and $h_\varepsilon \circ \Phi_\varepsilon$ also depend smoothly on ε

$$f_\varepsilon \circ \Phi_\varepsilon = f_0 + \varepsilon f_1 + \varepsilon^2 f_R(\varepsilon), \tag{4.6}$$

$$h_\varepsilon \circ \Phi_\varepsilon = h_0 + \varepsilon h_1 + \varepsilon^2 h_R(\varepsilon). \tag{4.7}$$

Inserting these expansions together with

$$\mathbf{n}_\varepsilon \circ \Phi_\varepsilon = \mathbf{n}_0 + \varepsilon \dot{\mathbf{n}} + \varepsilon^2 \mathbf{n}_R(\varepsilon) \tag{4.8}$$

and the formal ansatz

$$(u_\varepsilon \circ \Phi_\varepsilon)(x) = u_0(x) + \varepsilon \dot{u}(x) + O(\varepsilon^2) \tag{4.9}$$

into (4.3) and comparing the terms of the order $O(\varepsilon)$ we obtain a boundary value problem for the material derivative $\dot{u}$

$$
\begin{aligned}
-\mathrm{div}\sigma(\dot{u}) &= f_1 - L_1 u_0 && \text{in} \quad \Omega, \\
\dot{u} &= 0 && \text{on} \quad \Gamma^D, \\
\sigma(\dot{u})\mathbf{n}_0 &= h_1 - \sigma_1(u_0)\mathbf{n}_0 - \sigma(u_0)\dot{\mathbf{n}} && \text{on} \quad \Gamma^N.
\end{aligned}
\tag{4.10}
$$

The ansatz (4.9) has to be justified, i.e. we have to show that the function $\dot{u}$ in (4.9) coincides with the material derivative $\dot{u}$ defined by (4.1). The correctness of (4.9) can be easily proved with the help of the *a priori* estimate (3.4). Indeed, the following Theorem holds:

THEOREM 4.1. *Suppose that the Taylor expansions* ((4.6), (4.7)) *are valid with* $f_\varepsilon \circ \Phi_\varepsilon, f_0, f_1, f_R \in [V^1_\beta(\Omega)]^2$, $h_\varepsilon \circ \Phi_\varepsilon, h_0, h_1, h_R \in [V^{3/2}_\beta(\Gamma^N)]^2$ *and* $\beta := 2 - a_0 + \delta$ *with a small positive* δ. *Then the following estimate is valid*

$$
\|u_\varepsilon \circ \Phi_\varepsilon - u_0 - \varepsilon \dot{u}\|_{[V^3_\beta(\Omega)]^2} \leqslant c\varepsilon^2 \tag{4.11}
$$

with a positive real constant c.

P r o o f: From the formal ansatz (4.9) and the Taylor expansions (4.4) – (4.8) follows that the function $v := u_\varepsilon \circ \Phi_\varepsilon - u_0 - \varepsilon \dot{u}$ satisfies the following elliptic boundary value problem:

$$
\begin{aligned}
L^\varepsilon(v) &= \varepsilon^2(f_R - L_R u_0) + O(\varepsilon^3) && \text{in} \quad \Omega, \\
v &= 0 && \text{on} \quad \Gamma^D, \\
\sigma^\varepsilon(v)(\mathbf{n}_\varepsilon \circ \Phi_\varepsilon) &= \varepsilon^2(h_R - \sigma(u_0)\mathbf{n}_R - \sigma(\dot{u})\dot{\mathbf{n}} - \sigma_R(u_0)\dot{\mathbf{n}} \\
&\quad -\sigma_R(\dot{u})\mathbf{n}_0 - \sigma_R(u_0)\mathbf{n}_0) + O(\varepsilon^3) && \text{on} \quad \Gamma^N.
\end{aligned}
\tag{4.12}
$$

From Theorem 3.2 applied to (4.10) it follows that $\dot{u} \in [V^3_\beta(\Omega)]^2$. Since $f_R \in [V^1_\beta(\Omega)]^2$, $h_R \in [V^{3/2}_\beta(\Gamma^N)]^2$, the right-hand sides of (4.12) satisfy the assumptions of Theorem 3.2. Applying the *a priori* estimate (3.4) to (4.12) we obtain the assertion. □.

