JOURNAL OF COMPUTATIONAL PHYSICS 64, 459–472 (1986)

On the Numerical Treatment of Boundary Singularities in Elliptic Problems

TIMOTHY N. PHILLIPS*

Department of Applied Mathematics, University College of Wales, Aberystwyth SY23 3BZ, U.K.

Received March 1, 1985; revised August 14, 1985

Techniques are considered for improving the numerical approximation to a problem which possesses corner singularities. The particular problem considered here is taken from solid state electronics. Refined numerical solutions are obtained using two techniques. The first employs a non-uniform grid with a smaller spacing of the mesh points in the neighbourhood of the singularities. The second technique involves a transformation of the problem to one which is free from singularities. The dynamic ADI method, which needs no a priori relaxation parameters to accelerate convergence, is used to solve the discretized problem in both cases.

1. INTRODUCTION

In solid state electronics the designers of PIN diodes are interested in measuring the performance of the diode subject to changes in various design parameters. Of particular interest is the variation of the effective lifetime of the diode as a function of its base-width. There are obvious advantages in producing a good mathematical model since carrying out these tests in the laboratory could be a lengthy and expensive process. A description of the problem together with the derivation of the equations used in this paper are to be found in Aitchison and Berz [2]. The model gives rise to a coupled pair of elliptic partial differential equations. This problem has been solved numerically by Aitchison [1] who used Newton's method and a sparse matrix routine and by Phillips [7] who used the dynamic ADI method. Both these papers ignored the corner singularities.

In this paper we consider numerical techniques to treat the corner singularities which the problem possesses. In Section 2 we introduce the differential equations and discuss the nature of the singularities. The method of discretization, which uses a finite difference approximation on a non-uniform mesh, is described in Section 3. In Section 4 we review the dynamic ADI (DADI) method for solving a system of algebraic equations. In Section 5 a transformation of the problem to one which has no singularities is described. We make our concluding remarks in Section 6.

* This work was supported by the Science and Engineering Research Council while the author was in residence at Oxford University Computing Laboratory and Merton College, Oxford.

0021-9991/86 $3.00

2. The Governing Differential Equations

The problem is formulated in terms of the carrier density $c(x, y)$ and a stream function $u(x, y)$. The behaviour of diodes which are effectively 2-dimensional and of rectangular cross section can be described by the equations

$$\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}=c, \tag{1}$$

$$\frac{\partial}{\partial x}\left(\frac{1}{c}\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{1}{c}\frac{\partial u}{\partial y}\right)=0, \tag{2}$$

in the region $R=\{(x, y): 0\leqslant x\leqslant 2, 0\leqslant y\leqslant 4\}$. The associated boundary conditions are

$$\frac{\partial c}{\partial x}=\frac{b}{(1+b)}\frac{\partial u}{\partial y}, \frac{\partial u}{\partial x}=(1+b)\frac{\partial c}{\partial y} \qquad \text{on} \quad x=0, \tag{3}$$

$$\frac{\partial c}{\partial x}=\frac{-1}{(1+b)}\frac{\partial u}{\partial y}, \frac{\partial u}{\partial x}=-\frac{(1+b)}{b}\frac{\partial c}{\partial y} \qquad \text{on} \quad x=2, \tag{4}$$

$$\frac{\partial c}{\partial y}=0, \qquad u=0 \qquad \text{on} \quad y=0, \tag{5}$$

$$\frac{\partial c}{\partial y}=-sc, \qquad u=-1 \qquad \text{on} \quad y=4, \tag{6}$$

where s and b are positive constants. The particular values used in this paper are 5.0 and 2.7 respectively.

