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Numerical methods for shape identification problems

by

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Abstract: The paper concerns the class of shape optimization problems for linear partial differential equations. A small set inside the domain of integration of an elliptic equation is identified by minimization of an integral cost functional. In the two-dimensional case an existence result for the problem is given. The material derivative method of shape optimization is used to derive the first and the second order derivatives of the cost functional. For numerical solution of the elliptic equation the integral equations are introduced and the boundary element method of approximation is used. Numerical methods of optimization are described and results of computations are presented. In particular, superlinear methods are implemented.

1. Introduction

In the present paper a class of shape identification problems is considered. Such problems arise, e.g. in non-destructive identification of inclusions or voids in solids. The available information (data) are given on a part of the geometrical boundary of the solid (geometrical domain) and the inclusion is to be determined in the interior of the geometrical domain.

In the present paper we restrict ourselves to the class of problems associated with the stationary heat conduction. We refer the reader to e.g. Abda (1993), for a description of the problem and results on the identifiability of cracks on the basis of boundary measurements.

An existence result is established for the class of problems under considerations by an application of a recent result in Sverak (1993). Unfortunately, the result is based on the properties of harmonic functions and is valid only for 2–D problems.

The material derivative method, Sokołowski and Zolesio (1992), is used to derive the first and the second order optimality conditions for the shape identification problem. Finally, the boundary element method is applied to solve numerically the resulting shape optimization problem. The following notation is used.

$\Omega \subset \mathrm{I\!R}^N$ is an open set with the boundary $\partial\Omega = \Gamma \cup \Sigma$. We assume that Γ is smooth, and Σ is Lipschitz. In section 2, $\Omega = D \setminus S$, where S is a compact set and D is an open set with the boundary ∂D. The Sobolev space $H^1(\Omega)$ is defined in the standard way, Grisvard (1985),

$$H^1(\Omega) = \{\varphi \in L^2(\Omega) | \frac{\partial \varphi}{\partial x_i} \in L^2(\Omega),\ i = 1, ..., N\},$$

and by $H_0^1(\Omega)$ we denote the closure in $H^1(\Omega)$ of the space $\mathcal{D}(\Omega) = C_0^\infty(\Omega)$ of smooth functions with compact supports in Ω. If $\partial\Omega$ is sufficiently smooth, $H^{\frac{1}{2}}(\partial\Omega)$ denotes the space of traces of functions from $H^1(\Omega)$ on the boundary. $H^{\frac{1}{2}}(\partial\Omega)$ is a dense subspace of the space $L^{\frac{1}{2}}(\partial\Omega)$.

In the paper the weak solutions of elliptic partial differential equations are considered. In particular, for the equation

$$-\Delta\psi = E \text{ in } \Omega, \quad \psi = G \text{ in } \Sigma, \quad \frac{\partial \psi}{\partial n} = F \text{ in } \Gamma\ ,$$

the weak solution $\psi \in H^1(\Omega)$ minimizes the energy functional

$$\mathcal{I}(\Omega) = \inf_{\{\varphi \in H^1(\Omega) | \varphi = G \text{ in } \Sigma\}} \Big[\int_\Omega |\nabla\varphi|^2 dx - 2\int_\Omega E\varphi dx - 2\int_\Gamma F\varphi d\Gamma(x) \Big]$$

and satisfies the following integral identity, $\psi = G$ in Γ :

$$\int_\Omega \nabla\psi \cdot \nabla\varphi dx = \int_\Omega E\varphi dx + \int_\Gamma F\varphi d\Gamma(x) \quad \forall \varphi \in H_\Sigma^1(\Omega),$$

where $H_\Sigma^1(\Omega) = \{\varphi \in H^1(\Omega) | \varphi = 0 \text{ in } \Sigma\}$ and $E = E(x),\ x \in \Omega,\ \ G = G(x),\ x \in \Sigma,\ \ F = F(x),\ x \in \Gamma$, are given functions, defined in general as restrictions of functions defined in $\mathrm{I\!R}^N$.

We shall also use the material derivative method for the shape sensitivity analysis. The detailed description of the method can be found in the monograph, Sokołowski and Zolesio (1992). To this end a one-parameter family of domains $\{\Omega_s\} \subset D,\ s \in [0, \delta)$, is defined as follows :

$\Omega_s = T_s(\Omega)$ for $s \in [0, \beta)$ where $T_s = T_s(V) : \mathrm{I\!R}^N \mapsto \mathrm{I\!R}^N$, $N = 1, 2, 3$, is a smooth transformation. This transformation is given by a sufficiently smooth vector field $V(\cdot,\cdot)$ with $V(s, x) = \dfrac{\partial T_s}{\partial s} \circ T_s^{-1}(x)$.

We assume $V(\cdot,\cdot) \in C^1\big([0, \tilde\beta); C^2(\mathrm{I\!R}^N; \mathrm{I\!R}^N)\big)$, $\tilde\beta > \beta > 0$, and we denote $\partial\Omega_s = T_s(\partial\Omega)$.

The Eulerian semiderivative $d\mathcal{I}(\Omega; V)$ of the shape functional $\mathcal{I}(\Omega)$ is defined as,

$$d\mathcal{I}(\Omega; V) = \lim_{t \to 0} \frac{1}{s}(\mathcal{I}(\Omega_s) - \mathcal{I}(\Omega)),$$

whenever the limit exists. In the particular case of the energy functionals, first we differentiate the functional

$$I(\Omega) = \int_\Omega |\nabla\varphi|^2 dx - 2\int_\Omega E\varphi dx - 2\int_\Gamma F\varphi d\Gamma(x)$$

for a sufficiently smooth test function φ and obtain

$$dI(\Omega; V) =$$

$$\int_{\partial\Omega} [|\nabla\varphi|^2 - 2E\varphi] V(0, x) \cdot n(x) d\Gamma(x) - 2\int_\Gamma F\varphi\kappa V(0, x) \cdot n(x) d\Gamma(x)$$

where $\kappa = \mathrm{div}_\Gamma n$ is the tangential divergence of the normal vector field on Γ and F is the restriction to Γ of a given function defined in a neighbourhood of $\Gamma \subset \mathbb{R}^N$. Next, assuming that the solution $\psi = \psi(\Omega)$ is unique, we obtain

$$d\mathcal{I}(\Omega; V) = \int_{\partial\Omega} [|\nabla\psi(\Omega)|^2 - 2E\psi(\Omega)] V(0, x) \cdot n(x) d\Gamma(x)$$

$$-2\int_\Gamma F\psi(\Omega)\kappa V(0, x) \cdot n(x) d\Gamma(x) ,$$

where we should take into account that $\psi(\Omega) = G$ on Σ.

It means that we do not need to differentiate the solution $\psi(\Omega)$ with respect to Ω in order to obtain the derivative $d\mathcal{I}(\Omega; V)$. However, in the case of the second derivative of the shape functional $d^2\mathcal{I}(\Omega; V, W)$, it turns out that we have to use the derivative $\psi'(\Omega; W)$ of the solution $\psi(\Omega)$ in the direction of the vector field W.

We refer the reader to Sokołowski (1993), Bendsoe and Sokołowski (1995), El Yacoubi and Sokołowski (1996), Pierre, Roche (1993), Novruzi, Roche (1995) for applications of energy functionals in shape optimization. The results were presented at the IFIP Conference in Rabat (Maroc), Roche, Sokołowski (1994).

2. Shape identification

For the sake of simplicity we assume that $N = 2$, however, most of the results hold for $N = 3$ as well.

Given a bounded domain $D \in \mathbb{R}^2$ with the boundary ∂D, denote

$$D_\rho = \{x \in D | \mathrm{dist}(x, \partial D) > \rho\}$$

and define family of open sets Ω of the form

$$\mathcal{U}_{ad} = \{\Omega \subset D | \Omega = D \setminus S, \ S \subset D_\rho\}$$

for $\rho > 0$, ρ small enough.
Consider the following cost functional

$$J(\Omega) = \int_\Omega |\nabla(w-u)|^2 + \alpha\|w-u\|^2_{H^{\frac{1}{2}}(\Gamma)}$$

where $\alpha \geq 0$ is a constant, $w, u \in H^1(D)$ are given as the unique solutions to the following elliptic equations,

(I) Dirichlet problem

$$\Delta w = 0 \quad \text{in } \Omega \tag{1}$$

$$w = g \quad \text{on } \partial D \tag{2}$$

$$w = 0 \quad \text{on } S \tag{3}$$

(II) Dirichlet–Neumann problem

$$\Delta u = 0 \quad \text{in } \Omega \tag{4}$$

$$\frac{\partial u}{\partial n} = f \quad \text{on } \partial D \tag{5}$$

$$u = 0 \quad \text{on } S \tag{6}$$

Here $g, f \in C^1(\partial D)$ are given functions, i.e. data of the identification problem under considerations. In particular, such a shape optimization problem results in identification of voids or inclusions in solids when one uses as data the temperature and flux distributions on the boundary of solids.

