Finite difference solution to the Poisson equation at an intersection of interfaces

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Abstract

We consider the solution u to Poisson's equation $L(pu) = f$ on a polygonal domain $\Omega \in R^2$, which itself is composed of polygonal subdomains Ω_i, where L is the Laplacian operator and the coefficient p is piecewise constant, with value p_i in region Ω_i. At a point S of intersection of the interfaces between Ω_i and adjacent regions the solution may have singular components. These, if present, may be severe and will degrade the convergence of the basic methods of numerical approximation to the solution u in the locality of S. Elaborate methods are required to accurately estimate the singular components, or stress intensity factors, or to improve the accuracy of the numerical solution near S. When the interfaces are straight lines on a Cartesian grid,

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with homogeneous interface conditions, we show that a remarkable pattern of symmetries of the singular components leads to a simple finite difference solution at the point of intersection S, and to an estimate of the stress intensity factors enabling extraction of the singular components and improved accuracy at points close to S.

Contents

1 Introduction

We shall study the solution u to Poisson's equation

$$L(pu) = f \quad \text{on } \Omega \in R^2\,, \tag{1}$$

with boundary conditions $Bu = g$ on $\partial\Omega$, the boundary of Ω, with L the Laplacian operator, and B specifying Dirichlet, von Neumann or mixed boundary conditions. Ω may be subdivided into discrete regions Ω_i on which p, which is piecewise constant, assumes the positive value p_i. The interface, the line Γ_{ij}, is the common boundary of adjoining regions Ω_i and Ω_j across which we require homogeneous interface conditions

$$u|_{\Gamma_{ij-}} = u|_{\Gamma_{ij+}} \tag{2}$$

and

$$p_i \left.\frac{\partial u}{\partial \tau_{ij}}\right|_{\Gamma_{ij-}} = -p_j \left.\frac{\partial u}{\partial \tau_{ji}}\right|_{\Gamma_{ij+}}, \tag{3}$$

where Γ_{ij-} and Γ_{ij+} indicate the limiting values in Ω_i and Ω_j respectively at Γ_{ij}, and τ_{ij} is the outer unit normal to Γ_{ij} from Ω_i. Elliptic boundary value problems may have singular solutions which, even if the data f and g are smooth, may arise at irregular points, termed vertices, which include: corners on $\partial\Omega$; points on $\partial\Omega$ where the boundary conditions change; corners on an interface and points where interfaces meet or intersect another interface or the boundary [3]. With few restrictions the solution u may be decomposed

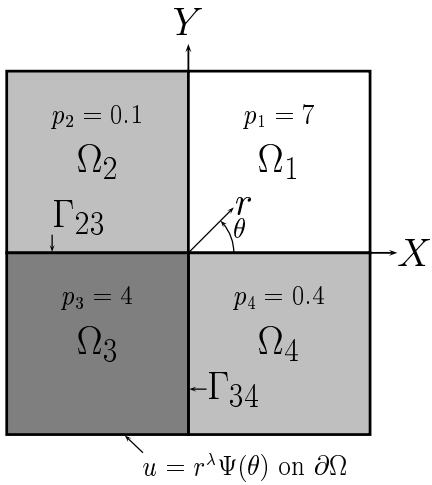
$$u = w + \sum_S v_S \,, \tag{4}$$

where w is a regular part whose smoothness depends on the smoothness of f and g, and v_S the singular part associated with each vertex S [6, 7]. v_S is composed of the eigenfunctions, solutions to $L(pu) = 0$, in the vicinity of S. If S is the origin of polar coordinates r, θ, with θ denoted θ_i within Ω_i, and ω_i the internal angle included by the boundary of Ω_i at S, then the eigenfunctions v_S with eigenvalue λ, in the vicinity of S have the form:

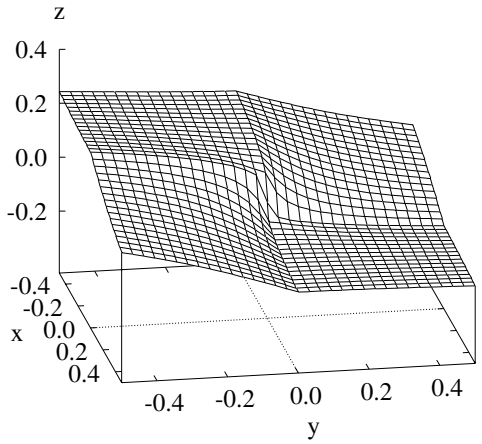
$$u(r,\theta) = \zeta(r) r^\lambda \Psi(\theta) \quad \text{where} \quad \lambda \notin N\,; \tag{5}$$

$$u(r,\theta) = \zeta(r) r^\lambda \left\{\ln(r)\Psi(\theta) + (\theta/\lambda)\Psi'(\theta)\right\} \quad \text{where} \quad \lambda \in N\,. \tag{6}$$

