Numerische Mathematik 6, 185—199 (1964)

Direct Solution of Partial Difference Equations by Tensor Product Methods

By
ROBERT E. LYNCH, JOHN R. RICE and DONALD H. THOMAS

1. Introduction

The tensor product method was presented in [5] and this paper contains an elaboration of the application of this method to the direct solution of partial difference equations. Since the results reported in [5] were obtained, we have found that EGERVÁRY [12] applied tensor products to the analysis of the five-point approximation of Poisson's equation. His computational scheme is not feasible for large problems.

We describe a method for the direct and explicit solution of the partial difference equations arising from a large class of problems. This class includes all second order separable elliptic partial difference equations. The approach is a natural and classic one. If the problem is separable, then the solution can be expressed in terms of *tensor products* (direct products) of solutions of lower dimensional (and hence much simpler) problems. This implies that the matrices involved in the corresponding partial difference equation can also be expressed in terms of tensor products of lower order matrices. In the simplest cases the difference equations can be written in the form

$$(I \otimes A + B \otimes I)\, u = g \tag{1.1}$$

where A, B and I are matrices and u and g are vectors. If A and B are $n \times n$ matrices then the matrix $I \otimes A + B \otimes I$ is $n^2 \times n^2$. We show how this $n^2 \times n^2$ matrix can be explicitly inverted in terms of the eigenvectors and eigenvalues of the matrices A and B.

It is, of course, no surprise that this can be done. We merely obtain the solution of (1.1) by the analog of the usual method involving the Green's function. The surprise is that this *exact* solution may be evaluated numerically with *fewer* operations than required by the common overrelaxation iterative schemes. There are no numerical instabilities in this evaluation.

This approach also leads to a simple and direct method for the analysis of alternating direction implicit schemes for solving (1.1). This analysis is presented elsewhere [6].

Section 2 contains a brief resume of pertinent results concerning tensor products and matrices. In the next section general second order separable partial difference equations are defined, analyzed, and an explicit expression for the solution of boundary value problems is obtained. Finally, it is shown how to efficiently evaluate the explicit form of the solution (one does *not*, as proposed in [12], compute the inverse of the matrix in (1.1) even though this inverse is explicitly available). Several types of possible generalizations are investigated in

Section 4. These include equations of higher order, including the biharmonic, equations with more than two independent variables, and *recursively separable equations*. The latter equations may be solved, by the method of separation of variables, yet the solution is not a sum of tensor products of solutions of one dimensional problems. Section 5 contains a detailed comparison of the effort required to solve Laplace's equation on a square by three methods: i) successive overrelaxation (SOR), ii) tensor product (TP), iii) alternating direction implicit (ADI). It is shown that, for a square with n mesh points in each direction, the number of operations required are, for large n, $14n^3 \log n$, $4n^3$ and $40n^2 \log^2 n$, respectively. That the ADI method is superior to the TP method is to be expected, since the ADI method is an approximate method based on the tensor product form of the solution [5]. Several examples are analyzed in Section 6. The equations considered are the Helmholtz equation, a general second order separable elliptic equation, the biharmonic equation and the three dimensional Helmholtz equation in spherical coordinates. The final section presents a brief indication of the application of the tensor product method to implicit parabolic partial difference equations.

2. Tensor Products and Matrices

Let A and B be matrices of order $K \times L$ and $M \times N$, respectively, and with elements a_{ij}, b_{ij}. The *tensor product (Kronecker product, direct product)* $A \otimes B$ of A and B is the matrix of order $KM \times LN$:* [4, 7]

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \dots & a_{1L}B \\ a_{21}B & a_{22}B & \dots & a_{2L}B \\ \dots & & & \\ a_{K1}B & a_{K2}B & \dots & a_{KL}B \end{pmatrix}. \tag{2.1}$$

Matrix multiplication is indicated by juxtaposition such as AB and the symbol $+$ indicates matrix addition.

We shall, from time to time, consider tensor products with several factors, e.g., $A \otimes B \otimes \cdots \otimes C$. In order to avoid cumbersome notation, we will not, in general, specify the sizes of the matrices involved in tensor products. *It is assumed throughout that the sizes of the various matrices and vectors are compatible with the indicated matrix operations; in particular I denotes the identity matrix of the appropriate order.*

The elementary properties of the tensor product are listed below:

$$\begin{aligned} &(A+C) \otimes B = A \otimes B + C \otimes B, \qquad (A \otimes B)^T = A^T \otimes B^T, \\ &(A \otimes B)\,(C \otimes D) = AC \otimes BD, \qquad (A \otimes B)^{-1} = A^{-1} \otimes B^{-1}. \end{aligned} \tag{2.2}$$

Here A^T and A^{-1} denote the transpose and inverse, respectively, of A.

For the special case $L = N = 1$, the matrices A and B in (2.1) are column vectors. Their tensor product is a KM component column vector.

* In fact the tensor product of A and B can be defined as the tensor C of rank four where $C = \{c_{klmn}\}$ and

$$c_{klmn} = a_{kl} b_{mn};$$

but in this paper we do not use this approach.

If e and f are eigenvectors of A and B with eigenvalues λ and μ, respectively, then $e \otimes f$ is an eigenvector of $A \otimes B$ with eigenvalue $\lambda\mu$.

The *direct sum* $A \oplus B$ of the matrices A and B is defined by

$$A \oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix},$$

and, in general

$$A_1 \oplus A_2 \oplus \cdots \oplus A_k = \begin{pmatrix} A_1 & 0 & \ldots & 0 \\ 0 & A_2 & \ldots & 0 \\ & \ldots & & \\ 0 & 0 & \ldots & A_k \end{pmatrix}. \tag{2.3}$$

A considerable portion of this analysis depends on the diagonalization of matrices. We present a brief resumé of known results concerning the diagonalization of matrices.