This problem possesses singularities at the points $P(0, 4)$ and $Q(2, 4)$. To establish this we present the following argument. Consider the point P. The region R is translated so that this point lies at the origin. This situation is illustrated in Fig. 1. On $0x$ we have $\partial u/\partial x=0$ since $u=-1$. Therefore $\partial u/\partial x\to 0$ at the origin. On

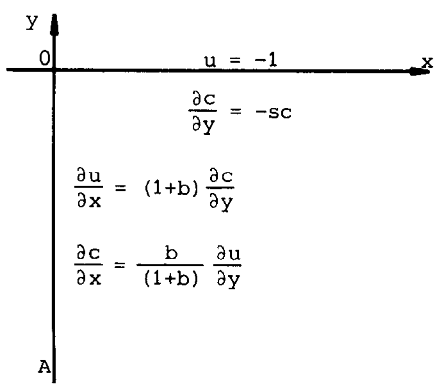

Figure 1

$0A$ we have that $\partial u/\partial x = (1+b)\,\partial c/\partial y$. Therefore, since $\partial u/\partial x \to 0$ at 0, we have $\partial c/\partial y \to 0$ at 0. On $0x$ we have $\partial c/\partial y = -sc$ and therefore $c \to 0$ at 0. However we know from the model that $c(0,0) \neq 0$. This means that the boundary conditions are not compatible at this point and so a boundary singularity occurs. So one or both of the following holds:

(i) $\lim_{x\to 0+}(\partial u/\partial x) \neq \lim_{y\to 0-}(\partial u/\partial x)$,

(ii) $\lim_{x\to 0+}(\partial c/\partial y) \neq \lim_{y\to 0-}(\partial c/\partial y)$.

If the limit of $\partial u/\partial x$ at 0 does not exist then $\partial^2 u/\partial x^2$ is unbounded near 0. Similarly $\partial^2 c/\partial y^2$ is unbounded near 0 if the limit of $\partial c/\partial y$ does not exist there. Since $\nabla^2 c = c$ this means that $\partial^2 c/\partial x^2$ is also unbounded near 0. Similarly $\partial^2 u/\partial y^2$ is unbounded if $\partial^2 u/\partial x^2$ is unbounded near 0.

We can perform a similar analysis for the corner at the point Q to establish that there is a singularity there of the same type. Numerical results can be obtained by ignoring the singularities. However the quality of the solution is likely to be poor in the vicinity of the singularities.

Attempts to determine the behaviour of the singularity in closed form failed due to the coupling of the dependent variables through the differential equations and boundary conditions.

3. Finite Difference Approximation on a Non-uniform Grid

In most elliptic problems singularities that occur on the boundary do not penetrate into the interior of the region. However, the solution may change very rapidly near the singularity and one or more of its higher derivatives becomes very large, which is the case with the problem being considered. The local truncation error of the finite difference equations involves terms like h^p multiplying some pth derivative, and if these get large near the singularity we would like to make h correspondingly smaller in these regions. To maintain the order of accuracy in our approximation in situations like these a uniform grid with an extremely fine mesh may be used to obtain a sufficient number of points in the vicinity of the singularity. This is wasteful and expensive since the points are distributed densely away from these regions, where they may not be needed. Kálnay de Rivas [6] suggested a different approach in which a change of independent variable is made which maps the domain into a new coordinate system where the variations of the solution are not so rapid. This approach is sketched out below.

The grid intervals are varied by defining stretched coordinates ξ and η such that $x = x(\xi)$ and $y = y(\eta)$ where the grid intervals $\Delta\xi$ and $\Delta\eta$ are constant and x and y are the old physical coordinates. Kálnay de Rivas [6] and Jones and Thompson [5] show how to express derivatives in terms of the stretched coordinates. For example, we can express the first derivatives in terms of ξ in the following manner

$$\frac{\partial v}{\partial x}=\frac{\partial v}{\partial \xi}\cdot\frac{d\xi}{dx}. \tag{7}$$

Equation (7) can be discretized using central differences to give the following approximation:

$$\frac{\partial v}{\partial x}\simeq\frac{v_{i+1,j}-v_{i-1,j}}{2\,\Delta\xi}\cdot\left.\frac{d\xi}{dx}\right|_{x_i},$$

where $v_{i,j}$ is the value of v at the grid point (x_i, y_j) with $x_i=x(i\,\Delta\xi)$ and $y_j=y(j\,\Delta\eta)$. The transformation can be differentiated numerically using central differences to obtain the following approximation to the first derivative

$$\frac{\partial v}{\partial x}\simeq\frac{v_{i+1,j}-v_{i-1,j}}{2\,\Delta\xi}\cdot\frac{2\,\Delta\xi}{x_{i+1}-x_{i-1}}=\frac{v_{i+1,j}-v_{i-1,j}}{x_{i+1}-x_{i-1}}. \tag{8}$$

Finite difference approximations for higher order derivatives are obtained in a similar way.

