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Techniques of Water-Resources Investigations
of the United States Geological Survey

Chapter A1

A MODULAR THREE-DIMENSIONAL FINITE-DIFFERENCE GROUND-WATER FLOW MODEL

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Book 6

MODELING TECHNIQUES

CHAPTER 12

STRONGLY IMPLICIT PROCEDURE PACKAGE

Conceptualization and Implementation

General Theory

The discussion of the Strongly Implicit Procedure (SIP) presented here utilizes certain general concepts of matrix algebra and numerical analysis which may be reviewed in any standard reference, including those noted earlier by Peaceman (1977), Crichlow (1977) or Remson, Hornberger and Molz (1971). In addition to general background material, these three references provide descriptions of the Strongly Implicit Procedure itself which may be consulted to supplement the discussion presented here.

SIP is a method for solving a large system of simultaneous linear equations by iteration. The finite difference equation for a single cell, i,j,k, was shown in Chapter 2 to be of the form

$$\begin{aligned} &CV_{i,j,k-1/2}h_{i,j,k-1} + CC_{i-1/2,j,k}h_{i-1,j,k} + CR_{i,j-1/2,k}h_{i,j-1,} \\ &+ (-CV_{i,j,k-1/2} - CC_{i-1/2,j,k} - CR_{i,j-1/2,k} \\ &- CR_{i,j+1/2,k} - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k})h_{i,j,k} \\ &+ CR_{i,j+1/2,k}h_{i,j+1,k} + CC_{i+1/2,j,k}h_{i+1,j,k} \\ &+ CV_{i,j,k+1/2}h_{i,j,k+1} = RHS_{i,j,k}. \end{aligned} \tag{79}$$

One equation of this form is written for each cell in the finite-difference grid, expressing the relationship among the heads at node i,j,k, and at each of the six adjacent nodes at the end of a time step. Because each equation may involve up to seven unknown values of head, and because the set of unknown head values changes from one equation to the next through the grid, the equations for the entire grid must be solved simultaneously at each time step. The solution consists of one value of head for each node, for the end of the step.

The discussion of the SIP procedure presented here is based on the notation of Weinstein, Stone and Kwan (1969), the developers of SIP. Using their notation, equation (79) may be written.

$$Z_{i,j,k}h_{i,j,k-1} + B_{i,j,k}h_{i-1,j,k} + D_{i,j,k}h_{i,j-1,k} + E_{i,j,k}h_{i,j,k} + F_{i,j,k}h_{i,j+1,k} + H_{i,j,k}h_{i+1,j,k} + S_{i,j,k}h_{i,j,k+1} = Q_{i,j,k}. \quad (80)$$

The coefficients in equation (80) all are labelled with the index i,j,k to show that they are associated with the equation for node i,j,k. Thus $Z_{i,j,k}$ of equation (80) is equivalent to $CL_{i,j,k-1/2}$ of equation (79); $E_{i,j,k}$ of equation (80) is equivalent to the expression $(-CV_{i,j,k-1/2} - CC_{i-1/2,j,k} - CR_{i,j-1/2k} - CR_{i,j+1/2k} - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k})$ of equation (79); and so on.

As pointed out in Chapter 2, the entire set of equations of the form of (80) can be summarized in matrix form as

$$[A]\{h\} = \{q\} \quad (81)$$

where [A] is the matrix of coefficients of head, {h} is a vector of head values, and {q} is a vector of the right-hand terms of equation (80). Figure 46 shows the elements of the coefficient matrix and of the two vectors for a mesh of three rows, four columns and two layers. Notice that the matrix [A] is sparse--i.e., that there are very few nonzero elements--and that these are all located on just seven diagonals, as indicated in figure 47.

Examination of equations (79) and (80) will show that the term $CL_{i,j,k-1/2}$ of equation (79) appears both as the coefficient Z in equation (80) for node i,j,k, and as the coefficient S in the corresponding equation for node i,j,k-1, that is