1. If the square matrix A has distinct eigenvalues, then there is a non-singular square matrix B such that

$$B^{-1} A B = \Lambda(A), \tag{2.4}$$

where $\Lambda(A)$ is a diagonal matrix of eigenvalues $\lambda_i(A)$ of A.

2. If A is normal ($A^T A = A A^T$) then B of (2.4) can be made unitary ($B B^* = I$ where I is the identity matrix and B^* is the conjugate transpose of B).

3. If A is real symmetric of order $N \times N$ and has N linearly independent eigenvectors, then B of (2.4) can be made real orthogonal ($B^T = B^{-1}$).

4. If A is symmetric positive definite and C is positive semidefinite, then there is a nonsingular matrix B such that

$$\begin{aligned} B^T A B &= I, \\ B^T C B &= \Lambda(A^{-1} C). \end{aligned} \tag{2.5}$$

The solutions of partial difference equations presented in this paper are given in terms of certain eigenvectors and eigenvalues. For some of the common equations, such as the Laplace, Helmholtz, and biharmonic in Cartesian coordinates on a rectangular domain, these quantities are known explicitly. These quantities are also explicitly known for any circulant matrix [7]. For less common partial difference equations (or nonuniformly spaced meshes), one may have to compute these quantities numerically. Even in this case the computations are greatly simplified since the matrices involved are band matrices (i.e., $a_{ij} = 0$ for $|i-j| > m$ for some small value of m). The numerical determination of eigenvalues and eigenvectors is discussed in [9, 11].

3. Second Order Separable Partial Difference Equations

In this section we consider difference equations derived from a partial differential equation of the form*

$$-a_2(x)\, v_{xx} + a_1(x)\, v_x - b_2(y)\, v_{yy} + b_1(y)\, v_y + \big(a_0(x) + b_0(y)\big)\, v = f(x, y), \tag{3.1}$$

* Alternately,

$$-(a_2(x)\, v_x)_x + a_1(x)\, v_x - (b_2(y)\, v_y)_y + b_1(y)\, v_y + (a_0(x) + b_0(y))\, v = f(x, y).$$

with $a_2, b_2 > 0$ on the square

$$R = \{(x, y) |\ 0 \leqq x \leqq 1,\ 0 \leqq y \leqq 1\}.$$

We assume for simplicity that we have Dirichlet type boundary conditions, though the analysis is readily extended to problems with periodic and mixed boundary values. This is done for an example in Section 6.

The difference equations are derived by replacing the differential operators by difference operators. For integers M and N, a mesh of points

$$\{(x_i, y_j) |\ x = ih_x,\ y = jh_y;\ i = 1, 2, \ldots, N;\ j = 1, 2, \ldots, M\},$$

is placed in R. Here $h_x = (N+1)^{-1}$, $h_y = (M+1)^{-1}$. We denote the value $v(x_i, y_j)$ by v_{ij} and similarly for other functions. Let D_{xx}, D_x, D_{yy}, D_y and I denote the difference operators used to approximate the differential operator in (3.1). We obtain the partial difference equation

$$-a_2 D_{xx} u + a_1 D_x u - b_2 D_{yy} u + b_1 D_y u + (a_0 + b_0) I u = f. \tag{3.2}$$

Difference operators which yield partial difference equations approximating (3.1) to order $h_x^2 + h_y^2$ are

$$h_x^2 D_{xx} u\,|_{ij} = u_{i-1,j} - 2u_{ij} + u_{i+1,j}, \tag{3.3}$$

$$2h_x D_x u\,|_{ij} = u_{i+1,j} - u_{i-1,j}, \tag{3.4}$$

and similarly for D_{yy} and D_y. Define the matrices

$$X_k = \{a_k(i\,h_x)\,\delta_{ij}\}, \qquad Y_k = \{b_k(i\,h_y)\,\delta_{ij}\},\ k = 0, 1, 2.$$

The equation (3.2) is then

$$\left\{\frac{1}{h_x^2}\left[-X_2 D_{xx} + h_x X_1 D_x + h_x^2 X_0\right] + \frac{1}{h_y^2}\left[-Y_2 D_{yy} + h_y Y_1 D_y + h_y^2 Y_0\right]\right\} u = g, \tag{3.5}$$

where the matrices D_{xx}, etc., are identified with difference operators (3.3) and (3.4) and g includes the values of f and the boundary conditions. Since the difference operators D_{xx} and D_x (D_{yy} and D_y) are independent of the y-coordinate (x-coordinate), it is readily verified that (3.5) is of the form

$$[I \otimes A + B \otimes I]\, u = g. \tag{3.6}$$

The matrices A and B are of order $N \times N$ and $M \times M$, respectively. It should be noted that this form depends *essentially* on the fact that R is rectangular [2]. Note that for h_x and h_y sufficiently small, the matrices A and B are diagonally dominant.