Since we have used central differences in deriving formulae like (8), they are formally second order in $\Delta\xi$. Jones and Thompson [5] give the exact form of the local truncation error of this approximation. They also point out that these errors will be small provided that the stretching function has the property that its derivatives are small where the derivatives of the solution are large, and vice versa.

Consider a function defined in the interval $0\leqslant x\leqslant 1$ with a singularity at the point $x=0$. The stretching function should possess the following properties:

(a) $dx/d\xi=0$ at $x=0$. This will ensure a concentration of grid points near $x=0$. Elsewhere we should have $dx/d\xi\neq 0$.

(b) $dx/d\xi$ should be finite over the whole interval since if $dx/d\xi$ becomes infinite at some point then the mapping $x=x(\xi)$ will give poor resolution near that point. This resolution cannot be improved by increasing the number of points since

$$\Delta x\simeq\left(\frac{dx}{d\xi}\right)\Delta\xi.$$

The following are examples of good stretching functions:

(i) $x(\xi)=\xi^2$. This is a suitable function if there is a singularity or boundary layer at $x=0$.

(ii) $x(\xi)=\sin^2(\frac{1}{2}\pi\xi)$. This mapping produces concentrations of grid points near the points $x=0$ and $x=1$.

(iii) $x(\xi)=\tan^{-1}(\pi(\xi-\frac{1}{2}))$. This has a similar effect as (ii).

Let $x(\xi)$ and $y(\eta)$ be two grid stretching functions with constant grid intervals $\Delta\xi$ and $\Delta\eta$, respectively. The region R is covered with a variable grid defined by the above mappings. We define $c_{i,j}$ and $u_{i,j}$ to be the values of $c(x, y)$ and $u(x, y)$ respectively at the grid point (x_i, y_j). The finite difference equations are constructed using the integration method of Varga [8]. This method was used by Aitchison [1] and Phillips [7] who solved the problem on a uniform grid. This technique is used because the conservative form of Eq. (2) is retained in the finite difference scheme.

Let the region $r_{i,j}$ be that part of the rectangle $\frac{1}{2}(x_i + x_{i-1}) \leqslant x \leqslant \frac{1}{2}(x_i + x_{i+1})$, $\frac{1}{2}(y_j + y_{j-1}) \leqslant y \leqslant \frac{1}{2}(y_j + y_{j+1})$ which lies within R. Let $s_{i,j}$ be the boundary of the region $r_{i,j}$. Integrating equations (1) and (2) over the region $r_{i,j}$ and applying Green's theorem we obtain

$$\int_{s_{i,j}} \frac{\partial c}{\partial n}\, ds - \iint_{r_{i,j}} c\, dx\, dy = 0, \tag{9}$$

$$\int_{s_{i,j}} \frac{1}{c} \frac{\partial u}{\partial n}\, ds = 0, \tag{10}$$

where n is the outward drawn normal. At internal points we obtain the following approximations, making use of the approximation (8),

$$\begin{aligned} &\frac{(c_{i+1,j} - c_{i,j})}{2(x_{i+1} - x_i)} (y_{j+1} - y_{j-1}) + \frac{(c_{i-1,j} - c_{i,j})}{2(x_i - x_{i-1})} (y_{j+1} - y_{j-1}) \\ &\quad + \frac{(c_{i,j+1} - c_{i,j})}{2(y_{j+1} - y_j)} (x_{i+1} - x_{i-1}) + \frac{(c_{i,j-1} - c_{i,j})}{2(y_j - y_{j-1})} (x_{i+1} - x_{i-1}) \\ &\quad - \tfrac{1}{4} c_{i,j} (x_{i+1} - x_{i-1})(y_{j+1} - y_{j-1}) = 0, \end{aligned} \tag{11}$$

