INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING, VOL 20, 1085–1109 (1984)

THE POST-PROCESSING APPROACH IN THE FINITE ELEMENT METHOD—PART 1: CALCULATION OF DISPLACEMENTS, STRESSES AND OTHER HIGHER DERIVATIVES OF THE DISPLACEMENTS†

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SUMMARY

This is the first in a series of three papers in which we discuss a method for 'post-processing' a finite element solution to obtain high accuracy approximations for displacements, stresses, stress intensity factors, etc. Rather than take the values of these quantities 'directly' from the finite element solution, we evaluate certain weighted averages of the solution over the entire region. These yield approximations are of the same order of accuracy as the strain energy. We obtain error estimates, and also present some numerical examples to illustrate the practical effectiveness of the technique. In the third paper of this series we address the matters of adaptive mesh selection and *a posteriori* error estimation.

1 INTRODUCTION

1.1. *The role of post-processing*

In many instances the primary aim of a finite element analysis is to obtain the values of a few important quantities with a rather high accuracy. For instance, in structural mechanics, the values of displacements, stresses or stress intensity factors at a small number of critical sites in the structure are important design criteria. Decisions on whether the structure meets design specifications, or whether it is safe, are made on the basis of these few quantities. The bulk of the remaining numerical output of the finite element analysis is generally not scrutinized so closely, but rather is looked at from a more qualitative viewpoint. It may, for instance, be used to identify the critical points in the construction, to obtain a graphical display of the structure's deformation or to examine the solution's plausibility with a view to replacing, if necessary the particular mathematical model or constitutive law employed.

These considerations suggest that some thought should be paid to how the solution should be 'post-processed' to obtain values for these quantities. Since only a few quantities ever need to be calculated, we should be willing, if necessary, to expend a modest amount of computational effort on any post-processing calculation. The standard approach to post-porcessing is usually to take the displacements or stresses directly as they are output from the finite element

† This work was partially supported by ONR Contract N00014-77-C-0623. The computations were carried out with support from the Computer Science Center of the University of Maryland, College Park, MD, U.S.A.

0029–5981/84/061085–25$02.50

Received 20 December 1982
Revised 21 March 1983

computations; or for stress intensity factor calculations, to fit the finite element solution to known asymptotic expansions. There are, however, more sophisticated techniques which are currently implemented in some commercial codes. We mention, for instance, the calculation of stresses at the Gaussian points of certain element types, and the use of the 'stiffness derivative' method of Parks[1] or the 'J-integral' method of Rice[2] for the determination of stress intensity factors.

We shall show in this and two succeeding papers that there are post-processing procedures available which give an accuracy for many physically important quantities of the same order as the error in the energy of the finite element approximation. For example, in solving the plate problem (i.e. the two-dimensional biharmonic equation) with conforming elements of degree $p \geqslant 5$ it is possible (with an appropriate finite element mesh) to determine at any point the displacement, rotation, moment and shear force, all with an order of accuracy $O(N^{-(p-1)})$, where N is the number of degrees-of-freedom of the finite element model. Compare this with the 'direct' approach which gives displacements to $O(N^{-(p+1)/2})$, rotation to $O(N^{-(p/2)})$ and moments to $O(N^{-(p-1)/2})$. The fact that the standard approach results in different accuracies for displacements, rotation and moments is widely known. We remark also that the post-processing approaches that we shall outline can be well understood from within the standard 'energy' theory of finite elements. This contrasts with the complex mathematical theory which is needed to analyse the direct approach to the determination of pointwise quantities.

1.2 *A general form for post-processing calculations*

Let us denote by Φ the quantity (e.g. stress at a point) which we wish to determine. We shall write $\Phi(w)$ for Φ to indicate that Φ relates to a problem whose exact solution is w. Now, let us suppose that we know a function ζ so that

$$\Phi = \Phi(w) = \int_\Omega w\zeta \, \mathrm{d}\Omega + R \tag{1}$$

where Ω is the region on which our problem is posed, and R is an integral which may be computed using only the problem's input data (applied tractions and forces, etc.). We shall refer to ζ as an extraction function and call R the load term. As a simple illustration of what (1) may dexcribe, consider the case where Φ is the value of w at some given point. Were the influence function (Green's function) known for this point, then we could take $\zeta = 0$ and Φ would be expressible in terms of the input data alone. So (1) would only contain a load term. Of course, the influence function is not in general available. At the other extreme, if we take ζ to be the Dirac delta function at the point under consideration, then we could set the load term $R = 0$ and formally write $\Phi = \int_\Omega w\zeta \, \mathrm{d}\Omega$. This is simply a formal way of saying, evaluate w directly at the point. However, as we shall see later, there are many choices for the extraction function ζ between these two extremes. Let us also mention that the form of (1) can be generalized. We may introduce integrals containing derivatives of w. Each such integral will have its own extraction function. The well-known J-integral of Rice[2] could be thought of as arising from such a generalized version of (1). The path independence property of the J-integral then corresponds to different choices for the associated extraction functions.

Having (1) suggests an obvious method of approximation for Φ. If $\tilde{w}$ is a finite element approximation to w, then we could try to approximate $\Phi = \Phi(w)$ by

$$\tilde{\Phi} = \tilde{\Phi}(\tilde{w}) = \int_\Omega \tilde{w}\zeta \, \mathrm{d}\Omega + R \tag{2}$$

The difference between Φ and $\tilde{\Phi}$ is given by

$$e = \Phi - \tilde{\Phi} = \int_{\Omega} (w - \tilde{w})\zeta \, d\Omega \tag{3}$$

and we see clearly that the choice of ζ affects the magnitude of this difference. If ζ is the Dirac delta function, then $\tilde{\Phi}$ is the point value of $\tilde{w}$ and e is the pointwise difference between w and $\tilde{w}$. If, however, ζ is not concentrated at one point, then e becomes some weighted average of $w - \tilde{w}$. It is well known that the finite element method appears more reliable when its accuracy is measured in an average, rather than a pointwise, sense. Spurious oscillation which may cause serious loss of accuracy in pointwise values of the approximate solution (especially of its higher derivatives) are filtered out by averaging. This is especially the case with the p-version of the finite element method. So, even at this early stage, we see that choices of ζ's which have large support are likely to give superior approximations $\tilde{\Phi}$. A good choice for ζ is an important feature of any successful implementation of (2). Numerical experience, however, has shown that provided ζ meets a few simple criteria, $\tilde{\Phi}$ is quite insensitive to the choice of ζ.

Another implementation issue that we shall address is the optimal choice of mesh (and consequently of $\tilde{w}$) for use in (2). This is especially significant for adaptive finite element codes, where some adaptive criteria must be set. Obviously, if a good approximation to Φ is our ultimate goal, this adaptive criteria should be directed towards producing a $\tilde{w}$ that performs well in (2).

From a computational point of view, evaluation of $\tilde{\Phi}$ needs at most $O(N)$ operations, while the solution of the finite element problem itself usually needs about $O(N^2)$ operations in two dimensions and $O(N^{7/3})$ in three dimensions. Since only a few evaluations are ever needed, the computational effort entailed is relatively insignificant.

1.3 Outline of the paper

This is the first of a series of three papers which deal with post-processing in the finite element method. In this paper we detail some particular applications of the general theory outlined in Subsection 1.2. In Section 2 we treat the example of a one-dimensional, elastic supported beam. Here we shall be interested in post-processed values for the displacement, rotation, moment and shear force at certain points, along with the average displacement over a subsection of the beam. Section 3 deals with the simple two-dimensional problem of a membrane on an elastic support. For this problem we shall be interested in the displacements and stresses at certain points. In Section 4 we briefly describe some post-processing procedures for a seepage analysis. Finally, in Section 5 we discuss a numerical example related to the problem treated in Section 3.

The second paper of the series will be devoted to applications in linear fracture mechanics. In particular, we shall be concerned with the computation of stress intensity factors (including both k_1 and k_2 for mixed mode fracture). In the third paper we address the issues of *a posteriori* error estimates for $\tilde{\Phi}$ and adaptive mesh selection for $\tilde{w}$.

2. A ONE-DIMENSIONAL EXAMPLE

2.1 Formulation of the example

By way of a one-dimensional application of the techniques outlined in Subsection 1.2 we shall consider the problem of a clamped beam (of unit length) on an elastic support which offers string-like and spring-like reactions. Such a problem would model the situation illustrated in Figure 1.