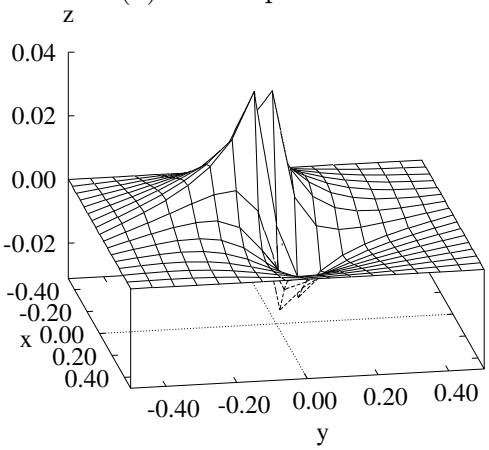
$\zeta(r)$ is a smooth cut-off function with value 1 for $0 \le r < r_0$ and smoothly decays to 0 for $r > r_b > r_0$ where r_b is less than the radial distance to any other vertex, boundary or interface. The value of λ, which determines the severity of the singularity, will depend on the included angle ω_i, and if S is at an interface, the values of p_j belonging to all Ω_j for which $S \in \bar{\Omega}_j$. The basic finite element method (FEM) has impaired accuracy and convergence in the presence of singular solutions, as shown in Figure 1 [1, 8]. In this paper we show that by a remarkable pattern of symmetries of the singular solutions finite difference (FD) methods are valid and will converge at the intersection S with order h, at points adjacent to S with order h^λ, and that



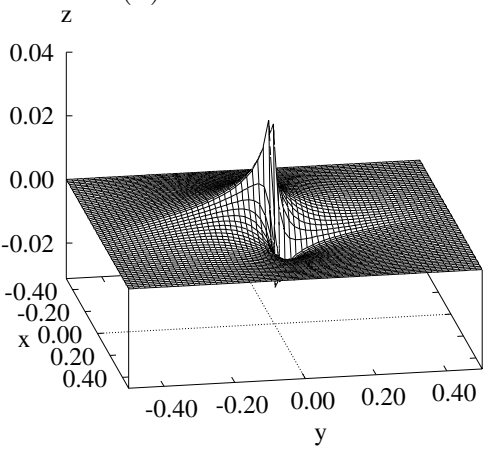
(a) Model problem



(b) Exact solution



(c) Error, $h = 1/16$



(d) Error, $h = 1/64$

FIGURE 1: (a) The region Ω and subregions Ω_i. $\Psi(\theta)$ (see equations (8)–(12)) with the lowest eigenvalue $\lambda \approx 0.27$ determines the value on the boundary at $x, y = \pm 0.5$, and satisfies $L(pu) = 0$ on Ω. (b) The exact solution. (c) and (d) are the error of the approximation by basic FEM, identical to the FD solution, on a regular grid of size h. The error is greatest at the nodes adjacent to the origin, and converges only slowly with decreasing h.

the most singular components are reliably estimated from point values close to S by exploiting a discrete p-orthogonality of the eigenfunctions. The latter may be used in FD or FEM to extract the singular components leading to a more accurate solution.

2 Singular solutions at interface intersection

Let all Ω_i be rectangular. At any intersection of interfaces S not on $\partial\Omega$ there will be four regions Ω_i, $i = 1, 2, 3, 4$ proceeding anticlockwise around S, with the line $\theta = 0$ coincident with Γ_{14}. $\Psi(\theta)$ in (5) is the solution to, and λ an eigenvalue of, the periodic Sturm–Liouville system

$$\frac{\partial^2 \Psi(\theta_i)}{\partial \theta_i^2} + \lambda^2 \Psi(\theta_i) = 0 \quad \text{for} \quad i = 1, 2, 3, 4\,, \tag{7}$$

