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On the Use of Singular Functions with Finite Element Approximations

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Finite element approximations to elliptic problems tend to converge poorly in the presence of singularities. This is especially true of spline functions. A scheme is given for efficiently modeling singularities in conjunction with such approximating functions. Three sample physical problems are chosen to illustrate the techniques.

1. INTRODUCTION

Over the past decade, "finite element" methods using piecewise polynomial approximating functions have solved many engineering problems with adequate accuracy, especially in the areas of solid and structural mechanics. However, if one wishes to achieve greater accuracy or if the exact solution involves even a mild "singularity," such as is typically the case in domains with edges or corners, to use piecewise polynomial functions exclusively is very inefficient.

One of us has recently[1] explored the possibility of achieving greater accuracy by supplementing a basis of piecewise polynomial "finite elements" by appropriate "singular functions" so chosen as to match *all* the leading terms of the exact solution near singular points. The method yielded satisfactory results, but several computational questions remain unresolved, and we shall deal with these in this paper in terms of the following three physical models: (i) the accurate computation of the rigidity and deformation of a cracked square elastic beam under torsion; (ii) the very accurate computation of the eigenvalues of an L-shaped membrane; and (iii) the flux distribution in an idealized square nuclear reactor consisting of a homogeneous square core surrounded by a square reflector, in the one-group diffusion approximation.

The first computational problem we consider concerns the most efficient class of

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[1] See [10] and [4]; also Wait and Mitchell [19].

piecewise polynomial functions to use in combination with "singular functions." More precisely, given an error tolerance $\epsilon > 0$, which approximating subspace gives this error with the least amount of work. This of course is a very broad question to which we can at best give only partial answers. The situation is further complicated by the various possible measures that can be used for computational work. In this paper we have chosen the number N of unknown parameters as our criterion. This is somewhat of an over simplification, but an entirely reasonable one for the type of finite element approximations discussed here.

The first conclusion we have drawn from our experiments is that *cubic elements are far more efficient than linear elements when singular functions are used.* For example, in the torsion problem (Section 2) linear elements with singular functions give approximations having 5% relative errors with 30–40 unknowns, while with the same number of unknowns the cubic elements yield errors of order. 1% (see Table I in Section 2).

In addition, we found that suitably modified *splines to be the most efficient cubic element* to use with singular functions. Each of the cubic elements (with singular functions) gave approximations with roughly the same errors for a given mesh size. The spline space, therefore, proved to be the most efficient, since it has least number of unknown parameters for a given mesh. For example, in torsion problems five place accuracy was obtained with the splines with 59 unknowns while the Hermite space required 132 unknowns, the mesh length being the same for both spaces (see Table I).

Finally, *each of the above schemes proved to be more efficient than local mesh refinement with triangular elements.* In the torsion problem, for example, local mesh refinement with linear elements gave relative errors of order 20% near the singularity; with two singular functions the error was 5% with 33 unknowns as noted above.

The addition of singular functions to a finite element basis of course destroys the band structure of the matrix. In addition, the condition number is greatly increased. Nevertheless, in Section 5 it is shown how the bordering techniques of Faddeev and Faddeeva [9] can be used to avoid both problems.

It should be noted that each of the three problems we have chosen have rectangular boundaries. Rectangular elements such as splines, however, are not confined to such configurations, and for example can be used for more general boundaries with Lagrange multipliers [26] or least-square techniques [27]. Another possibility is to use isoparametric splines near curvilinear boundaries [17]. We presume that the conclusion we have reached in this paper will not be drastically changed for such problems.

2. Torsion Problems

Consider the torsion of the cracked beam with square cross-section Ω shown in Fig. 1. The governing differential equation in terms of the stress function u is

$$-\Delta u = F \text{ in } \Omega, \tag{2.1}$$

$$u = 0 \text{ on } \partial\Omega, \tag{2.2}$$

where $\partial\Omega$ denotes the boundary of Ω and F is a constant.

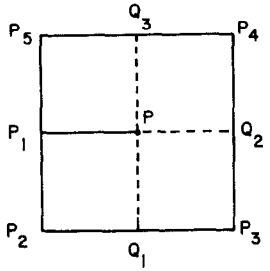


FIG. 1. Cracked square.

The solution u has a singularity at P with leading term $r^{1/2} \sin \theta/2$, where (r, θ) are polar coordinates. More precisely, it follows from Lehman's Theorem [2] that

$$u - \sum_{j=0}^{\infty} c_j r^{\nu_j} \sin \nu_j \theta, \qquad \nu_j = (2j + 1)/2, \tag{2.3}$$

is analytic in a neighborhood of P for suitable constants c_j.[2] Indeed, (2.3) is analytic everywhere in the closure $\bar{\Omega}$ of Ω except for the corners $P_1, \ldots, P_5$ at which it also has singularities of the form $\rho_i^2 \ln \rho_i$, ρ_i being the distance from P_i.

