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STATE DIFFUSION PROBLEMS
CONTAINING SINGULARITIES

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NUMERICAL SOLUTION OF STEADY STATE
DIFFUSION PROBLEMS CONTAINING SINGULARITIES

by

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Summary

A study is made of steady state diffusion in two-component composites made up of isolated islands of impermeable material in a continuum. Advantage is taken of symmetry so that only a problem in an L-shaped subregion need be considered. However, this problem contains a boundary singularity which causes numerical solutions calculated with standard finite element and finite difference methods to be inaccurate. The modification of these standard methods through the inclusion of terms having the form of the singularity or by local mesh refinement to provide applicable error analysis and to increase accuracy is discussed. Finite element results are given, and these are compared with those obtained with finite-difference methods and with a numerical conformal transformation method.

1. INTRODUCTION AND PHYSICAL PROBLEM

In the study of steady state diffusion in heterogeneous mixtures some property of the mixture, for example permeability or thermal conductivity, has to be determined. This property is itself related to a characteristic of the physical situation. Thus permeability is related to concentration of diffusing substance and thermal conductivity to temperature. In this paper the mixtures under consideration are two-component composites made up of isolated islands of impermeable material in a continuum.

We consider a two dimensional model situation of the type described above in which the function $u(x,y)$ represents either concentration of diffusing substance or temperature. In the composite it is assumed for simplicity that rectangular impermeable blocks are present on a regular lattice in an isotropic substance, see Figure.1, and that u is held constant on the sides of the composite. Advantage can be taken of the symmetry so that only a section of the problem in an L-shaped subregion, such as $\overline{OBCDEFO} = \Omega$ with boundary $\partial\Omega$ as in Figure 1, need be considered see[5], where $\overline{OB} = \overline{BC} = \overline{EF} = \overline{FO} = \frac{1}{2}\overline{CD} = \overline{DE} = 1$

The problem therefore becomes that of finding, $u(x,y)$, the solution of the harmonic mixed boundary value problem

$$-\Delta[u(x,y)] = 0, \quad (x,y) \in \Omega, \quad (1.1)$$

$$u(x,y) = 1, \quad (x,y) \in CD, \quad (1.2)$$

$$u(x,y) = 0, \quad (x,y) \in EF, \quad (1.3)$$

$$\frac{\partial u(x,y)}{\partial x} = 0, \quad (x,y) \in \overline{OB}, \quad (1.4)$$

$$\frac{\partial u(x,y)}{\partial x} = 0, \quad (x,y) \in \overline{BC} \cup \overline{DE} \cup \overline{FO}, \quad (1.5)$$

where the Dirichlet boundary conditions are taken for convenience

as zero and unity and can be scaled as necessary. We define the

two disjoint parts of the boundary $\partial\Omega_1 \equiv \overline{CD} \cup \overline{EF}$ and $\partial\Omega_2 \equiv \overline{OB} \cup \overline{BC} \cup \overline{DE} \cup \overline{FO}$

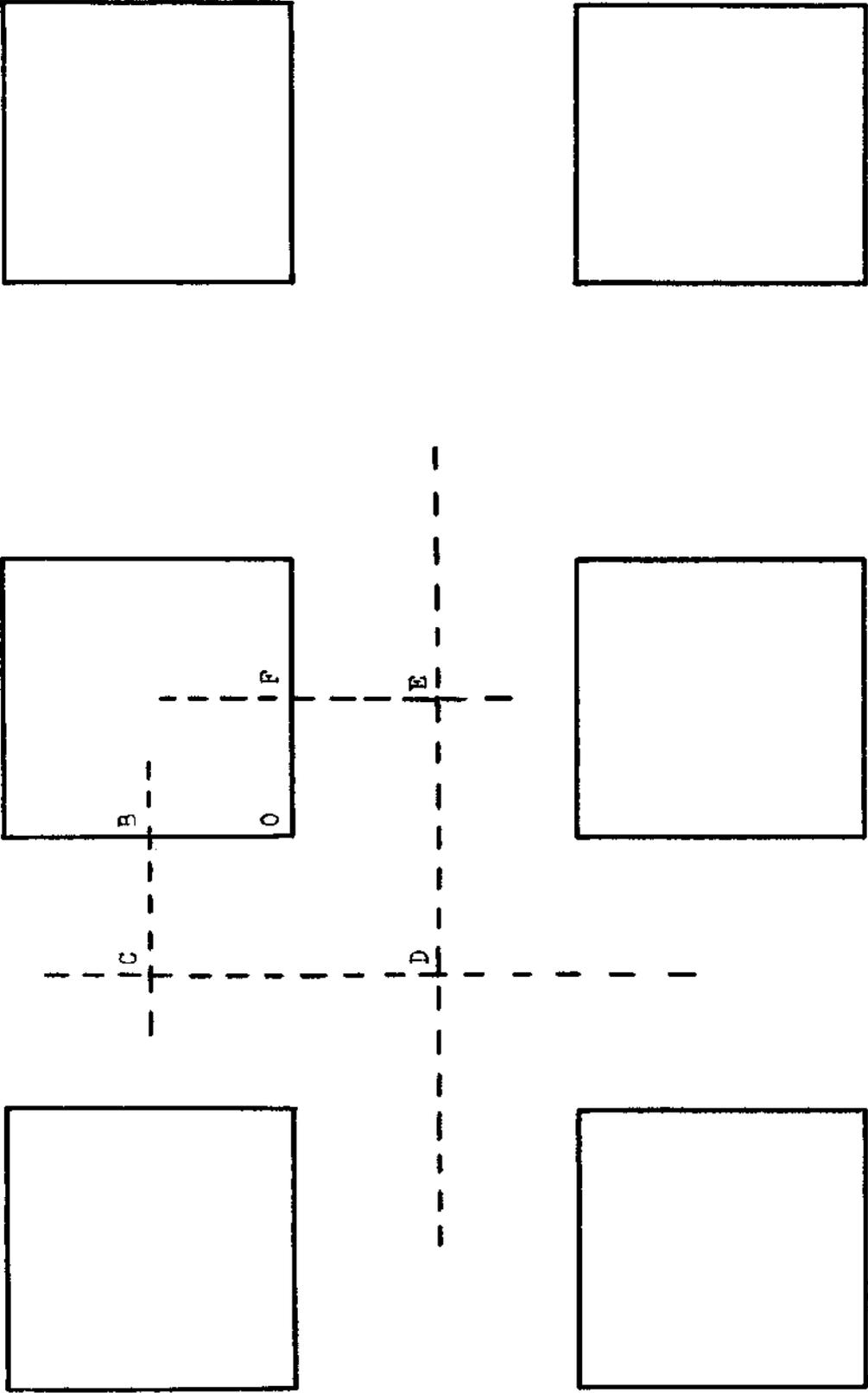


Figure 1.

and let $\Omega \equiv \Omega \cup \partial\Omega$.

The region Ω contains a re-entrant corner at 0 with internal angle $3\pi/2$, and as a result u possesses a boundary singularity in that it has derivatives which are unbounded at the corner. This is illustrated by the use of an asymptotic expansion of the solution due to Wasow [22] which was later adapted by Lehman [14]. In terms of local polar co-ordinates (r, θ) , with origin at the corner and zero angle along one of the arms of the corner, the asymptotic form of u is

$$\begin{aligned} u(r, \theta) &= \sum_i a_i \Phi_i(r, \theta) \\ &= a_1 r^{2/3} \cos \frac{20}{3} + a_2 r^{4/3} \cos \frac{40}{3} + \dots \end{aligned} \quad (1.6)$$

From (1.6) it is clear that $\partial u / \partial r$ is unbounded at $r=0$.