$$Z_{i,j,k} = S_{i,j,k-1} \quad (82)$$

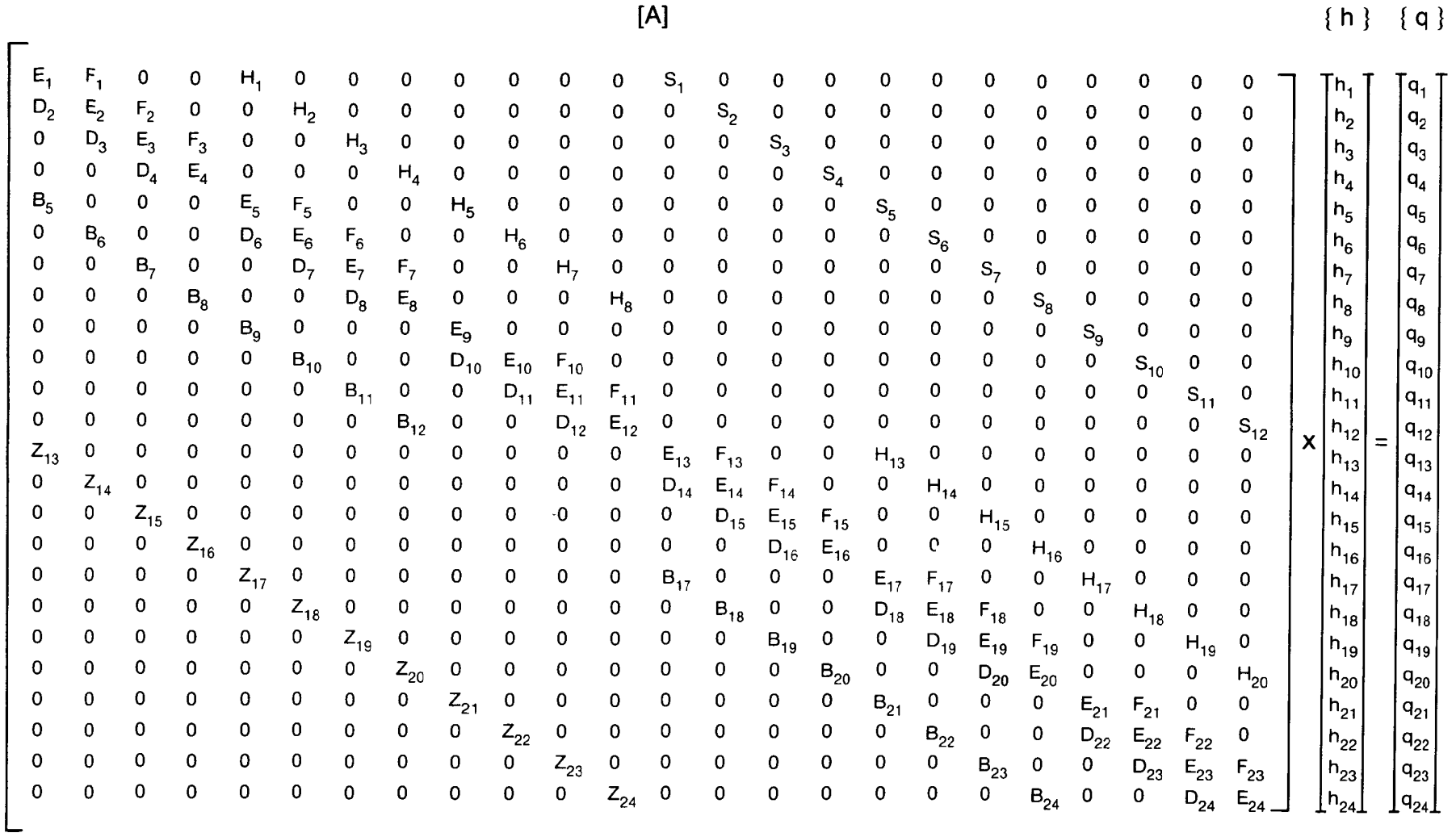
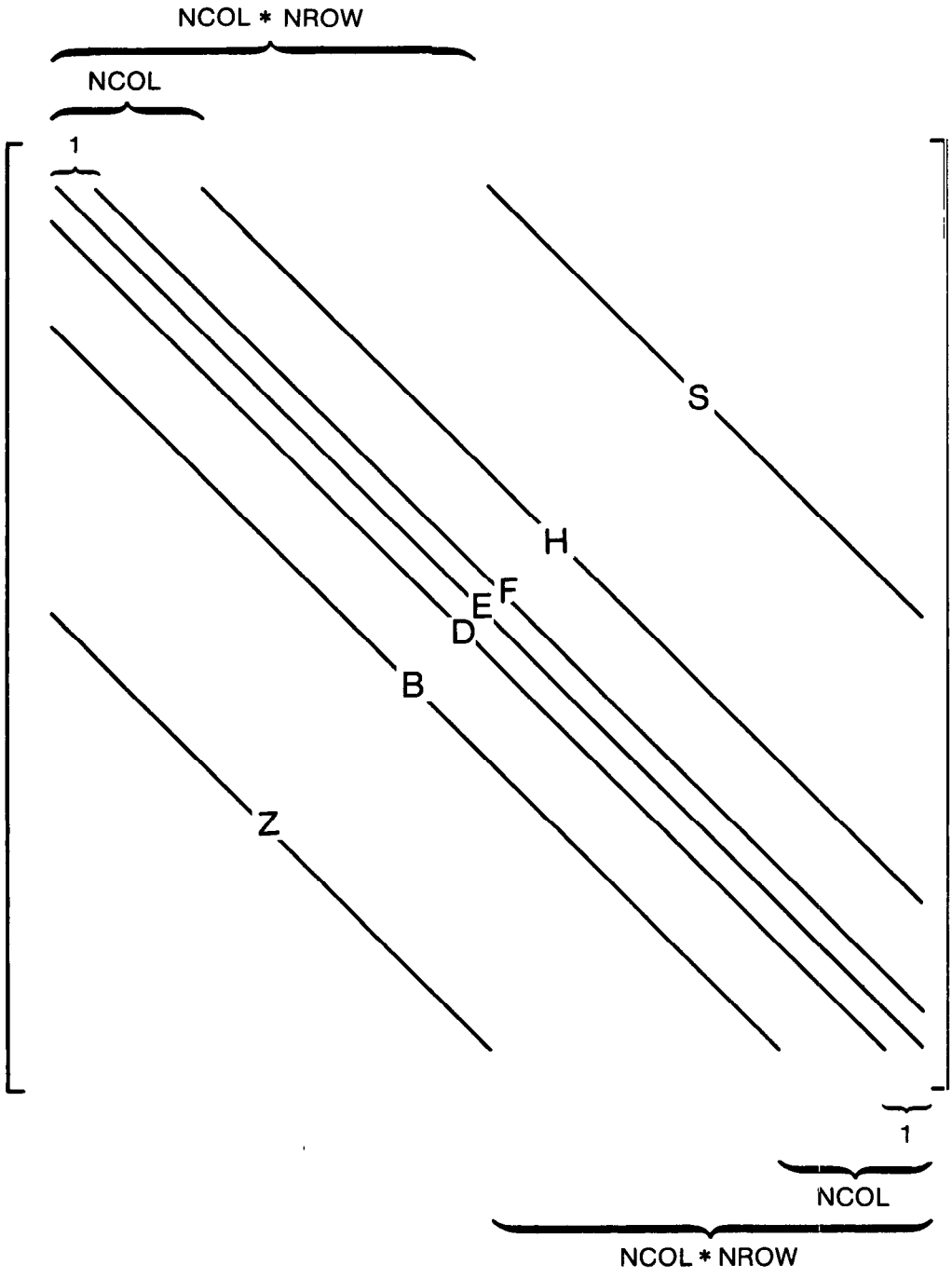


Figure 46.—Correspondence between the finite-difference equations and the matrix equation for a grid of three rows, four columns, and two layers.



Brackets indicate horizontal spacing, in matrix columns, between nonzero diagonals (e.g., diagonals E and F are adjacent).

Figure 47.—Structure of coefficient matrix showing nonzero diagonals.

Similarly,

$$B_{i,j,k} = H_{i-1,j,k} \tag{83}$$

and

$$D_{i,j,k} = F_{i,j-1,k}. \tag{84}$$

Replacing each Z, B, and D coefficient in the matrix of Figure 46 with the equivalent S, H, or F element, as defined by equations (82) - (84), yields the matrix of Figure 48, which is readily seen to be symmetric. Thus the coefficient matrix [A] of equation (81) is symmetric as well as sparse.

A system of equations of the form of (81) can be solved by direct methods if [A] can be factored into two matrices [L*] and [U*], such that [L*] is in lower triangular form (all nonzero elements are on or below the main diagonal), while [U*] is in upper triagular form (all nonzero elements are on or above the main diagonal), and all elements on the main diagonal of [U*] are equal to one. Figure (49) illustrates the characteristics of [L*] and [U*] relative to [A] for a 3 x 3 matrix [A]. Once this factoring has been accomplished, a technique known as "backward and forward substitution" can be used to complete the solution. However, a difficulty arises in that, even though [A] is a sparse matrix, [L*] and [U*] are generally not sparse, and a great deal of computer memory and time may be needed to calculate all of their nonzero elements. In addition, round-off errors may become unacceptably large.

The Strongly Implicit Procedure seeks to find a matrix [B] such that the sum matrix [A + B] can be factored easily into two matrices [L] and [U], where [A + B], [L], and [U] meet the following conditions:

(1) [A + B] is "close" to [A];

(2) [L] is in lower triangular form while [U] is in upper triangular form, and all entries along the main diagonal of [U] are equal to unity;

$E_{1,1,1}$	$F_{1,1,1}$	0	$H_{1,1,1}$	0	0	$S_{1,1,1}$	0	0	0	0	0
$F_{1,1,1}$	$E_{1,2,1}$	$F_{1,2,1}$	0	$H_{1,2,1}$	0	0	$S_{1,2,1}$	0	0	0	0
0	$F_{1,2,1}$	$E_{1,3,1}$	0	0	$H_{1,3,1}$	0	0	$S_{1,3,1}$	0	0	0
$H_{1,1,1}$	0	0	$E_{2,1,1}$	$F_{2,1,1}$	0	0	0	0	$S_{2,1,1}$	0	0
0	$H_{1,2,1}$	0	$F_{2,1,1}$	$E_{2,2,1}$	$F_{2,2,1}$	0	0	0	0	$S_{2,2,1}$	0
0	0	$H_{1,3,1}$	0	$F_{2,2,1}$	$E_{2,3,1}$	0	0	0	0	0	$S_{2,3,1}$
$S_{1,1,1}$	0	0	0	0	0	$E_{1,1,2}$	$F_{1,1,2}$	0	$H_{1,1,2}$	0	0
0	$S_{1,2,1}$	0	0	0	0	$F_{1,1,2}$	$E_{1,2,2}$	$F_{1,2,2}$	0	$H_{1,2,2}$	0
0	0	$S_{1,3,1}$	0	0	0	0	$F_{1,2,2}$	$E_{1,3,2}$	0	0	$H_{1,3,2}$
0	0	0	$S_{2,1,1}$	0	0	$H_{1,1,2}$	0	0	$E_{2,1,2}$	$F_{2,1,2}$	0
0	0	0	0	$S_{2,2,1}$	0	0	$H_{1,2,2}$	0	$F_{2,1,2}$	$E_{2,2,2}$	$F_{2,2,2}$
0	0	0	0	0	$S_{2,3,1}$	0	0	$H_{1,3,2}$	0	$F_{2,2,2}$	$E_{2,3,2}$