We *assume* for the remainder of this section that the matrices A and B are non-singular and have distinct eigenvalues. It is conceivable that, for certain equations and certain values of h_x and h_y, this assumption is not always satisfied. However, with this assumption, we have that there exist matrices P and Q such that

$$\begin{aligned} Q^{-1} A Q &= \Lambda(A), \\ P^{-1} B P &= \Lambda(B). \end{aligned} \tag{3.7}$$

It follows then that

$$P^{-1} \otimes Q^{-1} (I \otimes A + B \otimes I)\, P \otimes Q = I \otimes \Lambda(A) + \Lambda(B) \otimes I,$$

and hence

$$[I\otimes A + B\otimes I]^{-1} = P\otimes Q\,[I\otimes\Lambda(A) + \Lambda(B)\otimes I]^{-1}\,P^{-1}\otimes Q^{-1}. \tag{3.8}$$

The matrix $[I\otimes\Lambda(A)+\Lambda(B)\otimes I]$ is diagonal and its inverse is obtained trivially. Thus the solution* of (3.6) is

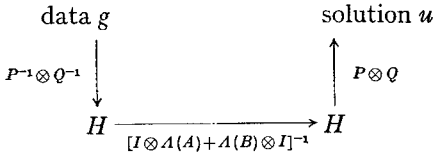
$$u = P\otimes Q\,[I\otimes\Lambda(A)+\Lambda(B)\otimes I]^{-1}\,P^{-1}\otimes Q^{-1}\,g. \tag{3.9}$$

Equation (3.9) gives the *exact* solution of the *partial* difference equation (3.2) in terms of tensor products of quantities associated with *ordinary* difference equations. That is to say that the $NM\times NM$ matrix $I\otimes A + B\otimes I$ is *directly inverted* in terms of the eigenvectors and eigenvalues of A and B**, which are only $N\times N$ and $M\times M$ matrices. Furthermore, for the difference operators in (3.5), the equations (3.7) are of a particularly tractible form. Indeed, since A and B are tridiagonal matrices, their eigenvectors and eigenvalues are relatively easily computed.

The formula given in (3.9) is of a familiar form and indeed indicates that we have merely obtained the *Green's function*, subject to the given boundary conditions, for the partial difference equation. If one examines (3.9) in a special case, such as Laplace's equation, where the Green's function is known for the differential problem, the similarity is clear. It is readily shown, in such a case, that the matrix operator of (3.9) tends to the Green's function operator of the continuous problem as h_x and h_y tend to zero.

There is another interpretation of (3.9) which is of some interest. Rather than viewing (3.9) as one matrix operating on g, consider it as a sequence of three operations. Each of these is represented by a matrix and each has a separate interpretation. The first matrix, $P^{-1}\otimes Q^{-1}$ projects the function (vector) g onto a set of orthonormal coordinates. One can consider these as coordinates in a Hilbert space. Thus it determines the components of g in terms of a system of unit vectors associated naturally with the problem, namely eigenvectors of $I\otimes A + B\otimes I$. The second matrix $[I\otimes\Lambda(A)+\Lambda(B)\otimes I]^{-1}$ represents the effect of the operator $(I\otimes A + B\otimes I)^{-1}$ acting on these unit vectors. Thus it changes coordinates in the Hilbert space. The third matrix $P\otimes Q$ is the inverse of the first matrix and transforms the result back into a function (vector) in the coordinate system of g. This is the solution. This interpretation is illustrated graphically below

(3.10)



where H is the vector space with eigenvectors as unit vectors. The key to the usefulness of this process is that, in H, the inverse of the partial difference operator is diagonal and easily computed.

* We do not recommend computing the inverse matrix (3.8). The computation required to multiply the inverse by g — regardless of the computation necessary to obtain the inverse — is greater than the computation required to solve the whole problem by using (3.11).

** The matrices Q, Q^{-1}, P, P^{-1} are the matrices formed from the eigenvectors of A, A^T, B, B^T, respectively.

To actually compute the solution of (3.6), one follows the procedure (3.10) rather than forming explicitly the inverse of $I \otimes A + B \otimes I$. Set

$$P = \{p_{ij}\}, \quad P^{-1} = \{p'_{ij}\}, \quad Q = \{q_{ij}\}, \quad Q^{-1} = \{q'_{ij}\},$$
$$\Lambda(A) = \{\lambda_\alpha(A)\,\delta_{\alpha i}\}, \quad \Lambda(B) = \{\lambda_\beta(B)\,\delta_{\beta i}\}.$$

Then (3.9) can be written in terms of matrix elements as

$$u_{ij} = \sum_{\alpha=1}^{M} p_{i\alpha} \sum_{\beta=1}^{N} q_{j\beta} \frac{1}{\lambda_\alpha(A) + \lambda_\beta(B)} \sum_{m=1}^{M} p'_{\alpha m} \sum_{n=1}^{N} q'_{\beta n}\, g_{mn}. \tag{3.11}$$

The solution u can be found by successively computing three intermediate matrices, each of order $N \times M$. These, together with the solution U, are

$$R = \{r_{m\beta} = \sum q'_{\beta n}\, g_{mn}\}, \tag{3.12}$$

$$S = \left\{s_{\alpha\beta} = \frac{1}{\lambda_\alpha(A) + \lambda_\beta(B)} \sum p'_{\alpha m}\, r_{m\beta}\right\}, \tag{3.13}$$

$$T = \left\{t_{\alpha j} = \sum_{\beta=1}^{M} q_{j\beta}\, s_{\alpha\beta}\right\}, \tag{3.14}$$

$$U = \left\{u_{ij} = \sum_{\alpha=1}^{N} p_{i\alpha}\, t_{\alpha j}\right\}. \tag{3.15}$$

We observe that the storage required for this computation is one block of storage for an $N \times M$ matrix and blocks for P, P^{-1}, Q, Q^{-1}. If the differential equation is self-adjoint then $P^T = P^{-1}$ and $Q^T = Q^{-1}$. In many cases of practical application the differential equation has constant coefficients, in which case the matrices P and Q contain at most $2N+1$ and $2M+1$ distinct elements. If the differential equation is homogeneous, then the matrices R and S may be obtained with an order of magnitude less effort. If, in addition, the solution is required only at one point (or at a very few points) it can be obtained with an order of magnitude less effort than required to solve the complete problem. A detailed comparison of the effort required for this method and other commonly used methods is given in Section 5 for a model problem.