For the shape optimization problem the following results can be established.

(i) The existence of a solution to the problem.
(ii) The first order necessary optimality conditions by using the material derivative method.
(iii) Numerical methods of solution by using the integral equations on $\partial\Omega$, i.e. BEM.

3. Existence of an optimal domain

Consider the following family of admissible domains

$$\mathcal{O}_\ell = \{\Omega \quad | \quad \Omega \in \mathcal{U}_{ad}, \quad \#S \leq \ell\}$$

where $\#S$ denotes the number of connected components of compact S.

THEOREM 3.1 *For $\alpha > 0$ and any finite ℓ there exists a solution $\tilde{\Omega} \in \mathcal{O}_\ell$ to the shape identification problem under considerations, i.e.,*

$$J(\tilde{\Omega}) = \min_{\Omega \in \mathcal{O}_\ell} J(\Omega)$$

REMARK 3.1 *The proof of this theorem is based on properties of harmonic functions in $\mathbb{R}^2$ and uses the same argument as given in Sverak (1993), for a slightly different shape optimization problem. In particular, the method cannot be directly applied in $\mathbb{R}^N$ for $N \geq 3$.*

Proof of Theorem 3.1. Let $\{\Omega_i\} = \{D \setminus S_i\}$, $i = 1, 2, ...$, be a minimizing sequence for the problem under consideration.

Since the cost functional is bounded by a constant, $J(\Omega_i) \leq J(\Omega_1)$, the corresponding sequences of solutions $\{u_i\}$, $\{w_i\}$, are bounded, i.e.

$$\|u_i\|_{H^1(D)} \leq C \tag{7}$$
$$\|w_i\|_{H^1(D)} \leq C \tag{8}$$

There exists a function $W \in H^1(D)$ such that $w_i - W \in H_0^1(\Omega_i)$. On the other hand, denote by $\tilde{U}_i \in H^1(D \setminus D_{\frac{\varrho}{2}})$ a solution to the following elliptic equation

$$\Delta\tilde{U}_i = \Delta\eta u_i + 2\nabla\eta \cdot \nabla u_i \text{ in } D \setminus D_{\frac{\varrho}{2}} \tag{9}$$
$$\frac{\partial\tilde{U}_i}{\partial n} = f \text{ on } \partial D \tag{10}$$
$$\tilde{U}_i = 0 \text{ on } \partial D_{\frac{\varrho}{2}} \tag{11}$$

and denote

$$U_i = \begin{cases} \tilde{U}_i & \text{in } D \setminus D_{\frac{\varrho}{2}} \\ 0 & \text{in } D_{\frac{\varrho}{2}} \end{cases}$$

where the function $\eta \in C_0^\infty(\mathbb{R}^2)$ satisfies the following conditions

$$0 \leq \eta(x) \leq 1 \text{ in } \mathbb{R}^2 \tag{12}$$
$$\eta(x) = 0 \text{ in } D_{\frac{\varrho}{3}} \tag{13}$$
$$\eta(x) = 1 \text{ in } D \setminus D_{\frac{\varrho}{6}}. \tag{14}$$

Therefore $\Delta\eta u_i + 2\nabla\eta \cdot \nabla u_i \in L^2(\Omega_i)$ for $i = 1, 2, ...$ Then, for $f \in H^{\frac{1}{2}}(\Gamma)$, it follows that

$$\tilde{U}_i \in H^2(D \setminus D_{\frac{\varrho}{2}}) \text{ and} \tag{15}$$
$$U_i \in H^1(D) \text{ for } i = 1, 2, ... \tag{16}$$
$$U_i \rightharpoonup \overline{U} \text{ in } H^1(D) \tag{17}$$
$$u_i - U_i \in H_0^1(\Omega_i) \text{ for } i = 1, 2, ... \tag{18}$$

The result in Sverak (1993) can be formulated in the following way. There exists a subsequence, still denoted by $\{S_i\}$, which converges to $\overline{S}$ in the Hausdorff metric, such that the sequence of metric projections

$$\mathcal{P}_i \,:\, H_0^1(D) \mapsto H_0^1(\Omega_i)$$

converges strongly to the metric projection

$$\overline{\mathcal{P}} \,:\, H_0^1(D) \mapsto H_0^1(D \setminus \overline{S})$$

Therefore, we can pass to the limit in both sides of the following equalities

$$w_i - W = \mathcal{P}_i(w_i - W) \tag{19}$$

$$u_i - U_i = \mathcal{P}_i(u_i - U_i) \tag{20}$$

and we obtain for the weak limits

$$w_i - W \rightharpoonup \overline{w} - W \text{ in } H^1(D) \tag{21}$$

$$u_i - U_i \rightharpoonup \overline{u} - \overline{U} \text{ in } H^1(D) \tag{22}$$

the following equality

$$\overline{w} - W = \overline{\mathcal{P}}(\overline{w} - W) \tag{23}$$

$$\overline{u} - \overline{U} = \overline{\mathcal{P}}(\overline{u} - \overline{U}) \tag{24}$$

which completes the proof of Theorem 1. ■

REMARK 3.2 *In order to obtain an existence result for $N = 3$ we should assume that the family of admissible domains $\mathcal{U}_{\rm ad}$ satisfies the following compactness condition.*

For any sequence $\Omega_i \in \mathcal{U}_{\rm ad}$, $i = 1, 2, \ldots$, there exists a subsequence, still denoted by $\Omega_i = D \setminus S_i$ such that the sequence of compacts S_i converges in the Hausdorff metric to the compact S and the associated sequence of the metric projections $\mathcal{P}_i : H_0^1(D) \mapsto H_0^1(\Omega_i)$ converges strongly to the metric projection $\mathcal{P} : H_0^1(D) \mapsto H_0^1(D \setminus S)$. For such family of admissible domains there exists a solution to the shape identification problem in $\mathbb{R}^3$.

The sufficient conditions for the hypothesis usually require some uniform regularity of boundaries Σ, e.g. the so-called cone condition or more complicated conditions involving the so-called capacity. We refer the reader to e.g. Henrot, Horn and Sokołowski (1996), for a review of the results on the stability of solutions to the Dirichlet problem and to Bucur, Zolesio (1995), for the latter approach to the existence problems.

4. Optimality conditions

In order to derive the first order necessary optimality conditions by using the shape derivatives (instead of material derivatives) we assume that an optimal solution $\Omega = D \setminus S \in \mathcal{O}_\ell$ is a domain with the Lipschitz boundary $\Sigma = \partial S$. In the case of a crack given by a Lipschitz curve i.e., with the Lebesgue measure $|S| = 0$, the optimality conditions can be obtained by an application of the material derivative method, taking into account the singularity coefficients at the tips of the crack.

THEOREM 4.1 *Assume that $\alpha = 0$ and $\ell = 1$. If $\Omega \in \mathcal{O}_1$, $\Omega = D \setminus S$, is an optimal solution, then*

$$\frac{\partial u}{\partial n} = \frac{\partial w}{\partial n} \quad \text{on } \Sigma = \partial S \tag{25}$$

The proof of the theorem is based on the fact that for $S \subset D_\rho$ the shape derivative of the cost functional $J(\cdot)$ is given in the following form

$$dJ(\Omega; V) = \int_\Sigma \left[\left(\frac{\partial u}{\partial n}\right)^2 - \left(\frac{\partial w}{\partial n}\right)^2 \right] V \cdot n d\sigma \tag{26}$$

for any vector field $V(\cdot,\cdot)$ with the compact support in D, n denotes a unit normal vector on $\partial\Omega$ directed outside Ω.

Indeed, the cost functional takes the form

$$\begin{aligned} J(\Omega) &= \inf_{\varphi \in H_0^1(\Omega)+g} \int_\Omega |\nabla\varphi|^2 dx \\ &- \inf_{\varphi \in H_S^1(\Omega)} \left[\int_\Omega |\nabla\varphi|^2 dx - 2\int_\Gamma f\varphi d\Gamma(x) \right] - 2\int_\Gamma gf d\Gamma(x) \end{aligned} \tag{27}$$

where

$$\Omega = D \setminus S \tag{28}$$

$$\partial\Omega = \partial D \cup \partial S, \ \partial D = \Gamma \tag{29}$$

$$H_S^1(\Omega) = \{\varphi \in H^1(D) | \varphi = 0 \text{ on } S\} \tag{30}$$

$$H_0^1(\Omega) + g = \{\varphi \in H_S^1(\Omega) | \varphi = g \text{ on } \Gamma\} \tag{31}$$

therefore, the form of the shape derivative $dJ(\Omega; V)$ is obtained in a standard way for the energy type shape functionals.

