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The Optimisation of Approximate-Factorisation Schemes for Solving Elliptic Partial Differential Equations in Three Dimensions, Featuring a New Two-Factor Scheme

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Current three-dimensional approximate-factorisation schemes do not appear capable of the same degree of optimisation as their two-dimensional counterparts. This is due principally to the greater complexity engendered by the third factor that arises in going from two to three dimensions. A new two-factor scheme is proposed which may be optimised with much greater ease and gives reliable and rapid convergence for all problems so far attempted. Applications include numerical grid generation and the calculation of transonic potential flow. © 1988 Academic Press, Inc.

1. INTRODUCTION

Approximate-factorisation (AF) schemes have been used widely for the numerical solution of elliptic partial differential equations (PDEs), particularly those found in the field of computational fluid dynamics. Two examples of where elliptic PDEs arise in this subject are in grid generation [1, 2] (where solutions of Laplace or Poisson equations are frequently used to obtain a smoothly varying computational grid that conforms to the boundaries of the computational region) and in the solution of potential flow problems. Ballhaus *et al.* [3] introduced the two types of AF schemes regularly used for two-dimensional (2D) steady flow problems and named them the AF1 and AF2 schemes. The simpler scheme, AF1, appears to be less suited to transonic flow problems than AF2, and the latter scheme has enjoyed considerable success (see Holst [4] and Baker [5]). Catherall [6] presented an analysis of the AF1 and AF2 schemes and showed how to optimise them so that rapid convergence was assured.

For three-dimensional problems rapid convergence has been much more difficult to achieve. Holst's [7] scheme has been the most successful for certain problems. Attempts by Baker and Forsey [8] to produce a version of Holst's scheme with faster convergence were only partially successful, the actual speed of convergence obtained depending on the particular problem being solved.

In this report a theoretical analysis of the three-dimensional version of AF1 and Holst's version of AF2 is described. It is shown that the analytical optimisation that

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was possible for the two-dimensional schemes [6] is impractical for the three-dimensional schemes. Another three-dimensional version of AF2 is then introduced, but having only two factors rather than three. This two-factor scheme can readily be optimised and is shown to give rapid convergence for all examples tested. A discussion is included on the important matter of what boundary conditions should be applied during the intermediate stages of a multifactor scheme.

2. Two-Dimensional AF Schemes

As a convenient introduction to AF schemes in general, a brief resumé of the two-dimensional schemes will be given. (For a more detailed exposition of the various techniques used, see Ref. [9], which provides a valuable introduction to the subject.)

The finite-difference equation,

$$L(\phi_{i,k}) = (A\,\vec{\delta X}\,\overleftarrow{\delta X} + C\,\vec{\delta Z}\,\overleftarrow{\delta Z} + D)\,\phi_{i,k} = 0 \tag{1}$$

results from replacing the derivatives in the general partial-differential equation,

$$\left(A\frac{\partial^2}{\partial X^2} + C\frac{\partial^2}{\partial Z^2} + D\right)\phi(X, Z) = 0$$

by central differences. A and C are positive, but not necessarily constant terms. They may be functions of ϕ and its first derivatives and they often contain transform derivatives resulting from a transformation from physical, Cartesian, space (x, z) to computational space (X, Z). The term D contains all the mixed and lower order derivatives (and thus their finite-difference analogs). Backward and forward differences are denoted above by $\overleftarrow{\delta X}$ and $\vec{\delta X}$, $\vec{\delta X}\,\phi_i \equiv \phi_{i+1} - \phi_i$; $\overleftarrow{\delta X}\,\phi_i \equiv \phi_i - \phi_{i-1}$; hence $\vec{\delta X}\,\overleftarrow{\delta X}\,\phi_i \equiv \phi_{i+1} - 2\phi_i + \phi_{i-1}$.

Equation (1) cannot be solved directly, by virtue of the complexity of the complete equation set that it represents and its possible nonlinear nature. Recourse must be made to iterative schemes for the solution of the equation. An iterative procedure is introduced of the form

$$N(\Delta) = L(\phi^n), \tag{2}$$

where the superscript n indicates the stage or level of the iteration, Δ is defined as $\phi^{n+1} - \phi^n$, the increment in solution during the iteration cycle. N is an operator that is simpler (in some sense) than the original operator L. In the approximate factorisation (AF) procedure N consists of two factors, each of which is easily inverted.

The AF1 scheme, originally devised by Peaceman and Rachford [10], may be written as

AF1:

$$\lambda^{-1}(\alpha - \lambda A\, \vec{\delta X}\, \overleftarrow{\delta X})(\alpha - \lambda C\, \vec{\delta Z}\, \overleftarrow{\delta Z})\, \Delta_{i,k} = \alpha\sigma L(\phi^n_{i,k}), \tag{3}$$

where α is termed an acceleration parameter, σ a relaxation parameter, and λ is a function of A and C, the precise form of which is crucial in determining the speed of convergence of the iterative method. The actual procedure used at each stage of the iteration is to solve in turn the two sets of equations

$$\lambda^{-1}(\alpha - \lambda A\, \vec{\delta X}\, \overleftarrow{\delta X})\, F_{i,k} = \alpha\sigma L(\phi^n_{i,k}) \tag{4a}$$

$$(\alpha - \lambda C\, \vec{\delta Z}\, \overleftarrow{\delta Z})\, \Delta_{i,k} = F_{i,k} \tag{4b}$$

for all points (i, k) to obtain Δ for each point, then increment the solution to obtain $\phi^{n+1} = \phi^n + \Delta$ and go onto the next iteration. The cycle of iterations is terminated when the maximum value of Δ is below some predefined tolerance. Each of Eqs. (4a) and (4b) is easily solved, and careful choice of σ, λ, and a sequence of values for α results in rapid convergence. In Ref. [6] optimum forms of the AF1 scheme are shown to exist, one with $\lambda = 1/C$, and $\sigma = 2$ and the other having $\lambda = 1/\sqrt{AC}$ and $\sigma = \frac{4}{3}$.

An alternative decomposition or factorisation of the finite-difference equation (1) with two factors, called AF2, may be written as

AF2:

$$\lambda^{-1}(\alpha - \lambda A\, \vec{\delta X})(\alpha\, \overleftarrow{\delta X} - \lambda C\, \vec{\delta Z}\, \overleftarrow{\delta Z})\, \Delta_{i,k} = \alpha\sigma L(\phi^n_{i,k}). \tag{5}$$

In Ref. [6] it is shown that the optimum version of AF2 has $\lambda = 1/\sqrt{AC}$ with $\sigma = \frac{4}{3}$, and a geometric series as a sequence of values for α. This result is still valid if the order of the factors is reversed, the roles of X and Z are interchanged, or if the splitting of the second difference into two first differences is performed in the reverse way. AF2 has usually been found to be faster than AF1, particularly when used to calculate transonic flows. In Ref. [6] it is demonstrated that a slight modification of the optimum form that avoids the evaluation of square roots resulting from the form of λ may be made, while retaining the rapid convergence of the original form. The important feature is the way in which the transform derivatives are split between the factors.

3. Three-Dimensional AF Schemes

In this section three schemes are considered, two of them having three factors and the third being a new scheme containing only two factors. In searching for other three-dimensional schemes, the following principle emerged from empirical and analytical investigations:

While it is beneficial to split one of the second differences between different fac-

tors (cf. AF1 and AF2), in that it speeds convergence particularly when calculating transonic flows, stability cannot be assured if more than one of the second differences is split.

The analysis in this section will be confined to the homogeneous difference problem

$$L(\phi_{i,j,k}) \equiv (A\,\vec{\delta X}\,\overleftarrow{\delta X} + B\,\vec{\delta Y}\,\overleftarrow{\delta Y} + C\,\vec{\delta Z}\,\overleftarrow{\delta Z})\,\phi_{i,j,k} = 0 \tag{6}$$

with A, B, and $C \geqslant 0$. Lower order terms and cross-derivatives may be present in practice; their inclusion does not appear to impair significantly the performance of an optimised scheme.

