Differentiability of strongly singular BIE formulations with respect to boundary perturbations

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1 Introduction

In e.g. shape design analysis, inverse problems or fracture mechanics, one is often faced with the need of computing sensitivities of functional or physical variables with respect to perturbations of the shape of the geometrical domain Ω under study. This goal is often achieved using analytical material differentiation followed by discretization, in the form of either the adjoint variable approach or the direct differentiation. In a BEM context, the latter is based on material differentiation of the relevant governing BIE formulation, so that a governing BIE for the field sensitivities is available.

This has led some investigators to consider the material differentiation of strongly singular BIE formulations (e.g. Barone and Yang [1], Mellings and Aliabadi [2]). The actual validity of the material differentiation process when applied to Cauchy principal value (CPV) singular integrals have not been previously questioned, although other kinds of analytic manipulations on these have sometimes proven tricky in the past (e.g. domain integrals associated with initial strains or stresses [3]). In the present communication, of a theoretical nature, it is established that the usual material differentiation formula for surface integrals actually yields the correct result when applied to a BIE-type strongly singular integral, the result being also taken in the CPV sense. This result encompasses a wide range of singular kernels, including most usual fundamental solutions used in static or dynamic BIE formulations.

2 Material differentiation

Let us consider, in the three-dimensional Euclidean space $\mathbf{R}^3$ equipped with a Cartesian orthonormal basis $(\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3)$, a body $\Omega_{\boldsymbol{p}}$ whose shape depends on a finite

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number of shape parameters $\boldsymbol{p} = (p_1, p_2, \ldots)$. The latter are treated as time-like parameters using a continuum kinematics-type lagrangian description and the "initial" configuration $\Omega = \Omega_0$ conventionally associated with $\boldsymbol{p} = \boldsymbol{0}$:

$$\boldsymbol{y} \in \Omega_0 \rightarrow \boldsymbol{y}^p = \boldsymbol{\Phi}(\boldsymbol{Y}; \boldsymbol{p}) \in \Omega^p \quad \text{where} \quad (\forall \boldsymbol{y} \in \Omega)\ \boldsymbol{\Phi}(\boldsymbol{y}; \boldsymbol{0}) = \boldsymbol{y} \tag{1}$$

A given domain evolution considered as a whole, as is the case e.g. in shape optimization, admits many different representations (1), with different *geometrical transformations* $\boldsymbol{\Phi}$.

As first-order derivatives with respect to $\boldsymbol{p}$ are considered here, attention is focused without loss of generality to the effect of infinitesimal variations δp about $p = 0$ of a generic shape parameter p while the others are kept fixed. The *initial transformation velocity* $\boldsymbol{\theta}(\boldsymbol{y})$ is defined by

$$\boldsymbol{\theta}(\boldsymbol{y}) = \frac{\partial}{\partial p}\boldsymbol{\Phi}(\boldsymbol{y}; 0) \tag{2}$$

In other words, the geometrical transformation (1) has the form

$$\boldsymbol{y} \rightarrow \boldsymbol{y}^{\delta p} = \boldsymbol{y} + \boldsymbol{\theta}(\boldsymbol{y})\delta p + \boldsymbol{o}(\delta p)$$

The material derivative $\overset{\star}{f}(\boldsymbol{y})$ of a generic field $f(\boldsymbol{y}, p)$ in the domain transformation, taken at $p = 0$, is defined as:

$$\overset{\star}{f}(\boldsymbol{y}) = \lim_{\delta p \rightarrow 0} \frac{1}{\delta p}[f(\boldsymbol{y}^{\delta p}, \delta p) - f(\boldsymbol{y}, 0)] = \frac{\partial}{\partial p} f(\boldsymbol{y}) + \boldsymbol{\nabla} f(\boldsymbol{y}).\boldsymbol{\theta}(\boldsymbol{y}) \tag{3}$$

The material derivatives of the unit normal $\boldsymbol{n}$ and the differential area $\mathrm{d}S$ on a surface S^p changing according to (1) are given [4], [5] by:

$$\overset{\star}{\mathrm{d}S} = \mathrm{div}_S \boldsymbol{\theta}\, \mathrm{d}S \qquad \overset{\star}{\boldsymbol{n}} = -\boldsymbol{n}.\boldsymbol{\nabla}_S \boldsymbol{\theta} \tag{4}$$

where div_S denote the surface divergence of a vector. The material derivative of a generic regular integral over S^p is then given by the formula (see e.g. Petryk and Mroz [4]):

$$\frac{d}{dp}\int_S f\, \mathrm{d}S = \int_S \left\{ \overset{\star}{f} + f \mathrm{div}_S \boldsymbol{\theta} \right\} \mathrm{d}S \tag{5}$$

Note that in formulas (3), (4), (5) and the sequel, all p-derivatives are understood for $\boldsymbol{p} = \boldsymbol{0}$. The argument p is omitted for brevity when $p = 0$.

