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CONDITIONS IN APPROXIMATE FACTORIZATION SCHEMES

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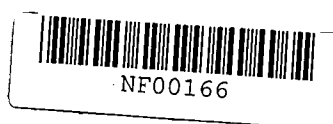
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STABILITY ANALYSIS OF INTERMEDIATE BOUNDARY CONDITIONS
IN APPROXIMATE FACTORIZATION SCHEMES

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Dedicated to Milton E. Rose
on Occasion of his 60th Birthday

Abstract

The paper discusses the role of the intermediate boundary condition in the AF2 scheme used by Holst for simulation of the transonic full potential equation. We show that the treatment suggested by Holst led to a restriction on the time step and suggest ways to overcome this restriction. The discussion is based on the theory developed by Gustafsson, Kreiss, and Sundström and also on the von Neumann method.

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INTRODUCTION

Approximate factorization schemes are widely used to obtain efficient solutions to problems in Computational Fluid Dynamics. In many cases, they have provided a significant increase in efficiency over previously-used solution methods in particular problems. Some outstanding examples are the classical Alternating-Direction-Implicit method of Peaceman and Rachford [1], the Briley-McDonald Linearized Block Implicit scheme [2], and the Beam and Warming [3] Approximate Factorization (AF) scheme for the compressible Navier-Stokes equations. In the transonic potential-flow area, some AF schemes which have significantly improved solution efficiency are the work of Ballhaus and Steger [4], Ballhaus et al. [5], Holst [6], [7], and Jameson [8].

All of these schemes have the common feature that the solution procedure is broken down into a sequence of easily-implemented stages; i.e., easily-inverted matrix factors. Each of the stages usually requires boundary conditions for an "intermediate" variable (vector) which is not always a consistent approximation to the solution function desired. This feature can make satisfaction of implicit boundary conditions difficult, at best, and impossible, at worst. Dwyer and Thames [9] demonstrated serious boundary-condition problems associated with the class of AF schemes called "Locally One-Dimensional," even in explicit schemes.

The present paper further highlights the importance of intermediate boundary conditions by focusing on a specific example--a boundary-induced stability restriction in Holst's AF2 scheme [6] for the transonic full-potential equation. An analysis of the effect of the intermediate boundary condition is given by use of the usual von Neumann method and also the methods of Gustaffson, Kreiss, and Sundstrom [10] and Osher [11].

ANALYSIS

Holst's scheme is a variation of the AF2 schemes presented in References 4 and 5. It will be referred to herein as "AF2Y," since in its implementation the y-operator is split, rather than splitting the x-operator as in References 4 and 5. For the purpose of analyzing the intermediate boundary-condition problem, it is illuminating to study the application of AF2Y to the two-dimensional (2-D) Laplace's equation in a rectangle. The present analysis is valid only for the subsonic flow condition, which is simpler by far than the transonic case. However, it is reasonable to assume that if boundary-induced instability is present in the subsonic case, it will also occur in the transonic case. In practice this was true.

The Discrete Problem

The following thin-airfoil problem is thus considered: We wish to solve the Laplace difference equation for the disturbance velocity potential

$$L\phi_{jk} = (a\delta_{xx} + b\delta_{yy})\phi_{jk} = 0 \quad (1)$$

where a and b are constant coefficients and δ_{xx} and δ_{yy} are central difference operators; e.g.,

$$\delta_{xx}\phi_{jk} = \phi_{j+1,k} - 2\phi_{jk} + \phi_{j-1,k} \quad (2)$$

The boundary conditions are set on a rectangular region with Dirichlet conditions, $\phi = 0$, set on three sides (left, top, and right), representing vanishing disturbances, and a Neumann condition at the bottom boundary,

representing a thin-airfoil flow-tangency condition:

$$\phi_y = s(x) \quad \text{at } y = 0. \quad (3)$$

A discrete analog of Eq. (3) at $k = 1$ can be written as:

$$(\delta_y^+ + \delta_y^-)\phi_{j,1} = 2\Delta y s(x) \quad (4)$$

where we use the following notation for one-sided, two-point differences:

$$\delta_y^+ \phi_{jk} = \phi_{j,k+1} - \phi_{jk} \quad (5)$$

$$\delta_y^- \phi_{jk} = \phi_{jk} - \phi_{j,k-1}. \quad (6)$$

The difference operator (1) requires evaluation of $\delta_{yy}\phi_{j,1}$ at the boundary $k = 1$. Since this operator can be written as:

$$\delta_{yy} = \delta_y^+ - \delta_y^-, \quad (7)$$

Equation (4) is used to eliminate $\delta_y^+ \phi_{j,1}$, which calls for a value of ϕ_{jk} below the boundary $k = 1$. Thus, the difference operator at $k = 1$ is:

$$L_B \phi_{j,1} = (a\delta_{xx} + 2b\delta_y^-)\phi_{j,1} - 2b\Delta y s(x). \quad (8)$$

