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Shape derivative of cost function for singular point: Evaluation by the generalized J integral

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Abstract

This paper presents analytic solutions of the shape derivatives (Fréchet derivatives with respect to domain variation) for singular points of cost functions in shape-optimization problems for the domain in which the boundary value problem of a partial differential equation is defined. A design variable is given by a domain mapping. Cost functions are defined as functionals of the design variable and the solution to the boundary value problem. The analytic solutions for singular points such as crack tips and boundary points of the mixed boundary conditions on a smooth boundary are obtained by using the generalized J integral.

Keywords calculus of variations, boundary value problem, shape optimization, generalized J integral, H1 gradient method

Research Activity Group Mathematical Design

1. Introduction

Determining the optimum shape of the domain in which a boundary value problem of a partial differential equation is defined is called a shape-optimization problem. One way to formulate this problem is to choose the domain mapping as the design variable. Cost functions are defined as functionals of the design variable and the solution to the boundary value problem. The shape derivatives, which are defined as the Fréchet derivatives with respect to domain variation, of the cost functions can be evaluated assuming appropriate regularity in the boundary value problem. Solution using the shape derivative is presented in [1].

On the other hand, in research of evaluating the singularity of a crack, the generalized J integral was proposed [2], and its relation to the shape derivative of a cost function has been presented [3–5]. However, the analytic solution at the singular point has not been shown.

The present paper is dedicated to obtaining the analytic solutions of the shape derivatives for singular points such as crack tips and boundary points of the mixed boundary conditions on a smooth boundary by the use of the generalized J integral.

2. Set of design variable

Let Ω_0 depicted in Fig. 1 be a two-dimensional bounded domain, where the boundary $\partial\Omega_0$ consists of Dirichlet boundary $\Gamma_{\mathrm{D}0} \subset \partial\Omega_0$ and Neumann boundary $\Gamma_{\mathrm{N}0} = \partial\Omega_0 \setminus \bar{\Gamma}_{\mathrm{D}0}$.

For $j \in \Theta_{\mathrm{N}} = \{1, \ldots, |\Theta_{\mathrm{N}}|\}$, let $\boldsymbol{x}_{j0}$ (note, $\boldsymbol{x}_{10}$ is hidden in Fig. 1) be corner points on $\Gamma_{\mathrm{N}0}$ having concave angles of $\alpha_{0j} \in (\pi, 2\pi]$. In the same manner, for $j \in \Theta_{\mathrm{D}} = \{|\Theta_{\mathrm{N}}| + 1, \ldots, |\Theta_{\mathrm{N}}| + |\Theta_{\mathrm{D}}|\}$, let $\boldsymbol{x}_{j0}$ be corner

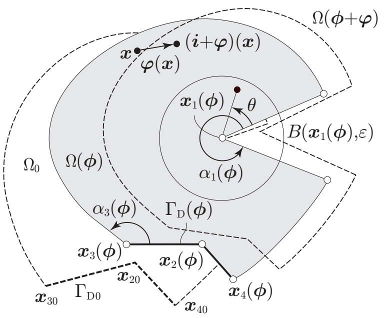

Fig. 1. Varying 2-dimensional domain with corner points.

points inside of $\Gamma_{\mathrm{D}0}$ with $\alpha_{0j} \in (\pi, 2\pi]$. Moreover, for $j \in \Theta_{\mathrm{M}} = \{|\Theta_{\mathrm{N}}| + |\Theta_{\mathrm{D}}| + 1, \ldots, |\Theta_{\mathrm{N}}| + |\Theta_{\mathrm{D}}| + |\Theta_{\mathrm{M}}|\}$, let $\boldsymbol{x}_{j0}$ be corner points on the boundary of the mixed boundary conditions having an opening angle of $\alpha_{0j} \in (\pi/2, 2\pi]$. In the present paper, we call these points the singular points, and define the set of their indexes as $\Theta = \Theta_{\mathrm{N}} \cup \Theta_{\mathrm{D}} \cup \Theta_{\mathrm{M}}$. The remaining part of the boundary is assumed to be sufficiently smooth.

