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Material derivative of potential energies and its application for design sensitivity by BIE

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Introduction.

There are many studies about the differentiation of the potential energies with respect to variable domains (see e.g. Haug, Choi and Komkov[2], Petryk and Mróz[5]), mostly in field of shape design. In this paper we calculate rigorously the derivative of potential energies with respect to variable domains and variable interfaces for the mixed boundary value problems. Next, the obtained result is applied for the shape design problem under the condition; volumes of materials are constant. In the last, an algorithm that find optimal shape is proposed by the use of the boundary integral equation (BIE).

In Pironneau[6], it is explained that the boundary element method has an advantage over other methods.

1. Material derivative of potential energies.

Let Ω be a domain in $\mathbb{R}^n$ with smooth boundary Γ. Let $\Phi_\tau, 0 \le \tau \le T$ be a family of C^∞-diffeomorphisms from $\mathbb{R}^n$ onto $\mathbb{R}^n$. We assume that the map $(x, \tau) \mapsto \Phi_\tau(x) : \mathbb{R}^n \times [0,1] \to \mathbb{R}^n$ is of class C^2.

A typical example of the above situation is the perturbation of domains. Let $U_\delta(\Gamma)$ be an open neighborhood of the surface Γ in $\mathbb{R}^n$, consisting of points whose distance from Γ is less than δ (see Fig. 1).

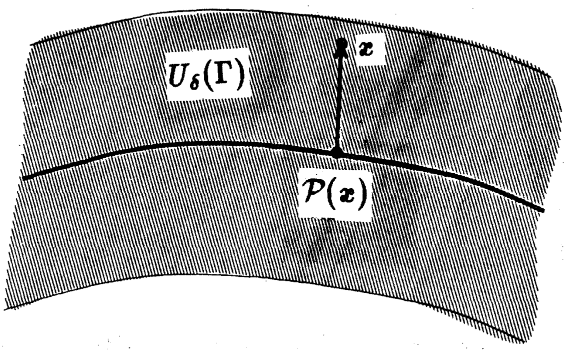

Fig. 1. Neighborhood $U_\delta(\Gamma)$ and $\mathcal{P}(x)$

We can take for δ so that, for each point $x \in U_\delta(\Gamma)$, there will exist a unique point $\mathcal{P}(x) \in \Gamma$ such that $|x - \mathcal{P}(x)| = \min_{y \in \Gamma} |x - y|$. Let h be a function defined on Γ. We consider the surface $\Gamma_{\tau,h}$ defined by

$$\Gamma_{\tau,h} = \{x + \tau h(x)\vec{n}(x) | x \in \Gamma\}$$

and let $\Omega_{\tau,h}$ the domain enclosed by $\Gamma_{\tau,h}$. Let β be a function in $C_0^\infty(U_\delta(\Gamma))$ such that $\beta \geq 0, \beta = 1$ near Γ. Setting

$$\Phi_{\tau,h} = \begin{cases} x + \tau\beta(x)h(\mathcal{P}(x))\vec{n}(\mathcal{P}(x)) & \text{for } x \in U_\delta(\Gamma), \\ x & \text{for } x \in \mathbf{R}^n \backslash U_\delta(\Gamma), \end{cases} \tag{1.1}$$

we get the C^∞-diffeomorphisms from $\mathbf{R}^n$ onto $\mathbf{R}^n$, satisfying that $\Phi_{\tau,h}(\Omega) = \Omega_{\tau,h}$. In this case,

$$\vec{X}(x) = \frac{d}{d\tau}\Phi_{\tau,h}(x) = \beta(x)h(\mathcal{P}(x))\vec{n}(\mathcal{P}(x)). \tag{1.2}$$

Let $f(x, \tau)$ be a function defined on $\Omega_\tau = \Phi_\tau(\Omega)$, for each $\tau > 0$. Let $\Psi_\tau = \Phi_\tau^{-1}$, then $f(\Psi_\tau(x), \tau)$ is the function defined on Ω. The *pointwise material derivative* of f is defined by

$$\dot{f}(x) = \lim_{\tau \to 0} \frac{1}{\tau}[f(\Phi_\tau(x), \tau) - f(x, 0)]. \tag{1.3}$$

