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SINGULARITIES IN TWO- AND THREE-DIMENSIONAL ELLIPTIC PROBLEMS AND FINITE ELEMENT METHODS FOR THEIR TREATMENT

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1. INTRODUCTION

The effective use of finite element methods for treating elliptic boundary value problems involving singularities is well recognised. As a result considerable effort has been expended by mathematicians and engineers in developing special finite element techniques which can produce accurate approximations to the solutions of problems involving singularities.

The work of mathematicians has been mainly in the context of two-dimensional Poisson problems. It has exploited and relied on known theoretical results concerning the regularity of solutions of weak forms of problems of this type, and has produced significant finite element error estimates for this limited class of problems. Comparable progress has not been made in the finite element treatment of three-dimensional problems involving singularities, mainly on account of the lack of theoretical results for the three-dimensional case. This is particularly relevant to the case of three-dimensional re-entrant vertices.

In this paper we present a survey of the finite element treatment of singularities. This is first done in the context of a model two-dimensional Poisson problem and estimates for various norms of the error are given. Some finite element techniques for singularities are then described, taking into account their effects on convergence rates and accuracy. In problems with singularities the approximation of secondary quantities by retrieval from approximations to the solutions (primary quantities) is of great importance,and so this is also treated here.Finally Poisson problems with singularities in three dimensions are presented and the state-of-the-art for this case is contrasted with that for two dimensions.

2. POISSON PROBLEMS INVOLVING SINGULARITIES

2.1. Two Dimensional Poisson Problems.

Let $\Omega \subset \mathbf{R}^2$ be a simply connected polygonal domain with boundary $\partial\Omega$. We consider first the much studied model problem in which the scalar function $u(\underline{x})$ satisfies

$$\begin{aligned} -\Delta[u(\underline{x})] &= f(\underline{x}), \quad \underline{x} \in \Omega, \\ u(\underline{x}) &= 0, \quad \underline{x} \in \partial\Omega, \end{aligned} \tag{2.1}$$

where $f \in L_2(\Omega)$. A weak form of (2.1) is defined in the usual Sobolev space $\mathring{H}^1(\Omega)$, and for this $u \in \mathring{H}^1(\Omega)$ satisfies

$$a(u,v) = F(v), \quad \forall\, v \in \mathring{H}^1(\Omega), \tag{2.2}$$

where

$$a(u,v) \equiv \int_\Omega \nabla u \nabla v \, d\underline{x}, \quad u,v \in \mathring{H}^1(\Omega), \tag{2.3}$$

and

$$F(v) \equiv \int_\Omega fv \, d\underline{x}, \quad v \in \mathring{H}^1(\Omega). \tag{2.4}$$

Problem (2.1) is treated by considering the weak form (2.2), where the bilinear form has the important properties that it is continuous, symmetric and elliptic on $\mathring{H}^1(\Omega)$, see Ciarlet [1].

For the finite element solution of (2.1) the region Ω is partitioned quasi uniformly into triangular elements Ω^e in the usual manner and the Galerkin method is applied to (2.2). Conforming trial and test functions are employed and the solution $u \in \mathring{H}^1(\Omega)$ is approximated by $u_h \in S^h$, where $S^h \subset \mathring{H}^1(\Omega)$ is a finite dimensional space of piecwise polynomial functions of degree p, $(p \geq 1)$, and u_h satisfies

$$a(u_h,v_h) = F(v_h) \quad \forall\, v_h \in S^h. \tag{2.5}$$

The well known best approximation property of the Galerkin solution gives the inequality

$$\|u - u_h\|_{1,\Omega} \leq \|u - w_h\|_{1,\Omega} \quad \forall\, w_h \in S^h, \tag{2.6}$$

where $\|v\|_{1,\Omega}$ is the energy norm $\|\nabla v\|_{L_2(\Omega)}$. Since (2.6) holds for all $w_h \in S^h$, we may take the interpolant $\tilde{u}_h \in S^h$ to u for w_h in (2.6) and, using approximation theory, it follows that

$$\|u - u_h\|_{1,\Omega} \leq Ch^\mu |u|_{k+1,\Omega} , \tag{2.7}$$

where $\mu = \min(p,k)$, whilst C is a constant. Throughout the paper all constants in the estimates are denoted by C.

