A NON-STANDARD POST-PROCESSING TECHNIQUE IN THE FINITE ELEMENT METHOD

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§1.1 INTRODUCTION

Often the principal purpose for which a partial differential equation is solved in practice is to obtain accurate values for a few physically important quantities. For instance in stress analysis, the values of stresses (i.e. derivatives of the solution) or stress intensity factors at a small number of critical sites in a structure are important design criteria. Decisions on whether a structure meets design and safety specifications are often made on the basis of these few quantities. Less is demanded of the mass of remaining solution information. It may be completely disregarded, or only examined qualitatively with a view to determining whether the solution is physically reasonable. These considerations suggest that some thought should be given to how these few specific quantities can be efficiently approximated.

In the finite element method the most straightforward way of obtaining approximations to solution values and derivatives is to directly evaluate the finite element solution or its derivative. However there are sometimes more sophisticated ways of "post-processing" the finite element solution than this. In this paper we shall discuss one such method. For a more detailed account than we are able to give here see [1] - [3]. The above straightforward post-processing technique of course has the advantage of being computationally fast. Let us note however, that since only a few quantities will usually ever need to be calculated, there is no real disadvantage in expending a modest amount of computational effort in any post-processing calculation.

The basic error estimate in the theory of the finite element method is the best approximation result

(1.1.1) $$\|w-\tilde{w}\|_E \leq \inf_{v\in\tilde{S}} \|w-v\|_E ,$$

where w is the exact solution of the problem, $\tilde{w}$ the finite element approximation from the finite element subspace $\tilde{S}$, and $\|\cdot\|_E$ is the energy norm associated with the problem. Typically $\|\cdot\|_E$ is an L_2 norm of first derivatives. The estimate (1.1.1) is relatively easy to obtain, and it highlights the special role that the energy norm plays in any analysis of the finite element method. Asymptotic estimates for pointwise errors in $\tilde{w}$ and its derivatives can be proved in some circumstances, however such proofs are considerably more involved than that of (1.1.1). Moreover, practical experience indicates that the behaviour of the pointwise error in $\tilde{w}$, and especially in its derivatives is not particularly robust. For instance, the errors can vary considerably within elements, or between elements, they may not decrease monotonically with mesh refinement, etc. While such effects may not be present to any significant extent in the case of smooth problems, they can cause serious problems in nonsmooth cases.

The post-processing technique to be discussed here will calculate approximations for pointwise values of the solution w and its derivatives, as well as other functionals of w, by global averaging of $\tilde{w}$. The errors in these approximations can be directly related to $\|w-\tilde{w}\|_E$. Because of this, the technique tends to be more robust than working directly from $\tilde{w}$. Moreover, the approximations are in most cases more accurate than those obtained by direct methods.

The technique can be applied to many linear problems, though for simplicity we shall only discuss it here in the context of a mixed boundary value problem for Poisson's equation, with a few brief comments about generalizations. This is all done in §2. In §3 we present some simple numerical examples to illustrate the theory of §2 and to demonstrate its practical viability.

§2.1 EXTRACTION EXPRESSIONS AND THEIR APPROXIMATIONS

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with sufficiently smooth boundary $\partial\Omega$. Suppose $\partial\Omega$ consists of two parts Γ_N and Γ_D (see Fig.1). Consider the boundary value problem:

$$\begin{aligned} -\nabla^2 w &= f \quad \text{in} \quad \Omega \\ w &= 0 \quad \text{on} \quad \Gamma_D \\ \nabla w\cdot\hat{n} &= g \quad \text{on} \quad \Gamma_N\,. \end{aligned} \tag{2.1.1}$$

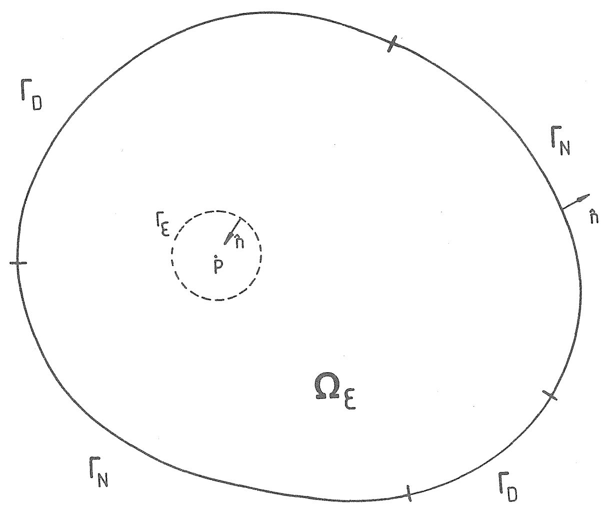

Figure 1.

For technical simplicity we suppose Γ_D is nonempty, though this is not essential.

The problem (2.1.1) has a Galerkin formulation as:

Find $w \in H = \{w \in W^{1,2}(\Omega) \; : \; w=0 \text{ on } \Gamma_D\}$ such that

$$\int_\Omega \nabla w\cdot\nabla v = \int_\Omega fv + \int_{\Gamma_N} gv \qquad \forall v \in H\,. \tag{2.1.2}$$

Letting $\tilde{S}$ be a (C°-conforming) finite element subspace of H, we can pose the corresponding finite element approximation of (2.1.2):

Find $\tilde{w} \in \tilde{S}$ such that

$$\text{(2.1.3)} \qquad \int_\Omega \nabla\tilde{w}\cdot\nabla v = \int_\Omega fv + \int_{\Gamma_N} gv \qquad \forall v \in \tilde{S} .$$

Subtracting (2.1.3) from (2.1.2) leads to the orthogonality relation

$$\text{(2.1.4)} \qquad \int_\Omega \nabla(w-\tilde{w})\cdot\nabla v = 0 \qquad \forall v \in \tilde{S}$$

from which follows the standard best approximation error estimate

$$\|w-\tilde{w}\|_E \leqq \inf_{v\in\tilde{S}} \|w-v\|_E$$

where

$$\|\cdot\|_E = \left(\int_\Omega |(\cdot)|^2\right)^{\frac{1}{2}}$$

is the energy norm associated with the problem (2.1.2)

Let us be interested in integral expressions for $w(P)$ and $\nabla w(P)$ where P is an interior point of Ω. Of course, if we knew the appropriate Green's function $G(\cdot,\cdot)$ for this geometry, we could immediately write down

$$\text{(2.1.5)} \qquad w(P) = \int_\Omega f(x)G(x,P)\,dx + \int_{\Gamma_N} g(s)G(s,P)\,ds .$$

(Similar expressions for the components of $\nabla w(P)$ could be obtained by differentiating (2.1.5) with respect to P.) However, except for the simplest geometries, $G(\cdot,\cdot)$ is not known explicitly. Nonetheless, integral expressions which are closely related to (2.1.5) can be readily obtained for quite general geometries.

