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The singular function boundary integral method for 3-D Laplacian problems with a boundary straight edge singularity

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ABSTRACT

Three-dimensional Laplace problems with a boundary straight-edge singularity caused by two intersecting flat planes are considered. The solution in the neighbourhood of the straight edge can be expressed as an asymptotic expansion involving the eigenpairs of the analogous two-dimensional problem in polar coordinates, which have as coefficients the so-called edge flux intensity functions (EFIFs). The EFIFs are functions of the axial coordinate, the higher derivatives of which appear in an inner infinite series in the expansion. The objective of this work is to extend the singular function boundary integral method (SFBIM), developed for two-dimensional elliptic problems with point boundary singularities [G.C. Georgiou, L. Olson, G. Smyrlis, A singular function boundary integral method for the Laplace equation, *Commun. Numer. Methods Eng.* 12 (1996) 127–134] for solving the above problem and directly extracting the EFIFs. Approximating the latter by either piecewise constant or linear polynomials eliminates the inner infinite series in the local expansion and allows the straightforward extension of the SFBIM. As in the case of two-dimensional problems, the solution is approximated by the leading terms of the local asymptotic solution expansion. These terms are also used to weight the governing harmonic equation in the Galerkin sense. The resulting discretized equations are reduced to boundary integrals by means of the divergence theorem. The Dirichlet boundary conditions are then weakly enforced by means of Lagrange multipliers. The values of the latter are calculated together with the coefficients of the EFIFs. The SFBIM is applied to a test problem exhibiting fast convergence of order $k + 1$ (k being the order of the approximation of the EFIFs) in the L^2 -norm and leading to accurate estimates for the EFIFs.

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1. Introduction

The solutions of elliptic equations, such as the Laplace and the biharmonic equations, in two-dimensional domains exhibit singularities at boundary corners and/or at boundary points where there is an abrupt change in the boundary condition. Such problems are of interest in many engineering fields, such as fracture and fluid mechanics. They have also attracted the attention of numerical analysts, since boundary singularities limit the regularity of solutions, even if the data are very smooth, leading to convergence difficulties to Galerkin and other standard numerical methods and thus causing inaccuracies in the numerical solutions. The latter are not always local and may propagate to the rest of the problem domain.

In the past few decades, several methods for treating elliptic boundary value problems with boundary singularities have been proposed. Among them one finds the so-called hybrid methods which incorporate, directly or indirectly, the form of the local asymptotic expansion for the solution in the approximation scheme. Knowledge of the leading singular coefficients of

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the local solution expansion, which in two-dimensional problems are also known as generalized stress intensity factors (SIFs) [30] or flux intensity factors [1], is of great importance in many applications, especially in fracture mechanics.

Many methods have been proposed in the literature for the effective and efficient approximation of singular coefficients, by postprocessing the numerical solution including high-order p/hp finite element methods [30,28] and special adaptive grid refinement schemes and multigrid algorithms [4,5]. The solution is first approximated on a refined grid designed especially to capture the singularity and the coefficients are obtained by an extraction formula which uses the computed solution. Methods that do not require any postprocessing and/or include information about the exact solution in the approximation scheme, such as Trefftz methods [20], are more attractive when the approximation of the coefficients is the main objective.

In Trefftz methods, which are also known as Boundary Approximation Methods (BAMs), the solution over the entire problem domain is approximated as a linear combination of certain particular solutions of the governing equation. As a result, only the boundary conditions need to be imposed in order to extract directly the unknown coefficients in the linear combination. Trefftz methods have been recently reviewed by Li and co-workers [20] who have also made comparisons with collocation and other boundary methods. Other recent reviews of methods used for solving elliptic boundary value problems with boundary singularities can be found in the articles of Bernal and Kindelan [3] who considered both global and local meshless collocation methods with multiquadratics as basis functions, and of Dosiyevev and Buranay [12] who employed the block method for solving Laplace problems on arbitrary polygons.