The AF2Y Scheme

The AF2Y scheme models a hyperbolic equation, $\sigma\phi_{yt} = \nabla^2\phi$, and is used as an iteration scheme:

$$(\alpha + b_1\delta_y^{\dagger})(- \alpha b_2\delta_y^{\dagger} - a\delta_{xx})\Delta\phi_{jk} = \alpha\omega L\phi_{jk}^n \quad (9)$$

where n is the iteration counter,

$$b_1 b_2 = b \quad (10)$$

and $\Delta\phi$ is the correction

$$\Delta\phi_{jk} = \phi_{jk}^{n+1} - \phi_{jk}^n. \quad (11)$$

The scheme is implemented in two stages:

$$(\alpha + b_1\delta_y^{\dagger})f_{jk} = \alpha\omega L\phi_{jk}^n \quad (12)$$

$$(- \alpha b_2\delta_y^{\dagger} - a\delta_{xx})\Delta\phi_{jk} = f_{jk}. \quad (13)$$

The intermediate variable f is defined by Eq. (13). The parameter α corresponds to a reciprocal "time" step, Δt^{-1} , and is usually cycled between small and large values to obtain rapid convergence. The parameter ω corresponds roughly to a relaxation factor which is usually close to 2.

The first stage (12) is bidiagonal, proceeding from the bottom boundary, $k = 1$, to the last interior row of mesh points, $k = K - 1$, for every j . The

second stage (13) is a tridiagonal solution which proceeds row-by-row, from $k = K - 1$ to $k = 1$, to obtain the correction $\Delta\phi_{jk}$. The second stage is initiated with the condition $\Delta\phi_{j,K} = 0$, corresponding to the vanishing disturbance, $\phi = 0$, at $k = K$.

The Intermediate Boundary Condition

The main problem in implementing the scheme is how to initiate the bidiagonal solution for f at $k = 1$. It seems reasonable, at first sight, to use a derivative condition on f at the boundary, as Holst [6] did; i.e.,

$$\delta_y^+ f_{j,1} = 0. \quad (14)$$

Comparison of Eqs. (14) and (12) implies that

$$f_{j,1} = \omega L_B \phi_{j,1}^n. \quad (15)$$

If this procedure is used with no further modification, it is unstable for small values of α (or large "time" steps) and fixed ω as described next.

Stability Analysis

A von Neumann (VN) analysis shows that the interior scheme (9) is stable for all modes under the restrictions

$$0 < \omega < 2 \quad (16)$$

$$\alpha > 0. \quad (17)$$

However, the boundary scheme, implied by Eqs. (15) and (13) taken together, is another matter.

A boundary condition more general than Eq. (14) for f can be considered. Let a "dummy-point" value for f be given as:

$$f_{j,0} = \gamma f_{j,1}. \quad (18)$$

Then the equation for $f_{j,1}$ is, from Eq. (12),

$$(\alpha + b_1)f_{j,1} = \alpha \omega L_B \phi_{j,1}^n + \gamma b_1 f_{j,1} \quad (19)$$

and Eq. (13) yields:

$$f_{j,1} = (-\alpha b_2 \delta_y^z - a \delta_{xx}) \Delta \phi_{j,1} = \Omega L_B \phi_{j,1}^n \quad (20)$$

where

$$\Omega = \frac{\alpha \omega}{\alpha + b_1(1-\gamma)}. \quad (21)$$

To carry out a VN analysis, we substitute into Eq. (20) trial solutions

$$\phi_{j,k}^n = G^n e^{i(jp\Delta x + kq\Delta y)} \quad (22)$$

where $i = \sqrt{-1}$, p and q are wave numbers, and G is the amplification factor, to obtain:

$$(\alpha B + 2Ab_1 - i\alpha E)(G - 1) = -2\Omega b_1(A + B - iE) \quad (23)$$

where

$$\left. \begin{aligned} A &= a (1 - \cos \xi) > 0 \\ B &= b (1 - \cos \eta) > 0 \\ E &= b \sin \eta \\ \xi &= p\Delta x \\ \eta &= q\Delta y \end{aligned} \right\} . \quad (24)$$