For the moment let ϕ be any sufficiently smooth function defined on $\bar{\Omega} - \{P\}$. Suppose ε is small enough to ensure that $\{x, |x-P| < \varepsilon\} \subset \Omega$. Let $\Omega_\varepsilon = \{x \in \Omega, |x-P| > \varepsilon\}$, and $\Gamma_\varepsilon = \{x, |x-P| = \varepsilon\}$. (see Fig.1). Multiply the first equation of (2.1.1) by ϕ and integrate by parts over Ω_ε to obtain

$$-\int_{\Omega_\varepsilon} f\phi = \int_{\Omega_\varepsilon} \nabla^2 w\phi = \int_{\partial\Omega_\varepsilon} (\nabla w\cdot\hat{n}\phi - \nabla\phi\cdot\hat{n}w) + \int_{\Omega_\varepsilon} \nabla^2\phi w ,$$

where $\hat{n}$ denotes the outward pointing unit normal to $\partial\Omega_\varepsilon$. Noting that $\partial\Omega_\varepsilon = \Gamma_\varepsilon \cup \Gamma_N \cup \Gamma_D$, and using the boundary conditions of (2.1.1) a simple rearrangement of the above gives

$$-\int_{\Gamma_\varepsilon} (\nabla w\cdot\hat{n}\phi - \nabla\phi\cdot\hat{n}w) = \int_{\Omega_\varepsilon} (\nabla^2\phi w + f\phi) + \int_{\Gamma_N \cup \Gamma_D} (\nabla w\cdot\hat{n}\phi - \nabla\phi\cdot\hat{n}w)$$

(2.1.6)
$$= \int_{\Omega_\varepsilon} (\nabla^2\phi w + f\phi) + \int_{\Gamma_N} (g\phi - \nabla\phi\cdot\hat{n}w)$$
$$+ \int_{\Gamma_D} (\nabla w\cdot\hat{n}\phi) .$$

Now let us be more specific about ϕ . Suppose in addition that

(2.1.7a)
$$\phi(x) = -\frac{1}{2\pi} \log|x-P| + \phi_0(x)$$

where ϕ_0 , $|\nabla\phi_0| = o(|x-P|^{-1})$ as $x \to P$;

(2.1.7b)
$$\phi = 0 \quad \text{on} \quad \Gamma_D ;$$

(2.1.7c) $(\nabla^2\phi)$ extends smoothly to all of Ω , $\nabla\phi\cdot\hat{n}$ smooth on Γ_N .

Take the limit as $\varepsilon \to 0$ in (2.1.6). Because of (2.1.7a)

(2.1.8)
$$\lim_{\varepsilon\to 0} -\int_{\Gamma_\varepsilon} (\nabla w\cdot\hat{n}\phi - \nabla\phi\cdot\hat{n}w) = w(P) ,$$

whilst (2.1.7c) ensures that

$$\lim_{\varepsilon\to 0} \int_{\Omega_\varepsilon} \nabla^2\phi w = \int_\Omega \nabla^2\phi\, w$$

exists. In the limit (2.1.6) therefore becomes

(2.1.9)
$$w(P) = \lim_{\varepsilon\to 0} \int_{\Omega_\varepsilon} f\phi + \int_{\Gamma_N} g\phi + \int_\Omega \nabla^2\phi w - \int_{\Gamma_N} \nabla\phi\cdot\hat{n}w$$

on using (2.1.7b). This expression is quite similar to (2.1.5) in that it involves integrals of the loading data f and g, but it also contains terms which are weighted integrals over Ω and Γ_N of the solution w itself.

In the particular case where (2.1.7c) reduces to $\nabla^2\phi = 0$ in $\Omega - \{P\}$, $\nabla\phi\cdot\hat{n} = 0$ on Γ_N, then $\phi(x) = G(x,P)$, the Green's function for the field point P, and (2.1.9) is identical with (2.1.5). The presence of integrals of w on the right hand side of (2.1.9) of course means that in general it no longer gives an explicit formula for $w(P)$. However, it provides a means of relating the pointwise value $w(P)$ to certain averages of w over Ω and Γ_N. Since intuitively we might expect a finite element solution to behave better in an average sense than in a pointwise sense, it would seem natural to try to approximate $w(P)$ by

$$(2.1.10) \qquad \tilde{w}_P = \lim_{\varepsilon\to 0} \int_{\Omega_\varepsilon} f\phi + \int_{\Gamma_N} g\phi + \int_{\Omega} \nabla^2\phi\tilde{w} - \int_{\Gamma_N} \nabla\phi\cdot\hat{n}\tilde{w} ,$$

rather than by the pointwise value $\tilde{w}(P)$ of the finite element solution itself. We shall discuss the accuracy of $\tilde{w}_P$ as an approximation to $w(P)$ in §2.2.

We shall refer to any expression of the form of the right hand side of

$$(2.1.11) \qquad \Lambda = Q(f,g) + \int_{\Omega} aw + \int_{\Gamma_N} bw$$

where $Q(f,g)$ is a quantity involving only integration of the data f,g, and a,b are sufficiently smooth functions on Ω and Γ_N respectively, as an extraction expression. The functions a and b will be called the corresponding volume and boundary extraction functions. If the terms of (2.1.11) take the particular forms

$$(2.1.12)\qquad \begin{cases} Q(f,g) = \int_\Omega f\phi + \int_{\Gamma_N} g\phi \\ a = \nabla^2\phi \\ b = -\nabla\phi\cdot\hat{n} \end{cases}$$

for some function ϕ which vanishes on Γ_P, then ϕ will be called a generalized Green's function. Often ϕ will have some kind of singular behaviour at a point of Ω or $\partial\Omega$. In these cases (2.1.12) may need to be interpreted appropriately. For instance, the integrals of $Q(f,g)$ may only exist in a principle value sense; while $a = \nabla^2\phi$ may need to be understood as meaning that $\nabla^2\phi$ (which may not exist in a classical sense at all points of Ω), can be extended smoothly by a to all of Ω. Likewise for $\nabla\phi\cdot\hat{n}$ on Γ_N.