From an engineering standpoint, the most interesting quantity is not the values of the stress function u but rather the constant (called the stress intensity factor)

$$\sigma_0 = \lim_{r \to 0} r^{-1/2}[u(r, \pi) - u(0, \pi)], \tag{2.4}$$

since it is a commonly accepted measure of the amount of torsion the beam can endure before fracture occurs [13].

[2] A more general treatment is given by Kondrat'ev [28]. This work is of central importance since in it is developed the form of the singularity for a rather wide class of elliptic problems.

To avoid the physically uninteresting logarithmic singularities we change the problem slightly and replace (2.2) with

$$u = 0 \quad \text{on} \quad \overline{PP_1}, \overline{P_2P_3}, \text{ and } \overline{P_4P_5}, \tag{2.2'}$$

$$\frac{\partial u}{\partial n} = 0 \quad \text{on} \quad \overline{P_1P_2}, \overline{P_3P_4}, \text{ and } \overline{P_5P_1}, \tag{2.2''}$$

where $\partial/\partial n$ is the normal derivative. Such a change of boundary conditions is typically justified in the engineering literature by the Sain-Venant principle [13]—the behavior of the stress function near P is not affected by boundary conditions away from P. Moreover, it follows from the results in [22], that the solution u to (2.1), (2.2'), 2.2'') has a singularity only only at P which is of the form (2.3). For simplicity we take $F = 1$, and appeal to symmetry to reduce the problem to the rectangle shown in Fig. 2.

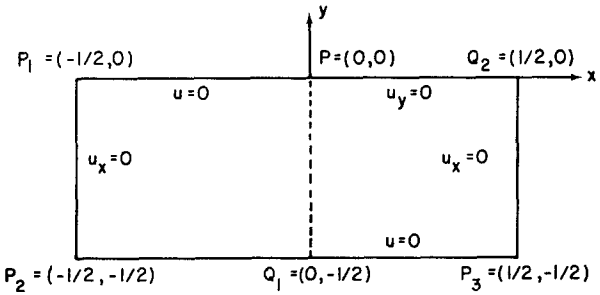


FIG. 2. Symmetrized region.

Four different types of finite elements will be considered. The first three arise from a partition of the region into subsquares with side length h and are as follows:

(i) S_h^L denotes the space of continuous functions which are *bilinear polynomials* $a + bx + cy + dxy$ in each subsquare of Ω. The unknowns are the values of the solution at the nodal points, and, hence, the dimension of this space is

$$\dim S_h^L = h^{-2} + 0(h^{-1}). \tag{2.5}$$

(ii) S_h^H is the *bicubic Hermite space* consisting of C^1 functions which are bicubic polynomials $\sum_{i=0}^{3}\sum_{j=0}^{3} a_{ij}x^iy^j$ in each subcube. There are four unknowns per interior point (the values of u, u_x, u_y, u_{xy}), hence the dimension of this space is

$$\dim S_h^H = 4h^{-2} + 0(h^{-1}). \tag{2.6}$$

(iii) S_h^{SL} (called the *spline-Lagrange* space below) is the space consisting of piecewise bicubic polynomials of class C^2 everywhere except across the line PQ_1, where they are only continuous. The dimension of this space is

$$\dim S_h^{SL} = h^{-2} + O(h^{-1}). \tag{2.7}$$

The reason for assuming only continuity along the vertical line intersecting P is related to the boundary condition (2.2′). In particular, this condition is essential [24] and must be satisfied by all trial functions in the approximating space. It is impossible for a smooth piecewise polynomial function, and in particular a C^2 bicubic spline function, to vanish along the line $\overline{P_1P}$ and be nonzero in the region exterior to this line. The solution u does this, but its derivatives have singularities at P. To avoid this difficulty, we weaken the smoothness requirements along $\overline{PQ_1}$, requiring only continuity here. A patch basis[3] of the form

$$\psi_{jk}(x, y) = \psi_j(x)\,\psi_k(y)$$

for S_h^{SL} is easily constructed using the divided difference formulas for the one dimensional B-splines $\psi_l(t)$ of Schoenberg [7] (see also [17]).

(iv) $S_{h,\delta}^{L}$ denotes the space of continuous functions which are *piecewise linear* in a triangulated subdivision of Ω (see Fig. 3), h signifying the maximum side length and δ the minimum side length.

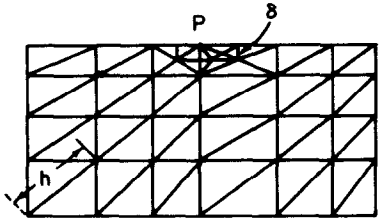


FIG. 3. Triangulation of Ω.