The above theorem states that the material derivative $\dot{u}$ exists and belongs to the space $[V^3_{2-a_0+\delta}(\Omega)]^2$. It means, both u_0 and $\dot{u}$ behave at least as $O(r^{a_0})$ in the vicinity of singular points. Furthermore, we obtain immediately the existence and the regularity of the shape derivative u'. Indeed, from the identity

$$
u' = \dot{u} - \mathbf{D}u_0 \cdot \Phi \tag{4.13}
$$

follows that u' belongs to $[V^2_{2-a_0+\delta}(\Omega)]^2$ and it behaves at least as $O(r^{a_0-1})$ near the singular points. If $a_0 < 1$ and the perturbation mapping Φ does not vanish near the singular points, then u' is a displacement field of infinite potential energy, $u' \notin [H^1(\Omega)]^2$. From now on, we will assume that the given body and surface forces do not depend on the parameter ε, i.e. there exist functions f, L defined on R^2 such that $f_\varepsilon = f|_{\Omega_\varepsilon}$, $h_\varepsilon = h|_{\Gamma^N_\varepsilon}$.

Inserting (4.13) into (4.10) we find out that the shape derivative u' satisfies the following boundary value problem (see e.g. [18, Chapter 3.1.5]):

$$
\begin{aligned}
-\mathrm{div}\sigma(u') &= 0 && \text{in } \Omega,\\
u' &= -\langle \Phi, \mathbf{n}_0\rangle \partial_{\mathbf{n}} u_0 && \text{on } \Gamma^D,\\
\sigma(u')\mathbf{n}_0 &= \langle \Phi, \mathbf{n}_0\rangle (f + \kappa h) - \mathrm{div}_\Gamma(\langle \Phi, \mathbf{n}_0\rangle \sigma_T(u_0)) && \text{on } \Gamma^N.
\end{aligned}
\tag{4.14}
$$

Here we denote by $\partial_n u_0$ the normal derivative of u_0 on $\partial\Omega$, $\sigma_T(u_0)$ is the tangential component of the stress tensor on $\partial\Omega$, κ is the curvature of $\partial\Omega$ and the tangential divergence operator div_Γ is defined by

$$
\mathrm{div}_\Gamma v = \mathrm{div} v - \langle \mathbf{D}v \cdot \mathbf{n}_0, \mathbf{n}_0\rangle. \tag{4.15}
$$

REMARK 4.1. The boundary value problem (4.14) is in general not suitable for the numerical computation of u' because $u' \notin [H^1(\Omega)]^2$ is not a variational solution of (4.14). The right-hand sides of (4.14) depend on the derivatives of $u_0 \in [H^{1+a_0}(\Omega)]^2$ and are also singular if $a_0 < 1$. However, in the following we use only the information on the dependence of the boundary values of u' on the boundary values of $\partial_{\mathbf{n}} u_0, \sigma_T(u_0)$ and $\langle \Phi, \mathbf{n}_0\rangle$.

5. Sensitivity of functionals by the method of adjoint problems

In this and in the following sections we write shortly σ_0 for $\sigma(u_0)$ and denote by $\dot{\sigma}, \sigma'$ the material and the shape derivative of $\sigma(u_\varepsilon)$, respectively.

5.1. Sensitivity via the material derivative

Let us assume that the scalar function F in (2.5) is continuously differentiable with respect to all its arguments and satisfies the growth conditions (2.6). Standard formulae for the sensitivity of integrals over varying domains yield [17, 14]

$$
dJ(\Omega, \Phi_\varepsilon) = \int_\Omega \{\langle \partial_u F(u_0, \sigma_0), \dot{u}\rangle + \partial_\sigma F(u_0, \sigma_0) : \dot{\sigma} + F(u_0, \sigma_0)\mathrm{div}\,\Phi\}\, dx. \tag{5.1}
$$

This formula is valid without any restrictions on the strength of the stress singularities. However, the expression (5.1) depends on the values of Φ inside Ω.

