JOURNAL OF COMPUTATIONAL PHYSICS 5, 229–243 (1970)

On the Comparison of Multistep Formulations of the Optimized Lax-Wendroff Method for Nonlinear Hyperbolic Systems in Two Space Variables

A. R. GOURLAY* AND J. LL. MORRIS

Department of Mathematics, University of Dundee, Dundee, Scotland

Received March 17, 1969

Schemes recently introduced by Strang [13], [14] are investigated with regard to the introduction of boundary conditions. Several numerical experiments are conducted, and a comparison of Strang's schemes with the Richtmyer scheme [12] and a generalization proposed by Gourlay and Morris [2] is reported.

I. OPTIMAL DIFFERENCE SCHEMES

The Lax-Wendroff method [10] for the one space dimensional system of conservation laws

$$\partial \mathbf{u}/\partial t + \partial \mathbf{f}/\partial x = 0, \tag{I.1}$$

where $\mathbf{u}$ is a vector and $\mathbf{f}$ is a vector function of the components of the unknown $\mathbf{u}$, has received considerable attention in recent years. In [12], Richtmyer showed how the Lax-Wendroff scheme could be written as a two step procedure in such a way that the scheme was computationally efficient and its high accuracy was maintained. The stability condition for these one dimensional schemes coincided with the well-known Courant-Friedrichs-Lewy condition, namely $p \mid \lambda \mid \leqslant 1$ for stability, where p is the mesh ratio and $\mid \lambda \mid$ is the maximum modulus eigenvalue of the Jacobian matrix of $\mathbf{f}$. In such a situation, the difference scheme is said to be optimally stable.

The natural extension of the Lax-Wendroff scheme in one space dimension to the system in two space dimensions,

$$\partial \mathbf{u}/\partial t + \partial \mathbf{f}/\partial x + \partial \mathbf{g}/\partial y = 0 \tag{I.2}$$

[$\mathbf{g} = \mathbf{g}(\mathbf{u})$], was considered in [11] by Lax and Wendroff and in [12] by Richtmyer. It was found, in this case, that the stability condition was more severe, namely

$$p \max \{ \mid \lambda_A \mid, \mid \lambda_B \mid \} \leqslant \frac{1}{\sqrt{8}},$$

* From April 1, 1970, at Scientific Centre, IBM (United Kingdom) Ltd., Peterlee, Co. Darham.

where λ_A and λ_B are the maximum eigenvalues of the Jacobians of $\mathbf{f}$ and $\mathbf{g}$ with respect to $\mathbf{u}$, respectively. Efforts to alleviate the stability condition have been proposed by Burstein [1] but, in so doing, the resulting scheme is so complex as to completely invalidate any hoped-for improvement.

A more promising scheme for solving (I.2) has been proposed by Strang [13]. There the author proposes a scheme which alternates a one-dimensional Lax-Wendroff operator in the x direction with one in the y direction so that if L_x represents a one dimensional x-direction Lax-Wendroff operator and L_y the y direction operator, Strang's scheme is

$$\mathbf{u}_{m+1} = \tfrac{1}{2}(L_x L_y + L_y L_x)\,\mathbf{u}_m\,, \tag{I.3}$$

where $\mathbf{u}_{m+1} = \mathbf{u}[x, y, (m + 1)k]$, k being the mesh spacing in time, and where $x = ih$, $y = jh$ is a grid point in the (x, y) space, h being the mesh spacing in the x and y directions. The scheme is $O(k^2)$ accurate and has the stability condition.

$$\max\{p \mid \lambda_A \mid, p \mid \lambda_B \mid\} \leqslant 1$$

and is, hence, optimal.

The computational procedure of (I.3) has been given by Gourlay and Morris [6]. A further improvement of (I.3) has recently been given by Strang [14]. The improvement comes from the computational aspect of the method. Strang notices that while (I.3) is optimal, it takes approximately twice as long to implement as the standard Lax-Wendroff scheme and the improvement of the scheme, computationally, is thus marginal. However, by introducing

$$\mathbf{u}_{m+1} = L_{x/2} L_y L_{x/2}\,\mathbf{u}_m\,, \tag{I.4}$$

where $L_{x/2}$ is the Lax-Wendroff operator in the x direction with a $\frac{1}{2}k$ span in time rather than the usual k, the $O(k^2)$ accuracy is maintained and the scheme is still optimal. By applying the operator twice and using the fact that

$$L_{x/2} \cdot L_{x/2} \to L_x + O(k^3),$$

we obtain

$$\mathbf{u}_{m+2} = L_{x/2} L_y L_x L_y L_{x/2}\,\mathbf{u}_m \tag{I.5}$$

so that six operators have been compounded into five. Thus, one can compound the operators at will, the $L_{x/2}$ operators being required only at print-out. As Strang points out, this makes the scheme (I.5) comparable in efficiency with the Lax-Wendroff method in two dimensions and has the factor $\sqrt{8}$ in its favor from the stability condition. The scheme (I.4) would, therefore, seem to be the more attractive to use in practice.

The purpose of this section is to consider the effect of boundary conditions upon Strang's schemes (I.3) and (I.4) in an effort to ascertain their merits in practical use.