The actual value of μ is thus dependent both on the choice of p and on the regularity of the solution u of (2.2). Under the condition that $f \in L_2(\Omega)$ the regularity of u is determined by the shape of $\partial\Omega$. If Ω is a convex polygon, then $u \in \mathring{H}^1(\Omega) \cap H^2(\Omega)$, so that $k = 1$ in (2.7) and

$$\|u - u_h\|_{1,\Omega} \leq C\, h|u|_{2,\Omega} \tag{2.8}$$

In this case, see Schatz [2],

$$\|u - u_h\|_{L_2(\Omega)} \leq C\, h^2 |u|_{2,\Omega} , \tag{2.9}$$

so that there is an $O(h)$ convergence gain through changing from the 1-norm to the L_2-norm. The above two estimates are *optimal* in that they are the best that can be obtained by approximating from S^h a function with the regularity of u. It has also been shown, see Nitsche [3] and Ciarlet [1], that for this case the L_∞-norm of the error has $0(h^2)$ convergence.

As has been stated in Section 1, problems with boundaries having re-entrant corners, and thus containing boundary singularities, are of main interest here. We thus consider again problem (2.1), but now in the situation where Ω is a non-convex polygonal domain with interior angles α_j, $1 \le j \le M$, where

$$0 < \alpha_1 \le \alpha_2 \le \ldots \le \pi < \alpha_m \le \ldots \le \alpha_M \le 2\pi .$$

In this case the solution u of (2.2) is such that $u \in \mathring{H}^1(\Omega) - H^2(\Omega)$, and it has been shown by Grisvard [4] that over Ω u can be written as

$$u = \sum_{j=m}^{M} a_j \chi_j (r_j) u_j (r_j, \theta_j) + w, \qquad (2.10)$$

where (r_j, θ_j) are local polar coordinates centred on the j^{th} corner of $\partial\Omega$, the χ_j are smooth cut-off functions for the corners, $w \in H^2(\Omega)$ and

$$u_j(r_j, \theta_j) = r_j^{\pi/\alpha_j} \sin \frac{\pi\theta_j}{\alpha_j} .$$

The regularity of u is clearly determined by the term in the summation in (2.10) associated with the M^{th} corner. In fact $u \in H^{1+\pi/\alpha_M - \varepsilon}(\Omega)$ for every $\varepsilon > 0$, see also Schatz and Wahlbin [5].

Since $\alpha_M > \pi$ and $u \in H^{1+\pi/\alpha_M-\varepsilon}(\Omega)$, it follows from (2.7) that

$$\| u - u_h \|_{1,\Omega} \le C\, h^{(\pi/\alpha_M - \varepsilon)} |u|_{1+\pi/\alpha_M-\varepsilon} , \qquad (2.11)$$

and, see Schatz [2], that

$$\| u - u_h \|_{L_2(\Omega)} \le C\, h^{2(\pi/\alpha_M - \varepsilon)} |u|_{1+\pi/\alpha_M-\varepsilon} . \qquad (2.12)$$

Whereas the convergence gain in the changing from the 1-norm to the L_2-norm is 0(h) for the case where Ω is a convex polygon, (2.8),(2.9), the gain is less for the re-entrant case.