We derive the form of the second order shape derivative of the shape functional under considerations which can be used to implement the Newton method. To this end we evaluate the material derivatives of solutions to the Dirichlet and the Dirichlet–Neumann problems. We assume that a vector field $W(\cdot,\cdot)$ is given with the compact support in D, and define the mapping $T_t = T_t(W)$. For the solution $w_t \in H^1(\Omega_t)$ of the Dirichlet problem defined in the domain $\Omega_t = T_t(\Omega)$ we have

$$\Delta w_t = 0 \text{ in } \Omega_t\,, \quad w_t = 0 \text{ on } S_t = T_t(S), \quad w_t = g \text{ on } \partial D \tag{32}$$

therefore, for $w^t = w_t \circ T_t \in H^1(\Omega)$,

$$\begin{aligned} -\text{div}\left(\gamma(t) DT_t^{-1} \cdot {}^*DT_t^{-1} \cdot \nabla w^t\right) = 0 \text{ in } \Omega\,, \\ w^t = 0 \text{ on } S, \quad w^t = g \text{ on } \partial D \end{aligned} \tag{33}$$

and the material derivative

$$\dot{w} = \dot{w}(S; W) = \lim_{t\to 0} \frac{1}{t}\left(w^t - w\right)$$

is given as the unique solution to the following elliptic equation

$$-\Delta\dot{w} = -\text{div}\left[(\text{div}W - DW - {}^*DW)\nabla w\right] \text{ in } \Omega\,, \tag{34}$$

$$\dot{w} = 0 \text{ on } S, \quad \dot{w} = 0 \text{ on } \partial D \tag{35}$$

In the same way the material derivative $\dot{u}$ of the solution to the Dirichlet–Neumann problem is obtained,

$$-\Delta \dot{u} = -\mathrm{div}\left[(\mathrm{div}W - DW - {}^*DW)\,\nabla u\right] \text{ in } \Omega\ , \tag{36}$$

$$\dot{u} = 0 \text{ on } S, \quad \frac{\partial \dot{u}}{\partial n} = 0 \text{ on } \partial D \tag{37}$$

5. Second order derivative

For $\Omega_t = T_t(W)(\Omega)$ we have the first order derivative in the direction $V(t)$

$$\begin{aligned} & dJ(\Omega_t; V(t)) \\ &= \int_{\Sigma_t} \left[\left(\frac{\partial u_t}{\partial n}\right)^2 - \left(\frac{\partial w_t}{\partial n}\right)^2\right] V(t)\cdot n_t d\sigma \\ &= \int_{\Sigma_t} G_t\ V(t)\cdot n_t d\sigma \\ &= \int_{\Sigma} G_t \circ T_t\ [V(t)\cdot n_t] \circ T_t\ \omega_t d\sigma \end{aligned} \tag{38}$$

where

$$G_t \circ T_t = \left[\left(\frac{\partial u_t}{\partial n}\right)^2 - \left(\frac{\partial w_t}{\partial n}\right)^2\right] \circ T_t.$$

Therefore

$$\begin{aligned} & dJ^2(\Omega; V, W) \\ &= \int_{\Sigma} \dot{G} V\cdot n + G[\dot{\omega} V\cdot n + \dot{V}\cdot n + V\cdot \dot{n}] d\Sigma \end{aligned} \tag{39}$$

where $\dot{G}, \dot{\omega}, \dot{n}$ denote respectively the material derivatives of functions G_t , ω_t , n_t defined on $\Sigma_t = T_t(W)(\Sigma)$ in the direction W.

When $\dot{V} = 0$ the second order derivative takes the following form

$$\begin{aligned} & \partial^2 J(\Omega; V(0), W(0)) \\ &= \int_{\Sigma} \dot{G} V\cdot n + G[\dot{\omega} V\cdot n + V\cdot \dot{n}] d\Sigma \end{aligned} \tag{40}$$

we refer to Khludnev, Sokolowski (1996), for the definition of $\partial^2 J(\Omega; V(0), W(0))$ in the general case and the properties of the second order shape derivatives using the material method.

In particular, the latter formula for the second order derivative holds whenever the method of the perturbations of identity is used for the computation of shape derivatives, since for this method the condition $\dot{V} = 0$ is always satisfied.

To evaluate $\dot{G}$ we need the material derivatives $\dot{u}, \dot{w}$ (or the shape derivatives u', w') in the direction of the vector field W of solutions u, w to elliptic equations. It follows that

$$\begin{aligned}\dot{G} &= \frac{\partial}{\partial t}[(n^t \cdot {}^*DT_t^{-1} \cdot \nabla u^t)^2 \\ &- (n^t \cdot {}^*DT_t^{-1} \cdot \nabla w^t)^2]_{|t=0} \\ &= 2[\nabla \dot{u} \cdot n + \nabla u \cdot \dot{n} - n \cdot {}^*DW \cdot \nabla u]\frac{\partial u}{\partial n} \\ &+ 2[\nabla \dot{w} \cdot n + \nabla w \cdot \dot{n} - n \cdot {}^*DW \cdot \nabla w]\frac{\partial w}{\partial n}\end{aligned} \tag{41}$$

6. Integral equations

In this section we introduce the integral equations used in our algorithm to compute the solution of the Dirichlet problem (I) and the Dirichlet-Neumann problem (II).

We start with the integral representation of the solution to the second order elliptic equation for the Laplace operator in a bounded domain $\Omega \subset \mathbb{R}^2$. Namely, if $w \in H^1(\Omega)$ is a solution to

$$-\Delta w = 0 \text{ in } \Omega$$

i.e. w is harmonic in Ω, w can be represented as

$$w(x) = \frac{1}{2\pi}\int_{\partial\Omega}[w(y)]\frac{\partial \ln}{\partial n_y}|x-y|d\sigma(y) - \frac{1}{2\pi}\int_{\partial\Omega}[\frac{\partial w}{\partial n_y}(y)]ln|x-y|d\sigma(y), \ x \in \Omega.$$

When $w = 0$ in $\Omega^c = \mathbb{R}^2 \setminus \Omega$ the jump relation on $\partial\Omega$ implies that the following equalities hold on the boundary $\partial\Omega$, see Kress (1982):

$$\begin{aligned}\frac{1}{2}w(x) &= \frac{1}{2\pi}\int_{\partial\Omega} w(y)\frac{\partial \ln}{\partial n_y}|x-y|d\sigma(y) \\ &- \frac{1}{2\pi}\int_{\partial\Omega}\frac{\partial w}{\partial n_y}(y)ln|x-y|d\sigma(y), \ x \in \partial\Omega\end{aligned} \tag{42}$$

and

$$\begin{aligned}\frac{1}{2}\frac{\partial}{\partial n_x}v(x) &= \frac{1}{2\pi}\frac{\partial}{\partial n_x}\int_{\partial\Omega} v(y)\frac{\partial\, ln}{\partial n_y}|x-y|d\sigma(y) \\ &- \frac{1}{2\pi}\frac{\partial}{\partial n_x}\int_{\partial\Omega}\frac{\partial v}{\partial n_y}ln|x-y|d\sigma(y), \ x \in \partial\Omega\end{aligned} \tag{43}$$

Therefore, for a solution to the Dirichlet problem (I) the following integral equation is obtained for the unknown density $\phi \in H^{-\frac{1}{2}+\sigma}(\partial\Omega)$

$$\int_\Gamma (g(y) - g(x))\frac{\partial \ln}{\partial n_y}|x-y|d\sigma(y) \tag{44}$$

$$= \int_\Gamma \phi \ln|x-y| d\sigma(y) + \int_\Sigma \phi \ln|x-y| d\sigma(y).$$

The associated integral operator is denoted by

$$(V_{\partial\Omega}\phi)(x) \quad = \quad \frac{1}{2\pi}\int_{\partial\Omega} ln|x-y|\phi(y)d\sigma(y). \tag{45}$$

The latter boundary integral operator from $H^{-\frac{1}{2}+\sigma}(\partial\Omega)$ into $H^{\frac{1}{2}+\sigma}(\partial\Omega)$ is continuous if $|\sigma| \le \frac{1}{2}$. Let us recall that this integral operator is not always invertible. For $N = 2$ the invertibility of $V_{\partial\Omega}$ depends on $\partial\Omega$.

