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MODIFIED FINITE-DIFFERENCE
APPROXIMATIONS NEAR THE SINGULARITY
IN THE PROBLEM OF MOTZ

by

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ABSTRACT

A simple, modified finite-difference method is described for solving Laplace's equation with boundary singularities of the infinite derivative type. Modified approximations for the derivatives of the Laplacian equation are employed near the singularity. These are developed from a truncated series form of the local analytical solution. The method is applied to the problem of Motz. The numerical results compare favourably with those obtained by other techniques.

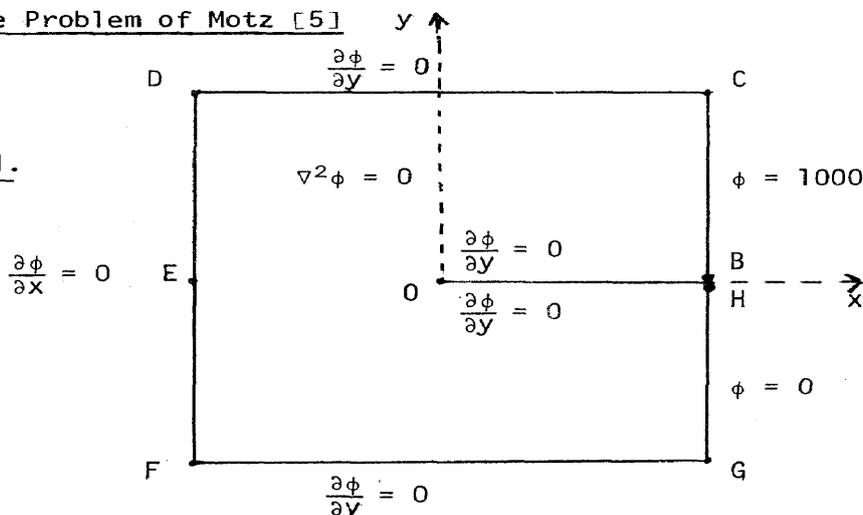
1. Introduction

The problem of Motz [5], with its singularity due to a re-entrant corner of internal angle 2π (Figure 1), has been treated by many authors to demonstrate the effectiveness of their singularity treatments. An alternative formulation of the problem, based on its antisymmetric properties, was given by Woods [15] (Figure 2), and it is in this form that the problem is treated in the literature [4, 6, 7, 9 - 14].

In this report the nature of the singularity is discussed and a new method proposed for obtaining numerical solutions near the singularity. The proposed method is based on that used by Motz in that it uses modified finite-difference approximations near the singularity which are developed from a local truncated series form of the solution. The method differs in that the modified approximations are developed from the derivatives in the governing Laplacian equation rather than, as done by Motz, from algebraic equations for the solution values. The method also differs in the set of neighbouring points used to approximate the unknown coefficients in the truncated series approximations for the derivatives. The method is an extension of the method of Bell and Crank [3].

2. The Problem of Motz [5]

Figure 1.



The problem of Motz is to solve

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \quad (2.1)$$

in the square containing a slit (Figure 1). The slit represents a re-entrant corner of internal angle 2π with Neumann boundary conditions on the arms OB and OH. Converting to local polar co-ordinates $x = \rho \cos \theta$, $y = \rho \sin \theta$, centred on 0,

$$\frac{\partial^2 \phi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \phi}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 \phi}{\partial \theta^2} = 0, \quad (2.2)$$

With $\frac{\partial \phi}{\partial \theta} = 0$ on $\theta = 0$ and $\theta = 2\pi$. (2.3)

Motz sought the local, variable-separable solution of (2.2),

$$\phi(\rho, \theta) = R(\rho)\psi(\theta), \quad (2.4)$$

Which gave

$$\left. \begin{aligned} \psi &= A \cos n\theta + B \sin n\theta \\ R &= C \rho^n \end{aligned} \right\} n, A, B, C \text{ arbitrary constants} \quad (2.5)$$