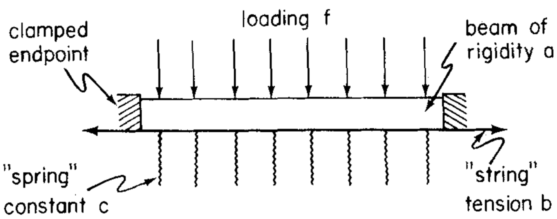

Figure 1. Model for a clamped bean on an elastic support

The governing differential equation is

$$(aw'')'' - (bw')' + cw = f \quad \text{on } (0, 1) \tag{4}$$

with the boundary conditions

$$w(0) = w'(0) = 0 \quad \text{and} \quad w(1) = w'(1) = 0 \tag{5}$$

We shall assume that a, b, c and f are smooth functions which satisfy

$$\begin{aligned} &a(t) \geqslant \alpha > 0 \qquad (0 < t < 1) \\ &b(t), c(t) \geqslant 0 \end{aligned} \tag{6}$$

The coefficient a is the rigidity of the beam, while b and c relate to the elastic properties of the support. For this problem we shall be interested in the evaluation of the following five important mechanical quantities:

1. The displacement of the beam $\Phi_1 = \Phi_1(w) = w$ at $0 < \bar{t} < 1$.
2. The rotation of the beam $\Phi_2 = \Phi_2(w) = w'$ at $0 < \bar{t} < 1$.
3. The bending moment $\Phi_3 = \Phi_3(w) = aw''$ at $0 \leqslant \bar{t} \leqslant 1$.
4. The shear force $\Phi_4 = \Phi_4(w) = (aw'')' - bw'$ at $0 \leqslant \bar{t} \leqslant 1$.
5. The average displacement of the subsection $t_1 \leqslant t \leqslant t_2$ of the beam,

$$\Phi_5 = \Phi_5(w) = (t_2 - t_1)^{-1} \int_{t_1}^{t_2} w \, dt$$

2.2 *Extraction expression for* $\Phi_i (i = 1, \ldots, 4)$

For the moment, let ϕ be any function defined on $(0, 1)$ which satisfies the boundary conditions (5). Suppose also that ϕ is sufficiently smooth to allow any operations that we carry out. Now, multiply (4) by ϕ and integrate by parts four times over the entire interval,

$$
\begin{aligned}
\int_0^1 f\phi \,\mathrm{d}t &= \int_0^1 ((aw'')''\phi - (bw')'\phi + cw\phi)\,\mathrm{d}t \\
&= [(aw'')'\phi - aw''\phi' + aw'\phi'' - w(a\phi'')']_{\bar t+0}^{\bar t-0} \\
&\quad -[bw'\phi - bw\phi']_{\bar t+0}^{\bar t-0} + \left(\int_0^{\bar t} + \int_{\bar t}^1\right) L[\phi]w\,\mathrm{d}t \\
&= [w(-(a\phi'')' + b\phi') + w'(a\phi'') + aw''(-\phi') \\
&\quad +((aw'')' - bw')\phi]_{\bar t+0}^{\bar t-0} + \left(\int_0^{0} + \int_{\bar t}^{0}\right) L[\phi]w\,\mathrm{d}t
\end{aligned}
\tag{7}
$$

where

$$L[\phi] = (a\phi'')'' - (b\phi')' + c\phi$$

and $[\cdot]_{\bar t+0}^{\bar t-0}$ denotes the jump in a quantity at $\bar t$ from right $(\bar t+0)$ to left $(\bar t-0)$.

Let us now be more specific about the behaviour of ϕ near $\bar t$. Depending upon which derivatives of ϕ are continuous at $\bar t$, (7) will form the basis of our expressions for Φ_i $(i=1,\dots,4)$. We shall refer to ϕ as the post-processing generating function, or simply the generating function.

Case I. Displacement expression. Suppose that

$$[\phi^{(i)}]_{\bar t+0}^{\bar t-0} = 0 \quad (i=0,1,2)$$

while

$$[\phi^{(3)}]_{\bar t+0}^{\bar t-0} = -a(\bar t)^{-1} \tag{8a}$$

where $\phi^{(0)} = \phi$, $\phi^{(1)} = \phi'$, $\phi^{(2)} = \phi''$, etc. Substituting in (7) gives

$$\Phi_1(w) = w(\bar t) = -\left(\int_0^{\bar t} + \int_{\bar t}^1\right) L[\phi]w\,\mathrm{d}t + \int_0^1 f\phi\,\mathrm{d}t$$

This is exactly in the form (1) with load term $R = \int_0^1 f\phi\,\mathrm{d}t$ and extraction function $\zeta = -L[\phi]$. Notice that $L[\phi]$ will, in general, be discontinuous at $\bar t$. We shall see later that from a numerical point of view it is important that ζ be smooth on $(0, 1)$. So let us append to (8a) the condition

$$[L[\phi]^{(j)}]_{\bar t+0}^{\bar t-0} = 0 \quad j=0,\dots,n \tag{8b}$$

where n is some integer, which, for the moment, will remain arbitrary.

If we select for the generating function ϕ the influence function (Green's function), then (8a) and (8b) are satisfied. Indeed, $L[\phi]=0$ on $(0,\bar t)$ and $(\bar t, 1)$, and we have $\Phi_1(w) = \int_0^1 f\phi\,\mathrm{d}t$. Of course, in general, we cannot find the influence function. Nevertheless, functions ϕ which satsify (8a) and (8b) are readily constructed, as the following example shows:

Example 1. We shall construct a generating function ϕ which fulfils all the necessary conditions, with $n=1$ in (8b). The construction is done in a number of steps. First, define

$$\phi_0(t) = \begin{cases} 0 & 0 < t \leq \bar t \\ a(\bar t)^{-1} & \bar t < t < 1 \end{cases}$$

and then set

$$\phi_1(t) = \int_0^t \int_0^y \int_0^x \phi_0(s)\,\mathrm{d}s\,\mathrm{d}x\,\mathrm{d}y$$

So $\phi_1(t)$ satisfied (8a). To meet the requirement (8b) with $n=1$ we define

$$\phi_2(t)=\begin{cases}\phi_1(t)+\alpha(t-\bar{t})^4+\beta(t-\bar{t})^5 & 0<t\leq\bar{t}\\ \phi_1(t) & \bar{t}<t<1\end{cases}$$

where the coefficients α and β are to be chosen so that (8b) holds. It is easy to see that this needs

$$\alpha=\frac{1}{4!a(t)}L[\phi_1]|_{\bar{t}+0}$$

and

$$\beta=\frac{1}{5!a(t)}(L[\phi_1]^{(1)}|_{\bar{t}+0}-3a'(\bar{t})4!\alpha)$$

(This step can be extended in an obvious fashion to handle $n>1$.)

We now have a function that satisfies (8); however, it may not yet satisfy the boundary conditions (5). There are many ways this can be remedied. Two possibilities are:

(i) Let χ be a smooth function which vanishes, along with its first derivative, at $t=0$ and $t=1$, but has a value of 1 in an interval about $\bar{t}$. Then $\phi=\chi\phi_2$ meets all the requirements. We shall refer to χ as a cut-off function.
(ii) Let ϕ_2 be a smooth function such that $\phi_3^{(i)}(0)=\phi_2^{(i)}(0)$ and $\phi_3^{(i)}(1)=\phi_2^{(i)}(1)$ $(i=0,1)$. Then we may set $\phi=\phi_2-\phi_3$. We shall refer to ϕ_3 as a blending function. Various mixtures of these two techniques are possible; for example, using a cut-off function to impose the boundary condition at one end, and a blending function approach to handle the other endpoint. □

The above example typifies a general method of constructing generating functions that we shall employ throughout this series of papers. First, a relatively simple function is constructed that behaves in some prescribed 'singular' manner near a given point. This function must then be modified to ensure that it satisfies a set of boundary conditions on the entire boundary of the region of interest. Either cut-off function, blending function or a combination of these techniques may be used to achieve this. Let us note, at this point, that blending function techniques will often lead to a smoother modified function than will the use of a cut-off function. For this reason, in a numerical setting, the blending function approach is to be preferred.

Case II. Rotation expression. Suppose that

$$\begin{aligned}&[\phi^{(i)}]_{\bar{t}+0}^{\bar{t}-0}=0 \qquad (i=0,1)\\ &[\phi'']_{\bar{t}+0}^{\bar{t}-0}=a(\bar{t})^{-1}\end{aligned}\tag{9a}$$

and

$$[-(a\phi'')'+b\phi']_{\bar{t}+0}^{\bar{t}-0}=0$$

then (7) gives

$$\Phi_2(w)=w'(\bar{t})=-\left(\int_0^{\bar{t}}+\int_{\bar{t}}^1\right)L[\phi]w\,dt+\int_0^1 f\phi\,dt$$

As for Case I, it will turn out to be important to add the condition

$$[L[\phi]^{(j)}]_{\bar{t}+0}^{\bar{t}-0}=0 \qquad j=0,\ldots,n\tag{9b}$$

Example 2. We shall construct a generating function ϕ that meets our requirements. We proceed much as in Example 1. First we define ϕ_0 as in that example, but now set

$$\phi_1(t) = -\int_0^t \int_0^x \phi_0(s)\,\mathrm{d}s\,\mathrm{d}x$$

To satisfy (9b) (with $n=1$, say) and the third part of (9a) we may define

$$\phi_2(t) = \begin{cases} \phi_1(t) + \alpha(t-\bar{t})^3 + \beta(t-\bar{t})^4 + \gamma(t-\bar{t})^5 & 0<t\leq\bar{t} \\ \phi_1(t) & \bar{t}<t<1 \end{cases}$$

where α, β and γ are to be chosen so that (9b) and the last part of (9a) hold. (That this may always be done follows since $a(\bar{t}) \neq 0$.) We then proceed to impose the boundary conditions (5) by the same methods described in Example 1. □

