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Boundary Conditions in Finite Difference Fluid Dynamic Codes

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This paper treats the question of extraneous boundary conditions in fluid dynamic computing. Several simple problems in one-dimensional gas dynamics are solved using different boundary schemes. Some surprising differences in the accuracy of the schemes are shown. A simple analytical investigation is proposed as a criterion for accuracy of boundary schemes.

1. INTRODUCTION

In fluid-dynamic and magnetohydrodynamic codes, the question of extraneous boundary conditions (i.e., boundary conditions needed by the difference equations but not by the differential equations) often results in difficulties and inaccuracies. This paper presents a series of test calculations addressed to this question.

The remarkable advances made in fluid computing during the past decade (see, e.g., [1–3]) corresponded to a vast increase in understanding of numerical analysis for pure initial-value problems. Knowledge of numerical stability, relation of stability to convergence, accuracy in terms of dissipation and dispersion of schemes, etc., have become by now rather well understood.

On the other hand, progress in understanding of mixed initial-boundary value problems is considerably slower. To begin with, convenient Fourier analysis (von Neumann criterion) is no longer applicable, and one must resort to energy methods or to operator-spectral methods (see, e.g., Richtmyer and Morton [4]). The latter methods, initially due to Godunov and Ryabenkii (see [4]), have been extended, improved, and applied with considerable vigor to numerous concrete cases by Kreiss and his coworkers [5–7]. Thus, only recently has our knowledge of the stability of schemes for mixed initial-boundary value problems become approximately comparable to that for pure initial-value problems; our knowledge of the accuracy and behavior of various schemes, involving dissipation and dispersion, etc., however, is still not well developed for these mixed initial-boundary value problems.

Naturally, most interesting fluid-dynamic calculations are precisely for mixed initial-boundary value problems, rather than for pure initial-value problems.

Well-known examples of such calculations include flow past bodies, flow in ducts, free surface flows, etc. These practical calculations have been carried out all this time, even though theoretical understanding may have lagged. The treatment of boundary conditions in these calculations, however, has generally been carried out in an ad hoc and unsystematic fashion. A notable example is the so-called "reflection principle", in which a variable, which may not be prescribed for the differential equation problem but which is needed for a difference scheme, is reflected or extrapolated near the boundary with virtually no justification. A number of fluid dynamicists, notably Cheng [9], Moretti [10], and Roache in his book [11], have objected to such procedures, and have proposed some remedies. On the whole, however, there is as yet no systematic study of such questions.

In pure initial-value problems paralleling the theoretical accuracy studies, the literature is also full of test calculations evaluating the relative merits of various schemes under fairly simple and controlled test conditions. (e.g., [12, 13]). Such calculations are valuable, not only in comparing with theoretical predictions of accuracy, but also in uncovering unexpected phenomena associated with the numerical schemes. For mixed initial-boundary value problems in fluid dynamics, even such test calculations are rare in the literature; and when they are done, e.g., Moretti [10], they usually are applied to relatively complex problems, so that comparison with exact results are spotty.

The present paper represents one simple series of such test calculations. The problem treated is the classical problem of one-dimensional isentropic gas flow in a tube. Various boundary conditions at the two ends represent various physical situations. Corresponding to each such mathematical boundary condition, a series of different finite-difference boundary conditions are applied and tested, and the results are compared with each other and with the exact solution. A similar study, applied to steady flow of a supersonic gas in two-dimensions, was recently made by Abbett [14]. Since one-dimensional unsteady gas flow and two-dimensional steady supersonic flow are similar phenomena (i.e., both represented by hyperbolic differential equations), we expect our conclusions to be compatible. They are indeed. Reference [14] contains many more subcases than in the present paper, but in our more simplified cases, they collapse to analogus cases treated here.

In Section 2, we describe the three different problems used to test various boundary conditions. The finite-difference scheme and various test boundary conditions are described in Section 3. In Section 4, we conclude by giving some theoretical analysis to explain the behavior of the various boundary conditions as evidenced in the computed results of the previous section.

In this paper, we confine our attention to one-dimensional problems only. The extension to unsteady flows in higher dimensions involve little conceptual change, but possibly give some different and unexpected results. This will be the subject of a later study.

