JOURNAL OF COMPUTATIONAL PHYSICS 26, 285–296 (1978)

The Numerical Solution of Elliptic and Parabolic Partial Differential Equations with Boundary Singularities

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Received April 13, 1976; revised March 21, 1977

A general numerical method is described for the solution of linear elliptic and parabolic partial differential equations in the presence of boundary singularities. The method is suitable for use with either a finite-difference or a finite-element scheme. Modified approximations for the derivatives are developed using the local analytical form of the singularity. General guidelines are given showing how the local analytical form can be found and how the modified approximations can be developed for many problems of mathematical physics. These guidelines are based on the reduction of the differential equation to the form $Au = gu + f$. The potential problem treated by Motz and Woods is taken as a numerical example. The numerical results compare favorably with those obtained by other techniques.

1. INTRODUCTION

The problem of boundary singularities in the numerical solution of elliptic and parabolic partial differential equations has received a great deal of attention. These singularities arise when sudden changes occur either in the direction of the boundary, as at a re-entrant corner, or they may be associated with mixed boundary conditions. Such singularities are found in a wide variety of physical problems, e.g., stress analysis in regions with cracks, discontinuities, point sources, etc. [8, 14, 43], flow around an obstacle [18], seepage through a dam [1], heat flow, diffusion or potential problems in regions with re-entrant corners, electrodes, heat sources or sinks [3–7, 11–15, 19–25, 27, 30–39, 42].

Special numerical schemes have been devised to obtain accurate solutions near boundary singularities without a large amount of computation. Some authors have used mesh refinement near the singularity [7, 12, 19, 32, 36, 39] and others have derived modified approximations to the governing differential equation and its solution near the singularity by using the local analytical form of the singularity, e.g., as in the Motz method [3–6, 8, 11, 14, 15, 17, 21, 35, 37, 42, 43]. Either approach may be part of, and dovetail readily into, a global finite-difference or finite-element scheme. The analytical forms needed for the second approach require some prior analysis but usually are readily available in the form of an asymptotic expansion by separable-variable [4, 17, 28, 43] or complex variable [20, 22, 40, 41] techniques. Alternative methods based on conformal transformations [23, 24, 29], modified

0021-9991/78/0263-0285$02.00/0

integral equations [31], modified collocation [29], power series [22], dual series [38], and removal of the singularity [34, 40–42] have been proposed.

In the following sections a new way of developing such modified approximations is given for differential equations of elliptic and parabolic type. The novel feature is that modified approximations for the derivatives in the governing equation are developed and take the place of the algebraic equations for the solution values as originally used by Motz [21]. The method is applied to the potential problem of Motz [21] and Woods [42].

2. Local Analytical Forms for Boundary Singularities

Separable-variable solutions for second-order equations of the form

$$\sum_{i=1}^{n} \kappa_i \frac{\partial^2 u}{\partial x_i^2} = gu + f, \tag{2.1}$$

where $\kappa_i = 0, 1,$ or -1 and u, g, f are functions of x_i only, and satisfying fairly general boundary conditions, have been given by Fox and Sankar [16, 17] for the case $n = 2$. These results may be summarized as

$$u = \phi_0(\rho, \theta) + \sum_{i=1}^{\infty} c_i \phi_i(\rho, \theta), \tag{2.2}$$

where the c_i are arbitrary constants, ρ, θ, are local polar coordinates centered on the boundary singularity. Each $\phi_i(\rho, \theta)$ is a linear combination of terms, some of which are singular, like

$$\rho^{\alpha+i} A_{\alpha,i}(\theta) \qquad \text{or} \qquad \rho^{\alpha+i}\{(\ln \rho)\, A_{\alpha,i}(\theta) + B_{\alpha,i}(\theta)\}, \tag{2.3}$$

where α is found by fitting the boundary conditions; A, B are trigonometric terms obtained from a sequence of ordinary differential equations with constant coefficients, e.g., for the first of (2.3)

$$\begin{aligned} A''_{\alpha,0} + \alpha^2 A_{\alpha,0} &= 0, \\ A''_{\alpha,1} + (\alpha + 1)\, A_{\alpha,1} &= 0, \\ A''_{\alpha,m+2} + (\alpha + m + 2)^2\, A_{\alpha,m+2} &= -\sum_{j=0}^{m} g_{m-j} A_{\alpha,j}, \qquad m = 0, 1, 2, \ldots . \end{aligned} \tag{2.4}$$