4. Generalizations

It is evident that there are several ways in which the analysis of the preceding section can be generalized. In this section some of these are indicated. In order to avoid excessive displays of partial difference equations, we shall consider matrix equations directly. One should keep in mind the interpretation of these equations as separable partial difference equations.

Thus we consider

$$Lu = g, \tag{4.1}$$

where L is a matrix. If L is of the form (3.6), then the analysis of Section 3 is applicable, regardless of whether (4.1) represents a partial difference equation or not.

A more general form for which this analysis can be made is

$$L = (B_2 \otimes A_1 + B_1 \otimes A_2), \tag{4.2}$$

where A_1 and B_1 are positive semidefinite and A_2 and B_2 are symmetric positive definite (all with distinct eigenvalues). With these assumptions, there are non-singular matrices P and Q such that

$$\begin{aligned} &Q^T A_1 Q = \Lambda(A_2^{-1} A_1), \qquad P^T B_1 P = \Lambda(B_2^{-1} B_1), \\ &Q^T A_2 Q = I, \qquad\qquad P^T B_2 P = I. \end{aligned} \tag{4.3}$$

Thus we have

$$L^{-1} = P \otimes Q [I \otimes \Lambda(A_2^{-1} A_1) + \Lambda(B_2^{-1} B_1) \otimes I]^{-1} P^T \otimes Q^T.$$

Note that the matrix $B_2^{-1} \otimes A_2^{-1} L$ is of the form (3.6).

If one is able to express L as a *product* of separable terms, then one can apply the same analysis. Thus if

$$L = \prod_{i=1}^{k} (I \otimes A_i + B_i \otimes I), \tag{4.4}$$

then

$$L^{-1} = \prod_{i=k}^{1} P_i \otimes Q_i [I \otimes \Lambda(A_i) + \Lambda(B_i) \otimes I]^{-1} P_i^{-1} \otimes Q_i^{-1} \tag{4.5}$$

where the P_i and Q_i are appropriately chosen.

A variation and simplification of (4.5) results when L is expressible in terms of polynomials of given matrices. Let $\pi_m(x)$ and $\pi_n(x)$ be polynomial functions and assume that

$$L = I \otimes \pi_m(A) + \pi_n(B) \otimes I. \tag{4.6}$$

Then

$$L^{-1} = P \otimes Q [I \otimes \pi_m(\Lambda(A)) + \pi_n(\Lambda(B)) \otimes I]^{-1} P^{-1} \otimes Q^{-1},$$

for appropriately chosen P and Q. A further variation on this theme occurs when L is of the form

$$L = \pi_m(I \otimes A + B \otimes I), \tag{4.7}$$

then

$$L^{-1} = P \otimes Q [\pi_m(I \otimes \Lambda(A) + \Lambda(B) \otimes I)]^{-1} P^{-1} \otimes Q^{-1}.$$

The matrix associated with the biharmonic equation (with the usual difference scheme) is of the form (4.7). One can analyze further generalizations formed from combinations of the forms (4.4), (4.6) and (4.7).

The analysis of Section 3 can be extended readily to separable equations in more than two variables. The matrix L for such a partial difference equation appears in the form

$$L = I \otimes I \otimes \cdots \otimes A + I \otimes \cdots \otimes B \otimes I + \cdots + C \otimes I \otimes \cdots \otimes I. \tag{4.8}$$

The inverse of L is

$$P \otimes \cdots \otimes Q \otimes R [\Lambda(A, B, \ldots, C)]^{-1} P^{-1} \otimes \cdots \otimes Q^{-1} \otimes R^{-1}, \tag{4.9}$$

where

$$\begin{aligned} P^{-1} C P &= \Lambda(C), \\ Q^{-1} B Q &= \Lambda(B), \\ R^{-1} A R &= \Lambda(A), \end{aligned}$$

and $\Lambda(A, B, \ldots, C)$ is the diagonal matrix formed in the natural way (i.e., as in (3.9) from $\Lambda(A), \Lambda(B), \ldots, \Lambda(C)$.

There are, of course, generalizations for matrices which are in the forms (4.4), (4.5) and (4.6) with more than two tensor product factors. These generalizations are not elaborated upon here.

The following type of problem with n independent variables (i.e., n factors in the tensor product) and n terms in the sum for L can also be analyzed. The matrix L has the decomposition

$$\left.\begin{aligned} L &= C_1 \otimes B_1 + I \otimes A_1 \\ C_1 &= C_2 \otimes B_2 + I \otimes A_2 \\ &\cdots \\ C_{n-2} &= C_{n-1} \otimes B_{n-1} + I \otimes A_{n-1} \end{aligned}\right\} n-1 \text{ decompositions.} \tag{4.10}$$

Such a problem is said to be *recursively separable*. To illustrate the form, we write L explicitly for $n=4$:

$$L = [[C_3 \otimes B_3 + I \otimes A_3] \otimes B_2 + I \otimes I \otimes A_2] \otimes B_1 + I \otimes I \otimes I \otimes A_1. \tag{4.11}$$

The Laplace equation in spherical coordinates is recursively separable and is considered in more detail in Section 6.

We have made no attempt to indicate the size of the matrices involved in (4.10) or in the following analysis. In order to keep the notation reasonably simple we assume that each matrix A_i, B_i and also C_{n-1} in (4.10) is $M \times M$. The analysis depends in no way on this assumption.