3.1. *Three-Dimensional Version of AF1*

The three-dimensional version of AF1 may be written as

3DAF1:

$$\lambda^{-1}(\alpha - \lambda A\,\vec{\delta X}\,\overleftarrow{\delta X})(\alpha - \lambda B\,\vec{\delta Y}\,\overleftarrow{\delta Y})(\alpha - \lambda C\,\vec{\delta Z}\,\overleftarrow{\delta Z})\,\Delta_{i,j,k} = \alpha^2 \sigma L(\phi^n_{i,j,k}). \tag{7}$$

As in two dimensions, the choice of λ, α, and σ will affect critically the speed of convergence. If the error after the nth iterative cycle is e^n (i.e., $\phi^n = \Phi + e^n$, where Φ is the exact solution of Eq. (6), then $\Delta = e^{n+1} - e^n$, and Eq. (7) may be written as

$$N(e^{n+1} - e^n) = \alpha^2 \sigma L(e^n), \tag{8}$$

where it is assumed, for simplicity, that L is a linear operator so that $L(\Phi + e^n) = L(\Phi) + L(e^n) = L(e^n)$, from Eq. (6). A von Neumann stability analysis [6] is performed by expressing the error as a multi-dimensional Fourier series

$$e^n(X, Y, Z) = \sum_{p,q,r} G^n(p, q, r) \exp(ipX) \exp(iqY) \exp(irZ). \tag{9}$$

(NB. Here i denotes the square root of -1, and not the index in the X direction.) Equation (9) is substituted in Eq. (8), and each Fourier component is considered separately. This analysis is only strictly valid for constant A, B, and C and for periodic boundary conditions, but in practice it often yields useful results for more complex situations. It may be shown, for the 3DAF1 scheme given by Eq. (7), that the amplification factor β is given by

$$\beta = \frac{G^{n+1}}{G^n} = \frac{\left[\begin{array}{l}(\alpha - 4\lambda AP)(\alpha - 4\lambda BQ)(\alpha - 4\lambda CR) \\ \quad + 4\alpha^2\lambda(AP + BQ + CR)(2 - \sigma) + 128\lambda^3 ABCPQR\end{array}\right]}{(\alpha + 4\lambda AP)(\alpha + 4\lambda BQ)(\alpha + 4\lambda CR)} \tag{10}$$

where $P = \sin^2(\frac{1}{2}p\,\Delta X)$, $Q = \sin^2(\frac{1}{2}q\,\Delta Y)$, $R = \sin^2(\frac{1}{2}r\,\Delta Z)$, and ΔX, ΔY, and ΔZ are the mesh spacings in the X, Y, and Z directions, respectively. For stability, which is a necessary condition for convergence, the amplification factor β must be

less than 1 in magnitude and this is assured for $\sigma \leqslant 2$. For rapid convergence $|\beta|$ must be as small as possible, and α, λ, and σ need to be chosen to make this so. In two dimensions (putting $B=0$ in Eq. (10)), β can be made equal to zero by setting $\sigma=2$ and $\alpha/\lambda=4CR$ (leading to the immediate annihilation of errors at particular frequencies and, hopefully, a reduction of errors at other frequencies). However, a similar result cannot easily be obtained for three-dimensional problems. Nevertheless, the choice $\sigma=2$ and $\alpha/\lambda=4CR$ can be expected to produce good, if not optimum, convergence for three-dimensional problems where the solution varies only slowly in either the X or Y direction, compared with the variation in the Z direction, and the initial approximation for ϕ is taken to be a constant at the start of the iterative sequence. This is not inconsistent with the common practice of setting ϕ to zero initially, apart from boundary values. In such cases, the error (Eq. (9)) is almost independent of X or Y, and G^n will be small for all finite values of p or q, respectively. Therefore it is only necessary to consider values of G corresponding to zero values of p or q, so that the final term in the numerator of Eq. (10) may be neglected because P or Q is zero. Hence a version of 3DAF1, which is moderately fast in certain cases, may be obtained from setting $\lambda=1/C$, $\alpha=4R$, and $\sigma=2$, i.e.,

$$(C\alpha - A\,\vec{\delta X}\,\overleftarrow{\delta X})(\alpha - B/C\,\vec{\delta Y}\,\overleftarrow{\delta Y})(\alpha - \vec{\delta Z}\,\overleftarrow{\delta Z})\,\Delta_{i,j,k} = 2\alpha^2 L(\phi^n_{i,j,k}). \tag{11}$$

The relation $\alpha=4R$ $(=4\sin^2(\frac{1}{2}r\,\Delta Z))$ is applied by choosing a geometric sequence of values for α ranging from $O(\Delta Z^2)$ to 4.

The solution at each iteration level proceeds in three stages:

$$(C\alpha - A\,\vec{\delta X}\,\overleftarrow{\delta X})\,F_{i,j,k} = 2\alpha^2 L(\phi^n_{i,j,k});$$

$$(C\alpha - B\,\vec{\delta Y}\,\overleftarrow{\delta Y})\,G_{i,j,k} = CF_{i,j,k};$$

$$(\alpha - \vec{\delta Z}\,\overleftarrow{\delta Z})\,\Delta_{i,j,k} = G_{i,j,k}.$$

This version of 3DAF1 has the added advantage of a particularly simple third stage, not involving A, B, or C.

3.2. *Three-Factor Version of AF2*

Equation (7) is an obvious extension of the two-dimensional version of AF1. The three-dimensional version of AF2 is, however, not so obvious. Holst [7] and Baker and Forsey [8] use the following scheme, here termed 3DAF3, where the final 3 is used to indicate that it is a three-stage factorisation,

3DAF3:

$$\lambda^{-1}[(\alpha - \lambda A\,\vec{\delta X}\,\overleftarrow{\delta X})(\alpha - \lambda B\,\vec{\delta Y}\,\overleftarrow{\delta Y}) - \alpha^2 E_z^{-1}](\alpha - \lambda C\,\vec{\delta Z})\,\Delta_{i,j,k} = \alpha^2\sigma L(\phi^n_{i,j,k}), \tag{12}$$

where E_z^{-1} is a shift operator, defined by $E_z^{-1}\Delta_k = \Delta_{k-1}$.

Application of a von Neumann stability analysis produces an expression for the

amplification factor β that is rather long and will not be repeated here. Again, stability is assured if $\sigma \leqslant 2$, but whereas in two dimensions an optimum choice of λ and α may be obtained by minimising β with respect to λ (or α), applying the same criteria in three dimensions becomes impossibly complicated. If the solution varies only slowly in the Y direction (BQ is small compared with AP and CR, following the argument in Section 3.1) then $\lambda = 1/\sqrt{AC}$ and $\alpha = 2\sqrt{P}$ is near optimum; whereas if the solution varies slowly in the X direction the appropriate values are $\lambda = 1/\sqrt{BC}$ and $\alpha = 2\sqrt{Q}$. In either case the problem is quasi-two-dimensional.

Holst [7] in his TWING code uses the full-potential equation to compute the flow over a wing using a grid based on cylindrical polar coordinates. With X taken as the angular ordinate around each spanwise section, Z the radial ordinate and Y the spanwise ordinate, Holst sets $\lambda = 1/C$, $\sigma = 1.8$, and $\alpha = 2\sqrt{P}$. This has the advantage that A, B, and C do not require evaluating in the third stage, but it is not clear why this should lead to rapid convergence. However, it was shown in Ref. [6] that for rapid convergence it is important to choose λ so that the factorisation is near optimum in the far-field. Furthermore, according to Baker and Forsey, who employ a similar coordinate system in Ref. [8], $A/C \to 1$ far from the wing. Accordingly, putting $\lambda = 1/C$ is a good approximation to $\lambda = 1/\sqrt{AC}$ which was shown, in the last paragraph, to be near optimum when there is only a small variation of the solution in the Y direction. Holst's scheme may therefore be expected to give rapid convergence for certain problems, but this cannot be guaranteed in general.