The presence of a nonzero f in (2.1) merely adds known terms to (2.2). Corresponding results for the time-dependent case of (2.1) are given in Bell [4]. An alternative way of expanding u is to split it into a well-behaved part plus a small number of singular terms as proposed by Woods [42] and used by Benzley [7] and Emery and Segedin [14, 15].

For more-general, second-order elliptic and parabolic equations of the form

$$\sum_{i,k=1}^{n} A_{ik} \frac{\partial^2 U}{\partial X_i \, \partial X_k} + \sum_{i=1}^{n} B_i \frac{\partial U}{\partial X_i} + CU + D = 0, \tag{2.5}$$

where A_{ik}, B_i, C, D are functions of X_i alone, the above techniques could be extended to cover the first- or cross-derivative terms; e.g., see Sankar [28] or Zak [43]. However, the presence of such terms, particularly if nonconstant coefficients are also present, considerably complicates the corresponding equation in polar coordinates and the sequence of equations for the functions of θ in (2.4). A more convenient way of proceeding is to reduce the general equation (2.5) to the simpler form (2.1) by transformations of the coordinates X_i to x_i and of the unknown function U to u and then seek a separable-variable solution. First, (2.5) is reduced to the canonical (normal) form

$$\sum_{i=1}^{n} \kappa_i \frac{\partial^2 U}{\partial x_i^2} + \sum_{i=1}^{n} b_i \frac{\partial U}{\partial x_i} = cU + d, \tag{2.6}$$

where $\kappa_i = 0$, 1, or -1, and b_i, c, d are functions of x_i, by the transformation of coordinates.

$$x_i = x_i(X_1, X_2, \ldots, X_n), \qquad i = 1, 2, \ldots, n; \tag{2.7}$$

see Courant and Hilbert [10, Chap. III, and p. 350]. Equation (2.6) is then reduced to form (2.1), which contains no first-derivative terms, by using the exponential transformation of Sankar [28]

$$u = U \exp\left\{\frac{1}{2} \sum_{i=1}^{n} \int b_i \, dx_i\right\}. \tag{2.8}$$

A similar transformation was given by Courant and Hilbert [10, p. 183] for the case when the b_i are constant.

Examples of such transformations have been given by

(i) Courant and Hilbert [10, p. 162] for Tricomi's equation (of special interest in high-velocity gas flows; Bers [9]).

(ii) Crank and Furzeland [11] for axially symmetric diffusion problems involving the numerical quadrature of a line integral across a singularity at the edge of a disk-shaped electrode (see also Duncan [13]).

(iii) Fox and Sankar [17] for the vortex theory of screw propellors.

3. Development of Modified Approximation Near the Singularity

As an example, consider the two-dimensional, elliptic case of (2.5) and assume that it is of such a form that it can be reduced using transformations (2.7) and (2.8) to the form

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - g(x, y)\, u - f(x, y) = 0, \tag{3.1}$$

where the transformation between U and u is given by, say,

$$U = L[u]. \tag{3.2}$$

Form (3.1) is most convenient for the analytical development of the modified approximations and keeps the number of derivative approximations needed to a minimum; no numerical computations with (3.2) are needed.