In order to invert L we define a sequence of matrices $Q(k)$ and $\Lambda(k)$, $k = n, n-1, \ldots, 1$ as follows:

i) $Q(n)$ is the $M \times M$ matrix such that

$$Q^{-1}(n)\, C_{n-1}\, Q(n) = \Lambda(n) = \Lambda(C_{n-1}). \tag{4.12}$$

ii) $Q(n-1)$ is the $M^2 \times M^2$ matrix such that

$$Q^{-1}(n-1)\, [\Lambda(n) \otimes B_{n-1} + I \otimes A_{n-1}]\, Q(n-1) = \Lambda(n-1), \tag{4.13}$$

where $\Lambda(n-1)$ is a diagonal matrix of eigenvalues of $\Lambda(n) \otimes B_{n-1} + I \otimes A_{n-1}$. We note that $Q(n-1)$ is the *direct sum* of M matrices $Q_j(n-1)$ each of order $M \times M$. The matrices $Q_j(n-1)$ are such that

$$Q_j^{-1}(n-1)\, [\lambda_j(n)\, B_{n-1} + A_{n-1}]\, Q_j(n-1) \tag{4.14}$$

is diagonal. Here $\lambda_j(n)$ is the j-th diagonal element of $\Lambda(n)$. Thus $Q(n-1)$ is of the form

$$Q(n-1) = Q_1(n-1) \oplus Q_2(n-1) \oplus \cdots \oplus Q_M(n-1).$$

iii) For a general index k we have

$$Q^{-1}(k)\, [\Lambda(k+1) \otimes B_k + I \otimes A_k]\, Q(k) = \Lambda(k),$$

where $\Lambda(k)$ is diagonal. Set $t = M^{(n-k)}$, then

$$Q(k) = Q_1(k) \oplus Q_2(k) \oplus \cdots \oplus Q_t(k),$$

where $Q_j(k)$ is the $M \times M$ matrix such that

$$Q_j^{-1}(k)\,[\lambda_j(k+1)\,B_k + A_k]\,Q_j(k),$$

is a diagonal matrix.

The matrices $Q(k)$, $k=n, n-1, \ldots, 1$ which are formed recursively in this manner are such that

$$\prod_{i=1}^{n}\left[Q^{-1}(i)\otimes\bigotimes_{j=0}^{i-1} I\right] L \prod_{i=n}^{1}\left[Q(i)\otimes\bigotimes_{j=0}^{i-1} I\right] = \Lambda(L). \tag{4.15}$$

where $\bigotimes_{j=0}^{i-1} I$ denotes $I\otimes\cdots(i-1)$ — times $\cdots\otimes I$ for $i>1$ and it denotes unity for $i=1$.

The matrix used to diagonalize L in (4.15) is more complicated than that found, for example, in (4.9). The justification for this analysis and development is the fact that *the exact solution of $Lu=g$ can be evaluated with exactly the same number of arithmetic operations whether L is separable of the form* (4.8) *or is recursively separable.* The number of operations required to evaluate the exact solution is of the order $2nM^{n+1}$. It is, presumably, more effort to compute the matrices $Q(k)$ for (4.15) than the matrices $P, Q, \ldots, R$ for (4.9).

5. Comparison of Methods for Solving Laplace's Equation

In this section we compare in detail the amount of computation to solve Laplace's partial difference equation on a square with Dirichlet boundary conditions. Three methods are considered: i) optimum Successive Overrelaxation (SOR), ii) Tensor Product (TP), iii) Alternating Direction Implicit (ADI).

The SOR and ADI methods are iterative rather than exact * and hence we must determine when to terminate the iterative process. We have chosen Laplace's equation as the problem because the asymptotic rates of convergence of the SOR and ADI methods are known exactly for this sample problem. Furthermore we have chosen to take

$$h_x = h_y = \frac{1}{N+1}. \tag{5.1}$$

Detailed comparisons made for Poisson's equation on a rectangle with $h_x \neq h_y$ lead to essentially the same conclusions as reached from the model problem considered here.

The number of iterations required for the SOR and ADI methods depends on the asymptotic rate of convergence and the accuracy required. We require that the accuracy in solving the difference equations be comparable with the truncation error of the partial difference equation approximation to the partial differential equation. Thus, for the usual second order finite difference scheme which we use, the iteration is terminated when the initial error has been reduced by a factor of h_x^2.

We briefly outline the equations pertinent for these two iterative methods. For more details see [*10*].

* The ADI method is exact in certain situations, however in practice one would not carry the calculations to the point where an exact solution is obtained.

i) SOR:

$$u_{ij}^{(k+1)} = (1 + 4\omega)\, u_{ij}^{(k)} - \omega\,[u_{i+1,j}^{(k)} + u_{i-1,j}^{(k+1)} + u_{i,j+1}^{(k)} + u_{i,j-1}^{(k+1)}].$$

The asymptotic rate of convergence is $2/(N+1)$. The number of arithmetic operations is $6N^2$ ($4N^2$ additions and $2N^2$ multiplications). The number of iterative sweeps required is $2.3\,N \log N$*.

ii) ADI (Peaceman-Rachford):

$$u_{i+1,j}^{(k+\frac{1}{2})} + u_{i-1,j}^{(k+\frac{1}{2})} - (2+\varrho_m)\, u_{ij}^{(k+\frac{1}{2})} = (2-\varrho_m)\, u_{ij}^{(k)} - u_{i,j+1}^{(k)} - u_{i,j-1}^{(k)},$$

$$u_{i,j+1}^{(k+1)} + u_{i,j-1}^{(k+1)} - (2+\varrho_m)\, u_{ij}^{(k+1)} = (2-\varrho_m)\, u_{ij}^{(k+\frac{1}{2})} - u_{i+1,j}^{(k+\frac{1}{2})} - u_{i-1,j}^{(k+\frac{1}{2})}.$$

The asymptotic rate of convergence with optimum parameters ϱ_m is $2/(.94 \log N)$ [3]. The number of arithmetic operations per iteration sweep is $18N^2$ ($10N^2$ additions, $4N^2$ multiplications, $4N^2$ divisions). The number of iteration sweeps required is $2.2 \log^2 N$.

