JOURNAL OF COMPUTATIONAL PHYSICS 26, 181–196 (1978)

Boundary Conditions for Multistep Finite-Difference Methods for Time-Dependent Equations*

DAVID GOTTLIEB

Institute for Computer Applications in Science and Engineering, NASA Langley Research Center, Hampton, Virginia 23665

AND

ELI TURKEL†

Courant Institute of Mathematical Sciences, New York University, New York, New York 10012

Received October 13, 1976; revised February 7, 1977

The stability and accuracy of various boundary treatments are analyzed for the two-step Richtmyer and MacCormack methods. Special attention is paid to ways of imposing the extra boundary conditions after the first step of the two-step process. The theory of Kreiss is used to study stability properties for both scalar and vector equations. The theory of Skollermo is used to compare accuracies of the various methods. Computations were also performed on both wavelike equations and on systems that approach a steady state. Several suggestions are given for more reliable boundary treatments.

1. INTRODUCTION

In recent years it has become popular to use two-level multistep methods for solving time-dependent problems in continuum mechanics. The schemes are chosen so that the pure initial-value problem is well posed. However, it is well known that most finite-difference schemes require more boundary data than those furnished by the given boundary conditions. Kreiss [6] and Gustafsson *et al.* [2] have established methods for deciding the stability of schemes with these additional numerical boundary conditions determined by various means. In the latter paper several applications were given for some of the well-known methods. Later Chu and Sereny [1] and Sundström [13] discussed other possibilities. Nevertheless for the procedures used in practice much is not known. In this study we analyze the stability of the Richtmyer and MacCormack two-step methods subject to a variety of techniques for specifying the additional boundary conditions.

* This paper was prepared as a result of work performed under NASA Contract NAS1-14101 while the authors were in residence at ICASE, NASA Langley Research Center, Hampton, Va. 23665.

† Also partially supported by ERDA Grant E(11-1)-3077-III.

0021-9991/78/0262-0181$02.00/0

2. Theoretical Background

We briefly review the stability theory of Kreiss for the initial boundary problem so as to make this paper self-contained. The reader is referred to the previously mentioned papers for further details. Consider the equation

$$u_t = au_x, \qquad 0 \leqslant x \leqslant 1, \quad t > 0, \tag{2.1}$$

with initial data $u(x, 0) = u_0(x)$. We assume that a is a real scalar constant. The theory can be extended to vector equations for strictly hyperbolic systems by diagonalizing the matrix. It has also been proved that these results apply for equations with variable coefficients.

When the constant a is positive, it is necessary to specify analytically a boundary condition at the right boundary, $x = 1$; while if a is negative the condition is specified at the left boundary, $x = 0$. Hence, in addition to Eq. (2.1), we specify boundary conditions.

$$\begin{aligned} u(0, t) &= g_0(t) \qquad \text{if} \quad a < 0, \\ u(1, t) &= g_1(t) \qquad \text{if} \quad a > 0. \end{aligned} \tag{2.2}$$

Popular methods for solving this equation are second-order three-point formulas of the form $u_j^{n+1} = F(u_{j-1}^n, u_j^n, u_{j+1}^n)$ for some function F. It is readily seen that numerically one needs boundary conditions at both $x = 0$ and $x = 1$. We assume that in addition to the analytically given conditions (2.1) and (2.2) a separate procedure is used to determine the extra boundary conditions. For example, if $a > 0$ then $u_0^{n+1} = G(u_0^n, u_1^n, \ldots)$ for some function G. The Kreiss stability theory for this case makes the ansatz $u_j^n = z^n \kappa^j$ for appropriate complex scalars z and κ. This substitution is made in both the difference scheme in the interior and on the boundary. The basic difference scheme is assumed stable and so the Von Neumann stability condition says that $|z| \leqslant 1$ for $|\kappa| = 1$. It is then proven that the initial-boundary scheme is stable if there are no nontrivial solutions of these equations with $|z| > 1$ and $|\kappa| < 1$. Conversely the scheme is unstable if there exist solutions with $|z| > 1$ but $|\kappa| < 1$. When $|z| = 1$, $|\kappa| = 1$ there are two cases to consider. If $z \neq 1$ the stability is not assured. When $z = 1$ it is called a generalized eigenvalue and to establish stability one must analyze the rate of growth. Kreiss [5] has shown that $\kappa = 1$ and $z = 1$ does not lead to any instabilities for the Lax–Wendroff type of scheme considered here. These concepts are applied to specific problems in the next sections. The extension of this technique to multilevel schemes or to methods that have a larger domain of dependence than three points is more difficult; the reader is referred to [2, 5] for details. Generalizations to parabolic equations have been proved by Varah [14].

3. Hyperbolic Stability

As concrete applications of this technique we consider several multistep methods. Historically, the first multistep method was proposed by Richtmyer and Morton [10] for equations in divergence form. For the simple equation (2.1) this method is given by

$$u_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \tfrac{1}{2}(u_{j+1}^{n} + u_j^{n}) + (a/2)(\Delta t/\Delta x)(u_{j+1}^{n} - u_j^{n}), \tag{3.1a}$$

$$u_j^{n+1} = u_j^{n} + a(\Delta t/\Delta x)(u_{j+\frac{1}{2}}^{n+\frac{1}{2}} - u_{j-\frac{1}{2}}^{n+\frac{1}{2}}). \tag{3.1b}$$

This set will be referred to as (R). We shall only consider the left boundary $x = 0$. The situation at the right boundary corresponds to interchanging x with $-x$ or equivalently a with $-a$. Kreiss has shown that it is sufficient to consider each boundary separately.