Assume that an analytical solution of form (2.2), valid near the boundary singularity at point 0, has been found. Taking the first N terms of (2.2) an approximation for u, valid near 0, is

$$u^*(\rho, \theta) = \phi_0(\rho, \theta) + \sum_{i=1}^{N} c_i \phi_i(\rho, \theta). \tag{3.3}$$

and the corresponding approximation for U is defined by

$$U^*(\rho, \theta) = L[u^*(\rho, \theta)] \equiv \psi_0(\rho, \theta) + \sum_{i=1}^{N} c_i \psi_i(\rho, \theta). \tag{3.4}$$

A neighborhood $N(0)$ near the singularity is chosen, and standard finite-difference or finite-element approximations are used for U and its derivatives in (2.5) for points outside $N(0)$. For points in $N(0)$, modified approximations for u and its derivatives in (3.1) are developed which take into account the nature of the singularity and these are in turn related to U values inside $N(0)$. The derivatives are approximated using the standard differential relations

$$\frac{\partial^2 u}{\partial x^2} = \cos^2\theta \frac{\partial^2 u}{\partial \rho^2} - \frac{\sin 2\theta}{\rho} \frac{\partial^2 u}{\partial \rho\, \partial \theta} + \frac{\sin^2\theta}{\rho^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\sin^2\theta}{\rho} \frac{\partial u}{\partial \rho} + \frac{\sin 2\theta}{\rho^2} \frac{\partial u}{\partial \theta}, \tag{3.5}$$

$$\frac{\partial^2 u}{\partial y^2} = \sin^2\theta \frac{\partial^2 u}{\partial \rho^2} + \frac{\sin 2\theta}{\rho} \frac{\partial^2 u}{\partial \rho\, \partial \theta} + \frac{\cos^2\theta}{\rho^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\cos^2\theta}{\rho} \frac{\partial u}{\partial \rho} - \frac{\sin 2\theta}{\rho^2} \frac{\partial u}{\partial \theta}, \tag{3.6}$$

where approximations for the ρ and θ derivatives are obtained by differentiating (3.3). Thus approximations for (3.5) and (3.6) can be expressed as

$$\left.\begin{aligned} \frac{\partial^2 u^*}{\partial x^2} &= w_0(\rho, \theta) + \sum_{i=1}^{N} c_i w_i(\rho, \theta) \qquad (3.7) \\ \frac{\partial^2 u^*}{\partial y^2} &= w_0'(\rho, \theta) + \sum_{i=1}^{N} c_i w_i'(\rho, \theta) \qquad (3.8) \end{aligned}\right\} \text{ with truncation error } O(\rho^{M-2}),$$

where M is the highest power of ρ in the $\phi_i(\rho, \theta)$ of (3.3).

The w_i, w_i' are readily found by following the above steps and the symmetry in (3.5) and (3.6) leads to symmetry between the w_i and w_i' (see the example in Section 4).

The N unknown constants c_i are approximated by fitting (3.4) to the set of U values $\{U_j : j = 1, 2, \ldots, N\}$ at N points in and near $N(0)$. More than N points can be used if a best-fit (e.g., least squares) technique is used. For each point n, say, in $N(0)$ the same set of points for the $\{U_j\}$ values can be used. In this case the set usually consists of points just outside $N(0)$, called "far" points; Motz [21]. Alternatively, a different set of points for each point n can be used. In this case the set usually consists of points surrounding the point n; Bell and Crank [6].

The proposed method is a variation of the latter type in that a different set of points is used for each x and y derivative for each point n. The method is illustrated by developing a modified five-point formula for the typical point 1 in $N(0)$; see Fig. 1, To construct a five-point formula approximations (3.3) and (3.4) are used with $N = 3$. Referring to Fig. 1, and denoting U_j^*, ρ_j, θ_j to be the corresponding U^*, ρ, θ

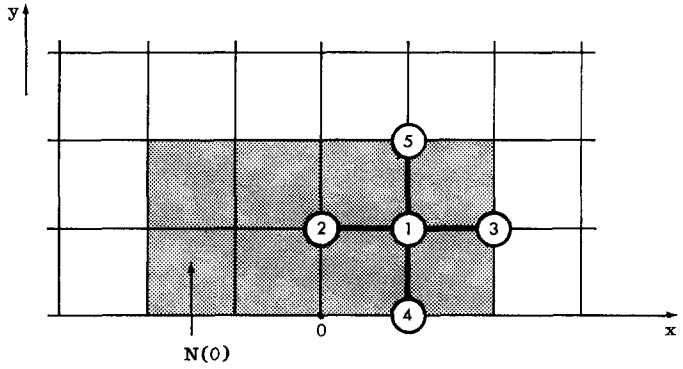

FIGURE 1

values at the points $j = 1$ to 5, then the most obvious choice of points to approximate the unknown constants c_i in (3.7) for $\partial^2 u^*/\partial x^2 \,|_{\text{point 1}}$ is to use points $j = 1, 2, 3$ in the horizontal direction. Using (3.4) this gives for the c_i the three equations