In Ref. [8], Baker and Forsey attempted to modify Holst's scheme by making some allowance for the effects of grid stretching. They chose $\lambda = Z\,\Delta Z(B\,\Delta Y^2)^{\nu}/C$ with $\nu = 0.1$ and Z measured in the radial direction. This worked extremely well for an isolated wing, but was much less successful when the computation of the flow about a wing-body combination was attempted.

In the examples given later in this paper Holst's [7] version of 3DAF3 (with $\lambda = 1/C$) is used for comparison with the new scheme detailed below.

3.3. *Two-Factor Version of AF2*

The major disadvantage of three-factor schemes is that they are difficult to optimise analytically unless the solution is quasi two-dimensional. This is clearly a severe limitation on any AF scheme. However, three-dimensional equivalents of two-dimensional AF schemes do *not* have to contain three factors. In contrast to AF1, there is a two-factor version of AF2 readily available:

$$[C/\lambda_3 - (A/\lambda_2)\,\vec{\delta X} - (B/\lambda_1)\,\vec{\delta Y}\,\overleftarrow{\delta Y}] \times [\lambda_1 + \lambda_2 \overleftarrow{\delta X} - \lambda_3\,\vec{\delta Z}\,\overleftarrow{\delta Z}]\,\Delta_{i,j,k} = \sigma L(\phi^n_{i,j,k}). \tag{13}$$

Application of a von Neumann stability analysis yields an expression for the amplification factor which can be minimised with respect to λ_1, λ_2, and λ_3 by setting $AC\lambda_1^2 = 4BCQ\lambda_2^2 = 16ABQR\lambda_3^2$. Details of some of the analysis may be found

in the Appendix. This result leads to the form (termed here 3DAF2 to denote that it is a two-stage scheme),

3DAF2:

$$(\alpha_1\alpha_2\sqrt{C}-\alpha_2\sqrt{A}\,\vec{\delta X}-\sqrt{B}\,\vec{\delta Y}\,\overleftarrow{\delta Y})(\alpha_1\alpha_2\sqrt{B}+\alpha_1\sqrt{A}\,\overleftarrow{\delta X}-\sqrt{C}\,\vec{\delta Z}\,\overleftarrow{\delta Z})\,\Delta_{i,j,k}$$
$$=\alpha_1\alpha_2\sigma L(\phi^n_{i,j,k}), \tag{14}$$

with $\alpha_1=2\sqrt{R}$ and $\alpha_2=2\sqrt{Q}$.

Stability is assured if $\sigma\leqslant 2$, but an optimum value for σ must be found by numerical experiment, unlike the result for two dimensions where optimum values for σ can be found by analysis. In the examples investigated in this report the value $\sigma=2$ has been found to give the most rapid convergence. The analysis detailed in the Appendix suggests that the best value for σ should lie in the range $1.5\leqslant\sigma\leqslant 2.0$. With a particular sequence of values for α_1 and α_2 the errors associated with the frequencies corresponding to these values will be reduced more rapidly than those of other frequencies. The overall speed of convergence will, however, depend on the largest amplification factor. In two-dimensional problems it is possible [6] to devise a sequence of values for the acceleration parameter which can be shown, analytically, to be near optimum. This does not appear to be possible in three dimensions, although there are indications that sequences similar to the two-dimensional ones may be applicable. These sequences are used in the following examples (Section 5).

4. Boundary Conditions

Boundary conditions will normally be applied at both ends of the X, Y, and Z ranges and will be either Dirichlet (ϕ prescribed) or Neumann (the derivative of ϕ normal to the boundary, ϕ_n, is prescribed). Most rapid convergence usually results from ensuring that all boundary conditions are implicitly satisfied at all stages of the iterative procedure. Thus at the start of the iterative cycle which progresses the solution from iteration level n to level $n+1$, ϕ^n can be assumed to satisfy all boundary conditions. The boundary condition prescribed for the increment, $\Delta\,(=\phi^{n+1}-\phi^n)$, is thus either $\Delta=0$ or $\Delta_n=0$ for Dirichlet or Neumann boundary conditions, respectively.

Boundary conditions are also required for the intermediate variables. For example, in order to solve Eq. (4a), boundary conditions on F need to be prescribed. If a Dirichlet condition is to be applied on ϕ at $i=1$ then $\Delta_{1,k}=0$ and from Eq. (4b)

$$F_{1,k}=(\alpha-\lambda C\,\vec{\delta Z}\,\overleftarrow{\delta Z})\,\Delta_{1,k}=0.$$

If a Neumann boundary condition is applied for ϕ at $i=1$ then the central difference form of the condition requires $\Delta_{0,k}=\Delta_{2,k}$. Thus, from Eq. (4b),

$$F_{2,k}-F_{0,k}=(\alpha-\lambda C\,\vec{\delta Z}\,\overleftarrow{\delta Z})(\Delta_{2,k}-\Delta_{0,k})=0.$$

This principle applies to any of the two-dimensional or three-dimensional factorisations, provided the appropriate difference expression is unsplit (i.e., a term $\vec{\delta X}\,\overleftarrow{\delta X}$ in $L(\phi)$ is matched explicitly by a term $\vec{\delta X}\,\overleftarrow{\delta X}$ in $N(\phi)$ (Eq. (2)), and it may be summarised as follows:

Where the difference equation to be solved for an intermediate dependent variable, F, retains unsplit differences for the independent variable, the boundary condition to be imposed on F is $F=0$ or $F_n=0$ when the boundary condition on ϕ is Dirichlet or Neumann, respectively. This type of boundary condition is termed straightforward.

Where differences are split (for example, the $\vec{\delta X}\,\overleftarrow{\delta X}$ terms in AF2), it is much more difficult to devise an appropriate intermediate boundary condition. South and Hafez [11], suggest how to devise a stable intermediate boundary condition for two-dimensional problems. If a Neumann boundary condition has to be applied at $z=0$ $(k=1)$ they suggest writing $G_{k-1}=\gamma G_k$ at $k=1$, where G is the intermediate variable whose boundary value is needed at $k=0$. By performing a stability analysis locally at the boundary, stability limits on the value of γ are found, and the above intermediate boundary condition enables the solution for G to be obtained during the first solution stage. Unfortunately, the technique cannot be extended to all three-dimensional problems. In particular, it cannot be applied to 3DAF3. Referring forward to Section 7, where the three solution stages are set out for 3DAF3, the condition $G_{k-1}=\gamma G_k$ needs to be applied at the first stage, but cannot be, since G is evaluated, not at this stage, but at the second.

Where differences are split, the following techniques are recommended for intermediate boundary conditions:

(i) Try to arrange for the intermediate boundary condition to apply at the "more innocuous" end of the computational range. For example, if one end of the computational region is a solid surface and the other a far-field boundary, then application of an intermediate boundary condition at the far-field boundary is less likely to induce instability.

(ii) If for any reason recommendation (i) cannot be followed, then the South and Hafez method should be attempted to determine an appropriate intermediate boundary condition.

(iii) If neither of the above is successful, put $F=0$ at the boundary and hope for the best!

5. The Three-Dimensional Factorisations Summarised

The following sequence of values for α was shown in Ref. [6] to be near optimum for two-dimensional (2D) problems and will be used in all the three-dimensional (3D) examples shown later:

$$\alpha_K=\alpha_h\left(\frac{\alpha_l}{\alpha_h}\right)^{(K-1)/(N_\alpha-1)} \qquad \text{for} \quad K=1, 2, ..., N_\alpha, \tag{15}$$

where α_l, α_h, and N_α are specified below. This sequence is repeated every N_α iterative cycles. In two-dimensions a slight improvement in convergence rate was obtained [6] by repeating the end points in this range, but this has not been investigated here.

The three-dimensional AF schemes which will be compared in the next two sections are now defined.

3DAF1: The factorisation given in Eq. (11) is used. In the sequence (15) $N_\alpha = 8$, $\alpha_h = 4$, $\alpha_l = \Delta Z^2$.

