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Comparative Test of Direct and Iterative Methods for Solving Helmholtz-Type Equations

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ABSTRACT—The Helmholtz-type equation arises in many areas of fluid dynamics, and, in recent years, there has been a rapid increase in the numerical procedures available for solving the equation. In this note, the various methods currently available are discussed, and representatives from the main categories are compared.

We suggest that for certain problems, the most important of which is Poisson's equation on a rectangle, direct methods are now available that are far superior to widely used iterative methods. For problems involving irregular domains, mixed boundary conditions, and variable Helmholtz coefficients, however, existing direct methods often cannot be used with the same flexibility as iterative methods; there is a continuing need to extend direct methods to these more general cases.

1. INTRODUCTION

One of the most frequently encountered equations of numerical weather prediction, and fluid dynamics generally, is the diagnostic equation

$$\nabla^2\phi-\alpha(x,y)\phi=f(x,y) \tag{1}$$

where ∇^2 is the two-dimensional Laplacian operator, $\alpha(x,y)$ is a non-negative function, and $f(x,y)$ is a forcing function. Included in the class of eq (1) are the equivalent barotropic vorticity equation [in which ϕ is the height of the 500-mb level and $\alpha(x,y)=\mu$, the Cressman correction factor]; the baroclinic filtered equation [where ϕ is the stream function tendency at some level and $\alpha(x,y)=0$]; the linear balance equation; and, most recently, the Helmholtz-type equations associated with the semi-implicit time differencing schemes.

When approximated in the usual way by a finite-difference analog, eq (1) reduces to a system of linear equations

$$\mathbf{Ax}=\mathbf{b} \tag{2}$$

where, for a finite-difference grid with $M\times N$ interior points, $\mathbf{A}$ is an $MN\times MN$ block tridiagonal matrix.

Many algorithms of varying generality, speed, accuracy, and efficiency have been devised for solving eq (2). They may be divided into two broad classes; namely, the iterative methods and the direct or "exact" methods. Some of these methods have been developed only recently, and a review of the procedures currently available is presented in the next section.

2. DISCUSSION OF AVAILABLE ALGORITHMS

Iterative Methods

The most widely used iterative methods are the Liebmann successive over-relaxation method (SOR) and the alternating direction implicit method (ADI) (Varga 1962, ch. 3 and 7). Because of its simplicity, the SOR method has found wide acceptance, particularly in its Sheldon-speeded form (Sheldon 1962); the superior speed of the ADI method has apparently not outweighed the associated coding difficulties and slightly increased storage requirements.

Direct Methods

By taking advantage of the special structure of the set of linear equations given in eq (2), researchers have devised many methods in recent years that are considerably faster and more accurate than the older iterative methods. Dorr (1970) has divided the direct methods, all of which avoid the excessive number of operations involved in solving eq (2) by standard elimination procedures, into four main categories:

1. Block methods, which use the fact that $\mathbf{A}$ is block tridiagonal. The "two-pass" recursion form (Lindzen and Kuo 1969) is the most familiar. Karlqvist (1952) has discussed this approach in detail for the Poisson equation. The block methods are generally slower than the other direct methods.

2. Cyclic reduction methods, which reduce the dimensions of the matrix problem to be solved. These methods rely on the matrix $\mathbf{A}$ being two-cyclic (Varga 1962, p. 126) thereby allowing the original matrix equation to be reduced in a recursive manner to a set of equations involving a much smaller matrix. This type of method is most efficient when the reduction procedure can be repeated until there is only one block of the original matrix remaining. This procedure places a restriction on the number of interior points of the $M \times N$ grid; either M or N should be equal to $2^{k+1}-1$ where k is an integer. In some cases, however, a combination of cyclic reduction and matrix decomposition (discussed later) is advantageous. For a more complete discussion, the reader is referred to Buzbee et al. (1970) and Hockney (1969).

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3. Matrix decomposition or tensor product methods, which depend on the use of coordinate transformations to reduce the problem to a simple tridiagonal form that has an easily computed solution. Lynch et al. (1964) have described the general form of this method. The dimension reduction method (DRM), as elaborated by Ogura (1969), is a particularly simple version that can be applied when a fast Fourier transform is available.

4. Fourier methods, as outlined by Hockney (1965), enable the fast Fourier transform to be applied directly in certain somewhat restrictive circumstances. The trigonometric interpolation method applied by Williams (1967) in his numerical experiments with a differentially heated rotating annulus is an example of the Fourier method.