We define design variable in a shape optimization problem by domain variation $\boldsymbol{\phi}$, with which a varied domain is created by continuous one-to-one mapping $\boldsymbol{i} + \boldsymbol{\phi} : \Omega_0 \to \mathbb{R}^2$ as $\Omega(\boldsymbol{\phi}) = \{(\boldsymbol{i} + \boldsymbol{\phi})(\boldsymbol{x}) \mid \boldsymbol{x} \in \Omega_0\}$. The symbol $\boldsymbol{i}$ is used as the identity mapping in the present paper. The notation $(\,\cdot\,)(\boldsymbol{\phi})$ is used as $\{(\boldsymbol{i} + \boldsymbol{\phi})(\boldsymbol{x}) \mid \boldsymbol{x} \in (\,\cdot\,)_0\}$ for domains and boundaries. To keep continuous one-to-one mapping property, we define the admissible set of $\boldsymbol{\phi}$ as

$$\mathcal{D} = \{\boldsymbol{\phi} \in Y \mid \|\boldsymbol{\phi}\|_Y < \sigma\}, \tag{1}$$

where Y is defined by $W^{1,\infty}(\mathbb{R}^2; \mathbb{R}^2)$, and $\sigma > 0$ is chosen such that $(\boldsymbol{i} + \boldsymbol{\phi})$ is a bijection [4, Proposition 1.39].

The domain of $\boldsymbol{\phi}$ is extended to $\mathbb{R}^2$ by Calderón's extension theorem [6]. In the present paper, Y is used as the Banach space for the perturbation $\boldsymbol{\varphi}$ of $\boldsymbol{\phi}$ in order to define the Fréchet derivatives as shown later.

3. Main problem

For simplicity, we use the Poisson problem as the main problem. The solution to the main problem is called the state variable in the shape optimization problem. We denote the outer unit normal by $\boldsymbol{\nu}$, and $\partial_\nu = \boldsymbol{\nu} \cdot \boldsymbol{\nabla}$.

Problem 1 (Main problem) *Let $b : \mathbb{R}^2 \to \mathbb{R}$ be a function not depending on $\boldsymbol{\phi}$ that is sufficiently smooth. For a given $\boldsymbol{\phi} \in \mathcal{D}$, find $u(\boldsymbol{\phi}) : \Omega(\boldsymbol{\phi}) \to \mathbb{R}$ such that*

$$-\Delta u(\boldsymbol{\phi}) = b \quad \text{in } \Omega(\boldsymbol{\phi}),$$
$$\partial_\nu u(\boldsymbol{\phi}) = 0 \quad \text{on } \Gamma_{\mathrm{N}}(\boldsymbol{\phi}),$$
$$u(\boldsymbol{\phi}) = 0 \quad \text{on } \Gamma_{\mathrm{D}}(\boldsymbol{\phi}).$$

If b is given appropriately, the weak solution $u(\boldsymbol{\phi})$ to Problem 1 lies within $U = H^1(\Omega(\boldsymbol{\phi}); \mathbb{R})$. The domain of $u(\boldsymbol{\phi})$ can be extended to $\mathbb{R}^2$ by Calderón's extension theorem. Moreover, in the present paper, we define the admissible set of the state variable $u(\boldsymbol{\phi})$ by

$$\mathcal{S} = W^{1,2q}\left(\mathbb{R}^2; \mathbb{R}\right) \tag{2}$$

for some $q > 2$. In [1], $u(\boldsymbol{\phi}) \in \mathcal{S}$ is used as a necessary condition in order to obtain the domain variation in Y without singular points by the H^1 gradient method. In the present paper, we clarify the conditions for singular points in order that $u(\boldsymbol{\phi})$ is included in $\mathcal{S}$.

4. Shape optimization problem

Using the design variable $\boldsymbol{\phi} \in \mathcal{D}$ and the state variable $u = u(\boldsymbol{\phi}) \in \mathcal{S}$, we define cost functions as

$$f_i(\boldsymbol{\phi}, u) = \int_{\Omega(\boldsymbol{\phi})} \zeta_i(\boldsymbol{\phi}, u, \boldsymbol{\nabla} u)\, \mathrm{d}x + c_i \tag{3}$$

for $i \in \{0, 1, \dots, m\}$, where ζ_i and their derivatives are sufficiently smooth, and $c_0, \dots, c_m$ are given constants. Among the $m+1$ cost functions, f_0 is called an objective function, and $f_1, \dots, f_m$ are called constraint functions.