Figure 48.—Symmetric coefficient matrix for a grid containing two rows, three columns, and two layers.

$$
\underset{[A]}{\begin{bmatrix} 1 & 2 & 1 \\ -1 & 1 & 2 \\ 3 & 2 & -2 \end{bmatrix}} \underset{\{h\}}{\begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix}} = \underset{\{q\}}{\begin{bmatrix} 1 \\ 2 \\ -3 \end{bmatrix}}
$$

$$
\underset{[L^*]}{\begin{bmatrix} 1 & 0 & 0 \\ -1 & 3 & 0 \\ 3 & -4 & -1 \end{bmatrix}} \underset{[U^*]}{\begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}} \underset{\{h\}}{\begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix}} = \underset{\{q\}}{\begin{bmatrix} 1 \\ 2 \\ -3 \end{bmatrix}}
$$

Figure 49.—Decomposition of a coefficient matrix into lower and upper triangular matrices.

(3) [L] and [U] are both sparse; and

(4) both [L] and [U] have just four nonzero diagonals.

Suppose a matrix [B] is constructed in an attempt to satisfy these conditions; the term [B] {h} can be added to each side of equation (81) to give

$$[A + B]\{h\} = \{q\} + [B]\{h\} \tag{85}$$

A solution vector {h} for equation (85) must also be a solution vector for equation (81). The presence of the vector {h} on both sides of equation (85) presents an immediate difficulty; however, if an iterative approach to the solution is utilized (chapter 2), values of h from the preceding iteration may be used in the head vector on the right. That is, equation (85) may be expressed in the form

$$[A + B]\{h^{\ell}\} = \{q\} + [B]\{h^{\ell-1}\} \tag{86}$$

where $\{h^{\ell}\}$ is a vector of head values from iteration ℓ, and $\{h^{\ell-1}\}$ a vector of head values from iteration ℓ-1. In equation (86), $\{h^{\ell-1}\}$ is actually used as an approximation to $\{h^{\ell}\}$. If the matrix [B] were known, solution of (86) would be straightforward; for according to the properties postulated above, [A + B] could be factored easily into the sparse matrices [L] and [U], allowing the use of forward and backward substitution. Thus the problem of solving equation (86) is equivalent to that of finding an appropriate matrix [B]. In practice, however, the solution is pursued in terms of the matrices [A], [A + B], [L] and [U]. The term $[A + B]\{h^{\ell-1}\}$ is subtracted from each side of (86) to yield

$$[A + B]\{h^{\ell}\} - [A + B]\{h^{\ell-1}\} = \{q\} - [A]\{h^{\ell-1}\} \tag{87}$$

or

$$[A + B]\{h^{\ell} - h^{\ell-1}\} = \{q\} - [A]\{h^{\ell-1}\} \tag{88}$$

In order that the conditions specified above for [L], [U], and [A + B] may be satisified, [A + B] must contain six nonzero diagonals which were not present in [A], as shown in figure 50; the effect of these additional nonzero diagonals is to introduce new terms into the equation for node i,j,k, involving heads at nodes not adjacent to i,j,k. The relationship between the elements of [A + B] and the elements of [L] and [U] is as given in the following equations, where as indicated in figures 50 and 51, a, b, c, and d, refer to elements of [L], e, f, and g, refer to elements of [U] above the main diagonal, and capital letters refer to elements of [A + B].

$$Z'_{i,j,k} = a_{i,j,k} \tag{89-a}$$

$$A'_{i,j,k} = a_{i,j,k}e_{i,j,k-1} \tag{89-b}$$

$$T'_{i,j,k} = a_{i,j,k}f_{i,j,k-1} \tag{89-c}$$

$$B'_{i,j,k} = b_{i,j,k} \tag{89-d}$$

$$C'_{i,j,k} = e_{i-1,j,k}b_{i,j,k} \tag{89-e}$$

$$D'_{i,j,k} = c_{i,j,k} \tag{89-f}$$

$$E'_{i,j,k} = a_{i,j,k}g_{i,j,k-1} + b_{i,j,k}f_{i-1,j,k} + e_{i,j-1,k}c_{i,j,k}+d_{i,j,k} \tag{89-g}$$

$$F'_{i,j,k} = d_{i,j,k}e_{i,j,k} \tag{89-h}$$

$$G'_{i,j,k} = f_{i,j-1,k}c_{i,j,k} \tag{89-i}$$

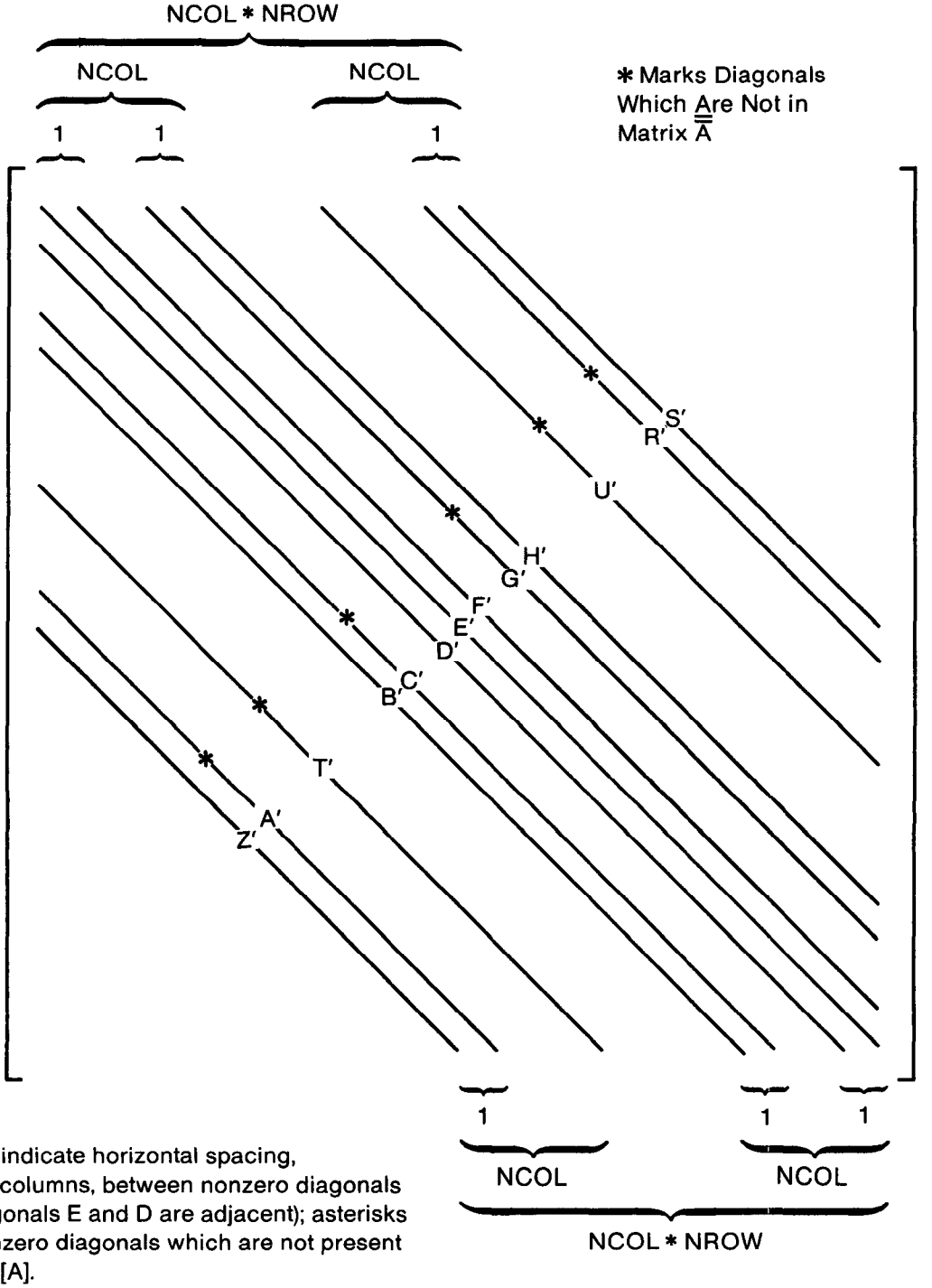
$$H'_{i,j,k} = f_{i,j,k}d_{i,j,k} \tag{89-j}$$