An independent method recently devised by Hirota et al. (1970) and referred to as the generalized sweep-out method (GSM) appears to combine flexibility with speed. This method requires the determination of residuals "swept out" after an initial guess has been inserted on a line (row) of the grid. It should be noted that this method can only compete with other methods when the inverse of the residual matrix arising in the problem has been calculated previously. In most cases, this is not expected to be a serious problem because the residual matrix depends only on the grid size and is independent of boundary conditions and forcing function.

In general, iterative methods have been easier to apply to irregular domains than have most direct methods. For nonrectangular domains, the matrix **A** of eq (2) is no longer in the block-tridiagonal form suitable for the most efficient direct methods. Buzbee et al. (1971) have shown, however, that it is possible to recast eq (2) into a form that is once again amenable to direct methods.

The nature of the Helmholtz coefficient is also of crucial importance in determining the applicability and performance of both direct and iterative methods for solving eq (1). When the Helmholtz coefficient is variable, as it frequently is in numerical weather prediction [e.g., $\alpha(x, y)$ may include variable map factor terms], then many direct methods can no longer be easily applied. Furthermore, when the Helmholtz term becomes large, the iterative methods converge rapidly because of the diagonal dominance of matrix **A** in eq (2). In view of the significance of the Helmholtz coefficient, it was decided to investigate the Poisson and Helmholtz equations separately, because each is important in its own right, and because general conclusions covering both are really not possible.

3. POISSON'S EQUATION

Poisson's equation $[\alpha(x,y)=0]$ is an extremely important special case of eq (1); the stream function-vorticity equation is one of the fundamental equations of classical incompressible fluid dynamics. Iterative methods have been widely used for solving Poisson's equation and the SOR method has been in favor from the time of the first attempts at numerical weather prediction in the early 1950s (e.g., Charney and Phillips 1953). With the rapid development of digital computer technology over the past 2 decades, fluid dynamicists began to attempt more ambitious modeling efforts, and new problems arose. Numerical modeling of the oceanic circulation, for example, required integration times of the order of months to model just the simple barotropic response (Veronis and Stommel 1956) which meant solving Poisson's equation many thousands of times. The accumulated errors associated with economically practicable error tolerances rendered SOR obsolete for this type of problem (Veronis 1966, Crowley 1970). Quicker, more accurate methods were needed, and there has been an intensive search for such algorithms in recent years. The situation has not been so acute in numerical weather prediction, which has typically involved integration periods of several days only. In such circumstances, SOR has remained popular. However, the recent interest in problems such as fine-mesh modeling and the increasing availability of efficient direct methods suggests that a comparison of direct and iterative methods is worthwhile so that some guidelines may be established.

Four of the methods discussed in section 2 were chosen for comparison in terms of speed and accuracy. The SOR method was used as a representative of the iterative methods, and the Buneman cyclic reduction method (DCR), the Ogura DRM, and the Hirota et al. GSM were selected to represent the direct methods in accordance with table 1.[1]

Each method was used to solve the Poisson equation

$$\nabla^2\phi_{i,j}=F_{i,j} \qquad \begin{matrix} 2\leq i\leq M \\ 2\leq j\leq N \end{matrix} \tag{3}$$

where

$$F_{i,j}=\phi^{(0)}_{i+1,j}+\phi^{(0)}_{i-1,j}+\phi^{(0)}_{i,j+1}+\phi^{(0)}_{i,j-1}-4\phi^{(0)}_{i,j}$$

is a forcing function derived from a 500-mb height field, $\phi^{(0)}_{i,j}$. The boundary conditions for eq (3) are the boundary values of $\phi^{(0)}_{i,j}$.

SOR

A flat, initial-guess field for SOR was provided by using the mean of the initial field. The iterative procedure was stopped when the relative error,

$$E^{(\tau)}_{i,j}=\frac{|\phi^{(\tau)}_{i,j}-\phi^{(0)}_{i,j}|}{\phi^{(0)}_{i,j}},$$

at the τth iteration was everywhere less than a prescribed δ. In table 2 the times taken to reach convergence on an IBM 360/65 computer[2] are shown plotted against selected values of δ. For values of δ less than 10^{-6}, double precision arithmetic was required. The number of iterations ranged from eight for $\delta=10^{-1}$ to 221 for $\delta=10^{-10}$ on a 65×65 grid. The corresponding number of iterations required on a 33×33 grid ranged from four for $\delta=10^{-1}$ to 111 for $\delta=10^{-10}$.