$$U_j^* = \psi_0(\rho_j, \theta_j) + \sum_{i=1}^{3} c_i \psi_i(\rho_j, \theta_j), \qquad j = 1, 2, 3, \tag{3.9}$$

whose solution can be denoted by

$$c_i = A_i + B_i U_2^* + C_i U_1^* + D_i U_3^*, \qquad i = 1, 2, 3. \tag{3.10}$$

Similarly, for the c_i in (3.8) for $\partial^2 u/\partial y^2 \,|_{\text{point 1}}$, points 4, 1, and 5 in the vertical direction are used and the solution is denoted by

$$c_i = A_i' + B_i' U_4^* + C_i' U_1^* + D_i' U_5^*, \qquad i = 1, 2, 3. \tag{3.11}$$

Substituting (3.10) and (3.11) in (3.7) and (3.8), and using (3.3) with the c_i given by

(3.10) for the term $g(x, y)\, u$ in (3.1), gives the following five-point approximation for (3.1) at the typical point 1 in $N(0)$:

$$\frac{\partial^2 u^*}{\partial x^2} + \frac{\partial^2 u^*}{\partial y^2} - gu^* - f = e_2 U_2^* + e_3 U_3^* + e_4 U_4^* + e_5 U_5^* + e_1 U_1^* + e_6 \simeq 0,$$

where

$$\begin{aligned}
e_1 &= \sum_{i=1}^{3} [C_i(w_i - g\phi_i) + w_i' C_i'], \\
e_2 &= \sum_{i=1}^{3} B_i(w_i - g\phi_i), \\
e_3 &= \sum_{i=1}^{3} D_i(w_i - g\phi_i), \\
e_4 &= \sum_{i=1}^{3} w_i' B_i', \\
e_5 &= \sum_{i=1}^{3} w_i' D_i', \\
e_6 &= w_0 + w_0' + \sum_{i=1}^{3} [A_i(w_i - g\phi_i) + A_i' w_i'] - g\phi_0 - f.
\end{aligned} \tag{3.13}$$

The functions w_i, w_i', ϕ_i, g, and f are evaluated at the point (ρ_1, θ_1). If the original differential equation (2.1) is equivalenced (via the zero right-hand side) to the reduced equation (3.1) then (3.12) represents a five-point approximation to the original equation which can be incorporated in either a finite-difference or a finite-element scheme.

The general way of writing approximations (3.7) and (3.8), so that the neighboring points chosen to approximate the c_i need not be on the same horizontal or vertical line, is useful in developing higher-order, multipoint modified approximations. It allows the number of terms included in the truncated series expansion, and the set of neighboring points used for any one point in $N(0)$, to be varied. The neighborhood $N(0)$ can include points away from 0 as long as approximations (3.3) and (3.4) remain valid (this may be checked as described in Motz [21]). The optimum size of $N(0)$ can be determined by comparison of the discretization error in the standard approximations used outside $N(0)$ with the truncation error in (3.7) and (3.8); see Section 4.

Five-point "molecules" differing from the one given in Fig. 1 are needed for points in $N(0)$ which involve the boundary. Two problems can arise. The first is that some of the five points required may, depending on the geometry of the problem, lie outside the region of solution. The second is that the values of $\psi_i(\rho, \theta)$ at the point (ρ_j, θ_j) may all be zero so that solutions to (3.9) for the c_i cannot be found. The remedy for both

problems is simply to choose alternative points near (ρ_j, θ_j) giving a new five-point molecule; e.g., see Section 4, Fig. 4–7.