Using the cost functions $f_0, \dots, f_m$, we define the shape optimization problem as follows.

Problem 2 (Shape optimization) *Let $\mathcal{D}$ and $\mathcal{S}$ be given by* (1) *and* (2)*, respectively, and $f_0, \dots, f_m$ be as defined in* (3)*. Find $\Omega(\boldsymbol{\phi})$ with $\boldsymbol{\phi}$ such that*

$$\boldsymbol{\phi} = \arg\min_{\boldsymbol{\phi} \in \mathcal{D}} \{ f_0(\boldsymbol{\phi}, u) \mid f_i(\boldsymbol{\phi}, u) \le 0 \quad \text{for } i \in \{1, \dots, m\},\ u \in \mathcal{S},\ \text{Problem 1} \}.$$

5. Shape derivative of cost functions

For $i \in \{1, \dots, m\}$, the Fréchet derivatives (we follow [4, Definition 1.8]) with respect to arbitrary domain variation $\boldsymbol{\varphi} \in Y$ of f_i are obtained in [1] as

$$\begin{aligned}\langle \boldsymbol{g}_i, \boldsymbol{\varphi} \rangle = \int_{\Omega(\boldsymbol{\phi})} \big[& \boldsymbol{\nabla} u \cdot (\boldsymbol{\nabla} \boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{\nabla} v_i) + \boldsymbol{\nabla} v_i \cdot (\boldsymbol{\nabla} \boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{\nabla} u) \\ & + (\zeta_{i\boldsymbol{\phi}}(\boldsymbol{\phi}, u, \boldsymbol{\nabla} u) + v_i \boldsymbol{\nabla} b) \cdot \boldsymbol{\varphi} \\ & + (\zeta_i - \boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v_i + b v_i)\, \boldsymbol{\nabla} \cdot \boldsymbol{\varphi} \big] \mathrm{d}x. \end{aligned} \tag{4}$$

Here, $v_i \in U$ is called the adjoint variable for f_i, and is given as the weak solution of the following problem.

Problem 3 (Adjoint problem for f_i) *For a given $\boldsymbol{\phi} \in \mathcal{D}$, let u be the solution to Problem 1 and ζ_i be the function in* (3)*. Find $v_i : \Omega(\boldsymbol{\phi}) \to \mathbb{R}$ such that*

$$-\Delta v_i(\boldsymbol{\phi}) = \zeta_{iu}(\boldsymbol{\phi}, u, \boldsymbol{\nabla} u) + \boldsymbol{\nabla} \cdot \zeta_{i\boldsymbol{\nabla} u}(\boldsymbol{\phi}, u, \boldsymbol{\nabla} u) \quad \text{in } \Omega(\boldsymbol{\phi}),$$
$$\partial_\nu v_i(\boldsymbol{\phi}) = 0 \quad \text{on } \Gamma_{\mathrm{N}}(\boldsymbol{\phi}),$$
$$v_i(\boldsymbol{\phi}) = 0 \quad \text{on } \Gamma_{\mathrm{D}}(\boldsymbol{\phi}).$$

In [1], it is shown that if u and v_i are in $\mathcal{S}$, $\boldsymbol{g}_i$ belongs to $L^q\left(\Omega(\boldsymbol{\phi}); \mathbb{R}^2\right)$, and the domain variation obtained by the H^1 gradient method belongs to Y without singular points.

In the present paper, we pay attention to the range of the opening angles for singular points in order that u and v_i are included in $\mathcal{S}$, and obtain the analytic solutions of the shape derivative at the crack tip and the boundary point of the mixed boundary conditions on smooth boundary.

6. Regularity of u and v_i at corner

For the regularities of u and v_i, the following results have been known [7–9].