When considering the times taken by SOR to reach convergence to a given error tolerance, one must remember that these times are inflated by the flat, first-guess field. In numerical weather prediction problems, a good guess is frequently available from the fields at the previous time

[1] No attempt was made to assess the trigonometric methods because of the detailed investigation carried out by Hockney (1969).

[2] Mention of a commercial product does not constitute an endorsement.

TABLE 1.—*Operational counts for the solution of Poisson's equation by various iterative and direct methods (based in part on tables 1 and 2 of Dorr 1970)*

Method	Operations count
Block (Karlqvist 1952)	$6N^3$
Cyclic Reduction (Buzbee et. al. 1970)	$\frac{9}{2}N^2\log_2 N$
Matrix Decomposition (Lynch et al. 1964)	$8N^3$
Matrix Decomposition (Ogura 1969)	$10N^2\log_2 N$
Fourier Series (Hockney 1965)	$5N^2\log_2 N$
SOR*	$\frac{3}{2}N^3\log_2 N$
ADI*	$4N^2(\log_2 N)^2$

*The operations counts for SOR and ADI are based on the assumption that the iterations are terminated when the initial error has been reduced by a factor of h^2, where h is the grid interval (Lynch et. al. 1964, p. 193, Dorr 1970, p. 259).

step, and the number of iterations is greatly reduced. Hockney (1969) has discussed the influence of the first guess on convergence for a variety of iterative methods.

DRM

The DRM takes only 0.29 and 1.25 s to solve the Poisson problem on the 33×33 and 65×65 grids, respectively, using single precision arithmetic. The maximum error is 1.1×10^{-6} and is effectively set by the single precision limit of the IBM 360/65. It is clear from table 2 that double precision arithmetic may be used to obtain very accurate solutions with only a very slight loss of speed but a possibly prohibitive increase in storage requirements.

DCR[3]

As may be expected from the operational counts given in table 1, DCR is faster than DRM, taking 0.21 s for the 33×33 grid and 0.89 s for the 65×65 grid, using single precision arithmetic (table 2). Again, these times are only marginally altered by double precision arithmetic.

GSM

Contrary to expectations, GSM failed to yield a solution on both the 33×33 and 65×65 grids. The extraordinary precision required in certain parts of the computation renders this method impractical for even moderate grid sizes with the computers generally available at present (McAvaney and Leslie 1972, Roache 1971). For an IBM 360/65, $N=20$ is the maximum array size that can be handled by GSM using double precision arithmetic. For larger N, greater than double precision arithmetic is needed, thereby removing some of the speed advantage and creating prohibitive storage requirements. Splitting the domain in the manner suggested by Hirota

[3] The version of DCR used in this investigation is the first published form (Buneman 1969). Buzbee et al. (1971) have given an alternative formulation which is slightly faster but requires more storage.

TABLE 2.—*Time required to solve the two-dimensional Poisson equation on a rectangular domain by the DCR, DRM, and SOR algorithms, using an IBM 360/65 machine, with Fortran IV level H, Opt=2 complier. Row (a) refers to single precision times and errors, row (b) to double precision. The bracketed figures in the first SOR column refer to the number of iterations required to reach the specified level of convergence.*

Mesh	DCR		DRM		SOR	
	Time (s)	Relative Error	Time (s)	Relative Error	Time (s)	Relative Error
33×33 (a)	0.21	10^{-6}	0.29	10^{-6}	5.6 [71]	10^{-6}
(b)	0.22	10^{-13}	0.30	10^{-13}	7.4 [111]	10^{-10}
65×65 (a)	0.89	10^{-6}	1.25	10^{-6}	42.3 [141]	10^{-6}
(b)	0.90	10^{-13}	1.27	10^{-13}	75.9 [221]	10^{-10}

et al. (1970, p. 166) offers no real alternative because one is faced with the task of inverting a $2N\times2N$ matrix to at least double, but most likely quadruple, precision accuracy. Even if such a task were considered worthwhile, it would still be necessary to use quadruple precision arithmetic (Roache 1971, p. 53, fig. 2) during the actual computation and once again the advantage will be lost.