Just as the approximation $\ddot{w}_P$ arose naturally from the extraction expression (2.1.9), so it would seem reasonable to approximate the value Λ of any extraction expression such as (2.1.11) by

$$(2.1.13)\qquad \tilde{\Lambda} = Q(f,g) + \int_\Omega a\tilde{w} + \int_{\Gamma_N} b\tilde{w}\ .$$

In the above terminology (2.1.9) is an extraction expression for $w(P)$ which is derived from the generalized Green's function ϕ of (2.1.7).

Extraction expressions analogous to (2.1.9), but which yield the components of $\nabla w(P)$ can be found by differentiating (2.1.9) with respect to P. Alternatively, the above derivation can be repeated, but with (2.1.7a) replaced by

$$(2.1.14)\qquad \phi(x) = \frac{1}{2\pi}\frac{x_1-P_1}{|x-P|^2} + \phi_0\ .$$

for the x_1 derivative, or by

(2.1.15) $$\phi(x) = \frac{1}{2\pi}\frac{x_2-P_2}{|x-P|^2} + \phi_0$$

for the x_2 derivative. Notice that the leading terms of (2.1.7a), (2.1.14) and (2.1.15) are simply the classical solutions of Poisson's equation in the entire plane corresponding to a point load, a dipole load oriented in the x_1 direction, and a dipole load oriented in the x_2 direction respectively.

For the approximation (2.1.10) to be practical, generalized Green's functions ϕ which satisfy (2.1.7) must be found. This does not usually present much difficulty. We shall briefly outline two quite general methods for constructing suitable functions ϕ :

(a) Cut-off function method: Let η be any sufficiently smooth function on Ω satisfying $\eta = 1$ in a neighbourhood of P , $\eta = 0$ on Γ_D . If we set

$$\phi(x) = \eta(x)\left(-\frac{1}{2\pi}\log|x-P|\right)$$

then (2.1.7) is satisfied. (See §3.1 for an example.)

(b) Blending function method: Choose ϕ^* to be sufficiently smooth on Ω and to satisfy $\phi^* = -\frac{1}{2\pi}\log|x-P|$, $x \in \Gamma_D$. Then

$$\phi(x) = -\frac{1}{2\pi}\log|x-P| - \phi^*$$

satisfies (2.1.7). (Again, see §3.1 for an example.)

Clearly there will be a wide choice for the cut-off function ψ or the blending function ϕ^* . Each such choice will lead to a different extraction expression. Of course, all these will yield the same result if applied to the exact solution w as in (2.1.9). However, this will not usually be the case for (2.1.10); different choices for ϕ will lead to different approximations $\tilde{w}_P$.

The above methods can similarly be applied to construct generalized Green's functions for the extraction of the derivatives. One need only replace the term $-\frac{1}{2\pi}\log|x-P|$ in (a) and (b) by the leading term of (2.1.14) or (2.1.15).

§2.2 THE ACCURACY OF $\tilde{\Lambda}$

If we suppose that $\tilde{\Lambda}$ is evaluated exactly, then subtracting (2.1.13) from (2.1.11) gives

$$|\Lambda-\tilde{\Lambda}| = \left| \int_\Omega a(w-\tilde{w}) + \int_{\Gamma_N} b(w-\tilde{w}) \right| .$$

To help estimate this error we make use of the following simple lemma:

LEMMA 2.2.1 *Let* $a \in L_2(\Omega)$, $b \in L_2(\Gamma_N)$ *say, and let* ψ *be the solution of*

$$\begin{aligned} -\nabla^2\psi &= a \quad \text{in } \Omega \\ \psi &= 0 \quad \text{on } \Gamma_D \\ \nabla\psi\cdot\hat{n} &= b \quad \text{on } \Gamma_N . \end{aligned} \tag{2.2.1}$$

Then

$$\left|\left(\int_\Omega aw + \int_{\Gamma_N} bw\right) - \left(\int_\Omega a\tilde{w} + \int_{\Gamma_N} b\tilde{w}\right)\right| \leq \|w-\tilde{w}\|_E \inf_{z\in\tilde{S}} \|\psi-z\|_E \tag{2.2.2}$$

where $\|\cdot\|_E = \left(\int_\Omega |\nabla(\cdot)|^2\right)^{\frac{1}{2}}$.

Proof: After an integration by parts and use of (2.2.1), we have

$$\int_\Omega \nabla\psi\nabla v = \int_\Omega av + \int_{\Gamma_N} bv \qquad \forall v \in H .$$

Choose $v = w-\tilde{w} \in H$ to find

$$E = \left(\int_\Omega aw + \int_{\Gamma_N} bw\right) - \left(\int_\Omega a\tilde{w} + \int_{\Gamma_N} b\tilde{w}\right) = \int_\Omega \nabla\psi\cdot\nabla(w-\tilde{w}) .$$

However by the fundamental orthogonality property (2.1.4)

$$\int_\Omega \nabla z \cdot \nabla (w-\tilde{w}) = 0$$

for any $z \in \tilde{S}$. Thus

$$(2.2.3) \qquad |E| = \left| \int_\Omega \nabla(\psi-\tilde{\psi}) \cdot \nabla(w-z) \right| \leq \|w-\tilde{w}\|_E \inf_{z \in \tilde{S}} \|\psi-z\|_E \ .$$

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Notice that (2.2.2) is only an upper bound as it fails to take account of any cancellation in the integral in (2.2.3).

The estimate (2.2.2) confirms the naturalness of the approximation $\tilde{\Lambda}$ in that it shows the accuracy of $\tilde{\Lambda}$ is directly related to the accuracy of the finite element solution $\tilde{w}$ as measured in $\|\cdot\|_E$. However the accuracy is also dependent upon how well the solution ψ of the auxiliary problem (2.2.1) can be approximated by functions from $\tilde{S}$, as measured by $\|\cdot\|_E$. Note that (2.2.1) is of precisely the same form as the original problem (2.1.1) but with different loading data. The loadings on Ω and Γ_N are now the volume and boundary extraction functions respectively.

