

A MODIFIED FINITE DIFFERENCE METHOD TO
SOLVE ELLIPTIC PARTIAL DIFFERENTIAL
EQUATIONS WITH REENTRANT CORNERS

By

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CHAPTER I

INTRODUCTION

This thesis explores numerical methods of approximating the solution to boundary value problems involving elliptic partial differential equations. The particular problems considered here concern equations over planar regions which have angular singularities along their boundaries. The examples used in this thesis primarily involve Laplace's equations ($U_{xx} + U_{yy} = 0$), but the techniques developed should be applicable to other types of partial differential equations.

Elliptic partial differential equations are encountered frequently in science and are usually solved over a closed region with some information known about the solution at each point of the boundary of the region. This information could consist of either the function values (Dirichlet), normal derivatives (Neumann), or some mixture of values and derivatives.

The boundaries of the problems considered here contain interior angles greater than π radians. At these reentrant corners a low order derivative of the solution does not exist. These singularities are often ignored; however, a severe loss of accuracy can occur when numerical schemes

such as the finite difference method or the finite element method are used to approximate the solutions. In this thesis a means of modifying the finite difference method is developed which accounts for these singularities and improves the accuracy of the approximation. Using this modification, the order of accuracy for a region with a reentrant corner approaches that expected in regions with no singularities.

Other approaches to modifying the finite difference method for problems with reentrant corners can be found in references [1] - [9], while references [10] - [13] concern modifications to the finite element method for these problems.

CHAPTER II

FINITE DIFFERENCE METHOD

One of the most common numerical methods used to approximate the solution of partial differential equations is known as the finite difference method. In this method the region over which the partial differential equation is to be solved is first overlaid with a grid of vertical and horizontal lines. An approximation to the solution is then found for the points of intersection which lie inside the region of interest, along with the points of intersection of these lines with the boundary (if these values are not specified in the boundary conditions). A set of independent equations is then developed using Taylor series expansions at each of the points of intersection. The variables for the equations are the solution values at the intersection points. There is generally one equation for each point to be determined.

To develop the equations needed to approximate the solution, each term in the partial differential equation is approximated by differences. The difference approximations for each derivative term are then assembled into a single expression representing the partial differential equation. This approximating equation for each point usually involves

the solution values at that point along with the values at neighboring points. The points needed for the approximation vary according to the derivatives to be approximated, the order of accuracy desired, and the position of the point with respect to the boundary.

To illustrate the development of the approximating equations, consider solving Laplace's equation ($U_{xx} + U_{yy} = 0$) over the region bounded by $X = 0$, $X = 1$, $Y = 0$, and $Y = 1$. For boundary conditions suppose $U_x = 0$ if $x = 0$ or 1 , and $U(x,y) = g(x,y)$ when $y = 0$ or 1 as in Figure 1.

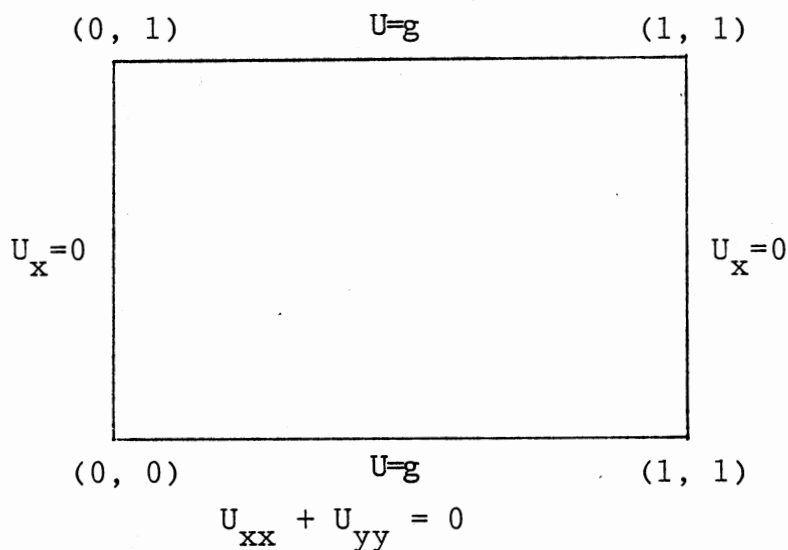


Figure 1. Sample Finite Difference Problems

When the region is overlaid with vertical and horizontal lines, the spacing between adjacent lines is arbitrary. However, a regular net is usually the easiest to

use, and for this example, the distance (h) between lines is 0.2 as shown in Figure 2.

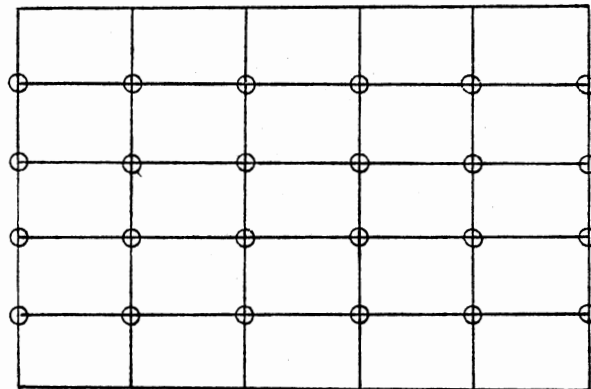


Figure 2. Sample Finite Difference Grid

An approximation to the solution is now sought for the 24 points of intersection which are circled. At each of these points an approximation to the partial differential equation is developed in terms of other nearby points. If the y value were fixed, the Taylor's series expansion for points to the right and left of an intersection point could be written as:

$$U(x+h,y) = U(x,y) + hU_x(x,y) + \frac{h^2}{2}U_{xx}(x,y) + \dots \quad (2-1)$$

and

$$U(x-h,y) = U(x,y) - hU_x(x,y) + \frac{h^2}{2}U_{xx}(x,y) - \dots \quad (2-2)$$

Adding these equations gives:

$$U(x+h,y) + U(x-h,y) = 2U(x,y) + h^2U_{xx}(x,y) + O(h^4),$$

or

$$U_{xx}(x,y) = (U(x+h,y) + U(x-h,y) - 2U(x,y))/h^2 + O(h^2). \quad (2-3)$$

Fixing x similarly would yield:

$$U_{yy}(x,y) = (U(x,y+h) + U(x,y-h) - 2U(x,y))/h^2 + O(h^2). \quad (2-4)$$

If Equation (2-3) were added to Equation (2-4) and $U_{xx}(x,y) + U_{yy}(x,y)$ set to 0,

$$\begin{aligned} U(x+h,y) + U(x-h,y) + U(x,y+h) + U(x,y-h) - 4U(x,y) \\ = O(h^4). \end{aligned} \quad (2-5)$$

Each interior point (x,y) is now associated with the approximating Equation (2-5). This equation will be valid only for interior points since for boundary points one of the neighbors will fall outside the area. To develop an equation for the right and left boundaries, Equation (2-2) is first subtracted from Equation (2-1) giving:

$$U_x(x,y) = (U(x+h,y) - U(x-h,y))/2h + O(h^2). \quad (2-6)$$

Since $U_x(x,y) = 0$ for $x = 0$ or 1 ,

$$U(x+h,y) = U(x-h,y) + O(h^3) \quad (2-7)$$

for points along the right or left hand boundaries. So if a term of Equation (2-5) falls outside the region, that term could be replaced using Equation (2-7). Thus when $x = 0$, Equation (2-5) becomes:

$$U(h,y) + (U(h,y) + O(h^3)) + U(0,y+h) + U(0,y-h) - 4U(0,y) = O(h^4),$$

or,

$$2U(h,y) + U(0,y+h) + U(0,y-h) - 4U(0,y) = O(h^3). \quad (2-8)$$

When $x = 1$, Equation (2-5) becomes:

$$2U(1-h,y) + U(1,y+h) + U(1,y-h) - 4U(1,y) = O(h^3). \quad (2-9)$$

Although this treatment at the boundary decreases the order of accuracy of the approximating equation, it does not cause a corresponding loss in accuracy in the overall solution. (Appendix B discusses the accuracy of the final solution.)