$$U'_{i,j,k} = b_{i,j,k}g_{i-1,j,k} \tag{89-k}$$

$$R'_{i,j,k} = g_{i,j-1,k}c_{i,j,k} \tag{89-l}$$

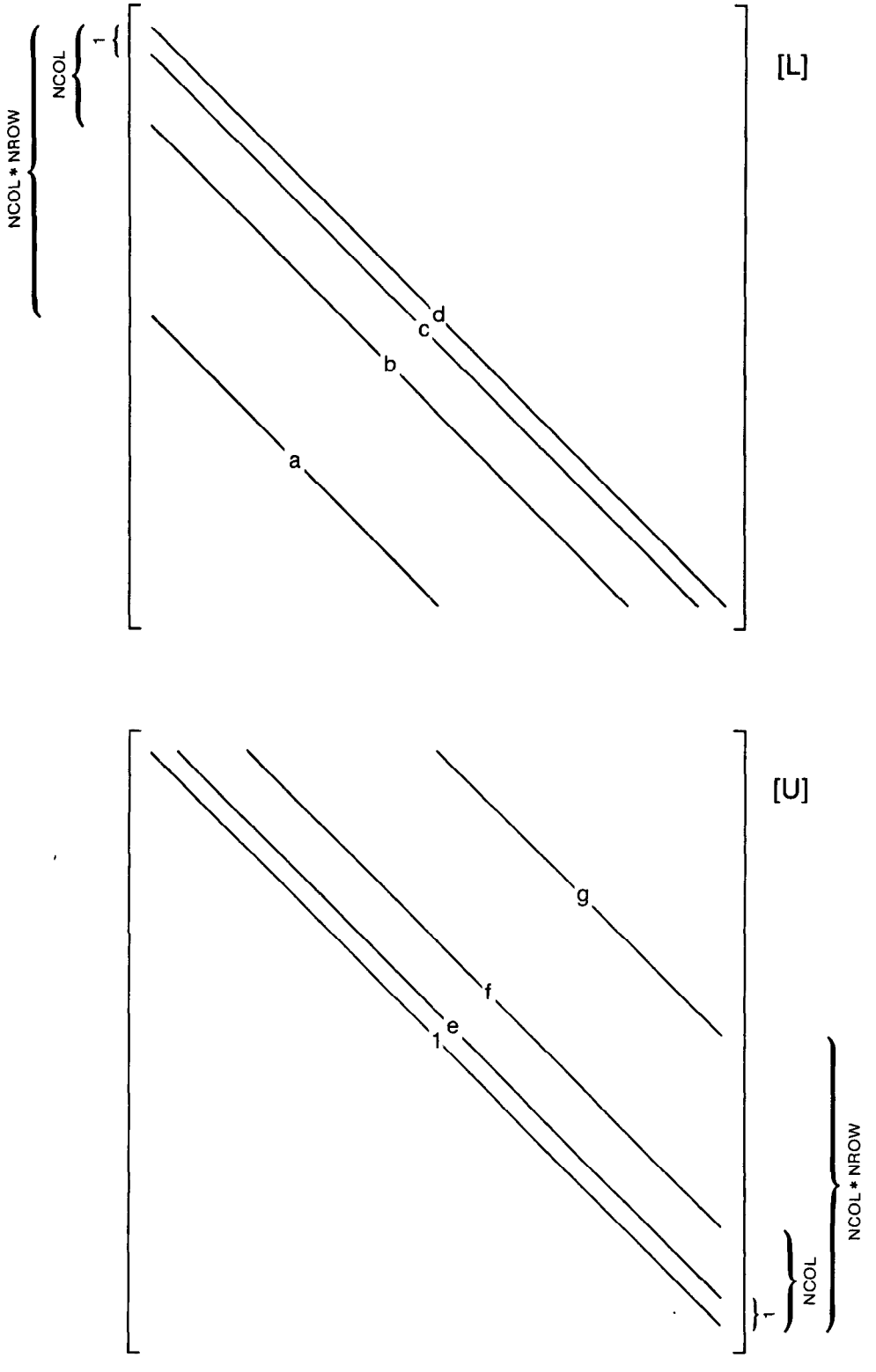
$$S'_{i,j,k} = g_{i,j,k}d_{i,j,k} \tag{89-m}$$

If the subscript of an element in equations (89-a...m) places the element outside of the grid boundary, the element is assumed to be equal to zero. The 13 equations contain 20 unknown values, the elements of [L], [U], and



Brackets indicate horizontal spacing, in matrix columns, between nonzero diagonals (e.g., diagonals E and D are adjacent); asterisks mark nonzero diagonals which are not present in matrix [A].

Figure 50.—Structure of matrix [A+B] showing nonzero diagonals.



Brackets indicate vertical spacing, in matrix rows, between nonzero diagonals (e.g., diagonals d and e are adjacent).

Figure 51.—Structure, showing nonzero diagonals, of the lower triangular factor [L] and the upper triangular factor [U] of matrix [A+B].