5.2. Sensitivity via shape derivative

Let us assume that the constant a_0 which determines the regularity of the displacement field u_0 and of the derivatives $\dot{u}, u'$ is not less than 1/2. Otherwise we have to require that the mapping Φ vanishes in the neighbourhood of singular points where the stress singularities are stronger. Replacing the material derivatives $\dot{u}, \dot{\sigma}$ in (5.1) by the corresponding shape derivatives u', σ' using the identity (4.13), we obtain an expression for $dJ(\Omega, \Phi_\varepsilon)$ which depends only on the boundary values of the perturbation mapping Φ [17, 14]

$$dJ(\Omega,\Phi_\varepsilon) = \int_\Omega \left\{ \langle \partial_u F(u_0,\sigma_0), u' \rangle + \partial_\sigma F(u_0,\sigma_0) : \sigma' \right\} dx + \int_{\partial\Omega} F(u_0,\sigma_0)\langle \Phi, \mathbf{n}_0 \rangle ds_x. \tag{5.2}$$

The assumption $a_0 \geqslant 1/2$ and the growth conditions (2.6) ensure that all integrals in (5.2) exist.

5.3. Boundary expression for the sensitivity

The expression (5.2) still contains a domain integral. It can be transformed to a boundary integral using the method of adjoint problems [2, 3]. Here we assume that $a_0 > 1/2$. The interesting case of elastic bodies with cracks, where $a_0 = 1/2$, requires a more careful investigation and will be treated in the next section. Furthermore, we assume that the function F is twice continuously differentiable. Following the ideas from [3] we replace $\partial_\sigma F(u_0, \sigma_0) : \sigma'$ in (5.2) by $\partial_\sigma F(u_0, \sigma_0) : (\mathbf{C} : e(u'))$ and use Green's first formula (9.1) applied to a field v with $\sigma(v) = \mathbf{C} : \partial_\sigma F(u_0, \sigma_0)$ and to the field u'

$$\int_\Omega (\mathbf{C} : \partial_\sigma F(u_0,\sigma_0)) : e(u') dx = \int_{\partial\Omega} \langle u', (\mathbf{C} : \partial_\sigma F(u_0,\sigma_0))\mathbf{n}_0 \rangle ds_x - \int_\Omega \langle u', \operatorname{div}(\mathbf{C} : \partial_\sigma F(u_0,\sigma_0)) \rangle dx. \tag{5.3}$$

In this way we obtain

$$dJ(\Omega,\Phi_\varepsilon) = \int_\Omega \langle \partial_u F(u_0,\sigma_0) - \operatorname{div}(\mathbf{C} : \partial_\sigma F(u_0,\sigma_0)), u' \rangle dx + \int_{\partial\Omega} \left\{ F(u_0,\sigma_0)\langle \Phi, \mathbf{n}_0 \rangle + \langle (\mathbf{C} : \partial_\sigma F(u_0,\sigma_0))\mathbf{n}_0, u' \rangle \right\} ds_x. \tag{5.4}$$

We introduce an adjoint displacement field w as the solution of the boundary value problem

$$
\begin{aligned}
-\mathrm{div}\sigma(w) &= \partial_u F(u_0,\sigma_0) - \mathrm{div}(\mathbf{C} : \partial_\sigma F(u_0,\sigma_0)) && \text{in} \quad \Omega, \\
w &= 0 && \text{on} \quad \Gamma^D, \\
\sigma(w)\mathbf{n}_0 &= (\mathbf{C} : \partial_\sigma F(u_0,\sigma_0))\mathbf{n}_0 && \text{on} \quad \Gamma^N.
\end{aligned}
\tag{5.5}
$$

LEMMA 5.1. *Let the assumptions of Theorem 4.1 be satisfied. Then the boundary value problem* (5.5) *has a unique weak solution w which belongs to* $[V^3_{2-a_0+\delta}(\Omega)]^2$.

Proof: Under the assumptions of Theorem 4.1 we have $u_0 \in [V^3_{2-a_0+\delta}(\Omega)]^2$, $\sigma_0 \in [V^2_{2-a_0+\delta}(\Omega)]^2$. Therefore $\partial_u F(u_0,\sigma_0), \mathrm{div}(\mathbf{C} : \partial_\sigma F(u_0,\sigma_0)) \in [V^1_{2-a_0+\delta}(\Omega)]^2$ and $(\mathbf{C} : \partial_\sigma F(u_0,\sigma_0))\mathbf{n}_0 \in [V^{3/2}_{2-a_0+\delta}(\Gamma^N)]^2$ because of the growth conditions (2.6). Thus we can apply Theorem 3.2 and obtain the assertion. □

The domain integral in (5.4) can now be transformed to a boundary integral by using second Green's formula (9.2) applied to the displacement fields u' and w. Note that in case of cracked bodies, where $a_0 = 1/2$, all integrals in (9.2) exist but the formula (9.2) is not valid any more.