Let us consider the solutions of the two-dimensional system of conservation laws

$$\partial \mathbf{u}/\partial t + \partial \mathbf{f}/\partial x + \partial \mathbf{g}/\partial y = 0 \tag{I.6}$$

subject to

$$\begin{aligned} \mathbf{u}(x, y, 0) &= \mathbf{U}_0(x, y) \qquad 0 \leqslant x, y \leqslant 1, \\ \mathbf{u}(0, y, t) &= \mathbf{U}_1(y, t) \qquad 0 \leqslant y \leqslant 1, \ t > 0, \\ \mathbf{u}(x, 0, t) &= \mathbf{U}_2(x, t) \qquad 0 \leqslant x \leqslant 1, \ t > 0, \end{aligned}$$

where $\mathbf{u}$ is an unknown vector of x, y, and t; $\mathbf{f}$ and $\mathbf{g}$ are known vector functions of the components of $\mathbf{u}$. $\mathbf{U}_0$, $\mathbf{U}_1$, and $\mathbf{U}_2$ are known functions. We assume, for convenience, that all the eigenvalues of the Jacobians of $\mathbf{f}$ and $\mathbf{g}$ with respect to $\mathbf{u}$ are positive so that (I.6) together with the initial and boundary conditions constitutes a well-posed problem.

The method (I.3), written using the format suggested by Gourlay and Morris [6], is

$$\begin{aligned} \mathbf{V}_{(1)}^{m+1} &= \mu_y \mathbf{u}^m - p/2\, \delta_y \mathbf{g}^m \\ \mathbf{V}_{(2)}^{m+1} &= \mathbf{u}^m - p\, \delta_y \mathbf{g}_{(1)}^{m+1} \\ \mathbf{V}_{(3)}^{m+1} &= \mu_x \mathbf{V}_{(2)}^{m+1} - p/2\, \delta_x \mathbf{f}_{(2)}^{m+1} \\ \mathbf{V}_{(4)}^{m+1} &= \mathbf{V}_{(2)}^{m+1} - p\, \delta_x \mathbf{f}_{(3)}^{m+1}, \end{aligned} \tag{I.7}$$

$$\begin{aligned} \mathbf{W}_{(1)}^{m+1} &= \mu_x \mathbf{u}^m - p/2\, \delta_x \mathbf{f}^m \\ \mathbf{W}_{(2)}^{m+1} &= \mathbf{u}^m - p\, \delta_x \mathbf{f}_{(1)}^{m+1} \\ \mathbf{W}_{(3)}^{m+1} &= \mu_y \mathbf{W}_{(2)}^{m+1} - p/2\, \delta_y \mathbf{g}_{(2)}^{m+1} \\ \mathbf{W}_{(4)}^{m+1} &= \mathbf{W}_{(2)}^{m+1} - p\, \delta_y \mathbf{g}_{(3)}^{m+1}, \end{aligned} \tag{I.8}$$

$$\mathbf{u}^{m+1} = \tfrac{1}{2}(\mathbf{V}_{(4)}^{m+1} + \mathbf{W}_{(4)}^{m+1}), \tag{I.9}$$

where the notation $\mathbf{u}^m = \mathbf{u}_{ij}^m = \mathbf{u}(ih, jh, mk)$, $\mathbf{g}^m = \mathbf{g}_{ij}^m = \mathbf{g}(\mathbf{u}_{ij}^m)$, $\mathbf{f}_{(1)}^{m+1} = \mathbf{f}(\mathbf{W}_{(1)}^{m+1})$ has been used and the difference operators δx, δy are the usual difference operators defined by

$$\delta_x \mathbf{u}_{ij}^m = \mathbf{u}_{i+1/2j}^m - \mathbf{u}_{i-1/2j}^m, \qquad \delta_y \mathbf{u}_{ij}^m = \mathbf{u}_{ij+1/2}^m - \mathbf{u}_{ij-1/2}^m,$$

and μ_x, μ_y are the usual averaging operators defined by

$$\mu_x \mathbf{u}_{ij}^m = \tfrac{1}{2}(\mathbf{u}_{i+1/2j}^m + \mathbf{u}_{i-1/2j}^m) \qquad \text{and} \qquad \mu_y \mathbf{u}_{ij}^m = \tfrac{1}{2}(\mathbf{u}_{ij+1/2}^m + \mathbf{u}_{ij-1/2}^m).$$

The scheme (I.4) may be written in a similar format to {(I.7), (I.8), (I.9)}, namely,

$$\begin{aligned}
\mathbf{V}_{(1)}^{m+1} &= \mu_x \mathbf{u}^m - p/4\, \delta_x \mathbf{f}^m \\
\mathbf{V}_{(2)}^{m+1} &= \mathbf{u}^m - p/2\, \delta_x \mathbf{f}_{(1)}^{m+1} \\
\mathbf{V}_{(3)}^{m+1} &= \mu_y \mathbf{V}_{(2)}^{m+1} - p/2\, \delta_y \mathbf{g}_{(2)}^{m+1} \\
\mathbf{V}_{(4)}^{m+1} &= \mathbf{V}_{(2)}^{m+1} - p\, \delta_y \mathbf{g}_{(3)}^{m+1} \\
\mathbf{V}_{(5)}^{m+1} &= \mu_x \mathbf{V}_{(4)}^{m+1} - p/4\, \delta_x \mathbf{f}_{(4)}^{m+1} \\
\mathbf{V}_{(6)}^{m+1} &= \mathbf{V}_{(4)}^{m+1} - p/2\, \delta_x \mathbf{f}_{(5)}^{m+1},
\end{aligned} \tag{I.10}$$