The method can be extended to the parabolic, time-dependent case since the form of the boundary singularity depends on the space coordinates rather than on the time coordinate. Thus seeking a separable-variable solution one finds that the time-dependent form of (3.3) can be expressed as

$$u^*(\rho, \theta, t) = \phi_0(\rho, \theta, t) + \sum_{i=1}^{N} c_i(t)\, \phi_i(\rho, \theta), \tag{3.14}$$

and so the above methods can be applied with the c_i being reevaluated at each time level; see Bell and Crank [4–6].

4. Application of the Method to the Problem of Motz and Woods

The problem of Motz [21] requires the solution of Laplace's equation in a rectangle with a slit, i.e., a re-entrant corner of internal angle 2π. It has been treated by many authors to demonstrate the effectiveness of their singularity treatments. Woods [42] gave an alternative formulation based on the fact that $u - 500$ is antisymmetric about the line BE containing the slit and, by imposing the boundary condition $u = 500$ on EO, only needed to consider the top half of the rectangle (Fig. 2). It is in this form that the problem is treated in the literature [3, 19, 22, 23, 32, 35–39].

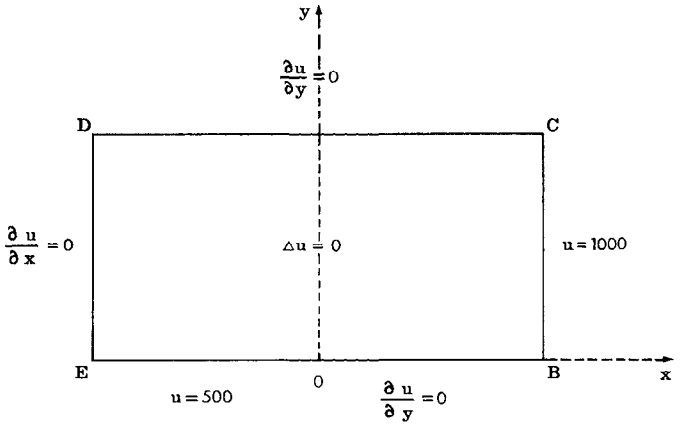

FIGURE 2

Examples of such singularities occur in potential problems concerning transmission lines with microstrips (Daly [12]) and in diffusion problems with narrow-band-type electrodes (Saito [27]). Since the governing Laplacian equation is already in the simple form (2.1) with $g = f = 0$ there is no need for a transformation of coordinates or an unknown function. (For an application of the method to a problem where such a

transformation is necessary see Crank and Furzeland [11].) In the Woods formulation the singularity is associated with the mixed boundary conditions

$$\partial u/\partial y = 0, \qquad x > 0; u = 500, \qquad x \leqslant 0 \text{ on } y = 0. \tag{4.1}$$

A separable-variable solution of the polar coordinate form of Laplace's equation yields the local analytic form

$$u = 500 + \sum_{i=1}^{\infty} c_i \rho^{(2i-1)/2} \cos \frac{(2i-1)}{2} \theta. \tag{4.2}$$

The problem of Fig. 2 is scaled by setting

(i) $$v = u - 500, \tag{4.3}$$

(ii) $$B = (1, 0); C = (1, 1); D = (-1, 1); E = (-1, 0), \tag{4.4}$$

and standard five-point finite-difference approximations are used for the discretized region of Fig. 3 with $\delta x = \delta y = h$. To enable comparisons the choice of discretization follows that of Motz and Woods, although this choice results in unequal intervals near the edges and so the discretisation error is only $O(h)$ for these points. For points