In engineering, the material derivative of potential energies are calculated by the use of Reynolds formulas

$$\begin{aligned} \frac{d}{d\tau}\int_{\Omega_\tau} f(x,\tau)dx &= \int_\Omega \dot{f}(x) + f(x)\mathrm{div}\vec{X}(x) \\ &= \int_\Omega \frac{\partial f}{\partial \tau}(x) + \mathrm{div}(f\vec{X})(x)dx, \end{aligned} \tag{1.4}$$

$$\frac{d}{d\tau}\int_{\Gamma_\tau} g(x,\tau)dx = \int_\Gamma [\dot{g}(x) + Hg(x)(\vec{X}, \vec{n})]d\gamma, \tag{1.5}$$

where $\vec{X}(x) = \frac{d}{d\tau}\Phi_\tau(x)\big|_{\tau=0}$, H the mean curvature of Γ, $\vec{n}$ the outward unit normal on Γ.

Such calculations appear in shape design sensitivity analysis (see e.g. [2]), assuming the pointwise material derivative to be able.

For the elliptic boundary value problems, we check material derivability in terms of functional analysis. As a matter of convenience, we try to check them the following simple boundary value problems defined on $\Omega_\tau = \Phi_\tau(\Omega)$,

$$
\begin{cases} -\Delta u_\tau = f_{\Omega_\tau} & \text{in } \Omega_\tau, \\ u_\tau = 0 & \text{on } \Gamma_{D,\tau}, \\ T(u_\tau) = 0 & \text{on } \Gamma_{N,\tau}, \end{cases} \tag{1.6}
$$

where f_{Ω_τ} is the restriction of $f \in L^2(\mathbb{R}^n)$ on Ω_τ, $\Gamma_{D,\tau} = \Phi_\tau(\Gamma_D)$ and $T(u_\tau)$ the normal derivative $\partial u_\tau/\partial n$.
In *generalized* sense, u_τ is said to satisfy (1.6), if u_τ minimize the potential energy functional

$$
\mathcal{E}(v; f, \Omega_\tau, \Gamma_{D,\tau}) = \int_{\Omega_\tau} \frac{1}{2}|\nabla v|^2 - fv\, dx
$$

over the functional space

$$
V(\Omega_\tau, \Gamma_{D,\tau}) = \{v \in H^1(\Omega_\tau) | v = 0 \text{ on } \Gamma_{D,\tau}\},
$$

where $H^1(\Omega_\tau)$ stands for Sobolev space of order 1 defined on Ω_τ. The potential energy is defined by

$$
\mathcal{E}(f, \Omega_\tau, \Gamma_{D,\tau}) = \int_{\Omega_\tau} \frac{1}{2}|\nabla u_\tau|^2 - fu_\tau\, dx. \tag{1.7}
$$

By the change of variables $\Phi_\tau^* v(x) = v(\Phi_\tau(x))$ for $v \in H^1(\Omega_\tau)$, we have for $v, w \in H^1(\Omega_\tau)$,

$$
\int_{\Omega_\tau} \nabla(\Phi_\tau^* v) \cdot \nabla(\Phi_\tau^* w) dx = \int_\Omega \big((\nabla\Phi_\tau)\Phi_\tau^*(\nabla v)\big) \cdot \big((\nabla\Phi_\tau)\Phi_\tau^*(\nabla w)\big) J_\tau dx,
$$

where J_τ is the Jacobian $\det\nabla\Phi_\tau$.

Then we obtain the following lemma.

Lemma 1.1(Ohtsuka[4]). *There exists a constant C independent of τ such that*

$$
\|\Phi_\tau^* u_\tau - u\|_{1,\Omega} \le C\tau, \tag{1.8}
$$

where $\|\cdot\|_{1,\Omega}$ is the norm of $H^1(\Omega)$ and $u = u_0$.

Remark: In Nečas[3], there are analogue of estimations in Lemma 1.1. The differentiation with respect to domains is discussed in Simon[7].