A problem of this type containing a slit has recently been considered by Rosser and Papamichael [18]. For this the re-entrant angle at the tip of the slit is 2π . They show that the series expansion about the tip of the slit, corresponding to (1.6), is convergent throughout the region of the problem so that in their case the exact rather than asymptotic form of u is given.

2. WEAK PROBLEM AND GALERKIN METHOD

Let $W_2^1(\Omega)$ be the Sobolev space of functions which together with their generalized derivatives of order one are in $L_2(\Omega)$. The subspace of functions in $W_2^1(\Omega)$ which satisfy a homogeneous boundary condition on $\partial\Omega_1$ is written $W_2^1(\Omega) \cap (\partial\Omega_1)_0$; that is for $v \in W_2^1(\Omega) \cap (\partial\Omega_1)_0$, $v \in W_2^1(\Omega)$ and $v = 0$ on $\partial\Omega_1$.

The weak problem corresponding to (1.1) - (1.5) is :

find $u \in \psi + W_2^1(\Omega)$ such that

$$a(u, v) = 0 \quad \forall v \in W_2^1(\Omega) \cap (\partial\Omega_1)_0, \quad (2.1)$$

were $\phi \in W^1_2(\bar{\Omega})$ with $\phi = 0$ on \overline{EF} . The notation

$u \in \psi + W^1_2(\Omega)$ means that $u = \psi + v$, where $v \in W^1_2(\Omega) \cap (\mathbb{F}\Omega_1)_0$. In (2.1) the "bilinear functional $a(u, v)$ is defined as

$$a(u, v) = \iint_{\Omega} \left(\frac{\partial u}{\partial x} \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \frac{\partial v}{\partial y} \right) dx dy \quad \square \quad u, v \in W^1_2(\Omega).$$

The energy norm $\|v\|_E$ is defined by

$$\|v\|_E = (a(v, v))^{1/2}. \quad (2.2)$$

The region Ω is discretized into elements, either entirely into triangles or entirely into rectangles so that there are m interior mesh points (nodes), n mesh points on and p mesh points on $\mathbb{F}\Omega_2$.

The elements have generic length h . In similar manner to that in

Barnhill and Whiteman [3] $\{B_i(x, y)\}_{i=1}^{m+p}$ and $\{C_j(x, y)\}_{j=1}^n$ are defined

To be two sets of functions which are biorthonormal (see Davis 10],)

with respect to point evaluations at the nodes. The B_i and C_j are

basis functions for our approximation. They are here taken so that,

with triangular elements each is linear in x and y , whilst with

rectangular elements each is bilinear in x and y .

The set $S^h \in \psi^h + W^1_2(\Omega)$, (i.e. elements of S^h are in $W^1_2(\Omega)$ and

take value unity at nodes in \overline{CD} and zero at nodes in \overline{EF} is defined

to be $m + p$ dimensional set elements of which can be written in the form

$$s(x, y) = \sum_{i=1}^{m+p} A_i B_i(x, y) + \sum_{j=1}^n \phi_j^h C_j(x, y). \quad (2.3)$$

In (2.3) in B_i , ψ_y^h and C_j are known and the A_i are to be found.

The $m + p$ dimensional space spanned by the B_i is written S_o^h . Note

that elements of S_o^h take on zero value on $\partial\Omega_1$ and that $S_o^h \subset W^1_2(\Omega) \cap (\partial\Omega_1)_0$.

In the Galerkin method used here we seek

$U \in S^h$ such that

$$a(U, B_k) = 0, \quad k = 1, 2, \dots, m + p. \quad (2.4)$$

The technique (2.4) for determining U is a special case of the more general method in which the test functions are all $V \in S_0^h$. Substitution of (2.3) for U in (2.4) leads to the system of linear equations for the A_i ,

$$\sum_{i=1}^{m+p} A_i a(B_i, B_k) = - \sum_{j=1}^n \varphi_j^h a(c_j, B_k), \quad k = 1, 2, \dots, m+p. \quad (2.5)$$

A best approximation property for the Galerkin solution is proved in the Lemma of [3] for the case $\partial\Omega_2 = \emptyset$. When that Lemma is applied here, it is found that the Galerkin solution U to (2.4) is the best approximation to the weak solution u of (2.1) from S^h in the energy norm (2.2).

Thus

$$\|u - U\|_E \leq \|u - w\|_E \quad \forall w \in S^h. \quad (2.6)$$

Taking for w in (2.6) the function $u \in S^h$ which interpolates u at the $m + n$ nodes in $\Omega \cup \Omega_1$, we obtain

$$\|u - U\|_E \leq \|u - u\|_E. \quad (2.7)$$

Many bounds for interpolation errors using rectangular and triangular elements have been given: see for example Birkhoff, Schultz and Varga [7] or Ciarlet and Raviart [9]. Under assumptions on the shape of both the triangular and rectangular elements, for the trial functions mentioned above, bounds of the form

$$\|u - u\|_E \leq X h |u|_2 \quad \forall Kh |u|_2 \quad (2.8)$$

can be found, where X is a constant and

$$|u|_2 = \left\{ \left\| \frac{\partial^2 u}{\partial x^2} \right\|_{L^2(\Omega)}^2 + \left\| \frac{\partial^2 u}{\partial x \partial y} \right\|_{L^2(\Omega)}^2 + \left\| \frac{\partial^2 u}{\partial y^2} \right\|_{L^2(\Omega)}^2 \right\}^{\frac{1}{2}}$$

Galerkin solutions to the weak problem (2.1) have been calculated using (2.4) with partitions of consisting either entirely of

rectangular or entirely of right triangular elements, as in Figure 2. Numerical results are given in Figure 3, and from these it is seen that the numerical solutions are inaccurate in the neighbourhood of 0 so that there they are being adversely affected by the boundary singularity. In addition it is clear from (1.6) that $u \in W_{\frac{1}{2}}(\Omega) - W_{\frac{2}{2}}(\Omega)$ so that for problem (2.1) equations (2.7) and (2.8) do not together constitute a meaningful bound for the Galerkin error.

In order that the shortcomings of inaccuracy of the Galerkin approximation and inapplicability of the error analysis for the standard Galerkin method in this context may be overcome, two modifications are now proposed. These are

- (i) local mesh refinement in the neighbourhood of 0,
- (ii) inclusion of singular terms from (1.6) in the trial functions in elements near 0.

Local Mesh Refinement

Functions contained in $W_{\frac{1}{2}}(\Omega)$ possess certain continuity properties which, since $S^h \subset W_{\frac{1}{2}}(\Omega)$, also have to be exhibited by functions in S^h . The continuity condition which must be satisfied is the conforming condition. and in this case it is that $S^h \subset C^0(\Omega)$. Thus to be conforming the global approximating functions of Section 2 for both triangular and rectangular meshes must be continuous over Ω . For a standard triangular mesh with linear interpolation to the function values at the vertices of each triangle, or a standard rectangular mesh with bilinear interpolation to the function values at the four corners of each rectangle, the global approximating functions are in $C^0(\Omega)$. Thus the results of Section 2 have been derived with conforming functions.