By using either Equation (2-5), (2-8), or (2-9), an equation is developed which corresponds to each of the unknown intersection points. To illustrate the form of these equations the example of Forsythe and Wasow [14] is followed. First designate the approximation to the solution at point P as $V(P)$. The approximation of the points to the right, left, top, and bottom of P are then designated $V(E)$, $V(W)$, $V(N)$, and $V(S)$, respectively, where the letter in parentheses represents a compass direction (top of the page

is north). To develop these equations, the error terms in Equations (2-5), (2-8), and (2-9) are dropped and the approximation V is substituted for the true solution U . Thus Equation (2-5) is used as a pattern for interior points and becomes:

$$V(E) + V(W) + V(N) + V(S) - 4V(P) = 0.$$

For points on the left boundary Equation (2-8) becomes:

$$2V(E) + V(N) + V(S) - 4V(P) = 0.$$

Similarly Equation (2-9) becomes:

$$2V(W) + V(N) + V(S) - 4V(P) = 0.$$

The linear equations (one for each unknown $V(p)$) are now assembled and solved using either a direct method such as Gaussian elimination or an iterative procedure. Since the set of equations has a unique solution, either method will provide the answer. However, the solution obtained is only an approximation to the solution of the original problem. Appendix B discusses how the solution to the approximating equations involving V differs from the solution to the original equations involving U . A more traditional approach to error estimates for the finite difference method can be found in references [15] - [17] as well as in many textbooks on numerical analysis.

A brief summary of iterative methods used to solve approximating equations which occur in the application of the finite difference method can be found in Appendix A.

CHAPTER III

IMPROVEMENTS IN ACCURACY

If the difference scheme developed in the previous chapter were applied to the sample problem, the solution $U(x,y)$ would be determined to within $O(h^2)$ at each of the grid points. A discussion of this error term can be found in references [15] - [17], and also in Appendix B. However, Richardson [18] goes beyond just giving the order of accuracy and asserts that the error, ϵ_h , can be represented by the following series:

$$\epsilon_h(x,y) = f_1(x,y)h^2 + f_2(x,y)h^4 + f_3(x,y)h^6 + \dots \quad (3-1)$$

The important thing to notice is that the functions, f_i , are independent of h . Thus, one obvious method to reduce the error is to use a smaller h . However, as h becomes smaller, the number of points and thus the number of equations becomes larger. As the number of equations increases, more computer time and storage is required. Also, as the number of equations increase, the error from machine roundoff increases until h reaches a critical size at which the minimum total error occurs. Richardson not only found the form of the error term, but also devised a method to exploit the

form of the error. His method was to first solve the problem for two or more different values of h . These solutions are then used to eliminate the f 's of the lower order terms in the series. For example, suppose V_h and $V_{\frac{h}{2}}$ were the solutions obtained by using h and $\frac{h}{2}$ for step sizes. Then,

$$\epsilon_h = V_h - U = f_1 h^2 + f_2 h^4 + \dots,$$

and

$$\epsilon_{\frac{h}{2}} = V_{\frac{h}{2}} - U = f_1 \left(\frac{h}{2}\right)^2 + f_2 \left(\frac{h}{2}\right)^4 + \dots$$

By algebraically eliminating f_1 and solving for U ,

$$U = (4V_{\frac{h}{2}} - V_h)/3 + f_2 \frac{h^4}{4} + \dots$$

Thus, by using two approximations of order h^2 an approximation of order h^4 is developed. If 3 different h 's had been used, both f_1 and f_2 could be eliminated to obtain an order h^6 approximation. This method of extrapolation only works when the form of the error is known.

Another method of improving the solution is to use a higher order method. The order h^2 5-point method developed earlier is one of many that could be used. The other most frequently used method, the 9-point rule, has an error of order h^6 when Laplace's equation is solved using a uniform grid if the solution is sufficiently differentiable.

The iterative form of the 9-point rule is:

$$U(P) = [U(NE) + U(NW) + U(SE) + U(SW) + 4(U(N) + U(S) + U(E) + U(W))] / 20,$$

where the points are defined by compass directions mentioned earlier. This method, like the 5-point rule, has the property that the commonly used iterative methods used to solve the resulting equations converge regardless of the starting values used. Programming the 9-point rule is as easy as programming the 5-point rule, but the accuracy for a given step size is much superior. Also, to further improve the accuracy of the approximation obtained by using the 9-point rule, Richardson's method could be used to eliminate the higher order error terms of its error series. However, when Richardson's method is used with two different grids, the improved accuracy is achieved only on the coarser grid. Fox's method of deferred corrections [2] is superior to Richardson's method in that it attains the improved accuracy on the finer grid.

CHAPTER IV

BOUNDARY SINGULARITIES

In the previous discussions it was assumed that the true solution, U , had sufficient derivatives to justify using Taylor's series expansions. It is known that the partial derivatives of harmonic functions exist everywhere in the open region. However, singularities can occur on the boundary, as is the case when the boundary is not sufficiently smooth. If the boundary is composed of line segments, the intersection points can produce singularities. In general, the larger interior angles (above 180°) will produce lower degrees of continuous partial derivatives at the vertex of the boundary angle. References [19] - [24] discuss the development and consequences of these singularities for various partial differential equations.

For Laplace's equation, differential equation theory can be used to derive the form of the solution at a corner, and thus determine the form of the singularity.

Let $U_{xx} + U_{yy} = 0$ over the region depicted in Figure 3. Boundary conditions will be discussed later. In polar coordinates Laplace's equation becomes:

$$U_{rr} + \frac{1}{r} U_r + \frac{1}{r^2} U_{\theta\theta} = 0, \quad (4-1)$$

where $0 \leq \theta \leq \alpha \pi$.

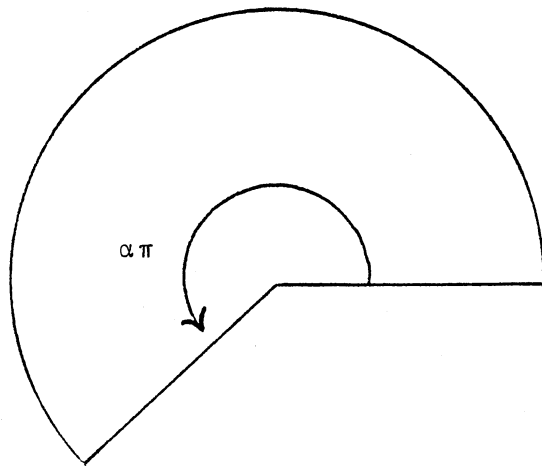


Figure 3. Reentrant Corner

The method of separation of variables is used, and it is assumed that the solution can be written as:

$$U(r, \theta) = T(\theta) \cdot R(r), \quad (4-2)$$

where T is a function of θ only and R is a function of r only. Substituting the partial derivatives from Equation (4-2) into Equation (4-1) gives:

$$R'' T + \frac{1}{r} R' T + \frac{1}{r^2} R T'' = 0,$$

or

$$r^2 \frac{R''}{R} + r \frac{R'}{R} = - \frac{T''}{T} = \lambda,$$

where λ is the separation constant. By requiring U to be bounded as $r \rightarrow 0$, the solutions to the ordinary differential equations become:

$$R(r) = c_1 r^\lambda \quad (\lambda \geq 0),$$

and

$$T(\theta) = k_1 \sin \lambda \theta + k_2 \cos \lambda \theta,$$

so that

$$U(r, \theta) = c_1 r^\lambda (k_1 \sin \lambda \theta + k_2 \cos \lambda \theta).$$