satisfying (2) and (3) at a constant radius $r < r_0$ from S [6]. Although (6) satisfies (7), it cannot simultaneously satisfy (2) and (3), and thus the only singular solutions are given by (5). The general form of $\Psi(\theta)$ with the interfaces being two straight lines intersecting at angle $0 < \varphi \leq \pi/2$ with supplementary angle $\psi = \pi - \varphi$ is given by Kellogg [5]:

$$\Psi(\theta) = \begin{cases} \cos(\lambda_n(\psi - b_1))\cos(\lambda_n(\theta - \varphi + a_1))\,, & 0 \leq \theta \leq \varphi\,, \\ \cos(\lambda_n a_1)\cos(\lambda_n(\theta - \pi + b_1))\,, & \varphi \leq \theta \leq \pi\,, \\ \cos(\lambda_n b_1)\cos(\lambda_n(\theta - \pi - a_1))\,, & \pi \leq \theta \leq \pi + \varphi\,, \\ \cos(\lambda_n(\varphi - a_1))\cos(\lambda_n(\theta - \varphi - \pi - b_1))\,, & \pi + \varphi \leq \theta \leq 2\pi\,. \end{cases} \tag{8}$$

With the aid of computerised algebraic manipulation and trigonometric identities when $\varphi = \pi/2$ we derived explicit expressions for $\Psi(\theta)$ and λ: define

$$\chi_1 = \sqrt{p_1p_2p_3 + p_1p_4p_3 + p_1p_4p_2 + p_4p_2p_3}\,; \quad \chi_2 = \sqrt{p_1 + p_2 + p_3 + p_4}\,; \tag{9}$$

and let

$$\gamma = \frac{2}{\pi}\tan^{-1}\left(\frac{\chi_1\chi_2}{p_1p_3 - p_2p_4}\right) \quad \text{for} \quad p_1p_3 \neq p_2p_4\,. \tag{10}$$

The eigenvalues λ of $\Psi(\theta)$ are then the positive values of

$$\lambda_n \in \{\lambda : \lambda = 2m \pm \gamma,\ m = 0, 1, 2, 3\ldots,\ \lambda > 0\}\,, \quad n = 0, 1, 2, 3, \ldots\,, \tag{11}$$

with

$$a_1 = \pm\frac{1}{\lambda_n}\tan^{-1}\left(\frac{p_2\chi_2}{\chi_1}\right)\,, \quad b_1 = \mp\frac{1}{\lambda_n}\tan^{-1}\left(\frac{p_3\chi_2}{\chi_1}\right)\,, \tag{12}$$

where the sign on γ in (11) corresponds with the sign in a_1 and its inverse in b_1. Kellogg's second set of equations similar to (8) for sin functions are identical to (8) when $\varphi = \pi/2$. Symmetries in these eigenfunctions valid for all λ_n are:

$$\frac{\Psi(0)}{\Psi(\pi)} = -\frac{p_2 + p_3}{p_1 + p_4}\,; \quad \frac{\Psi(\pi/2)}{\Psi(3\pi/2)} = -\frac{p_3 + p_4}{p_1 + p_2}\,; \tag{13}$$

$$p_1\Psi(\pi/4) + p_2\Psi(3\pi/4) + p_3\Psi(5\pi/4) + p_4\Psi(7\pi/4) = 0\,; \tag{14}$$

$$\Psi(\pi/4) - \Psi(3\pi/4) + \Psi(5\pi/4) - \Psi(7\pi/4) = 0\,. \tag{15}$$

When φ is a rational fraction of π there are solutions to (7) with integral eigenvalues. These eigenfunctions or their derivatives have a value of zero on the interfaces. Let $\varphi_i = (i-1)\pi/2\,,\ i = 1, 2, \ldots, 5\,$. These non-singular eigenfunctions, which are members of w in (4), for $i = 1, 2, 3, 4\,$, are:

$$w_A(\theta) = (1/p_i)\cos(\lambda_{A,n}(\theta_i - 3\pi/4))\,, \qquad \varphi_i \le \theta_i \le \varphi_{i+1}\,; \tag{16}$$

$$w_B(\theta) = \sin(\lambda_{B,n}(\theta_i - 3\pi/4))\,, \qquad \varphi_i \le \theta_i \le \varphi_{i+1}\,; \tag{17}$$