Since $\mathrm{div}\sigma(u') = 0$, we obtain finally

$$
dJ(\Omega,\Phi_\varepsilon) = \int_{\partial\Omega} F(u_0,\sigma_0)\langle\Phi,\mathbf{n}_0\rangle ds_x + \int_{\Gamma^N} \langle w, \sigma(u')\mathbf{n}_0\rangle ds_x
+ \int_{\Gamma^D} \langle(\mathbf{C} : \partial_\sigma F(u_0,\sigma_0))\mathbf{n}_0 - \sigma(w)\mathbf{n}_0, u'\rangle ds_x.
\tag{5.6}
$$

Inserting the boundary values of u' from (4.14) into (5.6) we get:

THEOREM 5.2. *Under previous assumptions we have*

$$
dJ(\Omega,\Phi_\varepsilon) = \int_{\partial\Omega} F(u_0,\sigma_0)\langle\Phi,\mathbf{n}_0\rangle ds_x + \int_{\Gamma^N} \langle w, \langle\Phi,\mathbf{n}_0\rangle(f+\kappa h)
-\mathrm{div}_\Gamma(\langle\Phi,\mathbf{n}_0\rangle\sigma_T(u_0))\rangle ds_x - \int_{\Gamma^D} \langle\Phi,\mathbf{n}_0\rangle\langle(\mathbf{C} : \partial_\sigma F(u_0,\sigma_0))\mathbf{n}_0
- \sigma(w)\mathbf{n}_0, \partial_\mathbf{n} u_0\rangle ds_x.
\tag{5.7}
$$

6. Method of adjoint problems for 2D crack problems

Let us consider an elastic body with a smooth crack (see e.g. Fig. 2). On the outer parts of the boundary, mixed boundary conditions are given, whereas the crack lips are stress-free. For the sake of simplicity we suppose that the material is isotropic, i.e. only two independent material constants λ, μ appear and

$$c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right). \tag{6.1}$$

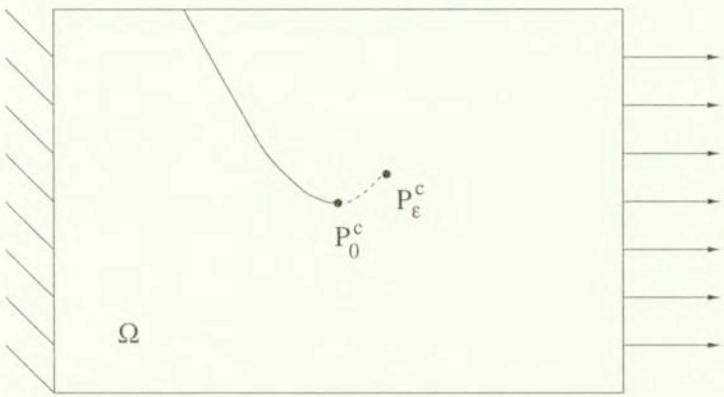

FIG. 2. A plate with a crack.

For every singular point P_i lying on the outer boundary we assume that there exists no eigenvalue α_j of $\mathcal{A}(P_i)$ with $0 < \mathrm{Re}\alpha_j \leqslant 1/2$, i.e. there is no stress singularity near P_i stronger than the singularity at the crack tip. Otherwise we must assume that the singular point P_i is not perturbed by Φ_ε. In this way we ensure that the crack tip singularity is dominating and we have $a_0 = 1/2$. Furthermore we suppose that the perturbed crack tip P^c_ε moves along a smooth curve and $\langle \Phi(x), \mathbf{n}_0(x) \rangle = O(|x - P^c_0|^{2\delta})$ with a small positive δ near the unperturbed crack tip P^c_0. Moreover, we can assume without loss of generality that the vector tangent to the crack curve at the unperturbed crack tip P^c_0 coincides with the vector $(1,0)^\top$. In this case the perturbation mapping has locally in the vicinity of P^c_0 the form

$$\Phi_\varepsilon \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} + \varepsilon \begin{pmatrix} 1 \\ 0 \end{pmatrix} + O(\varepsilon^2). \tag{6.2}$$