If the boundary conditions were:

$$U(r, 0) = U(r, \alpha\pi) = 0,$$

then

$$U(r, 0) = c_1 k_2 r^\lambda = 0,$$

which would force either c_1 or k_2 to be zero. If c_1 were zero, the solution would be trivial. Therefore $k_2 = 0$. Also

$$U(r, \alpha\pi) = c_1 r^\lambda \cdot k_1 \sin \lambda \alpha\pi = 0.$$

If c_1 or k_1 were 0, the solution would again be trivial so that $\sin \lambda \alpha\pi = 0$. But this requires $\lambda \alpha$ to be an integer so that $\lambda = \frac{n}{\alpha}$, where $n \in \{0, 1, 2, \dots\}$. Thus the solution for this set of boundary conditions is:

$$U(r, \theta) = \sum_{n=0}^{\infty} a_n r^{\frac{n}{\alpha}} \sin \frac{n\theta}{\alpha},$$

for $0 < \theta < \alpha\pi$.

If the boundary conditions had consisted of normal derivatives equal to 0 for $\theta=0$ and $\theta=\alpha\pi$, the solution would have been:

$$U(r, 0) = \sum_{n=0}^{\infty} a_n r^{\frac{n}{\alpha}} \cos \frac{n}{\alpha} 0.$$

When $\alpha > 1$, U_r becomes unbounded as $r \rightarrow 0$. Thus the error term developed using Taylor's series will not be valid. To see what error the 5-point rule generates at a reentrant corner, consider

$$U(r, 0) = \sum_{n=0}^{\infty} a_n r^{\frac{n}{\alpha}} \cos \frac{n}{\alpha} 0 \text{ for } \alpha = 3/2.$$

(If $\alpha < 3/2$ the 5-point rule cannot be used because one of the points would lie outside the domain.) Expanding each of the relevant points by the solution series gives:

$$U(P) = U(0, 0) = a_0,$$

$$U(N) = U(h, \frac{\pi}{2}) = a_0 + a_1 h^{\frac{2}{3}} \cos \frac{\pi}{3} + a_2 h^{\frac{4}{3}} \cos \frac{2\pi}{3} + \dots,$$

$$U(S) = U(h, \frac{3\pi}{2}) = a_0 + a_1 h^{\frac{2}{3}} \cos \pi + a_2 h^{\frac{4}{3}} \cos 2\pi + \dots,$$

$$U(E) = U(h, 0) = a_0 + a_1 h^{\frac{2}{3}} \cos 0 + a_2 h^{\frac{4}{3}} \cos 0 + \dots,$$

$$U(W) = U(h, \pi) = a_0 + a_1 h^{\frac{2}{3}} \cos \frac{2\pi}{3} + a_2 h^{\frac{4}{3}} \cos \frac{4\pi}{3} + \dots$$

Substituting these expansions in the 5-point rule gives:

$$4 U(P) - (U(N) + U(S) + U(E) + U(W)) = a_2 h^{\frac{4}{3}} + O(h^2).$$

Thus the 5-point rule at this reentrant corner gives

an approximation equation of order $h^{\frac{4}{3}}$ instead of the order h^4 which occurs at the interior points. The presence of even a single $\frac{3\pi}{2}$ reentrant corner in the region will change the error in the solution from order h^2 to order $h^{\frac{4}{3}}$.

If the reentrant angle had been $\frac{7\pi}{4}$, the error would have been of order $h^{\frac{4}{7}}$ instead of order $h^{\frac{4}{3}}$. It was fortunate that the 5-point rule eliminated the a_1 terms as well as the a_0 terms. (This only happens when $\cos \frac{\pi}{2}\alpha = -1, 0,$ or $\frac{1}{2}$.) If, however, a different rule could be developed for the reentrant corner which would eliminate the $a_0, a_1,$ and a_2 terms, the method would be an order h^2 method. A replacement rule for the reentrant corner is therefore sought having the form:

$$0 = C_P U(P) + C_N U(N) + C_S U(S) + C_E U(E) + C_W U(W),$$

that would eliminate the $a_0, a_1,$ and a_2 terms in the expansion. The following expansion results from substituting the series representations at each point into the general rule above:

$$0 = a_0 (C_P + C_N + C_S + C_E + C_W) + a_1 h^{\frac{2}{3}} (C_N/2 - C_S + C_E - C_W/2) +$$

$$\begin{aligned}
 & a_2 h^{\frac{4}{3}} (-C_N/2 + C_S + C_E - C_W/2) + \\
 & a_3 h^2 (-C_N - C_S + C_E + C_W) + \\
 & a_4 h^{\frac{8}{3}} (-C_N/2 + C_S + C_E - C_W/2) + \dots
 \end{aligned}$$

If each of the coefficients were equated to 0, a set of five linear equations in the unknowns C_P , C_N , C_S , C_E , and C_W would result. These equations are homogeneous, but the third and fifth are linearly dependent. Thus the set can be solved in terms of any one of the variables. If a value of K were assigned to C_P , the matrix form of the equations would be:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1/2 & -1 & 1 & -1/2 \\ -1/2 & 1 & 1 & -1/2 \\ -1 & -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} C_N \\ C_S \\ C_E \\ C_W \end{bmatrix} = \begin{bmatrix} -K \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

which has a solution:

$$C_N = C_W = \frac{-K}{3} \text{ and } C_S = C_E = \frac{-K}{6}.$$

This suggests the following rule for the reentrant corner using $K = -6$:

$$-6 U(P) + 2 U(N) + 2 U(W) + U(S) + U(E) = 0.$$

If this rule is used at the reentrant corner in place of

the 5-point rule, the error terms involving $h^{\frac{2}{3}}$, $h^{\frac{4}{3}}$, h^2 , and

$h^{\frac{8}{3}}$ are eliminated. As a bonus, the $h^{\frac{10}{3}}$ -term is also eliminated, but the h^4 terms remain. Thus by using an altered rule at the reentrant corner, the order of accuracy for the 5-point rule over a region with no singularities would be regained.

For higher order rules such as the 9-point rule, a more accurate rule for the $\frac{3\pi}{2}$ reentrant corner could be developed by using other neighboring points and eliminating the higher order terms. A rule compatible with the 9-point rule for a $\frac{3\pi}{2}$ reentrant corner is:

$$V(P) = [4(V(W) + V(N)) + 2(V(E) + V(S)) + V(NW) + V(SW) + V(NE)]/15.$$

CHAPTER V

THE CROSS SHEET-RESISTOR

The two reentrant corners which have precipitated the most interest are $3\pi/2$ and 2π radians. A reentrant corner of 2π radians is used to describe cracks in structures. Problems with $3\pi/2$ radians reentrant corners also abound in nature. Some examples concern the "flowing" of heat, electric charge, or any incompressible fluid around a 90° bend as illustrated in Figure 4.