The stability condition, $|G|^2 < 1$, reduces to:

$$\Omega \{ (A + B) [(2 - \Omega) b_1 A + (\alpha - \Omega b_1) B] + (\alpha - \Omega b_1) E^2 \} > 0. \quad (25)$$

To maintain the inequality (25) the following stability restrictions are easily deduced:

$$0 < \Omega < 2 \quad (26)$$

$$\alpha > b_1 \Omega. \quad (27)$$

For the case $\gamma = 1$, corresponding to the backward-Neumann condition on f (Eq. (14)), restrictions (26) and (27) reduce to Eq. (16) and

$$\alpha > b_1 \omega \quad (\gamma = 1). \quad (28)$$

The restriction (27) enforces a "time" step limitation on the scheme for fixed Ω , which will slow convergence; or a reduction in Ω , according to:

$$\Omega < \min \left(2, \frac{\alpha}{b_1} \right) \quad (29)$$

which in fact yields fast convergence and ensures stability.

It is noted that another useful type of boundary condition for f is given by

$$f_{j,0} = \frac{\alpha\beta}{b_1} L_B \phi_{j,1}^n \quad (30)$$

which gives the same form as Eq. (20) for $f_{j,1}$ with

$$\Omega = \frac{\alpha(\omega + \beta)}{\alpha + b_1} . \quad (31)$$

Both classes of schemes are implemented by initiating the bidiagonal march for f using Eq. (20), under restriction (29).

The restriction (29) was verified numerically in both a constant-coefficient, Cartesian-coordinate computer code for Laplace's equation and in the "TAIR" code [12] by using fixed values for α (i.e., no α -cycling) and Ω , and for various values of the coefficient b_1 . In all cases, convergence was obtained when the restriction (29) was obeyed; and divergence occurred when it was violated.

The experiments with the TAIR code were especially interesting, since the coefficient b_1 varies along the airfoil surface. The test case chosen was the default "0"-type mesh for an NACA 0012 airfoil. It was found that the arithmetic mean of b_1 along the surface presented the crucial condition, rather than the maximum value, as might be expected.

The question arises as to why the TAIR code, which implements the AF2Y scheme with the boundary condition (14), operates so well since α is cycled between small values, which violate the restriction (28) and large values. The answer seems to be that α is increased within several rows adjacent to

the boundary to a value which (in the default mesh) meets the restriction (28), when smaller values of α are used in the remaining interior field. This "fix" was developed empirically by the authors of Reference 12; without this fix the code diverges. This procedure is not recommended in general, since it requires a discontinuous change in α . The assumption in the development of the factored scheme (9) is that α is constant throughout the mesh.

A seemingly attractive scheme, involving a discontinuity in α at the boundary, is as follows: Initiate the solution for f using Eq. (15) with $\omega = 1$, and change the second stage (13) at the boundary to:

$$(-2b_2^+ \delta_y - a\delta_{xx}) \Delta \phi_{j,1} = f_{j,1} = L_B^n \phi_{j,1}. \quad (32)$$

This procedure exactly annihilates the boundary residual (in the linear case) and represents a fully implicit satisfaction of the surface boundary condition. However, the factored operator at line $k = 2$ is no longer the interior-point operator, since the term $-ab_2^+ \delta_y$ in the inner factor is changed to $-2b_2^+ \delta_y$ discontinuously. It is possible to analyze such a scheme by the methods presented herein, but the line $k = 2$ must be considered as part of the boundary scheme. No details will be given here, but the analysis shows that setting $\omega < 4/3$ at $k = 2$ guarantees linear stability of the overall scheme. However, the amplification factor modulus $|G|$ exceeds unity only in a narrow frequency range of small η (Eq. (24)) when $\omega > 4/3$. Numerical experiments showed no sensitivity to the value of ω at $k = 2$. This scheme was always stable in tests with a constant-coefficient Cartesian-mesh code, even with $\omega = 1.8$ at $k = 2$. If the scheme was unstable for

highly stretched grids, setting $\omega < 4/3$ at $k = 2$ did not stabilize the scheme. In the variable-coefficient, nonlinear case, such a scheme is no faster than, and not as robust as, the scheme (20) with restriction (29).