$$\begin{aligned} &\frac{(y_{j+1} - y_{j-1})(u_{i+1,j} - u_{i,j})}{(c_{i+1,j} + c_{i,j})(x_{i+1} - x_i)} + \frac{(y_{j+1} - y_{j-1})(u_{i-1,j} - u_{i,j})}{(c_{i-1,j} + c_{i,j})(x_i - x_{i-1})} \\ &\quad + \frac{(x_{i+1} - x_{i-1})(u_{i,j+1} - u_{i,j})}{(c_{i,j+1} + c_{i,j})(y_{j+1} - y_j)} + \frac{(x_{i+1} - x_{i-1})(u_{i,j-1} - u_{i,j})}{(c_{i,j-1} + c_{i,j})(y_j - y_{j-1})} = 0, \end{aligned} \tag{12}$$

where $0 < i < N$, $0 < j < 2N$. The finite difference approximation around the boundary is constructed in a similar manner.

The system of finite difference equations are solved using the DADI method which we describe in the next section. The problem is solved on the following non-uniform grids:

(a) $x(\xi) = 1 + \tan^{-1}(\xi - 1/2)/\tan^{-1}(1/2)$,

$$y(\eta) = 4 \tan^{-1}(5\eta)/\tan^{-1}(5). \tag{13}$$

(b) $x(\xi) = 2 \sin^2(\tfrac{1}{2}\pi\xi)$,

$$y(\eta) = 4\{1 - (1 - \eta)^2\}. \tag{14}$$

TABLE I

Number of DADI Steps

Mesh	Uniform grid	Grid (a)	Grid (b)
5×9	204	312	348
9×17	288	372	708
17×33	552	540	1548

These grid stretching functions are chosen to give a smaller spacing of the grid points in the neighbourhoods of the singularities. The following constant grid intervals are chosen:

(i) $\Delta\xi=0.25, \quad \Delta\eta=0.125;$

(ii) $\Delta\xi=0.125, \quad \Delta\eta=0.0625;$

(iii) $\Delta\xi=0.0625, \quad \Delta\eta=0.03125.$

These grids defined by (i), (ii), and (iii) have respectively 5×9, 9×17, and 17×33 points.

We compare the results obtained on these non-uniform grids with those obtained on a uniform grid with the same number of grid points in each direction. We use as our stopping criterion that the maximum value of the difference between successive iterates at the grid points is less than 10^{-6} in magnitude.

Table I gives the number of DADI steps required to attain the tolerance. The values of $c(x, y)$ at points P and Q are given in Table II. From these results we see that the DADI method with grid (b) takes longer to converge than with grid (a). This is because in grid (b) the points are closer together in the neighbourhoods of the singularities. In Section 6 we show by consideration of the local truncation error and also an analysis of difference tables that the approximation obtained on grid (a) is more accurate in the neighbourhoods of the singularities.

TABLE II

Values of $c(x, y)$ in the Top Corners

Mesh	Values	Uniform grid	Grid (a)	Grid (b)
5×9	$c(0, 4)$	0.0591	0.0581	0.0629
	$c(2, 4)$	0.0196	0.0188	0.0194
9×17	$c(0, 4)$	0.0682	0.0693	0.0758
	$c(2, 4)$	0.0203	0.0200	0.0208
17×33	$c(0, 4)$	0.0749	0.0766	0.0819
	$c(2, 4)$	0.0209	0.0209	0.0216

4. A Dynamic ADI Method

Here we describe how the DADI method of Doss and Miller [3] can be used to obtain a numerical solution to this problem. The ADI approach first converts Eqs. (1) and (2) to the parabolic equations

$$\frac{\partial c}{\partial t}=\frac{\partial^2 c}{\partial x^2}+\frac{\partial^2 c}{\partial y^2}-c, \tag{15}$$

$$\frac{\partial u}{\partial t}=\lambda\left\{\frac{\partial}{\partial x}\left(\frac{1}{c}\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{1}{c}\frac{\partial u}{\partial y}\right)\right\}, \tag{16}$$

whose steady state solution, if one exists, solves Eqs. (1) and (2). The parameter λ controls the interaction between the equations. When these equations are discretized in time it means that, effectively, we use different time steps for the two equations when $\lambda \neq 1$. The value of λ is chosen to be 0.05 in all our calculations, after some experimentation.