For any given $\xi \in \mathbb{R}$ the augmented integral equation,

$$V_{\partial\Omega}\phi - w \quad = \quad 0 \tag{46}$$

$$\int_{\partial\Omega} \phi(y)d\sigma(y) \quad = \quad \xi \tag{47}$$

has a unique solution $\phi \in H^{-\frac{1}{2}}(\partial\Omega)$, $w \in \mathbb{R}$. The map $\xi \to w$ being linear, there is a well-defined constant such that $w = c_{\partial\Omega}\xi$. By definition, the logarithmic capacity $cap(\partial\Omega)$ satisfies, see Costabel, Dauge (1995):

$$-\frac{1}{2\pi} log(cap(\partial\Omega)) = c_{\partial\Omega}. \tag{48}$$

The operator $V_{\partial\Omega}$ is invertible if and only if $c_{\partial\Omega} \neq 0$ and positive definite on $H^{-\frac{1}{2}}(\partial\Omega)$ if and only if $c_{\partial\Omega} > 0$, Costabel, Dauge (1995).
For example if $\partial\Omega$ is a circle of radius R, $V_{\partial\Omega}$ is non-invertible if and only if $R = 1$. In general $V_{\partial\Omega}$ is non-invertible if and only if the logarithmic capacity is equal to 1, see also Schmidt (1994), Symm (1967).
In the case of the Dirichlet–Neumann problem (II) the integral equations take the following form:

For $x \in \Gamma$,

$$\frac{1}{2}\frac{\partial u(x)}{\partial n_x} - \frac{1}{2\pi}\frac{\partial}{\partial n_x}\int_\Gamma u(y)\frac{\partial \ln}{\partial n_y}|x-y| d\sigma(y) \tag{49}$$

$$+ \quad \frac{1}{2\pi}\int_\Sigma \frac{\partial u(y)}{\partial n_y}\frac{\partial \ln}{\partial n_x}|x-y| d\sigma(y) = h(x)$$

with the right-hand side,

$$h(x) \quad = \quad -\frac{1}{2\pi}\int_\Gamma f(y)\frac{\partial \ln}{\partial n_x}|x-y| d\sigma(y). \tag{50}$$

Furthermore, for $x \in \Sigma$,

$$\frac{1}{2\pi}\int_\Gamma u(y)\frac{\partial \ln}{\partial n_y}|x-y| d\sigma(y) \tag{51}$$

$$- \quad \frac{1}{2\pi}\int_\Sigma \frac{\partial u(y)}{\partial n_y} \ln|x-y| d\sigma(y) = m(x)$$

where

$$m(x) = \frac{1}{2\pi} \int_{\Gamma} f(y) \ln |x - y| d\sigma(y). \tag{52}$$

The following boundary integral operators are related to the above system of integral equations,

$$(K_{\partial\Omega}\phi)(x) = -\frac{1}{2\pi} \int_{\partial\Omega} \frac{\partial \ln}{\partial n_y} |x - y| \phi(y) d\sigma(y), \tag{53}$$

$$(K'_{\partial\Omega}\phi)(x) = -\frac{1}{2\pi} \frac{\partial}{\partial n_x} \int_{\partial\Omega} \ln |x - y| \phi(y) d\sigma(y), \tag{54}$$

$$(D_{\partial\Omega}\phi)(x) = -\frac{1}{2\pi} \frac{\partial}{\partial n_x} \int_{\partial\Omega} \frac{\partial \ln}{\partial n_y} |x - y| \phi(y) d\sigma(y). \tag{55}$$

It is well known, Costabel and Stephan (1988), that the following integral operators are continuous for $|\sigma| \leq \frac{1}{2}$,

$$K_{\partial\Omega} : H^{\frac{1}{2}+\sigma}(\partial\Omega) \to H^{\frac{1}{2}+\sigma}(\partial\Omega) \tag{56}$$

$$K'_{\partial\Omega} : H^{-\frac{1}{2}+\sigma}(\partial\Omega) \to H^{-\frac{1}{2}+\sigma}(\partial\Omega) \tag{57}$$

$$D_{\partial\Omega} : H^{\frac{1}{2}+\sigma}(\partial\Omega) \to H^{\frac{1}{2}+\sigma}(\partial\Omega) \tag{58}$$

With this notation the integral equations (46) and (47) can be rewritten in the following form

$$[D_\Gamma u](x) + [K'_\Sigma \frac{\partial u}{\partial n}](x) = [(I + K'_\Gamma) f](x) \text{ if } x \in \Gamma \tag{59}$$

$$[K_\Gamma u](x) + [V_\Sigma \frac{\partial u}{\partial n}](x) = [-V_\Gamma) f](x) \text{ if } x \in \Sigma. \tag{60}$$

When the boundary Σ posseses the property that the operator ${V_\Sigma}^{-1}$ from $H^{\frac{1}{2}}(\Sigma)$ in $H^{-\frac{1}{2}}(\Sigma)$ is well defined, there exists the unique solution in $H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Sigma)$ of equations (49)(51), we refer the reader to Costabel and Stephan (1985), for the proof.

6.1. Integral equations in the 3-dimensional case

For $N = 3$ and $\Omega \subset \mathbb{R}^3$ a bounded domain, if $w \in H^1(\Omega)$ is a harmonic function in Ω i.e. $\Delta w = 0$, the following jump relation on $\partial\Omega = \Gamma \bigcup \Sigma$ is obtained, see Nedelec (1977).

$$\begin{aligned} \frac{w(x)|_{int} + w(x)|_{ext}}{2} &= \frac{1}{4\pi} \int_{\partial\Omega} [w(y)] \frac{\partial}{\partial n_y} \frac{1}{|x - y|} d\sigma(y) \\ &- \frac{1}{4\pi} \int_{\partial\Omega} [\frac{\partial w(y)}{\partial n_y}] \frac{1}{|x - y|} d\sigma(y) \text{ if } x \in \partial\Omega. \end{aligned} \tag{61}$$

Here $q(y) = [\frac{\partial w(y)}{\partial n_y}] = \frac{\partial w(y)}{\partial n_y}|_{int} - \frac{\partial w(y)}{\partial n_y}|_{ext}$ denotes the jump of the normal derivative on $\partial\Omega$. For the function w sufficiently regular in the boundary $\partial\Omega$ we have

$$w(x) = -\frac{1}{4\pi}\int_{\partial\Omega} q(y)\frac{1}{|x-y|}d\sigma(y), \qquad x \in \mathbb{R}^3. \tag{62}$$

Given $g \in H^{\frac{1}{2}}(\partial\Omega)$ the interior Dirichlet problem (I) in integral formulation has a unique solution with respect to the unknown density $q \in H^{-\frac{1}{2}}(\partial\Omega)$. Moreover, the following variational formulation is obtained,

$$b(q, q') = \langle g, q'\rangle \qquad \forall q' \in H^{-\frac{1}{2}}(\partial\Omega) \tag{63}$$

where the bilinear form is given by

$$b(q, q') = \frac{1}{4\pi}\int_{\partial\Omega}\int_{\partial\Omega}\frac{q(x)q'(y)}{|x-y|}d\sigma(x)d\sigma(y). \tag{64}$$

The bilinear form is coercive, i.e. there exists a constant $c > 0$ such that

$$b(q, q) \geq c||q||^2_{H^{-\frac{1}{2}}(\partial\Omega)} \qquad \forall q \in H^{-\frac{1}{2}}(\partial\Omega). \tag{65}$$

So the solution to the Dirichlet problem (I) is given by (62), where q is the unique solution to (63). In the three-dimensional case there is no restriction on the capacity of $\partial\Omega$ to assure the invertibility of the integral operator associated with the Dirichlet problem. In the same way as in the two-dimensional case, assuming that $u = 0$ in Ω^c, for $x \in \Gamma$ we have the following integral equation

$$\begin{aligned} &\frac{1}{2}\frac{\partial u(x)}{\partial n_x} - \frac{1}{4\pi}\frac{\partial}{\partial n_x}\int_\Gamma u(y)\frac{\partial}{\partial n_y}\frac{1}{|x-y|}d\sigma(y) \\ + &\frac{1}{4\pi}\int_\Sigma \frac{\partial u(y)}{\partial n_y}\frac{\partial}{\partial n_x}\frac{1}{|x-y|}d\sigma(y) = h(x) \end{aligned} \tag{66}$$

where

$$h(x) = -\frac{1}{4\pi}\int_\Gamma f(y)\frac{\partial}{\partial n_x}\frac{1}{|x-y|}d\sigma(y). \tag{67}$$

Furthermore, for $x \in \Sigma$,

$$\begin{aligned} &\frac{1}{4\pi}\int_\Gamma u(y)\frac{\partial}{\partial n_y}\frac{1}{|x-y|}d\sigma(y) \\ - &\frac{1}{4\pi}\int_\Sigma \frac{\partial u(y)}{\partial n_y}\frac{1}{|x-y|}d\sigma(y) = m(x) \end{aligned} \tag{68}$$

where

$$m(x) = \frac{1}{4\pi}\int_\Gamma f(y)\frac{1}{|x-y|}d\sigma(y). \tag{69}$$

By the same argument as for the two-dimensional problem the existence and uniqueness of the solution to the equations (63)(64) can be shown, see Nedelec (1977).

It is important for our purposes, that the weak solution to the system of integral equations (63), (64) satisfy the integral identities in the following form.