$$\mathbf{u}^{m+1} = \mathbf{V}_{(6)}^{m+1}. \tag{I.11}$$

The compounding of (I.10) is obvious and is omitted. It is immediately obvious that schemes {(I.7), (I.8), (I.9)} and {(I.10), (I.11)} require boundary conditions on $x = 1$, $0 \leqslant y \leqslant 1$, and $y = 1$, $0 \leqslant x \leqslant 1$, in order that the schemes are feasible. It is also obvious that such boundary conditions are not forthcoming from the differential equation and, furthermore, that the boundary conditions given on $x = 0, 0 \leqslant y \leqslant 1, y = 0, 0 \leqslant x \leqslant 1$ cannot be used in the intermediate levels as boundary conditions since the intermediate levels bear no relation to the differential Eq. (I.6). This means, therefore, that we must implement some technique for introducing the extra data required at *all* the intermediate boundaries and at the final time level at the upper boundaries. This procedure will also apply to the operators that are compounded, that is to the $L_{x/2}L_{x/2} \to L_x + O(k^3)$ operators, for the *given* boundary conditions again bear no relation to the difference scheme in this case. The techniques for introducing the extra boundary conditions can be derived following the procedure outlined by Gourlay and Morris [4]. For (I.7) and (I.8) the boundary techniques become

$$\begin{aligned}
\mathbf{V}_{(1)_0}^{m+1} &= \tfrac{1}{2}(\Delta_y^2 + 2)\, \mathbf{u}_0^m - p/2(2\Delta_y - \Delta_y^2)\, \mathbf{g}_0^m \\
\mathbf{V}_{(1)_N}^{m+1} &= \tfrac{1}{2}(\nabla_y^2 + 2)\, \mathbf{u}_N^m - p/2(2\nabla_y + \nabla_y^2)\, \mathbf{g}_N^m \\
\mathbf{V}_{(2)_0}^{m+1} &= \mathbf{u}_0^m - p(2\Delta_y - \Delta_y^2)\, \mathbf{g}_{(1)_0}^{m+1} \\
\mathbf{V}_{(2)_N}^{m+1} &= \mathbf{u}_N^m - p(2\nabla_y + \nabla_y^2)\, g_{(1)_N}^{m+1} \\
\mathbf{V}_{(3)_0}^{m+1} &= \tfrac{1}{2}(\Delta_x^2 + 2)\, \mathbf{V}_{(2)_0}^{m+1} - p/2(2\Delta_x - \Delta_x^2)\, \mathbf{f}_{(2)_0}^{m+1} \\
\mathbf{V}_{(3)_N}^{m+1} &= \tfrac{1}{2}(\nabla_x^2 + 2)\, \mathbf{V}_{(2)_N}^{m+1} - p/2(2\nabla_x + \nabla_x)\, \mathbf{f}_{(2)_N}^{m+1} \\
\mathbf{V}_{(4)_0}^{m+1} &= \mathbf{V}_{(2)_0}^{m+1} - p(2\Delta_x - \Delta_x^2)\, \mathbf{f}_{(3)_0}^{m+1} \\
\mathbf{V}_{(4)_N}^{m+1} &= \mathbf{V}_{(4)_N}^{m+1} - p(2\nabla_x + \nabla_x^2)\, \mathbf{f}_{(3)_N}^{m+1},
\end{aligned} \tag{I.12}$$

and

$$
\begin{aligned}
\mathbf{W}_{(1)_0}^{m+1} &= \tfrac{1}{2}(\Delta_x^2 + 2)\,\mathbf{u}_0^m - p/2(2\Delta_x - \Delta_x^2)\,\mathbf{f}_0^m \\
\mathbf{W}_{(1)_N}^{m+1} &= \tfrac{1}{2}(\nabla_x^2 + 2)\,\mathbf{u}_N^m - p/2(2\nabla_x + \nabla_x^2)\,\mathbf{f}_N^m \\
\mathbf{W}_{(2)_0}^{m+1} &= \mathbf{u}_0^m - p(2\Delta_x - \Delta_x^2)\,\mathbf{f}_{(1)_0}^{m+1} \\
\mathbf{W}_{(2)_N}^{m+1} &= \mathbf{u}_N^m - p(2\nabla_x + \nabla_x^2)\,\mathbf{f}_{(1)_N}^{m+1} \\
\mathbf{W}_{(3)_0}^{m+1} &= \tfrac{1}{2}(\Delta_y^2 + 2)\,\mathbf{W}_{(2)_0}^{m+1} - p/2(2\Delta_y - \Delta_y^2)\,\mathbf{g}_{(2)_0}^{m+1} \\
\mathbf{W}_{(3)_N}^{m+1} &= \tfrac{1}{2}(\nabla_y^2 + 2)\,\mathbf{W}_{(2)_N}^{m+1} - p/2(2\nabla_y + y_y^2)\,\mathbf{g}_{(2)_N}^{m+1} \\
\mathbf{W}_{(4)_0}^{m+1} &= \mathbf{W}_{(2)_0}^{m+1} - p(2\Delta_y - \Delta_y^2)\,\mathbf{g}_{(3)_0}^{m+1} \\
\mathbf{W}_{(4)_N}^{m+1} &= \mathbf{W}_{(2)_N}^{m+1} - p(2\nabla_y + \nabla_y^2)\,\mathbf{g}_{(3)_N}^{m+1},
\end{aligned}
\tag{I.13}
$$