Since Eqs. (15) and (16) are parabolic they may be advanced in time by a direct method and the complete solution procedure may be regarded as a single iterative scheme. Our interest is not in solving the parabolic equations (15) and (16) accurately for finite times but to reach the steady state as quickly as possible. Therefore the DADI method is used since it uses a strategy that attempts to keep the time step Δt within a region where convergence is fast. An advantage of using an automatic step size changer is that it avoids the necessity of choosing a priori iteration parameters.

Each step of the DADI method comprises two double sweeps of the ADI iteration with time step Δt together with a book-keeping double sweep of the ADI iteration. At the end of the step we use a computerized strategy to determine how to change Δt for the next step. The strategy of Doss and Miller [3] attempts to recognise instabilities as they start to occur and to bypass them by decreasing Δt. In their paper Doss and Miller give theoretical justification of this strategy for a model problem. Although their analysis of the step size strategy rests on rigid assumptions, they obtain good results in situations where these no longer hold.

The reader is referred to Phillips [7] for an outline of the algorithm used to solve this problem by the DADI method on a uniform grid. The extension to a non-uniform grid is straightforward. Detailed discussions of the ADI method and its implementation can be found in Varga [8] and Young [9].

5. Transformation Method

In this section we use a suitable transformation to map the problem in the neighbourhoods of the singularities to one which is free from singularities. To start with we assume that we have solved this problem in the region R using a uniform grid. We aim to improve the accuracy of our approximation near the singularities.

Consider the singularity at the point $P(0, 4)$. The rectangle R is translated so that this point lies at the origin. Let the sector S_M be defined by

$$S_M = \{(r, \theta): 0 \leqslant r \leqslant Mh, -\tfrac{1}{2}\pi \leqslant \theta \leqslant 0\},$$

where M is a positive integer and h is the mesh size of the uniform grid. This situation is illustrated in Fig. 2. By means of the transformation

$$\rho = -\log r, \qquad \theta = \tan^{-1}(y/x), \tag{17}$$

where $r^2 = x^2 + y^2$, the sector S_M is transformed to the semi-infinite strip T_M, where

$$T_M = \{(\rho, \theta): -\log(Mh) \leqslant \rho < \infty, -\tfrac{1}{2}\pi \leqslant \theta \leqslant 0\}.$$

With the change of variable (17) the partial differential equations (1) and (2) become

$$\frac{\partial^2 c}{\partial \rho^2} + \frac{\partial^2 c}{\partial \theta^2} = e^{-2\rho} c, \tag{18}$$

$$\frac{\partial}{\partial \rho}\left(\frac{1}{c}\frac{\partial u}{\partial \rho}\right) + \frac{\partial}{\partial \theta}\left(\frac{1}{c}\frac{\partial u}{\partial \theta}\right) = 0. \tag{19}$$

As $\rho \to \infty$, $r \to 0$, so for a sufficiently large value of ρ, say P, we are sufficiently close to the origin for both c and u to be constant along the arc $r = e^{-P}$, $-\frac{1}{2}\pi \leqslant \theta \leqslant 0$. So we close off the semi-infinite strip at $\rho = L$ where $L > -\log(Mh)$. Let $T_{M,L}$ be the rectangle

$$\{(\rho, \theta): -\log(Mh) \leqslant \rho \leqslant L, -\tfrac{1}{2}\pi \leqslant \theta \leqslant 0\}.$$

This is illustrated in the $\rho - \theta$ plane in Fig. 3.