Let us describe precisely the behaviour of the displacement fields u_ε and u'. Under the previous assumptions on the regularity of given forces, the displacement field u_ε belongs to $[V^3_{3/2+\delta}(\Omega_\varepsilon)]^2$ and admits in the neighbourhood of the perturbed crack tip P^c_ε the asymptotics (see e.g. [9, 10])

$$u_\varepsilon(r_\varepsilon, \omega_\varepsilon) = \sum_{j=1}^{2} K_j(u_\varepsilon) r_\varepsilon^{1/2} \varphi_j(\omega_\varepsilon) + O(r_\varepsilon) \tag{6.3}$$

with

$$\varphi_1(\omega) = \frac{1}{4\mu\sqrt{2\pi}} \begin{pmatrix} -\cos(3\omega/2) + (2\tau - 1)\cos(\omega/2) \\ \sin(3\omega/2) - (2\tau + 1)\sin(\omega/2) \end{pmatrix}, \tag{6.4}$$

$$\varphi_2(\omega) = \frac{1}{4\mu\sqrt{2\pi}} \begin{pmatrix} 3\sin(3\omega/2) - (2\tau - 1)\sin(\omega/2) \\ 3\cos(3\omega/2) - (2\tau + 1)\cos(\omega/2) \end{pmatrix}, \tag{6.5}$$

where $\tau = (\lambda+3\mu)(\lambda+\mu)^{-1}$. Here, $(r_\varepsilon, \omega_\varepsilon)$ are polar coordinates with origin in P_ε^c and the angular variable ω_ε is oriented in such a way that the crack lips correspond to the angles $\pi, -\pi$. Furthermore we have written the singular functions $\varphi_j, j = 1, 2$, in polar components $\varphi_j = (\varphi_j^r, \varphi_j^\omega)^\top$. The coefficients $K_1(u_\varepsilon)$ and $K_2(u_\varepsilon)$ are called stress intensity factors of Mode I and Mode II, respectively, and are given by

$$K_j(u_\varepsilon) = \int_{\Omega_\varepsilon} f_\varepsilon \cdot \zeta_{j,\varepsilon} dx_\varepsilon + \int_{\Gamma_\varepsilon^N} h_\varepsilon \cdot \zeta_{j,\varepsilon} ds_{x_\varepsilon}, \tag{6.6}$$

where the weight functions $\zeta_{j,\varepsilon} \in [V_{3/2+\delta}^2(\Omega_\varepsilon)]^2$, $j = 1, 2$, satisfy the problem (2.4) in Ω_ε with vanishing body and boundary forces and admit the asymptotics

$$\zeta_{j,\varepsilon}(r_\varepsilon, \omega_\varepsilon) = r_\varepsilon^{-1/2} \psi_j(\omega_\varepsilon) + O(r_\varepsilon^{1/2}). \tag{6.7}$$

with

$$\psi_1(\omega) = \frac{1}{(1+\tau)\sqrt{8\pi}} \begin{pmatrix} -3\cos(\omega/2) + (2\tau + 1)\cos(3\omega/2) \\ 3\sin(\omega/2) - (2\tau - 1)\sin(3\omega/2) \end{pmatrix}, \tag{6.8}$$

$$\psi_2(\omega) = \frac{1}{(1+\tau)\sqrt{8\pi}} \begin{pmatrix} \sin(\omega/2) - (2\tau + 1)\sin(3\omega/2) \\ \cos(\omega/2) - (2\tau - 1)\cos(3\omega/2) \end{pmatrix}. \tag{6.9}$$

The following theorem plays the key role in the application of the adjoint method to problems with cracks.

THEOREM 6.1. *Let* $\gamma = (1+\tau)/(4\mu)$ *and* $\langle \Phi(x), \mathbf{n}_0(x) \rangle = O(|x - P_0^c|^{2\delta})$ *near the crack tip* P_0^c. *Then the shape derivative* $u' \in [V_{3/2+\delta}^2(\Omega)]^2$ *has the following decomposition*:

$$u' = \gamma \sum_{i=1}^{2} K_i(u_0) \zeta_{i,0} + \tilde{u}' \tag{6.10}$$

with $\tilde{u}' \in [V_{3/2-\delta}^2(\Omega)]^2$.