We shall leave more specific discussion of the accuracy of $\tilde{\Lambda}$ to §3 where we shall illustrate the high accuracy of extracted approximations by way of some simple numerical examples. In this section we shall restrict our discussion to some general comments:

(a) In many cases one can expect $\|w-\tilde{w}\|_E$ and $\inf_{z \in \tilde{S}} \|\psi-z\|_E$ to be comparable, at least for some class of finite element subspaces $\tilde{S}$. In such a case (2.2.2) shows that $|\Lambda-\tilde{\Lambda}| = O(\|w-\tilde{w}\|_E^2)$. In particular, using the extraction expressions of §2.1 we can obtain extracted approximations for both pointwise solution values and derivatives, both to an accuracy of $O(\|w-\tilde{w}\|_E^2)$. Contrast this situation to that of direct evaluation of the pointwise values and derivatives of $\tilde{w}$ where the derivatives are usually one order of mesh size less accurate than the solution values. In addition, one can usually expect no better accuracy in the pointwise derivatives of $\tilde{w}$ than $O(\|w-\tilde{w}\|_E)$.

(b) A number of factors may influence the magnitude of the quantity $\inf_{z\in\tilde{S}} \|\psi-z\|_E$ in the estimate (2.2.2), but a major consideration is the smoothness of the data of (2.2.1). In cases where the extraction functions are derived from a generalized Green's function ϕ by means of (2.1.12), then the smoothness of the extraction function will obviously depend in some way on ϕ. For example, using the techniques outlined in §2.1 it is usually not too difficult to construct generalized Green's functions which yield appropriately smooth extraction functions provided the point P is far enough from $\partial\Omega$. However if P is "close" to $\partial\Omega$ this may not be the case. Unless special care is taken in the construction of ϕ, the singular behaviour demanded of ϕ at P by (2.1.7a), (2.1.14) or (2.1.15) will usually result in unacceptable volume or boundary extraction functions. An approach that overcomes this problem will be illustrated by way of an example in §3.2.

§2.3 EXTRACTION EXPRESSIONS AT BOUNDARY POINTS

In §2 so far we have only considered extraction expressions for solution values and derivatives at points P in the interior of Ω. We now want to handle points on $\partial\Omega$. For definiteness, suppose that $O \in \partial\Omega$ and that O is not an endpoint of either Γ_N or Γ_D. Suppose further that the x_2-axis is tangent to $\partial\Omega$ at O (see Fig.2.) and that we are interested in extraction expressions for $\Lambda = w(O)$ (if $O \in \Gamma_N$), or $\Lambda = \nabla w \cdot \hat{n}(O)$ (if $O \in \Gamma_D$).

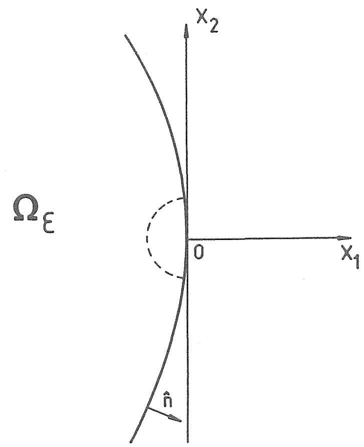


Figure 2.

Proceeding along similar lines to the derivation in §2.1 we may obtain extraction expressions for Λ of the form

$$\Lambda = \lim_{\varepsilon\to 0}\left(\int_{\Omega_\varepsilon} f\phi + \int_{\Gamma_{N,\varepsilon}} g\phi\right) + \int_{\Omega} \nabla^2\phi w - \int_{\Gamma_N} \nabla\phi\cdot\hat{n}w$$

where now $\Omega_\varepsilon = \{x\in\Omega : |x| > \varepsilon\}$, $\Gamma_{N,\varepsilon} = \begin{cases}\{x\in\Gamma_N\ ,\ |x|>\varepsilon\} & \text{if } 0\in\Gamma_N \\ \Gamma_N & \text{if } 0\in\Gamma_D\end{cases}$,

(2.4.1a) $$\begin{cases}\phi(x) = -\dfrac{1}{\pi}\log|x| + \phi_0(x) & (\text{for } w(0)\ ,\ 0\in\Gamma_N) \\ \phi(x) = \dfrac{1}{\pi}\dfrac{x_1}{|x|^2} + \phi_0(x) & (\text{for } \nabla w\cdot\hat{n}(0)\ ,\ 0\in\Gamma_D)\ .\end{cases}$$

where $\phi_0\ ,\ |\nabla\phi_0| = o(|x|^{-1})$ as $x\to 0$,

(2.4.1b) $\phi = 0$ on Γ_D (on $\Gamma_D - \{0\}$ if $0\in\Gamma_D$) .

(2.4.1c) $\nabla^2\phi$ extends smoothly to all of Ω ; $\nabla\phi\cdot\hat{n}$ extends smoothly to all of Γ_N .

Notice that the leading terms of (2.4.1a) are now the classical half-plane solutions for a point loading on a homogeneous Neumann boundary and a dipole loading on a homogeneous Dirichlet boundary.

As before, functions ϕ satisfying (2.4.1) are readily constructed using blending and cut-off function techniques. Provided O is reasonably distant from any endpoint of Γ_N or Γ_D, the resulting extraction functions $a = \nabla^2\phi$ and $b = -\nabla\phi\cdot\hat{n}$ can easily be ensured sufficiently smooth. For instance, in the case of an extraction expression for $w(0)$ one possibility would be

$$\phi(x) = \frac{-1}{\pi}\log|x| - \phi^*$$

where ϕ^* is any sufficiently smooth function satisfying $\phi^* = \frac{-1}{\pi}\log|x|$ on Γ_D. One point to note in connection with evaluating $\nabla\phi\cdot\hat{n}$ on Γ_N near 0 in this case, is that $\nabla\phi$ of course becomes singular as $x \to 0$. However provided Γ_N is smooth near 0, then $\nabla\phi\cdot\hat{n}$ is well behaved as a function of arclength along Γ_N. The practical consequence of this is that some care needs to be exercised in numerically evaluating $\nabla\phi\cdot\hat{n}$ here. Likewise in the case of extraction expressions for $\nabla w\cdot\hat{n}(0)$, the leading term of (2.4.1a) although singular as $x \to 0$ is smooth as a function of arclength along Γ_D.

§2.4 EXTRACTION EXPRESSIONS FOR STRESS INTENSITY FACTORS

It is well known that in the neighbourhood of certain critical boundary points (e.g. angular boundary points, points where Γ_N and Γ_D meet) the derivatives of the solution of (2.1.1) may exhibit some form of singular behaviour. Often it is of practical importance to know the "strength" of these singular terms. As an example, consider (2.1.1) in the particular case of the slit domain shown in Fig.3. Here the line $\theta = 0, 2\pi$ is a two-sided part of Γ_N. If the loading data f and g are smooth enough, then the solution w of (2.1.1) is known to have the following asymptotic representation:

(2.4.1) $$w(x) = kr^{\frac{1}{2}}\cos\theta/2 + w_0(x)$$

where w_0, $|\nabla w_0| = O(1)$ as $x \to 0$.