The singular function boundary integral method (SFBIM), developed by Georgiou et al. [17,13–16,7,8] for two-dimensional Laplacian and biharmonic problems with a boundary singularity is a Trefftz method, the basic feature of which is that the solution is approximated by the leading terms of the asymptotic expansion around the singular point. These singular functions are also used to discretize the governing elliptic equation in the Galerkin sense. The discretized equations are then reduced to boundary integrals by means of Green's theorem. A second feature of the SFBIM is that Dirichlet conditions are weakly enforced by means of Lagrange multipliers. It has been demonstrated both numerically [7] and theoretically [31] that for two-dimensional Laplacian problems, the SFBIM converges exponentially as the number of singular functions used in the approximation of the solution is increased. The method (and its convergence proof) has also been extended to biharmonic problems in two-dimensions arising from solid and fluid mechanics [8,14].

The main advantages of the SFBIM are: (a) the dimension of the problem is reduced by one, leading to considerable computational savings, and (b) the singular coefficients are calculated directly, hence avoiding the need for post-processing (and extra computational cost). However, formulating the SFBIM requires the knowledge of the singular function representation and this limits the range of applicability of the method. On the other hand, it is clear that in problems where calculation of SIFs is desired, the knowledge of the local solution is a prerequisite for their definition. Moreover, the problem domain must be a subset of the convergence domain of the local solution expansion. Otherwise, the method may be applied locally using another standard numerical method in the rest of the domain with appropriate conditions at the interface of the two subdomains (see, e.g. [26]).

Singularities in three-dimensional Laplacian problems have received less attention in the literature, mainly due to their complexity. Different forms of singularities may appear depending on the boundary geometry and conditions. In applications, both edge [23,36] and vertex [18,29,21] singularities are of interest. Of course, there are also other types of singularities. For example, Kozlov et al. [19] studied singularities near cusp tips of peak-shaped domains and Nazarov et al. [22] considered cuspidal edges and rotational cusps. Two very recent books by Costabel et al. [11] and Yosibash [35] contained unified analyses of singularities in two- and three-dimensional linear elliptic systems.

Yosibash et al. [32] studied the case of edge singularities; they presented the solution to the Laplace operator in three-dimensional domains in the vicinity of straight edges in the form of an asymptotic expansion involving eigenpairs and having as coefficients the so-called edge flux intensity functions (EFIFs). It turns out that the eigenpairs are those of the two-dimensional problem over a plane perpendicular to the edge. Edge singularities appear, for example, in V-notched solids loaded by static loads, in which the assumption of plane stress or plane strain condition is not valid. For the solution of such problems, few methods have been proposed, such as the methods of Costabel et al. [10] and Yosibash et al. [32] in which the EFIFs are computed by post-processing the solution obtained with a p -version finite element scheme. Edge singularities also appear in electrical conductors in micro-electromechanical systems (MEMS) [25].

Vertex singularities appear in electromagnetic fields, in magnetic recording, heat transfer, elasticity, fluid mechanics, as well as in multimaterial problems [36]. Among the earliest analyses of Laplacian solutions in the neighbourhood of a vertex are those of Stephan and Whiteman [29] and Beagles and Whiteman [2] who used finite elements for the computation of the eigenvalues; see also [27] for an approach using the boundary element method. Recently, Zaltzman and Yosibash [36] derived explicit analytical expressions for the local solution of the Laplace equation in the neighbourhood of a vertex. They also considered vertices at the intersection of a crack front and a free surface and provided numerical estimates of the eigenpairs obtained by extending a modified Steklov method.

The objective of the present work is to extend the SFBIM to 3-D Laplacian problems with a boundary straight-edge singularity and calculate the EFIFs directly. These are approximated locally by low-degree polynomials, the coefficients of which are primary unknowns of the method. To our knowledge, the only methods found in the literature for the calculation of the EFIFs are based on post-processing the numerical solution and/or using extraction formulae [24,32–34].