Refinement of the mesh will not make the above error analysis applicable to singular problems. However, as would be expected, refinement

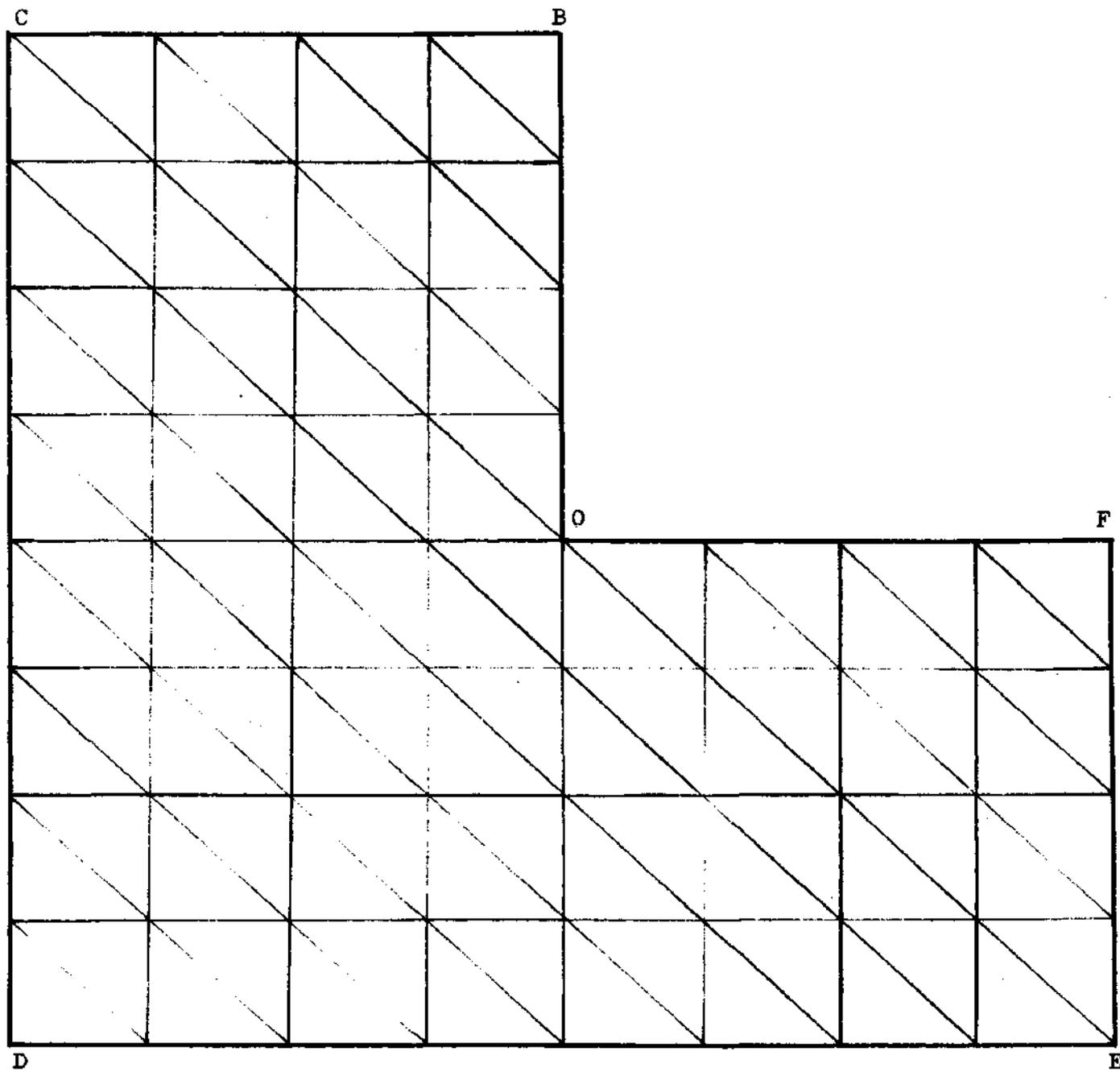


Figure 2.

1.0000	0.9698	0.9425	0.9202	0.9055	0.9005	At each mesh point P the numbers				
	0.9687	0.9401	0.9166	0.9011	0.8955	the significance.				
	0.9669	0.9366	0.9120	0.8958	0.8902					
1.0000	0.9686	0.9398	0.9163	0.9007	0.8953	CTM [17]				
	0.961k	0.9374	0.9127	0.8960	0.8900					
	0.965	0.9337	0.9077	0.8903	0.8843					
1.0000	0.9647	0.9319	0.9044	0.8856	0.8787	See section 4				
	0.9636	0.9296	0.9007	0.8803	0.8725	Finite elements with isoscles				
	0.9614	0.9253	0.8944	0.8731	0.8653	right triangles, h=0.1				
1.0000	0.9584	0.9188	0.8839	0.8581	0.8482	Finite elements with				
	0.9573	0.9166	0.8802	0.8521	0.8394	squares, h=0.1				
	0.9551	0.9119	0.8725	0.8409	0.8296					
1.0000	0.9502	0.9013	0.8548	0.8146	0.7948					
	0.9472	0.8992	0.8513	0.8085	0.7808					
	0.9472	0.8950	0.8440	0.7953	0.7928					
1.0000	0.9411	0.8816	0.8207	0.7560	0.6663	0.4884	0.3580	0.2371	0.1170	0.0000
	0.9402	0.8797	0.8173	0.7498	0.6667	0.5003	0.3653	0.2405	0.1196	
	0.9389	0.8771	0.8135	0.7456	0.6635	0.5118	0.3674	0.2418	0.1201	
1.0000	0.9324	0.8632	0.7897	0.7066	0.6026	0.4788	0.3555	0.2355	0.1174	0.0000
	0.9319	0.8622	0.7885	0.7068	0.6096	0.4847	0.3602	0.2386	0.1189	
	0.9311	0.8606	0.7864	0.7043	0.6048	0.4891	0.3637	0.2401	0.1195	
1.0000	0.9254	0.8487	0.7672	0.6774	0.5760	0.1616	0.3490	0.2326	0.1162	0.0000
	0.9253	0.8486	0.7676	0.6794	0.5803	1.4685	0.3522	0.2348	0.1174	
	0.9247	0.8474	0.7658	0.6768	0.5780	0.4693	0.3541	0.2362	0.1180	
1.0000	0.9204	0.8388	0.7528	0.6605	0.5606	0.4539	0.3428	0.2294	0.1149	0.0000
	0.9206	0.8393	0.7540	0.6627	0.5637	0.4569	0.3453	0.2311	0.1158	
	0.9200	0.8382	0.7523	0.6607	0.5621	0.4567	0.3460	0.2319	0.1163	
1.0000	0.9175	0.8331	0.7450	0.6516	0.5524	0.4477	0.3387	0.2271	0.1139	0.0000
	0.9179	0.8340	0.7465	0.6538	0.5550	0.4502	0.3408	0.2286	0.1147	
	0.9173	0.8328	0.7449	0.6520	0.5536	0.4496	0.3410	0.2290	0.1149	
1.0000	0.9163	0.8315	0.7426	0.6486	0.5500	0.4452	0.3376	0.2257	0.1140	0.0000
	0.9170	0.8323	0.7440	0.6510	0.5522	0.4480	0.3393	0.2277	0.1142	
	0.9164	0.8311	0.7425	0.6193	0.5509	0.4473	0.3393	0.2279	0.1145	