Fitting the boundary condition (2.3) gave

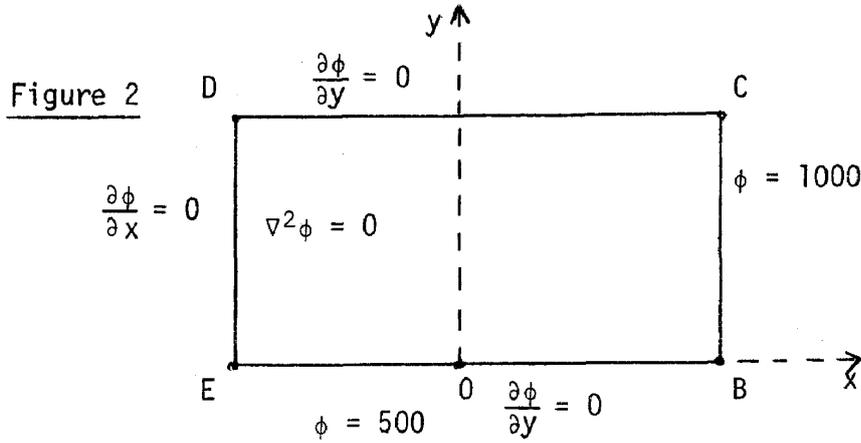
$$B = 0; n = \frac{k}{2}, \quad k = 0, 1, 2, \dots \quad (2.6)$$

Thus the local series form of the solution near the singularity at 0 is

$$\phi = c_0 + c_1 \rho^{\frac{1}{2}} \cos \frac{\theta}{2} + c_2 \rho \cos \theta + c_3 \rho^{\frac{3}{2}} \cos \frac{3\theta}{2} + \dots \quad (2.7)$$

where the c_i are unknown constants (to be found).

3. An antisymmetric Formulation, Woods [15]



Woods used the fact that $\phi - 500$ is antisymmetric about the line BE containing the slit and, by imposing the boundary condition $\phi = 500$ on E0, only needed to consider the top half of the square (Figure 2). However, this can lead to some confusion in that the local series form of the solution is altered since the re-entrant corner now has to be regarded as having an internal angle of π with boundary conditions

$$\frac{\partial \phi}{\partial \theta} = 0 \quad \text{on} \quad \theta = 0 ; \quad \phi = 500 \quad \text{on} \quad \theta = \pi . \quad (3.1)$$

Application of (3.1) to (2.5) gives

$$B = 0 ; \quad n = k + \frac{1}{2} , \quad k = 0, 1, 2, \dots \quad (3.2)$$

This gives the new local series form

$$\phi = c_0 + c_1 \rho^{\frac{1}{2}} \cos \frac{\theta}{2} + c_2 \rho^{\frac{3}{2}} \cos \frac{3\theta}{2} + c_3 \rho^{\frac{5}{2}} \cos \frac{5\theta}{2} + \dots \quad (3.3)$$

Comparing this with (2.7) we note that there are no longer any terms in integer powers of ρ and multiples of θ , but that the first two terms are the same. The difference in forms did not affect the work of Woods since he used only the first singular term, c_1 . Wait and

Mitchell [10], however, used an asymptotic expansion of the form (2.7) up to powers of $\rho^{\frac{3}{2}}$ for the antisymmetric form of the problem, - strictly speaking they should have used an expansion of the form (3.3).