$$w_C(\theta) = \cos(\lambda_{C,n}(\theta_i - 3\pi/4))\,, \qquad \varphi_i \le \theta_i \le \varphi_{i+1}\,; \tag{18}$$

$$w_D(\theta) = (1/p_i)\sin(\lambda_{D,n}(\theta_i - 3\pi/4))\,, \qquad \varphi_i \le \theta_i \le \varphi_{i+1}\,; \tag{19}$$

with $\lambda_{A,n} = \lambda_{B,n} = 4n + 2\,,\ \lambda_{C,n} = \lambda_{D,n} = 4n\,,\ n = 0, 1, 2, 3, \ldots\,$. Together with (8) they form a complete p-orthogonal basis of functions, which may be used to expand $u(r, \theta)$ at a fixed radius $r < r_0$ from the origin at S. If we let

$\phi_k(\theta)$, $k = 0, 1, 2, \ldots$, be a member of the complete set of eigenfunctions (8), (16)–(19) for all λ, then in the locality of S at radius $r < r_0$

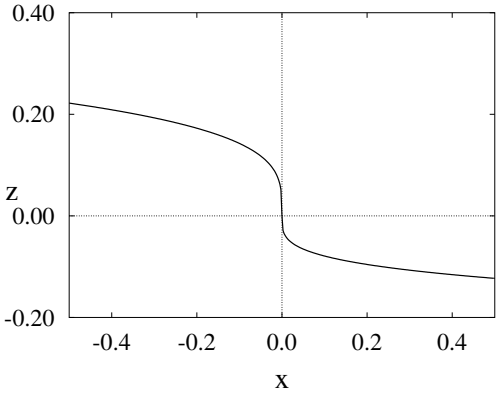
$$u(r,\theta)|_r = w + \sum_n c_n r^{\lambda_n} \Psi_n(\theta) = \sum_{k=0}^{\infty} \kappa_k^\star r^{\lambda_k} \phi_k(\theta) = \sum_{k=0}^{\infty} \kappa_k \phi_k(\theta)\,. \tag{20}$$

If $\phi_k(\theta)$ is member $\Psi_n(\theta)$ in (5), then $c_n r^{\lambda_n} \approx \kappa_k$, with the accuracy of the approximation depending on how much of w, which depends on f, is composed of Ψ_n at radius r in the series (20), and this by how much f varies with r in the interval $[0, r]$. From the symmetries (13)–(15) and the values of (16)–(19) the eigenfunctions $\phi_k(\theta)$ also satisfy a limited discrete p-orthogonality when evaluated at $\theta = j\pi/4$, $j = 0, 1, 2, \ldots, 7$. If we restrict the set ϕ_k of eigenfunctions to those of the lowest four eigenvalues of (8) and the lowest eigenvalue in each of (16)–(19), then

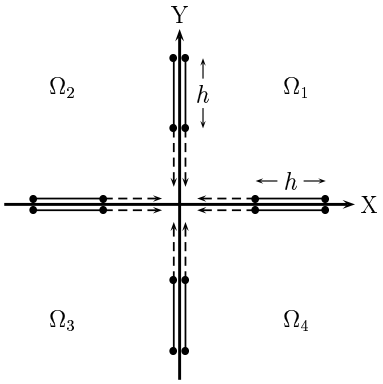
$$\sum_{j=0}^{7} p_j^* \phi_k(\theta_i)\phi_m(\theta_i) = \begin{cases} 0\,, & k \neq m \text{ or } \phi_k, \phi_m \in \{w_D(\theta)\}\,, \\ M \neq 0\,, & k = m\,, \quad \phi_k, \phi_m \notin \{w_D(\theta)\}\,, \end{cases} \tag{21}$$

$$p_j^* = \begin{cases} p_i\,, & i = (j+1)/2\,, \quad j \text{ odd}, \\ (p_i + p_{i+1})/2\,, & i = j/2\,, \quad p_0 \equiv p_4\,, \quad j \text{ even}\,. \end{cases}$$

The discrete p-orthogonality fails for $w_D(\theta)$, for on $\theta = j\pi/4$, $w_D(\theta) = 0$. The coefficients c_n are estimated from κ_k in (20) by using (21). The coefficients of the higher order eigenfunctions in each class will be aliased into the lower order coefficient, but from (20) their contribution will be reduced by the ratio $r^{\lambda_n+4m}/r^{\lambda_n} \ll 1$ for $r < 1$, $m = 1, 2, 3, \ldots$. In real situations the highly oscillatory singular eigenfunctions are unlikely, and it is those of the lowest order which are most likely and which cause the greatest degradation in convergence. Estimating the coefficient enables the value of the singular eigenfunctions to be extracted in the region of S, permitting improved accuracy by a second approximation on the remaining smooth components, as employed in multigrid FEM [2], and explained in Figure 3(b).