3 Strongly singular integral on a changing surface

Let us consider CPV singular integrals of the form

$$I_S(p) = PV \int_{S^p} K(\boldsymbol{x}, \boldsymbol{y}) u(\boldsymbol{y}; p)\, dS_y \tag{6}$$

where u is regular and possibly depends on p, either explicitely or implicitely (e.g. u is the field variable which solves a boundary-value problem over the changing domain Ω) and K is the strongly singular kernel given by

$$K(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{|\boldsymbol{y}-\boldsymbol{x}|^2}\frac{(y_i-x_i)}{|\boldsymbol{y}-\boldsymbol{x}|}\frac{(y_j-x_j)}{|\boldsymbol{y}-\boldsymbol{x}|}\frac{(y_k-x_k)}{|\boldsymbol{y}-\boldsymbol{x}|} \tag{7}$$

In the BIE context, the surface S^p is any portion of the (changing) boundary $\partial\Omega$ containing the singular point $\boldsymbol{x}$, which is also assumed to move according to (1).

CPV integrals are defined as the result of a limiting process where a *spherical* exclusion neighbourhood $v_\varepsilon(\boldsymbol{x})$ of vanishing radius ε centered at $\boldsymbol{x}$ is removed around $\boldsymbol{x}$. The difficulty that arises when a changing domain is considered is that the geometrical transformation (1) is likely to alter the shape of $v_\varepsilon(\boldsymbol{x})$, which is not allowed by the definition of CPV convergence. One remedy to this is the introduction of a parametrization of the initial surface S on a parameter space Δ:

$$\boldsymbol{\xi} = (\xi_1,\xi_2) \in \Delta \rightarrow \boldsymbol{y}(\boldsymbol{\xi}) \in S \tag{8}$$

This allows the changing surface S^p to be also parametrized on the fixed domain Δ:

$$(\boldsymbol{\xi} \in \Delta, p \geq 0) \rightarrow \boldsymbol{y}^p(\boldsymbol{\xi}) = \boldsymbol{\Phi}(\boldsymbol{y}(\boldsymbol{\xi});p) \in S^p \tag{9}$$

so that one can perform the change of variable $\boldsymbol{y} \rightarrow \boldsymbol{\xi}$ in both $I_S(0)$ and $I_S(\delta p)$. Of course, $v_\varepsilon(\boldsymbol{x})$ is also distorted in this process. However, this particular difficulty has been solved by Guiggiani and Gigante [6]; as a consequence, a rigorous and computable expression of I_S using the parametrization (9) is available and indeed provides a sound basis for the present discussion.

The latter result, which we now recall, is based upon the introduction of polar coordinates (ρ,α), centered at the image $\boldsymbol{\eta}$ of the singular point $\boldsymbol{x}$ in the parameter space Δ

$$\xi_1 = \eta_1 + \rho\cos\alpha \qquad \xi_2 = \eta_2 + \rho\sin\alpha$$

so that $\boldsymbol{\xi} \in \Delta \Leftrightarrow 0 \leq \rho \leq \rho(\alpha)$ (no loss of generality occurs in assuming that Δ is star-shaped around $\boldsymbol{\eta}$). Then a Taylor expansion about $\rho = 0$, i.e. $\boldsymbol{y} = \boldsymbol{x}$, gives [6]:

$$\boldsymbol{y}^p - \boldsymbol{x}^p = \rho\boldsymbol{A}^p(\alpha;p) + O(\rho^2) \tag{10}$$

$$\boldsymbol{A}^p(\alpha;p) = \frac{\partial \boldsymbol{y}^p}{\partial\xi_1}|_{\xi=\eta}\cos\alpha + \frac{\partial \boldsymbol{y}^p}{\partial\xi_2}|_{\xi=\eta}\sin\alpha \tag{11}$$

and the kernel function $K(\boldsymbol{x},\boldsymbol{y})$ takes the form

$$\begin{aligned} K(\boldsymbol{x}^p,\boldsymbol{y}^p) &= \frac{1}{\rho^2}\left\{\frac{1}{A^2(\alpha;p)}\frac{A_i(\alpha;p)A_j(\alpha;p)A_k(\alpha;p)}{A_3(\alpha;p)} + O(\rho)\right\} \\ &= \frac{1}{\rho^2}\{k(\alpha;p) + O(\rho)\} \end{aligned} \tag{12}$$