We now introduce the boundary conditions used to solve the differential equations (18) and (19) in the rectangle $T_{M,L}$. The lines $x = 0$ $(-Mh \leqslant y \leqslant 0)$ and $y = 0$ $(0 \leqslant x \leqslant Mh)$ are mapped under the transformation to the lines $\theta = -\frac{1}{2}\pi$ and

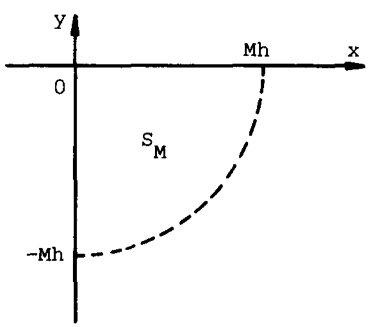

FIGURE 2

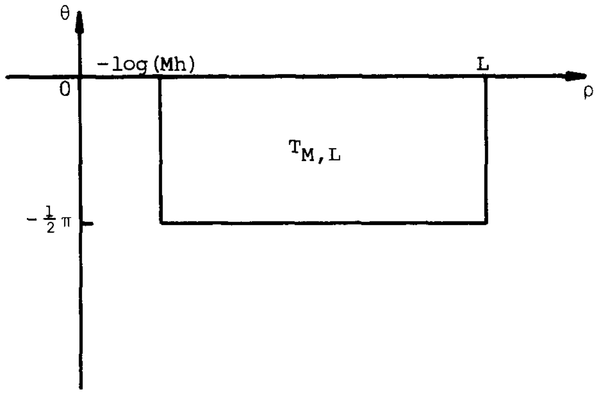

FIGURE 3

$\theta = 0$, respectively, for $-\log(Mh) \leqslant \rho \leqslant L$. Therefore the boundary conditions along these lines are given by

$$\frac{\partial c}{\partial \theta} = \frac{b}{(1+b)} \frac{\partial u}{\partial \rho}, \qquad \frac{\partial u}{\partial \theta} = (1+b) \frac{\partial c}{\partial \rho} \qquad \text{on} \quad \theta = -\tfrac{1}{2}\pi,$$

$$\frac{\partial c}{\partial \theta} = -se^{-\rho} c, \qquad u = -1 \qquad \text{on} \quad \theta = 0.$$

Along the line $\rho = L$ we impose the conditions

$$\frac{\partial c}{\partial \rho} = 0, \qquad \frac{\partial u}{\partial \rho} = 0,$$

since both c and u tend to some limiting value as $\rho \to \infty$. Along the line $\rho = -\log(Mh)$ we obtain values of c and u at certain points by bilinear interpolation. These points will be the mesh points lying on $\rho = -\log(Mh)$ and details of the interpolation will be given later.

We are now in a position to solve the partial differential equations (18) and (19) together with the associated boundary conditions in the rectangle $T_{M,L}$. $T_{M,L}$ is covered with a rectangular mesh with mesh length h_1 in the ρ-direction and h_2 in the θ-direction. The problem is discretized using the technique described in Section 3. The resulting difference equations are solved by the DADI method.

The corner situated at the point $Q(2, 4)$ is treated in a similar fashion. Let W be the region which is formed from R be removing squares of side $(M-1)h$ from the top right- and left-hand corners. The details of the procedure we use to obtain more accurate approximations near the singularities are given in the following algorithm.

ALGORITHM. (a) Solve Eqs. (1) and (2) in the region R using a uniform grid. The DADI method is used to solve the discretized equations.

(b) Set u^I and c^I to be the vectors of the current values of u and c respectively at the grid points. Let N_1 and N_2 be integers such that $N_1 h_1 = L + \log(Mh)$ and $N_2 h_2 = \frac{1}{2}\pi$. We require the values of u and c at the points of intersection of the lines $y = -k\pi/(2N_2)$, $k = 0, 1, \ldots, N_2$, with the boundary $r = Mh$ of the sector S_M. These will then be the values at the mesh points on the line $\rho = -\log(Mh)$ in the $\rho - \theta$ plane. This procedure refers to the transformation of the left-hand sector. A similar procedure is performed for the right-hand sector. The interpolation is described for the particular case shown in Fig. 4. Since we can determine the positions of the points A and B we can find the values of u and c at these points by linearly interpolating values at C and D, and D and E, respectively. We then linearly interpolate these values at A and B to obtain values at F.