The rest of the paper is organized as follows: in Section 2 we present a 3-D Laplacian problem with an edge singularity and its asymptotic local solution expansion. In Section 3 the three-dimensional version of the SFBIM is formulated. Numerical results on a model problem are presented and discussed in Section 4. Finally, our conclusions are summarized in Section 5.

2. A three dimensional problem with a straight edge singularity

To demonstrate the analogy with the two-dimensional case, we first consider the Laplace equation over a circular sector, as shown in Fig. 1. A boundary singularity arises at the origin O , which is due not only to the presence of a corner in the boundary, but also to the fact that the boundary conditions along boundaries S_1 and S_2 are different: $u = 0$ along $\theta = 0$ and $\partial u / \partial \theta = 0$ along $\theta = \alpha\pi$, where $0 < \alpha < 2$. The local solution in polar coordinates (r, θ) , centered at the singular point O , is of the general form

$$u_{2D}(r, \theta) = \sum_{j=1}^{\infty} \alpha_j r^{\mu_j} f_j(\theta), \tag{1}$$

where μ_j and f_j are, respectively, the eigenvalues and eigenfunctions of the problem with $\mu_{j+1} > \mu_j$, and α_j are the constant singular coefficients which are unknown. The eigensolution (μ_j, f_j) is uniquely determined by the geometry and boundary conditions along the boundary parts S_1 and S_2 sharing the singular point:

$$\mu_j = \frac{2j - 1}{2\alpha} \tag{2}$$

and

$$f_j(\theta) = \sin(\mu_j \theta). \tag{3}$$

The unknown singular coefficients α_j are determined by the boundary conditions in the remaining parts of the boundary. As already mentioned, these coefficients are called generalized stress intensity factors [30] and, in many applications, are the main unknowns.

Let us now move to the three-dimensional space using cylindrical coordinates (r, θ, z) . We consider a Laplacian problem in the three-dimensional domain $\Omega = [0, 1] \times [0, \alpha\pi] \times [-1, 1]$, as shown in Fig. 2:

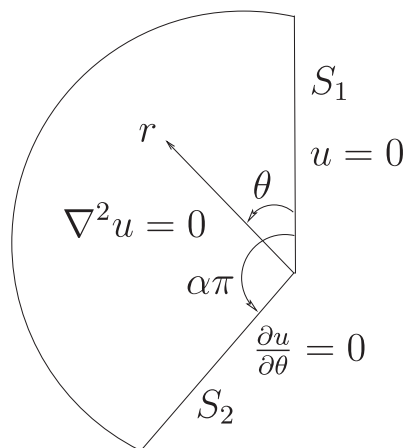


Fig. 1. A two-dimensional Laplacian problem with a boundary singularity at point O .

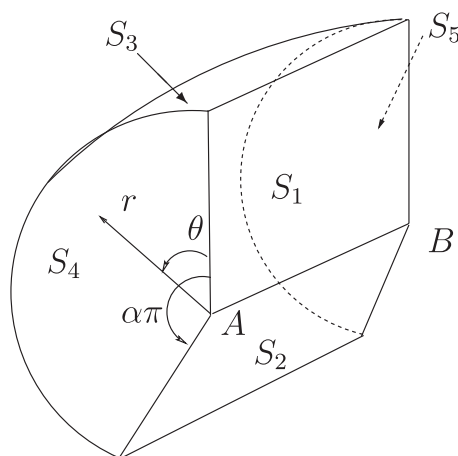


Fig. 2. A model three-dimensional domain $\Omega = [0, 1] \times [0, \alpha\pi] \times [-1, 1]$ with a straight edge AB .

$$\nabla^2 u = 0 \quad \text{in } \Omega, \tag{4}$$

with

$$\left. \begin{aligned} u &= 0 && \text{on } S_1 \\ \frac{\partial u}{\partial \theta} &= 0 && \text{on } S_2 \\ u &= g(r, \theta, z) && \text{on } S_3 \\ \frac{\partial u}{\partial z} &= q_1(r, \theta) && \text{on } S_4 \\ \frac{\partial u}{\partial z} &= q_2(r, \theta) && \text{on } S_5 \end{aligned} \right\}, \tag{5}$$

where $\partial\Omega = \bigcup_{i=1}^5 S_i$. S_1 and S_2 are quadrilateral surfaces intersecting at a straight edge AB , S_3 is a cylindrical surface of unit radius, and S_4 and S_5 are unit-circular sectors of angle $\alpha\pi$.