We suppose that $\partial\Omega(\boldsymbol{\phi}) \setminus \{\boldsymbol{x}_j(\boldsymbol{\phi})\}_{j \in \Theta}$ is sufficiently smooth in the following argument. If we let $B(\boldsymbol{x}_j(\boldsymbol{\phi}), \epsilon)$ be the disc of radius ϵ centered at $\boldsymbol{x}_j(\boldsymbol{\phi})$, then u has the expression for a point $\boldsymbol{x} - \boldsymbol{x}_j(\boldsymbol{\phi}) = r\mathrm{e}^{\mathrm{i}\theta} \in B(\boldsymbol{x}_j(\boldsymbol{\phi}), \epsilon) \cap \Omega(\boldsymbol{\phi})$ of

$$u\left(r\mathrm{e}^{\mathrm{i}\theta}\right) = k_j(\boldsymbol{\phi})\, r^{\frac{\pi}{\alpha_j(\boldsymbol{\phi})}} \cos \frac{\pi}{\alpha_j(\boldsymbol{\phi})}\theta + u_{\mathrm{R}} \quad \text{for } j \in \Theta_{\mathrm{N}}, \tag{5}$$

$$u\left(r\mathrm{e}^{\mathrm{i}\theta}\right) = k_j(\boldsymbol{\phi})\, r^{\frac{\pi}{\alpha_j(\boldsymbol{\phi})}} \sin \frac{\pi}{\alpha_j(\boldsymbol{\phi})}\theta + u_{\mathrm{R}} \quad \text{for } j \in \Theta_{\mathrm{D}}, \tag{6}$$

$$u\left(r\mathrm{e}^{\mathrm{i}\theta}\right) = k_j(\boldsymbol{\phi})\, r^{\frac{\pi}{2\alpha_j(\boldsymbol{\phi})}} \sin \frac{\pi}{2\alpha_j(\boldsymbol{\phi})}\theta + u_{\mathrm{R}} \quad \text{for } j \in \Theta_{\mathrm{M}}, \tag{7}$$

where $k_j(\boldsymbol{\phi})$ are constants, and u_{R} stands for the term in $H^2(B(\boldsymbol{x}_j(\boldsymbol{\phi}), \epsilon) \cap \Omega(\boldsymbol{\phi}); \mathbb{R})$.

A derivative of $u = r^\omega \psi(\theta)$ behaves as a finite sum of functions $r^{\omega-1}\tilde{\psi}(\theta)$, where $\psi(\theta)$ and $\tilde{\psi} \in C^\infty([0, \alpha_j]; \mathbb{R})$. The p-th power of $r^{\omega-1}\tilde{\psi}(\theta)$ is integrable in $B(\boldsymbol{x}_j(\boldsymbol{\phi}), \epsilon) \cap \Omega(\boldsymbol{\phi})$ iff $p(\omega - 1) + 1 > -1$. This means

$$u \in W^{1,p}(B(\boldsymbol{x}_j(\boldsymbol{\phi}), \epsilon) \cap \Omega(\boldsymbol{\phi}); \mathbb{R}) \quad \text{for } \omega > 1 - \frac{2}{p}. \tag{8}$$

We now obtain the following.

Theorem 4 (Regularity of u and v_i at corner) *For $j \in \Theta_{\mathrm{N}} \cup \Theta_{\mathrm{D}}$, the weak solutions u and v_i to Problem 1 and Problem 3, respectively, come into lie within $\mathcal{S}$ if $\alpha_j(\boldsymbol{\phi}) \in (0, 2\pi)$. For $j \in \Theta_{\mathrm{M}}$, the weak solutions u and v_i come into lie within $\mathcal{S}$ if $\alpha_j(\boldsymbol{\phi}) \in (0, \pi)$.*

The case $\alpha_j(\boldsymbol{\phi}) = 2\pi$ in $j \in \Theta_{\mathrm{N}} \cup \Theta_{\mathrm{D}}$ corresponds to the crack. The case $\alpha_j(\boldsymbol{\phi}) = \pi$ in $j \in \Theta_{\mathrm{M}}$ corresponds to the boundary point of the mixed boundary conditions on smooth boundary, which we call the smooth mixed boundary. In the next section, we shall show how to evaluate the shape derivative $\boldsymbol{g}_i$ in these cases.