Cases III and IV. Bending moment and shear force expressions. If $\bar{t}$ is internal to the interval, then selecting

$$\begin{aligned} [\phi]_{\bar{t}+0}^{\bar{t}-0} &= 0 \\ [\phi']_{\bar{t}+0}^{\bar{t}-0} &= -1 \\ [a\phi'']_{\bar{t}+0}^{\bar{t}-0} &= 0 \\ [-(a\phi'')' + b\phi']_{\bar{t}+0}^{\bar{t}-0} &= 0 \end{aligned} \tag{10}$$

and

$$[L[\phi]^{(j)}]_{\bar{t}+0}^{\bar{t}-0} = 0 \qquad j=0,\ldots,n$$

gives

$$\Phi_3(w) = aw''(\bar{t}) = -\left(\int_0^{\bar{t}} + \int_{\bar{t}}^1\right) L[\phi]w\,\mathrm{d}t + \int_0^1 f\phi\,\mathrm{d}t$$

with smooth $L[\phi]$. While choosing ϕ to satisfy

$$\begin{aligned} [\phi]_{\bar{t}+0}^{\bar{t}-0} &= 1 \\ [\phi']_{\bar{t}+0}^{\bar{t}-0} &= 0 \\ [a\phi'']_{\bar{t}+0}^{\bar{t}-0} &= 0 \\ [-(a\phi'')' + b\phi']_{\bar{t}+0}^{\bar{t}-0} &= 0 \end{aligned} \tag{11}$$

and

$$[L[\phi]^{(j)}]_{\bar{t}+0}^{\bar{t}-0} = 0 \qquad (j=0,\ldots,n)$$

leads to the expression

$$\Phi_4(w) = ((aw'')' - bw')(\bar{t}) = -\left(\int_0^{\bar{t}} + \int_{\bar{t}}^1\right) L[\phi]w\,\mathrm{d}t + \int_0^1 f\phi\,\mathrm{d}t$$

for $\Phi_4(w)$.

To treat these two cases when $\bar{t}$ is one of the endpoints we need a slightly different argument. For definiteness, suppose that $\bar{t}$ is the right-hand endpoint $\bar{t}=1$. We now let ϕ be a smooth function on $(0,1)$ which satisfies the boundary condition $\phi(0)=\phi'(0)=0$. Analogous to (7) we now have

$$\int_0^1 f\phi \, dt = \int_0^1 ((aw'')''\phi - (bw')'\phi + cw\phi) \, dt$$

$$= ((aw'')'\phi - aw''\phi')|_{t=1} + \int_0^1 L[\phi]w \, dt \tag{12}$$

If we further set

$$\phi(1)=0 \quad \text{and} \quad \phi'(1)=-1 \tag{13}$$

we obtain, after rearranging (12),

$$\Phi_3(w) = aw''(1) = -\int_0^1 L[\phi]w \, dt + \int_0^1 f\phi \, dt$$

while, using in place of (13)

$$\phi(1)=1 \quad \text{and} \quad \phi'(1)=0 \tag{14}$$

leads to the expression

$$\Phi_4(w) = (aw'')'(1) = -\int_0^1 L[\phi]w \, dt + \int_0^1 f\phi \, dt$$

Generating functions ϕ satisfying (10), (11), (13) or (14) and the appropriate boundary conditions are readily constructed using techniques like those described in Examples 1 and 2.

The expressions derived in this section are summarized in Tables I and II.

Table I. Extraction expressions for Φ_i $(i=1,\ldots,4)$ at an interior point $\bar{t}$:

$$\Phi(w) = -\left(\int_0^{\bar{t}} + \int_{\bar{t}}^1\right) L[\phi]w \, dt + \int_0^1 f\phi \, dt$$

$$(L[\phi] = (a\phi'')'' - (b\phi')' + c\phi)$$

(To find the properties required of the generating function ϕ associated with, for example, the rotation Φ_2 of the beam at $\bar{t}$, read down the second column of the table. The entries indicate that ϕ should be continuous at $\bar{t}$, ϕ' should be continuous, ϕ'' should have a right to left jump discontinuity of $a(\bar{t})^{-1}$, $-(a\phi'')' + b\phi'$ should be continuous, and $L[\phi]$ should have a certain number of derivatives continuous at $\bar{t}$.)

$[\cdot]_{\bar{t}+0}^{\bar{t}-0}$	Φ_1 (displacement)	Φ_2 (rotation)	Φ_3 (bending moment)	Φ_4 (shear force)
ϕ	0	0	0	1
ϕ'	0	0	−1	0
ϕ''	0	$a(\bar{t})^{-1}$	—	—
ϕ'''	$-a(\bar{t})^{-1}$	—	—	—
$-(a\phi'')' + b\phi'$	—	0	0	0
$a\phi''$	—	—	0	0
$L[\phi]^{(j)}$ $j=0,1,\ldots,n$	0	0	0	0
	$\phi(0)=\phi'(0)=0=\phi(1)=\phi'(1)$			

Table II. Extraction expressions for Φ_3 and Φ_4 at an endpoint:

$$\Phi(\omega) = -\int_0^1 L[\phi]\omega \, \mathrm{d}t + \int_0^1 f\phi \, \mathrm{d}t$$

$$(L[\phi] = (a\phi'')'' - (b\phi') + c\phi)$$

(To find the properties required of the generating function ϕ associated with, for example, the bending moment Φ_3 at $\bar{t}=0$, read down the first column of the table. The entries indicate that ϕ should have a value 0 at $\bar{t}$ and ϕ' a value of 1 at $\bar{t}$.)

	Φ_3 (bending moment) $\bar{t}=0$	$\bar{t}=1$	Φ_4 (shear force) $\bar{t}=0$	$\bar{t}=1$
$\phi(\bar{t})$	0	0	-1	1
$\phi'(\bar{t})$	1	-1	0	0
	$\phi(\bar{\bar{t}}) = \phi'(\bar{\bar{t}}) = 0$; $\bar{\bar{t}}=1$ when $\bar{t}=0$, $\bar{\bar{t}}=0$ when $\bar{t}=1$			

2.3 *An extraction expression for Φ_5 (average displacement)*

The definition of Φ_5 in Subsection 2.1 is already in the form (1), for we may certainly write

$$\Phi_5 = \Phi_5(w) = \int_0^1 w\zeta_0 \, \mathrm{d}t \tag{15}$$

where

$$\zeta_0 = \begin{cases} (t_2 - t_1)^{-1} & y_1 \leqslant t \leqslant t_2 \\ 0 & \text{otherwise} \end{cases}$$

However, from our point of view, this is an unsuitable expression for Φ_5 since the extraction function ζ_0 is not smooth. To overcome this failing we may proceed as follows. Define

$$\phi_1(t) = \int_0^t \int_0^{s_4} \frac{1}{a(s_3)} \int_0^{s_3} \int_0^{s_2} \zeta_0(s_1) \, \mathrm{d}s_1 \, \mathrm{d}s_2 \, \mathrm{d}s_3 \, \mathrm{d}s_4$$

Let ϕ_2 be a smooth blending function that satisfies the boundary conditions

$$\phi_2^{(i)}(0) = \phi_1^{(i)}(0) \quad \text{and} \quad \phi_2^{(i)}(1) = \phi_1^{(i)}(1) \qquad (i = 0, 1)$$

and set $\phi = \phi_1 - \phi_2$. Multiply (4) by ϕ and integrate by parts four times over the entire interval,

$$\begin{aligned} \int_0^1 f\phi &= \int_0^1 (aw'')''\phi - (bw')\phi + c\phi w \, \mathrm{d}t \\ &= \int_0^1 L[\phi] w \, \mathrm{d}t \\ &= \int_0^1 (L[\phi_1]w - L[\phi_2]w) \, \mathrm{d}t \\ &= \int_0^1 (\zeta_0 w - (b\phi_1')' w + c\phi_1 w - L[\phi_2]w) \, \mathrm{d}t \end{aligned}$$

Upon rearrangement, then,

$$\Phi_5 = \Phi_5(w) = \int_0^1 ((b\phi_1')' - c\phi_1 + L[\phi_2]w \, \mathrm{d}t + \int_0^1 f\phi \, \mathrm{d}t$$

which is of the form discussed in Subsection 1.2 with extraction function and load term

$$\zeta = (b\phi_1')' - c\phi_1 + L[\phi_2] \quad \text{and} \quad R = \int_0^1 f\phi \, \mathrm{d}t$$

In contrast to ζ_0, notice that the extraction function ζ has a continuous first derivative (although, in general, a discontinuous second derivative at t_1 and t_2). A ζ with more smoothness can be constructed by iterating the above process.

2.4 Natural boundary conditions

If the essential (geometric) boundary conditions (5), which describe a clamped beam, are replaced by the natural (force) boundary conditions

$$\begin{aligned} aw''(0) &= ((aw'')' - bw')(0) = 0 \\ aw''(1) &= ((aw'')' - bw')(1) = 0 \end{aligned} \tag{16}$$

which correspond to a beam with free ends, then there is no need for any specific boundary behaviour to be imposed on the generating function ϕ. Thus, it is not necessary to introduce cut-off or blending functions, as we did in Subsections 2.2 and 2.3 to obtain some required boundary behaviour of ϕ. In such a case, however, we have slightly different extraction expressions for the $\Phi_i's$, which now must include some endpoint terms. For instance, the displacement expression for Φ_1 given in Subsection 2.2 will become

$$\Phi_1(w) = w(\bar{t}) = -\left(\int_0^{\bar{t}} + \int_{\bar{t}}^1\right) L[\phi]w \, \mathrm{d}t + \int_0^1 f\phi \, \mathrm{d}t - [w - (a\phi'')' + b\phi') + w' a\phi'']_0^1$$

with ϕ only needing to satisfy (8a) and (8b). This expression and the corresponding ones for the other Φ_i's are derived by the same approach we took in Subsections 2.2 and 2.3, taking care that the integration by parts formula (7) should now contain endpoint terms.