Another set of two-step algorithms was proposed by MacCormack [8]. The first variant, which we refer to as (FB), is given by

$$u_j^{(1)} = u_j^{n} + a(\Delta t/\Delta x)(u_{j+1}^{n} - u_j^{n}), \tag{3.2a}$$

$$u_j^{n+1} = \tfrac{1}{2}(u_j^{n} + u_j^{(1)}) + \tfrac{1}{2}a(\Delta t/\Delta x)(u_j^{(1)} - u_{j-1}^{(1)}). \tag{3.2b}$$

With this variant one can calculate $u^{(1)}$ at the boundary $x = 0$, but not u^{n+1}. The second variant of MacCormack's method, referred to as (BF), is given by

$$u_j^{(1)} = u_j^{n} + a(\Delta t/\Delta x)(u_j^{n} - u_{j-1}^{n}), \tag{3.3a}$$

$$u_j^{n+1} = \tfrac{1}{2}(u_j^{n} + u_j^{(1)}) + \tfrac{1}{2}a(\Delta t/\Delta x)(u_{j+1}^{(1)} - u_j^{(1)}). \tag{3.3b}$$

With this variant one can no longer calculate $u^{(1)}$ at $x = 0$ but once it is determined by some other method one can calculate u^{n+1} at $x = 0$. The situation at the right boundary corresponds to interchanging the two variants. For linear equations with constant coefficients all three basic schemes (R), (FB), and (BF) are identical.

As previously discussed when a is positive, it is necessary to use separate numerical procedures to determine u^{n+1} at the left boundary $x = 0$. We consider the following techniques for determining u_0^{n+1}.

I. $u_0^{n+1} = 2u_1^{n+1} - u_2^{n+1}$.

This is linear extrapolation at time $t + \Delta t$, i.e., $u_{xx}^{n+1}|_{x=0} = 0$.

IIa. $u_{-1}^{n} = 2u_0^{n} - u_1^{n}$,

IIb. $u_0^{n+1} = u_0^{n} + a(\Delta t/\Delta x)(u_1^{n} - u_0^{n})$,

IIc. $u_0^{n+1} = u_0^{(1)}$. (FB)

Technique IIa is linear extrapolation at time t to a point outside the domain; IIb is

an approximation of the differential equation using differences forward in time and space finite; IIc applies only to (FB) and equates u_0^{n+1} to the approximation at the middle step, which is a first-order approximation to $u(0, t + \Delta t)$. These are grouped together since they are identical for equations with constant coefficients. Techniques IIb and IIc are identical even for nonlinear problems; IIc, when applicable, is the easiest to use computationally.

$$\text{IIIa.} \quad u_{-\frac{1}{2}}^{n+\frac{1}{2}} = 2u_{\frac{1}{2}}^{n+\frac{1}{2}} - u_{\frac{3}{2}}^{n+\frac{1}{2}}, \tag{R}$$

$$\text{IIIb.} \quad u_0^{n+1} = u_1^{n+1} + u_0^n - u_1^n.$$

Method IIIa is linear extrapolation outside the domain for the middle step of the Richtmyer method; IIIb is the equivalent of $u_{xt} = 0$ at the boundary.

$$\text{IVa.} \quad u_{-1}^{(1)} = 2u_0^{(1)} - u_1^{(1)}, \tag{FB}$$

$$\text{IVb.} \quad u_0^{n+1} = \tfrac{1}{2}(u_0 + u_0^{(1)}) + \tfrac{1}{2}a(\Delta t/\Delta x)(u_1^{(1)} - u_0^{(1)}), \tag{FB}$$

$$\text{IVc.} \quad u_0^{(1)} = u_0^n + a(\Delta t/\Delta x)(u_1^n - u_0^n). \tag{BF}$$

Methods IVa, IVb are only applicable to (FB), IVa being linear extrapolation outside the domain at the intermediate step and IVb similar to (3.2) with the backward difference replace by a forward difference at the boundary. If the extrapolation in IVa is done on the fluxes then IVa and IVb are equivalent even for nonlinear problems. Method IVc applies only to (BF) and is similar to (3.3a), again with the backward difference replaced by a forward difference.

$$\text{V.} \quad u_0^{(1)} = 2u_1^{(1)} - u_2^{(1)}. \tag{BF}$$

This is linear extrapolation in the middle step of (BF).

$$\text{VI.} \quad u_0^{n+1} = 2u_1^{(1)} - u_2^{(1)}. \tag{BF}$$

This is a composite of V and $u_0^{n+1} = u_0^{(1)}$.

Remark. We have concentrated on first-order methods since Gustafsson [3] has shown that this is sufficient for second-order convergence of the scheme. In the computational section we also consider zeroth and quadratic extrapolations.