7. Evaluation of $\boldsymbol{g}_i$ by generalized J-integral

To evaluate the shape derivative $\boldsymbol{g}_i$ in the cases that $\alpha_j(\boldsymbol{\phi}) = 2\pi$ in $j \in \Theta_{\mathrm{N}} \cup \Theta_{\mathrm{D}}$ and $\alpha_j(\boldsymbol{\phi}) = \pi$ in $j \in \Theta_{\mathrm{M}}$, we use the generalized J integral. The generalized J integral is defined in terms of the solution to an elliptic boundary value problem and domain variation. Here, using the solution $u = u(\boldsymbol{\phi}) \in U$ to Problem 1 and domain variation $\boldsymbol{\varphi} \in Y$, and following [3–5], we define the generalized J integral as

$$\mathscr{J}(\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u) = \mathscr{P}(\partial\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u) + \mathscr{R}(\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u), \tag{9}$$

where

$$\mathscr{P}(\partial\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u) = \int_{\partial\Omega(\boldsymbol{\phi})} \left[\frac{1}{2}(\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} u)\boldsymbol{\nu} \cdot \boldsymbol{\varphi} - \partial_\nu u \boldsymbol{\nabla} u \cdot \boldsymbol{\varphi}\right] \mathrm{d}\gamma \tag{10}$$

$$\mathscr{R}(\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u) = -\int_{\Omega(\boldsymbol{\phi})} \left[b\boldsymbol{\nabla} u \cdot \boldsymbol{\varphi} - \boldsymbol{\nabla} u \cdot \left(\boldsymbol{\nabla}\boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{\nabla} u\right) + \frac{1}{2}(\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} u)\boldsymbol{\nabla} \cdot \boldsymbol{\varphi}\right] \mathrm{d}x. \tag{11}$$

For $\mathscr{J}$, the following properties have been obtained [3].

Theorem 5 (Properties of gen. J-integral) *For $\boldsymbol{\phi} \in \mathcal{D}$, let $\mathscr{J}(\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)$ be defined in (9) with the weak solution $u \in U$ to Problem 1 and domain variation $\boldsymbol{\varphi} \in Y$. For all $\boldsymbol{\varphi} \in Y$, the following hold.*

(1) $\mathscr{R}(\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)$ has finite value for $u \in U$.

(2) For a Lipschitz domain $\Sigma \subset \mathbb{R}^2$, if $u|_{\Sigma\cap\Omega(\boldsymbol{\phi})}$ is of class H^2, then

$$\mathscr{J}(\Sigma \cap \Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u) = 0 \tag{12}$$

holds.

(3) Let $\Sigma \subset \mathbb{R}^2$ be separated into Σ_1 and Σ_2 such that $\Sigma_1 \cap \Sigma_2 = \emptyset$ and $\bar{\Sigma} = \bar{\Sigma}_1 \cup \bar{\Sigma}_2$. If u is of class H^2 on neighborhood of $\partial\Sigma_1$ and $\partial\Sigma_2$, then

$$\mathscr{J}(\Sigma \cap \Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u) = \mathscr{J}(\Sigma_1 \cap \Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u) + \mathscr{J}(\Sigma_2 \cap \Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u) \tag{13}$$

holds.

Let us rewrite $\boldsymbol{g}_i$ using the properties in Theorem 5. The partial Fréchet derivatives of $\mathscr{P}$ and $\mathscr{R}$ with respect to arbitrary variation $v_i \in U$ of u can be written as

$$-\mathscr{P}_u(\partial\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)[v_i] = \int_{\partial\Omega(\boldsymbol{\phi})} \left[(\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v_i)\boldsymbol{\nu} \cdot \boldsymbol{\varphi} - \partial_\nu u \boldsymbol{\nabla} v_i \cdot \boldsymbol{\varphi} - \partial_\nu v_i \boldsymbol{\nabla} u \cdot \boldsymbol{\varphi}\right] \mathrm{d}\gamma \tag{14}$$

$$\mathscr{R}_u(\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)[v_i] = -\int_{\Omega(\boldsymbol{\phi})} \left[b\boldsymbol{\nabla} v_i \cdot \boldsymbol{\varphi} - \boldsymbol{\nabla} u \cdot \left(\boldsymbol{\nabla}\boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{\nabla} v_i\right) - \boldsymbol{\nabla} v_i \cdot \left(\boldsymbol{\nabla}\boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{\nabla} u\right) + (\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v_i)\boldsymbol{\nabla} \cdot \boldsymbol{\varphi}\right] \mathrm{d}x. \tag{15}$$