P r o o f. Since $-1/2$ is the only eigenvalues of $\mathcal{A}(P_0^c)$ in the interval $(-\frac{1}{2}-\delta, -\frac{1}{2}+\delta)$, we can apply the general theory of elliptic systems in domains with corners [8, 9] to the problem (4.14). The condition $\langle \Phi(x), \mathbf{n}_0(x)\rangle = O(|x-P_0^c|^{2\delta})$ implies that the right-hand sides of (4.14) belong to $[V^{3/2}_{3/2-\delta}(\Gamma^D)]^2 \times [V^{1/2}_{3/2-\delta}(\Gamma^N)]^2$ and we obtain the decomposition

$$u' = \sum_{i=1}^{2} c_i \zeta_{i,0} + \tilde{u}' \tag{6.11}$$

with $\tilde{u}' \in [V^2_{3/2-\delta}(\Omega)]^2$ and real coefficients c_1, c_2 to be determined.

Let us calculate these coefficients. To this end we calculate the singular terms in the asymptotics of u' near the crack tip using the identity (4.13). Since $\dot{u} \in [V^3_{3/2+\delta}(\Omega)]^2$, the main parts of the asymptotics of the functions u' and $-\mathbf{D}u_0\cdot\Phi$ coincide. Furthermore $\mathbf{D}u_0\cdot\Phi = \partial_{x_1}u_0$ near the crack tip P_0^c because of the special form (6.2) of the perturbation mapping Φ_ε. Using the identity (see e.g. [9, 10])

$$\partial_{x_1}(r_0^{1/2}\varphi_j(\omega_0)) = -\gamma r_0^{-1/2}\psi_j(\omega_0), \quad j=1,2, \tag{6.12}$$

we obtain from (6.3) with $\varepsilon = 0$

$$\partial_{x_1}u_0(r_0,\omega_0) = -\gamma\sum_{j=1}^{2} K_j(u_0) r_0^{-1/2}\psi_j(\omega) + O(r_0^{1/2}) \tag{6.13}$$

and the assertion follows. □

THEOREM 6.2. *Under the assumptions of the previous theorem we have*

$$\begin{aligned} dJ(\Omega,\Phi_\varepsilon) = \gamma\sum_{i=1}^{2}K_i(u_0)K_i(w) &+ \int_{\partial\Omega} F(u_0,\sigma_0)\langle\Phi,\mathbf{n}_0\rangle ds_x \\ &+ \int_{\Gamma^N}\langle w, \langle\Phi,\mathbf{n}_0\rangle(f+\kappa h) - \operatorname{div}_\Gamma(\langle\Phi,\mathbf{n}_0\rangle\sigma_T(u_0))\rangle ds_x \\ &- \int_{\Gamma^D}\langle\Phi,\mathbf{n}_0\rangle\langle(\mathbf{C}:\partial_\sigma F(u_0,\sigma_0))\mathbf{n}_0 - \sigma(w)\mathbf{n}_0, \partial_n u_0\rangle ds_x. \end{aligned} \tag{6.14}$$

P r o o f. We insert the decomposition (6.10) into (5.3). The integrals with the weight functions $\zeta_{i,0}$ can be interpreted as $\gamma\sum_{i=1}^{2}K_i(u_0)K_i(w)$ due to formula (6.6). The remaining integrals with $\tilde{u}'$ are reduced to the boundary as described in Section 5.3 because $\tilde{u}' \in [V^2_{3/2-\delta}(\Omega)]^2$ is regular enough in order to apply the method of adjoint problems. Thus (6.14) follows. □

7. Examples

Let us apply the results of the last section to calculate the sensitivity of some special functionals. The resulting formulae have a particularly simple form if we assume that the crack tip moves along a straight line and the remaining boundary is fixed. In this case we have $\langle \Phi, \mathbf{n}_0 \rangle = 0$ on the whole boundary and formula (6.14) simplifies to

$$dJ(\Omega, \Phi_\varepsilon) = \gamma \sum_{i=1}^{2} K_i(u_0) K_i(w). \tag{7.1}$$

A formula similar to (7.1) was obtained in [13] for the mixed boundary value problem for the Laplace equation in a smooth domain with collision points (i.e. points where the boundary conditions change) moving along the boundary.