3DAF3: The Holst version of the scheme (from Ref. [7]) in Eq. (12) is used, so that $\lambda = 1/C$, $\sigma = 1.8$, $N_\alpha = 8$, $\alpha_h = 2$, and $\alpha_l = \Delta X$, except for the transonic flow problem in Section 7, where better results were obtained with $\alpha_l = 2\,\Delta X$.

3DAF2: The factorisation given in Eq. (14) is used, with $\sigma = 2.0$, $N_\alpha = 6$, $\alpha_{1h} = \alpha_{2h} = 2$, $\alpha_{1l} = \Delta Z$, and $\alpha_{2l} = \Delta Y$, except in the transonic flow problem (Section 7), where $\alpha_{1l} = 1.75\,\Delta Z$ and $\alpha_{2l} = 1.75\,\Delta Y$ produced faster convergence.

The values chosen for all the schemes described above are the result of numerical experiments to determine those combinations giving the fastest convergence rate for the examples in the next section.

6. Example—Solution of the Three-Dimensional Laplace Equation on a Stretched Computational Mesh

Laplace's equation

$$\phi_{XX} + \phi_{YY} + \phi_{ZZ} = 0$$

is to be solved inside a unit cube with boundary conditions defined below. To investigate the ability of the various AF schemes to respond to non-uniformity in meshes the following stretchings are applied:

$$X = \frac{1}{2} + \frac{[\tan^{-1}(a(2x-1))]}{(2\tan^{-1} a)},$$

$$Y = \frac{(\tan^{-1}(by))}{\tan^{-1} b},$$

$$Z = \frac{(\tan^{-1}(cz))}{\tan^{-1} c}.$$

A consequence of these stretchings is that the difference equation (6) will have

$$A=\left(\frac{X_x}{\Delta X}\right)^2$$

$$B=\left(\frac{Y_y}{\Delta Y}\right)^2$$

$$C=\left(\frac{Z_z}{\Delta Z}\right)^2$$

and $L(\phi)$ (but not $N(\Delta)$) will contain some first derivatives. In the examples shown here a, b, and c are all set equal to 5 and there are 64, 24, and 16 grid intervals in the X, Y, and Z directions, respectively. Other variations were tried, but not reported here, with similar comparative results emerging. Two problems are considered.

PROBLEM 1. Solution with rapid z variation. With boundary conditions $\phi=0$ on $x=0$, $x=1$, $y=1$, and $z=1$,

$$\phi_y=0 \qquad \text{on} \quad y=0$$

$$\phi_z=-\left(\frac{\pi\sqrt{5}}{2}\right)\cosh\left(\frac{\pi\sqrt{5}}{2}\right)\sin(\pi x)\cos\left(\frac{\pi y}{2}\right) \qquad \text{on} \quad z=0,$$

the exact solution is

$$\phi(x, y, z)=\sin(\pi x)\cos\frac{\pi y}{2}\sinh\left(\frac{\pi\sqrt{5}}{2}(1-z)\right).$$

This solution varies much more rapidly in the z direction than in either the x or y directions.

Figure 1 shows the convergence history of the three schemes used for Problem 1

$|L(\phi)|$ at that point divided by the maximum value of $|L(\phi)|$ at the start of the computation. Initially ϕ is set to zero inside the unit cube and on the boundary of the cube, the Neumann boundary conditions being enforced by the use of dummy points outside the unit cube.

The other set of curves is for a typical quantity obtained from the solution, in this case the value of ϕ at $x=\frac{1}{2}$, $y=z=0$, divided by its finally converged value. For this problem the three AF schemes yield similar levels of performance. 3DAF2 is the fastest, but it is closely followed by 3DAF3 and even 3DAF1 performs quite well. The values used for the various parameters (σ, N_α, etc.) are those given in the previous section and offer the fastest rates of convergence determined by numerical experiments. Reversing the direction of sweep in the z direction for 3DAF3 slowed the convergence rate slightly.

It is interesting to observe the effect of using a constant value for the acceleration

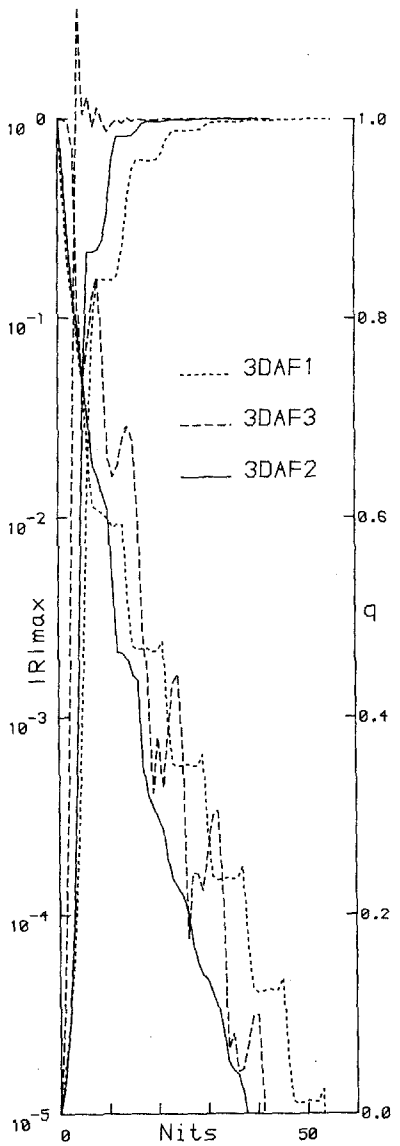

FIG. 1. Problem 1: Laplace's equation with rapid z variation.

parameter. In Fig. 2, instead of using a sequence of values of α_1 and α_2 as in Eq. (15), the performance of 3DAF2 is shown when constant values for Eq. (15) are chosen. It emerges that the most rapid convergence for the quantity q is achieved for $K=6$ (α_1 and $\alpha_2=\Delta Z$ and ΔY, respectively), but that the residual reduces fastest for the fourth value in the sequence (in this case $\alpha_1=4\,\Delta Z$ and $\alpha_2=4.7\,\Delta Y$). This exercise demonstrates that it is important to use a sequence (such as Eq. (15))

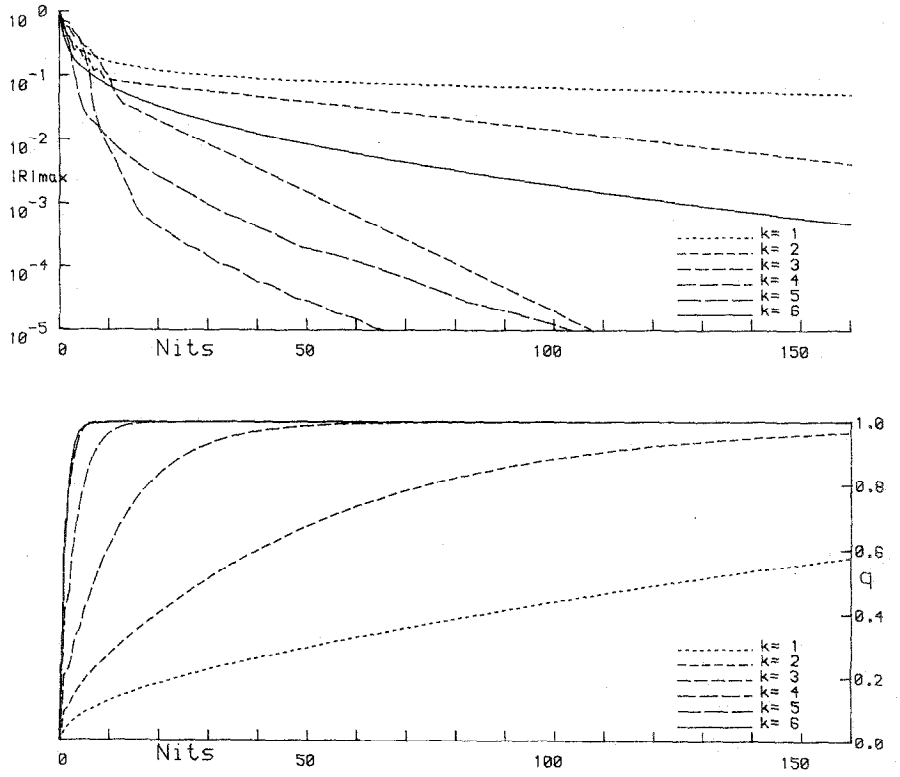

FIG. 2. Problem 1: 3DAF2 with constant values of acceleration parameter: top, residual; bottom, q.