As pointed out by Yosibash et al. [32], once the eigen-pairs for the 2-D Laplacian problem are obtained, the full series expansion solution for the 3-D Laplacian operator in the vicinity of straight edges may be constructed. The solution can be decomposed as follows:

$$u(r, \theta, z) = \sum_{j=1}^J \sum_{\ell=1}^L \alpha_{j\ell}(z) r^{\mu_j} (\ln r)^\ell f_{j\ell}(\theta) + v(r, \theta, z), \tag{6}$$

where the exponents μ_j are identical to the eigenvalues of the 2-D problem given by Eq. (2) and are now called edge eigenvalues, $\alpha_{j\ell}$ are the edge flux intensity functions (EFIFs) which are analytic in z up to the vertices, $f_{j\ell}$ are the edge eigenfunctions which are analytic in θ , and v is a sufficiently smooth function. $L \geq 0$ is an integer which is zero except when μ_j is an integer. In the present work it is assumed that $\mu_j, j \leq J$ are not integers. Therefore, (6) is reduced to

$$\bar{u}(r, \theta, z) = \sum_{j=1}^J \alpha_j(z) r^{\mu_j} f_j(\theta) + v(r, \theta, z), \tag{7}$$

where $f_j(\theta)$ are the eigenfunctions of the 2-D problem given by Eq. (3). As demonstrated in [32], good choices for the function v so that u satisfies identically the 3-D Laplace equation are

$$v_j(r, \theta, z) = r^{\mu_j} f_j(\theta) \sum_{i=1}^{\infty} \frac{d^{2i}}{dz^{2i}} (\alpha_j(z)) \frac{r^{2i} (-1/4)^i}{\prod_{n=1}^i (\mu_j + n)}, \quad j = 1, 2, \dots, J. \tag{8}$$

Thus, the solution (7) takes the form

$$u(r, \theta, z) = \sum_{j=1}^J \alpha_j(z) r^{\mu_j} f_j(\theta) + \sum_{j=1}^J v_j(r, \theta, z)$$

or

$$u(r, \theta, z) = \sum_{j=1}^J r^{\mu_j} f_j(\theta) \left\{ \alpha_j(z) + \sum_{i=1}^{\infty} \frac{d^{2i}}{dz^{2i}} (\alpha_j(z)) \frac{r^{2i} (-1/4)^i}{\prod_{n=1}^i (\mu_j + n)} \right\}. \tag{9}$$

The calculation of the EFIFs $\alpha_j(z), j = 1, 2, \dots, J$ is the main objective of the present work.

3. Formulation of the SFBIM

The basic assumption for the development of the SFBIM for 3-D Laplacian problems with edge singularities is the use of piecewise low-degree ($k = 0$ or 1) polynomial approximations for the EFIFs by partitioning the interval $[-1, 1]$ into M sub-intervals and writing

$$\bar{\alpha}_j(z) = \sum_{m=1}^{M_\phi} \alpha_{jm} \phi_m(z), \quad j = 1, 2, \dots, N, \tag{10}$$

where α_{jm} are unknown coefficients, $\phi_m(z)$ are (piecewise polynomial) basis functions, and M_ϕ is the number of basis functions (e.g. $M_\phi = M$ for constant, $M_\phi = M + 1$ for linear basis functions, etc.). Thus, the inner sum in Eq. (9) is eliminated and the solution can be approximated as follows:

$$\bar{u}(r, \theta, z) = \sum_{j=1}^N \bar{\alpha}_j(z) r^{\mu_j} f_j(\theta), \tag{11}$$

or

$$\bar{u}(r, \theta, z) = \sum_{j=1}^N \sum_{m=1}^{M_\phi} \alpha_{jm} W_j^m(r, \theta, z), \tag{12}$$

where

$$W_j^m(r, \theta, z) = r^{\mu_j} f_j(\theta) \phi_m(z), \quad j = 1, 2, \dots, N, \quad m = 1, 2, \dots, M_\phi. \tag{13}$$

It is worthy to note that the functions W_j^m satisfy identically the governing equation and the boundary conditions on boundaries S_1 and S_2 sharing the edge AB . In order to calculate the $N_\alpha = NM_\phi$ unknown coefficients α_{jm} , we discretize the problem by weighting the governing equation over Ω by means of the functions W_j^m . Applying Green's theorem (twice) one gets:

$$\iint_{S_3 \cup S_4 \cup S_5} \left(\frac{\partial \bar{u}}{\partial n} W_j^m - \frac{\partial W_j^m}{\partial n} \bar{u} \right) dS = 0, \quad j = 1, 2, \dots, N, \quad m = 1, 2, \dots, M_\phi. \tag{14}$$

The Neumann conditions on boundaries S_4 and S_5 are weakly imposed by simply substituting the functions q_1 and q_2 , respectively. The Dirichlet boundary condition on S_3 is imposed by means of a Lagrange multiplier function $\lambda(\theta, z)$ which replaces the normal derivative of the solution. In this work, λ is approximated by means of locally polynomial (depending on the choice for ϕ_m) basis functions Ψ_i :

$$\lambda(\theta, z) = \frac{\partial \bar{u}}{\partial r} \Big|_{r=1} = \sum_{i=1}^{N_\lambda} \lambda_i \Psi_i(\theta, z), \tag{15}$$

where $\lambda_i, i = 1, 2, \dots, N_\lambda$ are the unknown discrete Lagrange multipliers. To define the basis functions Ψ_i , the two-dimensional domain $[0, \alpha\pi] \times [-1, 1]$ is partitioned into $N_\theta \times M_\phi$ elements, which means that $N_\lambda = M_\phi N_\theta$ or $M_\phi(N_\theta + 1)$ for, respectively, constant or bilinear Lagrange multipliers. The additional required equations are obtained by weighting the Dirichlet condition $u = g(\theta, z)$ on S_3 by means of the basis functions Ψ_i . The following linear system of $N_\alpha + N_\lambda$ discretized equations is obtained:

$$\iint_{S_3} \left(\lambda W_j^m - \bar{u} \frac{\partial W_j^m}{\partial r} \right) dS + \iint_{S_4} \bar{u} \frac{\partial W_j^m}{\partial z} dS - \iint_{S_5} \bar{u} \frac{\partial W_j^m}{\partial z} dS = \iint_{S_4} q_1 W_j^m dS - \iint_{S_4} q_1 W_j^k dS$$

for $j = 1, 2, \dots, N, \quad m = 1, 2, \dots, M_\phi$ (16)

and

$$\iint_{S_3} \bar{u} \Psi_i dS = \iint_{S_3} g \Psi_i dS, \quad i = 1, 2, \dots, N_\lambda. \tag{17}$$