Find $q = (q_1, q_2) \in H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Sigma)$ such that,

$$\begin{aligned}
& \frac{1}{4\pi}\int_\Gamma \frac{\partial}{\partial s} q_1^1(x) \int_\Gamma \frac{\partial}{\partial s} q_1(y) \frac{1}{|x-y|} d\sigma(y) d\sigma(x) \\
+ & \frac{1}{4\pi}\int_\Gamma q_1^1(x) \int_\Sigma q_2(y) \frac{\partial}{\partial n_x} \frac{1}{|x-y|} d\sigma(y) d\sigma(x) \\
= & \frac{1}{4\pi}\int_\Gamma q_1^1(x) f(x) d\sigma(x) \\
+ & \frac{1}{4\pi}\int_\Gamma q_1^1(x) \int_\Sigma f(y) \frac{\partial}{\partial n_x} \frac{1}{|x-y|} d\sigma(y) d\sigma(x)
\end{aligned} \tag{70}$$

and

$$\begin{aligned}
& \frac{-1}{4\pi}\int_\Sigma q_2^1(x) \int_\Gamma q_1(y) \frac{\partial}{\partial n_x} \frac{1}{|x-y|} d\sigma(y) d\sigma(x) \\
+ & \frac{1}{4\pi}\int_\Sigma q_2^1(x) \int_\Sigma q_2(y) \frac{1}{|x-y|} d\sigma(y) d\sigma(x) \\
= & \frac{-1}{4\pi}\int_\Sigma q_2^1(x) \int_\Gamma f(y) \frac{1}{|x-y|} d\sigma(y) d\sigma(x)
\end{aligned} \tag{71}$$

for all test functions $q = (q_1^1, q_2^1) \in H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Sigma)$. Note, that in (70), (71) we have the tangential derivatives $\frac{\partial}{\partial s} q_1^i$, $\frac{\partial}{\partial s} q_1$ instead of normal derivatives.

The numerical method combines the boundary element technique with Quasi-Newton method in shape optimization.

7. Numerical method

For the numerical methods the continuous problem is approximated by a family of finite dimensional problems. To this end the integral equations are solved by the finite element technique. The resulting optimization problem is solved by an appropriate variant of Newton or Quasi-Newton methods.

7.1. Approximation of continuous problem

An optimal domain satifies the necessary optimality conditions in the form of the following equation,

$$dJ(\Omega; V) = 0$$

for all admissible vector fields $V(.,.)$. The equation is obtained by an application of the material derivative method, Sokołowski (1993), and can be used also in the framework of the so-called perturbation of identity technique for shape optimization. It means that the admissible vector fields are defined in such a way that admissible domains coincide with those constructed by the latter technique. The relation between both techniques is described in Sokołowski (1993). Numerically, we want to evaluate an approximation of the optimal domain i.e. such that the continuous shape derivative of the cost functional (27) vanishes for all admissible vector fields. To this end we construct a minimizing sequence of domains Ω^k, more precisely, we consider a sequence of domains defined by their boundaries $\Gamma^k \cup \Sigma^k$. In practice, in the two dimensional case, by Γ^k we mean the piecewise linear closed Jordan curve with n edges $[x_i^k, x_{i+1}^k] = L_i$, $i = 1, ..., n$ and $x_{n+1}^k = x_1^k$. In the same way Σ_k is defined as a piecewise linear closed Jordan curve with m edges $[y_i^k, y_{i+1}^k] = N_i$; $j = 1, ..., m$. In fact, at each iteration we set $\Gamma^k = \Gamma^0$, but Σ^k changes by local perturbations of vertex. To each vertex y_j^k of Σ^k is associated the direction $\hat{Z}_j^k \in \mathbb{R}^2$, $\hat{Z}_j^k$ is the mean value between the normal vector associated to two finite elements with y_j^k as vertex. We construct a continuous piecewise linear function $Z_j^k : \Gamma^k \to \mathbb{R}^2$ such that:

$$Z_i^k(y_j^k) = \hat{Z}_i^k \delta_{ij} \quad i, j = 1, ...m,$$

where δ_{ij} is the Kronecker symbol. The support of Z_i^k is equal to $[y_{i-1}^k, y_i^k] \cup [y_i^k, y_{i+1}^k]$. Given the surface Σ^k, at iteration $k+1$ we compute the vector field $Z^k(y) := \sum_{i=1}^n s_i Z_i^k(y)$, $y \in \Sigma^k$. The surface Σ^{k+1} is constructed in the following way,

$$\Sigma^{k+1} = \{X = x + \sum_{i=1}^{m} s_i Z_i^k(x); s_i \in \mathbb{R}, x \in \Sigma^k\} \tag{72}$$

where $\bar{s}^t = (s_1, ...s_m)$ is the vector of unknown parameters which determine the form of the surface Σ^{k+1}. This procedure gives the family of domains Ω^{k+1}, $k = 1, 2, ...$, with the piecewise linear boundaries Σ^{k+1} corresponding to $(s_1, ..., s_m) \in \mathbb{R}^m$. In the 3-dimensional case Γ^0 is the piecewise linear approximation of the exterior boundary Γ. Σ^k, $k = 1, 2, ...$, is the approximation of the inclusion boundary in the form of the union of triangles T_l in $\mathbb{R}^3$. Each triangle is parametrized with the help of a reference triangle in coordinates ξ and η. The vertices of the triangle T_l are denoted by $x^{l,1}, x^{l,2}, x^{l,3}$ so that if $x \in T_l$, the function defined on T_l can be expressed in the following way

$$x = x(\xi, \eta) = \sum_{i=1}^{3} x^{l,i} N_i(\xi, \eta) \tag{73}$$

where $N_i(.,.)$ are given functions,

$$N_1(\xi, \eta) = 1 - \xi - \eta; \; N_2(\xi, \eta) = \xi; \; N_3(\xi, \eta) = \eta. \tag{74}$$

where $DL'(\bar{s}_k, \Lambda_k)$ is given by:

$$DL'(\bar{s}_k, \Lambda_k) = \begin{pmatrix} H_k(\bar{s}_k) & d_s\omega(\bar{s}_k) \\ d_s\omega(\bar{s}_k)^t & 0 \end{pmatrix} \tag{95}$$

the matrix $H_k(\bar{s}_k)$ evaluated at $\bar{s}_k$ by the B.F.G.S. algorithm is an approximation of the Hessian of the cost function $J(\bar{s})$. Therefore, we obtain the following shape identification algorithm:

Algorithm;

Data. Initial guess for Σ^0 and r^0. The exterior boundary Γ. The boundary data g and f on Γ.

For $k = 0, \ldots$ until convergence test
Step 0. Initialise $H_k = Identity$ matrix in $\mathbb{R}^m \times \mathbb{R}^m$
Step 1. Compute the gradient of J.
i) Solve the Dirichlet problem;

$$\Delta w = 0 \quad \text{in } \Omega^k \tag{96}$$
$$w = g \quad \text{on } \Gamma \tag{97}$$
$$w = 0 \quad \text{on } \Sigma^k \tag{98}$$

ii) Solve the Dirichlet-Neumann problem;

$$\Delta u = 0 \quad \text{in } \Omega^k \tag{99}$$
$$\frac{\partial u}{\partial n} = f \quad \text{on } \Gamma \tag{100}$$
$$u = 0 \quad \text{on } \Sigma^k \tag{101}$$

iii) Compute the shape gradient of J. For $l = 1, .., m$

$$\{dJ_s(\bar{s})\}_l = \int_{\Sigma^k} \left[\left(\frac{\partial u_k}{\partial n}\right)^2 - \left(\frac{\partial w_k}{\partial n}\right)^2 \right] Z_l \cdot n_k d\sigma \tag{102}$$

Step 2. Compute the descent direction using a B.F.G.S. approximation of the Hessian of J_s.

For $g_k = dJ_s(\bar{s}_k) - dJ_s(\bar{s}_{k-1})$ and $\delta_k = \bar{s}_k - \bar{s}_{k-1}$ we compute the update H_{k+1}.

$$H_{k+1} = H_k + \frac{g_k^t g_k}{\delta_k^t g_k} - \frac{H_k \delta_k \delta_k^t H_k}{\delta_k^t g_k} \tag{103}$$

Step 3. Compute $\delta\bar{s}_k$ and $\delta\Lambda_k$ solution of the linear system.

$$\begin{pmatrix} H_{k+1}(\bar{s}_k) & d_s\omega(\bar{s}_k) \\ d_s\omega(\bar{s}_k)^t & 0 \end{pmatrix} \begin{pmatrix} \delta\bar{s}_k \\ \delta\Lambda_k \end{pmatrix} = - \begin{pmatrix} d_{\bar{s}}J(\bar{s}_k) + \Lambda_k d_{\bar{s}}\omega(\bar{s}_k) \\ \omega(\bar{s}_k) \end{pmatrix} \tag{104}$$

REMARK 7.1 *The first value r^0 for the penalty parameter r must be chosen in such a way that the penalty term is of the same order as the gradient of J, otherwise numerical instabilities may occur. After solving the unconstrained problem J_{r^0} only two or three steps in the parameter r are neccesary to reach numerical convergence.*

REMARK 7.2 *This algorithm requires the periodical reinitialisation of the matrix H_k by the identity matrix in order to obtain a minimisation procedure even in the case where H_k is not positive definite. At each iteration the condition $\delta_k^t g_k \geq 0$ should be verified to assure that H_{k+1} is positive definite. If it is not the case a gradient iteration is performed and afterwards the matrix H_k is set to be the identity matrix.*

7.3. Lagrange-Newton Method

We describe briefly another numerical method based on the Kuhn-Tucker optimality conditions for the minimization problem. The method can be applied in the case of equality constraints. We introduce the following Lagrangian:

$$L(\bar{s}, \Lambda) = J(\bar{s}) + \Lambda(\omega(\bar{s})) \tag{91}$$

where $\bar{s} \in \mathrm{I\!R}^m$ and $\Lambda \in \mathrm{I\!R}$.