4. Standard Finite-difference Solution for Woods' Form

The problem of Figure 2 is scaled by setting

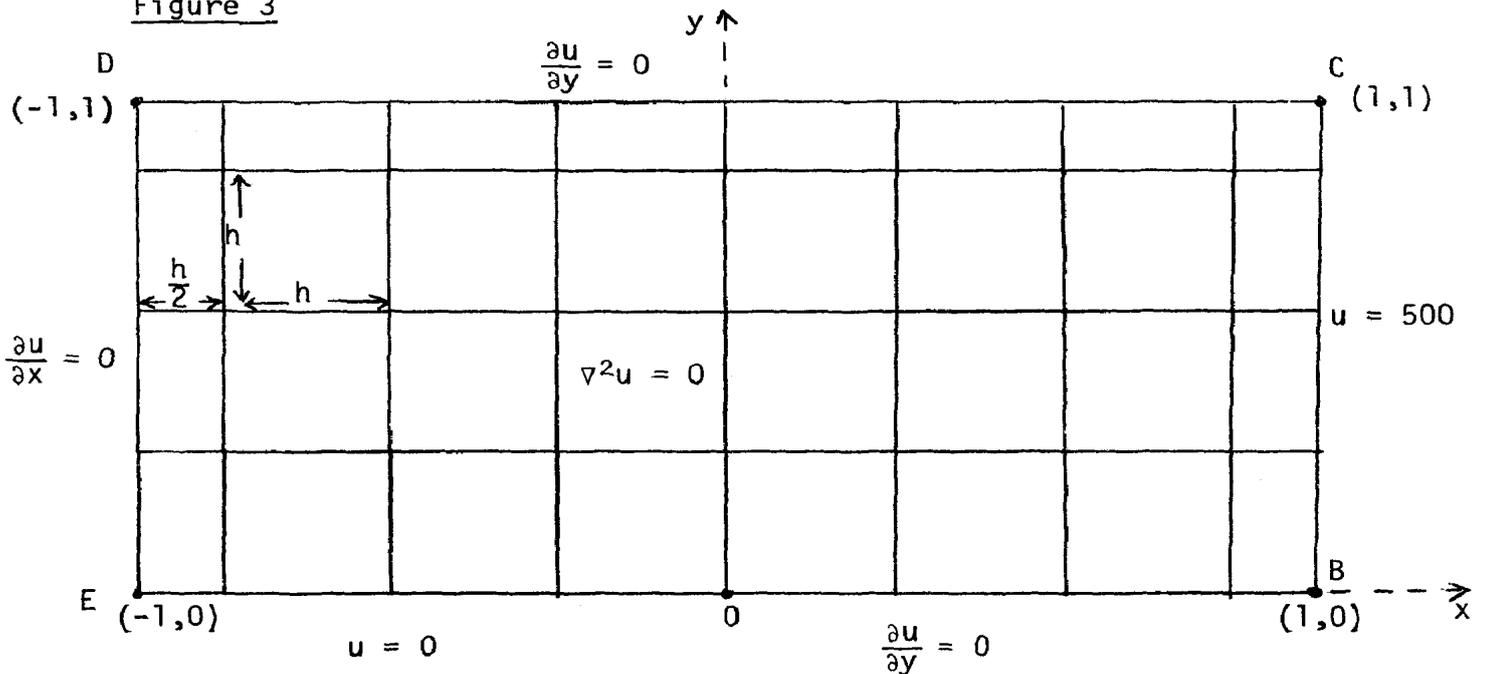
$$(i) \quad u = \phi - 500 \tag{4.1}$$

$$(ii) \quad B = (1,0) ; \quad c = (1,1) ; \quad D = (-1,1) ; \quad E = (-1,0) . \tag{4.2}$$

To enable comparisons with the work of Motz and Woods, the region is discretised as shown in Figure 3 with $\delta x = \delta y \equiv h = 2/7$.

This discretisation results in a mesh length of $h/2$ at the edges ED, DC and CB and, following Motz and Woods, values on ED and DC are not computed. Inspection of the Taylor series approximations for points on the mesh lines $h/2$ away from the edges ED, DC and CB shows that the discretisation error is only $O(h)$ for these points.

Figure 3



The governing equation is

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 . \quad (4.3)$$

Approximation of (4.3), using the standard, central-difference formulae, leads to the usual five-point approximations of $O(h^2)$

$$u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = 0 \quad (4.4)$$

for points (i,j) not involving the boundary, where

$$x = ih \quad , \quad i = 0,1,2,\dots \quad ; \quad y = jh \quad , \quad j = 0,1,2, \dots \quad (4.5)$$

For points involving the Neumann boundary condition the usual central difference approximations for the derivatives are used and the fictitious point argument applied. Figure 8 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 [7]. The results show that a high degree of inaccuracy occurs near the singularity and illustrate the fact that inaccuracies spread throughout the entire region. This is called the pollution effect by Babuska and Aziz [1].