Eqs. (16) and (17) involve only two-dimensional integrals, which implies that the dimension of the problem has been reduced by one. This is an important advantage of the method, since the required computational cost is reduced dramatically. Moreover, it should be noted that the contributions over boundary parts S_1 and S_2 , i.e. the two boundary parts that cause the edge singularity, are identically zero. The contributions over boundary parts S_4 and S_5 are also zero when the basis functions ϕ_m are constant ($k = 0$). The system of Eqs. (16) and (17) can be written in block form as follows:

$$\begin{bmatrix} K & L \\ L^T & O \end{bmatrix} \begin{bmatrix} A \\ \Lambda \end{bmatrix} = \begin{bmatrix} B \\ C \end{bmatrix}, \tag{18}$$

where A is the vector of the unknown coefficients α_{jm} of the EFIFs and Λ is the vector of the unknown discrete Lagrange coefficients. It is easily observed that the stiffness matrix is symmetric and becomes singular if the number of Lagrange multipliers, N_λ , is greater than the number of the unknown coefficients, $N_\alpha < N_\lambda$, or, equivalently, when $N < N_\theta$ for constant ϕ_k and $N < N_\theta + 1$ for linear ϕ_k . In order to assure that the stiffness matrix is non-singular, in all the numerical results of this work we have chosen $N_\theta = \min\{M, N - 2, 20\}$.

4. Numerical results

Following Yosibash et al. [32], we construct test problems having analytical solutions of the form:

$$u_s(r, \theta, z) = \sum_{i=1}^J \left[(\alpha_{i1} + \alpha_{i2}z + \alpha_{i3}z^2) r^{\mu_i} \sin(\mu_i \theta) - \frac{\alpha_{i3}}{2(\mu_i + 1)} r^{\mu_i+2} \sin(\mu_i \theta) \right], \tag{19}$$

where $\alpha_{ij}, i = 1, \dots, J, j = 1, 2, 3$ are specified as desired. Any solution of the form (19) satisfies the 3D Laplace equation as well as the boundary conditions along S_1 and S_2 . Once the solution u_s is specified, it is straightforward to find the functions g, q_1 and q_2 that appear in Eq. (5):

$$g(\theta, z) = u(1, \theta, z) = \sum_{i=1}^J \left(\alpha_{i1} - \frac{\alpha_{i3}}{2(\mu_i + 1)} + \alpha_{i2}z + \alpha_{i3}z^2 \right) \sin(\mu_i\theta), \tag{20}$$

$$q_1(r, \theta) = \frac{\partial u_s}{\partial z}(r, \theta, -1) = \sum_{i=1}^J (\alpha_{i2} - 2\alpha_{i3})r^{\mu_i} \sin(\mu_i\theta), \tag{21}$$

$$q_2(r, \theta) = \frac{\partial u_s}{\partial z}(r, \theta, 1) = \sum_{i=1}^J (\alpha_{i2} + 2\alpha_{i3})r^{\mu_i} \sin(\mu_i\theta). \tag{22}$$

In what follows we investigate the implementation of the above method for $\alpha = 3\pi/4$. The eigenvalues and eigenfunctions in this case are:

$$\mu_j = \frac{2(2j-1)}{3}, \quad f_j(\theta) = \sin(\mu_j\theta) = \sin\left[\frac{2(2j-1)}{3}\theta\right]. \tag{23}$$

For the model test problem we consider here we take $J = 100$ with

$$\alpha_{i1} = \frac{1}{i^4}, \quad \alpha_{i2} = \frac{2}{i^4 + i^2}, \quad \alpha_{i3} = \frac{3}{i^4}, \quad i = 1, \dots, J. \tag{24}$$

Due to the form of the essential boundary condition (20), the SFBIM calculates directly the EFIFs, which are given by

$$\alpha_i(z) = \alpha_{i1} - \frac{\alpha_{i3}}{2(\mu_i + 1)} + \alpha_{i2}z + \alpha_{i3}z^2. \tag{25}$$