[A + B]. This indicates that there are many matrices [B] which can be added to [A] so that the sum can be factored into upper and lower triangular matrices of the form of [L] and [U]. However, the requirement that [A + B] must be "close" to [A], or equivalently that

$$[A + B]\{h\} \approx [A]\{h\} \tag{90}$$

has not yet been used. In terms of the elements of [A + B] {h} and [A] {h} associated with an individual node, i,j,k, equation (90) implies that

$$\begin{aligned}
&Z'_{i,j,k}h_{i,j,k-1} + A'_{i,j,k}h_{i,j+1,k-1} + T'_{i,j,k}h_{i+1,j,k-1} \\
&+ B'_{i,j,k}h_{i-1,j,k} + C'_{i,j,k}h_{i-1,j+1,k} + D'_{i,j,k}h_{i,j-1,k} \\
&+ E'_{i,j,k}h_{i,j,k} + F'_{i,j,k}h_{i,j+1,k} + G'_{i,j,k}h_{i+1,j-1,k} \\
&+ H'_{i,j,k}h_{i+1,j,k} + U'_{i,j,k}h_{i-1,j,k+1} + R'_{i,j,k}h_{i,j-1,k+1} \\
&+ S'_{i,j,k}h_{i,j,k+1} \approx Z_{,j,k}h_{i,j,k-1} + B_{i,j,k}h_{i-1,j,k} \\
&+ D_{i,j,k}h_{i,j-1,k} + E_{i,j,k}h_{i,j,k} + F_{i,j,k}h_{i,j+1,k} + H_{i,j,k}h_{i+1,j,k} \\
&+ S_{i,j,k}h_{i,j,k+1}
\end{aligned} \tag{91}$$

Equation (91) can be rearranged so that the terms from the six nonzero diagonals not present in [A] are all on the right side, while the left side is made up of differences between elements of matrix [A] and corresponding elements of matrix [A + B], i.e.

$$\begin{aligned}
&(Z_{i,j,k}-Z'_{i,j,k})h_{i,j,k-1} + (B_{i,j,k}-B'_{i,j,k})h_{i-1,j,k} \\
&+ (D_{i,j,k}-D'_{i,j,k})h_{i,j-1,k} + (E_{i,j,k}-E'_{i,j,k})h_{i,j,k} \\
&+ (F_{i,j,k}-F'_{i,j,k})h_{i,j+1,k} + (H_{i,j,k}-H'_{i,j,k})h_{i+1,j,k} \\
&+ (S_{i,j,k}-S'_{i,j,k})h_{i,j,k+1} \approx A'_{i,j,k}h_{i,j+1,k-1} \\
&+ T'_{i,j,k}h_{i+1,j,k-1} + C'_{i,j,k}h_{i-1,j+1,k} + G'_{i,j,k}h_{i+1,j-1,k} \\
&+ U'_{i,j,k}h_{i-1,jk+1} + R'_{i,j,k}h_{i,j-1,k+1}
\end{aligned} \tag{92}$$

The terms on the right side of (92), corresponding to the six nonzero diagonals of [A + B] not appearing in [A], are all derived from the matrix B, and all involve the heads at nodes not adjacent to node, i,j,k; by contrast,

the terms on the left side of (92) are derived from both [A] and [B], and involve the heads at i,j,k and the six adjacent nodes.

To reduce the effect of the terms corresponding to nodes not adjacent to i,j,k, three parameters, here termed α, β and γ, and all chosen between zero and one, are introduced as multipliers of the terms on the right side of equation (92). Ultimately, as the solution of the matrix equations ((85) or (86)) is implemented, these multipliers take on the role of iteration parameters. They are brought into equation (92) as follows:

$$(Z_{i,j,k}-Z'_{i,j,k})h_{i,j,k-1} + (B_{i,j,k}-B'_{i,j,k})h_{i-1,j,k}$$
$$+ (D_{i,j,k}-D'_{i,j,k})h_{i,j-1,k} + (E_{i,j,k}-E'_{i,j,k})h_{i,j,k}$$
$$+ (F_{i,j,k}-F'_{i,j,k})h_{i,j+1,k} + (H_{i,j,k}-H'_{i,j,k})h_{i+1,j,k}$$
$$+ (S_{i,j,k}-S'_{i,j,k})h_{i,j,k+1} \approx \alpha A'_{i,j,k}h_{i,j+1,k-1}$$
$$+ \beta T'_{i,j,k}h_{i+1,j,k-1} + \gamma C'_{i,j,k}h_{i-1,j+1,k}$$
$$+ \gamma G'_{i,j,k}h_{i+1,j-1,k} + \beta U'_{i,j,k}h_{i-1,jk+1}$$
$$+ \alpha R'_{i,j,k}h_{i-1,k+1} \qquad (93)$$

Next the heads on right side of (93), corresponding to nodes not adjacent to i,j,k, are expressed in terms of heads at nodes which are adjacent to i,j,k. This is done by noting that, for example, node i, j+1, k-1 lies at the corner of a rectangle, the other three corners of which are: i,j,k-1; i,j+1,k; and i,j,k. Thus using the rules in interpolation illustrated in figure 52, $h_{i,j+1,k-1}$ is given approximately by

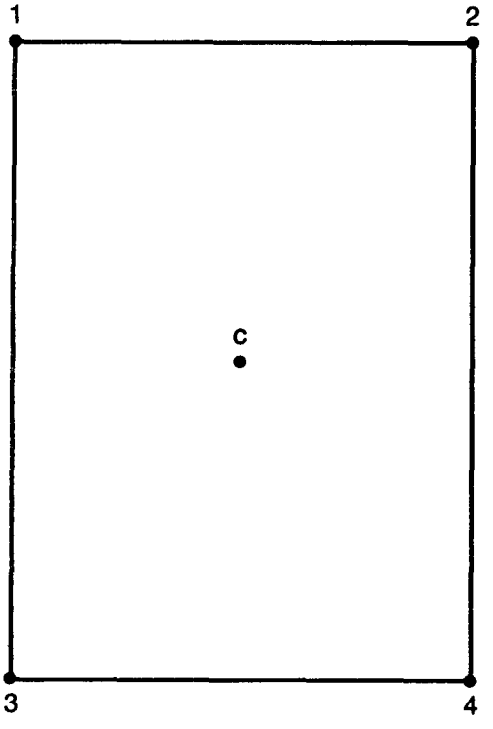
$$h_{i,j+1,k-1} = h_{i,j+1,k} + h_{i,j,k-1} - h_{i,j,k}. \qquad (94\text{-a})$$

Similarly,

$$h_{i+1,j,k-1} = h_{i,j,k-1} + h_{i+1,j,k} - h_{i,j,k} \qquad (94\text{-b})$$

$$h_{i-1,j+1,k} = h_{i-1,j,k} + h_{i,j+1,k} - h_{i,j,k} \qquad (94\text{-c})$$

Suppose the Function f Is Known at 2, 3 and 4.