5. Modified Five-point Approximations near the Singularity

Instead of applying the standard finite-difference approximations throughout the entire region, a neighbourhood $N(0)$ near the singularity is chosen and, for points in $N(0)$, modified approximations are developed which take into account the nature of the singularity. These modified approximations are formed by approximating each of the derivatives in (4.3) using the local polar co-ordinate series

form

$$u(\rho, \theta) = c_1 \rho^{\frac{1}{2}} \cos \frac{\theta}{2} + c_2 \rho^{\frac{3}{2}} \cos \frac{3\theta}{2} + c_3 \rho^{\frac{5}{2}} \cos \frac{5\theta}{2} + \dots \quad (5.1)$$

which is obtained by comparison with (3.3). A five-point approximation is formed by taking the following three-term truncated form of (5.1) :

$$u^*(\rho, \theta) = \sum_{i=1}^3 c_i f_i(\rho, \theta) \text{ where } f_i(\rho, \theta) = \rho^{\frac{2i-1}{2}} \cos \frac{(2i-1)\theta}{2} . \quad (5.2)$$

Using the standard differential relations

$$\frac{\partial^2 u}{\partial x^2} = \cos^2 \theta \frac{\partial^2 u}{\partial \rho^2} - \frac{\sin 2\theta}{\rho} \frac{\partial^2 u}{\partial \rho \partial \theta} + \frac{\sin^2 \theta}{\rho^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\sin^2 \theta}{\rho} \frac{\partial u}{\partial \rho} + \frac{\sin 2\theta}{\rho^2} \frac{\partial u}{\partial \theta} , \quad (5.3)$$

$$\frac{\partial^2 u}{\partial y^2} = \sin^2 \theta \frac{\partial^2 u}{\partial \rho^2} - \frac{\sin 2\theta}{\rho} \frac{\partial^2 u}{\partial \rho \partial \theta} + \frac{\cos^2 \theta}{\rho^2} \frac{\partial^2 u}{\partial \theta^2} + \frac{\cos^2 \theta}{\rho} \frac{\partial u}{\partial \rho} + \frac{\sin 2\theta}{\rho^2} \frac{\partial u}{\partial \theta} , \quad (5.4)$$

where approximations for the ρ and θ derivatives are obtained by differentiating (5.2), the following three-term series approximations

for $\frac{\partial^2 u}{\partial x^2}$, $\frac{\partial^2 u}{\partial y^2}$ are found:

$$\left. \begin{aligned} \frac{\partial^2 u^*}{\partial x^2} &= \sum_{i=1}^3 c_i w_i(\rho, \theta) \\ \frac{\partial^2 u^*}{\partial y^2} &= \sum_{i=1}^3 c_i w_i'(\rho, \theta) \end{aligned} \right\} \text{with truncation error } O(\rho^{\frac{3}{2}}) , \quad (5.5)$$

$$\left. \begin{aligned} \text{where } w_1 &= -\frac{\cos 3\theta/2}{4\rho^{\frac{3}{2}}} ; w_2 = \frac{3\cos\theta/2}{4\rho^{\frac{1}{2}}} ; w_3 = \frac{15\rho^{\frac{1}{2}} \cos\theta/2}{4} \\ w_i' &= -w_i \quad , i = 1, 2, 3. \end{aligned} \right\} \quad (5.7)$$

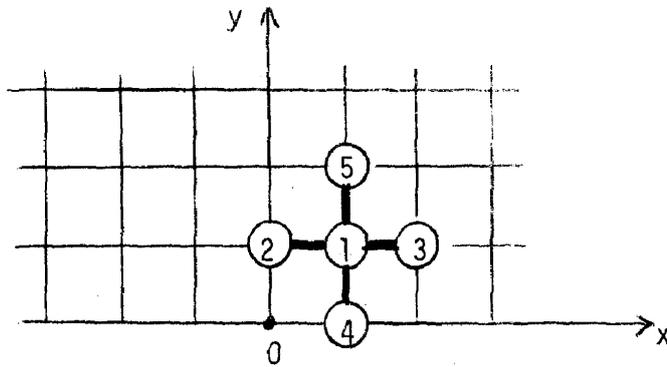
The symmetry of the w_i arises from the symmetry of (5.3) and (5.4).