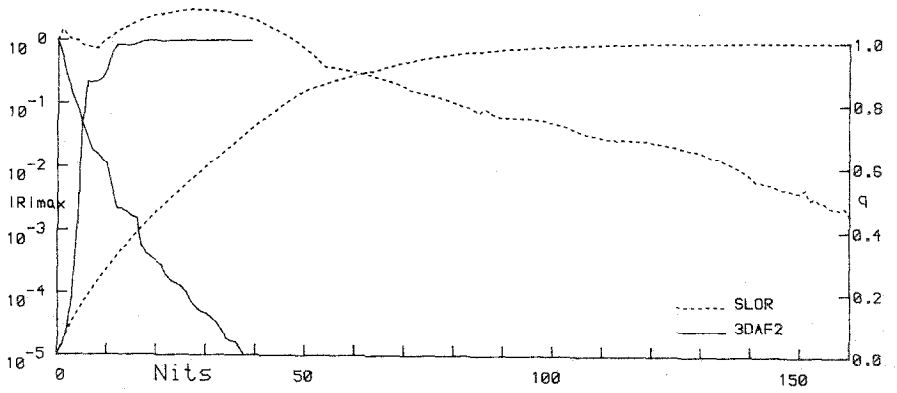

FIG. 3. Problem 1: 3DAF2 versus SLOR.

rather than constant values for α. It may well be that further improvement in convergence rates is possible by varying σ as well as α, but this has not been investigated here.

In Fig. 3 the performance of 3DAF2 is compared with the more conventional successive line over-relaxation method (SLOR). A relaxation factor of 1.95 (which gives the fastest convergence rate for this example) has been used. It is apparent that 3DAF2 offers a dramatic speed improvement over even this optimised SLOR.

PROBLEM 2. Solution with rapid y variation. This problem is identical to

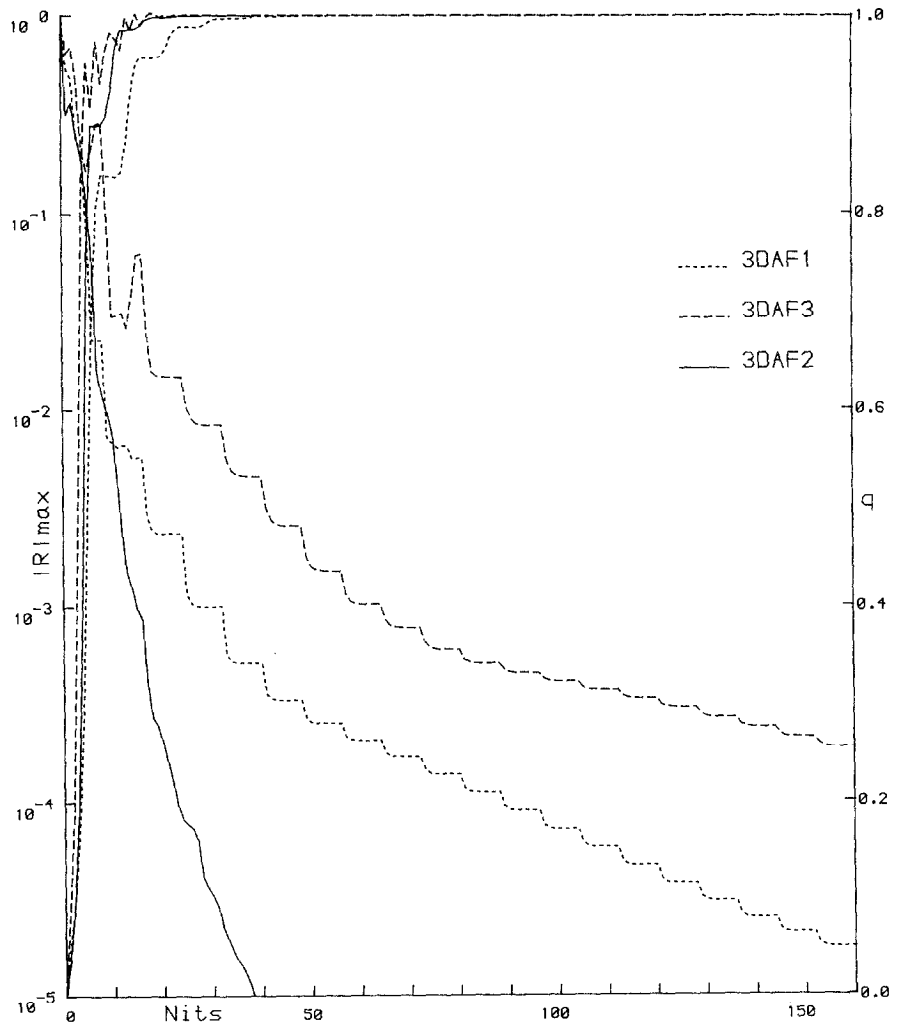

FIG. 4. Problem 2: Laplace's equation with rapid y variation.

Problem 1, except that the boundary conditions at $y=0$ and $z=0$ are changed as follows:

$$\phi_y = -\left(\frac{\pi\sqrt{5}}{2}\right)\cosh\left(\frac{\pi\sqrt{5}}{2}\right)\sin(\pi x)\cos\left(\frac{\pi z}{2}\right) \quad \text{on} \quad y=0$$

$$\phi_z = 0 \quad \text{on} \quad z=0.$$

The analytic solution for Problem 2 is the solution for Problem 1 with the roles of y and z interchanged. The solution thus varies rapidly in the y direction. Figure 4 shows the convergence history for the three schemes, and it may be seen that only 3DAF2 maintains its performance, whereas the other two schemes show a degradation in rate of residual reduction for this problem. This demonstrates that 3DAF2 is in some sense problem independent, whereas the other two schemes are only quasi-optimum for certain problems. No improvement can be obtained for 3DAF1 and 3DAF3 by varying parameters such as σ, N_z, or α.

7. Example—Solution of the Quasi-Conservative Small Disturbance Potential Equation for Transonic Flow

We take the simplest form of the three-dimensional small disturbance potential equation for compressible flow near $M_\infty = 1$,

$$(\beta^2 - K\phi_x)\,\phi_{xx} + \phi_{yy} + \phi_{zz} = 0,$$

where $\beta^2 = 1 - M_\infty^2$, $K = M_\infty^2(2 + (\gamma - 1)$, M_∞ is the free-stream Mach number, and γ the ratio of specific heats ($=1.4$).