If at one end of the beam essential boundary conditions are imposed, while at other natural boundary conditions apply, then the generating function ϕ need only satisfy the essential boundary conditions at the appropriate end. No specific behaviour is demanded at the other endpoint.

2.5 The accuracy of the approximations $\tilde{\Phi}_i$ $(i = 1, \ldots, 5)$

In Subsections 2.2 and 2.3 we derived some integral expressions for the Φ_i. These fitted into the general pattern discussed in Subsection 1.2. We shall now address the important question of the accuracy of the approximations $\tilde{\Phi}_i = \Phi_i(\tilde{w})$ which arise when the finite element solution $\tilde{w}$ is used in place of w in these expressions.

To be definite, suppose we have set up a finite element model of (4)/(5) using C^1 polynomial elements of degree $p(\geq 3)$. Write $I_1, \ldots, I_N$ for the intervals which comprise the finite element mesh. Denote by S the set of all admissible finite element functions. Let $h = \max_k$ (length I_k). In the case of the problem (4)/(5) the fundamental orthogonality property of the finite element error $w-\tilde{w}$ takes the specific form

$$\int_0^1 (a(w-\tilde{w})''v''+b(w-\tilde{w})'v'+c(w-\tilde{w})v\,\mathrm{d}t=0 \tag{17}$$

for all v in S. Denoting by $E(\cdot)$ the energy expression

$$E(\cdot)=\int_0^1 (a((\cdot)'')^2+b((\cdot)')^2+c(\cdot)^2)\,\mathrm{d}t$$

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the standard finite element error estimate may be written as

$$E(w-\tilde{w})\leqslant \min_{v^*\in S} E(w-v^*) \tag{18}$$

where the minimum is taken over all v^* from S.

辅助函数

For the purposes of the analysis, we need to introduce the auxiliary function ψ which satisfies

$$L[\psi]=\zeta \quad \text{on } (0,1) \qquad (a\psi'')''-(b\psi')'+c\psi=\zeta$$

and

$$\psi(0)=\psi'(0)=0=\psi(1)=\psi'(1) \tag{19a}$$

or what, after integration by parts, is the same thing

$$\int_0^1 (a\psi''u''+b\psi'u'+c\psi u)\,\mathrm{d}t=\int_0^1 \zeta u\,\mathrm{d}t \tag{19b}$$

for all u with boundary values as in (5). Now, recalling (3), we have the following estimate for the error $\Phi=\tilde{\Phi}$:

$$\boxed{e=\Phi-\tilde{\Phi}=\int_0^1 \zeta(w-\tilde{w})\,\mathrm{d}t}$$

$$=\int_0^1 (a(w-\tilde{w})''\psi''+b(w-\tilde{w})'\psi'+c(w-\tilde{w})\psi)\,\mathrm{d}t$$

(putting $u=w-\tilde{w}$ in (19b)

$$=\int_0^1 (a(w-\tilde{w})''(\psi-v)''+b(w-\tilde{w})'(\psi-v)'+c(w-\tilde{w})(\psi-v))\,\mathrm{d}t$$

for any v from S (by (17)). So

$$|\Phi-\tilde{\Phi}\leqslant \min_{v\in S}\left(\int_0^1 (a(w-\tilde{w})''(\psi-v)''+b(w-\tilde{w})'(\psi-v)'+c(w-\tilde{w})(\psi-v))\,\mathrm{d}t\right)$$

$$\leqslant \min_{v\in S}(E(w-\tilde{w})^{1/2}E(\psi-v)^{1/2})$$

$$\leqslant \min_{v^*\in S}(E(w-v^*)^{1/2})\min_{v\in S}(E(\psi-v)^{1/2}) \tag{20}$$

using (18). In words, then, the error in Φ is bounded by the product of the energy norm difference between w and its best approximation from S, and the energy norm difference between ψ and its best approximation from S. The importance of the smoothness of ζ can now be appreciated. Smooth functions ζ will give smooth auxiliary functions ψ, and these will be approximated well by the functions in S.

Let us now try to obtain an asymptotic rate of convergence for $\tilde{\Phi}$ which will be applicable to both the h- and p-versions of the finite element method. First, recall the approximation result (see Reference 3): If z is a function defined on $(0, 1)$ and if the smoothness measuring quantity

$$\|z\|_s = \left(\sum_{l=0}^{s} \sum_{k=1}^{N} \int_{I_k} \left| z^{(l)} \right|^2 \mathrm{d}t \right)^{1/2}$$

is finite for some integer $s \geqslant 2$, then

$$\min_{v \in S} E(z-v) \leqslant C_1 \frac{h^{2m}}{p^{2(s-2)}} \|z\|_s^2 \tag{21}$$

where C_1 is a constant which does not depend on the function z, the finite element mesh or the order of elements used; and $m = \min(p-1, s-2)$. If the load f in (4) and the function ζ are smooth enough to guarantee that $\|f\|_{s_1} < \infty$ and $\|\zeta\|_{s_2} < \infty$ for some integers s_1, $s_2 \geqslant 2$, then, provided the coefficients a, b and c are sufficiently smooth, it may be shown that

$$\|w\|_{s_1+4} \leqslant C_2 \|f\|_{s_1} \quad \text{and} \quad \|\psi\|_{s_2+4} \leqslant C_3 \|\zeta\|_{s_2} \tag{22}$$

where C_2 and C_3 do not depend on f and ζ, respectively. Having these smoothness properties of w and ψ, we may make use of the approximation bounds (21) in (20) to obtain

$$\begin{aligned} |\Phi - \tilde{\Phi}| &\leqslant C_1 \frac{h^{(m_1+m_2)}}{p^{(s_1+s_2+4)}} \|w\|_{s_1+4} \|\psi\|_{s_1+4} \\ &\leqslant C_1 C_2 C_3 \frac{h^{(m_1+m_2)}}{p^{(s_1+s_2+4)}} \|f\|_{s_1} \|\zeta\|_{s_2} \end{aligned} \tag{23}$$

where $m_i = \min\,(p-1, s_i+2) (i = 1, 2)$. Likewise (18) gives

$$E(w - \tilde{w}) \leqslant C_1 C_2^2 \frac{h^{2m_1}}{p^{2(s_1+2)}} \|f\|_{s_1}^2$$

We mentioned in Subsections 2.2 and 2.3 that the relevant extraction function ζ could be made arbitrarily smooth (i.e. n in (8b), etc., was arbitrary). For large values of n this could become laborious. Note that (23) allows discontinuities at mesh points without any adverse effects on the accuracy of $\tilde{\Phi}$. What is important is that ζ be smooth in the interior of each of the I_k. In the h-version of the finite element method, there would, at least from our analysis, seem to be no reason to proceed any further than the stage at which $s_2 + 2 = p - 1$. At this stage $|\Phi - \tilde{\Phi}| = O(h^{m_1+p-1})$, and this rate would not be improved by increasing s_2. Comparing this with $E(w - \tilde{w}) = O(h^{2m_1})$, we see, as was previewed in Section 1, that the error $|\Phi - \tilde{\Phi}|$ is at least of the same order as the energy of the error in the finite element solution. For the p-version there would seem to be no such limit. We may increase s_2 indefinitely, always improving the convergence rate for $\tilde{\Phi}$ as we go. Here we have $|\phi - \tilde{\phi}| = O(p^{-(s_1+s_2+4)})$ and $E(w - \tilde{w}) = O(p^{-2(s_1+2)})$.

Of course, actual computations must be carried out working from only a limited range of non-zero h's and finite p's. In such a setting, the asymptotic rate of convergence alone is not necessarily a good indication of an approximation's accuracy. As (23) shows, the error in $\tilde{\Phi}$ is related not only to p and h, but also to $\|\zeta\|_{s_2}$ and the constants C_i. As s_2 increases, the numerical values of these quantities may also increase dramatically, with the net effect that there is a loss of accuracy in $\tilde{\Phi}$. In practice, it is usually more important to ensure that the numerical value of $\|\zeta\|_{s_2}$ is reasonable, than to construct ζ's with high orders of continuity. Recall also our comment earlier that blending function techniques are generally superior to cut-off function methods in this respect.

Another important practical consideration is the choice of a finite element mesh. As (20) shows, the accuracy of $\tilde{\Phi}$ is related to the approximability of both w and ψ. So, an optimal mesh for calculating $\tilde{\Phi}$ would be one which was, in some way, simultaneously good for both the original problem (4)/(5) and the auxiliary problem (19a). We shall explore this question in the third of this series of papers. The sorts of concerns touched upon in this paragraph are of great importance in two-dimensional problems. For many such problems there is no complete analogue (22), and we are denied the luxury of being able to make ψ as smooth as we wish.

In summary then, the accuracy of the post-processed value is related to how well the finite element subspace can approximate simultaneously the solutions of the primary problem and the auxiliary problem. As far as the choice of extraction function is concerned, the approximability of the solution of the auxiliary problem is influenced by:

1. The smoothness of the extraction function ζ. When kinematic boundary conditions apply in the primary problem, the manner in which these are imposed on the generating function ϕ can have a significant effect on the smoothness of ζ. The blending function approach is often superior to a cut-off function method in this respect.
2. How well the finite element mesh takes account of any lack of smoothness in the extraction function ζ. A mesh refinement in the vicinity of any unsmooth portion of ζ will improve the accuracy of the post-processed value.