Figure 3

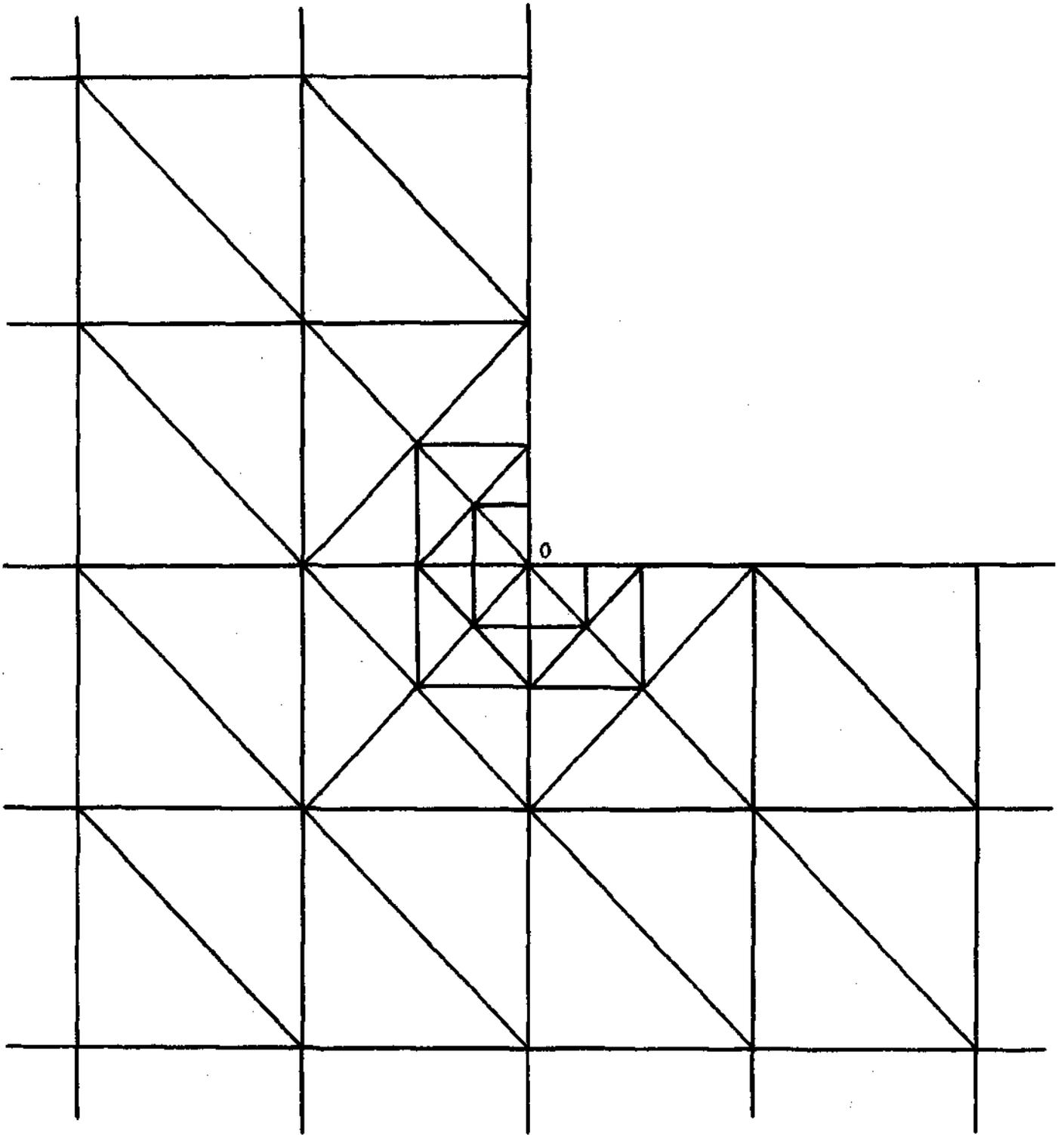


Figure 4.

10.

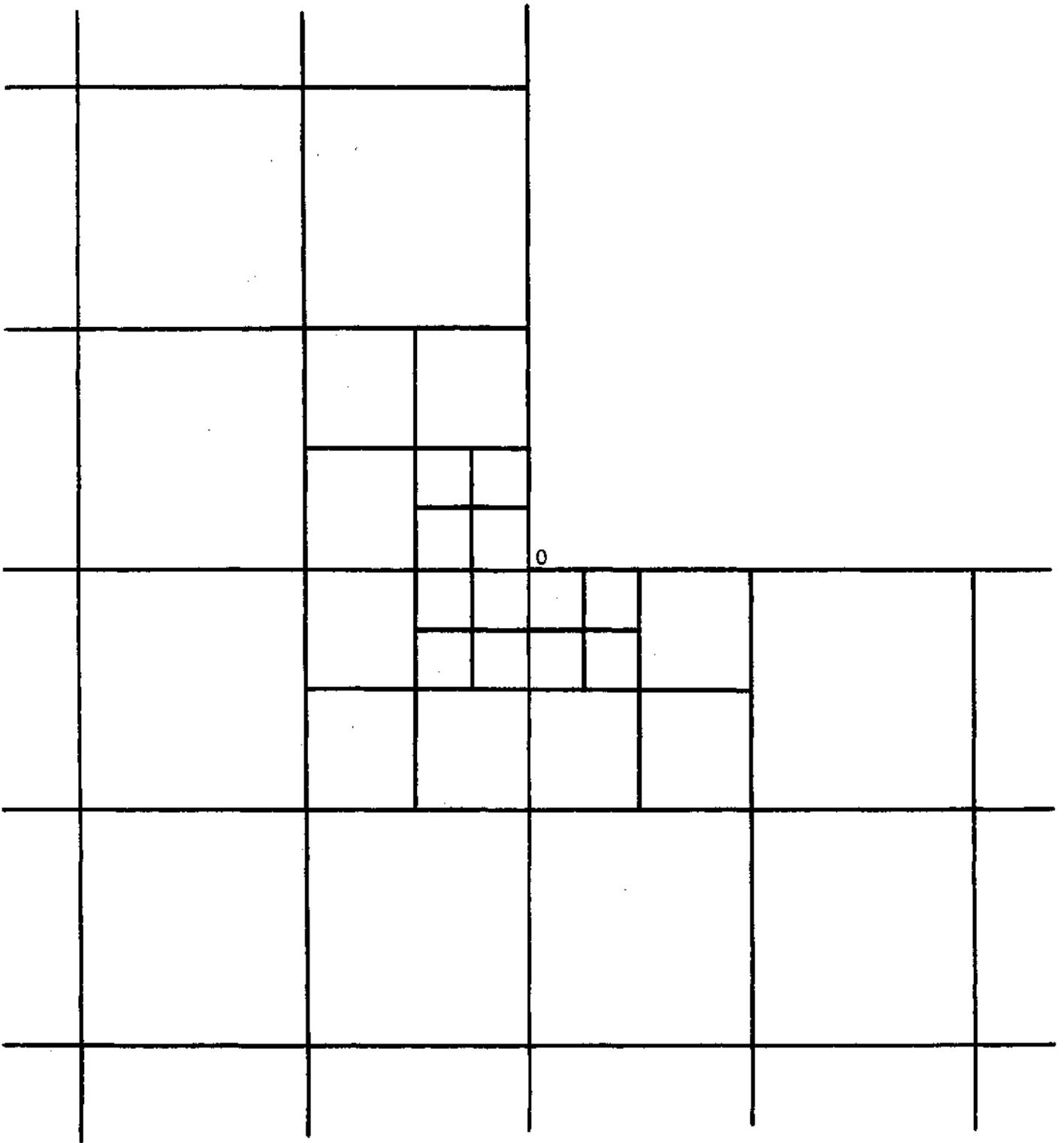


Figure 5.