The final comparison is shown in the Table**.

Table. *The number of arithmetic operations required to solve Laplace's equation for three methods*

Method	SOR	TP	ADI
Arithmetic Operations	$14N^3 \log N$	$4N^3$	$40N^2 \log^2 N$

The TP method uses (3.12)—(3.15). The matrices T and U require $2N^3$ (N^3 additions, N^3 multiplications) operations, while R and S require $8N^2$ operations. The p_{ij}, q_{ij} are given by

$$p_{ij} = q_{ij} = \sqrt{\frac{2}{N}} \sin \frac{ij\pi}{N+1} = p'_{ij} = q'_{ij},$$

and there are N distinct values.

Only the highest order (in N) terms are included in the Table and hence the comparison is valid only for large values of N.

The TP method has been used to solve a selection of problems with up to 10,000 mesh points. No numerical instabilities have been observed and we know of no theoretical arguments which would lead one to expect such instabilities. We have also experimented with the direct calculation of the inverse matrix (3.8). We have computed sample elements in the inverse for problems with 10,000 mesh points. The inverse matrix contains 100,000,000 elements (in general non-zero) in this case. No numerical instabilities or excessive round off effects were detected.

6. Examples

In this section we consider several specific examples of partial difference equations which can be solved in terms of tensor products. We consider only

* The factor 2.3 is ln 10, since asymptotic rates of convergence refer to natural logarithms.

** By using special properties of $\sin x$ and a special choice of N, HOCKNEY [13] is able to directly solve POISSON's equation with fewer operations than required for the ADI method.

the usual equally spaced finite difference operators, which are represented by the following matrices.

$$A = \begin{pmatrix} 2 & -1 & & & & 0 \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & & \ddots & & \\ 0 & & & & -1 & 2 \end{pmatrix} \quad \text{second difference,} \tag{6.1}$$

$$B = \tfrac{1}{2}\begin{pmatrix} 0 & 1 & & & & 0 \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & & \ddots & & \\ 0 & & & & -1 & 0 \end{pmatrix} \quad \text{first difference.} \tag{6.2}$$

It should be noted that, contrary to what one might expect, there is no simple relationship between B^2 and A. For further simplicity we assume that the problem is posed for the square

$$R = \{(x, y) \mid 0 \leqq x \leqq 1,\ 0 \leqq y \leqq 1\},$$

and $h_x = h_y = h$. The partial difference equations are written in the notation of partial differential equations, i.e., the corresponding differential equations are written.

a) Helmholtz Equation

The nonhomogeneous Helmholtz equation is

$$-(v_{xx} + v_{yy}) + \sigma v = f(x, y), \tag{6.3}$$

where σ is assumed to be constant. With Dirichlet boundary conditions, this leads to a system of linear equations of the form

$$(I \otimes A + A \otimes I + \sigma h^2 I \otimes I)\, u = g. \tag{6.4}$$

The boundary conditions and h^2 have been absorbed into g on the right side of (6.4). Another way of writing (6.4) is

$$(I \otimes (A + \sigma h^2 I) + A \otimes I)\, u = g. \tag{6.5}$$

The eigenvectors of (6.5) (and hence the matrices P and Q of (3.9)) are the same as for Laplace's equation. The eigenvalues are readily obtained.

If periodic boundary conditions are used then the matrix A is modified by the insertion of -1 in the lower left and upper right corners. This is a circulant matrix and its eigenvectors and values are known [7].

One may also consider the mixed boundary values

$$\begin{aligned} v(x, y) + \alpha(x)\, v_x(x, y) &= \gamma(x, y), \qquad x = 0, 1, \\ v(x, y) + \beta(y)\, v_y(x, y) &= \delta(x, y), \qquad y = 0, 1. \end{aligned} \tag{6.6}$$

There are several ways to incorporate these values into the finite difference equations. Each of them leads to a system of tensor product form where the first

and last rows of A are modified. In this case, one would, in general, have to numerically compute the eigenvectors and eigenvalues required for the formation of the matrices P and Q.

The so-called *nine-point formula* [*10*] may also be expressed in tensor product form. One obtains

$$[I\otimes A + A\otimes A/6 + A\otimes I + h^2\,\sigma\, I\otimes I]\, u = g. \tag{6.7}$$

The matrices P and Q are the same as for (6.5). The eigenvalues are $\mu_{\alpha\beta} = \lambda_\alpha(A) + \lambda_\alpha(A)\,\lambda_\beta(A)/6 + \lambda_\beta(A) + h^2\,\sigma$, $\alpha, \beta = 1, \ldots, N$. If $\mu_{\alpha\beta}$ is substituted for $\lambda_\alpha(A) + \lambda_\beta(B)$ in (3.11), then (3.11) gives the solution of (6.7). Consequently, *the amount of computation required to solve exactly the nine-point approximation* (6.7) *to* (6.3) *is only slightly more than that required to solve the five-point approximation* (6.4).

b) Second Order Elliptic Equations

We consider the equations (3.1) and (3.5). With usual finite differences (6.1) and (6.2), equation (3.5) is of the form

$$[I\otimes(X_2\,A + h\,X_1\,B + h^2\,X_0) + (Y_2\,A + h\,Y_1\,B + h^2\,Y_0)\otimes I]\, u = g. \tag{6.8}$$

Here g contains the right side of (3.1) and the Dirichlet boundary conditions. For h sufficiently small, each matrix in parentheses in (6.8) is diagonally dominant. The eigenvalues and eigenvectors are not, of course, known explicitly for this general form. However, they may be determined relatively easily by the methods referenced in Section 2.