(c) Solve the transformed equations (18) and (19) in each of the rectangles $T_{M,L}$ starting from some initial guess. When we come to step (c) other than for the first time we use the previous values to start the iteration. Again we use the DADI method to solve the discretized equations. The stopping criterion is that the maximum modulus of the difference in successive iterates is less than 10^{-4}.

(d) Use linear interpolation to calculate values of u and c at points of $T_{M,L}$ which correspond to mesh points of R lying within the sectors S_M. This updates the values of u and c at the mesh points within S_M.

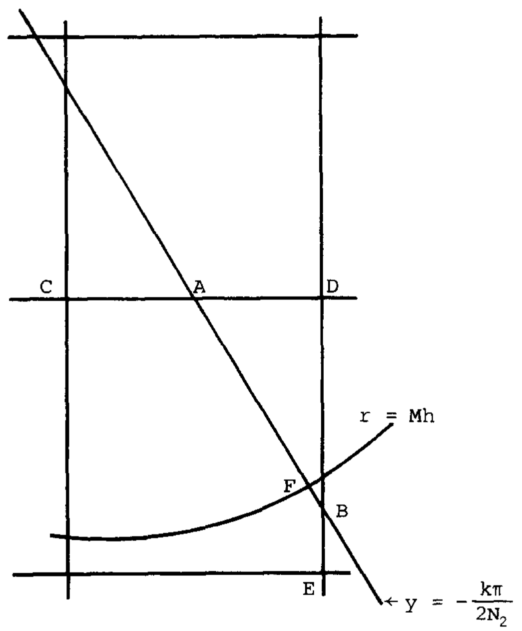

FIGURE 4

TABLE III

Variation of Corner Values with M

M	$c(0, 4)$	$c(2, 4)$
2	0.0831	0.0211
3	0.0789	0.0210
4	0.0767	0.0211
5	0.0768	0.0209
6	0.0769	0.0212

(e) Solve the discretized forms of Eqs. (1) and (2) in W using the DADI method. We use the same stopping criterion as in step (c). Set u^F and c^F to be the vectors of the current values of u and c respectively at the grid points of R.

(f) If $\|u^F - u^I\|_\infty < \varepsilon$ and $\|c^F - c^I\|_\infty < \varepsilon$, where ε is some tolerance, then the algorithm is terminated. If not, go to step (b).

Numerical results obtained using the above algorithm are shown above. The mesh length, h, of the uniform grid on R was chosen to be $\frac{1}{8}$. The values of N_1, N_2, and h_1 are chosen to be 37, 4, and $\frac{1}{4}$, respectively. This means that in the case when $M=2$ we have that $L=10.63$. This value of L corresponds to the value of $r=2.4\times10^{-5}$. We experimented with the position of L so that c and u did indeed tend to some limiting value as $\rho\to\infty$. The tolerance, ε, is chosen to be 10^{-4}. The value of M is chosen so that the two sectors S_M do not intersect, i.e., $M\leqslant 7$. The values of c at the points P and Q are shown in Table III for various values of M.

6. Conclusions

The iterative solution of finite difference equations constructed on a nonuniform grid usually presents great difficulties. This is due to the problem of finding suitable parameters for the acceleration of convergence of any selected iterative method. Hence, an advantage of the DADI method over standard iterative methods for solving problems of this type is that we do not require an a priori choice of parameters to accelerate convergence.

Although the local truncation error of the finite difference approximation to the first derivative on the non-uniform grid is formally second order in $\Delta\xi$, the term of $O(\Delta\xi^2)$ contains derivatives of the stretching function which will be large in certain areas if there is strong mesh stretching and large variation in the grid. The local truncation error of the first derivative is given by the expression

$$-(\Delta\xi)^2\left\{\frac{1}{4}\frac{d^2x}{d\xi^2}\frac{\partial^2 v}{\partial x^2}+\frac{1}{6}\left(\frac{dx}{d\xi}\right)^2\frac{\partial^3 v}{\partial x^3}\right\}+O(\Delta\xi^3).$$