3 TWO-DIMENSIONAL PROBLEMS (MEMBRANE PROBLEM)

3.1 *Formulation of the problem*

To illustrate the ideas of Subsection 1.2 in a two-dimensional setting, we shall consider in some detail the simple model example of

$$\nabla^2 w - kw = f \quad \text{in } \Omega\text{, a polygonal region} \tag{24}$$

with the boundary condition

$$w = 0 \quad \text{on } \partial\Omega\text{, the boundary of } \Omega \tag{25}$$

Here we suppose that $k \geqslant 0$ and assume, for simplicity, that k is a constant and f a smooth function. The problem (24)/(25) could, for example, be thought of as describing a polygonal membrane on an elastic support that is fixed along its edges. (In the case of $k=0$ and $f=-1$ (24)/(25) also models the torsion problem.) We shall be concerned with evaluating the following quantities which are related to W:

1. The displacement $\Phi_1 = \Phi_1(w) = w(\bar{x})$ at a point $\bar{x} = (\bar{x}_1, \bar{x}_2)$ in Ω.
2. The stress $\Phi_2 = \Phi_2(w) = \nabla w \cdot \hat{n}(\bar{y})$ at a point $\bar{y} = (\bar{y}_1, \bar{y}_2)$ on $\partial\Omega$, which is 'far' from a corner point. (The case of $\bar{y}$ 'close' to a corner point will be discussed in Reference 5. The vector $\hat{n}$ is the outward pointing unit normal on $\partial\Omega$.

3.2 *An integral for Φ_1 (displacement at $\bar{x}$)*

Let $\phi(x)$ be an arbitrary function defined and sufficiently smooth on $\Omega - \{\bar{x}\}$, which vanishes on $\partial\Omega$. For $\varepsilon > 0$, small enough, denote by S_ε a disc with centre $\bar{x}$ and radius ε which lies in

Ω. Multiply (24) by ϕ and integrate over $\Omega - S_\varepsilon$. Using Green's theorem we obtain

$$\int_{\Omega - S_\varepsilon} f\phi \, \mathrm{d}A = \int_{\partial S_\varepsilon} (\nabla w \cdot n\phi - \nabla\phi \cdot \hat{n} w) \, \mathrm{d}s + \int_{\Omega - S_\varepsilon} L[\phi] w \, \mathrm{d}A \tag{26}$$

where $L[\cdot] = \nabla^2(\cdot) - k(\cdot)$ and $\hat{n}$ denotes the unit normal on ∂S_ε pointing towards $\bar{x}$. Now, impose the extra conditions

$$\left.\begin{aligned} \phi(x) &= (2\pi)^{-1} \log \bar{r}(x) + O(1) \\ \nabla\phi(x) &= \nabla((2\pi)^{-1} \log \bar{r}(x)) + o(\bar{r}(x)^{-1}) \end{aligned}\right\} \quad (\text{as } x \to \bar{x}) \tag{27}$$

where $\bar{r}(\dot{x}) = ((x_1 - \bar{x}_1)^2 + (x_2 - \bar{x}_2)^2)^{1/2}$. Notice that the leading term of ϕ is simply the influence function for a concentrated load in an infinite domain. Then, in the limit as $\varepsilon \to 0$, (26) yields

$$\Phi_1(w) = w(\bar{x}) = -\int_\Omega L[\phi] w \, \mathrm{d}A + \int_\Omega f\phi \, \mathrm{d}A \tag{28}$$

Note that the integrals appearing on the right-hand side of (28) are possibly singular. We see that (28) is precisely in the form given in (1) with extraction function $\zeta = -L[\phi]$, and load term $R = \int_\Omega f\Phi \, \mathrm{d}A$. Notice also that were ϕ the influence function (Green's function) for (24)/(25), then the first integral on the right-hand side of (28) vanishes. In general, of course, the influence function is not available.

Just as in Section 2, it will turn out that, from a numerical viewpoint, it is important for the extraction function to be smooth. The task of selecting a suitable ζ or, what is the same thing, of choosing the generating function ϕ, appropriately can be thought of as having two aspects. First, ensuring that $L[\phi]$ is smooth in the immediate neighbourhood of $\bar{x}$; and secondly, of imposing the boundary conditions on ϕ in such a way that no unsmooth behaviour of ϕ is introduced.

Let us talk in more detail about these points as they relate to our model problem. It is easy to verify that if

$$\tilde{\phi}(x) = (2\pi)^{-1}\left(1 + \frac{k}{4}\bar{r}(x)^2\right) \log \bar{r}(x) \tag{29}$$

then $L[\tilde{\phi}] = 0(\bar{r}^2 \log \bar{r})$ in the vicinity of $\bar{x}$. Now $\tilde{\phi}$ has the required asymptotic behaviour (27); however, it does not vanish on $\partial\Omega$, and so cannot be used directly for φ in (28). Let us suppose for a moment that $\bar{x}$ is not too close to $\partial\Omega$. Then, as for the one-dimensional case, there are a number of techniques for modifying $\tilde{\phi}$. We could, for instance, proceed in one of the following ways:

1. Let $\chi(x)$ be a smooth 'cut-off' function which vanishes on $\partial\Omega$, but is a constant, equal to 1, in a neighbourhood of $\bar{x}$. The, $\phi(x) = \chi(x)\tilde{\phi}(x)$ satisfies all our requirements.
2. Let $\phi_0(x)$ be a smooth 'blending' function on Ω which agrees with $\tilde{\phi}(x)$ on $\partial\Omega$. We could then take $\phi(x) = \tilde{\phi}(x) - \phi_0(x)$.
3. Use a combination of the above two techniques—'cut-off' functions to handle part of the boundary, and 'blending' functions for the remainder.

In the case where $\bar{x}$ is very close to $\partial\Omega$, method 1 is not a good method to use, as the 'cut-off' function χ would have large derivatives in the region between $\bar{x}$ and $\partial\Omega$. Methods 2 and 3 provide better ways of handling this case. Note, however, that although $L[\phi]$ is smooth near $\bar{x}$, $\tilde{\phi}$ is not. For an arbitrary 'blending' function ϕ_0, agreeing with $\tilde{\phi}$ on $\partial\Omega$ near $\bar{x}$, there is no reason to expect that $L[\phi_0]$ be smooth. One way around this, at least in the case when $\bar{x}$, although close to the boundary of Ω, is far from a corner point of the boundary, is to formally extend $\tilde{\phi}$ across the straight line segment of the boundary closest $\bar{x}$. Now let ψ be the reflection of this extension back into Ω. Then $L[\psi]$ is smooth, and ψ agrees with $\tilde{\phi}$ on the straight line segment of the boundary closest $\bar{x}$. Standard 'blending' techniques may then be used to deal with the reamining three sides of Ω. There are extensions of the above ideas to domains with curved boundaries.

If the kinematic (essential) boundary condition (25) were replaced by

$$\nabla w \cdot \hat{n} = g \quad \text{on } \partial\Omega$$

then we could proceed in much the same way as above. In this case, there is no need to impose any boundary conditions on the generating function ϕ. Instead of (28) we would have

$$\Phi_1(w) = w(\bar{x}) = -\int_\Omega L[\phi] w \, \mathrm{d}A + \int_\Omega f\phi \, \mathrm{d}A - \int_{\partial\Omega} g\phi \mathrm{d}s + \int_{\partial\Omega} \nabla\phi \cdot \hat{n} w \, \mathrm{d}s$$

which is an instance of a generalized version of (1) with load term $\int_\Omega f\phi \, \mathrm{d}A - \int_{\partial\Omega} g\phi \, \mathrm{d}s$ and extraction functions $-L[\phi]$ in Ω and $\nabla\phi \cdot \hat{n}$ on $\partial\Omega$. For our model problem we could take ϕ to be $\tilde{\phi}$ as given in (29). Note, however, that if $\bar{x}$ is close to $\partial\Omega$ then the function $\nabla\tilde{\phi} \cdot \hat{n}$ could become rather unsmooth. To remedy this we could, for instance, use a blending function approach and use as the generating function $\phi = \tilde{\phi} + \psi$, where ψ is as defined in the last paragraph.