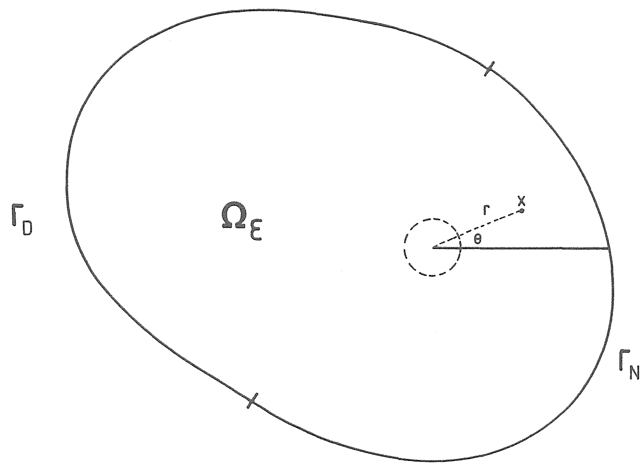


Figure 3.

Note that ∇w has an $r^{-\frac{1}{2}}$-type singularity as $x \to 0$. The coefficient k in (2.4.1) may, by analogy with fracture mechanics, be called the stress intensity factor. (In linear elastic fracture mechanics the stress intensity factor gives some indication of the tendency of a crack, as modelled by a slit, to extend under the applied loading data.)

Following exactly the same procedure as in §2.1 we can obtain an extraction expression for k :

(2.4.2) $$k = \underset{\varepsilon\to 0}{\mathrm{lmt}} \left(\iint_{\Omega_\varepsilon} f\phi + \int_{\Gamma_{N,\varepsilon}} g\phi \right) + \int_{\Omega} \nabla^2\phi w - \int_{\Gamma_N} \nabla\phi\cdot\hat{n}w$$

where now $\Omega_\varepsilon = \{x \in \Omega : |x|>\varepsilon\}$, $\Gamma_{N,\varepsilon} = \{x \in \Gamma_N , |x|>\varepsilon\}$ and

(2.4.3a) $$\phi(x) = \frac{1}{\pi} r^{-\frac{1}{2}}\cos\theta/2 + \phi_0(x)$$

where ϕ_0 , $|\nabla\phi_0| = o(r^{-\frac{1}{2}})$ as $x \to 0$.

(2.4.3b) $\phi = 0$ on Γ_D .

(2.4.3c) $\nabla^2\phi$ extends smoothly to all of Ω ; $\nabla\phi\cdot\hat{n}$ extends smoothly to all of Γ_N .

In (2.4.2) the line integrations treat the part $\theta = 0, 2\pi$ of Γ_N as two-sided. Note that the leading term of (2.4.3a) already satisfies

$$\nabla^2\left(\frac{1}{\pi} r^{\frac{1}{2}} \cos\frac{\theta}{2}\right) = 0 \quad \text{in } \Omega \quad \text{, and } \nabla\left(\frac{1}{\pi} r^{-\frac{1}{2}} \cos\frac{\theta}{2}\right)\cdot\hat{n} = 0 \quad \text{on} \quad \theta = 0, 2\pi$$

$(r\neq 0)$. Therefore functions ϕ satisfying (2.4.3) are readily constructed by the usual cut-off or blending function techniques.

§2.5 EXTRACTION EXPRESSIONS FOR INTEGRALS OF BOUNDARY FLUXES

Consider the case explicitly implied by Fig.1 where Γ_D has two components, Γ_D^0 and Γ_D^1 say. (We assume that Γ_0^D and Γ_D^1 are a non-zero distance apart.) Suppose we are interested in the quantities

(2.5.1) $$\Lambda_0 = \int_{\Gamma_D^0} \nabla w\cdot\hat{n}\, ds \quad \text{and} \quad \Lambda_1 = \int_{\Gamma_D^1} \nabla w\cdot\hat{n}\, ds \ .$$

In mechanical terms we can think of Λ_0 and Λ_1 as measuring how much of the total applied load $L\left(= \int_\Omega f + \int_{\Gamma_N} g\right)$ is carried by each of the fixed supports Γ_D^0 and Γ_D^1 respectively. (A simple integration by parts shows that $L = \Lambda_0 + \Lambda_1$.) Although the expressions of (2.5.1) for Λ_0, Λ_1 are already in some sense integrals of the solution, they are not of the proper form for an extraction expression as set out in (2.1.11). However it is not difficult to derive some appropriate extraction expressions.

Let $\phi_\alpha(\alpha=0,1)$ be any sufficiently smooth function defined on Ω which satisfies

$$(2.5.2)\qquad \begin{cases} \phi_0 = -1 \text{ on } \Gamma_D^0 \,, & \phi_0 = 0 \text{ on } \Gamma_D^1 \\ \phi_1 = -1 \text{ on } \Gamma_D^1 \,, & \phi_1 = 0 \text{ on } \Gamma_D^0 \,. \end{cases}$$

A simple integration by parts shows immediately that

$$(2.5.3)\qquad \Lambda_\alpha = \int_\Omega f\phi_\alpha + \int_{\Gamma_N} g\phi_\alpha + \int_\Omega \nabla^2\phi_\alpha w - \int_{\Gamma_N} \nabla\phi_\alpha \cdot \hat{n} w \qquad (\alpha=0,1) \,.$$

Finding smooth functions that satisfy (2.5.2) clearly presents no great difficulty. Obvious adaptations of cut-off function or blending function constructions could for instance be employed. (The smoothness of ϕ_α and the resulting extraction functions will obviously depend on how far Γ_D^0 and Γ_D^1 are apart.)

§2.6 MODIFIED VERSIONS OF THE PROBLEM (2.1.1)

In §2.1 we showed how to obtain extraction expressions for solution values and derivatives in a mixed boundary value problem (2.1.1) for Poisson's equation. These extraction expressions were constructed from the classical point source, and dipole solutions for the entire plane. An examination of the derivation in §2.1 shows that only the local behaviour of these solutions at P was essential to the argument. The fact that they also happened to be harmonic in $\Omega - \{P\}$ was more or less immaterial. This suggests that extraction expressions for solution values and derivatives for equations with (smooth) non-constant coefficients should be closely related to the corresponding extraction expressions for the equation with "frozen" coefficients at P .