so that the complete algorithm comprises (I.7), (I.8), (I.9), (I.12), and (I.13) where the constituent equations of (I.12) and (I.13) are used in the correct order with those of (I.7) and (I.8). That is, the first equation from (I.7) and the first two equations from (I.12) are used before going on to the next step, etc.

The corresponding boundary formulae for (I.10) are

$$
\begin{aligned}
\mathbf{V}_{(1)_0}^{m+1} &= \tfrac{1}{2}(\Delta_x^2 + 2)\,\mathbf{u}_0^m - p/4(2\Delta_x - \Delta_x^2)\,\mathbf{f}_0^m \\
\mathbf{V}_{(1)_N}^{m+1} &= \tfrac{1}{2}(\nabla_x^2 + 2)\,\mathbf{u}_N^m - p/4(2\nabla_x + \nabla_x^2)\,\mathbf{f}_N^m \\
\mathbf{V}_{(2)_0}^{m+1} &= \mathbf{u}_0^m - p/2(2\Delta_x - \Delta_x^2)\,\mathbf{f}_{(1)_0}^{m+1} \\
\mathbf{V}_{(2)_N}^{m+1} &= \mathbf{u}_N^m - p/2(2\nabla_x + \nabla_x^2)\,\mathbf{f}_{(1)_N}^{m+1} \\
\mathbf{V}_{(3)_0}^{m+1} &= \tfrac{1}{2}(\Delta_y^2 + 2)\,\mathbf{V}_{(2)_0}^{m+1} - p/2(2\Delta_y - \Delta_y^2)\,\mathbf{g}_{(2)_0}^{m+1} \\
\mathbf{V}_{(3)_N}^{m+1} &= \tfrac{1}{2}(\nabla_y^2 + 2)\,\mathbf{V}_{(2)_N}^{m+1} - p/2(2\nabla_y + \nabla_y^2)\,\mathbf{g}_{(2)_N}^{m+1} \\
\mathbf{V}_{(4)_0}^{m+1} &= \mathbf{V}_{(2)_0}^{m+1} - p(2\Delta_x - \Delta_x^2)\,\mathbf{g}_{(3)_0}^{m+1} \\
\mathbf{V}_{(4)_N}^{m+1} &= \mathbf{V}_{(2)_N}^{m+1} - p(2\nabla_y + \nabla_y^2)\,\mathbf{g}_{(3)_N}^{m+1} \\
\mathbf{V}_{(5)_0}^{m+1} &= \tfrac{1}{2}(\Delta_x^2 + 2)\,\mathbf{V}_{(4)_0}^{m+1} - p/4(2\Delta_x - \Delta_x^2)\,\mathbf{f}_{(4)_0}^{m+1} \\
\mathbf{V}_{(5)_N}^{m+1} &= \tfrac{1}{2}(\nabla_x^2 + 2)\,\mathbf{V}_{(4)_N}^{m+1} - p/4(2\Delta_x + \nabla_x^2)\,\mathbf{f}_{(4)_N}^{m+1} \\
\mathbf{V}_{(6)_0}^{m+1} &= \mathbf{V}_{(4)_0}^{m+1} - p/2(2\Delta_x - \Delta_x^2)\,\mathbf{f}_{(5)_0}^{m+1} \\
\mathbf{V}_{(6)_N}^{m+1} &= \mathbf{V}_{(4)_N}^{m+1} - p/2(2\nabla_x + \nabla_x^2)\,\mathbf{f}_{(5)_N}^{m+1}.
\end{aligned}
\tag{I.14}
$$

The difference operators Δ_x and ∇_x are defined by the relations

$$\Delta_x \mathbf{u}_{ij}^m = \mathbf{u}_{i+1/2j}^m - \mathbf{u}_{ij}^m, \qquad \nabla_x \mathbf{u}_{ij}^m = \mathbf{u}_{ij}^m - \mathbf{u}_{i-1/2j}^m$$

and similar definitions for Δ_y and ∇_y.

The merits of including such modifications are discussed in [4], together with certain generalizations. It should be noted that this procedure is slightly different from that suggested in several papers by Kreiss [7], [8], [9]. An alternative boundary procedure is given in [5], which maintains the uncoupled property of the Lax-Wendroff operator.