Approximations for the constants c_i , $i = 1,2,3$ are found in terms of neighbouring u values by using the three-term approximation (5.2). Referring to Figure 4, and denoting u^*_{j,ρ_j,θ_j} to be the corresponding u^* , ρ,θ , values at the points $j = 1,2,3,4,5$, then u^* values at three neighbouring points in the horizontal direction are used to find the

c_i in (5.5) for $\frac{\partial^2 u^*}{\partial x^2}$ / point 1. The most obvious choice, and that which leads to a five-point formula, is to use points $j = 1,2$ and 3 to give the following three equations for the c_i ,

$$u^*_j = \sum_{i=1}^3 c_i f_i(\rho_j, \theta_j), \quad j = 1,2,3. \quad (5.8)$$

Figure 4



The solution of (5.8) is denoted by

$$c_i = B_i u^*_2 + C_i u^*_1 + D_i u^*_3, \quad i = 1,2,3. \quad (5.9)$$

Similarly, to find the c_i in (5.6) for $\frac{\partial^2 u^*}{\partial y^2}$ / point 1, points 4, 1 and 5 are used in the vertical direction. The solution is denoted by

$$c_i = B'_i u^*_4 + C'_i u^*_1 + D'_i u^*_5, \quad i = 1,2,3. \quad (5.10)$$

Substitution of (5.9) and (5.10) in (5.5) and (5.6) respectively gives the five-point approximation

$$\nabla^2 u^* = \frac{\partial^2 u^*}{\partial x^2} \frac{\partial^2 u^*}{\partial y^2} = e_2 u_2^* + e_3 u_3^* + e_4 u_4^* + e_5 u_5^* + e_1 u_1^* = 0, \quad (5.11)$$

$$\text{whete } \left. \begin{aligned} e_2 &= \sum_{i=1}^3 w_i B_i, & e_3 &= \sum_{i=1}^3 w_i D_i, & e_4 &= \sum_{i=1}^3 w_i' B_i', \\ e_5 &= \sum_{i=1}^3 w_i' D_i', & e_1 &= \sum_{i=1}^3 w_i' C_i' + w_i' C_i', \end{aligned} \right\} \quad (5.12)$$

for a typical point 1 in $N(0)$, the w_i and w_i' being evaluated at the point 1.

The above technique of horizontal and vertical derivative replacement is based on that used by Bell and Crank [3] who

treated $\frac{\partial^2 u}{\partial y^2}$ as above but used the standard central difference

formula for $\frac{\partial^2 u}{\partial x^2}$. The method used above is a generalisation of

the ideas of Bell and Crank in that

- (i) both derivatives are treated
- (ii) the approximations (5.5) and (5.6) are written in a general way so that the neighbouring points chosen need not lie on the same horizontal or vertical line.

The generalisation (ii) is useful in developing higher-order, multi-point modified approximations by varying the number of terms included in the truncated series expression and the set of neighbouring points used for any one point in $N(0)$. The method can be extended to the time-dependent case by following Bell and Crank .

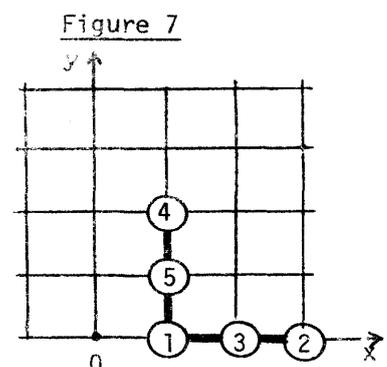
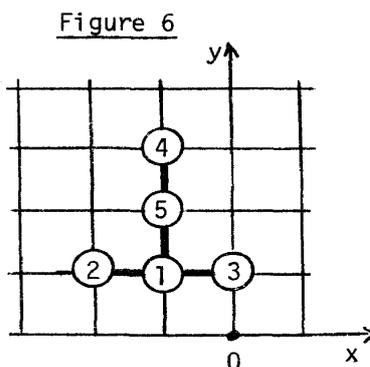
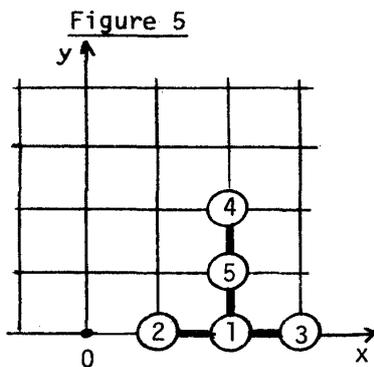
The neighbourhood $N(0)$ can include points away from the singularity at 0, as long as the three-term approximation (5.2) remains valid.