Periodic and mixed boundary conditions may be treated as described for the Helmholtz equation.

c) Biharmonic Equation

The nonhomogeneous biharmonic equation is

$$v_{xxxx} + 2\,v_{xxyy} + v_{yyyy} = f(x, y). \tag{6.9}$$

A common situation is for values of v and its second normal derivative to be given on the boundary. Note that we can, as is well-known, solve (6.9) by solving two Poisson equations. We can do this, of course, with the tensor product method described for the Helmholtz equation.

We can also solve (6.9) directly by noting the partial difference equation is of the form

$$(I\otimes A + A\otimes I)^2\, u = (I\otimes A^2 + 2A\otimes A + A^2\otimes I)\, u = g. \tag{6.10}$$

The equation (6.10) results only if the boundary conditions are treated in a particular way. The equation for the point (h, jh) adjacent to the boundary is, from (6.10),

$$5u_{1j} - 4u_{2j} + u_{3j} = g_{1j},$$

plus terms in the other direction. At an interior point one has (again for one direction only)

$$6u_{ij} - 4u_{i+1,j} + u_{i+2,j} = 4u_{i-1,j} - u_{i-2,j} + f_{ij}.$$

The given boundary values are u_{0j} and $u_{xx}(0, jh)$. Since

$$h^2 u_{xx}(0, jh) \approx u_{1j} - 2u_{0j} + u_{-1j},$$

the value $u_{-1,j}$ can be expressed in terms of u_{0j} and $u_{xx}(0, jh)$. We obtain, then,

$$5u_{1j} - 4u_{2j} + u_{3j} = 2u_{0j} - u_{xx}(0, jh) + f_{ij}.$$

Thus, the term g_{ij} on the right side of (6.10) is the right side of this equation.

The explicit formula for the solution of (6.10) is, with $h = (N+1)^{-1}$

$$u_{ij} = \sum_{\alpha=1}^{N} p_{i\alpha} \sum_{\beta=1}^{N} p_{j\beta} \frac{1}{\lambda_\alpha^2 + 2\lambda_\alpha \lambda_\beta + \lambda_\beta^2} \sum_{m=1}^{N} p_{\alpha m} \sum_{n=1}^{N} p_{\beta n} g_{mn}, \tag{6.11}$$

where λ_α, λ_β are the eigenvalues of A in (6.1) and $p_{i\alpha} = \sqrt{\frac{2}{N}} \sin\left(i\alpha\pi/(N+1)\right)$. The value g_{mn} for $m, n = 1, N$ includes the boundary conditions as described in the preceding paragraph. We see that we solve the nonhomogenous biharmonic equation with the stated boundary conditions, with essentially *no more effort than is required to solve the Poission equation.*

d) Helmholtz Equation in Spherical Coordinates

The nonhomogeneous Helmholtz equation in spherical coordinates can be written as

$$[r^2 v_r]_r + \frac{1}{\sin\vartheta}[\sin\vartheta\, v_\vartheta]_\vartheta + \frac{1}{\sin^2\vartheta} v_{\varphi\varphi} + r^2 \sigma v = f(r, \vartheta, \varphi), \tag{6.12}$$

with $r_1 \leqq r \leqq r_2$, $\vartheta_1 \leqq \vartheta \leqq \vartheta_2$, $\varphi_1 \leqq \varphi \leqq \varphi_2$. Define the matrix

$$B_2 = \left\{\frac{1}{\sin^2\vartheta_i}\, \delta_{ij}\right\},$$

and consider the finite difference operators

$$A_1 \approx [r^2 u_r]_r + r^2 \sigma u,$$

$$B_1 \approx \frac{1}{\sin\vartheta}[\sin\vartheta\, u_\vartheta]_\vartheta,$$

$$C_1 \approx u_{\varphi\varphi}.$$

Then the partial difference equation approximating (6.12) is

$$Lu = [(C_1 \otimes B_2 + I \otimes B_1) \otimes I + I \otimes I \otimes A_1]\, u = g. \tag{6.13}$$

The matrix L in (6.13) is recursively separable (see Section 4). It cannot be written in the form (4.8). Let R and P be the $N \times N$ orthogonal matrices such that

$$RC_1R = \Lambda(C_1), \qquad PA_1P = \Lambda(A_1).$$

Furthermore the N orthogonal $N \times N$ matrices Q_i are so that

$$Q_i[B_1 + \lambda_i(C_1)\, B_2]\, Q_i,$$

is diagonal. Then the inverse of L in (6.13) is

$$L^{-1} = [(Q_1 \oplus Q_2 \oplus \cdots \oplus Q_N)\,(R \otimes I)] \otimes P\,[\Lambda(L)]^{-1} \times [(R \otimes I)\,(Q_1 \oplus Q_2 \oplus \cdots \oplus Q_N)] \otimes P. \tag{6.14}$$

It should be noted that the procedure outlined here is the exact analog of the usual procedure [8] of separation of variables as applied to (6.12).

7. Application to Parabolic Equations

As is well-known, the solution of parabolic partial difference equations with implicit difference schemes leads to systems of linear equations similar to those discussed in Section 3. We briefly outline the development and application of tensor product methods to these problems. In particular we give a simple explanation of the method proposed by BAKER and OLIPHANT [1].