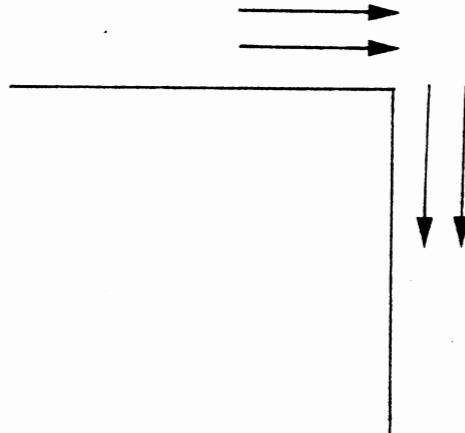


Figure 4. Singularity
in Flow

One such problem concerns calculating the voltage across a sheet resistor in the form of a Greek cross when voltages are applied at the center of two adjacent arms. (See Figure 5.) This problem was suggested by the National Bureau of Standards and is described in greater detail in reference [25] by David and Buehler. One nice property of this problem is that the current from A to B divided by the voltage difference between points C and D is a known constant. According to van de Pauw [26, 27],

$$I_{AB} / (V_C - V_D) = K\pi/\ln 2,$$

where K is a constant related to the resistance of the sheet. This fact provides a check for the absolute error in any numerical scheme.

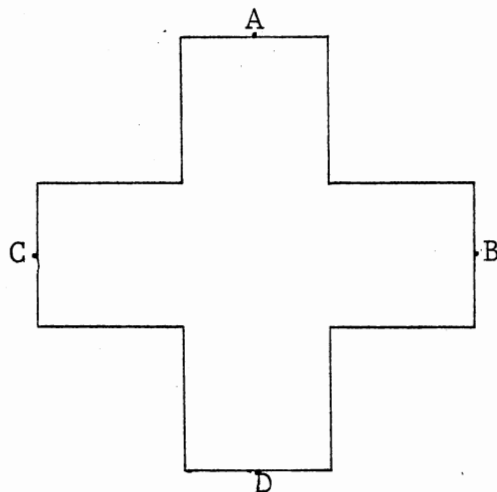


Figure 5. Cross Sheet-Resistor Geometry

Also, if the voltage applied at points A and B were 1 and -1, respectively, a symmetry would occur which would allow the problem to be defined as shown in Figure 6.

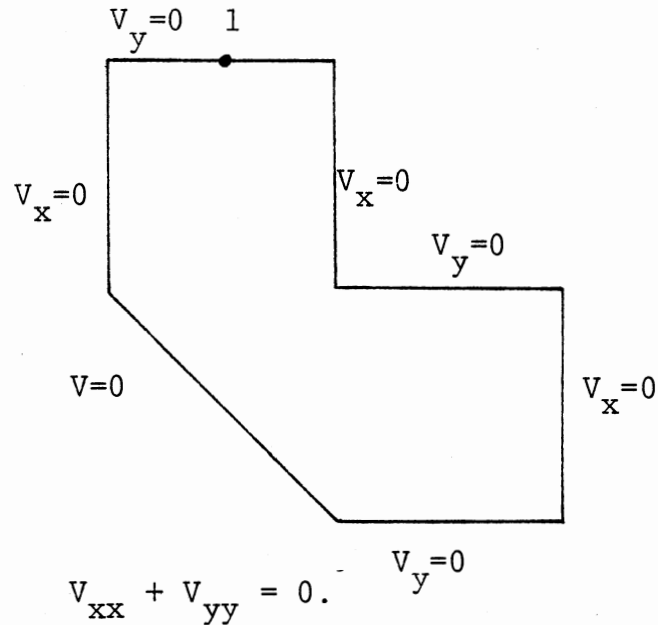


Figure 6. Simplified Cross Sheet-Resistor Geometry

After the problem is discretized and Laplace's equation is solved using the above boundary conditions, the current down the top arm is computed. To do this, the average potential is found along two adjacent rows near the middle (vertically) of the top arm. Let V_2 be the average potential of the middle row of the top arm and let V_1 be the average potential of the row just below that middle row of the grid.

By observing that the resistance between two rows of the grid is proportional to the distance between the rows, the current between the rows can be computed by Ohm's law using $I = (V_2 - V_1)/h$. Since Simpson's rule was used to estimate the integral in order to obtain an average potential, an error is introduced of order h^4 . (The error from Simpson's rule is $O(h^5)$ but dividing by h reduces the order of the error to $O(h^4)$.) The error from this computation could be reduced by using a higher order Newton-Coats formula to estimate the integrals.

The voltages were found using both finite difference methods with regular grids and finite element methods with uniform right isosceles elements. When polynomials of the form $A_0 + A_1 X + A_2 Y$ were used for the basis elements, the finite element method was identical to the 5-point rule finite difference method except at the reentrant corner. At the reentrant corner the rule became

$$U(P) = (U(N) + U(E) + 2U(W) + 2U(S))/6,$$

where the points are defined in Figure 7. This corner rule is the same as the one developed in Chapter III for the finite difference method at a $3\pi/2$ radian reentrant corner.

When basis polynomials of the form $A_0 + A_1X + A_2Y + A_3XY + A_4X^2 + A_5Y^2$ and regular isosceles elements with nodes added at the midpoint of each side were used, the finite element method was equivalent to a finite difference rule of the form

$$U(P) = 4(U(N) + U(E) + U(S) + U(W)) - U(NN) - U(EE) - U(SS) - U(WW)] / 12,$$

except at the reentrant corner. At the corner the rule is

$$U(P) = [8U(S) + 8U(W) + 4U(E) + 4U(N) - 2U(SS) - 2U(WW) - U(EE) - U(NN)] / 18.$$

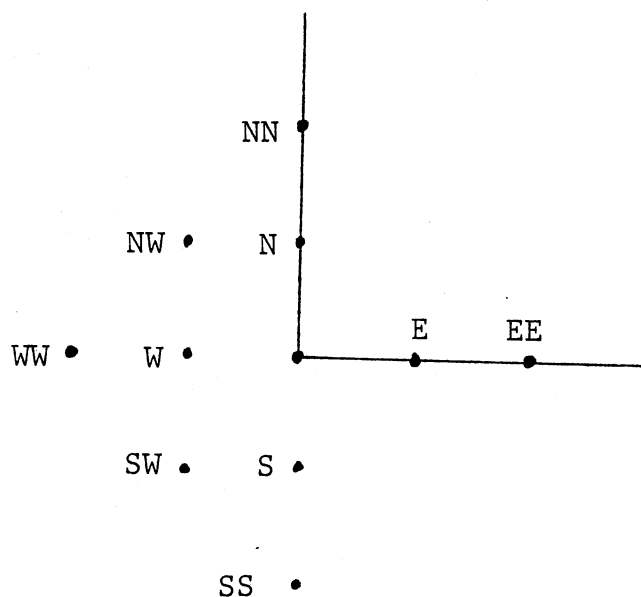


Figure 7. Nodes for the Cross Sheet-Resistor Reentrant Corner

A finite difference solution was found using the 5-point rule with both the normal 5-point rule and the modified 5-point rule at the reentrant corner. The modified rule for the corner was developed in Chapter III and is

$$U(P) = (U(N) + U(E) + 2U(W) + 2U(S)) / 6.$$

Three different reentrant rules were used with the finite difference 9-point rule. The 9-point rule cannot be used directly since it requires a point, $U(NE)$, which lies outside the region. Normally the derivative boundary conditions would allow the point outside the domain to be replaced by its reflection inside the domain. The point $U(NE)$, however, has two such points, $U(SE)$ and $U(NW)$. Thus one corner rule used was the regular 9-point rule with the value of $U(NE)$ replaced by the average of $U(SE)$ and $U(NW)$. The second corner rule used was the regular 5-point rule, and the third corner rule was the 9-point rule modification mentioned in Chapter III,

$$U(P) = [4U(S) + 4U(W) + 2U(E) + 2U(N) + U(NW) + U(SW) + U(SE)] / 15.$$

The problem was solved using a total of seven different methods using grid spacing of $1/6$, $1/12$, $1/24$, $1/48$, and $1/96$, where the cross fits into a one by one square. The results are listed in Table I.