does improve the accuracy of the numerical approximations, particularly in the neighbourhood of a singularity. The shortcoming of refining over the whole of the region Ω is that many mesh points remote from the singularity are introduced needlessly so that the resulting stiffness systems are unnecessarily large. In order to keep the total number of points in the discretization as small as possible, we refine only in the neighbourhood of 0 as indicated in Figures 4 and 5. With right triangular elements as many levels of refinement as required can be performed (in Figure 4 two levels are shown) and the elements are all triangles with nodes at the vertices. The linear trial function interpolating the function value at each node is used in each element. A piecewise linear trial function is again obtained which satisfies the conforming condition. For local refinement with rectangular elements the scheme of Figure 5 introduces mid-side nodes and special interpolants must be used in the five node rectangles so that the global approximating function may again be in C^0 . Five node interpolants of this type have been derived by Gregory and Whiteman in [12] and [13] so that merely the general form is given here. This is stated for a square element of unit side length, but can be scaled for a square of side h or for a rectangle.

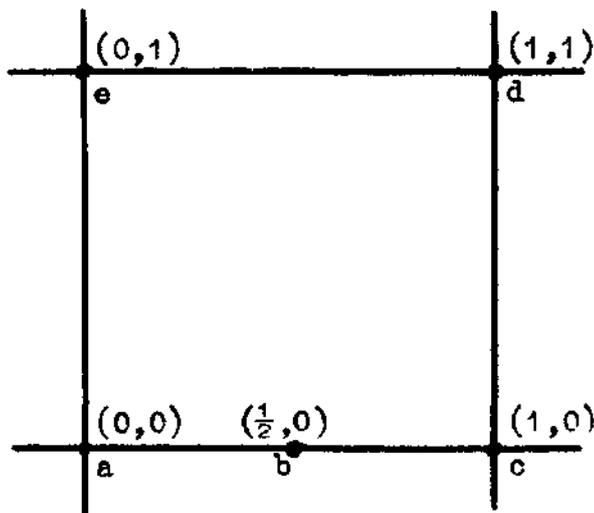


Figure 6.

12.

Consider the five node square element, Figure 6, with nodes at the points $a \equiv (0,0)$, $b = (\frac{1}{2},0)$, $c \equiv (1,0)$ $d \equiv (1,1)$ and $e \equiv (0,1)$. From [13] the trial function which is continuous throughout the element, which is bilinear for $0 \leq x \leq \frac{1}{2}$ and for $\frac{1}{2} \leq x \leq 1$, which interpolates the nodal values and which is linear along \overline{ab} , \overline{bc} , \overline{cd} , \overline{de} , and \overline{ea} , is

$$U(x,y) = (1-x)y U(0,1) + xy U(1,1) + \begin{cases} (1-2x)(1-y)U(0,0) + 2x(1-y)U(\frac{1}{2},0), & 0 \leq x \leq \frac{1}{2} \\ 2(1-x)(1-y)U(\frac{1}{2},0) + (2x-1)(1-y)U(1,0), & \frac{1}{2} \leq x \leq 1. \end{cases} \quad (2.9)$$

Incorporation of trial functions of the type (2.9) into the space S^h of piecewise bilinear functions will produce a C^0 global approximating function. Local rectangular mesh refinement can therefore be carried out in the manner of Figure 5, where two levels of refinement are shown.

The mid-side nodes are equivalent to the hanging points familiar in finite differences. We note that, if the equation corresponding to a point in the global stiffness system is considered as a difference equation, the resulting difference approximation at the point is inconsistent.

When refinement is done with triangular elements, no special procedure has to be adopted because the elements are all of the same form - isosceles right angled triangles. In our numerical experiments the mesh has been generated using an automatic mesh generation scheme due to A. Bykat [8], which demands as data only the co-ordinates of the boundary nodes. These nodes are thus concentrated near the re-entrant corner and the refined mesh so produced is in effect a graded mesh. This is one advantage over the method of refinement with rectangles where a problem defined peripheral node ordering scheme as in [13] has been used.

Results using local refinement schemes are given in Figure 7. We note that at the point of singularity itself the solution appears to have converged. This phenomenon occurs repeatedly with local mesh

1.0000	0.9698	0.9425	0.9202	0.9055	0.9005															
1.0000	0.9693	0.9414	0.9184	0.9034	0.8981															
	0.9693	0.9412	0.9182	0.9031	0.8977															
	0.9686	0.9398	0.9163	0.9007	0.8953															
1.0000	0.9681	0.9388	0.9146	0.8985	0.8927															
	0.9680	0.9386	0.9144	0.8981	0.8924															
	0.9647	0.9319	0.9044	0.8856	0.8787															
1.0000	0.9643	0.9310	0.9028	0.8832	0.8759															
	0.9641	0.9308	0.9025	0.8827	0.8755															
	0.9584	0.9188	0.8839	0.8581	0.8482															
1.0000	0.9580	0.9180	0.8824	0.8553	0.8448															
	0.9579	0.9178	0.8820	0.8549	0.8442															
	0.9502	0.9013	0.8548	0.8146	0.7948															
1.0000	0.9499	0.9006	0.8535	0.8112	0.7923															
	0.9497	0.9004	0.8531	0.8106	0.7913															
	0.9411	0.8816	0.8207	0.7560	0.6663	0.4884	0.3580	0.2371	0.1170	0.0000										
1.0000	0.9408	0.8810	0.8199	0.7553	0.6667	0.4894	0.3603	0.2379	0.1184	0.0000										
	0.9407	0.8809	0.8196	0.7548	0.6667	0.4904	0.3608	0.2382	0.1185	0.0000										
	0.9324	0.8632	0.7897	0.7066	0.6026	0.4788	0.3555	0.2355	0.1174	0.0000										
1.0000	0.9323	0.8629	0.7895	0.7077	0.6039	0.4811	0.3569	0.2365	0.1179	0.0000										
	0.9322	0.8628	0.7895	0.7077	0.6043	0.4817	0.3574	0.2376	0.1179	0.0000										
	0.9254	0.8487	0.7672	0.6774	0.5760	0.4646	0.3490	0.2326	0.1162	0.0000										
1.0000	0.9254	0.8488	0.7677	0.6787	0.5776	0.4659	0.3499	0.2312	0.1165	0.0000										
	0.9254	0.8488	0.7676	0.6788	0.5779	0.4663	0.3502	0.2334	0.1167	0.0000										
	0.9204	0.8388	0.7528	0.6605	0.5606	0.4539	0.3428	0.2294	0.1149	0.0000										
1.0000	0.9206	0.8392	0.7536	0.6618	0.5620	0.4550	0.3436	0.2298	0.1151	0.0000										
	0.9206	0.8392	0.7537	0.6619	0.5622	0.4553	0.3438	0.2300	0.1152	0.0000										
	0.9175	0.8331	0.7450	0.6516	0.5524	0.4477	0.3387	0.2271	0.1139	0.0000										
1.0000	0.9178	0.8337	0.7459	0.6528	0.5536	0.4487	0.3395	0.2275	0.1141	0.0000										
	0.9178	0.8338	0.7460	0.6529	0.5537	0.4489	0.3396	0.2277	0.1142	0.0000										
	0.9163	0.8315	0.7426	0.6486	0.5500	0.4452	0.3376	0.2257	0.1140	0.0000										
	0.9169	0.8319	0.7434	0.6500	0.5510	0.4466	0.3381	0.2267	0.1137											
	0.9169	0.8319	0.7435	0.6502	0.5514	0.4468	0.3382	0.2268	0.1138											

CTM [17]
P Finite elements with
isosceles
right triangles, h=0.1 plus
5 levels of local refinement.
Finite elements with
isosceles
right triangles, h=0.1 plus
2 levels of local refinement.