As an illustration consider the following generalization of (2.1.1)

$$- \nabla\cdot(k\nabla w) = f \quad \text{in } \Omega$$
$$w = 0 \quad \text{on } \Gamma_D$$
$$k\nabla w\cdot\hat{n} = g \quad \text{on } \Gamma_N$$

where k is a smooth function on Ω, $k(x) \geq k_0 > 0$ $(x \in \Omega)$. Again let us be interested in $w(P)$ and $\nabla w(p)$ for P an interior point of Ω.

Proceeding as in §2.1 we obtain extraction expressions of the form

(2.6.1) $$\lim_{\varepsilon \to 0} \int_{\Omega_\varepsilon} f\phi + \int_{\Gamma_N} g\phi + \int_{\Omega} \nabla\cdot(k\nabla\phi)w - \int_{\Gamma_N} k\nabla\phi\cdot\hat{n}w$$

for the quantities $w(P)$ and $\nabla w(P)$, where ϕ satisfies

(2.6.2a) $$\begin{cases} \phi(x) = \dfrac{-1}{2\pi k(P)} \log|x-P| + \phi_0 & \text{(for } w(P)\text{)} ; \\ \phi(x) = \dfrac{1}{2\pi k(P)} \dfrac{x_1-P_1}{|x-P|^2} + \dfrac{1}{4\pi(k(P))^2} \dfrac{\partial k}{\partial x_1}(P) \log|x-P| + \phi_0 & \text{(for } (\nabla w)_1(P)\text{)} ; \\ \phi(x) = \dfrac{1}{2\pi k(P)} \dfrac{x_2-P_2}{|x-P|^2} + \dfrac{1}{4\pi(k(P))^2} \dfrac{\partial k}{\partial x_2}(P) \log|x-P| + \phi_0 & \text{(for } (\nabla w)_2(P)\text{)} \end{cases}$$

where ϕ_0, $|\nabla\phi_0| = o(|x-P|^{-1})$ as $x \to P$.

(2.6.2b) $$\phi = 0 \text{ on } \Gamma_D .$$

(2.6.2c) $\nabla\cdot(k\nabla\phi)$ extends smoothly to all of Ω,

$k\nabla\phi\cdot\hat{n}$ smooth on Γ_N.

The task of constructing functions ϕ satisfying (2.6.2) is a little more difficult than that encountered in §2.1. The new difficulties arise from the first part of (2.6.2c). The operator $\nabla\cdot(k\nabla(\cdot))$ applied to the leading terms of (2.6.2a) no longer yields functions that can be smoothly extended to all of Ω. For instance, in the case of extraction expressions for $w(P)$,

$$\nabla_x\cdot k\left(\nabla_x\left[\frac{1}{2\pi k(P)} \log|x-P|\right]\right) = \frac{1}{|x-P|^2}((x-P)\cdot\nabla k)$$

which is singular at $x = P$. This problem may be overcome however by being a little more specific about the form of ϕ_0. If for example we take

$$\mu(x) = \frac{-1}{2\pi k^0}\left[\log R - \frac{1}{2k^0} k,{}_1^2 X_1 \log R + k,{}_2^0 X_2 \log R) + \frac{1}{8(k^0)^2}((k,{}_1^0)^2 + (k,{}_2^0)^2) R^2 \log R\right] \quad (2.6.3)$$

where $k^0 = k(P)$, $k,{}_i^0 = \frac{\partial k}{\partial x_i}(P)$, $R = |x-P|$, $X_i = x_i - P_i$ $(i=1,2)$ then $\nabla\cdot(k\nabla\mu)$ is bounded in a neighbourhood of P . By adding further terms of the form $X_j^m \log R$, $R^s \log R$ $(m,s \in \mathbb{N})$ with suitable coefficients, $\nabla\cdot(k\nabla\mu)$ can be made successively better behaved at P . We may now employ a cut-off function on blending function construction, just as in §2.1, to μ to obtain functions satisfying (2.6.2). Similar considerations apply to the cases of extraction expressions for $\nabla w(P)$.

Another modification of (2.1.1) that can be similarly handled is the inclusion of an absolute term. Consider for instance

$$\begin{aligned} -\nabla^2 w + cw &= f \quad \text{in} \quad \Omega \\ w &= 0 \quad \text{on} \quad \Gamma_D \\ k\nabla w\cdot\hat{n} &= g \quad \text{on} \quad \Gamma_N \end{aligned}$$

where $c \geqq 0$ is assumed for simplicity to be a constant. Again for this problem one can obtain extraction expressions for $w(P)$ and $\nabla w(P)$ $(P \in \Omega)$ of the form

$$\lim_{\varepsilon\to 0} \int_{\Omega_\varepsilon} f\phi + \int_{\Gamma_N} g\phi + \int_{\Omega} (\nabla^2\phi - c\phi)w - \int_{\Gamma_N} \nabla\phi\cdot\hat{n}\, w . \quad (2.6.4)$$

Here the generalized Green's functions ϕ are essentially the same as in §2.1, though again with a somewhat more specific form for ϕ_0 to ensure that $\nabla^2\phi - c\phi$ is smooth in a neighbourhood of P . For instance, in the case of an extraction expression for $w(P)$ if we take

$$\mu(x) = \frac{1}{2\pi}\left(1 + \frac{c}{4}R^2\right) \log R$$

then $\nabla^2\mu - c\mu = O(R^2 \log R)$ in the vicinity of P . The usual cut-off and blending function constructions applied to μ will yield a suitable generalized Green's function for use in (2.6.4).

§2.7 GENERALIZATIONS

The extraction expressions that were derived in §2.1, §2.3, and §2.4 depended on having certain singular solutions of Laplaces equation available explicitly. Clearly this sort of requirement places a limitation on the class of equations for which the techniques can be effectively generalized. However for some practically important equations such as the biharmonic, and those arising in linear elasticity, many of the required singular solutions are available in tractable form from classical sources. For instance in the case of plane linear elasticity, extraction expressions for pointwise displacements, stresses etc and for stress intensity factors can be readily derived with the help of the methods of [4]. As indicated in §2.6, once extraction expressions are available for a basic equation, then it may not be too difficult to obtain corresponding extraction expressions for slightly modified equations (e.g. equations with non-constant coefficients, equations with absolute terms etc.).