The example chosen here is non-lifting flow at a Mach number of 0.85 over a spherical bump (the three-dimensional equivalent of the circular arc aerofoil) whose maximum height, t, is 10% of its maximum chord. The boundary conditions are thus:

$$\phi \to 0 \quad \text{as} \quad x^2 + y^2 + z^2 \to \infty;$$

$$\phi_y = 0 \quad \text{on} \quad y=0 \quad \text{(a symmetry condition)};$$

$$\phi_z = 0 \quad \text{on} \quad z=0; \quad x^2 + y^2 > \tfrac{1}{4};$$

$$\phi_z = -x.2t/(0.25 - t^2) \quad \text{on} \quad z=0, \quad x^2 + y^2 \leqslant \tfrac{1}{4}.$$

The grid stretchings employed are

$$0 < X < \frac{1}{2}(1-a_x), \qquad x = -\frac{1}{2} + \left(\frac{b}{a_x}\right) \tan\left[\frac{(X - 1/2(1-a_x))}{b}\right],$$

$$\frac{1}{2}(1-a_x) \leqslant X \leqslant \frac{1}{2}(1+a_x), \qquad x = \frac{(X-1/2)}{a_x},$$

$$\frac{1}{2}(1+a_x) < X < 1, \qquad x = \frac{1}{2} + \left(\frac{b}{a_x}\right) \tan\left[\frac{(X - 1/2(1+a_x))}{b}\right],$$

with $b = (1-a_x)/\pi$ and $a_x = 0.5$;

$$0 \leqslant Y \leqslant \frac{1}{2}a_y, \qquad y = \frac{Y}{a_y},$$

$$\frac{1}{2}a_y < Y < 1, \qquad y = \frac{1}{2} + \left(\frac{\bar{b}}{a_y}\right) \tan\left[\frac{(Y - 1/2a_y)}{\bar{b}}\right],$$

with $\bar{b} = (2-a_y)/\pi$ and $a_y = 1.0$;

$$0 \leqslant Z < 1, \qquad z = \left(\frac{1}{a_z}\right) \tan\left(\frac{\pi Z}{2}\right)$$

with $a_z = 10$.

Three views of the grid are presented in Fig. 5. In Fig. 5a all grid lines (except, of course, for those at infinity) are shown in the plane $z = 0$ and in Fig. 5b a close-up of Fig. 5a is shown in the neighbourhood of the solid surface. Figure 5c shows a close-up in the plane $y = 0$.

In transformed space the small disturbance equation is now

$$(\beta^2 - KX_x\phi_X)\, X_x(X_x\phi_X)_X + Y_y(Y_y\phi_Y)_Y + Z_z(Z_z\phi_Z)_Z = 0, \tag{16}$$

the subscripts denoting differentiation.

A quasi-conservative finite difference solution results from solving, in conjunction with the boundary conditions, the set of difference equations

$$L(\phi_{i,j,k}) \equiv [\mu_i T_i \bar{A}_i \vec{\delta X}\, \bar{A}_{i-1/2} \overleftarrow{\delta X} + (1-\mu_{i-1})\, T_{i-1} \bar{A}_{i-1} \overleftarrow{\delta X}\, \bar{A}_{i-1/2} \overleftarrow{\delta X} + \bar{B}_j \vec{\delta Y}\, \bar{B}_{j-1/2} \overleftarrow{\delta Y} + \bar{C}_k \vec{\delta Z}\, \bar{C}_{k-1/2} \overleftarrow{\delta Z}]\, \phi_{i,j,k} = 0, \tag{17}$$

where

$$T_i = \beta^2 - K\bar{A}_i(\phi_{i+1,j,k} - \phi_{i-1,j,k})/2;$$

$$\mu_i = 1 \quad \text{if} \quad T_i \geqslant 0 \quad \text{and} \quad 0 \text{ otherwise};$$

$$\bar{A}_i = X_x(i)/\Delta X; \qquad \bar{B}_j = Y_y(j)/\Delta Y; \qquad \bar{C}_k = Z_z(k)/\Delta Z.$$

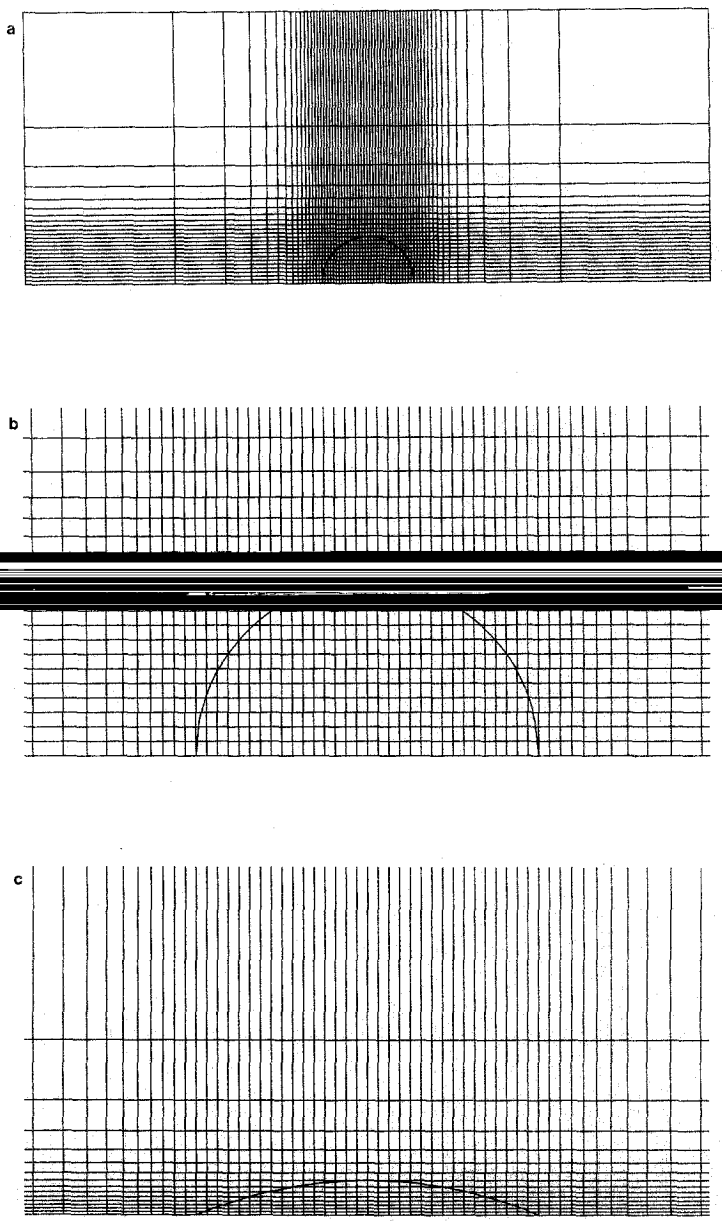

FIG. 5. (a) Grid in plane $z=0$ for transonic flow problem. (b) Close-up of Fig. 5a. (c) Close-up of grid in plane $y=0$ for transonic flow problem.

The three AF schemes under consideration now take the forms:

3DAF1:

$$[\bar{C}_k^2\alpha-\mu_i T_i \bar{A}_i \vec{\delta X}\,\bar{A}_{i-1/2}\,\overleftarrow{\delta X}-(1-\mu_{i-1})\,T_{i-1}\bar{A}_{i-1}\bar{A}_{i-1/2}\,\overleftarrow{\delta X}]\,F_{i,j,k}$$
$$=\alpha^2\sigma L(\phi^n_{i,j,k});$$
$$[\bar{C}_k^2\alpha-\bar{B}_j\,\vec{\delta Y}\,\bar{B}_{j-1/2}\,\overleftarrow{\delta Y}]\,G_{i,j,k}=\bar{C}_k^2 F_{i,j,k};$$
$$[\alpha-\vec{\delta Z}\,\overleftarrow{\delta Z}]\,\Delta_{i,j,k}=G_{i,jk}.$$

3DAF3:

$$[\bar{C}_k\alpha-\bar{\lambda}\{\mu_i T_i\bar{A}_i\,\vec{\delta X}\,\bar{A}_{i-1/2}\,\overleftarrow{\delta X}+(1-\mu_{i-1})\,T_{i-1}\bar{A}_{i-1}\bar{A}_{i-1/2}\,\overleftarrow{\delta X}\}]\,F_{i,j}$$
$$=\alpha^2\sigma L(\phi^n_{i,j,k})+\bar{C}_k^2\alpha^2 G_{i,j,k-1};$$
$$[\bar{C}_k\alpha-\bar{\lambda}\bar{B}_j\,\vec{\delta Y}\,\bar{B}_{j-1/2}\,\overleftarrow{\delta Y}]\,G_{i,j,k}=F_{i,j};$$
$$\left[\frac{\alpha}{(\bar{C}_k\bar{\lambda})}-\vec{\delta Z}\right]\Delta_{i,j,k}=G_{i,j,k};$$

with $\bar{\lambda}=1/\bar{C}_k$.