To the patch basis for each of the spaces S_h^L, S_h^H, S_h^{SL} we shall add singular functions of the form

$$\begin{aligned} \psi_l(r, \theta) &= r^{\nu_l} \sin \nu_l\theta \qquad \text{for} \quad 0 \leqslant r < r_0\,, \quad 0 \leqslant \theta < 2\pi, \\ &= p(r) \sin \nu_l\theta \qquad \text{for} \quad r_0 \leqslant r \leqslant r_1\,, \quad 0 \leqslant \theta < 2\pi, \\ &= 0 \qquad \text{for} \quad r > r_1\,, \end{aligned} \tag{2.8}$$

[3] A patch basis consists of functions $\psi_{jk}(x, y)$ which are locally supported; i.e., the area of region outside which ψ_{jk} is identically zero approaches zero as the maximum mesh length goes to zero. It is crucial to use such a basis in computations since they lead to sparse matrices.

where $\nu_l = (2l + 1)/2$ and $p(r)$ is a polynomial so chosen that ψ_l is of class C^4 or C^2 away from the point P depending on whether bicubic or bilinear elements are used. An alternate choice for this particular problem is to define ψ_l on all of Ω, for example,

$$\psi_l(r, \theta) = [1 - 4y^2]\, r^{\nu_l} \sin \nu_l \theta. \tag{2.9}$$

We found that (2.9) and (2.8) with $r_0 = 1/4$, $r_1 = 1/3$ gave substantially the same results.

For the spaces of piecewise bicubic functions S_h^H, S_h^{SL} we use ψ_l, $0 \leqslant l \leqslant 3$, since by Lehman's Theorem there are constants c_l, $0 \leqslant l \leqslant 3$, such that $u - \sum_{l=0}^{3} c_l \psi_l$ is of class C^4 and, hence can be approximated to fourth order by

TABLE I

Values of Approximate Solution

Space	Dimension (h)	$R_1 = (0, -1/24)$	$R_2 = (-11/24, -1/4)$	$R_3 = (11/24, -1/4)$
		0.027425	0.032877	0.070844
SS_h^{SL}	40 (1/6)	0.027438	0.032887	0.070835
	59 (1/8)	0.027429	0.032881	0.070847
	109 (1/12)	0.027426	0.032877	0.070844
SS_h^H	36 (1/4)	0.027402	0.032859	0.070895
	132 (1/8)	0.027423	0.032876	0.070848
	204 (1/10)	0.027424	0.032877	0.070844
SS_h^L	33 (1/8)	0.026459	0.033025	0.070385
	129 (1/16)	0.027153	0.032917	0.070721
	201 (1/30)	0.027289	0.032903	0.070780
$S_{h,\delta}^L$	7 ($h = 1/4, \delta = 1/4$)	0.006443	0.032483	0.065258
	15 ($h = 1/4, \delta = 1/16$)	0.017311	0.032696	0.068523
	32 ($h = 1/6, \delta = 1/6$)	0.009681		
	58 ($h = 1/6, \delta = 1/24$)	0.022079		
S_h^{SL}	36 (1/6)	0.020982	0.032643	0.069667
	55 (1/8)	0.022704	0.032712	0.069993
	105 (1/12)	0.024693	0.032771	0.070273
S_h^H	30 (1/4)	0.015593	0.032335	0.066730
	128 (1/8)	0.019681	0.032580	0.068872
	200 (1/10)	0.020980	0.032636	0.069275
S_h^L	7 (1/4)	0.007423		
	31 (1/8)	0.013700	0.032521	0.065258
	127 (1/16)	0.020686	0.032718	0.068174
	199 (1/20)	0.023306	0.032747	0.068523

bicubic elements [6, 7]. To use fewer functions would reduce the order to which the solution u can be approximated in the respective spaces. Similarly, we use ψ_l, $0 \leqslant l \leqslant 1$, with the bilinear elements. To distinguish the spaces with and without singular functions, we shall let $SS_h{}^L$, $SS_h{}^H$, and SS_h^{SL} denote the former.

No analytic expression for the exact solution of (2.1), (2.2′), (2.2″) is known, so to measure the accuracy in the linear and cubic elements we used even higher order elements. More precisely, we used a quintic spline-Lagrange element with six singular functions. The actual numbers computed with this space were very accurate; the maximum difference between the values at $h = 1/6$, $1/8$, and $1/10$ differed only in the seventh place. We, therefore, used the first six figures as the value of the exact solution.