§3.1 NUMERICAL EXAMPLE: A TORSION PROBLEM

Consider the boundary value problem

$$-\nabla^2 w = 1 \quad \text{in} \quad \Omega = (-1,1)^2$$

(3.1.1)

$$w = 0 \quad \text{on} \quad \partial\Omega\,(=\Gamma_D) \;.$$

We shall employ the theory of §2.1 and §2.3 for the calculation of approximate values for $w(0)$ and $(\nabla w)_1(1,0)$. A series solution for (3.1.1) can be found by the method of separation of variables, so exact values of $w(0)$ and $(\nabla w)_1(1,0)$ are available for comparison with any approximations.

The extraction expression (2.1.9) becomes in the current setting

(3.1.2) $$w(0) = \lim_{\varepsilon\to 0} \int_{\Omega_\varepsilon} \phi + \int_\Omega \nabla^2 \phi w \ .$$

We shall compute with three specific choices for the generalized Green's function ϕ .

CASE I $$\phi(x) = \eta(x)\left(\frac{-1}{2\pi} \log |x|\right)$$

where $$\eta(x) = \bar{\eta}(x_1)\bar{\eta}(x_2)$$

with $$\bar{\eta}(t) = \begin{cases} 1 & -\frac{1}{2} \leq t \leq \frac{1}{2} \\ 1-8(|t|-\frac{1}{2})^3 & \frac{1}{2} < |t| \leq 1 \end{cases}$$

CASE II $$\phi(x) = \frac{-1}{2\pi} \log |x| - \phi^*(x)$$

where $$\phi^*(x) = \frac{-1}{2\pi} \log \left[\frac{(1+x_1^2)(1+x_2^2)}{2}\right]^{\frac{1}{2}} \ .$$

Case I is a cut-off function construction, while in Case II a blending function method has been used. Ths third choice, Case III, also employs a blending function construction though space does not permit us to give complete details here.

Likewise from 2.3 we have the extraction expression of the form

(3.1.3) $$(\nabla w)_1(1,0) = \lim_{\varepsilon\to 0} \int_{\Omega_\varepsilon} \phi + \int_\Omega \nabla^2 \phi w \ .$$

Again we shall consider a number of choices for ϕ . Cases A and B will involve a combined cut-off function and blending function construction, while C and D just use blending function techniques. We shall only give details here of the construction of ϕ for Case B.

CASE B $$\phi(x) = \eta(x)\left(\frac{1}{\pi}\frac{x_1-1}{|x-(1,0)|^2} - \phi^*(x)\right)$$

where $$\eta(x) = \begin{cases} 1 & 0 \leqq x_1 \leqq 1 \\ 1-|x_1|^3 & -1 \leqq x_1 < 0 \end{cases}$$

and $$\phi^*(x) = \frac{x_1-1}{(x_1-1)^2+1} .$$

Notice that the singular term $\frac{1}{\pi}\frac{x_1-1}{|x-(1,0)|^2}$ already vanishes on $x_1 = 1$ $(x_2 \neq 0)$. To completely satisfy (2.4.1b) a blending function technique has been used to ensure that $\phi = 0$ on $x_2 = \pm 1$, and a cut-off function method to handle the edge $x_1 = -1$.

Because of the symmetry present in (3.1.1), when solving for the finite element approximation $\tilde{w}$ we need only work on the quarter segment $(0,1)^2$. A sequence of uniform square meshes employing bilinear elements was established on this quarter segment. The top portion of Table 1 shows the finite element error as measured by $\|w-\tilde{w}\|_E$ for each of these meshes. The remainder of Table 1 compares the accuracy of the direct approximations $\tilde{w}(0)$ and $(\nabla\tilde{w})_1(1,0)$, to the accuracy of approximations based on the extraction expressions (3.1.2) and (3.1.3). Notice that the first integral of (3.1.2) is strictly speaking improper, though in the computations it was evaluated using the standard 4-point Guassian quadrature on each element. However the first integral of (3.1.3) is more critical, and care is needed in its evaluation near (1,0). One possibility is to evaluate it analytically, though there are other possibilities.

Table 1 shows, as expected for bilinear elements and smooth solution w, (i) an $N^{-\frac{1}{2}}$ rate of convergence for both the global error as measured by $\|w-\tilde{w}\|_E$, and the error in $(\nabla\tilde{w})_1(1,0)$; and (ii) an N^{-1} rate of convergence

TABLE 1

NUMERICAL RESULTS FOR THE EXAMPLE OF §3.1

N (No of elements in quarter segment, uniform mesh.)	4	16	64
$\|w-\tilde{w}\|_E / \|w\|_E$	30.1%	15.2%	7.62%
Relative error in approximations for w(0):			
Direct Evaluation $\tilde{w}(0)$	5.4%	1.3%	0.31%
Extraction Expression (3.1.2)			
Case I	8.7%	2.5%	0.62%
II	2.5%	0.63%	0.16%
III	0.95%	0.25%	0.064%
Relative error in approximations for $(\nabla w)_1(1,0)$:			
Direct Evaluation $(\nabla\tilde{w})_1(1,0)$	29%	16%	8.7%
Extraction Expression (3.1.3)			
Case A	4.1%	0.49%	0.096%
B	1.3%	0.32%	0.076%
C	1.5%	0.37%	0.089%
D	0.59%	0.15%	0.038%

for $|w(0) - \tilde{w}(0)|$. Turning now to the errors in the extracted approximations based on (3.1.2) and (3.1.3), Table 1 shows that in all cases these errors are $O(N^{-1})$. This is consistent with the assertion made in §2.2 that these errors should all behave as $O(\|w-\tilde{w}\|_E^2)$. Notice in particular that for approximations to the derivative this is twice the order of accuracy of the derivative of the finite element solution itself. The fact that the rates of convergence for $\tilde{w}(0)$ and the cases I - III are the same is a consequence of our use of bilinear elements; quadratic elements would have produced $O(N^{-3/2})$ for $\tilde{w}(0)$, but a superior $O(N^{-2})$ rate for cases I - III . Nonetheless, even for bilinear elements cases II and III consistently give better accuracy than $\tilde{w}(0)$.

The variation of accuracies amongst the cases I, II and III, or amongst the cases A, B, C and D can, at least partially, be attributed to the relative smoothness of the respective extraction functions. For instance, one would expect the extraction function $b = \nabla^2\phi$ arising in case I to be more rapidly varying than that arising in case II. It is not surprising then, that case II yields a consistently more accurate approximation than case I.