3DAF2:

$$\left[\alpha_1\alpha_2\bar{C}_k-\left(\frac{\alpha_2}{\bar{\beta}}\right)\{\mu_i T_i\bar{A}_i\,\vec{\delta X}+(1-\mu_{i-1})\,T_{i-1}\bar{A}_{i-1}\}-\bar{B}_j\,\vec{\delta Y}\,\overleftarrow{\delta Y}\right]F_{i,j,k}$$
$$=\alpha_1\alpha_2\sigma L(\phi^n_{i,j,k});$$
$$[\alpha_1\alpha_2\bar{B}_j+\alpha_1\bar{A}_{i-1/2}\beta\,\overleftarrow{\delta X}-\vec{\delta Z}\,\bar{C}_{k-1/2}\,\overleftarrow{\delta Z}]\,\Delta_{i,j,k}=F_{i,j,k}.$$

The following points should be noted:

(i) The upwind differencing in the X direction when the flow is locally supersonic has not been fully simulated in any of the AF schemes. Nevertheless, because it is done correctly in $L(\phi)$ then, provided convergence is achieved, the solution should be unaffected. The reason for this omission in the first two cases is to maintain tridiagonality, so simplifying the matrix inversion problem. In the third case values of F are not available for lower values of i. The upwind differencing is, however, partially simulated in all cases: the term $(\overleftarrow{\delta X}\,\bar{A}_{i-1/2}\,\overleftarrow{\delta X})\,F_i$ when expanded becomes $\bar{A}_{i-1/2}(F_i-F_{i-1})-\bar{A}_{i-3/2}(F_{i-1}-F_{i-2})$. Omitting the second half of this term is equivalent to using values for $\phi_x|_{i-3/2}$ from the previous iteration level. Similarly, if a forward difference (which occurs when treating the full-potential equation) were involved, $(\vec{\delta X}\,\bar{A}_{i+1/2}\,\vec{\delta X})\,F_i=\bar{A}_{i+3/2}(F_{i+2}-F_{i+1})-\bar{A}_{i+1/2}(F_{i+1}-F_i)$ and omission of the first half of the term would be equivalent to evaluating $\phi_x/_{i+3/2}$ from the previous iteration level. In practice, the omission of part of the upwind term from the factorisation has not been found to cause any problems.

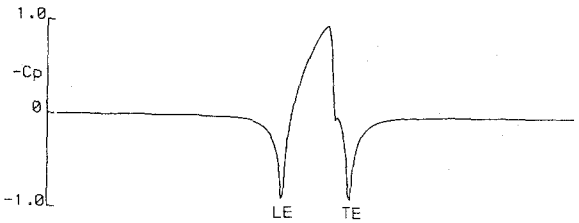

FIG. 6. Pressure distribution for transonic flow problem.

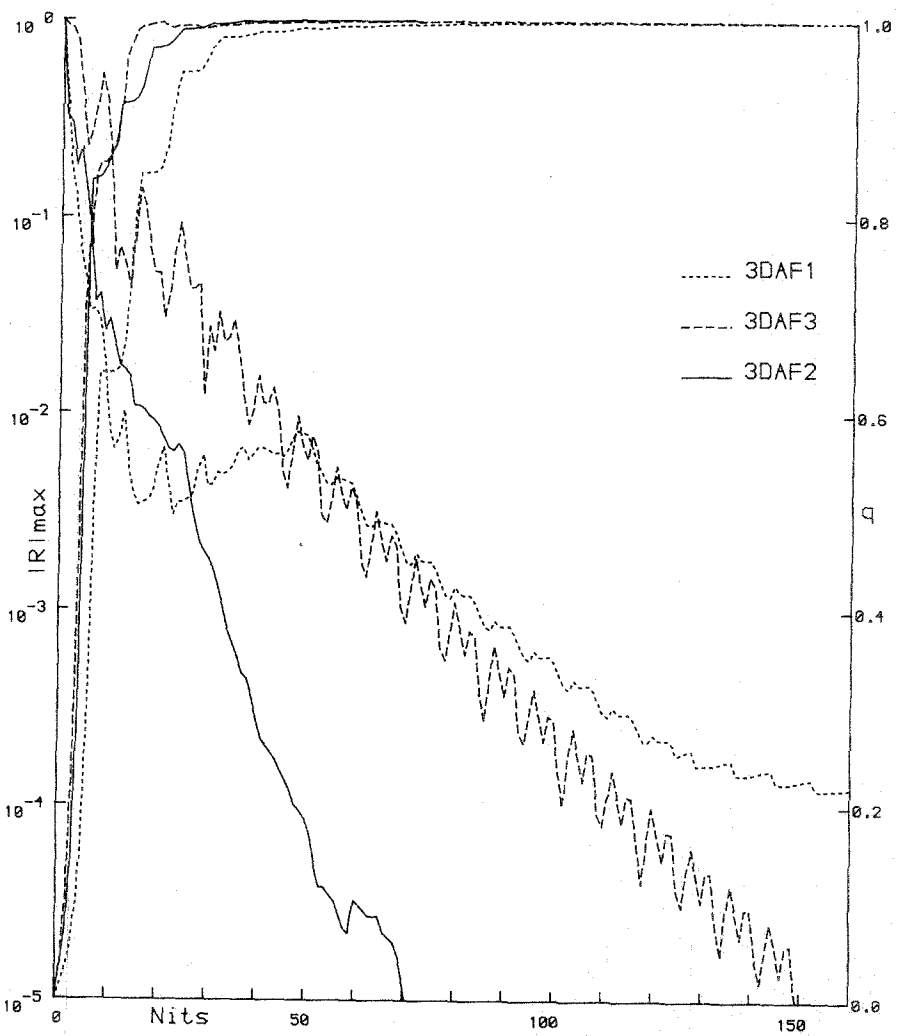

FIG. 7. Convergence of AF schemes for transonic flow problem.

(ii) In this quasi-conservative formulation it is not always convenient to evaluate transform derivatives within the factors precisely as within L; see, for example, the third factor of 3DAF1. In two-dimensional lifting flow it has sometimes been found important, for convergence, to have the same form within L, but in the present exercise it does not appear to matter. In fact, replacing $\alpha - \vec{\delta Z}\,\overleftarrow{\delta Z}$ in the third factor of 3DAF1 by $\alpha - (1/\bar{C}_k)\,\vec{\delta Z}\,\bar{C}_{k-1/2}\,\overleftarrow{\delta Z}$ actually made convergence slower.

(iii) In 3DAF2 the X second difference is split between the two factors, and, according to the earlier analysis, T_i as well as $\bar{A}_i^2$ should be split between the two factors. This would be most inconvenient to apply since it would involve evaluating T_i during the second as well as the first stage (where it has to be evaluated for inclusion in $L(\phi)$) and also involve costly square roots. In Ref. [6] it was shown that the most important feature affecting convergence speed is the correct splitting between the factors in the far-field. Here $T_i \sim \bar{\beta}^2$ in the far-field and this should be split, as above, so that $T_i/\bar{\beta}$ is included in the first factor and $\bar{\beta}$ in the second.

The pressure distribution on $y = z = 0$ for this problem (the pressure coefficient C_p is evaluated as $C_p = -2\phi_x$) is shown in Fig. 6, the two dips in the distribution corresponding to the leading and trailing edges, and the convergence of the three schemes is compared in Fig. 7. In this case the quantity q which is plotted is the value of C_p at the top of the bump (at $x = y = z = 0$ in the small disturbance simulation) divided by its converged value. Once again 3DAF2 produces the most rapid convergence, with 3DAF1 performing the worst. Many other cases were run, varying the Mach number, height of bump, grid stretchings, and the grid dimensions, and in every case 3DAF2 out-performed the other two schemes, as it also did with the non-conservative small disturbance equation.