Estimates of the type (2.11) and (2.12), being global, reflect the worst behaviour of the solution over Ω. The situation may not be so bad locally, in particular away from the corners where from (2.10) $u \in H^2$. Thus we now consider L_∞-estimates. Suppose that at the j^{th} vertex z_j of $\partial\Omega$ the intersection of Ω with a disc centred at z_j and containing no other corner is Ω_j and that $\Omega_0 \equiv \Omega \backslash (\bigcup_{j=1} \Omega_j)$. It has been shown by Schatz and Wahlbin [5] that

$$\| u - u_h \|_{L_\infty(\Omega_0)} \le C\, h^{\min(p+1, 2\pi/\alpha_M) - \varepsilon} \qquad (2.13)$$

$$\|u - u_h\|_{L_\infty(\Omega_M)} \le C\,h^{\pi/\alpha_M - \varepsilon} \qquad (2.14)$$

Similar estimates were discussed by Oden and O'Leary [6]. It should be emphasised that all the above estimates are based on quasi-uniform meshes and piecewise p^{th} order polynomials.

Specific examples of estimates (2.11) - (2.14) are those where the region Ω contains a slit, $\alpha_M = 2\pi$, for which

$$u \in H^{3/2-\varepsilon}(\Omega),\ \|u - u_h\|_{1,\Omega} = O(h^{1/2-\varepsilon}),\ \|u - u_h\|_{L_2(\Omega)} = O(h^{1-\varepsilon})$$

$$\|u - u_h\|_{L_\infty(\Omega_0)} = O(h^{1-\varepsilon}),\ \|u - u_h\|_{L_\infty(\Omega_M)} = O(h^{1/2-\varepsilon})$$

and where the region is L-shaped, $\alpha_M = 3\pi/2$, for which

$$u \in H^{5/3-\varepsilon}(\Omega),\ \|u - u_h\|_{1,\Omega} = O(h^{2/3-\varepsilon}),\ \|u - u_h\|_{L_2(\Omega)} = O(h^{4/3-\varepsilon})$$

$$\|u - u_h\|_{L_\infty(\Omega)} = O(h^{4/3-\varepsilon}),\ \|u - u_h\|_{L_\infty(\Omega_M)} = O(h^{2/3-\varepsilon})$$

2.2 Techniques for Singularities.

The error estimates of Section 2.1 indicate the deterioration from the *optimal* state caused by the presence of the singularity. On account of the practical importance of singularities, much effort has been expended in producing special finite element techniques fro treating singularities, and a considerable literature now exists. The approaches fall mainly into three classes; augmentation of the trial ans test spaces with functions having the form of the dominant part of the singularity, use of singular elements, use of local mesh refinement. These techniques and their effects are now reviewed briefly.

Since for problems of type (2.2) with re-entrant corners the form of the singularity is known, use of this can be made by augmenting the space S^h with functions having the form of the singularity. The solution u of (2.3) is in this case approximated by $u_h \in \text{Aug}S^h$. The technique, proposed by Fix [7] and used by Barnhill and Whiteman [8] and Stephan and Whiteman [9], enables estimates as for problems with smooth solutions to be obtained. It does, however, have the disadvantage of producing a system of linear equations in which the coefficient matrix has a more complicated structure than normal.

The technique of employing *singular* elements involves in elements near the singularity the use of local functions which approximate realistically the singular behaviour. Elements of this type have been proposed by Akin [10], Blackburn [11] and Stern and Becker [12], and their use can lead to significant increase in accuracy of u_h. O'Leary [13], specifically for the Stern-Becker element, has proved that use of the element produces no improvement in the rate of convergence in the error estimate. The increase in accuracy must therefore be produced by reduction in size of the constant in the estimate.

Local mesh refinement near a singularity was originally performed on an ad-hoc basis without theoretical backing. In recent years error analysis has been produced which indicates the grading which a mesh should have near a corner in order that the effect of a singularity may be nullified. Examples of such local mesh refinement are given by Schatz and Wahlbin [5] and Babuska and Osborn [14]. Another approach is to use *adaptive* mesh refinement involving a-posteriori error estimation.