TABLE IV

Differences of $c(1, y)$ with a Uniform Grid

y	$c(1, y)$		δ^2		δ^4
4.000	0.0133				
		82			
3.875	0.0215		−3		
		79		−3	
3.750	0.0294		−6		−4
		73		1	
3.625	0.0367		−5		−1
		68		0	
3.500	0.0435		−5		−1
		63		1	
3.375	0.0498		−6		1
		57		0	
3.250	0.0555		−6		0
		53		0	
3.125	0.0608		−6		
		47			
3.000	0.0655				

TABLE V

Differences of $c(0, y)$ with a Uniform Grid

y	$c(0, y)$		δ^2		δ^4
4.000	0.0749				
		240			
3.875	0.0989		−155		
		85		165	
3.750	0.1074		10		−186
		95		−21	
3.625	0.1169		−11		25
		84		4	
3.500	0.1253		−7		−3
		77		1	
3.375	0.1330		−6		0
		71		1	
3.250	0.1401		−5		−2
		66		−1	
3.125	0.1467		−6		
		60			
3.000	0.1527				

TABLE VI

Differences of $c(0, y)$ with Grid (a)

y	$c(0, y)$		δ^2		δ^4		δ^6
4.000	0.0766						
		58					
3.982	0.0824		−17				
		41		7			
3.963	0.0865		−10		−1		
		31		6		−3	
3.942	0.0896		−4		−4		6
		27		2		3	
3.920	0.0923		−2		−1		−2
		25		1		1	
3.897	0.0948		−1		0		1
		24		1		0	
3.872	0.0972		0		0		
		24		1			
3.845	0.0996		1				
		25					
3.816	0.1021						

TABLE VII

Differences of $c(0, y)$ with Grid (b)

y	$c(0, y)$		δ^2		δ^4		δ^6
4.000	0.0819						
		13					
3.996	0.0832		7				
		20		−3			
3.984	0.0852		4		5		
		24		2		−5	
3.965	0.0876		6		0		−3
		30		2		−8	
3.938	0.0906		8		−8		25
		38		−6		17	
3.902	0.0942		2		9		−31
		40		3		−14	
3.859	0.0982		5		−5		
		45		−2			
3.809	0.1027		3				
		48					
3.750	0.1075						

Near a singularity the higher derivatives of v become large and therefore the coefficient of $(\Delta\xi)^2$ is small provided that the derivatives of the stretching function are small there. For the grid transformation given by (14) this is not the case and so the coefficient of $O(\Delta\xi^2)$ of the local truncation error of the resulting approximation near the singularities is not small.

The results obtained using uniform grids mainly show a good agreement and the convergence is approximately quadratic except at the points P and Q. The bad results at these points are due to the singularities. This is illustrated in Tables IV and V which are difference tables of $c(1, y)$ and $c(0, y)$ respectively with y taking values between 3 and 4 at intervals of 0.125. We can see from Table IV that the differences of $c(1, y)$ are well behaved. Table V illustrates the fact that there is a singularity at the point P since the differences diverge there (see Fox [4]). Tables VI and VII are tables of differences of $c(0, y)$ in terms of equal intervals in the stretched coordinates given by (13) and (14), respectively. The differences in Table VI are reasonably well behaved suggesting that the approximation obtained using the grid given by (13) is fairly accurate. The differences in Table VII appear to be rather less satisfactory.

However, it is preferable to leave ourselves with the task of solving a nonsingular problem, when this is possible, for which numerical methods of finite difference type have a much sounder basis. This is an advantage of the transformation method which maps the problem in the vicinities of the singularities into a problem free of singularities. From Table V we see that the effects of the singularity are local in nature and so the finite difference approximation computed at points at a reasonable distance from the singularities is accurate.

From the above discussion we would expect the results from the DADI method with grid defined by (13) and the transformation method to be accurate and indeed there is good agreement between them. However, it is worth noting that the DADI method with a variable grid is easier to implement than the transformation method.

Acknowledgments

I am grateful to Dr. David Mayers for many useful discussions in connection with this work.

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