3.3 *An integral for Φ_2 (stress at $\bar{y}$)*

For definiteness, suppose that $\bar{y}$ lies on the straight line segment $((1, -1), (1, 1))$ which forms part of $\partial\Omega$. This time, let ϕ be an arbitrary, sufficiently smooth function defined on Ω, which vanishes on $\partial\Omega - \{\bar{x}\}$. For $\varepsilon > 0$, small enough, denote by $S_\varepsilon^+(\bar{x})$ a half-disc with centre $\bar{x}$ and radius ε, which lies in Ω. Multiply (24) by ϕ and integrate over $\Omega - S_\varepsilon^+$. Using Green's theorem we obtain

$$\int_{\Omega - S_\varepsilon^+} f\phi \, \mathrm{d}A = \int_{\Gamma_\varepsilon} (\nabla w \cdot \hat{n}\phi - \nabla\phi \cdot \hat{n} w) \, \mathrm{d}s + \int_{\Omega - S_\varepsilon^+} L[\phi] w \, \mathrm{d}A \tag{30}$$

where Γ_ε denotes the circular portion of the boundary of S_ε^+, and as usual $\hat{n}$ denotes a unit normal pointing towards the centre of S_ε^+ (see Figure 2). Now if we impose the extra conditions

$$\left.\begin{aligned} \phi(x) &= \frac{1}{\pi} \frac{\cos\bar{\theta}(x)}{\bar{r}(x)} + o(\bar{r}(x)^{-1}) \\ \nabla\phi(x) &= \nabla\left(\frac{1}{\pi} \frac{\cos\bar{\theta}(x)}{\bar{r}(x)}\right) + o(\bar{r}(x)^{-2}) \end{aligned}\right\} \quad \begin{array}{c} (\text{as } x \to \bar{y} \\ \text{from within } \Omega) \end{array} \tag{31}$$

where $\bar{r}(x)$, $\bar{\theta}(x)$ are plane-polar co-ordinates centred on $\bar{y}$ (see Figure 2), then,

$$\lim_{\varepsilon \to 0} \int_{\Gamma_\varepsilon} \nabla w \cdot \hat{n} \, \mathrm{d}s = \frac{1}{2} \frac{\partial w}{\partial x_1}(\bar{y})$$

and after expanding w in a Taylor series about $\bar{y}$ we find

$$\lim_{\varepsilon \to 0} \int_{\Gamma_\varepsilon} \nabla\phi \cdot \hat{n} w \, \mathrm{d}s = \frac{1}{2} \frac{\partial w}{\partial x_1}(\bar{y})$$

In the limit then, as $\varepsilon \to 0$, (30) gives

$$\Phi_2(w) = \frac{\partial w}{\partial x_1}(\bar{y}) = \int_\Omega L[\phi] w \, dA - \int_\Omega f\phi \, dA \tag{32}$$

This is in the form (1) with extraction function $\zeta = L[\phi]$ and load term $R = -\int_\Omega f\phi \, dA$. In general, the integrals on the right-hand side of (32) will be singular.

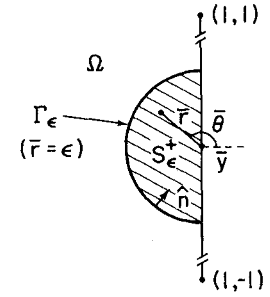


Figure 2. The region S^+_ε

As usual we should choose the generating function ϕ so that ζ is smooth. This problem can be approached in an analogous fashion to that outlined in Subsection 3.2. In our case, it can be verified that if

$$\tilde{\phi}(x) = \frac{\partial}{\partial x_1}\left(\frac{1}{\pi}\left(1 + \frac{k}{4}\bar{r}(x)^2\right)\log \bar{r}(x)\right) \tag{33}$$

then $L[\tilde{\phi}]$ is smooth about $\bar{x}$ (in fact, $L[\tilde{\phi}] = O(\bar{r}(x)\log \bar{r}(x))$. Now $\tilde{\phi}$ has the necessary asymptotic and boundary behaviour near $\bar{y}$, but it does not vanish everywhere on $\partial\Omega$. To construct suitable ϕ's based on $\tilde{\phi}$, we may use obvious adaptations of the 'cut-off' or 'blending' techniques outlined in Subsection 3.2.

3.4 *The accuracy of the approximations $\tilde{\phi}_1$, $\tilde{\phi}_2$*

Suppose that we set up a finite element model of the problem (24)/(25). In the usual way let us partition Ω into elements $E_1, E_2, \ldots, E_n$ say (we do not need to be specific about the shapes of the elements), and assume that on each element we represent $\tilde{w}$ by a polynomial of degree p. Conformity requires that these polynomials be continuous across the inter-element boundaries, and vanish on $\partial\Omega$. Denote by S the set of all such finite element functions. Let h_j be a characteristic linear dimension of E_j, and set $h = \max_j h_j$.

The finite element solution $\tilde{w}$ satisfies

$$\int_\Omega (\nabla \tilde{w} \nabla v + k\tilde{w}v) \, dA = -\int_\Omega fv \, dA \tag{34}$$

for all v from S; in addition, we have

$$\int_\Omega (\nabla(w - \tilde{w})\nabla v + k(w - \tilde{w})v \, dA = 0 \tag{35}$$

for all finite element functions v in S. Defining the strain energy expression by

$$E(\cdot)=\int_{\Omega}(\nabla(.)^2+k(.)^2)\,\mathrm{d}A$$

we have

$$E(w-\tilde{w})\leq\min_{v\in S}E(w-v) \tag{36}$$

In line with the general procedure outlined in Section 1, we consider approximations $\tilde{\Phi}_1=\tilde{\Phi}_1(\tilde{w})$ and $\tilde{\Phi}_2=\tilde{\Phi}(\tilde{w})$ to Φ_1 and Φ_2. In either case, we make an error of the form

$$e=\Phi-\tilde{\Phi}=\int_{\Omega}\zeta(w-\tilde{w})\,\mathrm{d}A \tag{37}$$

Now, just as for the one-dimensional case, introduce an auxiliary function $\psi(x)$ which satisfies

$$\nabla^2\psi-k\psi=-\zeta$$

$$\psi=0\quad\text{on }\partial\Omega$$

or equivalently,

$$\int_{\Omega}(\nabla\psi\nabla u+k\psi u)\,\mathrm{d}A=\int_{\Omega}\zeta u\,\mathrm{d}A$$

for all functions u which vanish on $\partial\Omega$ and for which $E(u)$ is finite. We may certainly choose $u=w-\tilde{w}$ to obtain, from (37),

$$e=\int_{\Omega}\nabla\psi\nabla(w-\tilde{w})+k\psi(w-\tilde{w})\,\mathrm{d}A$$

and using (35) we see that for any finite element function v from S

$$\begin{aligned}|e|&=\left|\int_{\Omega}(\nabla(\psi-v)\nabla(w-\tilde{w})+k(\psi-v)(w-\tilde{w})\,\mathrm{d}A\right|\\&\leq E(\psi-v)^{1/2}E(w-\tilde{w})^{1/2}\end{aligned}$$

So on choosing v to minimize $E(\psi-v)$, and recalling (36), we have

$$|e|\leq\min_{v\in S}E(\psi-v)^{1/2}\min_{v^*\in S}E(w-v^*)^{1/2} \tag{38}$$

This estimate is telling us, exactly as did (20) in the one-dimensional case, that the accuracy of $\tilde{\Phi}$ depends on how well both the solution w of the original problem, and the solution ψ of the auxiliary problem, can be approximated in the energy norm by the finite element functions in S.

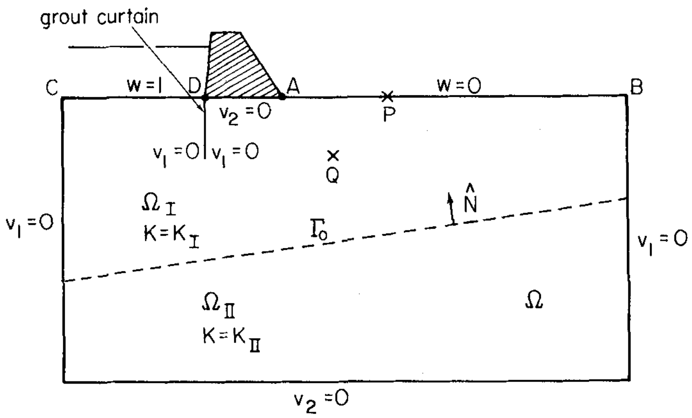
If we try to obtain rates of convergence for $\tilde{\Phi}$, we come up against some important differences between the one- and two-dimensional cases. In general, the analogue of (22) holds only if the boundary of Ω is smooth. If $\partial\Omega$ is not smooth then (22) must be modified to account for some special singular terms that arise because of corners of $\partial\Omega$ (see Reference 4). These singular terms govern the smoothness and approximability of w and ψ. The analogue of estimate (21) is also more complicated in the two-dimensional case (see Reference 3). None the less, if the mesh has the proper level of refinement around the corners of $\partial\Omega$, then similar results to those in the one-dimensional case can be achieved if the rate of convergence is now measured with respect to the number of degrees-of-freedom rather than p and h. To go into further details is beyond the scope of this paper (see, however, References 5 and 6).

4 TWO-DIMENSIONAL PROBLEM (SEEPAGE PROBLEM)

4.1 *Formulation of the problem*

We shall briefly discuss the problem illustrated in Figure 3. This models the seepage under a dam which has been fitted with a grout curtain. The mathematical model is based upon the following assumptions:

1. A linear relationship (Darcy's law) between flow velocity $v=(v_1, v_2)$ and the gradient of the piezometric head w, namely $v=-K\nabla w$, where $K>0$ is the permeability of the (isotropic) ground material.
2. The flow is incompressible, that is $\nabla \cdot v=0$.



$\nabla^2 w=0$ in Ω_{I} and Ω_{II}

$-Kv.\hat{N}$ continuous across the interface Γ_0

Figure 3. Model for the seepage beneath an impermeable dam with a grout curtain: w = piezometric head, K = permeability, $v=(v_1, v_2)$ = flow velocity = $-K\nabla w$ (Darcy's law)

We shall restrict our attention to the slit region Ω (the slit models the grout curtain). The region Ω is composed of two subregions Ω_{I} and Ω_{II} which meet along an oblique interface Γ_0. We suppose that the permeability is constant in each subregion (zone) taking the values K_{I} and K_{II} in Ω_{I} and Ω_{II}, respectively. The ground surface downstream from the dam is taken as the zero of piezometric head, and the value of w at the ground surface upstream has been scaled to unity. The region Ω is assumed large enough that a no-outflow condition is valid on all the below ground boundaries. Finally, the grout curtain and the dam base are assumed impermeable.