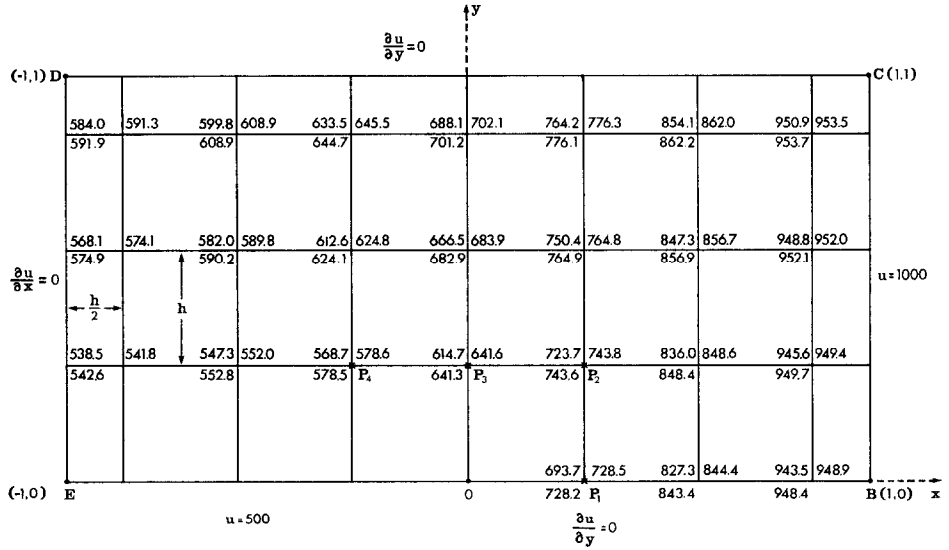

FIG. 3. Tabulation of values of u from the problem of Fig. 2. $DC = EB = 2$ units; $DE = BC = 1$ unit; $\delta x = \delta y = 2/7$ (except near ED, DC, CB). Key:

Finite-difference solution, *no* singularity treatment	Conformal transformation solution, Papamichael and Whiteman [29].
Crank and Furzeland modified formulas at points P_1–P_4.	

involving the Neumann boundary condition the usual central-difference approximations for the derivatives are used in conjunction with fictitious points. Figure 3 compares the numerical solution obtained using these standard finite-difference approximations with the highly accurate results produced by the conformal transformation method of Papamichael and Whiteman [23]. The results show that a high degree of inaccuracy occurs near the singularity and illustrate the fact that inaccuracies spread throughout the entire region, called "the pollution effect" [2]. Instead of applying the standard finite-difference approximations throughout the entire region, a neighborhood $N(0)$ near the singularity is chosen and for points in $N(0)$ modified approximations are developed which take into account the nature of the singularity given by (4.2). Following Section 3 the derivative approximations (3.7) and (3.8) with $N = 3$ lead to the modified five-point

$$g = f = 0, \qquad e_6 = 0,$$

$$w_1 = -\frac{\cos \frac{3}{2}\theta}{4\rho^{3/2}}; \qquad w_2 = \frac{3 \cos \frac{1}{2}\theta}{4\rho^{1/2}}; \qquad w_3 = \frac{15\rho^{1/2} \cos \frac{1}{2}\theta}{4}; \tag{4.5}$$

$$w_i' = -w_i, \qquad i = 1, 2, 3.$$

The approximate size of $N(0)$ can be determined by noting that the discretization error in the standard five-point approximations to Laplace's equation is $O(h^2)$, whereas it is easily verified that the modified approximations based on (3.7) and (3.8) with $N = 3$ contain a truncation error of $O(\rho^{3/2})$. Thus application of the modified approximations is advantageous as long as the truncation error does not exceed the discretization error. An approximate rule is then to choose $N(0)$ such that the maximum ρ value in $N(0)$, $\rho_{\max}$, say, is such that $\rho_{\max}^{3/2}$ is of the same order of magnitude as h^2. Practical experience suggests that $\rho_{\max}^{3/2} < 5h^2$ is a useful guide. In practice only a few points in $N(0)$ are needed.

Referring to Fig. 3, the four immediately neighboring points P_1, P_2, P_3, and P_4 around O are chosen for $N(0)$ since here $\rho_{\max}^{3/2} \approx 0.26$ and $h^2 \approx 0.08$. This choice of points is similar to that used by Motz and Woods and enables comparisons to be made with their results. Modified approximations of forms (3.12) and (4.5) are applied at points inside $N(0)$ and standard finite-difference approximations are used for points outside $N(0)$. The results obtained are comparable with those of Motz and Woods and give good agreement with the conformal transformation values of Papamichael and Whiteman [23], which are generally accepted to be of high accuracy.