Figure 7.

14.

refinement, where the effect of the singularity on the numerical solution has been removed by the refinement. However, it should be remembered that the approximation contains a discretization error which at points remote from the singularity is related to the original mesh length. Thus the apparent convergence will in all probability be to the wrong number,

2.2 Inclusion of Singular Terms

The idea of augmenting the trial function spaces (S^h of Section 2) with terms having the form of the singularity was proposed by Fix [11], who used rectangular elements to solve a second order self-adjoint elliptic problem in a rectangular region with homogeneous Dirichlet boundary conditions. The technique has been extended to triangular elements by Barnhill and Whiteman [2] and [3]. This modification of the standard finite element method is undertaken with two aims in mind; the adaptation of the error analysis of Section 2 and the increase of accuracy of the numerical solution.

Let the neighbourhoods $N(r_i) \subset \bar{\Omega}$ of the corner be defined as

$$N(r_i) \equiv \{ (r, \theta) ; 0 \leq r \leq r_i, 0 \leq \theta \leq 3\pi/2 \}, i = 0, 1$$

where $r_1 > 0$ is some fixed number and $r_0 = qr_1, 0 < q < 1$; (r, q) as in Section 1; (Note that $N(r) \subset N(r_1)$). The functions $w_i(r, \theta), i = 1, 2, \dots, N$ are constructed in $N(r_1)$, where the $w_i(r, \theta)$ have the form of the singularity in $N(r_0)$, are equal to zero in $(\bar{\Omega} - N(r_1))$ and are in $W_{\frac{2}{2}}(\bar{\Omega} - N(r_0))$. These last smoothness properties can be achieved by taking in $N(r_1) - N(r_0)$ the functions $w_i(r, \theta)$ as the product of a cubic Hermite polynomial in r and a suitable function of θ ; for details see [1].

The function

$$w = u - \sum_{i=1}^N a_i w_i(r, \theta)$$

can now be formed, such that w would be in $W_{\frac{2}{2}}(\Omega)$ if the a_i were known exactly. Thus w could then be approximated with the Galerkin solution $U \in S^h$, and clearly if the a_i were known the error bound formed by combining (2,7) and (2,8) would then apply.

However, the a_i cannot be found exactly, and in practice approximations \hat{a}_i are calculated by the method of augmenting with singular functions from (1.6) the trial functions spaces S^h . These augmented spaces are denoted by $\text{Aug } S^h$, and in each element the trial functions of $\text{Aug } S^h$ have the form :

for triangular elements :

$$a + bx + cy + \sum_{i=1}^N c_i w_i(r, \theta)$$

for rectangular elements :-

$$a + bx + cy + dxy + \sum_{i=1}^N c_i(r, \theta).$$

Galerkin approximations $\hat{U} \in \text{Aug } S^h$ to u are calculated, and the best approximation Lemma of [3] is now applied to $\text{Aug } S^h$. Thus it follows immediately that

$$\|u - \hat{U}\|_E \leq \|u - V\|_E \quad \forall v \in \text{Aug } S^h. \quad (2.10)$$

In particular let $\tilde{u} \in S^h$ interpolate to $u - \sum_{i=1}^N a_i w_i$ at the $m+p$ nodes in $\Omega \cup \Omega_1$ and take $v \in \text{Aug } S^h$ as

$$v = \sum_{j=1}^N a_j w_j(r, \theta) + \tilde{u}$$

Then (2.10) gives

$$\|u - \hat{U}\|_E \leq \left\| u - \left(\sum_{j=1}^N a_j w_j + \tilde{u} \right) \right\|_E = \left\| \left(u - \sum_{i=1}^N a_i w_i \right) - \tilde{u} \right\|_E. \quad (2.11)$$

The Ciarlet Raviart theorem can be applied so that

$$\left\| \left(u - \sum_{i=1}^N a_i w_i \right) - \tilde{u} \right\|_E \leq kh \left| u - \sum_{i=1}^N a_i w_i \right|_2. \quad (2.12)$$

As the a_i are the correct values of, and not approximations to,

the constants in the expansion (1.6), the function $u - \sum_{i=1}^N a_i w_i$

is in $W^{\frac{2}{2}}(\Omega)$ so that (2.11) and (2.12) combined give

an $O(h)$

bound on the Galerkin error.

Galerkin approximations have been calculated with the inclusion of singular functions in the trial function spaces for both triangular and rectangular elements. Augmentation with one singular function ($N = 1$) in each case causes considerable improvement in accuracy in the neighbourhood of 0. It is found that the inclusion of more singular terms does not appreciably further improve the accuracy. This conclusion is in agreement with that of Wait and Mitchell [21] who use a combination of mesh refinement and singular function augmentation with rectangular elements to solve a harmonic problem in a region containing a slit.

3. FINITE-DIFFERENCE METHODS

The systems of linear equations which result from the use of finite element methods, as considered in the previous Sections, can be thought of as systems of difference equations. Many well known finite-difference schemes can thus be produced by the use of the finite element method with appropriate trial functions on meshes of squares and right angled triangles. Clearly in such case error analyses as in Section 2 are applicable.

In particular the use of linear trial functions interpolating function values at the element vertices with a mesh of isosceles right triangles having short sides of length h , as in Figure 2, produces at a mesh point (x,y) the standard five-point finite-difference replacement for Laplace's equation

$$4U(x,y) - U(x+h,y) - U(x,y+h) - U(x-h,y) - U(x,y-h) = 0. \quad (3.1)$$

Thus the relevant results given in Figure 3 are exactly those obtained with this scheme for the problem (1.1)-(1.5) with the mesh length h as shown.

If bilinear trial functions are used in the same way with the square mesh of side h as in Figure 2, these lead to the non-standard nine-point finite-difference replacement for Laplace's equation, see [7],

$$8 U(x,y) - \{U(x+h,y) + U(x,y+h) + U(x-h,y) + U(x,y-h)\} - f\{U(x+h,y+h) + U(x-h,y+h) + U(x-h,y-h) + U(x+h,y-h)\} = 0. \quad (3.2)$$

Use of the replacement (3.2) therefore produces again the relevant results of Figure 3.

The standard nine-point replacement for Laplace's equation,

$$20 U(x,y) - 4\{U(x+h,y) + U(x,y+h) + U(x-h,y) + U(x,y-h)\} - \{U(x+h,y+h) + U(x-h,y+h) + U(x-h,y-h) + U(x+h,y-h)\}, \quad (3.3)$$

has also been used to produce numerical solutions to the problem (1.1)-(1.5). For completeness results obtained using (3.3) with a square mesh of length $h = 0.1$ are given in Figure 8. It is seen that these results are less accurate in the neighbourhood of the singularity than those obtained with (3.1) or (3.2). This might be expected since the truncation error in (3.3) involves the sixth derivatives of u , the solution of (1.1)-(1.5). Thus use of (3.3) implicitly assumes the continuity and boundedness of higher order derivatives of u than those presupposed by the use of (3.1) and (3.2). It was shown in Section 1 that the solution u does not possess these properties.