PROPOSITION 7.1 *Let $J(\bar{s})$ and $\omega(\bar{s})$ be two functions with the first derivatives continuous at $\bar{s}^*$. We suppose that $\omega(\bar{s}^*) = 0$ and $d_s\omega(\bar{s}^*) \neq 0$, then a necessary condition that s^* is a local minimum of $J(\bar{s})$ with the constraint $\omega(\bar{s}) = 0$ is the existence of the Lagrange multiplier $\Lambda^* \in \mathrm{I\!R}$ such that:*

$$d_s L(\bar{s}^*, \Lambda^*) = \nabla_s J(\bar{s}^*) + \Lambda^*(\nabla_s \omega(\bar{s}^*)) = 0 \tag{92}$$

see e.g. Fiacco, McCormick (1968) for a proof.

Then a numerical method to find a local critical point $\bar{s}^*$ of the cost functional $J(\bar{s})$ subject to the constraints $\omega(\bar{s}) = 0$ consists in computing a solution to the following set of the first order necessary conditions:

$$DL(\bar{s}, \Lambda) = \begin{pmatrix} d_s J(\bar{s}) + \Lambda d_s \omega(\bar{s}) \\ \omega(\bar{s}) \end{pmatrix} = 0 \tag{93}$$

A Quasi-Newton method to solve the Kuhn-Tucker equation (92) consists in computing a sequence of solutions $(\bar{s}_k, \Lambda^k)$ to the linearized equations obtained from (92). This leads to the following algorithm:

$$\left\{ \begin{array}{l} \text{Given } \bar{s}_0 \text{ and } \Lambda^0 \\ \text{Compute} \\ (\bar{s}_{k+1}, \Lambda_{k+1}) = (\bar{s}_k, \Lambda_k) + (\delta\bar{s}_k, \delta\Lambda_k);\ \delta\bar{s}_k \in \mathrm{I\!R}^m;\ \delta\Lambda_k \in \mathrm{I\!R} \\ \text{defined by:} \\ DL(\bar{s}_k, \Lambda_k) + DL'(\bar{s}_k, \Lambda_k)(\delta\bar{s}_k, \delta\Lambda_k) = 0 \end{array} \right. \tag{94}$$

The direction of the displacement at each vertex of Σ^k is given by a piecewise linear vector field

$$Z_k^i(x) = \begin{cases} \hat{Z}_k^i N_j(\xi,\eta) \text{ if } x \in T_l \text{ and } (\xi,\eta) = x^{l,j} \in T_l \\ 0 \text{ otherwise.} \end{cases} \tag{75}$$

Then, as in the two dimensional case, at the iteration $k+1$ the update of the boundary Σ^k is given by

$$\Sigma^{k+1} = (I + \sum_{i=1}^{m} s_i Z_i^k)(\Sigma^k), \ \bar{s}^t = (s_1, ..., s_m). \tag{76}$$

This method of evolution of the boundary has the important advantage that there is only one degree of freedom at each vertex, for $N = 2$ as well as for $N = 3$.
Finally, to perform the shape optimization, the vector $\bar{s}^{k+1} \in \mathbb{R}^m$ is computed at each iteration by a minimisation procedure in such a way that:

$$J(\bar{s}^{k+1}) \leq J(\bar{s}^k). \tag{77}$$

See Pierre, Roche (1993) for a related approximation technique in shape optimisation.

7.2. Penalty method

For the problem under considerations it is convenient to introduce constraints. Constraints on the position of the inclusion, can be introduced, for instance stipulating that the distance of the inclusion to the boundary is greater than a given constant $\epsilon > 0$. Another constraint can reflect the requirement that the surface of the inclusion is prescribed. We denote by $\omega(\bar{s}) = 0$ or $\omega(\bar{s}) \leq 0$ such constraints in terms of the parameter of optimization $\bar{s} \in \mathbb{R}^m$. Let us consider the following penalized cost functional

$$J_r(\bar{s}) = J(\bar{s}) + \frac{r}{2}(w(\bar{s}))^2 \tag{78}$$

for the equality constraint or, in the case of inequality constraints:

$$J_r(\bar{s}, t) = J(\bar{s}) + \frac{r}{2}(w(\bar{s}) - t)^2 \tag{79}$$

In both cases r is the parameter which is large enough, theoretically $r \nearrow \infty$, see e.g. Fletcher (1987), and Minoux (1983), for a description of such methods.

We propose the following scheme to evaluate the unknown crack boundary Σ by the penalization technique.

Algorithm;

Data. Given Σ^0 and r^0. The exterior boundary Γ. The boundary data g and f on Γ.

For $r = r^0, r^1, ...$ solve the unconstrained optimization problem.

$$(P_r) \qquad Min\{J_r(\bar{s}), \bar{s} \in \mathbb{R}^n\} \tag{80}$$

For $k = 0, ...$ until convergence test.

Step 0. Initialise $H_k = Identity$ matrix in $\mathbb{R}^m \times \mathbb{R}^m$
Step 1. Compute the gradient of J_r.
i) Solve the Dirichlet problem;

$$\Delta w = 0 \quad \text{in } \Omega^k \tag{81}$$
$$w = g \quad \text{on } \Gamma \tag{82}$$
$$w = 0 \quad \text{on } \Sigma^k \tag{83}$$

ii) Solve the Dirichlet-Neumann problem;

$$\Delta u = 0 \quad \text{in } \Omega^k \tag{84}$$
$$\frac{\partial u}{\partial n} = f \quad \text{on } \Gamma \tag{85}$$
$$u = 0 \quad \text{on } \Sigma^k \tag{86}$$

iii) Compute the shape gradient of J_r. For $l = 1, .., m$

$$\{dJ_r(\bar{s})\}_l = \int_{\Sigma^k} \left[\left(\frac{\partial u_k}{\partial n} \right)^2 - \left(\frac{\partial w_k}{\partial n} \right)^2 \right] Z_l \cdot n_k d\sigma \tag{87}$$

Step 2. Compute the descent direction using a B.F.G.S. approximation of the inverse of the Hessian of J_r.

For $g_k = dJ_r(\bar{s}_k) - dJ_r(\bar{s}_{k-1})$ and $\delta_k = \bar{s}_k - \bar{s}_{k-1}$ find the update H_{k+1}

$$H_{k+1} = H_k + [\frac{1 + g_k^t H^k \delta_k}{\delta_k^t g_k}] \frac{\delta_k \delta_k^t}{\delta_k^t g_k} - \frac{\delta_k^t g_k H_k + H_k g_k \delta_k^t}{\delta_k^t g_k} \tag{88}$$

Step 3. Compute $\bar{s}^{k+1}$.

$$\bar{s}_{k+1} = -\rho_k (H_k D J_r(\bar{s}_k)) \tag{89}$$

where ρ is found by of the Armijo's line search procedure.
Step 4. Update the boundary of Σ_k to obtain Σ_{k+1}.

$$\Sigma^{k+1} = (I + \sum_{l=1}^{m} \{\bar{s}_{k+1}\}_l Z_l)(\Sigma^k) \tag{90}$$

Go back to step 1.

Step 4. Compute $\bar{s}_{k+1} = \bar{s}_k + \rho^k \delta \bar{s}_k$ where ρ^k is found by the Armijo's line search procedure.
Step 5. Update the boundary of Σ^k to obtain Σ^{k+1}.

$$\Sigma^{k+1} = (I + \sum_{l=1}^{m} \{\bar{s}_{k+1}\}_l Z_l)(\Sigma^k) \tag{105}$$

Go back to step 1.

This scheme describes the algorithm with a superlinear rate of convergence if the first guess Σ^0 is close enough to the solution . In general, such a procedure starts with a steepest descent method to obtain Σ^0 and applies a Quasi-Newton technique to refine the result of optimization.

In the next section we are going to explain the numerical method which is used to find approximations of the solutions to the Dirichlet problem (I) and Dirichlet-Neumann problem (II) by the boundary element method.