We now find the regions of stability for the scalar equation (3.1). Gustasson *et al.* [2] have shown that the Lax–Wendroff method is stable if any order extrapolation is applied at the end and so we need not consider I. Similarly, they have shown that IIb is stable. Since each group is linearly equivalent we need not consider group II either. Hence, we begin with group III. Assuming $u_j^n = U\kappa^j z^n$ and substituting into either (3.1) or (3.2) or (3.3) we find that

$$z\kappa = \kappa + (\tau/2)(\kappa^2 - 1) + (\tau^2/2)(\kappa - 1)^2; \qquad \tau = a(\Delta t/\Delta x). \tag{3.4}$$

Using boundary conditions III we find that

$$z = 1 + (\tau/2)(\kappa^2 - 1) + (\tau^2/2)(\kappa - 1)^2. \tag{3.5}$$

Subtracting (3.5) from (3.4) yields $z(\kappa - 1) = \kappa - 1$. Hence, $z = 1$ and either $\kappa_1 = 1$ or $\kappa_2 = (\tau - 1)/(\tau + 1)$. As before, $\kappa_1 = 1$ creates no difficulty. However, κ_2 is now an eigenvalue since $|\kappa_2| < 1$ while $z = 1$. Gustaffson (personal communication) has shown that in this case the scheme is stable but there is a loss of accuracy.

Boundary conditions IV are equivalent to

$$z = 1 + \tau(\kappa - 1) + (\tau^2/2)(\kappa - 1)^2. \tag{3.6}$$

Multiplying (3.6) by κ and subtracting from (3.4) we have that $\kappa = 1$ or $\kappa = 1 - 1/\tau$. $\kappa = 1$ creates no difficulties while $\kappa = 1 - 1/\tau$ implies that $z = \frac{1}{2}$ and so there are no instabilities.

Boundary condition V implies that

$$z = \tfrac{1}{2}(1 + 2\kappa - \kappa^2) + \tau(\kappa - 1) + (\tau^2/2)(\kappa - 1)^2. \tag{3.7}$$

Subtracting (3.7) from (3.4) and assuming $\kappa \neq 1$ we have that $z = \frac{1}{2}[1 - \tau + \kappa(1 + \tau)]$. Hence, $|z| \leqslant \frac{1}{2}[|1 - \tau| + |1 + \tau|]$ since $|\kappa| \leqslant 1$. Since $|\tau| < 1$ for initial-value stability we have that $|z| < 1$ and no instabilities occur.

Finally, boundary condition VI implies that

$$z = 2\kappa - \kappa^2 + \tau(-2 + 3\kappa - \kappa^2). \tag{3.8}$$

Multiplying (3.8) by κ and subtracting from (3.4) we find that $\kappa = \tau(1 - \tau)/2(1 + \tau)$ so $|\kappa| < 1$. In this case $z = -(\tau/4)(\tau^2 + 3\tau + 4)$. Hence, for $\tau < 0.64$ we have $|z| < 1$ and stability. For this case the boundary treatment necessitates a smaller time step for stability than the pure initial-value problem required.

THEOREM. *Boundary conditions* I, II, IV, *and* V *are stable when* $\tau < 1$, *as for the initial-value problem. Boundary case* III *has an eigenvalue* $|\kappa| < 1$, $z = 1$ *while condition* VI *is only stable when* $\tau < 0.64$.

Both these latter facts are observed in the computational data.

We next consider the case when $a < 0$. Then the boundary condition is given analytically. In the MacCormack methods one of the two steps can be calculated at $x = 0$ without use of this boundary condition. Expansion in a Taylor series shows that the use of the boundary condition at both the intermediate and final steps makes (3.2) only first order at the mesh point nearest the boundary. Nevertheless, computational results indicate that it is much better to specify the boundary conditions at both levels. In fact the ability to specify the boundary conditions at both steps seems to be a major advantage of the MacCormack method over the Richtmyer scheme. A similar situation occurs in time-splitting methods (see [9]).

4. Systems of Equations

The previous section applies only to scalar equations or to a system of equations when the extra condition due to the difference method is calculated on the outgoing characteristic values. In this section we analyze some noncharacteristic specifications. We first consider the system

$$u_t = -u_x - 2v_x, \tag{4.1a}$$

$$v_t = -2u_x - v_x, \qquad 0 \leqslant x \leqslant 1, \quad t > 0. \tag{4.1b}$$

Let

$$q = \frac{u+v}{2}, \qquad r = \frac{u-v}{2}, \qquad u = q + r, \quad v = q - r, \tag{4.2}$$

$$q_t + 3q_x = 0, \tag{4.3a}$$

$$r_t - r_x = 0. \tag{4.3b}$$

This system was chosen since it has positive and negative eigenvalues and there are no obvious symmetries. It is necessary to give one boundary condition at both the left and right boundaries while the other boundary is given by a numerical technique. As before it is sufficient to consider only the boundary $x = 0$. If at $x = 0$ we calculate r by any of the methods of the previous section then all the conclusions of that section remain valid. However, a more usual procedure is to specify u at $x = 0$ and to calculate v by a numerical technique. Because of the complexity of the problem we shall consider only space extrapolation methods for determining v. Additional procedures are considered in the computations. As before we let

$$q = Q\kappa_1{}^j z^n, \qquad r = R\kappa_2{}^j z^n. \tag{4.4}$$

The initial-boundary problem is unstable if there exists a nontrivial solution of the above form to both the difference scheme and the boundary conditions with both $|\kappa_1| < 1$, $|\kappa_2| < 1$ and $|z| > 1$. As before, if κ is on the unit circle a more delicate treatment is required.