Review of the Stability Theory

It is well known that in general the von Neumann analysis at a single line is neither sufficient nor necessary for checking stability. Trapp and Ramshaw [13] pointed out the usefulness of the VN analysis to study boundary schemes but recognized that no theoretical justification was known.

We wish to review briefly the stability theory for finite-difference approximations to initial boundary-value problems. A necessary condition for the stability of such a scheme is the Ryabenkii-Godunov condition. It states that the numerical scheme is unstable if there exists a solution of the type

$$\phi_{j,k}^n = G^n \psi_{j,k}, \quad |G| > 1 \quad (33)$$

for the inner scheme and the boundary scheme. (It is also sufficient to check one boundary at a time.) Substituting (33) into (12) and (13) one finds that $\psi_{j,k}$ satisfies a constant coefficient second-order difference scheme whose solution is

$$\psi_{j,k} = \mu^k e^{i(j\rho\delta x)}. \quad (34)$$

Actually there are two possible μ 's, but it is readily verified that only one of them satisfies $|\mu| < 1$ for $|G| > 1$; and, therefore, it is not a valid solution for the quarter-plane problem.

In Appendix A we show that there exists a solution of the form (34) to (12), (13), and (20) such that $|G| > 1$ and $|\mu| < 1$ if (29) is not satisfied. This proves that the scheme is unstable. By instability here we mean that unbounded solution occurs after a fixed number of time steps for any mesh--it precludes the possibility of reaching steady state.

It should be noted here that VN analysis of the boundary scheme does not predict the existence of solutions of the form (33) with $|G| > 1$. In fact, Gottlieb and Turkel [15] gave an example of a boundary scheme (Scheme VI, p. 184 of Reference 15) coupled with a variant of MacCormack's scheme in the interior which is conditionally stable, yet the VN analysis of the boundary scheme shows unconditional instability. However, Goldberg and Tadmor showed that for a dissipative interior scheme (i.e., amplification--factor modulus bounded away from unity for all nonzero modes) VN stability of the boundary scheme excludes the possibility of an eigenvalue or a generalized eigenvalue. By an eigenvalue we mean a solution of the form (34) with $|G| > 1$ whereas a generalized eigenvalue is G such that $|G| = 1$. Thus, if the condition stated in (29) is satisfied no eigenvalue or generalized eigenvalue exists. In Appendix A we show it directly. The theory of Gustafsson, Kreiss, and Sundström [10] (see also, Osher [11]) states that for a system of first-order hyperbolic equations stability is assured if there is no eigenvalue or generalized eigenvalue. While their theory does not apply directly to the equation

$$\sigma_{yt} = \nabla^2 \rho,$$

it can be modified to include this case.

As a concluding remark we should note that stability here implies convergence in the sense of Lax--the numerical solution converges to the analytic one as the mesh size tends to zero for fixed time t . This is clearly only a necessary requirement to reach steady state.

Two-Dimensional Numerical Results

A limited number of numerical tests for cases involving stretched grids and nonlinear transonic flow have convinced us that the discontinuous- α schemes (e.g., Eq. (32)) are not as reliable as the scheme using Eq. (20) with restriction (29). Some numerical results are presented in Tables 1 and 2. In the tables, the following identification is used for the various boundary schemes:

Scheme I: Original TAIR scheme; Eqs. (13) and (15) at boundary, with α increased at 3 lines adjacent to boundary to satisfy restriction (28) with 10% safety margin.

Scheme II: Exact annihilation of boundary residual; Eqs. (15) and (32), with $\omega = 1$ at boundary only.

Scheme III: Eq. (20) and restriction (29) with 10% safety margin.

Table 1 shows a series of numerical tests for incompressible flow over a circle, with varying degrees of mesh stretching near the boundary. The TAIR code was used with $\omega = 1.8$ at all points except as noted in schemes II and III, and with the default settings for the α -cycle ($\alpha_{\min} = 0.07$, $\alpha_{\max} = 1.5$). The mesh contained 101 points uniformly spaced around the circle and 21 points in the radial direction with stretched spacing. The first column lists the cell aspect ratio at the boundary, $\Delta x / \Delta y (= b_1)$, for each case. The next

three columns show the number of iterations required to decrease the starting residual by 10^{-4} for three schemes previously discussed. Divergence is indicated by an entry "D." It is seen that scheme III is significantly less sensitive to grid stretching in the normal direction than are the discontinuous- α schemes, I and II.