II. Numerical Results

A number of numerical experiments were carried out to compare the schemes (I.3) and (I.4) using the formulation given in equations {(I.7), (I.8), (I.9)} and {(I.10), (I.11)}. We investigated the average saving in time using techniques (I.4) and (I.3) and, also, the effect of the method of incorporating the boundary conditions upon the accuracy of the methods. To these ends, we studied the numerical solution of the two space dimensional equation

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(\tfrac{1}{4}u^2) + \frac{\partial}{\partial y}(\tfrac{1}{4}u^2) = 0 \tag{II.1}$$

subject to the initial condition

$$u(x, y, 0) = \tfrac{1}{4}(x + y)^2 \tag{II.2}$$

and the boundary conditions

$$\begin{aligned} u(0, y, t) &= \left\{\frac{1 - \sqrt{1 + yt}}{t}\right\}^2 \qquad 0 \leqslant y \leqslant 1, \\ u(x, 0, t) &= \left\{\frac{1 - \sqrt{1 + xt}}{t}\right\}^2 \qquad 0 \leqslant x \leqslant 1. \end{aligned} \tag{II.3}$$

Equation (II.1), together with Eq. (II.2) and (II.3), has the theoretical solution

$$u(x, y, t) = \left\{\frac{1 - \sqrt{1 + (x + y)t}}{t}\right\}^2.$$

As a comparison with the novel schemes described in Section I, we also ran the problem (II.1, II.2, II.3) for the two step Lax-Wendroff method and the generalizations described in [2]: namely,

$$u^*_{m+1} = \tfrac{1}{2}(\mu_x + \mu_y)\, u_m - ap(H_x f_m + H_y g_m),$$

$$u_{m+1} = u_m - p/2[(1 - 1/(4a))(H_x f_m + H_y g_m) + 1/(4a)(H_x f^*_{m+1} + H_y g^*_{m+1})],$$

TABLE I

Scheme (I.3): Errors at 100 Time Steps

Expt.	h \ p	0.3	0.6	1.0	1.5	1.75	2.0	Average Time
1	0.1	10^{-1} uneven	10^{-1} uneven	10^{0} uneven	10^{0} very uneven	10^{0} very uneven	10^{0} very uneven	1 min
	0.2	10^{0} very uneven	10^{0} very uneven	10^{0} very uneven	10^{0} very uneven	10^{0} very uneven	10^{0} very uneven	52 sec
2	0.1	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	1 min
	0.2	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	56 sec
3	0.1	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	2 min
	0.2	10^{-3} even	10^{-3} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	3 sec
4	0.1	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	2 min
	0.2	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	6 sec

Experiment No. 1. All boundary conditions inserted as appropriate theoretical solution.

Experiment No. 2. All upper boundaries obtained using the appropriate formula from (I.12) and (I.13) and all lower boundaries given by appropriate theoretical solution.

Experiment No. 3. All upper boundaries given as in No. 2. All intermediate lower boundaries given by appropriate formula from (I.12) and (I.13). The lower $(m + 1)$ boundary given by appropriate theoretical solution.

Experiment No. 4. All boundaries given by appropriate equation in formulae from (I.12) and (I.13).

Note. The p quoted in these results $= 2 \times p$ quoted in text in Section 1. (For convenience we programmed the schemes on a double size grid.)

where

$$\mu_x u_m = \frac{u^m_{i+1j} + u^m_{i-1j}}{2}; \qquad H_x f_m = f^m_{i+1j} - f^m_{i-1j},$$

etc., and a is a parameter.

The result of the runs on a computer are given in Tables I–IV. The entries indicate the largest error that occurred over the region at one hundred time steps, and the comment with each entry in the table indicates the distribution of the errors.

TABLE II

Scheme I.4: Errors at 100 Time Steps

Expt.	h \ p	0.3	0.6	1.0	1.5	1.75	2.0	Average Time
1	0.1	10^{-2} uneven	10^{-2} uneven	10^{-2} uneven	10^{-2} uneven	10^{-2} uneven	10^{-2} uneven	1 min 30 sec
	0.2	10^{-1} uneven	10^{-1} uneven	10^{-1} uneven	10^{-0} uneven	10^{-0} very uneven	10^{-0} very uneven	
2	0.1	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	1 min 25 sec
	0.2	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	
3	0.1	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	1 min 21 sec
	0.2	10^{-3} even	10^{-3} even	10^{-3} even	10^{-4} even	10^{-4} even	10^{-4} even	
4	0.1	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	1 min 20 sec.
	0.2	10^{-3} even	10^{-3} even	10^{-4} even	10^{-4} even	10^{-4} even	10^{-4} even	

Experiment No. 1. Theoretical boundaries at all boundaries.

Experiment No. 2. All upper boundaries obtained using appropriate formula from (I.14) and all lower boundaries given by appropriate theoretical solution.

Experiment No. 3. All boundaries except $(m + 1)$ lower boundary given by appropriate formula from Eq. (I.14). The $(m + 1)$ lower boundary given by appropriate theoretical solution.

Experiment No. 4. All boundaries given by (I.14) except at print-out, when the theoretical solution at lower boundaries at the final level was substituted.

Note. The p quoted in the table $= 2 \times p$ quoted in Section I.