8. Computation Times

All the computational examples were run on a Cray 1-S computer. A particular advantage of the AF schemes when a vector processor is used is that *all* DO loops may be vectorised. For example, in 3DAF2, the evaluation of $L(\phi)$ and the coefficients of the unknowns $F_{i,j,k}$ can be performed in parallel for all points on an $i =$ constant plane. The resulting tridiagonal matrices may then be inverted in parallel along each $j =$ constant column. For a $62 \times 24 \times 16$ mesh (i.e.., nearly 25,000 points) the time taken for each of the AF schemes to advance one iteration level varied between 0.05 s for Problems 1 and 2 to 0.07 s for the transonic flow problem. Times for complete solution (a reduction in the maximum residual by five orders of magnitude) via the 3DAF2 scheme of the examples given varied between 2 and 5 s. The SLOR scheme applied to Problem 1 was actually slower per iteration cycle (0.075 s) than the AF schemes, because less of the code was vectorisable, and the complete solution time was about 20 s, ten times that for 3DAF2.

9. Concluding Remarks

The optimisation of three-dimensional approximate factorisation schemes has been addressed in the preceding sections. It has been shown that schemes involving three factors may be optimised in a very approximate sense for particular problems, but that the particular form of the schemes so obtained will not necessarily perform well on other problems. By contrast, the two-factor scheme described in its optimum form in this report, performs well on all problems that have been addressed so far. Applications for the method include numerical grid generation and subsonic or transonic potential flow calculation. The scheme has also been applied to three-dimensional transonic potential flow problems with similar success, though these are not reported here. An additional complication when treating the full potential equation is the presence of cross-derivative terms. These must, of course, be included in the residual $L(\phi)$, but it has not been found necessary to modify the AF factors to allow for them, even when the grid is not orthogonal (examples run have included regions with a 35° departure from orthogonality with no noticeable deterioration in performance).

Despite the advent of multigrid techniques, which are capable of achieving faster convergence rates (perhaps by a factor of 2 or more for a 4-level multigrid scheme) in terms of computation time than AF schemes without multigrid, by virtue of the reduction of low frequency errors on a coarse grid, AF schemes are still of great utility.

They are easy to program, easily produce vectorisable code, are more economic in computer storage than multigrid, are simple to apply, and are fast and efficient [redacted] optimum forms have been deduced and these two papers thus form user guides to the application of AF schemes in both two and three dimensions.

APPENDIX: Analysis of 3DAF2

Here a von Neumann stability analysis is performed (as in Section 3.1) for the 3DAF2 scheme described by Eq. (13). The analysis is simplified by the substitutions

$$\xi \equiv 2\sqrt{\frac{BQ}{A}}\cdot\frac{\lambda_2}{\lambda_1} > 0; \qquad \eta \equiv 4\sqrt{\frac{BQR}{C}}\cdot\frac{\lambda_3}{\lambda_1} > 0. \tag{A.1}$$

(One of the λs is effectively redundant.) After some algebra it may be shown that

$$\beta^2 = \left|\frac{G^{n+1}}{G^n}\right|^2 = \left[\left\{\left(\eta+\frac{1}{\eta}\right)\sqrt{BCQR}+\left(\frac{\xi}{\eta}+\frac{\eta}{\xi}\right)P\sqrt{ACR}\right.\right.$$
$$\left.\left.+P\left(\xi+\frac{1}{\xi}\right)\sqrt{ABQ}+(1-\sigma)(AP+BQ+CR)\right\}^2\right.$$

$$+P(1-P)\left\{\left(\frac{\xi}{\eta}-\frac{\eta}{\xi}\right)\sqrt{ACR}+\left(\xi-\frac{1}{\xi}\right)\sqrt{ABQ}\right\}^2\Bigg]$$

$$\div [\text{the same expression but with } \sigma=0]. \tag{A.2}$$

For stability we require $|\beta| \leqslant 1$, and this is assured if $0 \leqslant \sigma \leqslant 2$.

For rapid convergence we need to choose ξ and η so as to minimise $|\beta|$. Values of ξ and η which satisfy $\partial(\beta^2)/\partial\xi = \partial(\beta^2)/\partial\eta = 0$ are $\xi = \eta = 1$. This may be seen by writing Eq. (A.2) as

$$\beta^2 = \frac{(u-\sigma v)^2 + w^2}{u^2 + w^2},$$

where u and w are functions of ξ and η while v is not. Therefore $\partial(\beta^2)/\partial\xi = 0$ when

$$\left(\frac{\partial u}{\partial \xi}\right)(u^2 - w^2 - \sigma uv) + w\left(\frac{\partial w}{\partial \xi}\right)(2u - \sigma v) = 0,$$

with a similar expression, involving η derivatives, giving $\partial(\beta^2)/\partial\eta = 0$. One way of fulfilling these conditions is to set $w = \partial u/\partial\xi = \partial u/\partial\eta = 0$ and, by comparing with Eq. (A.2) it may be seen that this occurs when $\xi = \eta = 1$. This may not be the only solution but it has the virtue of simplicity. A simple solution is essential as it is necessary to express each λ as a function of A, B, and C multiplied by a function of P, Q, and R, as shown below.

It is easy to demonstrate that $\xi = \eta = 1$ minimises $|\beta|$ with respect to ξ and η, provided $\sigma \leqslant 1$. However, for $1 < \sigma \leqslant 2$ it has not been possible to prove that, in all cases, this solution gives a minimum rather than a maximum. It should be noted, however, that stability is still assured, by choosing $\sigma \leqslant 2$, even if the choice of ξ and η is not optimum in some small regions.

Setting $\xi = \eta = 1$ in Eq. (A.2) we obtain

$$\beta_{\min} = \left|1 - \frac{\sigma(AP + BQ + CR)}{2\sqrt{BCQR} + 2P\sqrt{ACR} + 2P\sqrt{ABQ} + AP + BQ + CR}\right|.$$

We shall attempt to minimise the largest value of $\beta_{\min}$ by a suitable choice of σ. First, stationary values of $\beta_{\min}$ with respect to BQ and CR are found. These occur when

$$CR = BQ = 0.25\sqrt{A}\,(1 + \sqrt{1+8P}),$$

giving

$$\beta_{\min} = \left|1 - \frac{1/2\sigma(1+\sqrt{1+8P})}{1+2P+\sqrt{1+8P}}\right|.$$

The maximum value of $\beta_{\min}$ will occur therefore either when $BQ = CR = 0$ (so that $\beta_{\min} = |1-\sigma|$), or when

$$BQ = CR = 0.25A(1+\sqrt{1+8P})$$

and

$$P = 0 \text{ or } 1 \qquad (\beta_{\min} = |1-\tfrac{1}{2}\sigma| \text{ or } |1-\tfrac{1}{3}\sigma|).$$

Whichever of these three values is largest depends on σ, and it would appear that $\beta = \frac{3}{2}$ should minimise the largest value. However, although P, Q, and R may take small values they are never zero, so $\beta_{\min}$ never takes the value $|1-\sigma|$, and so the best value for σ may be higher than $\frac{3}{2}$, reducing $|1-\sigma/2|$ and $|1-\sigma/3|$ at the expense of $|1-\sigma|$. It appears, then, that the best value for σ may depend on the problem and needs to be determined by numerical experiment. However, the present analysis indicates that it should lie between 1.5 and 2.0 (cf. the optimum value for σ of $\frac{4}{3}$ in two dimensions [6]).

With $\xi = \eta = 1$ we have, from Eq. (A.1)

$$\frac{\lambda_1}{\lambda_2} = 2\sqrt{BQ/A}; \qquad \frac{\lambda_1}{\lambda_3} = 4\sqrt{BQR/C}.$$

A convenient way of introducing these values into Eq. (13) is to separate out the frequency terms by writing

$$\frac{\lambda_1}{\lambda_2} = \alpha_2\sqrt{B/A}; \qquad \frac{\lambda_1}{\lambda_3} = \alpha_1\alpha_2\sqrt{B/C}.$$

On substitution into Eq. (13), Eq. (14) is obtained with $\alpha_1 = 2\sqrt{R}$ and $\alpha_2 = 2\sqrt{Q}$.

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