7.4. Integral equations

At each iteration we evaluate a numerical approximation of normal derivatives $\frac{\partial w}{\partial n}, \frac{\partial u}{\partial n}$ on Σ^k and $\frac{\partial w}{\partial n}$, u on Γ^k in order to approximate the continuous gradient and the value of the cost functional.

$$\begin{aligned} J(\Omega^k) &= \int_{\partial\Omega^k} g(x) \frac{\partial w^k(x)}{\partial n_x} d\sigma(x) \\ &+ \int_{\partial\Omega^k} f(x) u^k(x) d\sigma(x) - 2\int_{\partial\Omega^k} g(x) f(x) d\sigma(x) \end{aligned} \tag{106}$$

The integral equations for density $q(x)$ associated to the Dirichlet problem take the following form.
For $y \in \Gamma^k$,

$$\int_{\partial\Omega^k} (g(x) - g(y)) \frac{\partial \ln}{\partial n_x} |x-y| d\sigma(x) = \int_{\partial\Omega^k} q(x) \ln |x-y| d\sigma(x) \tag{107}$$

and for $y \in \Sigma^k$,

$$\int_{\partial\Omega^k} g(\dot{x}) \frac{\partial \ln}{\partial n_x} |x-y| d\sigma(x) = \int_{\partial\Omega^k} q(x) \ln |x-y| d\sigma(x) \tag{108}$$

In order to solve the above system of two integral equations, the Galerkin method, Costabel and Stephan (1985), Schmidt (1994), is used. In the continuous case the following variational fomulation is obtained,

$$q \in H^{-\frac{1}{2}} : \qquad b(q, q') = l(q') \forall q' \in H^{-\frac{1}{2}} \tag{109}$$

with

$$b(q, q') = \int_{\partial\Omega} \int_{\partial\Omega} q(y) q'(x) \ln |x-y| d\sigma(y) d\sigma(x) \tag{110}$$

and

$$l(q') = \int_\Gamma \int_\Gamma (g(y) - g(x)) \frac{\partial \ln}{\partial n_y} |x - y| d\sigma(x) \tag{111}$$

The bilinear form $b(.,.)$ is coercive, i.e. there exists a constant $c > 0$ such that

$$b(q,q) \geq c||q||_{H^{-\frac{1}{2}}}; c > 0 \tag{112}$$

for all $q \in H^{-\frac{1}{2}}(\partial\Omega)$ with $\int_{\partial\Omega} q(y)d\sigma(y) = 0$. Then, if $\partial\Omega$ has the property that there exists the inverse mapping $V_{\partial\Omega}^{-1}$, the equation has the unique solution in $H^{-\frac{1}{2}}(\partial\Omega)$. The same formulation is used for $\partial\Omega^k$ in the discrete case.

The equation (109) is discretized by using a finite element representation q^k of q. We introduce the basis functions $\{e_j\}_{j=1,\dots,n}$ on Γ^k and $\{f_j\}_{j=1,\dots,m}$, on Σ^k which are both piecewise constant.

Then, $q^k(x)$ for $x \in \Gamma$ is obtained as $q^k(x) = \Sigma_{j=1}^n q_j^1 e_j(x)$ and $q^k(x)$ for $x \in \Sigma^k$ takes the form $q^k(x) = \Sigma_{j=1}^n q_j^2 f_j(x)$ where $\{q_j^1\}_{j=1,..n} \in \mathbb{R}^n$ and $\{q_j^2\}_{j=1,..m} \in \mathbb{R}^m$ are the solutions of the following linear system:

$$\begin{pmatrix} A & B \\ & \\ C & D \end{pmatrix} \begin{pmatrix} q_1^1 \\ \cdot \\ q_i^1 \\ \cdot \\ \cdot \\ q_i^2 \\ \cdot \\ q_M^2 \end{pmatrix} = \begin{pmatrix} f_1 \\ \cdot \\ f_i \\ \cdot \\ \cdot \\ f_i \\ \cdot \\ f_{N+M} \end{pmatrix} \tag{113}$$

here

$$a_{ij} = \int_{L_i} \int_{L_j} \ln |x - y| d\sigma(x) d\sigma(y) \tag{114}$$

$$b_{ij} = \int_{L_i} \int_{N_j} \ln |x - y| d\sigma(x) d\sigma(y) \tag{115}$$

$$c_{ij} = \int_{N_i} \int_{L_j} \ln |x - y| d\sigma(x) d\sigma(y) \tag{116}$$

$$d_{ij} = \int_{N_i} \int_{N_j} \ln |x - y| d\sigma(x) d\sigma(y) \tag{117}$$

and

$$f_i = \begin{cases} \int_{L_i} \int_{\Gamma^k} (g(y) - g(x)) \frac{\partial \ln}{\partial n_x} |x - y| d\sigma(y) d\sigma(x) & 1 \leq i \leq N \\ \int_{N_i} \int_{\Gamma^k} g(y) \frac{\partial \ln}{\partial n_x} |x - y| d\sigma(y) d\sigma(x) & N \leq i \leq N + M \end{cases}$$

The above linear system is symmetric and the associated matrix is positive definite.

For the mixed Dirichlet-Neumann problem (II) we solve the integral equations (46) in Γ^k and (51) in Σ^k. This system of integral equations has a unique solution in $H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Sigma)$, see section 6 for details. We introduce now a variational formulation, find $(q_1, q_2) \in H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Sigma)$ such that for all test functions $(\varphi, \psi) \in H^{\frac{1}{2}}(\Gamma) \times H^{-\frac{1}{2}}(\Sigma)$ the following equations are satisfied.
For $x \in \Gamma^k$,

$$\begin{aligned} & \int_{\Gamma^k} \varphi(x) \frac{\partial}{\partial n_x} \int_{\Gamma^k} q_1(y) \frac{\partial \ln}{\partial n_y} |x-y| d\sigma(y) d\sigma(x) \\ + & \int_{\Gamma^k} \varphi(x) \frac{\partial}{\partial n_x} \int_{\Sigma^k} q_2(y) \ln |x-y| d\sigma(y) d\sigma(x) \\ = & \int_{\Gamma^k} \varphi(x) f(x) d\sigma(x) \\ + & \int_{\Gamma^k} \varphi(x) \frac{\partial}{\partial n_x} \int_{\Sigma^k} f(y) \ln |x-y| d\sigma(y) d\sigma(x) \end{aligned} \tag{118}$$

For $x \in \Sigma^k$

$$\begin{aligned} - & \int_{\Sigma} \psi(x) \int_{\Gamma} q_1(y) \frac{\partial \ln}{\partial n_x} |x-y| d\sigma(y) d\sigma(x) \\ + & \int_{\Sigma} \psi(x) \int_{\Sigma} q_2(y) \ln |x-y| d\sigma(y) d\sigma(x) \\ = & -\int_{\Sigma} \psi(x) \int_{\Gamma} f(y) \ln |x-y| d\sigma(y) d\sigma(x) \end{aligned} \tag{119}$$

This equations have unique solutions, Costabel and Stephan (1988), Schmidt (1994), if the mapping V_Σ is invertible. We introduce the basis functions $\{f_j\}_{j=1,n}$ where $f_j(x)$ are piecewise linear on Γ and satisfy the conditions $f_j(x_i) = \delta_{ij}$. We set $q_1(x) := \Sigma_{j=1}^n v_j^1 f_j(x)$ and we approximate $q_2(x)$ by the piecewise constant function $q_2(x) = \Sigma_{j=1}^m v_j^2 e_j(x)$ defined on Σ. Then the following linear system is obtained:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} v_1^1 \\ \cdot \\ v_i^1 \\ \cdot \\ \cdot \\ v_i^2 \\ \cdot \\ v_M^2 \end{pmatrix} = \begin{pmatrix} m_1 \\ \cdot \\ m_i \\ \cdot \\ \cdot \\ m_i \\ \cdot \\ m_M \end{pmatrix} \tag{120}$$

where

$$a_{ij} = \int_{L_{i-1} \cup L_i} \frac{\partial}{\partial s_x} f_i(x) \int_{L_{j-1} \cup L_j} (\frac{\partial}{\partial s_y} f_j(y)) \ln |x-y| d\sigma(y) d\sigma(x) \tag{121}$$

$$b_{ij} = -\int_{L_{i-1}\cup L_i} f_i(x) \int_{N_j} \frac{\partial \ln}{\partial n_x}|x-y| d\sigma(y) d\sigma(x) \tag{122}$$

$$c_{ij} = \int_{N_i} \int_{L_{j-1}\cup L_j} f_j(y) \frac{\partial \ln}{\partial n_y}|x-y| d\sigma(y) d\sigma(x) \tag{123}$$

$$d_{ij} = -\int_{N_i} \int_{N_j} \ln|x-y| d\sigma(y) d\sigma(x) \tag{124}$$

and the right–hand side is given by:

$$\begin{aligned} h_i &= \pi \int_{L_{i-1}\cup L_i} f_i(x) f(x) d\sigma(y) \\ &+ \int_{L_{i-1}\cup L_i} f_i(x) \int_{\Gamma} f(y) \frac{\partial \ln}{\partial n_x}|x-y| d\sigma(x) d\sigma(y) \end{aligned} \tag{125}$$

and

$$m_i = \int_{N_i} \int_{\Gamma} f(y) \ln|x-y| d\sigma(y) d\sigma(x) \tag{126}$$

The system (120) is symmetric and dense. It can be solved by LDL^t method, see Golub, Van Loan (1983).