If Richardson's [18] extrapolation is applied to these results, a further error reduction can be made. Also, a check on the order of accuracy can be made by using the three successive approximations and solving for the smallest exponent of h in the error expansion. If h , $h/2$, and $h/4$ were used for grid spacings, and the error term were written as,

$$e_h = V_h - U = f_1 h^\gamma + f_2 h^B + \dots,$$

then by dropping this higher order terms, α could be approximated by,

$$\gamma = \log_2 \left(\frac{V_h - V_{\frac{h}{2}}}{V_{\frac{h}{2}} - V_{\frac{h}{4}}} \right).$$

The estimated error exponents and the results of extrapolating the values from Table I are listed in Table II.

TABLE I
 A SUMMARY OF RESULTS FOR THE CROSS SHEET-RESISTOR PROBLEM
 (ACTUAL ANSWER $\pi/\ln 2 = 4.532360145$)

Basic Rule	Corner Rule	h=1/6	h = 1/12	h = 1/24	h = 1/48	h = 1/96	Error * 10 ⁵ For h = 1/96
5-point	5-point	3.6161322	4.0434452	4.3203311	4.4424094	4.4953464	3701.37
5-point	Modified 5-point	4.7307868	4.5740398	4.5510311	4.5374773	4.5336816	132.15
9-point	5-point	3.5363345	4.0663269	4.3346862	4.4512051	4.4997159	3264.42
9-point	Averaged 9-point	3.5246161	4.0918810	4.3488829	4.4573926	4.5022532	3010.69
9-point	Modified 9-point	4.3718954	4.5137948	4.5310890	4.5321613	4.5323285	3.16
Quadratic Finite Element	Quadratic Finite Element	4.4322917	4.5743166	4.5340915	4.5327211	4.5324234	6.33
Quadratic Finite Element	Modified 9-point	4.8596311	4.5821775	4.5351731	4.5327919	4.5324278	6.77

TABLE II
 EXTRAPOLATION OF THE RESULTS FOR THE CROSS SHEET-RESISTOR

Basic Rule	Corner Rule	Estimated Exponents	Exponents Used	Best Estimate Before Extrapolation	Extrapolated Value	Error * 10 ⁵ Before Extrapolation	Error * 10 ⁵ After Extrapolation
5-point	5-point	1.21	1.333333	4.4953464	4.5301770	3701.37	218.31
		1.44	2.0		4.5326585		29.84
5-point	Modified 5-point	1.84	2.0	4.5336816	4.5324164	132.15	5.63
		4.26	4.0		4.5323802		2.01
9-point	5-point	1.29	1.333333	4.4997159	4.5316342	3264.42	72.59
		2.14	2.0		4.5328889		52.88
9-point	Averaged 9-point	1.29	1.333333	4.5022532	4.5317698	3010.69	59.03
		1.86	2.0		4.5327638		40.37
9-point	Modified 9-point	3.45	4.0	4.5323285	4.5323396	3.16	2.05
Quadratic Finite Element	Quadratic Finite Element	2.2	4.0	4.5324234	4.5324036	6.33	4.35
Quadratic Finite Element	Modified 9-point	3.47	4.0	4.5324278	4.5324035	6.77	4.34

CHAPTER VI

THE TORSION PROBLEM

Another problem involving reentrant corners concerns computing the torsion of a cracked beam with a square cross section, Q . Fix, Galati, and Wakoff [28] describe a simplified version of this problem in terms of the stress function, S , where

$$S_{XX} + S_{YY} = -1 \text{ in } Q,$$

$$S_X(-1/2, Y) = 0, S_X(1/2, Y) = 0, S(X, -1/2) = 0,$$

$$S(X, 1/2) = 0, \text{ and } S(X, 0) = 0 \text{ if } X \leq 0$$

as shown in Figure 8.

By an appeal to symmetry, the problem becomes as shown in Figure 9.

In addition to the stress function S , the stress intensity factor σ_0 is sought. The symbol σ_0 is a measure of the amount of torsion the beam can endure before it fractures, and is given by,

$$\sigma_0 = \lim_{r \rightarrow 0^+} r^{-\frac{1}{2}} (S(r, 0) - S(0, 0)). \quad (6-1)$$

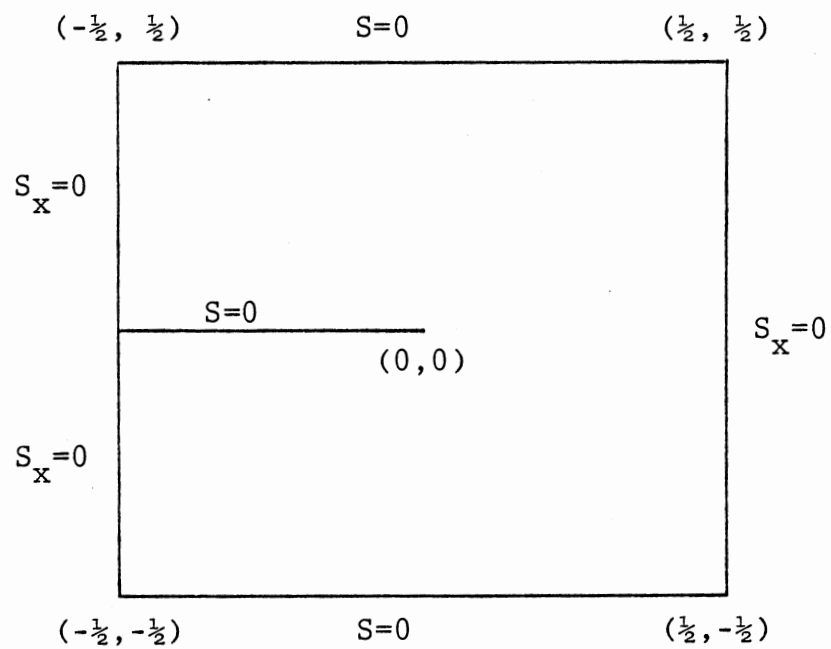


Figure 8. Torsion Problem Geometry

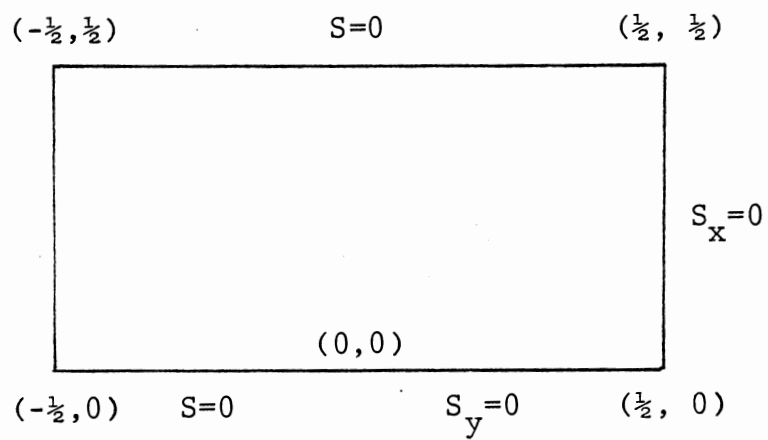


Figure 9. Simplified Torsion Geometry

The problem can be further transformed into a problem involving Laplace's equation by adding the function $Y^2/2$ to $S(X, Y)$. If $U(X, Y) = S(X, Y) + Y^2/2$, then $U_{XX} + U_{YY} = 0$. In terms of the function U the problem now becomes as shown in Figure 10.