Table 1. Number of Iterations to Reduce Residual by 10^{-4} .
Incompressible Circle Flow, 101 by 21 Mesh

$\frac{\Delta x}{\Delta y}$	Scheme		
	I	II	III
0.5	44	43	34
1	72	36	51
10	68	43	47
20	99	53	48
100	212	D	34
1000	400	D	127

As previously mentioned, the empirically-developed default settings in the TAIR code provide for an increased value of α near the surface; the default value satisfies the restriction (28) only for the first case in Table 1, $\Delta x/\Delta y = 0.5$. For that case, convergence is obtained; the scheme diverges for the other listed cases for which the default setting violates restriction (28). In scheme I, the value of α near the surface met the restriction, and convergence was obtained for all the listed cases.

It should be noted again that the stability analysis presented herein is valid only for subsonic flow, when the AF2Y scheme is guaranteed to be hyperbolic in time. When the flow becomes locally supersonic, the linearized Eq. (1) will have $a < 0$, and a term which simulates ϕ_{xt} must be added for stability [16]. The effect of including such a term (e.g., in the second factor of Eq. (9)) has not been studied at present. With that cautionary remark, we present results for transonic cases in the next table.

Table 2 presents results for two transonic cases for an NACA 0012 airfoil: (1) Zero incidence with free-stream Mach number $M_\infty = 0.85$ and (2) 2° incidence with $M_\infty = 0.75$. All cases were run with $\omega = 1.8$, but with different α -cycles. It can be seen that there is little difference in the convergence rate among the schemes, except that scheme II is noticeably slower than schemes I or III for case (2).

Table 2. Number of Iterations to Decrease Residual by 10^{-4} for Transonic Flow. NACA 0012, Default TAIR Mesh, 149 by 30

Flow Condition	Scheme		
	I	II	III
$M_\infty = 0.85$			
Zero incidence	190	174	187
$M_\infty = 0.75$			
2° incidence	190	360	226

Three-Dimensional Version of AF2Y

A three-dimensional (3-D) version of the AF2Y scheme is presented in Ref. 7. It is different from the 2-D version discussed up to now, in that the factors are reversed in order. That is, the scheme can be written in the present context as:

$$\left(\alpha - \frac{c}{b_2} \delta_{zz}\right) \left(b_2 - \frac{a}{\alpha} \delta_{xx}\right) \left(\alpha - b_1 \delta_y\right) \Delta \phi_{jkl} = \alpha \omega L \phi_{jkl}^n + \alpha b_2 \left(\alpha - b_1 \delta_y\right) \Delta \phi_{j,k-1,l} \quad (35)$$

where

$$L \phi_{jkl} = (a \delta_{xx} + b \delta_{yy} + c \delta_{zz}) \phi_{jkl}. \quad (36)$$

Because the factors are reversed, we will refer to this scheme as AF2YR.

Here the third coordinate direction is z , which can be thought of as the spanwise coordinate for a wing. The x - and y -coordinates are still the streamwise and normal coordinates as in the 2-D problem. The boundary operator corresponding to Eq. (8) is:

$$L_B \phi_{j,1,l} = (a \delta_{xx} + 2b \delta_y + c \delta_{zz}) \phi_{j,1,l} - 2b \Delta y s(x). \quad (37)$$

The scheme is implemented in three stages, as follows:

$$1. \quad \left(\alpha - \frac{c}{b_2} \delta_{zz}\right) g_{jl} = \alpha \omega L \phi_{jkl}^n + \alpha b_2 f_{j,k-1,l} \quad (38)$$

$$2. \quad \left(b_2 - \frac{a}{\alpha} \delta_{xx}\right) f_{jkl} = g_{jl} \quad (39)$$

$$3. \quad \left(\alpha - b_1 \delta_y\right) \Delta \phi_{jkl} = f_{jkl}. \quad (40)$$

The solution for f proceeds in planes, outward from the wing surface, using the tridiagonal Eqs. (38) and (39). The third stage (40) proceeds inward, solving for the correction in a bidiagonal march.