In both cases numerical errors of two types appear. The first one is the geometric representation error, the error of replacing Γ and Σ by Γ^k and Σ^k. The second one is the approximation error, between $q(x)$ and its piecewise linear approximation. An exhaustive analysis of numerical errors in boundary integral methods can be find in Nedelec (1977), Rannacher, Wendland (1985;1988).

8. Numerical example

In the first numerical example we consider as D a ball in $\mathbb{R}^2$ of radius R and centered at the origin. As the inclusion (void) S we consider a small ball of radius r and centered at the origin. A harmonic function $u(x), x \in \mathbb{R}^2 \setminus S$, can be constructed by taking $u(x) = \ln|x| - \ln(r)$.

To follow the evolution of the iterations of the algorithm we consider five parameters. The first one is $Cost_k/Cost_0$ which is the quotient of the value of the cost function in the k-th shape iteration to the value of the cost function at the initial shape guess. The second parameter is ∇_k/∇_0 which is the quotient of the L^2 norm of the gradient at the k-th step to the L^2 norm of the gradient at the initial iteration. The third parameter is $\|\frac{\partial w}{\partial n} - F\|_{L^2(\partial\Omega)}$ the L^2 error between the normal derivative of w computed by solving the Dirichlet problem (I) and the true value F. The fourth parameter $\|\frac{\partial u}{\partial n} - F\|_{L^2(\Sigma)}$ is the L^2 error between the normal derivative of u computed by solving the Dirichlet-Neumann problem (II) and the true value F on Σ. The fifth parameter $\|u - g\|_{L^2(\Gamma)}$ is the L^2 error

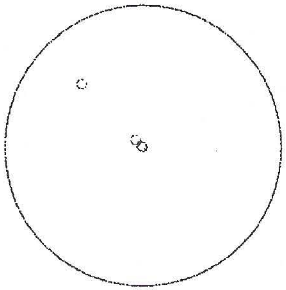

Figure 1.

between the approximation of u computed by solving the Dirichlet-Neumann problem and the true value g on Γ.

The boundary $\partial\Omega$ is discretised by piecewise linear finite element, and we obtain $\partial\Omega_h \equiv \Gamma_h \cup \Sigma_h$.

The numerical method consists in constructing a minimizing sequence (S_h^k, u_h^k, w_h^k) for the discrete shape functional $J_h(S_h)$. In fact we consider a discretised continuous gradient method, which means that we compute at each iteration a numerical approximation of the continuous gradient and not the gradient of the discrete problem. This implies that at each iteration we compute only an approximation of the gradient of the discrete problem.

In the first run we consider an initial guess Σ^0 such that it has the same shape as Σ^* (the solution) but is not in true position in D. We want to identify the position of the void. Then, the sequence of inclusions Σ_h^k is determined by a sequence in $\mathbb{R}^2$, since Σ_h^k depends on two parameters, the center $a^k = (a_1, a_2)$ of the circle Σ^k.

The minimizing sequence is obtained by locally optimal displacements of the vertex of the boundary Σ_h according to a given vector field V with translation.

For the vector field parametrized by x_0, y_0 the continuous gradient takes the following form:

$$dJ(\Omega; V) = \int_\Sigma \left[\left(\frac{\partial u}{\partial n}\right)^2 - \left(\frac{\partial w}{\partial n}\right)^2 \right] V \cdot n d\sigma = C(x_0, y_0, w, u) \quad (127)$$

In Figure 1 we plot the evolution of the iterations, the first guess Σ^0 is the most distant circle.

In Table 1 we can see the evolution of the five parameters described above. We observe that after fifteen iterations the algorithm reaches a good approximation of the real position of the void in the center of D. We spent twenty more iterations to improve this position identification. The errors of the computation stabilize after twenty five iterations, only the gradient decreases but the precision of the computation of u and w is stable because it depends on the

k	$Cost_k/Cost_0$	∇_k/∇_0	$\|\frac{\partial w}{\partial n} - F\|_{L^2(\partial\Omega)}$	$\|\frac{\partial u}{\partial n} - F\|_{L^2(\Sigma)}$	$\|u - g\|_{L^2(\Gamma)}$
0	1.	1.	2.8331	0.5476	2.1273
5	9.48e-03	9.23e-02	0.3131	6.10e-02	0.279
15	8.37e-03	2.21e-03	7.56e-03	2.19e-02	1.72e-02
25	8.38e-03	5.41e-05	5.76e-04	2.18e-02	1.58e-02
35	8.38e-03	1.32e-06	5.62e-04	2.18e-02	1.58e-02

Table 1. Example $n°$ 1, n=64.

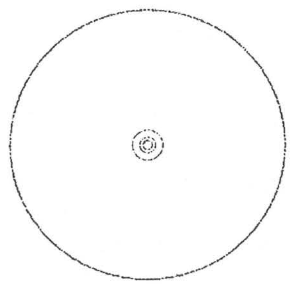

Figure 2.

number n of nodes in the representation of $\partial\Omega^k$.

In the second example a first guess is given by a circle of radius $r^0 > r$. In this case we apply the algorithm described in section 7.2, we have one degree of freedom for each vertex of Σ^k. Then the shape gradient $DJ(\Sigma^k, Z^k)$ at iteration k is given by:

$$\{DJ(\Omega^k; Z^k)\}_i = \int_\Sigma \left[\left(\frac{\partial u}{\partial n}\right)^2 - \left(\frac{\partial w}{\partial n}\right)^2\right] Z_i \cdot \nu d\sigma \tag{128}$$

In Figure 2 we observe the results of the subsequent iterations, here the position is known but the shape is the unknown.

In Table 2 we observe the evolution of the cost function with respect to the initial guess cost, the minimum is reached after thirty iterations. The minimum error in the numerical solution of the integral equations is also reached after thirty iterations because the error of numerical approximation is at that step greater than the error induced by the wrong shape. The last twenty iterations are used to improve the shape, then the gradient decreases.

In Figure 3 we consider an example where we add the two problems, the first guess is in a wrong position and it has a wrong radius r^0. In this case we have also one degree of freedom for each node of the Σ boundary.

In Table 3 we observe that the same precision is reached in the numerical

k	$Cost_k/Cost_0$	∇_k/∇_0	$\|\frac{\partial w}{\partial n} - F\|_{L^2(\partial\Omega)}$	$\|\frac{\partial u}{\partial n} - F\|_{L^2(\Sigma)}$	$\|u - g\|_{L^2(\Gamma)}$
0	1.	1.	8.44	48.8	6.16
5	0.47	0.61	4.74	38.27	5.19
10	0.19	0.40	2.20	24.6	3.68
20	3.62e-03	8.38e-02	0.15	2.79	0.47
30	7.88e-04	6.08e-06	3.87e-03	6.08e-02	2.31e-03
40	7.88e-04	2.00e-10	3.87e-03	6.08e-02	2.28e-03
50	7.88e-04	3.69e-14	3.87e-03	6.08e-02	2.28e-03

Table 2. Example $n°$ 2, n=64.

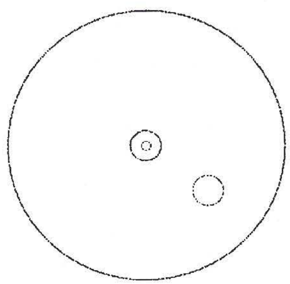

Figure 3.

k	$Cost_k/Cost_0$	∇_k/∇_0	$\|\frac{\partial w}{\partial n} - F\|_{L^2(\partial\Omega)}$	$\|\frac{\partial u}{\partial n} - F\|_{L^2(\Sigma)}$	$\|u - g\|_{L^2(\Gamma)}$
0	1.	1.	5.32	18.52	2.77
10	0.31	3.74e-02	1.44	18.49	2.67
20	9.68e-03	3.36e-03	1.55e-02	0.29	5.99e-02
30	9.94e-03	1.03e-05	3.88e-03	6.09e-02	2.28e-03
40	9.94e-03	7.35e-06	3.88e-03	6.09e-02	2.28e-03
50	9.94e-03	6.67e-06	3.88e-03	6.09e-02	2.28e-03

Table 3. Example n° 3, n=64.

approximation of the integral equations solutions as in example 2. The rate of convergence of the gradient is compared to example 2 because of the presence of translations and shape deformations in the shape perturbation vector fields.

In conclusion we observe that the presented shape optimisation technique will be able to identify the position and the shape of inclusion via boundary data.

As shown in Tables 1, 2 and 3 the precision of the results depends on the performance of the numerical solution of the integral equations. Computational errors in numerical approximation of u and w include errors in shape gradient and cost function computation which cause a lower rate of convergence of the optimization procedure.

The numerical technique proposed here can be used in other shape identification problems, for example electromagnetic casting, see Pierre, Roche (1993). Purely Newton techniques can be also used if the shape Hessian is available and its numerical computation is not too expensive in terms of floating point operations, see Novruzi, Roche (1995).

The computations were carried out with the Silicon Graphics Parallel computer of the C.C.H high performances computer center of Nancy, France.

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