Table I gives the values of the approximate solution at the points $R_1=(0, -1/24)$, $R_2 = (-11/24, -1/4)$, $R_3 = (11/24, -1/4)$, and Table II gives the values of the

TABLE II

Approximate Values of Stress Intensity Factor σ_0

Space	Dimension (h)	$\sigma_0{}^h$ (0.1917)
SS_h^{SL}	40 (1/6)	0.1925
	59 (1/8)	0.1920
	109 (1/12)	0.1918
$SS_h{}^H$	36 (1/4)	0.1902
	132 (1/8)	0.1915
	204 (1/10)	0.1916
$SS_h{}^L$	33 (1/8)	0.1830
	129 (1/16)	0.1867
	201 (1/20)	0.1877
$S_{h,\delta}^L$	7 ($h = 1/4, \delta = 1/4$)	0.0773
	15 ($h = 1/4, \delta = 1/16$)	0.1038
	17 ($h = 1/6, \delta = 1/6$)	0.0848
	58 ($h = 1/6, \delta = 1/24$)	0.1072

approximate stress intensity factor $\sigma_0{}^h$. The exact values are listed at the top of each column. Observe that the conclusions drawn in the introduction—namely that with singular functions cubic elements are superior to linear elements and both of these are superior to local mesh refinement—are readily confirmed from these tables.

We included the approximations from the spaces S_h^{SL}, $S_h{}^H$, $S_h{}^L$ without singular functions to illustrate the drastic improvements that result from the addition of

singular functions. Note that for these approximations the errors are worse, as expected, near the singularity. However, *there is serious "pollution" in the errors away from the singularity*, for example, the approximation at R_1 has about 40% accuracy with cubics and no singular functions; by adding four of the latter this error is reduced to about 1%.

3. The L-Shaped Membrane

Many attempts have been made to compute accurately the eigenvalues of an L-shaped membrane; see for example [2, p. 137; 10; 12]. The most accurate eigenvalues reported to date are those obtained using a collocation method by Fox, Henrici, and Moler [11]. However, their techniques are hard to generalize to other regions, even to other rectangular polygons with more than one reentrant corner.

In this section we shall present some new numerical results based on the Rayleigh–Ritz method with a space of modified splines with singular functions, like that used for the torsion problem in Section 2. The results are as accurate as those reported in [11], and much more accurate than those reported in [2, p. 137; 10] using spaces of bilinear and bicubic Hermite functions.

The problem to be solved is

$$\Delta u + \lambda u = 0 \text{ in } \Omega, \qquad u = 0 \text{ on } \partial\Omega, \tag{3.1}$$

where Ω is the L-shaped region shown in Fig. 4. To define the modified space of

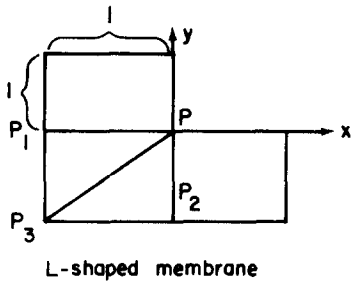


FIGURE 4

splines, which we shall call the *spline-Hermite space* and denote by S_h^{SH} for reasons that will be apparent shortly, we subdivide Ω into squares of side h. Then S_h^{SH} consists of those functions which are bicubic polynomials in each square, and which are of class C^2 in $\bar{\Omega}$ except along the lines $\overline{PP_1}$ and $\overline{PP_2}$ where they are C^1.

The weaker smoothness conditions along the lines $\overline{PP_2}$ and $\overline{PP_1}$ were introduced

for the reasons cited in Section 2. However, we found that C^1 continuity along these lines was sufficient for the L-shaped region; whereas, for cracked square discussed in Section 2 it was necessary to allow mere continuity. This is presumably due to the larger interior angle at the reentrant corner for the former case.

Sample calculations for the L-shaped region show that this type of modification is crucial, since approximations obtained with pure splines (and singular functions) are considerably less accurate than those reported here! See also [20, pp. 4–17]. In addition, the weaker smoothness conditions make the essential boundary condition [24] $u = 0$ on $\partial\Omega$ easier to satisfy.

From Lehman's Theorem [22] it follows that eigenfunctions u admit the development

$$u(r, \theta) = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} c_{kl} r^{2k/3+2l} \sin(2k\theta/3) \tag{3.2}$$

near P, and we used singular functions of the form

$$\psi_{kl}(r, \theta) = (1 - y^2)(1 - x^2)\, r^{2k/3+2l} \sin(2k\theta/3) \tag{3.3}$$

defined over all of Ω. To be consistent with the notation established in Section 2, we shall let SS_h^{SH} denote the space spanned by S_h^{SH} and appropriate singular functions.

For simplicity we have computed only the *even* symmetry class, i.e., the eigenfunctions which are symmetric about the line PP_3 in Fig. 4. For this case, the expansion (3.2) simplifies to

$$u(r, \theta) = \sum_{k=1,3,5,\ldots} \sum_{l=0}^{\infty} c_{kl} r^{2k/3+2l} \sin(2k\theta/3), \tag{3.2'}$$

and to obtain optimal order of accuracy it is necessary (and sufficient) to use only ψ_{11}, ψ_{12}, and ψ_{50}. See [10, Theorem 1] which applies to this case.