By interpolation the Function
at the Center Can be Approximated by

$$f_1(c) \approx \frac{f(2) + f(3)}{2}$$

and

$$f_2(c) \approx \frac{f(1) + f(4)}{2}$$

Suppose

$$f_1(c) \approx f_2(c)$$

Then

$$\frac{f(2) + f(3)}{2} \approx \frac{f(1) + f(4)}{2}$$

Therefore

$$f(1) \approx f(2) + f(3) - f(4)$$

Figure 52.—Estimation of a function at one corner of a rectangle in terms of the values of the function at the other three corners.

$$h_{i+1,j-1,k} = h_{i+1,j,k} + h_{i,j-1,k} - h_{i,j,k} \qquad (94\text{-d})$$

$$h_{i-1,j,k+1} = h_{i,j,k+1} + h_{i-1,j,k} - h_{i,j,k} \qquad (94\text{-e})$$

$$h_{i,j-1,k+1} = h_{i,j,k+1} + h_{i,j-1,k} - h_{i,j,k}. \qquad (94\text{-f})$$

Substituting equations (94-a...f) into equation (93) and reorganizing gives

$$\begin{aligned}
&(Z'_{i,j,k} - Z_{i,j,k} + \alpha A'_{i,j,k} + \beta T'_{i,j,k})\, h_{i,j,k-1} \\
&+ (B'_{i,j,k} - B_{i,j,k} + \gamma C'_{i,j,k} + \beta U'_{i,j,k})\, h_{i-1,j,k} \\
&+ (D'_{i,j,k} - D_{i,j,k} + \gamma G'_{i,j,k} + \alpha R'_{i,j,k})\, h_{i,j-1,k} \\
&+ (E'_{i,j,k} - E_{i,j,k} - \alpha A'_{i,j,k} - \beta T'_{i,j,k} - \gamma C'_{i,j,k} \\
&\quad - \gamma G'_{i,j,k} - \beta U'_{i,j,k} - \alpha R'_{i,j,k})\, h_{i,j,k} \\
&+ (F'_{i,j,k} - F_{i,j,k} + \alpha A'_{i,j,k} + \gamma C'_{i,j,k})\, h_{i,j+1,k} \\
&+ (H'_{i,j,k} - H_{i,j,k} + \beta T'_{i,j,k} + \gamma G'_{i,j,k}) h_{i+1,j,k} \\
&+ (S'_{i,j,k} - S_{i,j,k} + \beta U'_{i,j,k} + \alpha R'_{i,j,k}) h_{i,j,k+1} \approx 0 \qquad (95)
\end{aligned}$$

The relation expressed in equation (95) can be satisfied if each coefficient is approximately equal to zero. Setting these coefficients equal to zero yields the equations

$$Z'_{i,j,k} - Z_{i,j,k} + \alpha A'_{i,j,k} + \beta T'_{i,j,k} = 0 \qquad (96\text{-a})$$

$$B'_{i,j,k} - B_{i,j,k} + \gamma C'_{i,j,k} + \beta U'_{i,j,k} = 0 \qquad (96\text{-b})$$

$$D'_{i,j,k} - D_{i,j,k} + \gamma G'_{i,j,k} + \alpha R'_{i,j,k} = 0 \qquad (96\text{-c})$$

$$\begin{aligned}
E'_{i,j,k} - E_{i,j,k} &- \alpha A'_{i,j,k} - \beta T'_{i,j,k} \\
&- \gamma C'_{i,j,k} - \gamma G'_{i,j,k} \\
&- \beta U'_{i,j,k} - \alpha R'_{i,j,k} = 0
\end{aligned} \qquad (96\text{-d})$$

$$F'_{i,j,k} - F_{i,j,k} + \alpha A'_{i,j,k} + \gamma C'_{i,j,k} = 0 \qquad (96\text{-e})$$

$$H'_{i,j,k} - H_{i,j,k} + \beta T'_{i,j,k} + \gamma G'_{i,j,k} = 0 \qquad (96\text{-f})$$

$$S'_{i,j,k} - S_{i,j,k} + \beta U'_{i,j,k} + \alpha R'_{i,j,k} = 0 \qquad (96\text{-g})$$

Equations (96-a...g) and (89-a...m) form a system of 20 equations in 20 unknowns which when solved, will yield the entries of [A + B], [L] and [U] such that [A + B] is "close" to [A], and can be readily factored into

[L] and [U], where [L] and [U] are both sparse and have the required lower triangular and upper triangular forms. For example, substituting equations (89-a, -b, and -c) into equation (96-a) and rearranging yields

$$a_{i,j,k} = Z_{i,j,k}/(1 + \alpha e_{i,j,k-1} + \beta f_{i,j,k-1}). \tag{97-a}$$

Similarly,

$$b_{i,j,k} = B_{i,j,k}/(1 + \gamma e_{i-1,j,k} + \beta g_{i-1,j,k}) \tag{97-b}$$

$$c_{i,j,k} = D_{i,j,k}/(1 + \gamma f_{i,j-1,k} + \alpha g_{i,j-1,k}) \tag{97-c}$$

$$A'_{i,j,k} = a_{i,j,k} e_{i,j,k-1} \tag{97-d}$$

$$C'_{i,j,k} = e_{i-1,j,k} b_{i,j,k} \tag{97-e}$$

$$G'_{i,j,k} = f_{i,j-1,k} c_{i,j,k} \tag{97-f}$$

$$R'_{i,j,k} = g_{i,j-1,k} c_{i,j,k} \tag{97-g}$$

$$T'_{i,j,k} = a_{i,j,k} f_{i,j,k-1} \tag{97-h}$$

$$U'_{i,j,k} = b_{i,j,k} g_{i-1,j,k} \tag{97-i}$$

$$\begin{aligned} d_{i,j,k} = {} & E_{i,j,k} + \alpha A'_{i,j,k} + \beta T'_{i,j,k} \\ & + \gamma C'_{i,j,k} + \gamma G'_{i,j,k} + \beta U'_{i,j,k} \\ & + \alpha R'_{i,j,k} - a_{i,j,k} g_{i,j,k-1} - b_{i,j,k} f_{i-1,j,k} \\ & - e_{i,j-1,k} c_{i,j,k} \end{aligned} \tag{97-j}$$

$$e_{i,j,k} = (F_{i,j,k} - \alpha A'_{i,j,k} - \gamma C'_{i,j,k})/d_{i,j,k} \tag{97-k}$$

$$f_{i,j,k} = (H_{i,j,k} - \beta T'_{i,j,k} - \gamma G'_{i,j,k})/d_{i,j,k} \tag{97-l}$$

$$g_{i,j,k} = (S_{i,j,k} - \alpha R'_{i,j,k} - \beta U'_{i,j,k})/d_{i,j,k} \tag{97-m}$$

Using these relations to provide the elements of [L] and [U], [A + B] may be replaced with the product [L][U] in (88) to yield

$$[L][U] \{h^{\ell} - h^{\ell-1}\} = \{q\} - [A] \{h^{\ell-1}\} \tag{98}$$

where again the superscript ℓ refers to the current iteration level, and ℓ-1 to the preceding iteration level. We next define the vector $\{RES^{\ell}\}$ by

$$\{RES^{\ell}\} = \{q\} - [A]\{h^{\ell-1}\} \quad (99)$$

Using this notation equation (98) can be written

$$[L][U]\{h^{\ell}-h^{\ell-1}\} = \{RES^{\ell}\} \quad (100)$$

Equation (100) can now be solved by a process of forward and backward substitution. The first step involves forward substitution to solve for the vector $\{v\}$ in the equation

$$[L]\{v\} = \{RES^{\ell}\} \quad (101)$$

where $\{v\} = [U]\{h^{\ell}-h^{\ell-1}\}$. The vector $\{v\}$ determined in this way is then ultilized in a process of back substitution to solve for the vector $\{h^{\ell}-h^{\ell-1}\}$ in the equation