Using Lemma 1.1, we arrive at the result

$$(1.9)\qquad \frac{d}{d\tau}\mathcal{E}(f,\Omega_\tau,\Gamma_{D,\tau})|_{\tau=0} = -R_\Omega(u;\vec{X}) + \int_\Omega [(\vec{X}\cdot\nabla)(fu) + fu\mathrm{div}\vec{X}]dx$$

if $f \in H^1(\mathbb{R}^n)$.

The right-hand side of (1.9) is expressed as the surface integral defined on Γ, if $u \in H^2(\Omega)$.

GENERALIZED J-INTEGRAL. *Let ω be a domain in $\mathbb{R}^n$ and let $\mathcal{X}(\omega)$ be a set of all suitably smooth vector fields defined on $\overline{\omega}$. We call a domain ω "regular relative to Ω" if ω is a bounded domain in $\mathbb{R}^n$ and the divergence theorem holds on $\omega' = \omega\cap\Omega$, for all suitably smooth functions and all elements in $\mathcal{X}(\omega)$. Let us define GJ-integral $J_\omega(u;\vec{X})$ as a functional of all domains ω in $\mathbb{R}^n$ regular relative to Ω, all solutions u of (1.6) ($\tau = 0$) and $\vec{X}\in\mathcal{X}(\omega)$.*

$$P_\omega(u;\vec{X}) = -\int_{\partial\omega'} [W(u)(\vec{X}\cdot\vec{n}) - T(u)(\vec{X}\cdot\nabla u)]d\gamma,$$

$$R_\omega(u;\vec{X}) = \int_\omega \{\vec{X}\cdot\nabla_x W(x,u,\nabla u) - A_i(x,u,\nabla u)(D_iX_l)(D_lu) + W(u)div\vec{X} + f\cdot(\vec{X}\cdot\nabla u)\}dx$$

are finite, then Generalized J-integral $J_\omega(u;\vec{X})$ is defined by

$$J_\omega(u;\vec{X}) = P_\omega(u;\vec{X}) + R_\omega(u;\vec{X}),$$

where $\vec{n}$ is the outward unit normal to $\partial\omega'$ and $d\gamma$ the surface element of $\partial\omega'$.

For the problem (1.6), $W(x,u,\nabla u) = \frac{1}{2}|\nabla u|^2$, $\vec{X}\cdot\nabla_x W(x,u,\nabla u) = 0$ and $A_i(x,u,\nabla u) = \partial u/\partial x_i$.

Using the property;

$$u\in H^2(\omega\cap\Omega) \Rightarrow J_\omega(u;\vec{X}) = 0$$

we get for (1.6)
(1.10)

$$\begin{aligned}\frac{d}{d\tau}\mathcal{E}(f,\Omega_\tau,\Gamma_{D,\tau})|_{\tau=0} &= -\int_{\Gamma\backslash U(\Gamma_{DN})}\left[W(u) - fu - \left(\frac{\partial u}{\partial n}\right)^2\right](\vec{X}\cdot\vec{n})d\gamma \\ &+ R_{U(\Gamma_{DN})} \\ &+ \int_{\partial U(\Gamma_{DN})\cap\Omega}\left[W(u) - fu - \left(\frac{\partial u}{\partial n}\right)^2\right](\vec{X}\cdot\vec{n})d\gamma.\end{aligned}$$

where $\Gamma_{DN} = \overline{\Gamma_D} \cap \overline{\Gamma_N}$ and $U(\Gamma_{DN})$ an open neighborhood of Γ_{DN}. If the *interface* Γ_{DN} *does not move*, i.e.

$$\Phi_\tau(x) = x \text{ for all } \tau \qquad \Leftrightarrow \qquad \vec{X} = 0 \text{ near } \Gamma_{DN},$$

then we have

$$\frac{d}{d\tau}\mathcal{E}(f, \Omega_\tau, \Gamma_{D,\tau})\big|_{\tau=0} = -\int_\Gamma \left[W(u) - fu - \left(\frac{\partial u}{\partial n}\right)^2 \right] (\vec{X}\cdot\vec{n})d\gamma. \tag{1.11}$$