Example 1. Let $\tilde{u} \in L_2(\tilde{\Omega})$ where $\Omega_\varepsilon \subset \tilde{\Omega}\ \forall \varepsilon \in [0, \varepsilon_0]$ and let the functional J be defined by

$$J(\Omega_\varepsilon) = \frac{1}{2} \int_{\Omega_\varepsilon} (u_\varepsilon - \tilde{u})^2 dx_\varepsilon. \tag{7.2}$$

Here we obtain formula (7.1) with the adjoint field w satisfying the following boundary value problem:

$$\begin{aligned} -\mathrm{div}\sigma(w) &= u_0 - \tilde{u} \quad && \text{in} \quad \Omega, \\ w &= 0 && \text{on} \quad \Gamma^D, \\ \sigma(w)\mathbf{n}_0 &= 0 && \text{on} \quad \Gamma^N. \end{aligned} \tag{7.3}$$

Example 2. In case of the energy functional

$$J(\Omega_\varepsilon) = \frac{1}{2} \int_{\Omega_\varepsilon} \sigma(u_\varepsilon) : e(u_\varepsilon) dx_\varepsilon, \tag{7.4}$$

the adjoint field w coincides with the displacement field u_0. In this way we obtain the well known Irwin formula [15, 11, 4, 10]

$$dJ(\Omega, \Phi_\varepsilon) = \gamma \sum_{i=1}^{2} K_i(u_0)^2. \tag{7.5}$$

8. Conclusions

The occurence of stress singularities in elastic bodies demands in the sensitivity analysis the consideration of the regularity of underlying elastic fields. Since singular stresses belong only to $L_2(\Omega)$, it is necessary to impose restrictions on the class of admissible functionals. Integral functionals over singular stresses are well defined only if the integrands satisfy quadratic growth conditions with respect to the components of the stress tensor.

The sensitivity of integral functionals can be easily expressed with the help of the material derivatives of the elastic fields. In this case we do not need any restrictions on the strength of stress singularites but the resulting expression depends on the perturbation of the interior of the domain. If all stress singularities in a body are weaker than the singularities at a crack tip (all singular exponents greater than 1/2), then the sensitivity of the functionals can be expressed as boundary integrals using the method of adjoint problems. This method is based on the application of Green's formulae to the original displacement field and to the solution of an appropriately defined adjoint problem. In the limiting case of bodies with cracks, the sensitivity depends also on the stress intensity factors of the original and of the adjoint field. In case of stronger singularities, the method of adjoint problems can not be applied because the Green formulae are not valid.

The same approach can be also applied to three-dimensional elastic structures and to interface problems. The difficulty in the mathematical justification of the adjoint method in these cases stems from the necessity to define the weighted Sobolev spaces which take all possible stress singularities into accout (singularities at conical points, at smooth edges, intersections of edges etc.).

The problem how to reduce the sensitivity of the functionals to a boundary expression is still unsolved for problems where boundary points with very strong singularities (singular exponents smaller than 1/2) are perturbed. One should note that singular exponents smaller than 1/2 occur often in applications (change of boundary conditions at reentrant corners, interior interface corners etc.).

9. Appendix

In the literature, the Green integral formulae are usually formulated under assumptions on the regularity of underlying integrands which are too restrictive for the application in this paper. Therefore we give here precise assumptions which can be best formulated in weighted Sobolev spaces.