Modifications for improving accuracy of finite difference solutions can be performed as in Sections 2.1 and 2.2. Experiments using local and general mesh refinement have been performed and accuracy is increased. The technique of incorporating singular functions into finite-difference methods has also been much used ; see Motz [16], Woods [25], Whiteman [23] and Bernal and Whiteman [6],

For non-modified difference methods uniform convergence with decreasing mesh size of the finite difference solution to the exact solution of the problem defined in a rectangle containing a slit considered by Rosser and Papamichael [18] is proved by Whiteman and Webb [24]. However, in [24] they exploit the symmetry of the problem and reflect the region across those parts of the resulting boundary which meet at the singular point. Such reflecting cannot be used for the problem in the L - shaped region.

4. NUMERICAL CONFORMAL TRANSFORMATION METHOD.

As no closed form solution is available for the problem (1.1)-(1.5), an accurate approximation, obtained by transforming the problem into a simple problem which can be solved by inspection,

1.0000 0.9698 0.9425 0.9202 0.9055 0.9005

	0.9670	0.9367	0.9121	0.8159	0.8902						
1.0000	0.9686	0.9398	0.9163	0.9007	0.8953						
1.0000	0.9656	0.9339	0.9079	0.8905	0.8843						
	0.9647	0.9319	0.9044	0.8856	0.8787						
	0.9615	0.9255	0.8950	0.8736	0.8656						
1.0000	0.9584	0.9188	0.8839	0.8581	0.8482						
	0.9548	0.9118	0.8732	0.8431	0.8299						
1.0000	0.9502	0.9013	0.8548	0.8146	0.7948						
	0.9460	0.8940	0.8438	0.7969	0.7624						
1.0000	0.9411	0.8816	0.8207	0.7560	0.6663	0.4884	0.3580	0.2371	0.1170	0.0000	
	0.9344	0.8748	0.8115	0.7427	0.6559	0.5013	0.3639	0.2394	0.1190		
1.0000	0.9324	0.8632	0.7897	0.7066	0.6026	0.4788	0.3555	0.2355	0.1174	0.0000	
	0.9293	0.8584	0.7839	0.7011	0.6023	0.4830	0.3591	0.2377	0.1184		
1.0000	0.9254	0.8487	0.7672	0.6774	0.5760	0.4646	0.3490	0.2326	0.1162	0.0000	
	0.9237	0.8457	0.7638	0.6747	0.5755	0.4660	0.3508	0.2339	0.1169		
1.0000	0.9204	0.8388	0.7528	0.6605	0.5606	0.4539	0.3428	0.2294	0.1149	0.0000	
	0.9194	0.8370	0.7508	0.6590	0.5601	0.4543	0.3436	0.2301	0.1153		
1.0000	0.9175	0.8331	0.7450	0.6516	0.5524	0.4477	0.3387	0.2271	0.1139	0.0000	
	0.9168	0.8319	0.7436	0.6505	0.5518	0.4476	0.3391	0.2275	0.1141		
1.0000	0.9163	0.8315	0.7426	0.6486	0.5500	0.4452	0.3376	0.2257	0.1140	0.0000	
	0.9160	0.8303	0.7413	0.6479	0.5492	0.4455	0.3376	0.2266	0.1137		

CTM [17]

P Standard 9-point
finite-difference
replacement h = 0.1

Figure 8.

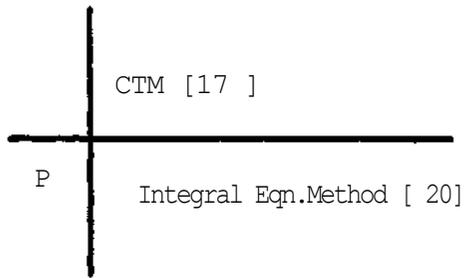
has been used throughout this paper for comparing the accuracy of the finite element and finite difference solutions. This method, the Numerical Conformal Transformation Method (NCTM), is given in Papamichael and Whiteman [17]. The NCTM consists of four successive conformal mappings, the first of which is performed numerically using a technique due to Symm [19] which involves the numerical solution of a Fredholm integral equation of the first kind with a logarithmic kernel. The results for problem (1.1)-(1.5) obtained in [17] have been displayed in each of Figures 3, 7 and 8. They are also quoted by Bell and Crank in [5]. Symm in [20] uses an integral equation technique modified to deal with the singularity to solve the boundary value problem (1.1)-(1.5) numerically. His results are given in Figure 9 together again with those obtained with the NCTM.

5. DISCUSSION

The results of the previous Sections show the shortcomings of the finite element and finite difference methods when boundary singularities are present. The success of the modifications to the finite element method in improving the accuracy of the numerical solutions is evident. Indeed with continued local mesh refinement the stage has been reached by Gregory and Whiteman in [13] in which the Galerkin solutions are more accurate near the singularity than they are at points in Ω remote from 0, The effect of the singularity on the numerical solution has thus been neutralized by the refinement. For problems of this type and magnitude there seems to be little to choose between the finite element and finite difference methods when comparing accuracy of solutions for a certain amount of computation. The NCTM produces accurate approximations in a fraction of the

At each mesh point P
the numbers represent :

1.0000	0.9698	0.9425	0.9202	0.9055	0.9005						
0.9999	0.9700	0.9427	0.9205	0.9060	0.9009						
1.0000	0.9686	0.9398	0.9163	0.9007	0.8953						
1.0000	0.9687	0.9400	0.9166	0.9012	0.8957						
1.0000	0.9647	0.9319	0.9044	0.8856	0.8787						
1.0000	0.9648	0.9322	0.9048	0.8860	0.8793						
1.0000	0.9584	0.9188	0.8839	0.8581	0.8482						
1.0000	0.9584	0.9191	0.8843	0.8587	0.8487						
1.0000	0.9502	0.9013	0.8548	0.8146	0.7948						
1.0000	0.9503	0.9015	0.8553	0.8154	0.7961						
1.0000	0.9411	0.8816	0.8207	0.7560	0.6663	0.4884	0.3580	0.2371	0.1170	0.0000	
1.0000	0.9412	0.8818	0.8210	0.7565	0.6667	0.4869	0.3579	0.2364	0.1177	0.0000	
1.0000	0.9324	0.8632	0.7897	0.7066	0.6026	0.4788	0.3555	0.2355	0.1174	0.0000	
1.0000	0.9325	0.8633	0.7898	0.7066	0.6019	0.4780	0.3549	0.2352	0.1172	0.0000	
1.0000	0.9254	0.8487	0.7672	0.6774	0.5760	0.4646	0.3490	0.2326	0.1162	0.0000	
1.0000	0.9254	0.8487	0.7671	0.6772	0.5756	0.4642	0.3486	0.2323	0.1161	0.0000	
1.0000	0.9204	0.8388	0.7528	0.6605	0.5606	0.4539	0.3428	0.2294	0.1149	0.0000	
1.0000	0.9204	0.8387	0.7527	0.6603	0.5604	0.4536	0.3425	0.2291	0.1147	0.0000	
1.0000	0.9175	0.8331	0.7450	0.6516	0.5524	0.4477	0.3387	0.2271	0.1139	0.0000	
1.0000	0.9175	0.8331	0.7449	0.6515	0.5521	0.4474	0.3385	0.2269	0.1133	0.0000	
1.0000	0.9163	0.8315	0.7426	0.6486	0.5500	0.4452	0.3376	0.2257	0.1140	0.0000	
1.0001	0.9166	0.8313	0.7424	0.6487	0.5495	0.4453	0.3371	0.2261	0.1134	0.0000	



computation time taken by the other methods. However, it is a much less general method and the range of problems to which it can be applied is limited.