TABLE III

Theoretical Boundary Data: Errors at 100 Time Steps

a		0.3	0.6	1.0	1.5	1.75	2.0	Average Time
0.25	0.1	10^{-3} even	10^{-2} even	10^{-2} uneven	10^{-1} uneven	10^{-1} very uneven	10^{-1} very uneven	
	0.2	10^{-1} uneven	10^{-1} uneven	10^{0} very uneven	10^{0} very uneven	10^{0} very uneven	10^{0} poor results	
0.5	0.1	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	
	0.2	10^{-2} even	10^{-2} even	10^{-2} even	10^{-1} uneven	10^{-1} uneven	10^{-1} uneven	2 min 20 sec

TABLE IV

Boundary Technique Applied: Errors at 100 Time Steps

a		0.3	0.6	1.0	1.5	1.75	2.0	Average Time
0.25	0.1	10^{-1} uneven	10^{-1} uneven	*	*	*	*	
	0.2	*	*	*	*	*	*	
0.5	0.1	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	10^{-3} even	
	0.2	10^{-2} even	10^{-3} even	10^{-3} even	*	*	*	2 min 37 sec

* Indicates nonlinear instability had developed.

From the computed results quoted in Tables I–IV, it was concluded that the most satisfactory procedures were those described in Experiments 3 and 4 in Table II and Experiment 3 in Table I. These schemes have a higher accuracy than the best schemes in Tables III and IV and, furthermore, the accuracy is greater when using $a = \frac{1}{2}$ than when $a = \frac{1}{4}$ in Tables III and IV. However, even the scheme with $a = \frac{1}{2}$ in table IV suffers from nonlinear instability for $h = 0.2$ and, thus, makes the scheme suspect. It is marked how even the errors are for Experiments 2, 3, and 4 in both Tables I and II.

A point that naturally arises in connection with the schemes (I.10) is its associated boundary technique when compounding of the operator takes place. In this case, boundary conditions on $x = 0$ which would be applied to the two operators $L_{x/2}$, $L_{x/2}$ separately cannot be applied to the operator L_x which results from the

compounding of $L_{x/2} \cdot L_{x/2}$. This means that a boundary technique similar to those quoted in Eqs. (I.14) should be used and Eq. (I.11), which introduces the physical boundary conditions, does not appear again until print-out. In these circumstances, it is obvious that there are grave dangers of the difference equations becoming unstable since, in effect, continued introduction of boundary data, using the boundary techniques on $x = 0$ and $y = 0$, means that the data are being introduced in a direction directly opposite to the direction of the characteristic curves on the lines $x = 0$ and $y = 0$. This problem arises *only* when the compounding of operators occurs. Since no such operation takes place in (I.7), (I.8), and (I.9), no problem of introducing 'wrong' boundary conditions takes place. To investigate the effect of the continual introduction of 'wrong' data when compounding the operators in (I.10), we considered the problem

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(\tfrac{1}{2}u^2) + \frac{\partial}{\partial y}(\tfrac{1}{2}u^2) = 0 \tag{II.4}$$

with the initial condition

$$u(x, y, 0) = \begin{cases} 1, & 0 \leqslant x \leqslant 0.1 \\ 0, & 0.1 < x \leqslant 0.5, \end{cases} \tag{II.5}$$

which is independent of y. This initial condition has a discontinuity which propagates into the field so that the shock front is parallel to the y axis and moves along the line

$$x = 0.1 + 0.5t.$$

Thus, we substituted the boundary conditions

$$u(0, y, t) = 1, \quad t > 0; \qquad u(x, 0, t) = \begin{cases} 1, & x \leqslant 0.1 + 0.5t \\ 0, & x > 0.1 + 0.5t. \end{cases} \tag{II.6}$$

The results of computing the solution of (II.4), (II.5), (II.6) using the algorithms defined by (I.7), (I.8), (I.9), and (I.10) are given in Table V, where the mesh ratio p was 1.0 and $h = 0.01$ for all the experiments.

The effect that incorrect data can have upon schemes (I.10), (I.11) (if compounding of the operators takes place with the associated boundary technique is clear from Table V); nonlinear instability can take place when print-out is suspended for more than two time steps. Thus, we must compound the operators

$$L_{x/2} \cdot L_{x/2} \rightarrow L_x$$

with caution and, hence, the hoped-for increase in efficiency is only marginal.

TABLE V

Solution at 20 Time Steps for $y = 0.25$

Grid Point No. \ Expt	1	2	3	4	5	6	7	8
1	1.000	1.000	1.000	*1	*2	*3	*4	1.000
2	0.993	1.016	1.007					1.003
3	0.929	0.812	0.882					0.9221
4	0.925	0.821	0.885					0.9233
5	1.078	1.153	1.108					1.084
6	1.077	1.158	1.109					1.085
7	1.003	0.989	1.000					1.000
8	1.002	0.992	1.002					1.000
9	0.751	0.629	0.695					0.744
10	0.751	0.629	0.695					0.744
11	1.287	1.380	1.326					1.294
12	1.287	1.380	1.326					1.260
13	1.259	1.264	1.264					1.260
14	1.259	1.264	1.264					0.153
15	0.154	0.149	0.152					0.153
16	0.154	0.149	0.152					0.153
17	0.000	0.000	0.000					0.000
18	0.000	0.000	0.000					0.000
19	0.000	0.000	0.000					0.000
	↓							
	Solution = 0.000 to grid point 50							

Experiment No. 1. Equations I.7, I.8, I.9.