Again, the main problem is how to initiate the first stage. In Reference 7, the boundary condition used for f is

$$f_{j,0,l} = 0. \quad (41)$$

We can again consider the more general boundary conditions studied previously,

$$f_{j,0,l} = \gamma f_{j,1,l} \quad (42)$$

or

$$f_{j,0,l} = \frac{\beta}{b_2} L_B \phi_{j,1,l} \quad (43)$$

corresponding to Eqs. (18) and (30), respectively. Actually, condition (42) can only be approximately modeled in the 3-D problem, with some splitting error in the first two factors. That is, we can approximate Eq. (42) by solving, at $k = 1$:

$$1. \quad \left(\alpha - \frac{c}{b_2} \delta_{zz} \right) g_{j\ell} = \alpha \omega L_B \phi_{j,1,l}^n \quad (44)$$

$$2. \quad \left[(1-\gamma) b_2 - \frac{a}{\alpha} \delta_{xx} \right] f_{j,1,l} = g_{j\ell}. \quad (45)$$

Equation (43) is easily implemented by replacing ω in Eq. (38) by $\omega + \beta$ and setting $f_{j,0,l} = 0$.

Stability Analysis of the 3-D AF2YR Scheme

A VN analysis of the 3-D interior scheme shows that VN stability is achieved under restrictions (16) and (17). VN analysis of the boundary scheme (42) shows that sufficient conditions for stability of the VN boundary scheme are:

$$0 < \omega < 1 - \gamma \quad (46)$$

and

$$\gamma < 1. \quad (47)$$

The same criteria are obtained in the 2-D counterpart of the AF2YR scheme with boundary condition (18). The corresponding criteria for boundary condition (43) are:

$$0 < \omega + \beta < 1. \quad (48)$$

At this time we have no numerical experiments to test the stability and convergence of the 3-D boundary conditions (42) or (43) and the criteria (46) or (48). However, some comments about the use of AF2YR versus AF2Y are in order.

In the AF2YR scheme, the use of boundary condition (42) or (43) makes the scheme parabolic at the surface; i.e., the time-like equation at the boundary is:

$$\sigma \phi_t = \nabla^2 \phi \quad (49)$$

where

$$\sigma = b_2 (1-\gamma)/\omega \quad (50)$$

for Eq. (42), and where

$$\sigma = b_2/(\omega + \beta) \quad (51)$$

for Eq. (43). In the case of AF2Y, the boundary equation remains hyperbolic, like the interior scheme, with

$$-\sigma \phi_{yt} = \nabla^2 \phi \quad (52)$$

where

$$\sigma = b_2/\Omega. \quad (53)$$

It is felt that for this reason AF2Y may lead to faster convergence. It would appear that there is no difficulty in implementing such a scheme in 3-D, as:

$$1. (\alpha + b_1 \delta_y) f_{jkl} = \alpha \omega L \phi_{jkl} \quad (54)$$

$$2. (\alpha b_2 - c \delta_{zz}) g_{jl} = f_{jkl} + \alpha b_2 \Delta \phi_{j,k+1,l} \quad (55)$$

$$3. (1 - \frac{a}{\alpha b_2} \delta_{xx}) \Delta \phi_{jkl} = g_{jl}. \quad (56)$$

The factors in the second and third stages could also be interchanged. The first stage is initiated by using Eq. (20), and the same stability and restrictions (26) and (27) hold.

CONCLUDING REMARKS

We have studied the stability of the AF2Y scheme with several boundary conditions for the intermediate variable. The von Neumann method provides a useful tool for this study in view of the Goldberg-Tadmor theorem, and the results were verified in the two-dimensional case by the more complete GKSO theory.

In general, the boundary schemes place a limitation on α and ω which is more restrictive than the requirements for the interior scheme. Since small α is desirable to damp low-frequency errors, one strategy involves increasing α at or near the boundary to meet the boundary restriction while using smaller α in the interior mesh. Such "discontinuous- α " schemes require further analysis of the stability at the line next to the discontinuity since the scheme there is no longer the interior scheme. They diverge on certain stretched grids. A safer strategy is to decrease ω at the boundary to conform to the restrictions. This results in a more robust scheme; and it does not appear to suffer much, if any, loss in convergence rate.

In regard to the 3-D AF2Y scheme, the current implementation in the TWING code involves a reversal of the factors from the 2-D TAIR code. We refer to this scheme as AF2YR. Although the reversal of the factors makes no difference in the interior (for the linear constant-coefficient case), there is a significant difference at the boundary. The AF2YR boundary scheme is parabolic in time as opposed to hyperbolic for AF2Y. For this reason, there may be a preference for the AF2Y, as in the TAIR code.