This may be checked as described in Motz [5]. The approximate s of $N(0)$ can be determined by noting that the discretisation error in the standard finite-difference approximations (4.4) is $O(h^2)$ whereas the modified approximations (5.5) and (5.6) contain a truncation error of $O(\rho^{\frac{3}{2}})$. Thus application of the modified approximations is advantageous as long as the truncation error does not exceed the discretisation error. An approximate rule is then to choose $N(0)$ such that the maximum ρ value in $N(0)$, ρ_{\max} .

say, is such that $\rho_{\max}^{\frac{3}{2}}$ is of the same order of magnitude as

h^2 , - practical experience suggests that $\rho_{\max}^{\frac{3}{2}} < 5h^2$ is a useful guide. In practice only a few points in $N(0)$ are needed.

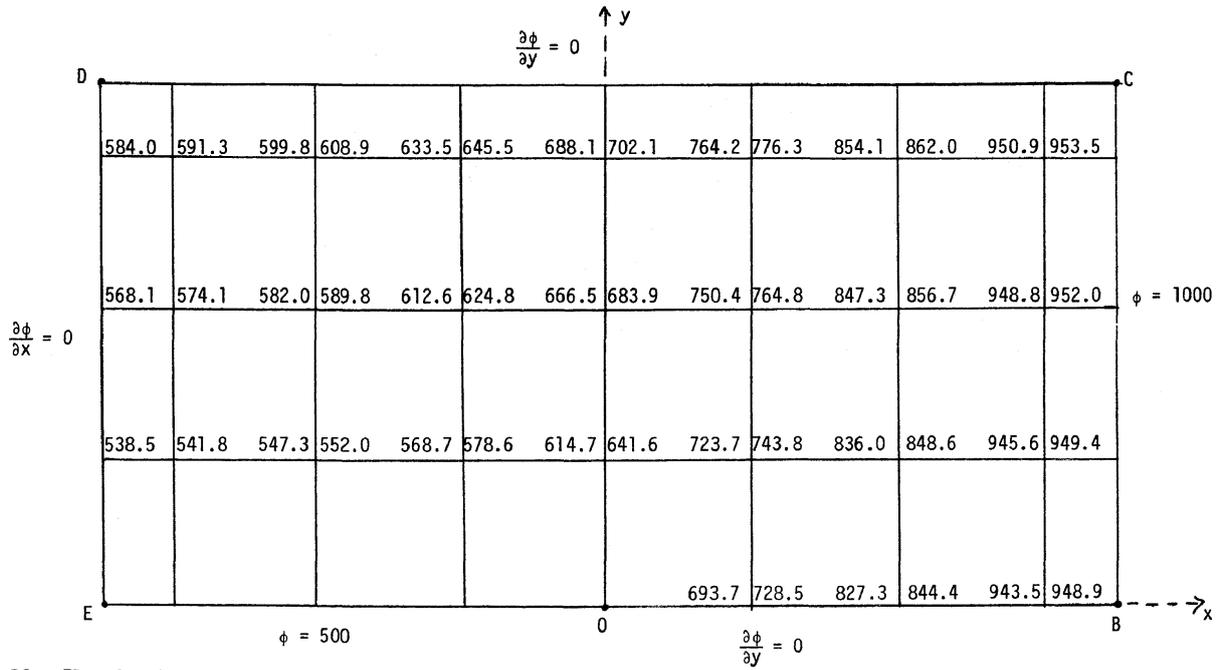
Five-point 'molecules' differing from that given in Figure 4 are needed for points in $N(0)$ which involve the boundary. Points to the right of 0 on $j = 0$ do not have a point at the $j-1$ level, necessitating a different molecule, e.g. Figure 5. Points to the left of 0 on $j = 1$ involve points on $j = 0$ for which $\theta = \pi$. The fact that $\theta = \pi$ means that each of the $f_1(\rho, \theta)$ in (5.2) are zero, and thus solutions to (5.8) cannot be found. A suggested alternative is given in Figure 6. The first point on the right of 0 on $j = 0$ involves both the above problems and a suggested molecule is given in Figure 7. The general form of the modified approximations allows for any combination of five neighbouring points provided $\theta \neq \pi$.