Substituting (4.4) into the Lax–Wendroff scheme for (4.3) we have

$$\kappa_1 z = \kappa_1 + (\tau_1/2)(\kappa_1{}^2 - 1) + (\tau_1{}^2/2)(\kappa_1 - 1)^2, \tag{4.5a}$$

$$\kappa_2 z = \kappa_2 + (\tau_2/2)(\kappa_2{}^2 - 1) + (\tau_2{}^2/2)(\kappa_2 - 1)^2, \tag{4.5b}$$

where $\tau_1 = -3\Delta t/\Delta x$ and $\tau_2 = \Delta t/\Delta x$. For initial-value stability we assume $|\tau_1| < 1$. Specifying u at $x = 0$, (4.2) yields that

$$Q + R = 0. \tag{4.6a}$$

Using $(j-1)$th-order space extrapolation at $x = 0$ together with (4.6a) we have

$$(\kappa_1 - 1)^j + (\kappa_2 - 1)^j = 0 \tag{4.6b}$$

or

$$\kappa_1 - 1 = w(\kappa_2 - 1), \tag{4.7}$$

where w is one of the jth roots of (-1). We first consider zeroth-order extrapolation, $v_0^{n+1} = v_1^{n+1}$. Then (4.7) becomes $\kappa_1 + \kappa_2 = 2$. The only roots of this with $|\kappa_1| \leqslant 1$, $|\kappa_2| \leqslant 1$ are $\kappa_1 = \kappa_2 = 1$. However, Kreiss has already shown that this causes no trouble and so we have stability. For general jth-order extrapolation we multiply (4.5a) by κ_2, (4.5b) by κ_1 and subtract. This gives a plynomial in κ_1 and κ_2. κ_1 can be eliminated by the boundary condition (4.7). The resulting polynomial in κ_2 can be solved numerically for a sequence of τ_1, τ_2. It was found that linear extrapolation is stable for this system while quadratic extrapolation is unconditionally unstable.

We next show that even zeroth-order extrapolation can be unstable if some non-characteristic variables are extrapolated. This occurs even though the initial-boundary problem for the differential equations is well posed.

Assume $q_t = \lambda_1 q_x$ and $r_t = \lambda_2 r_x$. Let $u = q + r$ and $v = q + \sigma r$. When $\sigma = 1$ the variables u and v are linearly dependent. When $\sigma \neq 0, 1$ and $\lambda_1\lambda_2 < 0$, the problem is well posed if one boundary condition is specified at each end of the x interval. We assume that we solve the equations using the Lax–Wendroff scheme; $u = 0$ at the left boundary and v is found by zeroth-order extrapolation, i.e., $v_0^n = v_1^n$. Let $\tau_1 = \lambda(\Delta t/\Delta x)$, $\tau_2 = \lambda_2(\Delta t/\Delta x)$, $q_j^n = \kappa_1{}^j z^n$, $r_j^n = \kappa_2{}^j z^n$. The boundary condition is then equivalent to

$$\kappa_1 = 1 = \sigma(\kappa_2 - 1), \qquad \sigma \text{ real}, \tag{4.8}$$

and the differential equation is represented by (4.5). Multiplying (4.5a) by κ_2, (4.5b) by κ_1, subtracting and using (4.8), we find that

$$\begin{aligned}&\sigma\kappa_2{}^2[\sigma\tau_1(1 + \tau_1) - \tau_2(1 + \tau_2)]\\ &\quad + \kappa_2[\sigma\tau_1(2 - \sigma - \sigma\tau_1) - \tau_2(1 - 2\sigma\tau_2 + \tau_2)] - (1 - \sigma)\,\tau_2(1 - \tau_2) = 0.\end{aligned} \tag{4.9}$$

Let $\sigma = 1 + \epsilon$, ϵ small; then a root of (4.9) is

$$\begin{aligned}\kappa_2 &= \frac{\epsilon\tau_2(1 + \tau_2)}{[\tau_1(1 + \tau_1) - \tau_2(1 + \tau_2)][\tau_1(1 - \tau_1) - \tau_2(1 - \tau_2)]} + O(\epsilon^2),\\ \kappa_1 &= \kappa_2 - \epsilon + O(\epsilon^2).\end{aligned} \tag{4.10}$$

This result holds if Δt is large enough that κ_2/τ_1 and κ_2/τ_2 are $O(\epsilon)$. If we substitute this into (4.5) we find that $z = O(1/\epsilon)$. Hence, if the specified and extrapolated values, u and v, are close to being linearly dependent then the time step required for stability with zeroth-order extrapolation is severely reduced. For example, if $\sigma = 1.1$, $\tau_1 = \frac{1}{2}$, $\tau_2 = -\frac{1}{2}$ (i.e., half the Courant number), then $\kappa_2 \simeq 0.02$, $\kappa_1 \simeq 0.07$ and $z \simeq 6.1$. Thus, even when ϵ is not very small the same conclusions may hold.

5. Accuracy

Until now we have discussed only the stability of the initial-boundary problem. Given the stable boundary approximations one wishes to compare the accuracy of the solutions. A start in this direction was given by Sköllermo [11]. As before we give a brief description of the procedure as it applies to the Lax–Wendroff scheme. Applications to multilivel schemes or schemes that require a larger domain of dependence are more involved. Let $f(z, \kappa) = 0$ be the boundary algorithm that is being tested. Let $\epsilon = f(z, \kappa)/f(z, \kappa_1)$, where $z = e^{2\pi i\omega \Delta t}$, $\kappa = e^{2\pi i\omega \Delta x/a}$ and κ_1 is the root inside the unit circle which corresponds to $z = 1$ for the basic difference scheme. For the Lax–Wendroff method $\kappa_1 = (\tau - 1)/(1 + \tau)$, $\tau = a\,\Delta t/\Delta x$. Defining $M = a/\omega\,\Delta x$, M is the number of points per wavelength. Expanding f for small ω we find f as a function of M. Given an error level ϵ we can find the number of points per wavelength required to make the error less than a given tolerance. The smaller the value of M, the more accurate the algorithm, according to this theory. For example, for boundary condition II of Section 2 (i.e., one-sided Euler)

$$f(z, \kappa) = z - 1 - \tau(\kappa - 1)$$

and so

$$\epsilon = \frac{z - 1 - \tau(\kappa - 1)}{z - 1 - \tau(\kappa_1 - 1)}, \qquad \kappa_1 = \frac{\tau - 1}{1 + \tau},$$

$$\simeq \frac{\pi^2(1 - \tau^2)}{M^2}.$$

In Table I we present the six sets of boundary conditions considered in Section 2. Since Sköllermo used an incorrect value for κ_1, our results differ from hers. In the