4. HELMHOLTZ-TYPE EQUATION

The Helmholtz-type equation $[\alpha(x,y)>0]$ arises in such numerical weather prediction models as the baroclinic filtered model, and models with semi-implicit time differencing (Robert et al. 1972, Gerrity and McPherson 1971). As noted earlier, the size of the Helmholtz coefficient is extremely important in determining the convergence rate of iterative methods. For large values[4] of α, the block matrix **A** of eq (2) is strongly diagonally dominant and few iterations are required by SOR. For small values of α, the convergence rate of SOR approaches that for solving Poisson's equation.

In barotropic models with Cressman phase correction or semi-implicit time differencing, the Helmholtz term is indeed small and the results of section 3 carry over with only slight modification.[5] Certain multilevel models, however, such as n-level models with semi-implicit time differencing, require n Helmholtz equations to be solved at each time step; one corresponding to the barotropic mode, and $n-1$ corresponding to the baroclinic modes. The Helmholtz coefficient is small for the barotropic mode but increases to very large for the slowest baroclinic modes. Thus, the best method for the fastest modes may not necessarily be the most suitable for the slower modes.

As a means of investigating the effect of the Helmholtz coefficient, the six-level, N30, primitive-equation model, developed at the Commonwealth Meteorology

[4] The finite-difference approximation to eq (1) using the conventional five-point Laplacian difference operator is

$$\phi_{i+1,j}+\phi_{i-1,j}+\phi_{i,j+1}+\phi_{i,j-1}-(4+\alpha h^2)\phi_{i,j}=h^2f_{i,j},$$

assuming a constant grid interval, h. Large α means $h^2\alpha>>4$, and small α means $h^2\alpha<<4$.

[5] In these cases, $h^2\alpha$ is about an order of magnitude smaller than 4. The convergence rate of SOR increases rapidly with increasing α; and, even for these models, convergence is measurably faster than for Poisson's equation.

TABLE 3.—*The variation in the Helmholtz parameter for each eigenmode appearing in a six-level primitive-equation model with semi-implicit time differencing*

	Eigenvalue number (n)					
	1	2	3	4	5	6
Eigenvalue α_n	4.4×10^{-16}	2.1×10^{-15}	1.7×10^{-14}	5.6×10^{-14}	1.3×10^{-13}	2.8×10^{-13}
Helmholtz coefficient $\alpha_n h^2$	3.1×10^{-1}	1.4×10^{0}	1.2×10^{1}	4.1×10^{1}	9×10^{1}	2.0×10^{2}

TABLE 4.—*Time (s) required to solve the two-dimensional Helmholtz equation on a rectangular domain (65×65) by the DCR, DRM, and SOR algorithms using an IBM 360/65 machine with the Fortran IV level H, Opt=2 compiler. The values of the Helmholtz coefficient for each eigenmode are given in table 3. In the case of SOR, the numbers in brackets are the number of iterations required to achieve the specified accuracy, δ. The total time taken to solve the Helmholtz equations for the set of six eigenmodes is given in the last column. The last line of the table shows the values of ω_b (the optimum relaxation parameter) used for the solution of each eigenmode using SOR.*

Method	Eigenmode						Totals
	1	2	3	4	5	6	
DCR	0. 89	0. 89	0. 89	0. 89	0. 89	0. 89	5. 3
DRM	1. 25	1. 25	1. 25	1. 25	1. 25	1. 25	7. 5
SOR ($\delta=10^{0}$)	0. 30 (1)	0. 30 (1)	0. 30 (1)	0. 30 (1)	0. 30 (1)	0. 30 (1)	1. 8
($\delta=10^{-2}$)	2. 10 (7)	1. 30 (4)	0. 91 (3)	0. 91 (3)	0. 60 (2)	0. 60 (2)	6. 4
($\delta=10^{-4}$)	4. 9 (16)	2. 10 (7)	1. 30 (4)	0. 91 (3)	0. 91 (3)	0. 91 (3)	11. 0
($\delta=10^{-6}$)	7. 6 (25)	3. 2 (10)	1. 6 (5)	1. 3 (4)	1. 3 (4)	1. 3 (4)	16. 3
ω_b	3.3955×10^{-1}	1.5689×10^{-1}	3.4649×10^{-2}	1.8546×10^{-2}	9.6224×10^{-3}	4.9211×10^{-3}	