with $A(\alpha;p) = |\boldsymbol{A}(\alpha;p)|$. The CPV integral (6) is then given by [6]:

$$I_S(p) = \int_0^{2\pi}\int_0^{\rho(\alpha)}\left[F(\rho,\alpha;p) - \frac{f(\alpha;p)}{\rho}\right]d\rho d\alpha + \int_0^{2\pi} f(\alpha;p)\ln[\rho(\alpha)A(\alpha;p)]d\alpha \tag{13}$$

with the notations

$$\left.\begin{array}{rcl} F(\rho,\alpha;p) & = & \rho K(\boldsymbol{x}^p,\boldsymbol{y}^p)u(\boldsymbol{y};p)J(\boldsymbol{\xi};p) \\ f(\alpha;p) & = & k(\alpha;p)u(\boldsymbol{x};p)J(\boldsymbol{\eta};p) \end{array}\right\} \quad (\boldsymbol{x}^p=\boldsymbol{\Phi}(\boldsymbol{x};p),\ \ \boldsymbol{y}^p=\boldsymbol{\Phi}(\boldsymbol{y}(\rho,\alpha);p))$$

$J(\boldsymbol{\xi};p)$ being the Jacobian of the parametrization (9). Note that the last term in (13) accounts for the preservation of the shape of $v_\varepsilon(\boldsymbol{x})$, and that $k(\alpha;p)$, eq. (12), has the following key property, strongly connected to the actual convergence in the CPV sense of the singular integral:

$$k(\alpha+\pi;p)=-k(\alpha;p) \tag{14}$$

4 Material derivative of the singular integral

The formula (13) holds for any fixed $p \geq \mathbf{0}$, the parameter space Δ being independent of $\boldsymbol{p}$; moreover the double integral is regular because of the singularity removal achieved through the introduction of $f(\alpha;p)$. Thus the derivative w.r.t. po of (13) can be taken:

$$\begin{aligned} \overset{\star}{I}_S &= \int_0^{2\pi}\int_0^{\rho(\alpha)}\left[\overset{\star}{F}(\rho,\alpha)-\frac{1}{\rho}\overset{\star}{f}(\alpha)\right]d\rho d\alpha+\int_0^{2\pi}\overset{\star}{f}(\alpha)\ln[\rho(\alpha)A(\alpha)]d\alpha \\ &\quad -\int_0^{2\pi} f(\alpha)\frac{\overset{\star}{A}(\alpha)}{A(\alpha)}d\alpha \end{aligned} \tag{15}$$

with

$$\overset{\star}{F}(\rho,\alpha) = \rho J(\boldsymbol{\xi})\left\{K(\boldsymbol{x},\boldsymbol{y})[\overset{\star}{u}(\boldsymbol{y})+u(\boldsymbol{y})\mathrm{div}_S\boldsymbol{\theta}(\boldsymbol{y})]+\overset{\star}{K}(\boldsymbol{x},\boldsymbol{y})u(\boldsymbol{y})\right\} \tag{16}$$

$$\overset{\star}{K}(\boldsymbol{x},\boldsymbol{y}) = [\theta_i(\boldsymbol{y})-\theta_i(\boldsymbol{x})]\frac{\partial K}{\partial y_i}(\boldsymbol{x},\boldsymbol{y}) \tag{17}$$

$$\overset{\star}{f} = J(\boldsymbol{\eta})\left\{\frac{\partial k}{\partial A_i}\overset{\star}{A}_i\,u(\boldsymbol{x})+u(\boldsymbol{x})\mathrm{div}_S\boldsymbol{\theta}(\boldsymbol{x})+\overset{\star}{u}(\boldsymbol{x})\right\} \tag{18}$$

(note that Δ, i.e the function $\rho(\alpha)$, does not depend on p). Moreover, the derivatives $\overset{\star}{\boldsymbol{A}}$ and $\overset{\star}{A}$ are given by

$$\overset{\star}{\boldsymbol{A}}(\alpha) = \frac{\partial}{\partial p}\left\{\frac{\partial \boldsymbol{y}^p}{\partial \xi_1}|_{\xi=\eta}\cos\alpha+\frac{\partial \boldsymbol{y}^p}{\partial \xi_1}|_{\xi=\eta}\sin\alpha\right\} \tag{19}$$

$$= \frac{\partial \boldsymbol{\theta}}{\partial \xi_1}|_{\xi=\eta}\cos\alpha+\frac{\partial \boldsymbol{\theta}}{\partial \xi_2}|_{\xi=\eta}\sin\alpha \tag{20}$$

$$= \boldsymbol{\nabla\theta}(\boldsymbol{x}).\boldsymbol{A}(\alpha) \tag{21}$$

$$\overset{\star}{A}(\alpha) = \frac{\boldsymbol{A}(\alpha).\boldsymbol{\nabla\theta}(\boldsymbol{x}).\boldsymbol{A}(\alpha)}{A(\alpha)} \tag{22}$$