Five-point "molecules" differing from that given in Fig. 1 are needed for points in $N(0)$ which involve the boundary. Five-point molecules for points to the left of 0 on $y = \delta y$ involve points on $y = 0$ for which $\theta = \pi$. The fact that $\theta = \pi$ means that, by comparing (4.2) with (3.9), each of the $\psi_i(\rho, \theta)$ is zero and thus solutions to (3.10) cannot be found. Suggested alternatives are given in Figs. 6 and 7. The first point on the right of O on $y = 0$ also involves a point for which $\theta = \pi$. Further, there is no $y - \delta y$ level, and so an alternative molecule such as that given in Fig. 4 is used. The

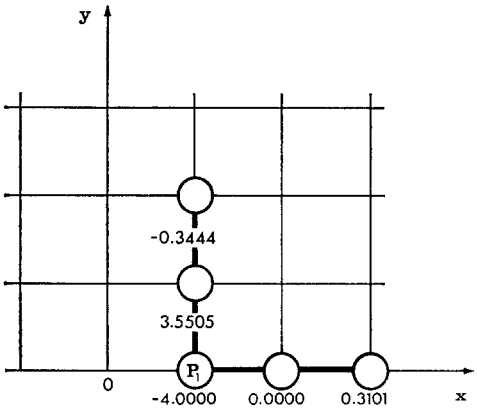

FIGURE 5

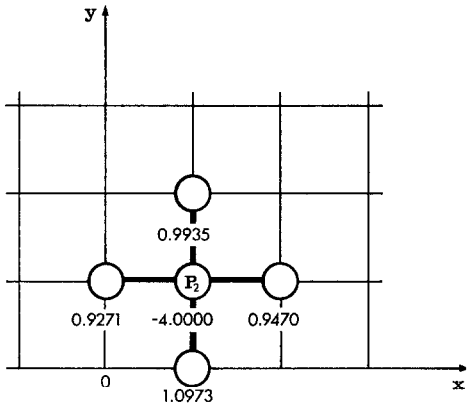

FIGURE 6

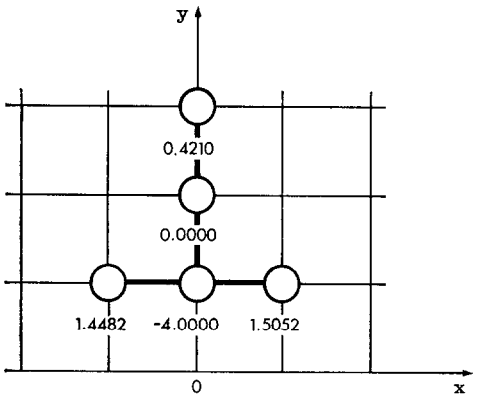

FIGURE 7

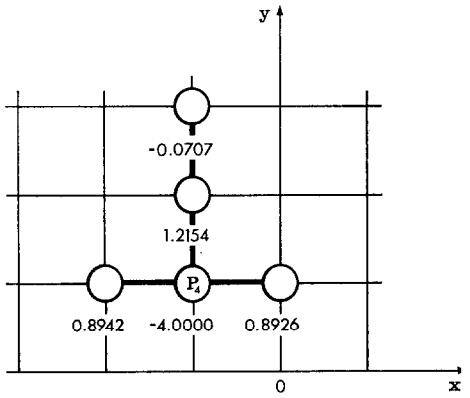

FIGURE 9

Note. The figures below the nodes represent the values of e_i in (3.12) for points P_1–P_4. These values are for $v = u - 500$ values; see (4.3).

general form of the modified approximations allows for any combination of five neighboring points provided $\theta \neq \pi$.

The values of the e_i in (3.12) are given in Fig. 4–7 for the points P_1–P_4 with $h = 2/7$. The values given have been scaled so that $e_1 = -4.0000$.

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