Experiment No. 2. Equations (I.10) (I.11) using theoretical data on $x = 0$ at print-out; print-out every time step.

Experiment No. 3. As in No. 2 except print-out every 2 time steps.

Experiment No. 4. As in No. 2 except print-out every 3 time steps.

Experiment No. 5. As in No. 2 except print-out every 4 time steps.

Experiment No. 6. As in No. 2 except print-out every 5 time steps.

Experiment No. 7. As in No. 2 except print-out every 10 time steps.

*1 indicates numbers order 10^{78} after 3 time steps.

*2 indicates numbers order 10^{78} after 8 time steps.

*3 indicates numbers order 10^{78} after 9 time steps.

*4 indicates numbers order 10^{78} between 10 and 20 time steps.

Experiment No. 8. Equations (I.10), (I.11) using "theoretical" data for all $x = 0$. This was possible in this example since the boundary data were time independent ($u = 1$ for all t at $x = 0$).

III. Generalizations

In Section II we assumed the Jacobian matrices of f and g had only positive eigenvalues. If this were not so and, corresponding to $(u_1\, u_2, \ldots, u_p)$, the

eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_p$ of A and $\mu_1, \mu_2, \ldots, \mu_p$ of B are positive, and the eigenvalues

$$\lambda_{p+1}, \lambda_{p+2}, \ldots, \lambda_n \text{ of } A \text{ and } \mu_{p+1}, \mu_{p+2}, \ldots, \mu_n \text{ of } B,$$

corresponding to the elements $(u_{p+1}, u_{p+2}, \ldots, u_n)$, are negative, then boundary conditions would be given for the first p components of $\mathbf{u}$ on $x = 0, 0 \leqslant y \leqslant 1$ and $y = 0, 0 \leqslant x \leqslant 1$ and for the next $(n - p)$ components of $\mathbf{u}$ on

$$x = 1, 0 \leqslant y \leqslant 1 \qquad \text{and} \qquad y = 1, 0 \leqslant x \leqslant 1.$$

(Other combinations are obviously possible.) In the cases where the eigenvalues are of mixed sign, it is theoretically possible to apply the procedures outlined in Section II using the boundary procedure on the boundaries which have no given data.

The techniques discussed in Section I can be extended, in a natural manner, to problems of a higher number of space dimensions. Thus, for example, the system

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial h}{\partial z} = 0,$$

where f, g, h are functions of u, x, y, z, t, the extension of (I.4) is

$$u_{m+1} = L_{x/2} L_{y/2} L_z L_{y/2} L_{x/2} u_m \tag{III.1}$$

and, as before, the $L_{x/2}$ operators combine. However, the process is obviously losing in efficiency. In [14], Strang suggests that the extension of (I.3) would involve all permutations of L_x, L_y, and L_z. In fact, this is not so. It is sufficient to use

$$u_{m+1} = \tfrac{1}{2}(L_x L_y L_z + L_z L_y L_x)\, u_m . \tag{III.2}$$

Notice that the computational advantage of (III.1) over (III.2) has now dropped to a factor of only 3/2. The advantage in general is reduced as the number of dimensions increases.

IV. Implicit Schemes

The attractive stability conditions of implicit methods has long been known and appreciated by practical workers in the field of fluid mechanics and other physical sciences. However, there is always the question of extra boundary data required by these implicit methods when used to solve hyperbolic systems of partial differential equations. In the past, this problem has been ignored and arbitrary data have been

included where the physical problem was not forthcoming with the necessary data.

In this section, we propose the use of explicit boundary schemes similar to those outlined by Gourlay and Morris [4] for the introduction of data at unknown boundary points.

Consider the solution of the one space dimensional hyperbolic system

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}}{\partial x} = 0$$

subject to

$$\begin{aligned} \mathbf{u}(x, 0) &= \mathbf{u}_0(x) \qquad 0 \leqslant x \leqslant 1, \\ \mathbf{u}(0, t) &= \mathbf{u}_1(t) \qquad t > 0, \end{aligned}$$

where $\mathbf{u}$ is an unknown $\mathbf{n}$ vector with components which are functions of x and t. $\mathbf{f}$ is a known vector function of the components of $\mathbf{u}$. We consider the implicit scheme given in [4], namely,

$$\begin{aligned} \mathbf{u}^*_{m+1} &= \mu_x \mathbf{u}_m - p/2 H_x \mathbf{f}_m \\ [I + p/4 H_x \tilde{\mathbf{A}}^*_{m+1}]\, \mathbf{u}_{m+1} &= \mathbf{u}_m - p/4 H_x \mathbf{f}_m , \end{aligned} \tag{IV.1}$$

where μ_x and H_x are difference operators defined by

$$\mu_x \mathbf{u}_i^m = \frac{\mathbf{u}^m_{i+1} + \mathbf{u}^m_{i-1}}{2} \qquad \text{and} \qquad H_x \mathbf{u}_i^m = \mathbf{u}^m_{i+1} - \mathbf{u}^m_{i-1} .$$