Research Centre (Gauntlett and Hincksman 1971) and currently being converted to semi-implicit time-differencing (Gauntlett 1971), was used to provide representative values of α. By using real initial data, we were able to provide good first guesses to SOR, thereby removing the bias in favor of the direct methods described in section 3. Each time step requires that six Helmholtz equations be solved, the Helmholtz coefficients varying from small to very large (table 3). The times taken to advance one time step forward; that is, to solve all six equations, was compared for a variety of combinations of direct and iterative methods (table 4). Variations of map factor have been ignored to ensure that α is constant; otherwise, the DCR and DRM methods may not be applied in their present form. Such an assumption is, of course, valid only for such limited-area grids as the Bushby-Timpson grid (Bushby and Timpson 1967). The implications of the present requirement of constant α for the fastest direct methods will be discussed next.

The times taken by DCR and SOR on a 65×65 rectangular subset of the original N30 hemispheric domian reveal that for an acceptable level of convergence (i.e., error tolerance no greater than 10^{-4}), SOR is still slower than applying DCR to all six equations (table 4). However, the difference is now not nearly so great as in section 3 because of the very rapid convergence for large values of the Helmholtz coefficient. The DCR method is about as fast as three iterations with SOR on the 65×65 grid; and, for the four slowest baroclinic modes, less than five iterations of SOR are needed for a relative error tolerance of 10^{-6}, which is approximately the accuracy of DCR on an IBM 360/65 using single precision arithmetic. The DCR method requires 5.3 s to solve all six equations on the 65×65 grid, while SOR takes 16.3 s for approximately the same level of accuracy, including 10.8 s for the two fastest modes. For a slightly lower relative error tolerance of 10^{-4} (one that is acceptable in many problems), SOR requires only 11.0 s. This suggests that, if the number of time steps was not too large, a case would still exist for the continued use of SOR, at least for some of the modes, even if the direct methods can be generalized to include variable Helmholtz coefficients and irregular domains (e.g., hemispheric models in which the domain is a circle). The simplicity of the SOR code compared with many direct methods (DCR being a notable exception) and the small additional storage demands are further factors in favor of the method.

5. SUMMARY

In section 3 it was seen that direct methods are available (such as DCR and DRM) that are clearly superior to SOR in terms of speed and accuracy, for solving Poisson's equation on a rectangular domain with specified boundary values. This conclusion was supported by a comparative evaluation of the methods with typical meteorological fields.[6] Another direct method, GSM, is intrinsically the fastest of all the methods discussed in section 2 but is not suitable for computers generally available at present because of its severe demands for precision. Only when modest accuracy is required and good first guesses are available does SOR seriously compete with the direct methods for the class of problems considered in section 3.

Speed and accuracy are, of course, not the only con-

[6] The investigation was repeated using a random field generated by the IBM pseudo-random-number generator subroutine, RANDU, and the results confirmed the conclusions reached in section 3.

siderations when a method is being assessed. Like most iterative methods, the SOR method is readily generalized to irregular domains and mixed boundary conditions. Furthermore, it is simple to code and involves little overhead storage cost. Direct methods, on the other hand, are not yet sufficiently flexible. Extensive additional coding is normally required to handle mixed boundary conditions, while the application to an irregular domain usually requires some type of transformation of either the coordinate system being used or the matrix arising in the formulation of the problem. Intensive research in recent years has produced some significant advances, however. For example, Buzbee et al. (1970, 1971) have shown how to generalize some direct methods to mixed boundary conditions and many types of irregular domains, and Le Bail (1972) has discussed the extension of Fourier methods to more general problems including mixed boundary conditions.

The conclusions reached regarding the choice of method for solving Helmholtz-type equations on a rectangular grid are not as definite as they were for the Poisson equation. As was discussed in section 4, the magnitude of the Helmholtz coefficient greatly influences the rate of convergence of the iterative methods. In particular, for large values of the Helmholtz coefficient, SOR required very few iterations to reach a high degree of accuracy. The relative flexibility of the iteractive methods was further illustrated in section 4, where it was seen that the fastest direct methods could not be applied to the case where the Helmholtz coefficient varies over the grid. In view of the growing importance of the Helmholtz equation in meteorology and other related fields, it is hoped that the current interest in extending direct methods will continue and that many of the present limitations will eventually be removed.

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