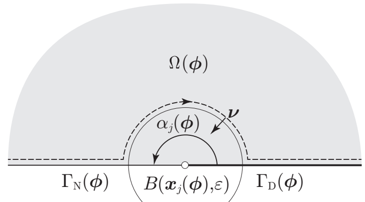

Fig. 2. Path for the boundary integral of $\mathscr{P}_u$.

Here, by comparing (4) and (15), we have

$$\langle \boldsymbol{g}_i, \boldsymbol{\varphi} \rangle = \mathscr{R}_u(\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)[v_i] + \langle \boldsymbol{g}_{i\mathrm{R}}, \boldsymbol{\varphi} \rangle, \tag{16}$$

where

$$\langle \boldsymbol{g}_{i\mathrm{R}}, \boldsymbol{\varphi} \rangle = \int_{\partial\Omega(\boldsymbol{\phi})} b v_i \boldsymbol{\nu} \cdot \boldsymbol{\varphi} \, \mathrm{d}\gamma + \int_{\Omega(\boldsymbol{\phi})} \left(\zeta_{i\boldsymbol{\phi}}(\boldsymbol{\phi}, u, \boldsymbol{\nabla} u) \cdot \boldsymbol{\varphi} + \zeta_i \boldsymbol{\nabla} \cdot \boldsymbol{\varphi}\right) \mathrm{d}x. \tag{17}$$

Moreover, denoting the ϵ-neighborhood of the singular points by $B_\Theta = \bigcup_{j\in\Theta} B(\boldsymbol{x}_i(\boldsymbol{\phi}), \epsilon)$, separating $\Omega(\boldsymbol{\phi})$ into $\Omega(\boldsymbol{\phi}) \setminus B_\Theta$ and $\Omega(\boldsymbol{\phi}) \cap B_\Theta$, and applying the properties of (ii) and (iii) in Theorem 5, we have

$$\mathscr{R}_u(\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)[v_i] = -\mathscr{P}_u(\partial(\Omega(\boldsymbol{\phi}) \setminus B_\Theta), \boldsymbol{\varphi}, u)[v_i] + \sum_{j\in\Theta} \mathscr{R}_u(B(\boldsymbol{x}_i(\boldsymbol{\phi}), \epsilon) \cap \Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)[v_i]. \tag{18}$$

The dotted line in Fig. 2 shows the path for the boundary integral of $\mathscr{P}_u$ around the boundary point of the mixed boundary conditions on the smooth boundary ($\alpha_j(\boldsymbol{\phi}) = \pi$). Here, when $\epsilon \to 0$, the second term on the right-hand side of (18) converges to 0. The first term on the right-hand side of (18) can be written as

$$-\mathscr{P}_u(\partial\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)[v_i] + \sum_{j\in\Theta} \langle \hat{\boldsymbol{g}}_{ij}, \boldsymbol{\varphi} \rangle, \tag{19}$$

where

$$\langle \hat{\boldsymbol{g}}_{ij}, \boldsymbol{\varphi} \rangle = \lim_{\epsilon\to 0} -\int_0^\alpha \left\{(\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v_i)\boldsymbol{\nu} \cdot \boldsymbol{\varphi} - \partial_\nu u \boldsymbol{\nabla} v_i \cdot \boldsymbol{\varphi} - \partial_\nu v_i \boldsymbol{\nabla} u \cdot \boldsymbol{\varphi}\right\} \epsilon \, \mathrm{d}\theta. \tag{20}$$

Hence, if the right-hand side of (20) converges, we have

$$\langle \boldsymbol{g}_i, \boldsymbol{\varphi} \rangle = -\mathscr{P}_u(\partial\Omega(\boldsymbol{\phi}), \boldsymbol{\varphi}, u)[v_i] + \sum_{j\in\Theta} \langle \hat{\boldsymbol{g}}_{ij}, \boldsymbol{\varphi} \rangle + \langle \boldsymbol{g}_{i\mathrm{R}}, \boldsymbol{\varphi} \rangle. \tag{21}$$

8. $\boldsymbol{g}_i$ at crack tip and smooth mixed boundary

Based on the result in (21), we show the analytic solutions of $\hat{\boldsymbol{g}}_{ij}$ in two cases as follows.