APPENDIX A

Application of the GKS0 Theory to the AF2Y Scheme

In the GKS0 theory [10], [11], the interior and boundary schemes are considered as a coupled problem. Instead of substituting the Fourier solutions as in Eq. (22), the class of trial solutions is extended to

$$\phi_{jk}^n = G^n e^{i(jp\Delta x)} \mu^k \quad (A1)$$

where μ is a complex number not restricted to lie on the unit circle in the complex plane. Fourier modes are retained in the direction tangential to the boundary under study. The trial solutions are substituted into the interior and boundary schemes, Eqs. (9) and (20), to obtain, respectively:

$$[\alpha + b_1(1 - \frac{1}{\mu})] [-\alpha b_2(\mu - 1) + 2A](G - 1) = \alpha \omega [-2A + b(\mu - 2 + \frac{1}{\mu})] \quad (A2)$$

and

$$[-\alpha b_2(\mu - 1) + 2A](G - 1) = \Omega [-2A + 2b(\mu - 1)], \quad (A3)$$

where Eq. (8) for $L_B \phi_{j,1}^n$ is used for the right-hand side of Eq. (A3) and where we have used the notation of Eq. (24).

Equations (A2) and (A3) are two simultaneous equations for the unknowns G and μ . In the theory, we are concerned only with values of μ inside the unit circle, i.e., only those solutions which decay away from the

boundary. If the solution of Eqs. (A2) and (A3) yield $G > 1$ for $\mu < 1$, the scheme is unstable.

If Eq. (A3) is divided into Eq. (A2), G is eliminated; and there results an equation for μ :

$$\Omega[\alpha\mu + b_1(\mu - 1)][-2A + 2b(\mu - 1)] = \alpha\omega[-2\mu A + b(\mu - 1)^2]. \quad (A4)$$

First, it will be shown that for

$$A = a(1 - \cos \xi) = 0 ,$$

there is a value of μ inside the unit circle. When $A = 0$, Eq. (A4) reduces to two linear factors:

$$(\mu - 1)\{[2\Omega(a + b_1) - \alpha\omega]\mu - 2b_1\Omega + \alpha\omega\} = 0. \quad (A5)$$

The root $\mu = 1$ is a solution of Eqs. (A2) and (A3) only when $\Omega = \omega$, corresponding to $\gamma = 1$. (See Eq. (21).) Then

$$G = 1 - \omega \quad (A6)$$

and the restriction (16) must be satisfied. The other root is:

$$\mu = \frac{2b_1\Omega - \alpha\omega}{2\Omega(\alpha + b_1) - \alpha\omega} \quad (A7)$$

which is less than 1.0 and is arbitrarily close to 1.0 as α approaches zero.

Using Eq. (A3), we can show that for any complex μ such that its real part is less than 1, $G < 1$ if and only if restrictions (26) and (27) are satisfied. Thus, let

$$\mu = \mu_R + i\mu_I \quad (\text{A8})$$

where μ_R and μ_I are the real and imaginary parts. Substitution of Eq. (A8) into (A3) and multiplication by b_1 gives:

$$[\alpha b (1 - \mu_R) + 2Ab_1 - i\alpha b\mu_I](G - 1) = -2\Omega b_1[A + b(1 - \mu_R) - i b\mu_I]. \quad (\text{A9})$$

The condition $G^2 < 1$ then yields:

$$\begin{aligned} &\Omega\{A^2 b_1(2 - \Omega) + Ab(1 - \mu_R)[\alpha - \Omega b_1 + (2 - \Omega)b_1] \\ &+ b^2(\alpha - \Omega b_1)[(1 - \mu_R)^2 + \mu_I^2]\} > 0. \end{aligned} \quad (\text{A10})$$

For $\mu_R < 1$, the restrictions (26) and (27) are sufficient to ensure the inequality (A10) for arbitrary positive values of A , b_1 , and b , regardless of the magnitude of μ_I . When $A = 0$, a value $\mu < 1$ always occurs, as shown by Eq. (A7); and the scheme will be unstable unless restriction (27) is satisfied. Thus, restriction (27) is necessary; and when it is satisfied (for small α), restriction (26) will also be satisfied.

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