We consider the equations arising from the solution of

$$-\frac{\partial v}{\partial t} = L v, \tag{7.1}$$

where L is a second order separable operator in two variables in a rectangular domain. The most common implicit schemes are Crank-Nicholson and the backward schemes. These lead to problems of the following forms, respectively,

$$-2(u_{n+1} - u_n)/\Delta t = (I \otimes A/h_x^2 + B \otimes I/h_y^2)\,(u_{n+1} + u_n), \tag{7.2}$$

$$-(u_{n+1} - u_n)/\Delta t = (I \otimes A/h_x^2 + B \otimes I/h_y^2)\,u_{n+1}, \tag{7.3}$$

in which u_n is the approximation to v at $t = n\Delta t$. In both cases, u_{n+1} satisfies an equation of the form

$$(I \otimes A/h_x^2 + B \otimes I/h_y^2 + \beta\, I \otimes I)\,u_{n+1} = f, \tag{7.4}$$

in which f is known and which may be solved explicitly in terms of tensor products.

We now discuss the factorization method of BAKER and OLIPHANT [1]. Consider the heat equation with two space variables

$$-\partial v/\partial t = -\nabla^2 v, \qquad \nabla^2 v = \partial^2 v/\partial x^2 + \partial^2 v/\partial y^2, \tag{7.5}$$

on a square. For simplicity, we consider equal mesh-lengths, $h_x = h_y = h$. Baker and Oliphant's idea was to construct a difference approximation similar to (7.4) but with the left side modified so that it factored. To obtain a matrix which factors, cross products must be used which lead to nine-point approximations to the spatial differential operator instead of the five-point approximations used in (7.4). Baker and Oliphant's scheme can be written as

$$[\beta\, I \otimes I + (I \otimes A + A \otimes I)/h^2 + A \otimes A/\beta\, h^4]\,u_{n+1} = f. \tag{7.6}$$

This is easy to solve as can be seen by writing (7.6) in the factored form

$$(\beta\, h^2\, I + A) \otimes (\beta\, h^2\, I + A)\,u_{n+1} = \beta\, h^4\, f.$$

The matrix $\beta\, h^2\, I + A$ is, of course, tridiagonal. The quantity $\beta\, h^2$ is equal to $\Delta x^2/\Delta t$ when $\partial u/\partial t$ is approximated by $(u_{n+1} - u_n)/\Delta t$. It is easily shown by

using Taylor's theorem with remainder that if u is sufficiently differentiable, then the left side of (7.6) is equal to

$$[\beta u + V^2 u + (\partial^4 u/\partial x^2 \partial y^2)/\beta]_{n+1} + O(h^2),$$

and since $1/\beta = O(\Delta t)$, it can be seen that this is a good approximation to the desired $(\beta u + V^2 u)_{n+1}$ only for small Δt.

This approximation can be improved by adding $(A \otimes A\, u/\beta h^4)_n$ to the right side to obtain

$$[\beta I \otimes I + (I \otimes A + A \otimes I)/h^2 + A \otimes A/\beta h^2]\, u_{n+1} = f + A \otimes A\, u_n/\beta h^2,$$

so that by Taylor's theorem this becomes

$$(\beta u + V^2 u)_{n+1} + O(h^2) = f + \{[-\partial^4 u_{n+1}/\partial x^2 \partial y^2 + \partial^4 u_n/\partial x^2 \partial y^2]/\beta\},$$

and the quantity in curly brackets is $O(h/\beta) = O(h \Delta t)$. But, a systematic study of ADI schemes yields better methods. One obtains efficient difference schemes which yield high accuracy with a relatively small amount of computation. These will be discussed in another paper [6].

References

[1] Baker, G. A., and T. A. Oliphant, Jr.: An implicit, numerical method for solving the two-dimensional heat equation. Quart. Appl. Math. **17**, 361–373 (1960).

[2] Birkhoff, G., and R. S. Varga: Implicit alternating direction methods. Trans. Amer. Math. Soc. **92**, 13–24 (1959).

[3] de Boor, C. W., and J. R. Rice: Chebyshev approximation by a $\Pi (x-r_i)/(x+s_i)$ and application to ADI iteration. J. Soc. Indust. Appl. Math. **11**, 159–169 (1963).

[4] Halmos, P. R.: Finite dimensional vector spaces, Chap. II. New York: D. van Nostrand 1958.

[5] Lynch, R. E., J. R. Rice, and D. H. Thomas: Tensor product analysis of partial difference equations. Bull. Amer. Math. Soc. **70**, 378—384 (1964).

[6] — Tensor product analysis of alternating direction implicit methods. (To appear.)

[7] Marcus, M.: Basic theorems in matrix theory. National Bureau of Standards Applied Mathematics Series **57** (1960).

[8] Morse, P. M., and H. Feshbach: Methods of mathematical physics. I. New York: McGraw-Hill 1953.

[9] Rutishauser, H., and H. R. Schwarz: The LR transformation method for symmetric matrices. Numer. Math. **5**, 273–289 (1963).

[10] Varga, R. S.: Matrix iterative analysis. Englewood Cliffs, N.T.: Prentice-Hall 1962.

[11] Wilkinson, J. H.: Calculation of the eigenvalues of a symmetric tridiagonal matrix by the method of bisection. Numer. Math. **4**, 362–367 (1962).

[12] Egerváry, E.: Über eine Methode zur numerischen Lösung der Poissonschen Differenzengleichung für beliebige Gebiete. Acta. Math. Acad. Sci. Hungar **11**, 341–361 (1960).

[13] Hockney, R. W.: A fast direct solution of Poisson's equation using Fourier analysis. Tech. Rept. CS 6, Computer Science Division, Stanford University, 1964.

Research Laboratories, General Motors Corporation
General Motors Corporation
12 Mile and Mound Roads
Warren, Michigan 48090/USA

(Received February 14, 1964)