One case is that of a crack tip on $\Gamma_{\mathrm{N}}(\boldsymbol{\phi}) \cup \Gamma_{\mathrm{D}}(\boldsymbol{\phi})$, i.e.,

$\boldsymbol{x}_j$ of $\alpha_j(\boldsymbol{\phi}) = 2\pi$ for $j \in \Theta_{\mathrm{N}} \cup \Theta_{\mathrm{D}}$. In a neighborhood of the point, we have the solution u to Problem 1 by (5) and the solution v_i to Problem 3 by

$$v_i\left(r\mathrm{e}^{\mathrm{i}\theta}\right) = l_{ij}(\boldsymbol{\phi})\, r^{\frac{\pi}{\alpha_j(\boldsymbol{\phi})}} \cos\frac{\pi}{\alpha_j(\boldsymbol{\phi})}\theta + v_{i\mathrm{R}}, \tag{22}$$

were $l_{ij}(\boldsymbol{\phi})$ is a constant, and $v_{i\mathrm{R}}$ is the term in $H^2(B(\boldsymbol{x}_j(\boldsymbol{\phi}),\epsilon) \cap \Omega(\boldsymbol{\phi}))$. In the following, we neglect the regular terms of u_{R} and $v_{i\mathrm{R}}$ by taking a sufficiently small ϵ. Here, putting $r = \epsilon$, $\alpha_j(\boldsymbol{\phi}) = 2\pi$, and calculating the derivatives of (5) and (22), we have

$$\boldsymbol{\nabla} u = \begin{pmatrix} \cos\theta \frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta} \\ \sin\theta\frac{\partial}{\partial r} + \frac{\cos\theta}{r}\frac{\partial}{\partial\theta} \end{pmatrix} u = \frac{k_j}{2\epsilon^{\frac{1}{2}}} \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) \end{pmatrix}, \tag{23}$$

$$\boldsymbol{\nabla} v_i = \frac{l_{ij}}{2\epsilon^{\frac{1}{2}}} \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) \end{pmatrix}. \tag{24}$$

From these results, we have

$$\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v_i = \frac{k_j l_{ij}}{4\epsilon}. \tag{25}$$

Then, for all $\boldsymbol{\varphi} = (\varphi_1, \varphi_2)^{\mathrm{T}} \in \mathbb{R}^2$,

$$\begin{aligned} &-\int_0^{2\pi} (\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} v_i)\, \boldsymbol{\nu} \cdot \boldsymbol{\varphi}\, \epsilon\, \mathrm{d}\theta \\ &\quad = \int_0^{2\pi} \frac{k_j l_{ij}}{4} (\varphi_1 \cos\theta + \varphi_2 \sin\theta)\, \mathrm{d}\theta = 0 \end{aligned} \tag{26}$$

holds. Moreover, we have

$$\begin{aligned} \partial_\nu u = \boldsymbol{\nu} \cdot \boldsymbol{\nabla} u &= \frac{k_j}{2\epsilon^{\frac{1}{2}}} \begin{pmatrix} -\cos\theta \\ -\sin\theta \end{pmatrix} \cdot \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) \end{pmatrix} \\ &= -\frac{k_j}{2\epsilon^{\frac{1}{2}}} \cos\left(\frac{\theta}{2}\right), \end{aligned} \tag{27}$$

$$\partial_\nu u \boldsymbol{\nabla} v_i = -\frac{k_j l_{ij}}{4\epsilon} \cos\left(\frac{\theta}{2}\right) \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) \end{pmatrix}. \tag{28}$$