In the case $n = 2$, Γ_{DN} consists of two points $\{\gamma_1, \gamma_2\}$. Let $D_\epsilon(\gamma_i)$ be the open disc of radius ϵ centered at γ_i, $i = 1, 2$. Then

$$\begin{aligned} \frac{d}{d\tau}&\mathcal{E}(f, \Omega_\tau, \Gamma_{D,\tau})\big|_{\tau=0} \\ &= -\lim_{\epsilon\to 0}\int_{\Gamma\setminus(D_\epsilon(\gamma_1)\cup D_\epsilon(\gamma_2))} \left[W(u) - fu - \left(\frac{\partial u}{\partial n}\right)^2 \right] (\vec{X}\cdot\vec{n})d\gamma \\ &\quad -\sum_{j=1}^{2} \frac{\pi}{8}\alpha_j(\vec{X}\cdot\vec{s}(\gamma_j)), \end{aligned} \tag{1.12}$$

where α_j is the coefficients of the singular term of u and $\vec{s}$ the tangential unit vector as in Fig. 2.

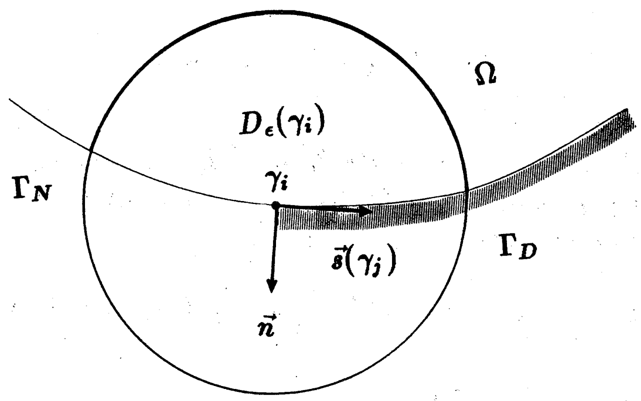

Fig. 2. The tangential vector $\vec{s}$ and $D_\epsilon(\gamma_i)$

2. Shape design problem.

In this section, we consider the problem:

PROBLEM 2.1. *For a given* $f \in H^1(\mathbb{R}^n)$, *find* $\Omega^{opt}, \Gamma_D^{opt}, u^{opt}$ *such that*

$$\min_{\Omega \subset \mathbb{R}^n} \mathcal{E}(f, \Omega, \Gamma_D) \text{ with Volume of } \Omega = \text{constant}.$$

In this situation, f represent the gravitational field, the electromagnetic field, the heat flow, etc. The problem 2.1 is not uniquely solvable. If, moreover, $\Gamma_{a,D} \subset \Gamma_{b,D}$, then we have from (1.12),

$$\mathcal{E}(f, \Omega, \Gamma_{a,D}) \leq \mathcal{E}(f, \Omega, \Gamma_{b,D}).$$

This indicates that the potential energy of Neumann problem is less than that of the mixed boundary value problem (1.6, $|\Gamma_D| \neq 0$). Here $|\Gamma_D|$ is the surface measure of Γ_D.

THEOREM 2.1. *If* Γ_{DN} *does not move and* Ω^{opt} *exists, then*

$$\int_\Gamma \left[W(u) - fu - \left(\frac{\partial u}{\partial n} \right)^2 \right] h d\gamma = 0 \tag{2.1}$$

for all function $h \in \delta\Gamma, h = 0$ *near* Γ_{DN},

$$\delta\Gamma = \left\{ h \in C^\infty(\Gamma) \middle| \int_\Gamma h d\gamma = 0 \right\}.$$

If, moreover, $W(u^{opt}) - fu^{opt} - (\partial u^{opt}/\partial n)^2$ *is continuous, then* $W(u^{opt}) - fu^{opt}$ *is constant on* Γ_N *and* $-\frac{1}{2}(\partial u^{opt}/\partial n)^2$ *is constant on* Γ_N. *Here we assumed connected component of* $\Gamma \backslash \Gamma_{DN}$ *are* Γ_D *and* Γ_N.