(a) model solution on x axis



(b) FD derivation at vertex

FIGURE 2: (a) The singularity of the solution in Figure 1: an unbounded gradient at the origin. (b) schematic of derivation of the FD formula at the origin. The dashed arrows indicate taking the inner points to the limit at the origin.

3 Finite difference formulation

3.1 Solution at the vertex

FD derived approximations to u are based upon its Taylor series (TS) expansion which has a remainder term R_n, which for a function $f_T(z)$ is

$$R_n(z) = \frac{h^n}{(n-1)!} \int_0^1 (1-t)^{n-1} f_T^{(n)}(z+th)\, dt\,. \tag{22}$$

It is generally required that $f_T^{(n-1)}(z)$ be absolutely continuous, thus bounded, in $[z, z+h]$ for $R_n(z)$ to be finite. The series converges if $\lim_{n\to\infty} R_n(z) = 0$. Figure 2(a) clearly shows that the x partial derivative of the singular solution of the model problem of Figure 1 is unbounded at the origin. For the moment we shall assume that u is sufficiently smooth in each region Ω_i

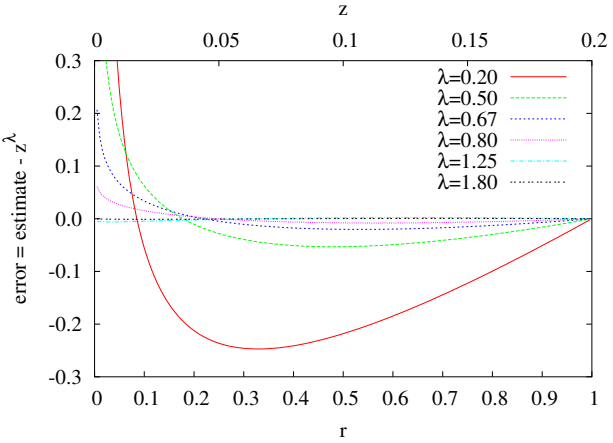
for TS expansion, and use Cartesian (x, y) coordinates with the axes on the interfaces and $\theta = 0$ being the $+x$ axis. By taking limits of u and its partial derivatives at points adjacent to the interfaces (see Figure 2(b)) and using the continuity and interface conditions (2)–(3), a FD expression is obtained to estimate $u(0,0)$ from values of u on the interfaces at distance h from S and the limiting values of f in each quadrant Ω_i at S:

$$\begin{aligned}&\frac{2}{h^2}\{(p_1+p_4)(u(h,0)-u(0,0))+(p_1+p_2)(u(0,h)-u(0,0))\\&\quad+(p_2+p_3)(u(-h,0)-u(0,0))+(p_3+p_4)(u(0,-h)-u(0,0))\}\\&=p_1f(0^+,0^+)+p_2f(0^-,0^+)+p_3f(0^-,0^-)+p_4f(0^+,0^-)+\mathcal{O}(h)\,.\end{aligned}\tag{23}$$

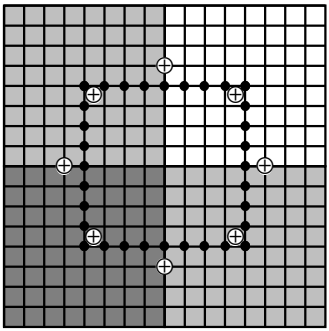
If u did have singular components, the symmetry (13) exactly cancels all the singular components (5) and all their derivatives in the derivation of (23). Thus (23) remains valid with singular components v_S in u. A similar limiting procedure on the diagonals, decomposing the partial derivatives along the diagonals into x and y partial derivatives, leads to a FD expression on $x = \pm y$:

$$\begin{aligned}&\frac{2}{h^2}\{p_1(u(h,h)-u(0,0))+p_2(u(-h,h)-u(0,0))\\&\quad+p_3(u(-h,-h)-u(0,0))+p_4(u(h,-h)-u(0,0))\}\\&=p_1f(0^+,0^+)+p_2f(0^-,0^+)+p_3f(0^-,0^-)+p_4f(0^+,0^-)+\mathcal{O}(h)\,,\end{aligned}\tag{24}$$