TABLE I

Sköllermo Predictions for Accuracy

Scheme	$\epsilon = \dfrac{f(z, \kappa)}{f(z, \kappa_1)}$	Number of points per wavelength for τ of			
		0.25	0.50	0.75	1.0
I	$\pi^2(1 + \tau)^2/M^2$	40	48	55	63
II	$\pi^2(1 - \tau^2)/M^2$	31	28	21	0
III[a]	$\pi(\tau + 1)/M$	393	472	550	629
IV	$\pi^2(1 + \tau)^2/M^2$	40	48	55	63
V	$\pi^2(1 - \tau)^2/M^2$	31	28	21	0
VI	$\pi^2(\tau^2 + \tau + 2)(\tau + 1)/M^2(\tau + 2)$	36	41	[b]	[b]

[a] presence of an eigenvalue at $z = 1$, $\kappa = (\tau - 1)/(\tau + 1)$.
[b] not stable.

second column we present ϵ for that scheme. In the following columns we present the M necessary to make the error less than 1% for $\tau = 0.25$, $\tau = 0.50$, $\tau = 0.75$, and $\tau = 1.0$. The general conclusion of this theory is that the best methods are II (one-sided Euler) and V (linear extrapolation for (BF) at the intermediate step). Method III (linear extrapolation for (R) at the intermediate step or equivalently $u_{xt} = 0$) is the worst of all the methods. This might be caused by the eigenvalue, as predicted by Gustaffson. The computational results of Section 7 confirm that group III is the worst method, but the other conclusions are not verified by the computations.

6. Parabolic Stability

For sufficiently viscous problems the parabolic portion of the equation will dominate and one can consider the equation

$$\begin{aligned} u_t &= bu_{xx}, \qquad 0 \leqslant x \leqslant 1, \quad b > 0, \\ u(x, 0) &= f(x), \\ u(0, t) &= g_0(t), \qquad u(1, t) = g_1(t). \end{aligned} \tag{6.1}$$

Boundary conditions are now given at both ends; however, the two-step scheme uses a five-point lattice at the previous time level and hence extra boundary information is required to determine the solution at the net points adjacent to the boundaries. It is difficult to generalize the Richtmyer method to this case since the intermediate level is at half-points. Hence, we consider only the MacCormack method.

$$\begin{aligned} u_j^{(1)} &= u_j{}^n + [b\,\Delta t/(\Delta x)^2](u_{j+1}^n - 2u_j{}^n + u_{j-1}^n), \\ u_j^{n+1} &= \tfrac{1}{2}(u_j{}^n + u_j^{(1)}) + [b\,\Delta t/2(\Delta x)^2](u_{j+1}^{(1)} - 2u_j^{(1)} + u_{j-1}^{(1)}). \end{aligned} \tag{6.2}$$

Let $\sigma = b\,\Delta t/(\Delta x)^2$; then the initial-value problem is stable if $0 < \sigma \leqslant \frac{1}{2}$. The modal analysis equation associated with Eq. (4.2) is given by

$$z\kappa^2 = \kappa^2 + \sigma\kappa(\kappa - 1)^2 + (\sigma^2/2)(\kappa - 1)^4. \tag{6.3}$$

As before we consider only the left boundary, $x = 0$; the situation at the right boundary, $x = 1$, follows by symmetry. Linear extrapolation no longer leads to a first-order approximation at the boundary. Linear extrapolation is equivalent to assuming that $u_{xx} = 0$. However, by Eq. (4.1) this implies $u_t = 0$, i.e., a zeroth-order approximation. We therefore consider the boundary conditions

(1) $u_{-1}^n = 3u_0{}^n - 3u_1{}^n + u_2{}^n$,

(2) $u_0^{(1)} = g_0(t + \Delta t)$,

(3) $u_0^{(1)} = 3u_1^{(1)} - 3u_2^{(1)} + u_3^{(1)}$,

$$(4)\quad u_0^{(1)} = u_0^n + \sigma(u_2^n - 2u_1^n + u_0^n),$$

$$(5)\quad u_1^{n+1} = u_1^{(1)},$$

$$(6)\quad u_1^{n+1} = \tfrac{1}{2}(u_0^{n+1} + u_2^{n+1}).$$

THEOREM 6.1. *All the above boundary conditions are stable when used in conjunction with scheme* (4.2).

The proof follows the same pattern as before and will not be given.

Remark 1. Algorithm (2) states that one should use the given data also at the intermediate step. As seen in the Section 7 this is also useful for the hyperbolic case whenever appropriate.

Remark 2. The above results apply only for truly parabolic systems. The hydrodynamic equations at high Reynolds numbers should be considered as a singular perturbation of a hyperbolic system (see [4, 11]).