To approximate the value of $S(X, Y)$, $Y^2/2$ is subtracted from the approximation of $U(X, Y)$. Using the standard numerical methods for solving Laplace's equation, $U(X, Y)$ can be approximated. However, U has a singularity at $(0, 0)$ which drastically reduces the order of accuracy normally expected from these methods.

The solution at this singularity in polar form is,

$$U(r, \theta) = \sum_{n=0}^{\infty} a_n r^{\frac{2n+1}{2}} \cos \frac{2n+1}{2} \theta, \quad (6-2)$$

where $0 \leq \theta \leq \pi$. If this expansion is applied to each point a distance of h from $(0, 0)$ on cardinal headings, the discretization error which would result from applying the 5-point rule at $(0, 0)$ can be determined.

$$U(P) = 0,$$

$$U(N) = U(h, \frac{\pi}{2}) = a_0 h^{\frac{1}{2}} \cos \frac{\pi}{4} + a_1 h^{\frac{3}{2}} \cos \frac{3\pi}{4} + \dots,$$

$$U(E) = U(h, 0) = a_0 h^{\frac{1}{2}} \cos 0 + a_1 h^{\frac{3}{2}} \cos 0 + \dots,$$

$$U(W) = U(h, \pi) = a_0 h^{\frac{1}{2}} \cos \frac{\pi}{2} + a_1 h^{\frac{3}{2}} \cos \frac{3\pi}{2} + \dots,$$

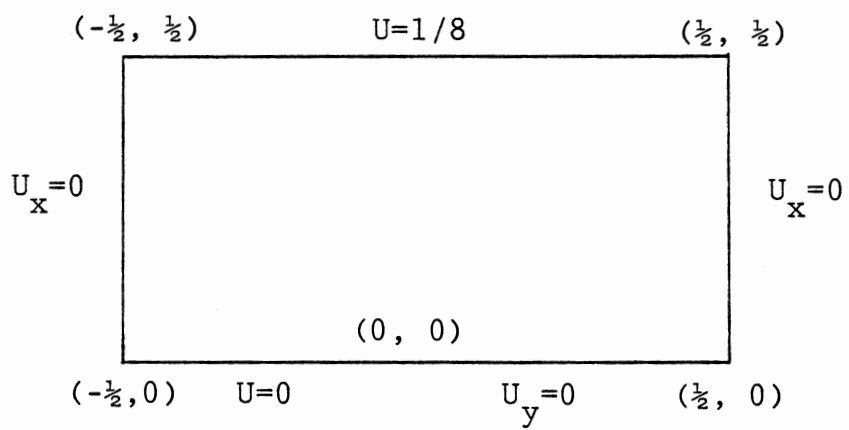


Figure 10. Transformed Torsion Problem

$$U(S) = U(N) \text{ (by symmetry).}$$

Thus the 5-point rule gives

$$4U(P) - U(N) - U(S) - U(E) - U(W) = \\ -a_0 h^{\frac{1}{2}} (1 + \sqrt{2}) - a_1 h^{\frac{3}{2}} (1 - \sqrt{2}) + \dots$$

This $h^{\frac{1}{2}}$ discretization error at (0,0) is much worse than the h^4 error normally expected.

To reduce the error introduced because of the singularity, new rules must be used in the infected area. The method of substituting a different rule at the singularity cannot be used in this case since the value at the singularity is specified in the boundary conditions. For the cross sheet-resistor problem, the value at the singular point had to be determined, so a modified rule was used at the singularity. For this problem, different rules need to be developed for points neighboring the singularity, especially points B and D in Figure 11.

In applying Taylor's expansion to points B and D, the singular point P was used. For example in developing the 5-point rule at point B, the following expansion was used,

$$U(X, Y-h) = U(X,Y) - hU_y(X,Y) + \dots \quad (6-3)$$

However, this Taylor's series expansion is invalid since the point $U(X, Y-h)$ represents the function value at the singularity. Thus to obtain a more accurate method, a rule

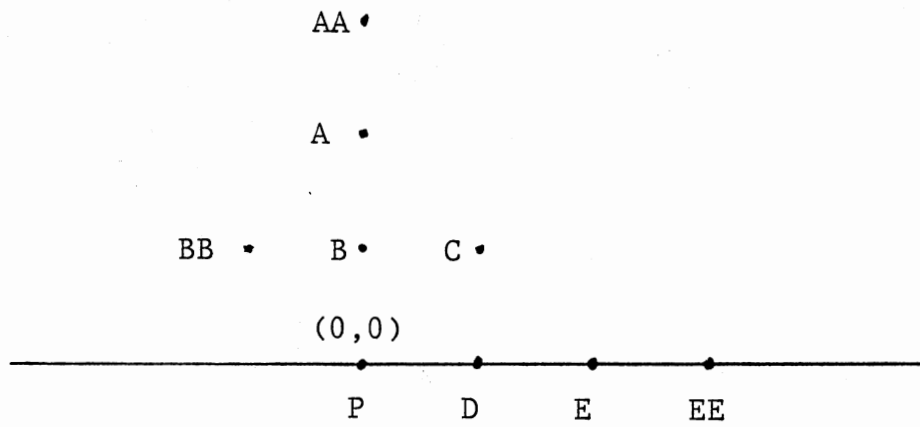


Figure 11. Nodes for the Torsion Reentrant Corner

which uses the form of the singularity could be developed for points B and D. As an example consider a rule for the point B of the form,

$$U(B) = K_A U(A) + K_D U(D). \quad (6-4)$$

To find K_A and K_D , the series expansion for the singularity is used to express $U(A)$, $U(B)$, and $U(D)$ in powers of h .

$$U(B) = U(h, \frac{\pi}{2}) = a_0 h^{\frac{1}{2}} \cdot \frac{\sqrt{2}}{2} - a_1 h^{\frac{3}{2}} \frac{\sqrt{2}}{2} + \dots,$$

$$U(A) = U(2h, \frac{\pi}{2}) = a_0 (2h)^{\frac{1}{2}} \cdot \frac{\sqrt{2}}{2} - a_1 (2h)^{\frac{3}{2}} \frac{\sqrt{2}}{2} + \dots,$$

$$U(D) = U(h, 0) = a_0 h^{\frac{1}{2}} + a_1 h^{\frac{3}{2}} + \dots$$

After these series are substituted into equation (6-4), the

$h^{\frac{1}{2}}$ and $h^{\frac{3}{2}}$ terms will be eliminated if

$$\frac{\sqrt{2}}{2} = K_A + K_D, \text{ and}$$

$$-\frac{\sqrt{2}}{2} = -2K_A + K_D.$$

Thus, $K_A = \sqrt{2}/3$ and $K_D = \sqrt{2}/6$. Therefore at point B the 5-point rule is replaced by

$$U(B) = (\sqrt{2}/6) (2U(A) + U(D)). \quad (6-5)$$

Similarly the 5-point rule at point D could be replaced by

$$U(D) = (\sqrt{2}/3) (U(B) + U(E)). \quad (6-6)$$

Another approach is to avoid the singularity by using Taylor series expansions for $U(A)$ and $U(AA)$ to estimate $U_{YY}(B)$ and expansions for $U(E)$ and $U(EE)$ to estimate $U_{XX}(D)$. Using this strategy, the rules at B and D are

$$U(B) = U(BB) + U(C) - 2U(A) + U(AA) \quad \text{and} \quad (6-7)$$

$$U(D) = 2U(C) - 2U(E) + U(EE). \quad (6-8)$$

The solutions obtained by these methods can be compared to the solutions obtained by Fix, Galati, and Wakoff as described in reference [28]. They use four different finite element methods with singular functions added to the basis elements for their first three methods.