Using the latter formulas and the expansion

$$\boldsymbol{\theta}(\boldsymbol{y})-\boldsymbol{\theta}(\boldsymbol{x})=\rho\boldsymbol{\nabla\theta}(\boldsymbol{x}).\boldsymbol{A}+O(\rho^2)$$

about $\rho = 0$, it is easy to show that $\overset{\star}{f}/\rho$ is indeed the singular part of $\overset{\star}{F}$, and also that $\overset{\star}{K}$ has the same degree of singularity than $K(\boldsymbol{x}, \boldsymbol{y})$. As a result, $\{\overset{\star}{F} - \overset{\star}{f}/\rho\}$ is regular. From (16), (18), it is then readily seen that the material derivative $\overset{\star}{I}_S$ as given by (15) has the form

$$\overset{\star}{I}_S = PV \int_S \{[Ku]^\star + Ku \mathrm{div}_S \boldsymbol{\theta}\} \, \mathrm{d}S + R \tag{23}$$

where the residual term, given by

$$R = -\int_0^{2\pi} f(\alpha) \frac{\overset{\star}{A}(\alpha)}{A(\alpha)} d\alpha \tag{24}$$

remains to be examinated. Indeed, from (22), one has

$$f(\alpha) \frac{\overset{\star}{A}(\alpha)}{A(\alpha)} = f(\alpha) \frac{\boldsymbol{A}(\alpha).\boldsymbol{\nabla}\boldsymbol{\theta}(\boldsymbol{x}).\boldsymbol{A}(\alpha)}{A^2(\alpha)}$$

and then, from property (14) and the definition (11) of $\boldsymbol{A}(\alpha)$:

$$f(\alpha+\pi) \frac{\overset{\star}{A}(\alpha+\pi)}{A(\alpha+\pi)} = -f(\alpha) \frac{\overset{\star}{A}(\alpha)}{A(\alpha)} \tag{25}$$

As a result, the residual integral R (24) vanishes:

$$R = -\int_0^{2\pi} f(\alpha) \frac{\overset{\star}{A}(\alpha)}{A(\alpha)} d\alpha = -\left\{\int_0^{\pi} + \int_\pi^{2\pi}\right\} f(\alpha) \frac{\overset{\star}{A}(\alpha)}{A(\alpha)} d\alpha = 0 \tag{26}$$

Thus we have proved that the material differentiation formula (5) is generalizable to CPV singular integrals with the kernel (7):

$$\begin{aligned} &\frac{d}{dp}\left\{PV \int_S K(\boldsymbol{x}, \boldsymbol{y}) u(\boldsymbol{y}) \, dS_y\right\} \\ &\quad = PV \int_S \{[K(\boldsymbol{x}, \boldsymbol{y}) u(\boldsymbol{y})]^\star + K(\boldsymbol{x}, \boldsymbol{y}) u(\boldsymbol{y}) \mathrm{div}_S \boldsymbol{\theta}(\boldsymbol{y})\} \, dS_y \end{aligned} \tag{27}$$

5 Concluding remarks

The present result is obviously also valid for any linear combination of kernels (7); also, the unit normal $\boldsymbol{n}(\boldsymbol{y})$ can be incorporated without difficulty in the regular factor $u(\boldsymbol{y})$ if present. Thus all usual potential or isotropic elastic BIE formulations, either static or dynamic, are encompassed by the present analysis. Also, the kernel (7) can be generalized to any combination of kernels of the form $|\boldsymbol{y} - \boldsymbol{x}|^{-2} (\boldsymbol{e}_r \otimes \ldots \otimes \boldsymbol{e}_r)$ where the unit vector $\boldsymbol{e}_r = (\boldsymbol{y} - \boldsymbol{x})/|\boldsymbol{y} - \boldsymbol{x}|$ appears an *odd* number of times in the tensor product, for which property (14) still holds.

The approach of [1] and others thus receives an *a posteriori* validation, at least when the free term present in singular BIE formulations remains constant under the

geometrical transformation (1). This is generally the case when dealing with smooth collocation points $\boldsymbol{x}$. Although the present analysis does not answer this issue, it is conjectured that the present result remains true for a corner or edge point $\boldsymbol{x}$, for which the free-term is likely to vary under the geometrical transformation.

Of course, material differentiation is also applicable to regularized BIE formulations (Bonnet [5], Zhang and Mukherjee [7]), and no complication arises at corner points in this case.

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