7. COMPUTATIONAL RESULTS

The theoretical conclusions of the sections on hyperbolic equations were tested on several problems. The first two cases concern the system

$$\begin{aligned} u_t &= -u_x - 2v_x, \\ v_t &= -2u_x - v_x, \qquad 0 \leqslant x \leqslant 1, \quad t > 0. \end{aligned} \tag{7.1}$$

This system has a solution

$$\begin{aligned} u &= f(\xi_1) + g(\xi_2), \\ v &= f(\xi_1) - g(\xi_2), \\ \xi_1 &= x - 3t, \qquad \xi_2 = x + t. \end{aligned} \tag{7.2}$$

This is solved using the MacCormack (FB) method, Eq. (3.2). Boundary conditions are imposed on u at both the left and right boundaries. The initial and boundary conditions used are given by (7.2). The first case considered is with f, g given by

$$f(x) = e^{\pi x} \sin 2\pi x, \qquad g(x) = e^{-2\pi x} \cos 2\pi x. \tag{7.3}$$

In this case the solution decays and at $t = 10$ the L_2 norm is about 1 % of the original energy. The second case is with

$$f(x) = \sin 2\pi x, \qquad g(x) = \cos 2\pi x. \tag{7.4}$$

In this case the solution is periodic but this fact is never used. For both cases it is necessary to calculate v at both the left and right boundaries. In Table II we present

TABLE II

Errors in the L_2 Norm for (7.1) with f Given by (7.3)[a]

Scheme	CFL = 0.9 Time = 1.0	CFL = 0.9 Time = 5.0	CFL = 0.9 Time = 10.0	CFL = 0.25 Time = 1.0	CFL = 0.25 Time = 5.0	CFL = 0.25 Time = 10.0
L = Z; R = Z	.0184	.0135	.0090	.0310	.0201	.0156
L = Z; R = V	.0101	.0088	.0077	.0125	.0119	.0113
L = Z; R = Q	.0070	.0062	.0055	.0092	.0081	.0076
L = I; R = Z	.0179	.0133	.0132	.0306	.0264	.0274
L = I; R = V	.0087	.0083	.0089	.0110	.0129	.0183
L = I; R = Q	.0045	.0043	.0043	.0072	.0076	.0096
L = Q; R = Z	.0178	.0124	.0109	.0305	.0253	.0238
L = Q; R = V	.0087	.0079	.0078	.0110	.0122	.0159
L = Q; R = Q	.0046	.0041	.0039	.0072	.0073	.0085
L = II; R = V	.0094	.0087	.0095	.0114	.0115	.0132
L = III; R = V	.0423	.1734	.3430	.0493	.1983	.3910
L = IV; R = V	.0088	.0074	.0069	.0114	.0110	.0123
L = I; R = IV	.0014	.0012	.0014	.0065	.0071	.0080
L = IV; R = IV	.0016	.0010	.0009	.0067	.0056	.0047
L = VI; R = V	U	U	U	.0110	.0130	.0180
L = ZT; R = ZT	.0054	.0040	.0036	.0263	.0169	.0129

[a] Analytic boundary conditions are imposed after both steps. U denotes an instability. CFL = $a(\Delta t/\Delta x)$.

TABLE III

Errors in the L_2 Norm for (7.1) with f Given by (7.3)[a]

	CFL = 0.9 Time = 1.0	CFL = 0.9 Time = 5.0	CFL = 0.9 Time = 10.0	CFL = 0.25 Time = 1.0	CFL = 0.25 Time = 5.0	CFL = 0.25 Time = 10.0
L = Z; R = Z	.0714	.0381	.0259	.0500	.0304	.0225
L = Z; R = V	.0538	.0638	.0885	.0206	.0208	.0214
L = Z; R = Q	.0325	.0285	.0252	.0128	.0116	.0106
L = I; R = Z	.0707	.0494	.0465	.0496	.0415	.0427
L = I; R = V	.0526	.1010	.2512	.0194	.0269	.0473
L = I; R = Q	.0308	.0384	.0603	.0107	.0125	.0174
L = Q; R = Z	U	U	U	U	U	U
L = Q; R = V	U	U	U	U	U	U
L = Q; R = Q	U	U	U	U	U	U
L = II; R = V	.0530	.0779	.1398	.0196	.0217	.0280
L = III; R = V	.1021	.2801	.5424	.0778	.2330	.4153
L = IV; R = V	.0530	.0660	.0997	.0196	.0210	.0260
L = I; R = IV	.0015	.0017	.0020	.0067	.0086	.0106
L = IV; R = IV	.0024	.0019	.0017	.0070	.0062	.0050
L = VI; R = V	U	U	U	.0496	.0421	.0439
L = ZT; R = ZT	.0083	.0057	.0054	.0498	.0307	.0176

[a] Analytic boundary conditions used only once per cycle. U denotes an instability. CFL = $a(\Delta t/\Delta x)$.