§3.2 NUMERICAL EXAMPLE: A SLIT DOMAIN PROBLEM

Consider the model problem (see Fig. 4.)

$$\nabla^2 w = 0 \quad \text{in} \quad \Omega$$

$$\nabla w \cdot \hat{n} = 0 \quad \text{on} \quad \Gamma_N^0 \quad \text{(considered two-sided)}$$

$$\nabla w \cdot \hat{n} = \frac{(1+3r)}{2} r^{\frac{1}{2}} \cos \theta/2 \quad \text{on} \quad \Gamma_N^1$$

where the boundary data has been chosen to give an exact solution

$$w = r^{\frac{1}{2}} \cos \theta/2 + r^{3/2} \cos 3\theta/2 .$$

Obviously the exact value of the stress intensity factor k associated with w is 1. (cf. §2.4)

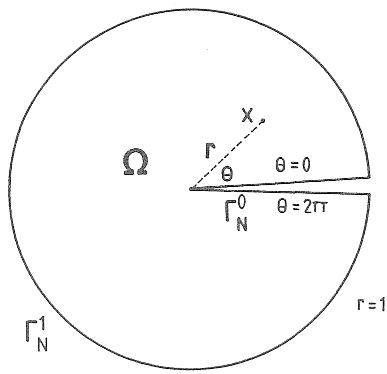


Figure 4.

Finite element approximations $\tilde{w}$ were computed for a sequence of specially refined meshes for this problem. Transformed bilinear square elements were used. The presence of a singularity at 0 means that uniform or quasi-uniform meshes are not appropriate for this problem. For each such approximation the extraction expression (2.4.2) was employed (with $\phi = \frac{1}{\pi} r^{-\frac{1}{2}} \cos \theta/2$) to extract an approximation $\tilde{k}$ from $\tilde{w}$. Some results are shown in Table 2. For the sake of comparison we also give the results of an alternative method for approximating k. This method is based on rewriting (2.4.1) as $k = \underset{\substack{x \to 0 \\ (\theta \neq \pi)}}{\mathrm{lmt}} \frac{w(x)}{r^{\frac{1}{2}} \cos \theta/2}$, and then approximating this limit by evaluating

(3.2.1) $$k^* = \frac{w(x)}{r^{\frac{1}{2}} \cos \theta/2}$$

at points x sufficiently close to 0.

The following two comments can be made concerning the results shown in Table 2:

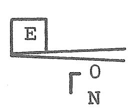
(a) The error in the extracted approximation $\tilde{k}$ behaves roughly like

TABLE 2

APPROXIMATIONS TO STRESS INTENSITY FACTOR k

N (No of degrees-of-freedom)	28	63	98
$\lVert w-\tilde{w} \rVert_E \,/\, \lVert w \rVert_E$	13.6%	8.7%	6.86%
Extraction Expression (2.4.2)	.9857	.9922	.9956
(relative error in parentheses)	(1.42%)	(0.77%)	(0.43%)
Method of (3.2.1) with			
(i) $(x_1,x_2) = (.125,0)$	(*) 1.038	1.067	1.093
(ii) (0,.125)	0.8144	0.8179	0.8486
(iii) (.125,.125)	0.9718	1.022	1.041
(iv) (.0625,0)		(*) 0.9887	1.009
(v) (0,.0625)		0.8735	0.8815
(vi) (.0625,.0625)		0.9411	0.9895
(vii) (.03125,0)			(*) 0.9632
(viii) (0,.03125)			0.9036
(ix) (.03125,.03125)			0.9262

(*) These points are vertices of the element E for this mesh.



$O(\|w-\tilde{w}\|_E^2)$. (The energy norm of the error $\|w-\tilde{w}\|_E$ itself has an experimental convergence rate of $N^{-\frac{1}{2}}$. This is a consequence of our use of "optimally" graded meshes.)

(b) For each mesh considered the extracted approximation is markedly better than those based on (3.2.1) which are seen to be sensitive to the point x used. The problem with (3.2.1) is that the non-leading terms of (2.4.1) will pollute k^* . To minimize this pollution one can try to move x closer to 0 , however $\tilde{w}(x)$ can then be expected to become less accurate.

We shall also use this example to illustrate the difficulties that may arise when the extraction expressions of §2.1 are applied at points P close to $\partial\Omega$. Suppose we wish to find the x_1 component of ∇w at $P = (.5,.05)$. If we apply the techniques of §2.1 in a straight forward manner using the generalized Green's function (2.1.14) with $\phi_0 = 0$, then we obtain the poor results shown in the first part of Table 3. The reason for these poor results is that the boundary extraction function $b = -\nabla\phi\cdot\hat{n}$ is changing rapidly along Γ_N^0 near P . As was remarked in §2.2 this will generally mean that the solution ψ of the auxiliary problem (2.2.1) will also not be well behaved near P . Thus the factor $\inf_{z\in\tilde{S}} \|\psi-z\|_E$ in the estimate (2.2.2) could well be quite large. Moreover, any rapid changes in b will have a bearing on the accuracy of any quadrature formula used. One way to overcome these difficulties is of course to locally refine the mesh near P . However this is probably not very practical. Another possibility is to slightly modify the generalized Green's function used above.

Let

$$\mu(x) = \frac{1}{2\pi}\left(\frac{x_1-P_1}{|x-P|^2} + \frac{x_1-P_1^*}{|x-P^*|^2}\right)$$

TABLE 3

APPROXIMATIONS TO x_1-DERIVATIVE AT (.5,.05)

N (No of degrees-of-freedom)	28	63	98
Approximation of $(\nabla w)_1$ using unmodified generalized Green's function.	8.2996	-1.5278	-1.5477
Approximation of $(\nabla w)_1$ using modified generalized Green's function. (relative errors in parentheses)	1.7681 (0.095%)	1.7693 (0.163%)	1.7677 (0.073%)

Exact Value: $(\nabla w)_1(.5,.05) = 1.7665$

where $P^* = (.5,-.05)$ is the image point of P in the x_1-axis. Then μ is harmonic (except at P and P^*) and $\nabla\mu\cdot\hat{n} = 0$ on the x_1 axis and so in particular on (both sides of) Γ_N^0. Clearly μ has the necessary asymptotic behaviour at P for a generalized Green's function (see (2.1.4)). To complete the modification we can apply any of a variety of cut-off or blending function constructions. For instance, if η is any sufficiently smooth function defined on Ω, satisfying $\eta = 1$ in a neighbourhood of P and $\eta = 0$ in a neighbourhood of P^*, then

$$\phi(x) = \eta(x)\mu(x)$$

is an appropriate generalized Green's function.

The extraction approximations resulting from such a modification are also shown in Table 3. The improvement in accuracy over the previous case is obvious.

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