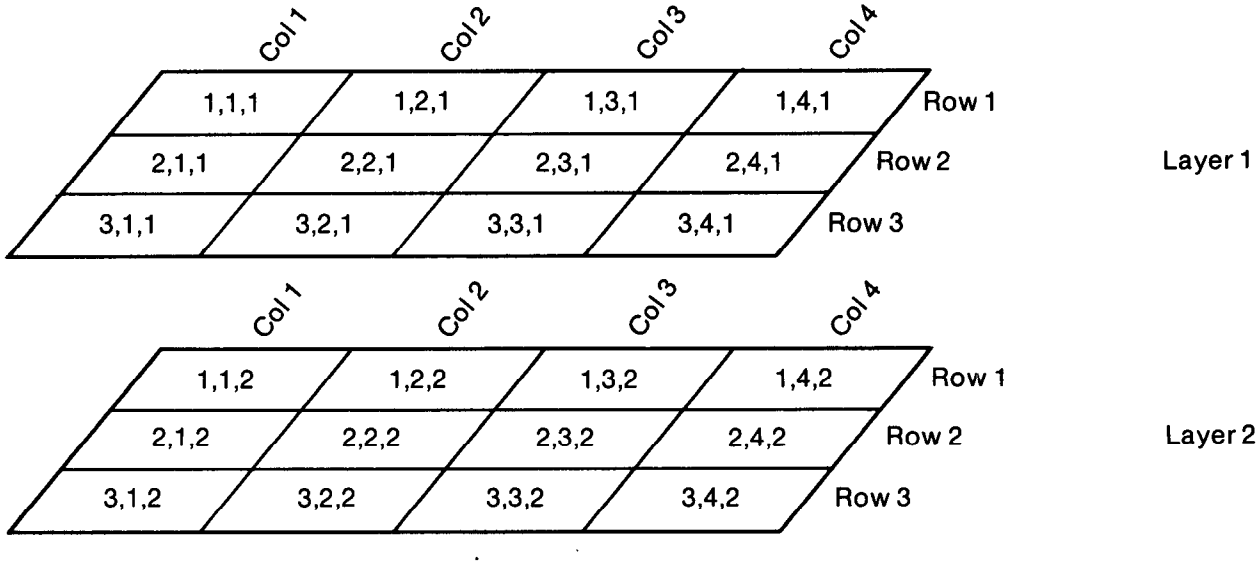
$$[U]\{h^{\ell}-h^{\ell-1}\} = \{v\} \quad (102)$$

In earlier discussions, the coefficients of the equations and hence the elements of the matrices were identified by the indices of the cells, as shown in figure 53-a. To illustrate the process of forward substitution, used to calculate the elements of the vector $\{v\}$, it is convenient to renumber the equations sequentially using a single index, as shown in figure 53-b. Because all elements in [L] above the main diagonal are zero, the first linear equation represented by matrix equation (101) is

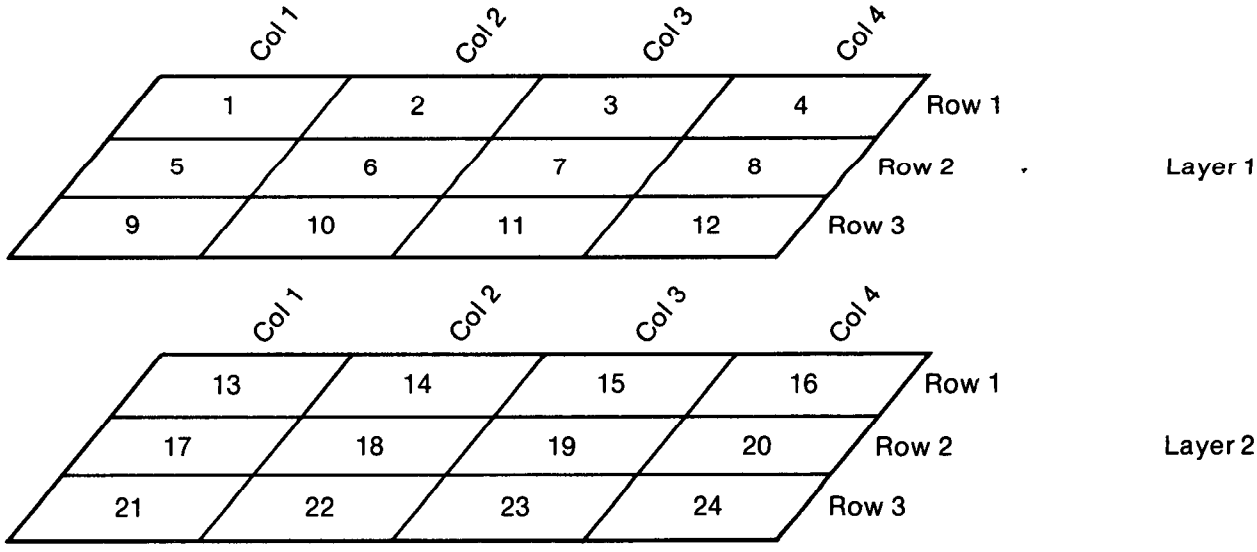
$$d_1 v_1 = RES_1^{\ell} \quad (103)$$

In equation (103), the term d_1 has been determined through equation (97-j), and RES_1^{ℓ} has been calculated through equation (99) as an element of the vector (RES^{ℓ}); thus (103) can be solved immediately for the value of v_1. The second equation represented by matrix equation (101) is

$$c_2 v_1 + d_2 v_2 = RES_2^{\ell} \quad (104)$$



(a) Cell Numbering With 3 Indices



(b) Cell Numbering With 1 Index

Figure 53.—Cell numbering schemes for a grid using three indices and using one index.

Again, c_2 and d_2 are known from equations (97), and RES_2^{ℓ} is known from equation (99); using the value of v_1 from the solution of equation (103), (104) can be solved for v_2.

The general equation for an element of $\{v\}$ has the form

$$v_n = (RES_n^{\ell} - a_n v_{n-NRC} - b_n v_{n-NCOL} - c_n v_{n-1})/d_n \qquad (105)$$

where NRC is the number of cells in the layer, NCOL is the number of columns in the model, the coefficeints a_n, b_n, c_n and d_n are all determined through equations (97) and RES_n^{ℓ} is determined through equation (99). The terms a_n and b_n are zero for the first and second eqations ((103) and (104)); and each equation involves elements of $\{v\}$ determined earlier in the sequence. This procedure of forward substitution, in which the elements of $\{v\}$ are determined in sequence, is possible because of the lower triangular form of the matrix [L]--i.e., because [L] has only zeros to the right of the main diagonal.

Back substitution is next used to calculate the elements of the vector $\{h^{\ell} - h^{\ell-1}\}$ from the elements of $\{v\}$, thus solving equation (102). The process of back substitution is similar to that of forward substitution except that, because the matrix [U] is upper triangular, the order of calculation is reversed. When the vector $\{h^{\ell} - h^{\ell-1}\}$ has been calculated, it is added to the vector $\{h^{\ell-1}\}$ to obtain $\{h^{\ell}\}$, the vector of head values corresponding to iteration ℓ.

In summary, the problem of solving the equation

$$[A]\{h\} = \{q\} \qquad (106)$$

has thus been converted into an iterative process in which: (1) the matrices [L] and [U] are determined using equations (97); (2) the vector $\{RES^{\ell}\}$ is calculated using the vector $\{q\}$, the matrix [A] and heads from the preceding iteration; (3) equation (100) is then solved using forward

and backward substitution to obtain the vector $\{h^{\ell}-h^{\ell-1}\}$; and (4) the vector $\{h^{\ell-1}\}$ is added to the vector $\{h^{\ell}-h^{\ell-1}\}$ to obtain the vector $\{h^{\ell}\}$. However, while these are the essential steps of the SIP procedure, several aspects of the method remain to be discussed.