TABLE IV

Errors in the L_2 Norm for (7.1) with f Given by (7.4)[a]

Scheme	CFL = 0.9 Time = 1.0	CFL = 0.9 Time = 5.0	CFL = 0.9 Time = 10.0	CFL = 0.25 Time = 1.0	CFL = 0.25 Time = 5.0	CFL = 0.25 Time = 10.0
L = Z; R = Z	.1099	.1448	.1438	.1474	.1679	.1550
L = Z; R = V	.1122	.2554	.2632	.1487	.3780	.3249
L = Z; R = Q	.1107	.2497	.2635	.1459	.3591	.3249
L = I; R = Z	.0607	.1156	.1049	.0882	.1418	.1383
L = I; R = V	.0295	.0355	.0372	.0348	.0998	.0764
L = I; R = Q	.0287	.0480	.0465	.0335	.0939	.0721
L = Q; R = Z	.0611	.1111	.0929	.0852	.1281	.1301
L = Q; R = V	.0359	.0575	.0402	.0371	.0946	.0509
L = Q; R = Q	.0358	.0701	.0516	.0366	.0947	.0544
L = II; R = V	.0802	.2264	.1471	.0543	.1388	.0648
L = III; R = V	.1802	.6109	1.110	.2240	.7425	1.268
L = IV; R = V	.0389	.0810	.0561	.0473	.1160	.0547
L = I; R = IV	.0297	.0595	.0530	.0332	.0912	.0667
L = IV; R = IV	.0361	.0559	.0413	.0443	.0866	.0476
L = VI; R = V	U	U	U	.0347	.1007	.0800
L = ZT; R = ZT	.1738	.3354	.2118	.1679	.2139	.1765

[a] Analytic boundary conditions are imposed after each step. U denotes an instability. CFL = $a(\Delta t/\Delta x)$.

TABLE V

Errors in the L_2 Norm for (7.1) with f Given by (7.4)[a]

Scheme	CFL = 0.9 Time = 1.0	CFL = 0.9 Time = 5.0	CFL = 0.9 Time = 10.0	CFL = 0.25 Time = 1.0	CFL = 0.25 Time = 5.0	CFL = 0.25 Time = 10.
L = Z; R = Z	.2375	.2611	.2596	.1851	.1845	.1907
L = Z; R = V	.2082	.6616	.9115	.1756	.4744	.4515
L = Z; R = Q	.1946	.5502	.7747	.1702	.4354	.4327
L = I; R = Z	.2015	.3966	.3010	.1337	.2404	.2012
L = I; R = V	.0688	.3344	.5924	.0401	.1388	.1310
L = I; R = Q	.0400	.1672	.2478	.0334	.1105	.0958
L = Q; R = Z	U	U	U	U	U	U
L = Q; R = V	U	U	U	U	U	U
L = Q; R = Q	U	U	U	U	U	U
L = II; R = V	.1101	.4563	.4528	.0582	.1717	.0834
L = III; R = V	.3139	1.132	1.976	.2636	.8901	1.504
L = IV; R = V	.0914	.3425	.2504	.0549	.1568	.0721
L = I; R = IV	.0257	.0500	.0667	.0331	.0941	.0768
L = IV; R = IV	.0533	.1208	.0806	.0468	.0949	.0498
L = VI; R = V	U	U	U			
L = ZT; R = ZT	.3182	.3732	.3512	.2103	.2244	.2266

[a] Analytic boundary conditions used only once per cycle. U denotes an instability. CFL = $a(\Delta t/\Delta x)$.

the L_2 norm of the difference between the numerical and analytic solutions for (7.3). This number is normalized by the initial energy of the solution.

In the first columns of Tables II through V the various boundary treatments are given. L and R denote the left and right boundaries, respectively. The numbers represent the groups of methods discussed in Section 3. Thus, L = II; R = V states that the left boundary was treated with a group II method while the right boundary was calculated with a group V method. In addition to these groups the additional cases of zeroth and quadratic extrapolation are denoted by Z and Q, respectively. Zeroth extrapolation in space and time, $v_0^{n+1} = v_1^n$, is denoted by ZT. Using the (FB) method (3.2) all boundary conditions at the left end were imposed after the second step. Boundary conditions at the right were imposed after the first step. For Tables II and IV, the analytically given boundary conditions were imposed after both steps. For the Richtmyer scheme it is difficult to impose the boundary data after each step and so only Tables III and V are relevant. In all these tables the errors are given for time steps $a\,\Delta t/\Delta x = \text{CFL} = 0.90$ and 0.25.

From Table II we see that at the intermediate level the higher-order extrapolations gave improved accuracy. Increasing the order of extrapolation at the end of both steps no longer is of any benefit. Zeroth-order extrapolation in space and time is advantageous for time steps near the stability limit. As predicted by Gustaffson, the use of group III methods is not advisable. This is because of the generalized eigenvalue that appears. The best results were obtained using group IV methods, which is no longer in agreement with the theory of Sköllermo. As shown by the scalar analysis of Section 3, boundary treatment VI is unstable for large time steps.

In Table III we consider the same case but with u specified only when it is not determined by the scheme and hence only once per boundary per cycle. For several boundary conditions the accuracy is decreased by an order of magnitude by this change. As predicted in Section 4, quadratic extrapolation at the end yielded unstable results. Use of the group VI boundary treatment was also unstable for sufficiently large time steps. In this case zeroth-order extrapolation was as good as the higher-order extrapolations except for short times. As before, the usefulness of zeroth-extrapolation increases for longer times. Table IV is similar to Table II but with the solution given by (7.4), while Table V considers the same solution specifying u at only one of the two steps. The general conclusions are similar to those of the previous case. The general error level is higher in the second case since the energy is no longer decaying.