Proof. Let $\Omega = \Omega^{opt}, u = u^{opt}$. By (1.1), (1.2) and (1.11), we have

$$\begin{aligned} 0 &= \frac{d}{d\tau} \mathcal{E}(f, \Omega_{\tau,h}, \Gamma_{\tau,h}) \\ &= -\int_\Gamma \left[W(u) - fu - \left(\frac{\partial u}{\partial n} \right)^2 \right] h d\gamma \quad \forall h \in \delta\Gamma. \end{aligned}$$

We note that

$$\begin{cases} W(u) - fu - (\partial u/\partial n)^2 = W(u) - fu & \text{on } \Gamma_N, \\ W(u) = -\frac{1}{2} (\partial u/\partial n)^2, u = 0 & \text{on } \Gamma_D. \end{cases}$$

If $W(u) - fu$ is not constant on Γ_N, there exists a number $k > 0$, points $x_1, x_2 \in \Gamma_N$ and neighborhoods $U(x_1), U(x_2)$ of x_1, x_2 respectively such that

$$\min_{x \in \overline{U(x_1)} \cap \Gamma} W(u(x)) - f(x)u(x) - \max_{x \in \overline{U(x_2)} \cap \Gamma} W(u(x)) + f(x)u(x) = k.$$

We can construct the function $h \in \delta\Gamma$ such that

$$\mathrm{supp} h \subset (U(x_1) \cup U(x_2)) \cap \Gamma \text{ and } \int_{U(x_i) \cap \Gamma} h d\gamma = (-1)^{i-1} 1, i = 1, 2.$$

Then

$$\int_{\Gamma_N} W(u) - fu d\gamma \ \geq \ k > 0.$$

This contradict the formula (2.1). ∎

We assume that there exists a domain Ω which approximates the optimal shape and the surface $\Gamma_D = \emptyset$ for simplify.

By the mean value theorem and Theorem 2.1,

$$\mathcal{E}(f, \Omega_{\tau,h}, \Gamma_D) - \mathcal{E}(f, \Omega, \Gamma_D) = -\theta\tau F(h), \quad 0 < \theta < 1, \quad \tau > 0$$

where

$$F(h) = \int_{\Gamma_N} [W(u) - fu] h d\gamma, h \in \delta\Gamma.$$

If the potential energy $\mathcal{E}(f, \Omega_{\tau,h}, \Gamma_D)$ is strictly lower than $\mathcal{E}(f, \Omega, \Gamma_D)$, then $F(h) > 0$, and the converse is true.

Let $E(x)$ be the fundamental solution, that is,

$$\Delta E(x) = \delta(x), \text{ where } \delta \text{ is Dirac function.}$$

We set

$$u_f(x) = \int_{\mathbb{R}^n} E(x - y) f(y) dy,$$

then $v = u + u_f$ satisfy

$$\begin{cases} \Delta v = 0 & \text{in } \Omega, \\ T(v) = T(u_f) & \text{on } \Gamma_N, \end{cases}$$

Step 1. Solve the boundary integral equation (BIE)

$$\frac{q(x)}{2} + \int_\Gamma q(y) \frac{\partial}{\partial n_x} E(x-y) d\gamma(y) = T(u_f)(x) \text{ on } \Gamma$$

(Solvability is proved in e.g. Dautray-Lions[1].)
Then

$$u(x) = \int_\Gamma E(x-y) q(y) dy + u_f(x). \tag{2.2}$$

Step 2. By the use of (2.2), calculate

$$F(h) = \int_\Gamma [W(v+u_f) - f(v+u_f)] h d\gamma \quad \text{for } h \in \delta\Gamma_{ad}.$$

If $\max_{h \in \delta\Gamma_{ad}} F(h) \le 0$, then stop. Otherwise, find $h_{max} \in \delta\Gamma_{ad}$ such that $F(h_{max}) = \max_{h \in \delta\Gamma_{ad}} F(h)$. where $\delta\Gamma_{ad}$ is a finite dimensional subset of $\delta\Gamma$.

Step 3. Let the domain enclosed by the surface $\{x + h(x)\vec{n}(x) | x \in \Gamma\}$ be the new approximation of Ω^{opt}.

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