Then, for all $\boldsymbol{\varphi} = (\varphi_1, \varphi_2)^{\mathrm{T}} \in \mathbb{R}^2$,

$$\begin{aligned} &\int_0^{2\pi} \partial_\nu u \boldsymbol{\nabla} v_i \cdot \boldsymbol{\varphi}\, \epsilon\, \mathrm{d}\theta \\ &\quad = \int_0^{2\pi} \partial_\nu v_i \boldsymbol{\nabla} u \cdot \boldsymbol{\varphi}\, \epsilon\, \mathrm{d}\theta = -\frac{k_j l_{ij}}{4} \begin{pmatrix} \pi \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \end{aligned} \tag{29}$$

holds. From these results, the analytic solution at the crack tip can be obtained by

$$\langle \hat{\boldsymbol{g}}_{ij}, \boldsymbol{\varphi} \rangle = -\frac{k_j l_{ij}}{2} \begin{pmatrix} \pi \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \tag{30}$$

We can confirm that $\hat{\boldsymbol{g}}_{ij}$ points to the crack plane.

The other one is the case of the boundary point of the mixed boundary conditions on smooth boundary, i.e., $\boldsymbol{x}_j$ of $\alpha_j(\boldsymbol{\phi}) = \pi$ for $j \in \Theta_{\mathrm{M}}$. In a neighborhood of the point, using (7) for $u\left(r\mathrm{e}^{\mathrm{i}\theta}\right)$, and (22) for $v_i\left(r\mathrm{e}^{\mathrm{i}\theta}\right)$ in which cos and $\alpha_j(\boldsymbol{\phi})$ are replaced by sin and $2\alpha_j(\boldsymbol{\phi})$, we use

$$\int_0^{\pi} \frac{k_j l_{ij}}{4} (\varphi_1 \cos\theta + \varphi_2 \sin\theta)\, \mathrm{d}\theta = \frac{k_j l_{ij}}{2} \varphi_2$$

instead of (26). Moreover, we have

$$\begin{aligned} \int_0^{\pi} \partial_\nu u \boldsymbol{\nabla} v_i \cdot \boldsymbol{\varphi}\, \epsilon\, \mathrm{d}\theta &= \int_0^{\pi} \partial_\nu v_i \boldsymbol{\nabla} u \cdot \boldsymbol{\varphi}\, \epsilon\, \mathrm{d}\theta \\ &= \frac{k_j l_{ij}}{8} \begin{pmatrix} \pi \\ -2 \end{pmatrix} \cdot \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \end{aligned}$$

instead of (29). Then, the analytic solution at the boundary point can be obtained as

$$\langle \hat{\boldsymbol{g}}_{ij}, \boldsymbol{\varphi} \rangle = \frac{k_j l_{ij}}{4} \begin{pmatrix} \pi \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \tag{31}$$

From the equations above, we have the following.

Theorem 6 ($\boldsymbol{g}_i$ at crack tip and s. mixed bound.) *If $\alpha_j(\boldsymbol{\phi}) = 2\pi$ at $\boldsymbol{x}_j(\boldsymbol{\phi})$ for $j \in \Theta_{\mathrm{N}} \cup \Theta_{\mathrm{D}}$, $\boldsymbol{g}_i$ defined by* (4) *is given by* (21)*, where $\hat{\boldsymbol{g}}_{ij}$ is given by* (30)*. If $\alpha_j(\boldsymbol{\phi}) = \pi$ at $\boldsymbol{x}_j(\boldsymbol{\phi})$ for $j \in \Theta_{\mathrm{M}}$, $\boldsymbol{g}_i$ defined by* (4) *is given by* (21)*, where $\hat{\boldsymbol{g}}_{ij}$ is given by* (31)*.*

From the calculation above, it becomes clear that the shape derivative is not evaluated in the case of an opening angle greater than π for the boundary point of the mixed boundary conditions, because $\hat{\boldsymbol{g}}_{ij} \to \infty$ as $\epsilon \to 0$.

9. Conclusions

In the present paper, we showed the following.

(1) If the assumption in Theorem 4 is satisfied, then the solutions to the main problem and the adjoint problem are included in the admissible set of state variable $\mathcal{S}$ in (2).

(2) The shape derivatives at the crack tip and the boundary point of the mixed boundary conditions on a smooth boundary are obtained as stated in Theorem 6.

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