THEOREM 9.1. *a) Let* $v \in [V_\alpha^{d+2}(\Omega)]^2$, $w \in [V_\beta^{d+1}(\Omega)]^2$, $d = 0, 1, 2, \ldots$ *and* $\alpha, \beta \in \mathbb{R}$ *with* $\alpha + \beta < 2d + 1$. *Then Green's first formula holds*

$$(9.1)\qquad \int_{\Omega} \sigma(v) : \epsilon(w)dx = \int_{\partial\Omega} \langle w, \sigma(v)\mathbf{n}_0\rangle ds_x - \int_{\Omega} \langle w, \mathrm{div}\sigma(v)\rangle dx$$

b) Let $v \in [V_{\alpha}^{d+2}(\Omega)]^2$, $w \in [V_{\beta}^{d+2}(\Omega)]^2$, $d = 0, 1, 2, \ldots$ and $\alpha, \beta \in \mathbb{R}$ with $\alpha + \beta < 2d + 2$. Then Green's second formula holds

$$(9.2)\qquad \int_{\Omega} \{\langle \mathrm{div}\sigma(v), w\rangle - \langle v, \mathrm{div}\sigma(w)\rangle\} dx = \int_{\partial\Omega} \{\langle \sigma(v)\mathbf{n}_0, w\rangle - \langle v, \sigma(w)\mathbf{n}_0\rangle\} ds_x.$$

References

1. J. APPELL and P.P. ZABREJKO, *Nonlinear superposition operators,* Cambridge University Press, Cambridge 1990.
2. K. DEMS and Z. MRÓZ, *Variational approach by means of adjoint systems to structural optimization and sensitivity analysis II. Structure shape variation,* Int. J. Solids Struct., **20**, 527–552, 1984.
3. K. DEMS and Z. MRÓZ, *Shape sensitivity in mixed Dirichlet–Neumann boundary-value problems and associated class of path-independent integrals,* Eur. J. Mech. A/Solids, **14**, 169–203, 1995.
4. P. DESTUYNDER and M. DJAOUA, *Sur une interprétation mathématique de l'integrale de Rice en théorie de la rupture fragile,* Math. Meth. Appl. Sci., **3**, 70–87, 1981.
5. P.R. GARABEDIAN and M. SCHIFFER, *Convexity of domain functionals,* J. d'Anal. Math., **2**, 281–368, 1952/53.
6. E.J. HAUG, K.K. CHOI and V. KOMKOV, *Design sensitivity analysis of structural systems,* Academic Press Inc., Orlando 1986.
7. S.N. KARP and F.C. KARAL, *The elastic-field behaviour in the neighbourhood of a crack of arbitrary angle,* Comm. Pure Appl. Math., **15**, 413–421, 1962.
8. V.A. KONDRAT'EV, *Boundary problems for elliptic equations in domains with conical or angular points,* Trans. Moscow Math. Soc., **16**, 209–292, 1967.
9. S.A. NAZAROV and B.A. POLYAKOVA, *Elliptic problems in domains with piecewise smooth boundaries,* Walter de Gruyter, Berlin 1994.
10. S.A. NAZAROV and O.R. POLYAKOVA, *Rupture criteria, asymptotic conditions at crack tips, and selfadjoint extensions of the Lamé operator,* Trans. Moscow Math. Soc., **57**, 13–66, 1996.
11. K. OHTSUKA, *Generalized J-integral and three-dimensional fracture mechanics I,* Hiroshima Math. J., **11**, 21–52, 1981.
12. K. OHTSUKA and M, BOCHNIAK, *Shape sensitivity analysis of stress intensity factors by generalized J-integrals,* Math. Meth. Appl. Sci., **21**, 1343–1363, 1998.
13. B. PALMERIO and A. DERVIEUX, *Hadamard's variational formula for a mixed problem and an application to a problem related to a Signorini-like variational inequality,* Numer. Funct. Anal. Optimiz., **1**, 113–144, 1979.

14. H. PETRYK and Z. MRÓZ, *Time derivatives of integrals and functionals defined on varying volume and surface domains*, Arch. Mech., **38**, 697–724, 1986.

15. J.R. RICE, *A path independent integral and the approximate analysis of strain concentration by notches and cracks,* J. Appl. Mech., **35**, 379–386, 1968.

16. A.-M. SÄNDIG, U. RICHTER and R. SÄNDIG, *The regularity of boundary value problems for the Lamé equations in a polygonal domain,* Rostocker Math. Kolloqium, **36**, 21–50, 1989.

17. J. SIMON, *Differentiation with respect to the domain in boundary value problems,* Numer. Funct. Anal. Optimiz., **2**, 649–687, 1980.

18. J. SOKOŁOWSKI and J.P. ZOLESIO, *Introduction to shape optimization,* Springer Verlag, Berlin 1992.

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