Transfer of Arrays

As noted previously, the coefficient matrix [A] is sparse, with only seven nonzero diagonals. Rather than passing the entire matrix to the SIP Package, only the nonzero diagonals are needed; and because of symmetry of the matrix, only the main diagonal and the three lower diagonals are needed. The three lower diagonals correspond to the conductance arrays CC, CR, and CV. The main diagonal is formed from the three conductance arrays and the array HCOF described in Chapter 2. The right hand side of the matrix equation, $\{q\}$, corresponds to the array RHS described in Chapter 2. The latest estimate of the head distribution $\{h^{\ell-1}\}$, corresponds to the array HNEW. As new estimates of head are calculated by SIP, they are stored in HNEW replacing the previous estimates. Thus input to SIP consists of the following arrays: CC, CR, CV, RHS, HCOF, and HNEW. Output from SIP consists of a new HNEW array. As explained in Chapter 3, the Formulate Procedure is inside the iteration loop; therefore, the input arrays may be modified at each iteration.

Order of Calculation

Experience has shown that if the finite-difference equations are solved in two different orders on alternate iterations, the number of iterations needed to converge to a solution is reduced. The order assumed in the discussion, to this point, has been to begin at the first column, the first row, and the first layer, and to proceed in ascending column order, ascending row order, and ascending layer order. An alternative is to start at the first column, the last row, and the last layer, and to proceed in ascending column order, descending row order, and descending layer order. Using the same ordering of diagonal names used in figure 51, equations similar to equations (97-a...m) can be developed. They are

$$a_{i,j,k} = Z_{i,j,k}/(1+\alpha e_{i,j,k+1}+\beta f_{i,j,k+1}) \tag{107-a}$$

$$b_{i,j,k} = B_{i,j,k}/(1+\gamma e_{i+1,j,k}+\beta g_{i+1,j,k}) \tag{107-b}$$

$$c_{i,j,k} = D_{i,j,k}/(1+\gamma f_{i,j-1,k}+\alpha g_{i,j-1,k}) \tag{107-c}$$

$$A'_{i,j,k} = a_{i,j,k} e_{i,j,k+1} \tag{107-d}$$

$$C'_{i,j,k} = e_{i+1,j,k} b_{i,j,k} \tag{107-e}$$

$$G'_{i,j,k} = f_{i,j-1,k} c_{i,j,k} \tag{107-f}$$

$$R'_{i,j,k} = g_{i,j-1,k} c_{i,j,k} \tag{107-g}$$

$$T'_{i,j,k} = a_{i,j,k} f_{i,j,k+1} \tag{107-h}$$

$$U'_{i,j,k} = b_{i,j,k} g_{i+1,j,k} \tag{107-i}$$

$$\begin{aligned} d_{i,j,k} = {} & E_{i,j,k} + \alpha A'_{i,j,k} + \beta T'_{i,j,k} \\ & + \gamma C'_{i,j,k} + \gamma G'_{i,j,k} + \beta U'_{i,j,k} \\ & + \alpha R'_{i,j,k} - a_{i,j,k} g_{i,j,k+1} - b_{i,j,k} f_{i+1,j,k} \\ & - e_{i,j-1,k} c_{i,j,k} \end{aligned} \tag{107-j}$$

$$e_{i,j,k} = (F_{i,j,k} - \alpha A'_{i,j,k} - \gamma C'_{i,j,k})/d_{i,j,k} \qquad (107\text{-k})$$

$$f_{i,j,k} = (H_{i,j,k} - \beta T'_{i,j,k} - \gamma G'_{i,j,k})/d_{i,j,k} \qquad (107\text{-l})$$

$$g_{i,j,k} = (S_{i,j,k} - \alpha R'_{i,j,k} - \beta U'_{i,j,k})/d_{i,j,k} \qquad (107\text{-m})$$

In the model described herein, equations (107-a...m) and equations (97-a...m) are in effect invoked alternately in successive iterations. The model program actually uses one general set of equations in which the variables are identified by single indices. The ordering of (97) or of (107) is then achieved through the sequence of values assigned to the indices. In the following list of these general equations, the index nll refers to the cell in the previous layer calculated, but in the same row and column as cell n; the indices nrl and ncl are defined analogously. Also, in these equations, the iteration parameters α, β and γ have each been replaced by a single parameter ω as explained in the following section. Note that one additional equation has been added to the list--the equation for v_n, the element of the vector $\{v\}$ corresponding to cell n. This equation can be added inasmuch as v_n can be calculated as soon as the n^{th} rows of the matrices [L] and [U] have been calculated. The equations are

$$a_n = Z_n/(1 + \omega(e_{nll} + f_{nll})) \qquad (108\text{-a})$$

$$b_n = B_n/(1 + \omega(e_{nrl} + g_{nrl})) \qquad (108\text{-b})$$

$$c_n = D_n/(1 + \omega(f_{ncl} + g_{ncl})) \qquad (108\text{-c})$$

$$A'_n = a_n e_{nll} \qquad (108\text{-d})$$

$$C'_n = b_n e_{nrl} \qquad (108\text{-e})$$

$$G'_n = c_n f_{ncl} \qquad (108\text{-f})$$

$$R'_n = c_n g_{ncl} \qquad (108\text{-g})$$

$$T'_n = a_n f_{nll} \qquad (108\text{-h})$$

$$U'_n = b_n g_{nrl} \qquad (108\text{-i})$$

$$d_n = E_n + \omega(A'_n + T'_n + C'_n + G'_n + U'_n + R'_n) - a_n g_{n11} - b_n f_{nrl} - c_n e_{ncl} \quad (108\text{-j})$$

$$e_n = (F_n - \omega(A'_n + C'_n))/d_n \quad (108\text{-k})$$

$$f_n = (H_n - \omega(T'_n + G'_n))/d_n \quad (108\text{-l})$$

$$g_n = (S_n - \omega(R'_n + U'_n))/d_n \quad (108\text{-m})$$

$$v_n = (RES_n - a_n v_{n11} - b_n v_{nrl} - c_n v_{ncl})/d_n \quad (108\text{-n})$$

Since the backward substitution requires all values of e_n, f_n, g_n, and v_n, space is allocated in the SIP Package for four arrays to store those values. Each of these arrays has as many elements as there are cells in the grid.

Iteration Parameters

While Weinstein, Stone and Kwan (1969) define three iteration parameters in their theoretical development, they utilize a single value in practice. Thus the terms α, β and γ of equation (93) are replaced by a single parameter, ω, which multiplies each term on the right side of the equation; however, ω must be cycled through a series of values in successive iterations to achieve satisfactory rates of convergence. In the model described herein, values of ω are calculated from the expression

$$\omega(\lambda) = 1-(WSEED)^{(\lambda-1)/(NPARM-1)} \qquad \lambda=1,2....NPARM \quad (109)$$

where NPARM is the total number of ω values to be used; λ is an index taking on integral values from 1 to NPARM; $w(\lambda)$ is the corresponding iteration parameter value; and WSEED is the iteration parameter "seed", calculated according to rules outlined below, and used as a basis for determining the sequence of ω values.

The value of WSEED is in turn developed as follows. The terms ρ_1, ρ_2, and ρ_3 are calculated for each cell in the mesh using the conductances between that cell and its neighbors, as follows