We have found that for these problems where there is considerable regularity of mesh the programming involved to produce the finite element solutions can be much simplified. The technique is to divide the totality of mesh points into several different classes, where each mesh point of a class has the same pattern of neighbouring mesh points. The linear equation derived with the finite element method for a particular point is then treated as a difference equation, and so one type of difference equation is associated with each class. This removes the need to generate local stiffness matrices ; a fact that will be hotly disputed by some as removing one of the main advantages of versatility possessed by the finite element method.

In this paper we started by considering a specific class of composites. We now return to the physical situation and note that an important application of composites of this type is in the production of materials that have "effective diffusion properties" which are equivalent to those of isotropic materials. In this way the isotropic material may be simulated. The pattern of flow in the composite is in general dependent on the arrangement of the impermeable islands in the continuum. The effect of different arrangements is discussed by Barrer [4]. In the study of the flow rates through a composite of the type under consideration here, the total flow across a section ($x = \text{constant}$) of the L-shaped region will be sought. This total flow is

$$\int_0^a \frac{\partial u(x,y)}{\partial x} ay,$$

$$\text{where } \alpha = \begin{cases} 1 & \text{for } 0 \leq x < \frac{1}{2} \\ \frac{1}{2} & \text{for } \frac{1}{2} \leq x < 1 \end{cases},$$

and can easily be approximated with a quadrature formula from the

numerical results for a particular value of x .

We have concentrated on trying to eliminate the effect of the singularity on the solution of a particular diffusion problem. Another important field is that of stress and deformation of this type of composite. Leissa, Claussen and Agrawal [15] have attempted an analysis of this using point matching techniques. In the stress situation the governing differential equation is biharmonic and, when the finite element method is used to solve this, the conforming condition is that the relevant finite dimensional subspace be contained in $C^1(\Omega)$. Gregory and Whiteman [13] have derived a C^1 element for the local mesh refinement scheme with rectangles as in Figure 4. Thus this local refinement scheme may again be used.

It is clear from the references made throughout this paper that much of this work has been done in collaboration with colleagues. I acknowledge with great pleasure the contributions of R.E.Barnhill, J.A.Gregory, N. Papamichael and J.Barkley Rosser, and also the programming assistance of A.Bykat and P.Theodorou. Many of the numerical results will appear in the dissertation of Theodorou for the degree of Master of Technology at Brunel University.

REFERENCES

1. Barnhill, R.E. and Whiteman, J.R. , Error Analysis of Finite Element Methods with Triangles for Elliptic Boundary Value Problems, pp.83-112 of J.R.Whiteman (ed.). The Mathematics of Finite Elements and Applications, Academic Press, London, 1973.
2. Barnhill, R.E. and Whiteman, J.R., Singularities Due to Re-Entrant Boundaries in Elliptic Problems. In L.Collatz (ed.), ISNM 19, Birkhauser-Verlag, Zurich (to appear).
3. Barnhill, R.E. and Whiteman, J.R., Error Analysis of Galerkin Methods for Dirichlet Problems Containing Boundary Singularities. Technical Report TR/19, Department of Mathematics, Brunei University, 1973.
4. Barrer, R.M., Diffusion and Permeation in Heterogeneous Media pp.165-217 of J.Crank and G.S.Park (eds.). Diffusion in Polymers, Academic Press, London, 1968.
5. Bell, G.E. and Crank, J., Diffusion in Composite Media. Part I: Steady State. Technical Report TR/23, Department of Mathematics, Brunel University, 1973.
6. Bernal, M.J.M. and Whiteman, J.R., Numerical treatment of biharmonic boundary value problems with re-entrant boundaries. Computer Journal 13, 87-91, 1970.
7. Birkhoff, G., Schultz, M.H. and Varga, R.S., Piecewise Hermite interpolation in one and two variables with applications to partial differential equations. Numer.Math. 11, 232-256, 1968.
8. Bykat, A., Automatic Triangulation of Two Dimensional Regions. Report ICSI 420, University of London, Institute of Computer Science, 1972.
9. Ciarlet, P.G., and Raviart, P.G., General Lagrange and Hermite interpolation in R^n with applications to finite element methods. Arch. Rat. Mech. Anal. 1.46, 177-199, 1972.
10. Davis, P.J., Interpolation and Approximation. Blaisdell, New York, 1963.
11. Fix, G., Higher-order Rayleigh-Ritz approximations. J.Math.Mech. 18, 645-657, 1969.
12. Gregory, J.A., Piecewise Interpolation Theory and Finite Element Analysis. Ph.D. Thesis, Department of Mathematics, Brunei University, (to appear).
13. Gregory, J.A., and Whiteman, J.R., Local Mesh Refinement with Finite Elements for Elliptic Problems. Technical Report TR/24, Department of Mathematics, Brunei University, 1973.
- 11+. Lehman, R.S. , Development at an analytic corner of solutions of elliptic partial differential equations. J.Math.Mech. 8, 727-760, 1959.
15. Leissa, A.W., Clausen, W.E. and Agrawal, G.K., Stress and deformation analysis of fibrous composite materials by point matching. Int.J.Numer.Meth.Eng. 3, 89-101, 1971.

16. Motz, H., Treatment, of singularities in partial differential equations by relaxation methods. *Q.Appl.Math.*4, 371-377, 1946.
17. Papamichael N. , and Whiteman, J.R. , A numerical conformal transformation method for harmonic mixed boundary value problems in polygonal domains. *Z.angew. Math.Phys.* 24, 304-316, 1973.
18. Rosser, J.B. and Papamichael, N., A Power Series Solution for a Harmonic Mixed Boundary Value Problem. Technical Report TR/35 Department of Mathematics, Brunel University, 1973.
19. Symm, G.T., An integral equation method in conformal mapping. *Numer.Math.*9, 250-258, 1966.
20. Symm, G.T., Treatment of Singularities in the Solution of Laplace's Equation by an Integral Equation Method. Report NAC31, National Physical Laboratory, 1973.
21. Wait, R. and Mitchell, A.R., Corner singularities in elliptic problems by finite element methods. *J.Comp.Phys.*8, 45-52, 1971 .
22. Wasow, W., Asymptotic development of the solution of Dirichlet's problem at analytic corners. *Duke Math.J.*24, 47-56, 1957.
23. Whiteman, J.R., Singularities Due to Re-entrant Corners in Harmonic Boundary Value Problems. Technical Report No.829, Mathematics Research Center, University of Wisconsin, Madison, 1967.
24. Whiteman, J.R. and Webb, J.C, Convergence of finite difference techniques for a harmonic mixed boundary value problem. *B.I.T.* 10, 366-374, 1970.
25. Woods, L.C., The relaxation treatment of singular points in Poisson's equation. *Q.J.Mech.Appl.Math.*6, 163-189, 1953.

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