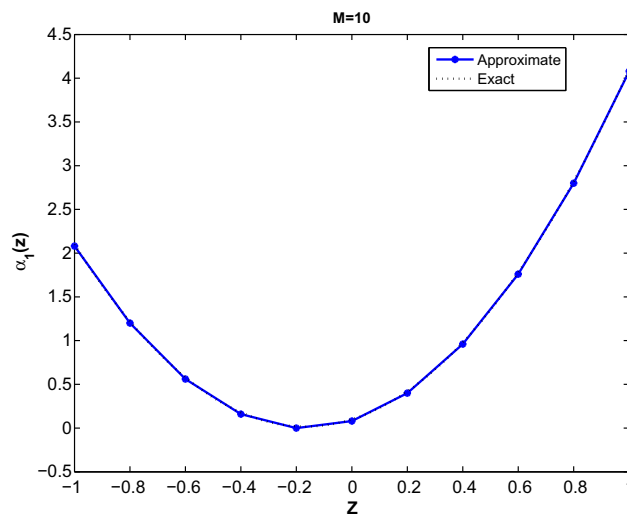


Fig. 3. The approximate first EFIF, $\alpha_1(z)$, calculated with $N = 15$ and $M = 10$ compared to the exact solution.

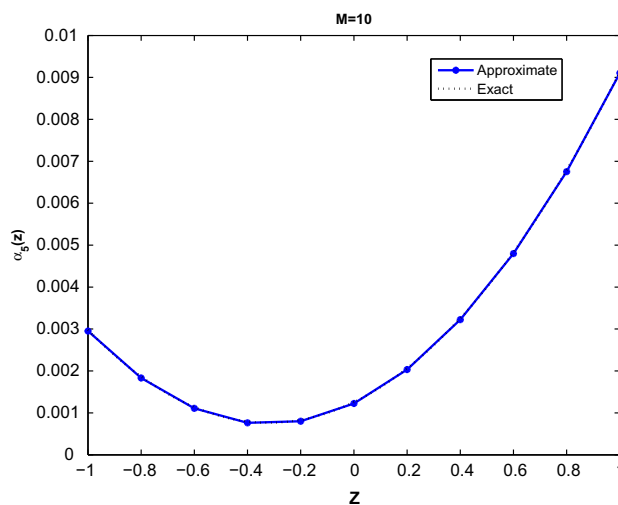


Fig. 4. The approximate fifth EFIF, $\alpha_5(z)$, calculated with $N = 15$ and $M = 10$ compared to the exact solution.

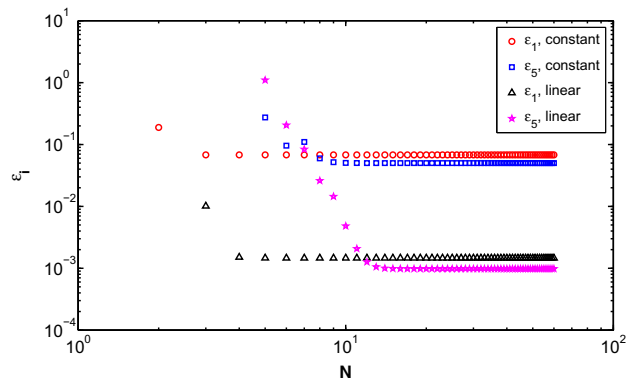


Fig. 5. The errors ϵ_1 and ϵ_5 for both constant and linear basis functions when $M = 20$.

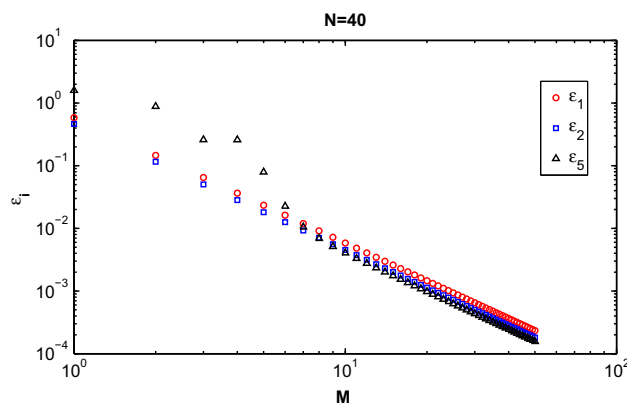


Fig. 6. Convergence of $\alpha_1(z)$, $\alpha_2(z)$ and $\alpha_5(z)$ with M when $N = 40$.