Table III lists our most accurate approximation values, together with those obtained by Fox, Henrici, and Moler [11]. The integer n in this table stands for the nth eigenvalue λ_n ordered by $\lambda_1 < \lambda_2 < \cdots < \lambda_n < \cdots$. We have found that the best way to obtain very high accuracy was not by refining the mesh but by adding more singular functions, and the numbers given in Table III were calculated with 14 singular functions. This reduces the constant C in the eigenvalue error bound

$$0 \leqslant \lambda^h - \lambda \leqslant Ch^6$$

(see [10] and [23]). Indeed, the use of more than three singular functions cannot

TABLE III

Approximate Eigenvalue of the L-Shaped Membrane Even Symmetric Class

Eigenvalue number n	Fox, Henrici, Moler upper and lower bounds		Ritz upper bounds $h = 1/8$, 14 singular functions
1	9.6397238	05 84	9.6397 23844
3	31.91263	31 88	31.9126 3607
4.	41.4745	039 159	41.4745 2424
6.	56.7096	02 18	56.7096 6596
7	—		71.0585 3953
9	—		89.3062 4622

TABLE IV

n	$h = 1/4$ $N_s = 0$	 $N_s = 3$	 $N_s = 11$
1	10.263 45261 96	9.639 73228 538	9.639 72387 301
2*	19.739 40065 32	19.739 40065 32	19.739 40065 32
3	33.240 56446 13	31.917 63099 60	31.912 64025 76
4	42.653 11016 15	41.497 70734 33	41.475 02450 21
5*	49.387 23635 23	49.387 23635 23	49.387 23635 23
n	$h = 1/8$ $N_s = 0$	 $N_s = 11$	 $N_s = 14$
1	9.887 34798 535	9.639 72384 432	9.6397 2384409
2*	19.739 21136 66	19.739 21136 66	19.739211366
3	32.481 62580 32	31.912 63607 34	31.912 63606 64
4	41.928 52875 62	41.474 52865 46	41.4745 2424 21
5*	49.348 42004 58	49.348 42004 58	49.348 42004 58

n = eigenvalue number; N_s = number of singular functions; * = eigenvalues of the square.

increase the exponent of h, which is best possible [23], but the effect on C can be rather significant. This is illustrated in Table IV. It is perhaps significant that this phenomenon would not be nearly so pronounced if we had defined the singular functions over a smaller subregion of Ω, as in (2.8).

Not all of the eigenfunctions of the L have singularities at the corner P. In particular, the eigenvalues of the square

$$(m^2 + n^2)\,\pi^2 \tag{3.4}$$

are also eigenvalues of the L and have *analytic eigenfunctions*. Singular functions are therefore not needed to approximate the latter. Refering to Table IV, we note that the second and fifth eigenvalues are of the form (3.4); the exact value of λ_2 is $2\pi^2$ and the exact value of λ_5 is $5\pi^2$. As expected the addition of singular functions do not change the approximations. In fact, the lack of any significant change confirms the stability of the numerical procedures discussed in Section 5.

Of course, efficiency with moderate accuracy is usually much more important than such extreme accuracy in engineering problems. With this in mind we turn to Table V where the approximations with three singular functions are given.

TABLE V

Three Singular Functions

n	$h = 1/4$	$h = 1/6$
1	9.639 73228 538	9.639 72449 886
2*	19.739 40065 32	19.739 22390 70
3	31.917 63099 60	31.912 99290 71
4	41.497 70734 33	41.476 04137 86
6	56.744 45703 31	56.711 95591 59
7	71.410 76701 53	71.078 80615 32

* = eigenvalues of the square.

Observe that even with the coarse mesh $h = 1/4$, five places of accuracy are obtained, which is typically sufficient for engineering purposes.

In Tables IV and V the digits which differ from the values listed in Table III are underlined.

4. One-Group, Two-Region Reactor

In the previous examples the introduction of auxiliary singular functions was essential to the success of the finite element method. In our final example, the boundary value problem associated with the one-group, two-region reactor, this

TABLE VI
Approximations to the first eigenvalue of (4.1)

h	Number of unknowns	λ
Bicubic spline-Lagrange space; no singular functions		
1/4	64	5.5841818
1/6	100	5.5833516
1/8	144	5.5829692
Bicubic spline-Lagrange space; one singular function		
1/4	65	5.5823256
1/6	101	5.5822830
1/8	145	5.5822736

$p_1 = 1, p_0 = 5, q = 0, \rho = 1, \nu = 0.784.$

does not appear to be the case. The solution u can be written $cv + dw$, where v is smooth and w has unbounded first derivatives at certain points. Fortunately the constant d is apparently small so that the error in the finite element approximation is quite acceptable (see Table VI) although the rate at which it converges to zero as the mesh is refined is quite slow.