and the symmetry (14) exactly cancels all singular components and their derivatives at all stages in the derivation. In (23) the symmetry (13) balances the singular components on the x axis independently of those on the y axis, so the solution may be split, but in (24) symmetry (14) requires the value on all axes for cancellation of the singular components, so may not be split. The symmetries (13) and (14), which permit FD formulation at S by cancellation of the singular components, apply only on the axes coincident with and at angle $\pi/4$ to the interfaces, as fortuitously used in most FEM schemes [8], and do not pertain to orthogonal axes at other orientations.



(a) Error $\left(\frac{R_1}{h_1} + \frac{R_2}{h_2}\right)$ versus $r = \frac{h_1}{(h_1+h_2)}$



(b) Extraction

FIGURE 3: (a) The error in the FD estimate of $f_T(z) = z^\lambda$, solution to $f_T''(z) = \lambda(\lambda-1)z^{\lambda-2}$, at $z = h_1$ from 'boundary' values $f_T(0)$ and $f_T(h_1 + h_2) = 0.2^\lambda$. (b) From an initial estimate of solution u to $L(pu) = f$, the value at points $\oplus$, at constant radius from the centre, enables estimation of the stress intensity factors and subtraction of the singular eigenfunctions from the initial estimate at the points $\bullet$, which become an inner 'boundary'. A new estimate of the remaining smooth components of u is found internal to this 'boundary', and the singular eigenfunctions are then added back to the points $\bullet$ and to the new estimate of u internal to them.

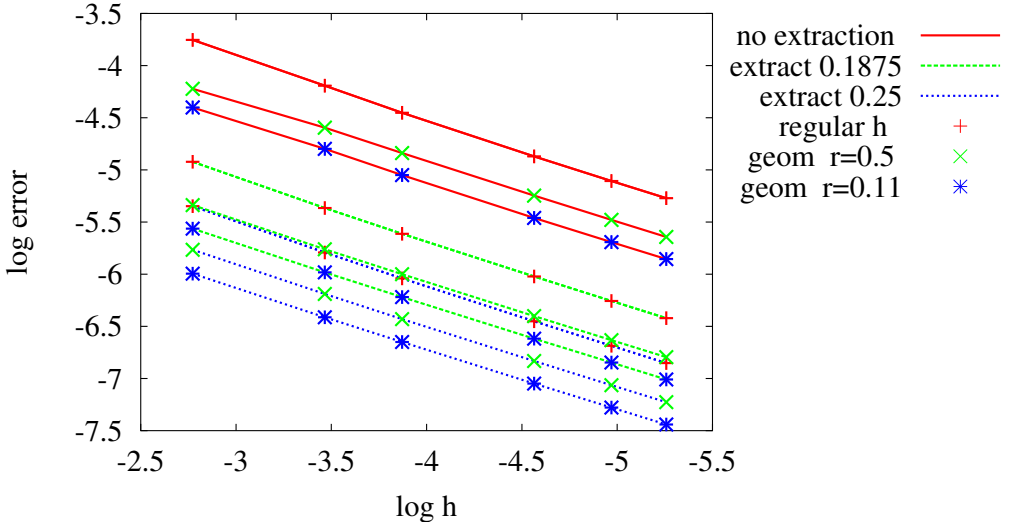


FIGURE 4: Convergence of solution u to the problem in Figure 1 at the point $(0.0625, 0)$ as h is refined, on combinations of a regular grid, a grid with the first interval h adjacent to the origin divided into two by h_1 with ratio $r = h_1/h$ of 0.5 and 0.11 , the latter determined by (28) with $h = h_1 + h_2$, and extraction of the singular component on squares of sides 0.1875 and 0.25 from origin. The slope is approximately -0.6 .