With adaptive mesh refinement the region Ω is partitioned initially and the local error in each element is estimated. If, for a particular element, this is greater than a prescribed tolerance, the element is subdivided thus causing the local refinement, see Babuska and Rheinboldt [15], [16]. Hierarchical finite elements have recently been incorporated into the technique, Craig, Zu und Zienkiewicz [17], as have multigrid methods Bank and Sherman [18] and Rivara [19].

2.3 Retrieved Quantities.

As has been stated in Section 1, for problems involving boundary singularities the approximation of secondary (retrieved) quantities is most important. Specifically the coefficients a_j in (2.10) of singular terms are of practical significance, so that ways must be found of approximating these accurately. Apart from the obvious approach of using collocation or least squares methods to fit terms to calculated results, it is often possible to exploit the mathematics of the original problem. An important case is that of a problem containing a slit, $\alpha_M = 2\pi$, and here use can be made of the "J-integral" concept to produce an integral expression for the a_M, see Destuynder et al.,[20]. This integral can be approximated using the calculated solution u_h. For piecewise linear test and trial functions on a mesh with local refinement, O(h) estimates are given in [20] for the absolute value in the error in the approximation to the singularity coefficient a_M.

Fro problem (2.2), when a singularity is present, the integrand of the "J-integral" involves derivatives of the solution u. Thus the accuracy of the approximation to the integral, and hence to the singularity coefficient, depends on the errors in the gradients of u_h.

A possibility exists here of exploiting superconvergence properties in the estimation of errors in gradients of u_h, provided local estimates can be obtained. To date the error estimates have depended on the global regularity of the solution u, see Levine [21].

2.4 Three Dimension Poisson Problems.

We consider again problems of the type (2.1), except that now $\Omega \subset \mathbf{R}^3$ is a polyhedral domain. The weak forms and the finite element method for the three-dimensional case can be described similarly, again with $\Omega \subset \mathbf{R}^3$. Singularities can in this case occur on account of re-entrant edges and vertices. The decomposition of the three dimensional weak solution corresponding to (2.10) has been shown, e.g. by Stephan [22] to have the form

$$u = \underset{(\text{vertices})}{\sum_{j=1}^{M} a_j \chi_j u_j} + \underset{(\text{edges})}{\sum_{k=1}^{N} f_k \Xi_k v_k} + w \qquad (2.15)$$

where $w \in H^2(\Omega)$, $\chi_j(r_j)$ and $\Xi_k(\rho_k)$ are cut-off functions respectively for the vertices and edges, whilst the u_j and v_k are functions associated also respectively with vertices and edges. For an edge the v_k have the two dimensional form for any plane orthogonal to the edge associated with the appropriate two dimensional problem, whilst the b_k are functions of z_k.

The singular function u_j for each vertex is found by solving a Laplace-Beltrami eigenvalue problem on that part of the surface of the unit ball centred on the vertex cut off by the faces of the vertex. When the vertex is such that the eigenvalue problem is separable (has a single coordinisation), there are special cases when the problem can be solved exactly, see Walden and Kellogg [23]. When this is not so, for example for a vertex made up from three mutually orthogonal planes, Beagles and Whiteman [24], a numerical approximation to the eigenvalue must be obtained with the result that the singular function will not be known exactly.

Clearly this lack of knowledge of the exact singular functions is very important from the finite element point of view, and in particular means that the error analysis of Section 2.1 cannot in general be transferred directly to the three-dimensional singular case. All the singularity methods described in Section 2.1 are affected, although all are used in the three-dimensional context. The augmentation technique is obviously adversely affected, although Beagles and Whiteman [25] have devised the technique of *non-exact augmentation*, whereby the trial and test function spaces in the

Galerkin procedure are augmented with the non- exact singular functions. As far as we are aware no method of the "J-integral" type exists for three-dimensional Poisson problems.

The above indicates that the state-of-the-art fro treating three-dimensional singularities with finite element methods is far less advanced than that for the two-dimensional case. This arises more from limitations in the theory of three-dimensional Poisson problem than from the finite element methods themselves.

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