The boundary value problem associated with the one-group, two-region ractor is

$$-\nabla(p\,\nabla u) + qu = \lambda\rho u. \tag{4.1}$$

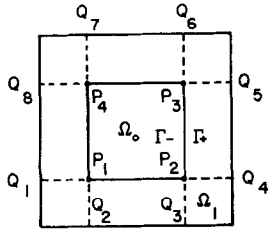


FIG. 5. Reactor with core.

This differential equation holds in the core Ω_0 and the reflector Ω_1 (see Fig. 5), and we require that energy flux u vanish on the outer boundary $\partial\Omega_1$:

$$u = 0 \text{ on } \partial\Omega_1 . \tag{4.2}$$

Typically the coefficients p, q, and ρ are regionwise constants. Thus, the curve Γ separating Ω_0 and Ω_1 is an interface, and we require that u, $p(\partial u/\partial n)$ be continuous across Γ, where n is the normal to Γ:

$$p \frac{\partial u}{\partial n}\Big|_{\Gamma+} = p \frac{\partial u}{\partial n}\Big|_{\Gamma-}, \qquad u|_{\Gamma+} = u|_{\Gamma-} . \tag{4.3}$$

The most important quantity to calculate is the eigenvalue of least magnitude λ which measures the criticality of the reactor [14].

Independent of any singularity the existence of interfaces fundamentally alters the best choice of an appropriate finite element space S^h. To use spaces of piecewise polynomial functions which are C^1 or better across Γ would clearly lead to poor approximations, since u has discontinuous derivatives across Γ. The use of trial functions satisfying the jump condition (4.3) as proposed in [20] leads to difficulties at the corners P_j , $j = 1, 2, 3, 4$. For example, at the point P_1 , if we force the trial functions $v^h(x, y)$ to satisfy

$$p_0 \frac{\partial v^h}{\partial y}\Big|_{\Gamma-} = p_1 \frac{\partial v^h}{\partial y}\Big|_{\Gamma+} \tag{4.4}$$

along $\overline{P_1P_2}$, where

$$p = \begin{cases} p_0 & \text{in } \Omega_0 \\ p_1 & \text{in } \Omega_1 , \end{cases}$$

then they will also satisfy (4.4) on a portion of $\overline{Q_1P_1}$ where the solution is smooth.

In light of the above considerations we decided to use a bicubic spline-Lagrange space for this problem. Before describing this space we first exploit the symmetry to reduce the region to the half square in Fig. 6, where a Neumann boundary condition $\partial u/\partial n = 0$ is used along $\overline{R_2R_3}$ and $\overline{R_3R_4}$. Subdividing the region

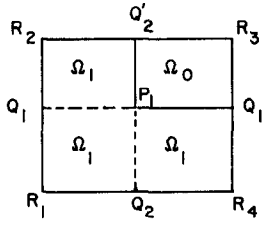


FIG. 6. Symmetrized region.

into squares with side lenth h, we let S_h^{S-L} denote the space of functions which are bicubic polynomials in each subsquare and which are of class C^2 except across the lines $\overline{Q_1Q_1'}$ and $\overline{Q_2Q_2'}$ where they are only continuous. We do not require that the trial functions satisfy the interface condition (4.3), which is permissible since this is a *natural boundary condition* [12].

The eigenfunction u associated with the first eigenvalue λ has singular derivatives at the point P_1 in Fig. 6. Indeed, Birkhoff [3] and Kellogg [25] have shown that the leading term in the asymptotic expansion near P_1 has the form

$$r^{\nu}\psi_{\nu}(\theta), \tag{4.5}$$

where $0 < \nu < 1$ and $\psi_{\nu}(\theta)$ is a periodic function of θ. As was mentioned at the beginning of this section, however, the coefficient of (4.5) is quite small and does not appreciably affect the size of the error as we shall show in the following examples.

The first case we consider is

$$p_0 = 5, \qquad p_1 = 1, \qquad q = 0, \qquad \rho = 1, \tag{4.6}$$

where $p = p_0$ in Ω_0 and $p = p_1$ in Ω_1. For this choice of coefficients the value of ν in (4.5) is

$$\nu = 0.783653104.$$

Thus [17], the error in the spline-Lagrange approximate eigenvalue is

$$0(h^{2\nu}) \simeq 0(h^{1.56}); \tag{4.7}$$

when one singular function is used this error is reduced to

$$0(h^{4+2\nu}) \simeq 0(h^{5.56}). \tag{4.8}$$

The numerical results listed in Table VI confirm the rates (4.7) and (4.8), but observe that the approximations without singular functions are quite good even though their rate of convergence is slow.