3.2 Solution adjacent to vertex

FD approximations to (1) across an interface at points away from S may be formed using limits of u and its derivatives at the interface, utilising the interface and continuity conditions [4]. At a point on an interface adjacent to S, for example $(h_1, 0)$, any FD expression will require the value $u(0,0)$. With singular components (5) with $\lambda < 1$, all partial derivatives $\partial^n u(r,\theta)/\partial r^n = \partial^n u(x,0)/\partial x^n$ are unbounded as r and $x \to 0^+$, as shown in Figure 2(a), violating the general requirements for the existence of R_n in (22). When $f_T(z) = z^\alpha$ with $\alpha > 0$, $\alpha \notin N$ it is possible to evaluate (22)

$$R_n(h_1) = \frac{(-1)^n h_1^{(\alpha)} (\alpha - 1)!}{(n-1)!(\alpha - n)!}, \tag{25}$$

but $\lim_{n\to\infty} R_{n+1}(h_1)/R_n(h_1) = 1$ and $\lim_{n\to\infty} R_n(h_1) \neq 0$ so that the TS does not converge. The TS with remainder R_n, however, is a correct representation of $f_T(z) = z^\alpha$. The complete FD expression of (1) at $(h_1, 0)$, with adjacent x axis points $(0,0)$ and $(h_1 + h_2, 0)$, is

$$\begin{aligned}\frac{p_1}{2} f(h1, 0^+) + \frac{p_4}{2} f(h1, 0^-) &= -(p_1 + p_4)\frac{(h_1 + h_2)}{(h_1^2 h_2)} u(h_1, 0) \\ &+ \frac{(p_1 + p_4)}{(h_1 + h_2)h_1} u(0,0) + \frac{(p_1 + p_4)}{(h_1 + h_2)h_2} u(h_1 + h_2, 0) + \frac{p_1}{h_1^2} u(h_1, h_1) \\ &+ \frac{p_4}{h_1^2} u(h1, -h_1) + \frac{(p_1 + p_4)}{(h_1 + h_2)} \left(\frac{R_1}{h_1} + \frac{R_2}{h_2} \right) + \frac{p_1 R_y^+ + p_4 R_y^-}{h_1^2}.\end{aligned} \tag{26}$$

R_1 and R_2 are the truncation error terms $R_n(z)$ in (22) with $n = 3$ for the x partial derivative TS of u at $(h_1, 0)$ expanded about $(0,0)$ and $(h_1 + h_2, 0)$ respectively, and R_y^+ and R_y^- are the error terms for the limits of the y partial derivative TS of u at $(h_1, 0)$ expanded about (h_1, h_1) and $(h_1, -h_1)$. Let $h = K\sqrt{h_1 h_2}$ and $h_1 = K_1 h_2$ for some bounded positive constants K, K_1. The convergence of (26) is determined by the R_1, R_2 and R_y terms. For bounded derivatives this is $\mathcal{O}(h)$. The v_S component of R_1 is given by (25)

so that $R_1/(h_1(h_1+h_2))$ would appear to be $\mathcal{O}(h^{\lambda-2})$ which does not converge for $\lambda < 2$ as $h \to 0$, but this truncation error arises in the approximation of $\partial^2 v_S/\partial x^2$ which is unbounded as $x \to 0$ rendering convergence by this criterion meaningless. The convergence of (26) is dominated by the largest error term, usually component v_S of u in R_1. In (26) let $u = v_S$, $f = 0$ and the values of v_S at $(0,0)$, (h_1,h_1), $(h_1,-h_1)$ and $(h_1+h_2,0)$ be regarded as known boundary values. The error in the estimate $\hat{v}_S(h_1,0)$ from (26) is then

$$v_S(h_1,0) - \hat{v}_S(h_1,0) = \frac{h_1^2 h_2}{(h_1+h_2)^2}\left(\frac{R_1}{h_1} + \frac{R_2}{h_2}\right) + \frac{h_2(p_1 R_y^+ + p_4 R_y^-)}{(p_1+p_4)(h_1+h_2)}. \quad (27)$$

The term with R_1 in (27) is $\mathcal{O}(h^\lambda)$, and usually determines the convergence of (26). This agrees with the pointwise convergence for basic FEM[1]. The ratio $q = h_2/h_1$ is chosen by solution to

$$-q\lambda^2 + q\lambda - 2q + 2(1+q)^\lambda - q^2\lambda(\lambda-1) - 2 = 0\,, \quad (28)$$

so that $R_1/h_1 = -R_2/h_2$, (Figure 3(a)), reducing the error. This is similar to h-FEM using geometric grid division in the interval(s) adjacent to the singularity [8]. Improved accuracy to the solution of the model problem using geometric division of the first interval h, and extraction, is shown in Figure 4.

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