Their first method, FGW1, uses square elements and bilinear basis polynomials of the form $a + bx + cy + dxy$.

Their second method, FGW2, uses square elements and bicubic basis polynomials $\sum_{i=0}^3 \sum_{j=0}^3 a_{ij} x^i y^j$. This method requires only the function to be continuous between elements.

Their third method, FGW3, is the same as the second with the added condition that the derivative of the function is required to be continuous at all interfaces except the vertical line passing through the singularity.

Their fourth method, FGW4, uses triangular elements with piecewise linear functions and mesh refinement in the area of the singularity. This is the only method for which

singular elements were not added to the basis elements.

They also solved the problem using the first three methods without adding singular elements to the basis, but these results are far inferior and are not reported here.

Although no analytic solution is known for this problem, Fix, Galati, and Wakoff use a quintic spline finite element method with six singular functions to obtain a value with which to compare the accuracy of these various methods. They report the value of the function $S(X,Y)$ at the points $(0, 1/24)$, $(-11/24, 1/4)$, and $(11/24, 1/4)$ as well as the value of the stress intensity factor σ_0 . Table III compares their results with the results obtained with the various finite difference methods developed here.

As these results indicate, the modification of the 5-point rule at points B and D give the best results for the finite difference methods. The result obtained by ignoring the singularity and not involving the value of the solution at the singularity was worse than the normal 5-point rule results. This modification also required the approximation equation to be solved explicitly, since the system diverged using iteration. The other modifications to the finite difference method converged using standard iteration methods.

TABLE III
A COMPARISON OF RESULTS FOR THE TORSION PROBLEM

Method	h	σ_0 [.1917]	Error ₄ *10	(0,1/24) [.027425]	Error ₆ *10	$(-\frac{11}{24}, \frac{1}{4})$ [.032877]	Error ₆ *10	$(\frac{11}{24}, \frac{1}{4})$ [.070844]	Error ₆ *10
Ignore Singularity	1/24	.2441	(524.)	.032968	(5543.)	.033182	(305.)	.072577	(1733.)
5-point	1/24	.1523	(394.)	.024912	(2513.)	.032780	(97.)	.070334	(510.)
5-point modified at B & D	1/24	.1886	(31.)	.027425	(<1.)	.032887	(10.)	.070861	(17.)
5-point modified at B,C & D	1/24	.1871	(46.)	.027226	(199.)	.032878	(1.)	.070842	(2.)
FGW1	1/12	.1918	(1.)	.027424	(1.)	.032877	(<1.)	.070844	(<1.)
FGW2	1/10	.1916	(1.)	.027424	(1.)	.032877	(<1.)	.070844	(<1.)
FGW3	1/30	.1877	(40.)	.027289	(136.)	.032903	(26.)	.070780	(64.)
FGW4	1/24	.1072	(845.)	.022079	(5346.)	.032696	(181.)	.068523	(2321.)

CHAPTER VII

CONCLUSIONS

Singularities in the form of reentrant corners can pose grave problems for traditional finite difference and finite element methods. The errors caused by these singularities are not confined to the area around the corners but also pollute the entire region. Increasing the order of the finite difference method has little effect on the error unless special provision is made for dealing with the singularity. However, after the form of the singularity has been determined using elementary differential equation theory, modifications to the finite difference method in the area of the reentrant corner can be made which will restore the order of accuracy expected from the original method.

Richardson extrapolation provides an effective means to further improve the accuracy of the results of these methods. However, the form of the error resulting from these methods must be derived before Richardson's extrapolation method is attempted.

In general, the finite element method was more effective for problems with reentrant corners than the finite difference method if the singularity was ignored. However, after modifying the finite difference method to account for

the singularity, the two methods gave similar results.

Further research could be done to improve the accuracy for both sample problems. For the cross sheet resistor, both the second application of Richardson extrapolation for the modified 5-point rule and the first application for the modified 9-point rule gave relatively little improvement in accuracy. This may have been caused by not treating the reentrant corner at point Q as shown in Figure 12. This point was ignored because of the symmetry involved, but may have had an influence in the higher orders of the error term.

Further research could also be done to develop a higher order finite difference method to solve the torsion problem. A modification at the singularity which was compatible with the 9-point rule might give results much superior to the modification of the 5-point rule discussed in this thesis.

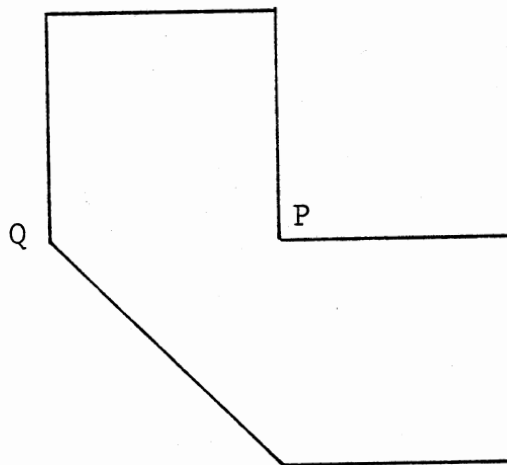


Figure 12. Reentrant corners for the Cross Sheet-Resistor

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APPENDICES

APPENDIX A

AN OVERVIEW OF RELAXATION METHODS

In order to use a relaxation method, the equation formed at each point is used to express the function value at the point in terms of other neighboring points. Thus for interior points using the 5-point rule,

$$V(P) = (V(N) + V(S) + V(E) + V(W)) / 4.$$

To begin the iteration process an initial guess is made for the function at each point to be solved. Then, using the approximating functions, the values are iteratively redefined until the values change less than a specified amount. For the Jacobi method, the current iteration and the previous iteration are stored in separate arrays. The new values are obtained from the values of the previous iteration. Using subscripts for the iteration number, K , the Jacobi method applied to the 5-point rule is:

$$V_{K+1}(P) = (V_K(N) + V_K(S) + V_K(E) + V_K(W)) / 4.$$

The Gauss-Seidel method is similar except that old values are immediately updated so that only one set of values needs to be stored at a time. Thus if the values were computed from top to bottom and from left to right, the Gauss-Seidel method would give:

$$V_{K+1}(P) = (V_{K+1}(N) + V_K(S) + V_K(E) + V_{K+1}(W)) / 4.$$

The successive overrelaxation method (SOR) modifies the Gauss-Seidel method by using a parameter, W , to accelerate the convergence process. This is done by first calculating

the Gauss-Seidel iterate, V_{k+1}^* , then moving the value further along the indicated direction of change. The formula used to do this is:

$$V_{K+1}(P) = V_K(P) + W (V_{K+1}^*(P) - V_K(P)).$$

The W is known as the relaxation factor and is usually chosen between 0 and 2. Carre', [29], gives a method to compute iteratively an approximation to the optimal W .

Other variations of these relaxation methods include symmetric successive overrelaxation (SSOR) for which an SOR sweep is made through the points followed by another SOR sweep reversing the order the points were relaxed. The unsymmetric SOR (USSOR) method is similar except the relaxation factor on the reverse pass differs from the factor used on the forward pass.

Other variations use both iteration and Gaussian-elimination by directly solving the equations from a line or block of points using the previous iteration values for the surrounding points. These methods are known as line and block relaxation.