The second case we consider has a larger variation in the coefficient p:

$$p_0 = 500, \qquad p_1 = 1, \qquad q = 0, \qquad \rho = 1. \tag{4.9}$$

For this case

$$\nu \simeq 2/3,$$

and as before the approximate eigenvalues have errors of order $0(h^{2\nu})$, $(0(h^{4+2\nu}))$ when no (one) singular functions are used. The results are listed in Table VII, and are similar to those obtained in the first case.

TABLE VII
Approximations to the First Eigenvalue of (4.1)

Bicubic spline-Lagrange space; no singular functions		
h	Number of unknowns	λ
1/4	64	5.799411
1/6	100	5.796708
1/8	144	5.795361

$p_1 = 1, p_0 = 500, q = 0, \rho = 1, \nu \cong 2/3.$

Observe that the difference between the eigenvalues for (4.6) and (4.9) is about 3 %; i.e., the first eigenvalue of (4.1) appears to depend very weakly on the value p_0 of the coefficient p in the core Ω_0. Presumably the associated eigenfunction is almost constant in Ω_0, a fact which partially explains the weak effects of the singularity.

The eigenvalue, however, depends quite strongly on the value p_1 of p in the reflector Ω_1. For example, if

$$p_0 = 1, \qquad p_1 = 500, \qquad q = 0, \qquad \rho = 1, \tag{4.10}$$

the value of λ is increased fourfold. See Table VIII.

TABLE VIII
Approximations to the first eigenvalue of (4.1)

Bicubic spline-Lagrange space; no singular functions		
h	Number of unknowns	λ
1/4	64	19.6798194
1/6	100	19.6797314
1/8	144	19.6797208

$p_1 = 500, p_0 = 1, q = 0, \rho = 1, \nu \cong 4/3.$

One cannot expect a weak effect from singularities for all geometrical configurations. For example, consider the region Ω shown in Fig. 7. For the choice of coefficients

$$q = 0, \qquad \rho = 1$$

$$p(x, y) = \begin{cases} 100 & \text{if } (x, y) \in \Omega_0 \cup \Omega_2, \\ 1 & \text{if } (x, y) \in \Omega_1 \cup \Omega_3, \end{cases} \tag{4.11}$$

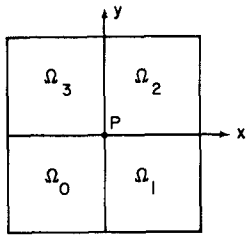


FIGURE 7

the approximate eigenvalues without singular functions is given in Table IX. Observe both size and rate of convergence of the error is very poor. Fortunately, *such configurations rarely occur in reactors*, the configuration given in Fig. 5 is the most typical.

TABLE IX

Approximations to the First Eigenvalue of (4.1)

Bicubic spline-Lagrange space; no singular functions		
h	Number of unknowns	λ
1/4	64	38.27058
1/6	100	37.29292
1/8	144	36.569080

p is given by (4.11), $q = 0$, $\rho = 1$.

5. Solution of Approximate Equations

That the addition of extra functions to a finite element basis can lead to numerical instability is not too surprising. The extra singular functions *can* be approximated by the finite elements, and this is especially true of, for example, the higher-order singular functions like $r^{7/2}\sin(7\theta/2)$ needed to obtain the full efficiency of the bicubic elements in the torsion problem. Thus, we have a "nearly dependent" (ill conditioned) basis for the space spanned by the finite elements and singular functions no matter what basis we use for the finite elements.

An equally serious difficulty is that the addition of singular functions destroys the band structure of the matrices generated by the finite element method. This can lead to extra operations in elimination ("fillin"), as well as extra storage requirements.

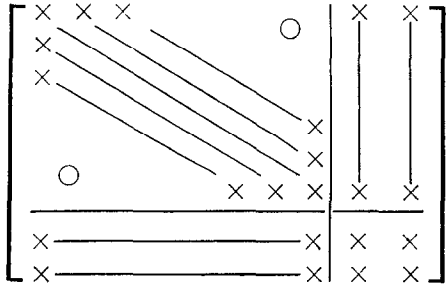
A closer look at the type of *sparsity structure* of the matrices associated with the spaces SS_h^L, SS_h^H, and SS_h^{SL} employing singular functions shows, however, that both of the above difficulties can be resolved by using ideas of Faddeev and Faddeeva [9, pp. 163–167] for handling *bordered matrices.*

Let us first consider the source problem (2.1), where the variational method leads to a system of linear equations

$$A\mathbf{u} = \mathbf{f}, \tag{5.1}$$

whose coefficient matrix A has the form

$$A = \begin{bmatrix} A_{11} & A_{12}^* \\ A_{12} & A_{22} \end{bmatrix} = \tag{5.2}$$



In (5.2), A_{11} is the matrix that arises from the finite elements without singular functions; its entries are inner products of B-splines. It is, therefore, a banded positive definite $N \times N$ matrix, whose bandwidth is $O(h^{-1})$ and whose dimension is $N = O(h^{-2})$. The entries of the $N_s \times N$ matrix A_{12}, N_s denoting the number of singular functions, are inner products of the B-splines with the singular functions, while A_{22} is the $N_s \times N_s$ positive definite matrix whose entries are the inner products of the singular functions with each other.