6. Numerical Results

Referring to Figure 9, the four immediately neighbouring points P_1, P_2, P_3 and P_4 around 0 are chosen for $N(0)$ since here $\rho_{\max}^{\frac{3}{2}} \approx 0.26$ 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 the form (5.11) are applied at points inside $N(0)$ using the suggested molecules of Figures 5 - 7 where appropriate. Standard finite-difference approximations (4.4) are used for points outside $N(0)$. The highly accurate values of Papamichael and Whiteman [7] based on a conformal transformation are used to represent exact values. The results obtained are comparable with those of Motz and Woods and give good agreement with the conformal transformation values.

The values of the e_i in (5.11) are given in Figures 10-13 for the points $P_1 - P_4$ with $h = 2/7$. The values given have been scaled so that $e_i = -4.0000$.



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 [7]

Figure 8

Figure 10

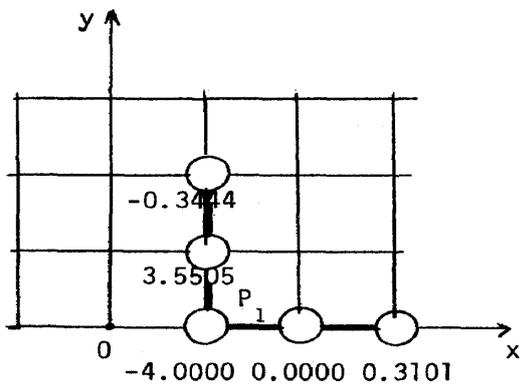


Figure 11

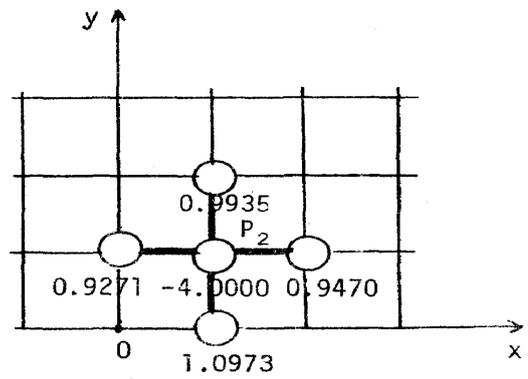


Figure 12

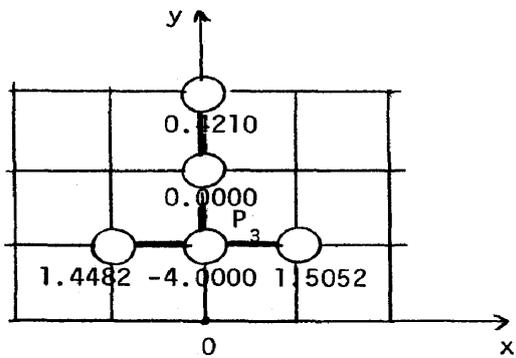
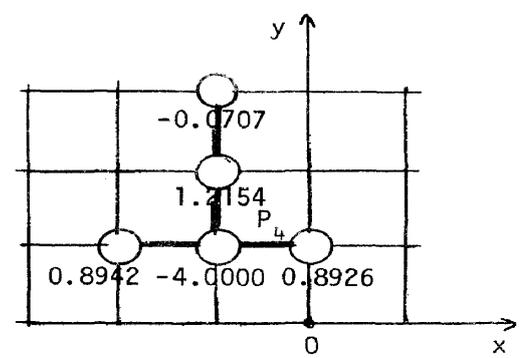


Figure 13



N.B. The above e_i values are for $u = \phi - 500$ values, see (4.1).

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