$\tilde{A}$ is defined by the relation

$$\tilde{A}(\mathbf{u}) \cdot \mathbf{u} = \mathbf{f}(\mathbf{u}).$$

Equation (IV.1) is unconditionally stable in the linearized sense and requires the inversion of a tridiagonal matrix for its solution. In order to invert this matrix, the value of $\mathbf{u}_{m+1}$ is required at $x = 1$. It is at this node that we propose to use an explicit boundary procedure. Any explicit procedure will do but we prefer the scheme

$$\begin{aligned} \underset{N}{\mathbf{u}^*_{m+1}} &= \tfrac{1}{2}(\nabla_x^{\,2} + 2)\, \underset{N}{\mathbf{u}_m} - p/2(2\nabla_x + \nabla_x^{\,2})\, \underset{N}{\mathbf{f}_m} , \\ \underset{N}{\mathbf{u}_{m+1}} &= \underset{N}{\mathbf{u}_m} - p/4[(2\nabla_x + \nabla_x^{\,2} + \nabla_x^{\,3})\, \underset{N}{\mathbf{f}_m} + (2\nabla_x + \nabla_x^{\,2} + \nabla_x^{\,3})\, \underset{N}{\mathbf{f}^*_{m+1}}]. \end{aligned} \tag{IV.2}$$

Equation (IV.2) is the method of introducing extra data at boundary points given in the explicit schemes considered in [4].

The results of using Eq. (IV.1) and (IV.2) and the conventional method of introducing boundary data are given in Table VI for the problem of Section II.

It was concluded that no loss in accuracy occurred by introducing the boundary data by (IV.2). Also, no advantage was gained by "inverting" the lower boundary at the predictor level; these boundary data were given by the same data as those for the implicit corrector formula.

It is straightforward to see that this technique can be generalized to a higher number of space dimensions. In particular, A.D.I. schemes (see [3], [4], for example) for hyperbolic systems in two space dimensions can then be used for physical problems without the need for introducing arbitrary data points.

TABLE VI

Errors at 100 time steps for schemes (4.1), (4.2)

Expt. No.	$h \backslash p$	0.1	0.3	0.6	1.0
1	0.1	10^{-4}	10^{-4}	10^{-4}	10^{-4}
2	0.1	10^{-4}	10^{-4}	10^{-4}	10^{-4}
3	0.1	10^{-4}	10^{-4}	10^{-4}	10^{-4}
4	0.1	10^{-4}	10^{-4}	10^{-4}	10^{-4}

1 = Theoretical boundaries.
2 = Theoretical boundaries except for inversion at top boundary of predictor formula.
3 = Upper boundaries given by (IV.2). Bottom boundaries given by theoretical solution.
4 = The same as 3, except the lower boundary of predictor level also "inverted."
Experiments 3 and 4, in fact, gave identical results.
The errors indicate the $\max^n$ error that occurred at the 100 time step level.

REFERENCES

1. S. Z. BURSTEIN, Numerical calculations of multidimensional shocked flows, *AIAA J.* **2** (1964), 211–217.
2. A. R. GOURLAY AND J. LL. MORRIS, Finite difference methods for nonlinear hyperbolic systems, *Math. Comp.* **22** (1968), 28–39.
3. A. R. GOURLAY AND A. R. MITCHELL, Alternating direction methods for hyperbolic systems, *Numer. Math.* **8** (1966), 137–149.
4. A. R. GOURLAY AND J. LL. MORRIS, Finite difference methods for non-linear hyperbolic systems II. *Math. Comp.* **22** (1968), 103, 549–556.
5. A. R. GOURLAY AND J. LL. MORRIS, Deferred approach to the limit in non-linear hyperbolic systems, Comput. J. **11** (1968), 1, 95–101.
6. A. R. GOURLAY AND J. LL. MORRIS, A multistep formulation of the optimized Lax-Wendroff method for non-linear hyperbolic systems in two space variables, *Math. Comp.* **22** (1968), 104, 715–719.

7. H. O. KREISS, "Difference Approximations for the Initial Boundary Value Problem for Hyperbolic differential Equations," *in* Numerical Solution of Nonlinear Differential Equations (D. Greenspan, Ed.) Wiley, New York, 1966.
8. H. O. KREISS, "Difference approximations for hyperbolic differential Equations," *in* Numerical Solution of Partial Differential Equations (J. H. Bramble, Ed.) Academic Press, New York 1966.
9. H. O. KREISS, Stability theory for difference approximations of mixed initial boundary value problems I, *Math. Comp.* **22** (1968), 104, 703–714.
10. P. LAX AND B. WENDROFF, Systems of conservation laws, *Comm. Pure Appl. Math.* **13** (1960), 217–237.
11. P. LAX AND B. WENDROFF, Difference schemes for hyperbolic equations with high order of accuracy, *Comm. Pure Appl. Math.* **17** (1964), 381–398.
12. R. D. RICHTMYER, A survey of difference methods for non-steady fluid dynamics, *N.C.A.R. Tech.*, Notes 63–2.
13. W. G. STRANG, Accurate partial difference methods II, Nonlinear problems, *Numer. Math.* **13** (1964), 37–46.
14. W. G. STRANG, On the construction and comparison of difference schemes, *SIAM J. Numer. Anal.* **5** (1968), 3, 506–517.