The governing differential equation is

$$\nabla^2 w = 0 \quad \text{in } \Omega_{\text{I}} \text{ and } \Omega_{\text{II}} \tag{39}$$

with boundary conditions on $\partial\Omega$ as shown in Figure 2. There is also an interface condition

$$(-K\nabla w.\hat{N})_{\text{I}} = (-K\nabla w.\hat{N})_{\text{II}} \quad \text{on } \Gamma_0 \tag{40}$$

where $\hat{N}$ is a unit normal to Γ_0, and the subscripts I, II indicate limiting values as Γ_0 is approached from within Ω_{I}, Ω_{II}, respectively.
The three quantities that we shall be interested in evaluating are:

1. The total outflow per unit time through the downstream surface AB,

$$\Phi_1 = -\int_{\text{AB}} K_{\text{I}} \frac{\partial w}{\partial x_2} \, \mathrm{d}s$$

2. The outflow speed $\Phi_2 = -K_{\text{I}}\, \partial w/\partial x_2$ at a point P on the downstream surface AB.
3. The piezometric head $\Phi_3 = w$ at a point Q in Ω_{I}.

4.2 An extraction expression for Φ_1

Suppose that ϕ is a smooth function which satisfied (i) $\phi = -1$ on AB and (ii) $\phi = 0$ on CD. Then an integration by parts shows

$$\int_\Omega K\nabla w.\nabla\phi \, \mathrm{d}A = \int_{\partial\Omega} K\nabla w.\hat{n}\phi \, \mathrm{d}s + \int_{\Gamma_0} [(K\nabla w.\hat{N})_{\text{II}} - (K\nabla w.\hat{N})_{\text{I}} \, \mathrm{d}s - \int_{\Omega_{\text{I}}\cup\Omega_{\text{II}}} K\nabla^2 w\phi \, \mathrm{d}A$$

where $\hat{n}$ is the outward pointing unit normal on $\partial\Omega$. Using (39), (40) the boundary conditions for w on $\partial\Omega$, we obtain the extraction expression

$$\Phi_1 = -\int_{\text{AB}} K_{\text{I}} \frac{\partial w}{\partial x_2} \, \mathrm{d}s = \int_\Omega K\nabla w.\nabla\phi \, \mathrm{d}A \tag{41}$$

Notice that this formula is an example of a generalized version of (1) since it entails the integration of the derivatives of w. It is not diffcult to see that there are many choices for the generating function ϕ which lead to smooth extraction functions in (41).

As usual, the extraction expression (41) suggests that we try to approximate Φ_1 by

$$\tilde{\Phi}_1 = \int_\Omega K\nabla\tilde{w}.\nabla\phi \, \mathrm{d}A$$

where $\tilde{w}$ is a finite element approximation to w.

4.3 An extraction expression for Φ_2

Setting

$$\phi = \frac{1}{\pi}\frac{\sin\theta}{r} \qquad (r, \theta \text{ polar co-ordinates central at } P) \tag{42}$$

and proceeding as in Subsection 3.3, we find

$$\Phi_2 = -K_{\text{I}} \frac{\partial w}{\partial x_2}(P) = \int_{\partial\Omega} K\nabla\phi.\hat{n}w \, \mathrm{d}s - (K_{\text{I}} - K_{\text{II}}) \int_{\Gamma_0} \nabla\phi.\hat{N}w \, \mathrm{d}s \tag{43}$$

where $\hat{n}$ is the outward pointing unit normal on $\partial\Omega$. Notice that this formula is another example of a generalized version of (1), needing only the evaluation of line integrals along $\partial\Omega$ and the interface Γ_0. (Since ϕ, as given in (42), already vanishes on the parts of $\partial\Omega$ where w is prescribed, there was no reason to explicitly introduce cut-off functions, blending functions, etc., to impose this condition.) Observe also, that the integral over $\nabla\Omega$ includes no contribution from AB, since $w=0$ there; and that the extraction functions in (43) are smooth as long as P is 'reasonably' distant from A or B. How to proceed when this is not the case is discussed in Reference 5.

Based on (43), we have the approximation

$$\tilde{\Phi}_2=\int_{\partial\Omega} K\nabla\phi.\hat{n}\tilde{w}\,\mathrm{d}s-(K_{\mathrm{I}}-K_{\mathrm{II}})\int_{\Gamma_0}\nabla\phi.\hat{N}\tilde{w}\,\mathrm{d}s$$

to Φ_2.

4.4 *An extraction expression for* Φ_3

Set $\phi=(1/2\pi K_{\mathrm{I}})(\log r-\phi_0)$ (r, θ polar co-ordinates centred on Q) where ϕ_0 is some smooth blending function which ensures that ϕ vanishes on AB and CD. Proceeding much as in Subsection 3.2, we find

$$\Phi_3=w(Q)=\int_{\partial\Omega} K\nabla\phi.\hat{n}w\,\mathrm{d}s-(K_{\mathrm{I}}-K_{\mathrm{II}})\int_{\Gamma_0}\nabla\phi.\hat{N}w\,\mathrm{d}s+\int_{\Omega}K\nabla^2\phi_0 w\,\mathrm{d}A \tag{44}$$

We could, for instance, use $\phi_0(x)=\log|Q-(x_1,d)|$ where $x_2=d$ is the equation of the BC. Then, provided Q is 'reasonably' distant from $\partial\Omega$ and Γ_0, the extraction functions appearing in (44) are smooth.

As usual, we may use (44) to obtain the approximation

$$\tilde{\Phi}_3=\int_{\partial\Omega} K\nabla\phi.\hat{n}\tilde{w}\,\mathrm{d}s-(K_{\mathrm{I}}-K_{\mathrm{II}})\int_{\Gamma_0}\nabla\phi.\hat{N}\tilde{w}\,\mathrm{d}s+\int_{\Omega}K\nabla^2\phi_0\tilde{w}\,\mathrm{d}A$$

4.5 *The accuracy of the approximation* $\tilde{\Phi}_i (i=1,2,3)$

Just as for the one- and two-dimensional problems already considered in Sections 2 and 3, the error $|\Phi_i-\tilde{\Phi}_i|$ is related to how well the finite element functions can simultaneously approximate both the solution of the primary problem (39), (40) and the solution of an auxiliary problem. The auxiliary problem in this case has the same form as (39), (40) except that there are now loadings on $\partial\Omega$, Γ_0 and Ω. These loadings are related to the corresponding extraction functions. The same comments we made in Sections 2 and 3 concerning the desirability of smooth extraction functions apply here also. In addition, the presence of the grout curtain and the change in the nature of the boundary condition at A gives rise to solutions having singular behaviour. Numerically this should be dealt with in a proper manner. We shall not go into detail here, (however, see References 5 and 6), except to say that with the appropriate mesh refinement these problems may be effectively overcome.

5 A NUMERICAL EXAMPLE

5.1 *Formulation of the example*

As a practical demonstration of the methods discussed in Section 3, we shall consider some numerical results for the problem modelling a square, uniformly loaded membrane which is fixed along its edges. More specificially, we deal with the problem governed by the differential equation

$$\nabla^2 w = -1 \quad \text{on } \Omega = (-1, 1)^2 \tag{45}$$

and boundary conditions

$$w = 0 \quad \text{on the boundary } \partial\Omega \text{ of } \Omega \text{ (See Figure 4)} \tag{46}$$

(This mathematical formulation also models the torsion problem for a square beam.)

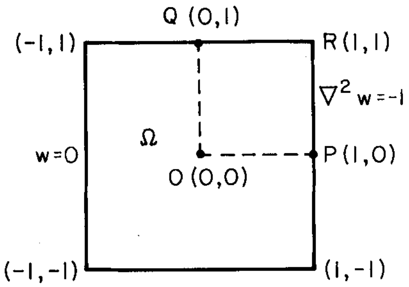


Figure 4. Model for the membrane problem

We shall employ the theory of Section 3 for the calculation of approximate values for:

1. The displacement at the centre of the membrane: $\Phi_1 = \Phi_1(w) = w(0)$.
2. The stress at the point $P(1, 0)$: $\Phi_2 = \Phi_2(w) = \partial w/\partial x_1(P)$.

By the method of separation of variables, an infinite series representation of w can be found. Using this series the following exact values (accurate to five significant figures) can be calculated:

$$E(w) = \int_\Omega |\nabla w|^2 \, dA = 0{\cdot}56231$$

$$\Phi_1(w) = w(0) = -0{\cdot}29469$$

$$\Phi_2(w) = \frac{\partial w}{\partial x_1}(P) = 0{\cdot}67531$$

Let us also note that the solution w is relatively smooth (in fact, it has square integrable second derivatives, although not square integrable third derivatives).