To solve (5.1), we use the Cholesky factorization

$$A = \begin{bmatrix} L_{11} & \\ L_{12} & L_{22} \end{bmatrix} \begin{bmatrix} \overbrace{L_{11}^*}^{N} & \overbrace{L_{12}^*}^{N_s} \\ & L_{22}^* \end{bmatrix} \begin{matrix} \}N \\ \}N_s \end{matrix},$$

where L_{11} and L_{22} are lower triangular matrices. The Cholesky factors are determined from

$$A_{11} = L_{11}L_{11}^*, \tag{5.3}$$

$$A_{12}^* = L_{11}L_{12}^*, \tag{5.4}$$

$$A_{22} - L_{12}L_{12}^* = L_{22}L_{22}^*. \tag{5.5}$$

The first factorization (5.3) is the usual Cholesky factorization of the (finite element)

matrix A_{11}. We backsolve with L_{11} to obtain the row vectors of L_{12} from (5.4), and, finally, the factor L_{22} is obtained by a Cholesky factorization of the $N_s \times N_s$ matrix $A_{22} - L_{12}L_{12}^*$.

To compute the solution $\mathbf{u}$ we first use the partition

$$\mathbf{u} = \begin{pmatrix} \mathbf{u}_1 \} N \\ \mathbf{u}_2 \} N_s \end{pmatrix}, \qquad \mathbf{f} = \begin{pmatrix} \mathbf{f}_1 \} N \\ \mathbf{f}_2 \} N_s \end{pmatrix},$$

and then backsolve using the triangular factors

$$\begin{aligned} L_{11}\mathbf{v}_1 &= \mathbf{f}_1, \\ L_{22}\mathbf{v}_2 &= \mathbf{f}_2 - L_{12}\mathbf{v}_1, \end{aligned} \tag{5.6}$$

$$\begin{aligned} L_{22}^*\mathbf{u}_2 &= \mathbf{v}_2, \\ L_{11}^*\mathbf{u}_1 &= \mathbf{v}_1 - L_{12}^*\mathbf{u}_2. \end{aligned} \tag{5.7}$$

First observe that it is necessary to store only the bands of A_{11} as well as A_{12}, A_{22}, $\mathbf{f}_1$, and $\mathbf{f}_2$. Thus, the addition to the storage requirement, which is $O(h^{-3})$ without singular functions, is only of order $O(h^{-2})$. The increase in the operation counts to solve (5.1) by (5.2)–(5.7) also makes a lower order contribution. Without singular functions, where (5.1) is replaced with $A_{11}\mathbf{u}_1 = \mathbf{f}_1$, $O(h^{-4})$ operations are required. Moreover the extra operations required from (5.2)–(5.7) result only from the matrix multiplications in (5.4), the factorization (5.5) and the backsolves in (5.6) and (5.7). This increase is, therefore, only of order $O(h^{-2})$.

In addition, backsolving only involves the Cholesky factor L_{11} of the finite element matrix A_{11}, and the small $N_s \times N_s$ matrix L_{22}. (Recall that $N_s = 2$ for linear elements and $N_s = 4$ for cubic elements.) The latter is the only place where numerical instabilities occur, and since the matrices involved are so small, rounding errors can be easily kept under control. Observe that with a standard "black box" elimination code, row pivoting would occur, the effect of which would be to put part of A_{12}^* into A_{11}—a disaster for stability!

Similar techniques can be used for the associated eigenvalue problem $A\mathbf{u} = \lambda B\mathbf{u}$, where B denotes the mass matrix. For example, in the Rayleigh quotient algorithm [21], which we have found to be the best scheme to solve for the first eigenvalue λ and eigenvector $\mathbf{u}$, iterations

$$A\mathbf{u}^{(n+1)} = \lambda^{(n)}B\mathbf{u}^{(n)}, \tag{5.8}$$

$$\lambda^{(n+1)} = \mathbf{u}^{(n+1)} \cdot A\mathbf{u}^{(n+1)} / \mathbf{u}^{(n+1)} \cdot B\mathbf{u}^{(n+1)} \tag{5.9}$$

are introduced. Thus, it is necessary only to factor A by (5.3)–(5.5) at the beginning of the calculation, and backsolve at each step to obtain $\mathbf{u}^{(n+1)}$ from $\mathbf{u}^{(n)}$ using (5.6)–(5.7).

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