As an additional case we consider the one-dimensional inviscid fluid dynamic equations for a converging–diverging nozzle. The two-dimensional effects are accounted for, since $A(x)$ appears in the equations. The solution approaches a steady state and so the nature of the problem is different from that of the previously considered cases. At the inlet the total pressure and total temperature are prescribed. At the outlet the flow is supersonic and so no conditions are given. With the parameters chosen no shocks appear. In Table VI we present the results for several boundary treatment at the inlet using the MacCormack (FB) scheme. As expected, changing

TABLE VI

Inviscid Equations for Converging-Diverging Nozzle[a]

Left boundary	Cycles to reach steady state	Error for M (throat)	Error for M (inlet)
Zero extrap.	426	.00561	.00248
Linear extrap. (I)	420	.00296	.00125
Quadratic extrap.	419	.00307	.00142
Euler (IIc)	Unstable		
Zero-Space-Time	427	.00553	.00247
IIIb	DID NOT CONVERGE IN 2000 CYCLES		
IVb	431	.00021	.00005
VI	420	.00284	.00114

[a] Steady state is considered to be reached when $| p_t/p | < 10^{-5}$. Right boundary was not varied. Error at steady state for Mach number is given.

the boundary treatment at the supersonic outlet did not have any large effect. The second column of Table VI gives the number of cycles required for $\max_x | p_t/p | < 10^{-5}$ In the next columns we present the error in the calculated Mach number at both the inlet and the throat.

The problem was also solved using the (BF) variant of the MacCormack method. This latter method was more accurate than the first variant. The difference between the two finite-difference methods was as important as the difference between the various boundary treatments. Differences between the two variants were analyzed by Lerat and Peyret [7] for shocked flows. Specifying the given variables at both steps again improved the accuracy. As before, the use of group IV methods led to the most accurate results while the group III method did not achieve steady state within 2000 cycles. The use of a one-sided Euler method (IIb or IIc) led to instabilities.

8. Conclusions

The theory of Kreiss is used to test the stability of various boundary treatments for both the Richtmyer and MacCormack methods. Analysis for a scalar equation shows that boundaries can cause instabilities even for the Lax-Wendroff type of schemes. Because of the complexity of the theory the results of the scalar equation are frequently applied to a system. Both analytic and computational results confirm that instabilities can occur in systems that do not occur for the scalar equations. This happens even for reasonable techniques, as extrapolation. Thus, whenever feasible, extrapolations should be performed on variables which approximate the outgoing characteristic variables. In this case the scalar theory is valid.

Comparisons of the accuracies of the different methods were made. The theory of Sköllermo [11] was found useful only for eliminating the least accurate of the methods. Imposing the analytic boundary conditions after each step of the method dramatically improved the accuracy of the method. As this is feasible only for the MacCormack methods, it is a disadvantage of the Richtmyer method. We note that imposing these conditions twice lowers the order of accuracy at the point adjoining the boundary from second-order to first-order accurate.

Zeroth-order extrapolation is seen to be a competitive method, especially for long-term integrations. Similar conclusions were reached by Chu and Sereny [1]. This of course is valid only for reasonable error tolerances. For sufficiently accurate answers the use of zeroth-order extrapolation is not recommended.

Section 3 discusses six groups of methods for treating the boundary. The general conclusion is that the group IV methods work best. In this group the one-sided difference operator in the MacCormack method is reversed at the edge. As this method is not applicable to the Richtmyer method, it again demonstrates the superiority of the MacCormack schemes for boundary problems. For the Richtmyer methods the most reasonable boundary treatment is extrapolation at the ends of both steps. Extrapolation, for the Richtmyer method, at the intermediate level is strongly discouraged.

These results can also be applied to the Navier–Stokes equations with a rigid wall condition. At the wall the velocities and temperature are given. One can then use the above techniques for the density equation, which does not contain any second-derivative terms.

The analysis and computations demonstrate that the boundary treatment must be investigated separately for each system of equations. For example, there are differences between the results of Sundström [13], who analyzed a fluid dynamic system, and the results presented in this study for a wave equation with nonequal sound speeds in the positive and negative directions. This may have important implications for non-isotropic flow such as occurs in plasticity or in plasma physics.

REFERENCES

1. C. K. CHU AND A. SERENY, *J. Computational Physics* **15** (1974), 476.
2. B. GUSTAFSSON, H. O. KREISS, AND A. SUNDSTRÖM, *Math. Comp.* **26** (1972), 649.
3. B. GUSTAFSSON, *Math. Comp.* **29** (1975), 396.
4. B. GUSTAFFSON AND A. SUNDSTRÖM, "Incompletely Parabolic Problems in Fluid Dynamics," Department of Computer Science Report, Uppsala, 1976.
5. KREISS, H. O., Difference approximations for the initial-boundary value problem for hyperbolic differential equations, *in* "Numerical Solutions of Nonlinear Differential Equations" (D. Greenspan, Ed.), p. 141, 1966.
6. H. O. KREISS, *Math. Comp.* **22** (1968), 703.
7. A. LERAT AND R. PEYRET, *Computers and Fluids* **2** (1974), 35.
8. MACCORMACK, R. W., "Lecture Notes in Physics," Vol. 8, p. 151, Springer–Verlag, New York, 1971.
9. G. R. MCGUIRE AND J. L. MORRIS, *J. Inst. Math. Appl.* **17** (1976), 53.

10. R. D. RICHTMYER AND K. W. MORTON, "Difference Methods for Initial Value Problems," 2nd ed., Interscience, New York, 1967.
11. G. SKÖLLERMO, Department Computer Science Report No. 63, Uppsala University, 1975.
12. J. C. STRIKWERDA, *Comm. Pure Appl. Math.* **30** (1977), 797.
13. A. SUNDSTRÖM, *J. Computational Physics* **17** (1975), 450.
14. J. M. VARAH, *SIAM J. Numer. Anal.* **8** (1971), 598.