5.2 *The finite element approximation*

We shall consider a simple finite element model of (45)/(46); namely, bilinear elements on a square uniform mesh. By the symmetry of the problem, we need only actually calculate using the quarter-segment *OQRP* of Ω (see Figure 4). For this problem we expect the following rates of convergence:

$O(h^2)$	for the energy $E(\tilde{w})$
$O(h)$	for the energy norm of the error $E(w-\tilde{w})^{1/2}$
$O(h^2)$	for the displacement $\tilde{w}(0)$
$O(h)$	for the stress $\dfrac{\partial \tilde{w}}{\partial x_1}(P)$

where, as usual, h denotes the length of the side of an element. Using a uniform mesh and elements of degree 2 or higher we would obtain

$$O(h^3) \qquad \text{for the energy } E(\tilde{w})$$

$$O(h^{2\cdot 5-\varepsilon}) \qquad \text{for the displacement } \tilde{w}(0)$$

and

$$O(h^{1\cdot 5-\varepsilon}) \qquad \text{for the stress } \frac{\partial \tilde{w}}{\partial x_1}(P)$$

where $\varepsilon > 0$ is an arbitrary small number. For the h–p version, it is possible by suitable refinement about the corner points to obtain arbitrarily large orders of convergence with respect to the number of degrees-of-freedom (see Reference 3).

5.3 Calculation of $\tilde{\Phi}_1(\tilde{w})$

In accordance with the theory developed in Subsection 3.2, we use the formula

$$\tilde{\Phi}_1(\tilde{w}) = -\int_\Omega \nabla^2\phi\tilde{w}\,\mathrm{d}A - \int_\Omega \phi\,\mathrm{d}A$$

where ϕ takes the generic form

$$\phi = X(x_1, x_2)\left[\frac{1}{2\pi}\log(x_1^2+x_2^2)^{1/2} - \phi_0(x_1, x_2)\right]$$

We consider two choices for ϕ:

Case (a): $X(x_1, x_2) = \bar{X}(x_1)\bar{X}(x_2)$, where

$$\bar{X}(t) = \begin{cases} 1 & 0 \leqslant |t| \leqslant \frac{1}{2} \\ 1 - 8(|t| - \frac{1}{2})^3 & \frac{1}{2} < |t| \leqslant 1 \end{cases}$$

(see Figure 5), and

$$\phi_0(x_1, x_2) = 0$$

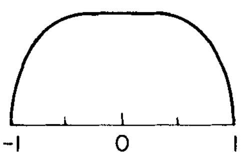


Figure 5. Cut-off function used in the evaluation of $\tilde{\Phi}_1$—case (a)

Case (b): $X(x_1, x_2) = 1$, and

$$\phi_0(x_1, x_2) = \frac{1}{2\pi}\left(\log\left(\frac{(1+x_1^2)(1+x_2^2)}{2}\right)^{1/2}\right)$$

In case (a) we have employed a cut-off function technique to enforce the boundary conditions on ϕ, while in case (b) a blending function method has been used. The first integral in the foregoing formula for $\tilde{\Phi}_1$ may be calculated by numerical quadrature. (We used Gaussian quadrature.) The second integrand is singular at 0. This integral may be evaluated analytically. However, it is also possible to calculate it numerically by the following procedure. Choosing ρ such that $\nabla^2\rho = 1$ (e.g. $\rho = \frac{1}{4}(x_1^2 + x_2^2)$), integration by parts gives

$$\int_\Omega \phi\nabla^2\rho \,\mathrm{d}A = \int_{\partial\Omega} \phi\nabla\rho.\hat{n}\,\mathrm{d}s - \int_{\partial\Omega} \nabla\phi.\hat{n}\rho\,\mathrm{d}s + \int_{\Omega-(0,0)} \nabla^2\phi\rho\,\mathrm{d}A + \rho(0,0)$$

All the integrals on the right-hand side are proper, and may be readily evaluated by numerical means.

Table III. Table of the results of the numerical calculations ((*): negative signs have been suppressed in this table. Percentages in parentheses are relative errors with respect to the appropriate exact value)

No. of elements in quarter-segment (uniform mesh)		4	16	64	Exact value
Energy norm error in $\tilde{w}$ $= \left(\frac{E(w-\tilde{w})}{E(w)}\right)^{1/2}$		30·1%	15·2%	7·62%	
Displacement: standard method, $\tilde{w}(0)$		(*) 0·310714	0·298393	0·295596	
		(5·4%)	(1·3%)	(0·31%)	
Displacement: post-processing method, $\tilde{\Phi}_1(\tilde{w})$ (see Subsection 5.3)	Case (a)	0·268783	0·287205	0·292751	0·29469
		(8·8%)	(2·5%)	(0·65%)	
	Case (b)	0·287306	0·292829	0·294220	
		(2·5%)	(0·63%)	(0·16%)	
Stress: standard method, $\frac{\partial w}{\partial x_1}(P)$		0·482142	0·565480	0·61687	
		(29%)	(16%)	(8·7%)	
Stress: post-processing method, $\tilde{\Phi}_2(\tilde{w})$ (see Subsection 5.4)	Case (a)	0·64758	0·67197	0·67463	
		(4·1%)	(0·49%)	(0·096%)	0·67528
	Case (b)	0·66623	0·67313	0·67477	
		(1·3%)	(0·32%)	(0·076%)	
	Case (c)	0·66482	0·67276	0·67468	
		(1·5%)	(0·37%)	(0·089%)	

The results of the computations are shown in the middle section of Table III. For comparison, we also list the value of the finite element solution $\tilde{w}$ at 0. Notice that $\tilde{w}(0)$ and both cases of $\tilde{\Phi}_1$ all show an $O(h^2)$ rate of convergence. This is as we would expect. Observe also the superiority of the post-processed value in case (b) over case (a). This is in line with our previous comment that blending function technqiues can usually be expected to perform better than cut-off function methods. (Looking at the definition of X in case (a) and examining Figure 5 shows that indeed X changes quite rapidly in the region $|x_2| > \frac{1}{2}$. In terms of the arguments we presented in Subsection 3.5, we should therefore not expect the corresponding ψ to be as well approximated from within our finite element subspace as it would be in case (b)—see (38).

The fact that the accruacies of $\tilde{w}(0)$ and $\tilde{\Phi}_1 \tilde{w})$ are comparable in this example is a consequence of our using bilinear elements. None the less, Table III shows that, in case (b), the $\tilde{\Phi}$ values are twice as accurate as the $\tilde{w}(0)$ values for the same number of elements. Putting this another way, for the same accuracy the 'direct' displacement method would require twice as many elements as the post-processing approach of case (b).

5.4 *Calculation of* $\tilde{\Phi}_2(\tilde{w})$

In the case of our model problem, the theory of Subsection 3.3 leads to

$$\tilde{\Phi}_2(\tilde{w}) = \int \nabla^2\phi\tilde{w}\,\mathrm{d}A + \int \phi\,\mathrm{d}A$$

where ϕ takes the generic form

$$\phi = X(x_1, x_2)\left(\frac{1}{\pi}\right)\left(\frac{x_1 - 1}{(x_1-1)^2 + x_2^2} - \phi_0(x_1, x_2)\right)$$

We shall treat three cases:

Case (a):

$$X(x_1, x_2) = \begin{cases} 1 & \frac{1}{2} \leqslant x_1 \leqslant 1 \\ 8(6x_1^4 - 8x_1^3 + 3x_1^2) & 0 \leqslant x_1 < \frac{1}{2} \\ 0 & -1 \leqslant x_1 < 0 \end{cases}$$

(see Figure 6(i))

$$\phi_0(x_1, x_2) = \frac{x_1 - 1}{(x_1 - 1)^2 + 1}$$

Case (b):

$$X(x_1, x_2) = \begin{cases} 1 & 0 \leqslant x_1 \leqslant 1 \\ 1 - |x_1|^3 & -1 \leqslant x_1 < 0 \end{cases}$$

(see Figure 6(ii))

$$\phi_0 = \frac{x_1 - 1}{(x_1 - 1)^2 + 1}$$

Case (c):

$$X(x_1, x_2) = 1$$

$$\phi_0 = \frac{x_1 - 1}{(x_1 - 1)^2 + 1} + (x_1 - 1)\left(\frac{1}{4 + x_2^2} - \frac{1}{5}\right)$$

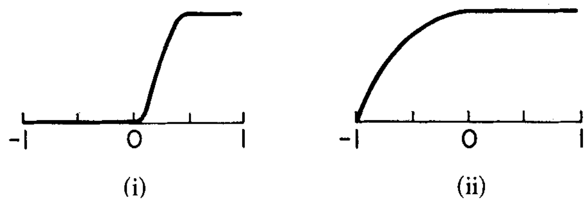


Figure 6. Cut off-functions used in the evaluation of $\tilde{\Phi}_2$: (i) case (a); (ii) case (b)

Cases (a) and (b) correspond to our using a blending function technique to satisfy the boundary condition on the edges $x_2 = \pm 1$, and a cut-off function method to handle the edge $x_1 = 1$. In case (c), a blending function method is used to handle the entire boundary. Conerning the actual evaluation of $\tilde{\Phi}_2(\tilde{w})$, the same comments made in Subsection 5.2 about $\tilde{\Phi}_1(\tilde{w})$ apply here also.

The results of the calculations are shown in the lower part of Table III, where, for comparison, we have also listed the corresponding values of $\partial \tilde{w}/\partial x_1(P)$. In contrast to the situation for the displacements, we see that the post-processed values for $\tilde{\Phi}_2$ are markedly more accurate than the 'direct' value $\partial \tilde{w}/\partial x_1(P)$. We see, as theory predicts, an $O(h)$ rate of convergence for the 'direct' value, but an $O(h^2)$ rate for $\tilde{\Phi}_2$.

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