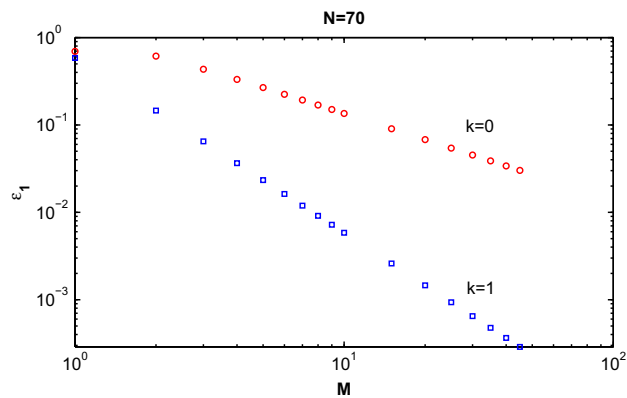


Fig. 7. The error $\epsilon_1(z)$ in the first EFIF when constant and linear basis functions are used; $N = 70$.

Figs. 3 and 4 show the exact and computed $\alpha_1(z)$ and $\alpha_5(z)$, respectively, obtained with $M = 10$, $N = 20$ using linear basis functions ($k = 1$). Other combinations of these parameters gave similar results, with higher values of M or N yielding better results, as expected. Analogous results have also been obtained using constant basis functions instead ($k = 0$). Fig. 5 compares the convergence in the approximations of α_1 and α_5 for $M = 20$ when constant and linear basis functions are used. The errors plotted are relative, i.e.,

$$\epsilon_i = \frac{\|\alpha_i - \bar{\alpha}_i\|_2}{\|\alpha_i\|_2},$$

where

$$\|f\|_2 = \left[\int_{-1}^1 f^2(z) dz \right]^{1/2}.$$

Of course, convergence with the linear elements is faster. However, the accuracy of the solution is limited by the type and number M of the elements employed in the approximation of the EFIFs. Hence, beyond a certain value, accuracy cannot be improved any further by increasing N .

Fig. 6 shows the convergence in the approximation of α_i , $i = 1, 2, 5$, when $N = 15$ and the number of linear elements M varies. As expected, the convergence is of order 2, as $M \rightarrow \infty$, since we are using piecewise linear functions and measuring the error in the L^2 -norm. It is well known from interpolation theory that if piecewise polynomials of degree k are used as basis functions then the error in the L^2 norm is of order $k + 1$ [6]. This is readily verified in Fig. 7 where we compare the errors in the first EFIF for $N = 70$ when constant ($k = 0$) and linear ($k = 1$) basis functions are employed; the slopes of the two curves are respectively 1 and 2.

5. Conclusions

We have extended the SFBIM to three-dimensional Laplacian problems with a boundary straight-edge singularity. The EFIFs are approximated locally by low degree polynomials of degree $k = 0, 1$ and the corresponding coefficients are primary unknowns along with the discrete Lagrange multipliers, which are employed in enforcing the Dirichlet boundary conditions. The method has been applied to a model Laplacian problem yielding accurate results for the EFIFs which converge with order $k + 1$ in the L^2 -norm. In other words, in three dimensions exponential convergence is not feasible, since the convergence rate is limited by the lower-order approximation of the EFIFs in the z-coordinate.

Our current research efforts focus on the application of the method to more realistic 3-D Laplacian problems, like those considered by Omer et al. [24], the theoretical convergence analysis of the method, and possible extensions to problems with vertex singularities similar to those considered by Zaltzman and Yosibash [36]. Another direction for future work is the extension of the method to three-dimensional elasticity problems with edges. Costabel et al. [9] presented a method to compute the singularity exponents and the associated singular functions, the knowledge of which is a prerequisite of the SFBIM, in the case of piecewise homogeneous media near three-dimensional edges.

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