APPENDIX B

A DISCUSSION OF THE ORDER OF CONVERGENCE
IN THE FINITE DIFFERENCE METHOD

In Chapter I the solution to Laplace's equation was approximated by solving a set of linear equations of the following type:

$$V(P) = (V(N) + V(S) + V(E) + V(W)) / 4$$

for interior points,

$$V(P) = (V(N) + V(S) + 2 V(E)) / 4$$

for points on the left boundary, and

$$V(P) = (V(N) + V(S) + 2 V(W)) / 4$$

for points on the right boundary. These equations were developed by dropping the error terms from the original equations in the function U . The error terms dropped from the equations in the conversion of U to V were of order h^4 , h^3 , and h^3 respectively. However, when the corresponding equations in V were solved, the final error $(V(X,Y) - U(X,Y))$ was of order h^2 .

To understand how the error term $V-U$ is related to the discretization error in changing from U to V , consider solving the set of linear equations in V by using Jacobi iteration. For starting values consider using the exact values for U at each grid point. The first Jacobi iteration would replace the value at each interior point, $U(P)$, with $(U(N) + U(E) + U(S) + U(W)) / 4$, which is equal to $U(P) + Mh^4$. Thus unless M is zero, we have moved away from the desired solution U toward the solution V . Similarly an

error of the form Mh^3 would be introduced at the boundary points where the normal derivative was specified. To observe what happens at subsequent iterations, let ϵ_p be the truncation error at point P. ϵ_p will have the form Mh^4 . At the second iteration the value at point P ($U_p + \epsilon_p$) would be replaced by $(U_N + \epsilon_N + U_E + \epsilon_E + U_S + \epsilon_S + U_W + \epsilon_W) / 4$, which equals $U_p + \epsilon_p + (\epsilon_N + \epsilon_E + \epsilon_S + \epsilon_W) / 4$. On the third iteration the value at P would be:

$$U_p + \epsilon_p + \epsilon_p/4 + (\epsilon_{NE} + \epsilon_{NW} + \epsilon_{SE} + \epsilon_{SW}) / 8 \\ + (\epsilon_{NN} + \epsilon_{EE} + \epsilon_{SS} + \epsilon_{WW}) / 16.$$

Thus the effect of the error at each point spreads to other points at each successive iteration. The error introduced at a single point during a single iteration is divided into fourths and distributed to the four neighboring points during the next iteration. At the following iteration the fourths are divided into sixteenths and again distributed to other neighboring points. Figure 13 follows the distribution of this error throughout the grid. At each iteration step an additional error, ϵ_p , is introduced at point P which is similarly distributed during future iterations. The total error in the system from the error introduced at point P during the first iteration remains in the system until a boundary point with a fixed value is reached. At that iteration, part of the error leaves the system.

The errors introduced at point A find their way to each

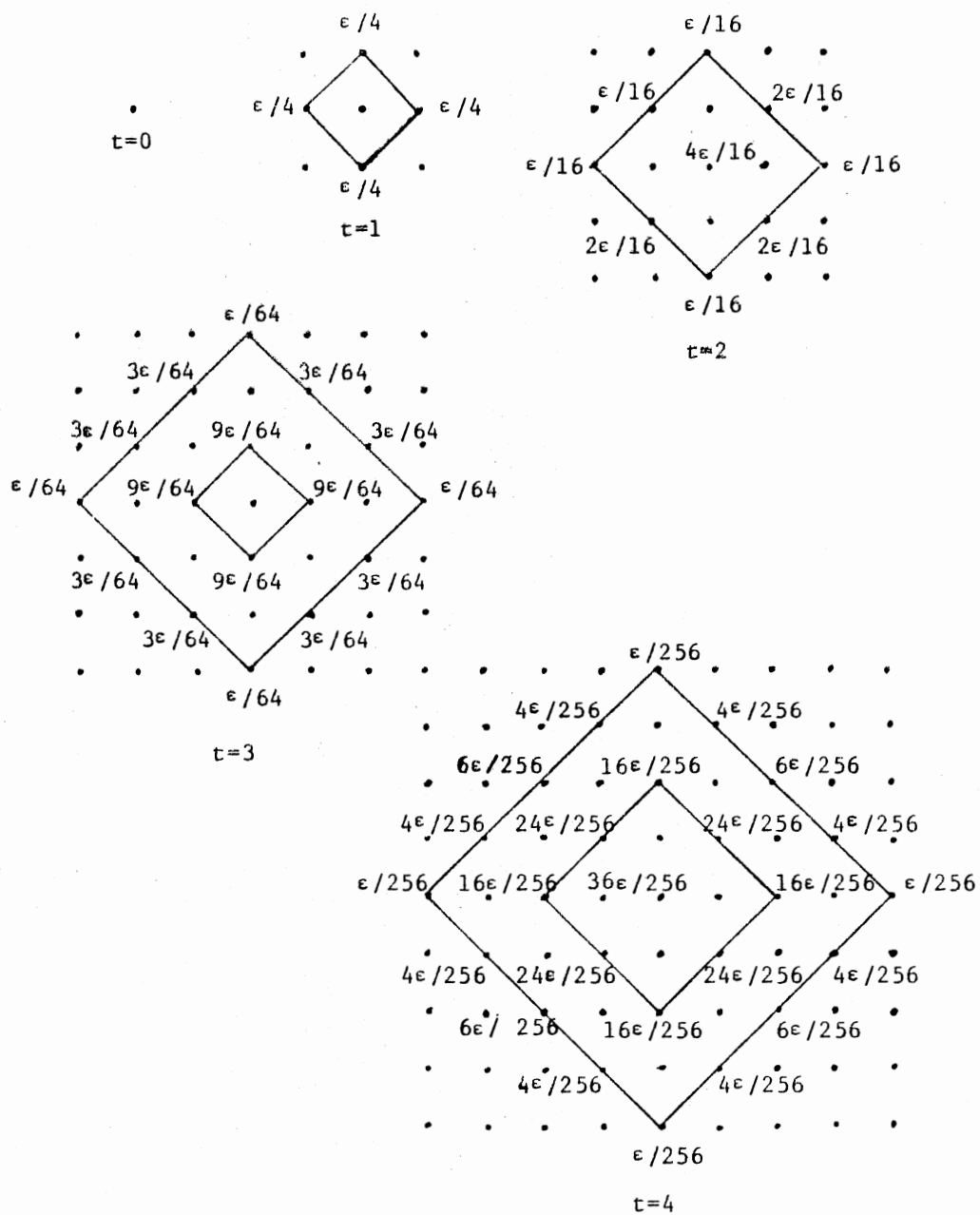


Figure 13. Combinational Pattern of the Error from Time=0 Followed to Time=4

of the points in the grid. The error at point B due to errors introduced at point A is $\epsilon_A \sum_{n=1}^{\infty} 4^{-n} P_{AB}^n$, where P_{AB}^n is

is the number of paths between A and B of length nh . (Paths consist only of horizontal and vertical point-to-point segments within the grid.) For bounded regions, the series will converge. However, the error at any point P when the solution V is attained will be an accumulation of errors from each of the unknown points in the grid. The total error at point P will be a sum of approximately n^2 errors from the interior points plus approximately $2n$ errors from unspecified boundary points. These n^2 errors of order h^4 plus $2n$ errors of order h^3 gives a total error term of order h^2 . (n is approximately $1/h$.)

From the above discussion it can be seen that if only one point had a discretization error of order h , that error would pollute every point in the grid and lower the accuracy at each point to order h .

2

VITA

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