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2. Test Problem for Gas Dynamics and Boundary Conditions

We shall use as a model the following class of problems: inviscid compressible gas initially at rest is placed in a tube with the following wall conditions: (A) Solid wall at left end, piston withdrawn at right end. (B) Solid wall at left end, constant pressure atmosphere at right end. (C) Piston at right end, no reflection at left end (i.e., a truncated infinite tube). In cases (A) and (C) the piston is drawn outward, and in case (B) the pressure of the atmosphere is lower than the pressure of the gas in the tube, so that in all cases, there are only expansion waves and no shocks. We do not wish to clutter the picture with additional difficulties of resolving shocks.

The differential equations governing the problem, as well as the initial and boundary conditions for the three problems, are well known:

$$\begin{aligned} \rho_t + (\rho u)_x &= 0, \\ u_t + u u_x + p_x/\rho &= 0, \end{aligned} \tag{1}$$

where ρ is the density, u the velocity, and p the pressure which equals $C\rho^\gamma$, γ being the ratio of the specific heats and C a constant depending on initial data. The speed of sound a is connected to the density by the well known relation $a^2 = \gamma p/\rho = \gamma C\rho^{\gamma-1}$. The assumption of constant entropy is a consequence of the absence of shocks. The boundary conditions are shown in Fig. 1.

As is well known, two pieces of data are given at $t = 0$, while only one piece is given on the boundaries (u or ρ or combination). The other variable, which is not prescribed on the boundary, comes out of the solution of the differential equation problem. If the difference scheme uses, for example, centered x-differences, then this additional variable is also needed at the boundary, and we may have to overspecify, or extrapolate, or reflect. This is the central question we want to investigate. Whatever we do naturally must first of all be stable, and additionally must be accurate.

We transform the problem into Lagrange coordinates, so that the domain of interest becomes a rectangular strip. In so doing, we avoid yet another separate question at the boundary: how to deal with interpolating when grid points do not coincide with the boundary curve. This problem requires some consideration of its own, but should not interfere with our consideration of overspecification in this paper.

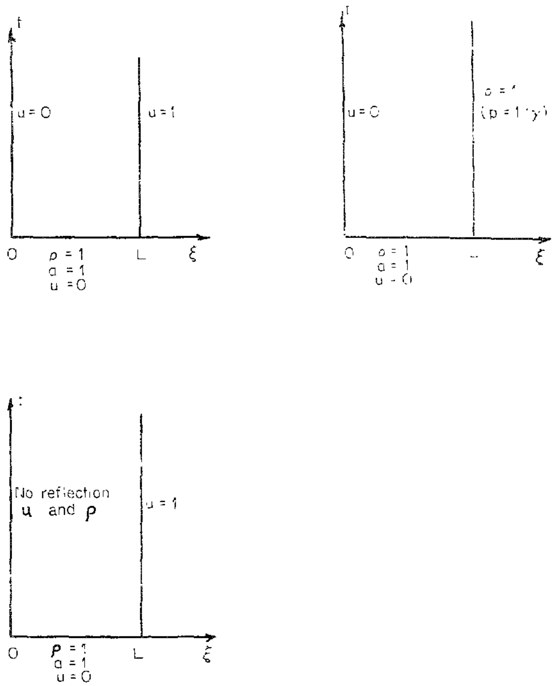

FIG. 1. Boundary conditions for problems A. (wall–piston); B. (wall–atmosphere); and C (nonreflecting end–piston).

In Lagrangian coordinates, the equations and boundary conditions become

$$\begin{aligned} V_t - u_\xi &= 0, \\ u_t + p_\xi &= 0, \end{aligned} \tag{2}$$

where $\xi = \int_0^\infty \rho(x')\,dx'$, $V = \rho^{-1}$. The boundary conditions are given in Fig. 1.

The characteristics of (2) are $d\xi/dt = \pm a\rho$. The Riemann invariants, which are constant along the characteristics, are the same as in Eulerian coordinates, being

$$R_\pm = u \pm 2a/(\gamma - 1), \text{ constant along } d\xi/dt = \pm a\rho, \text{ respectively.}$$

In addition to the simplicity of the domain shape, the differential equations (2) also become simpler than the corresponding equations (1) in that the convective terms have disappeared. Our conclusions and results obtained for Lagrangian coordinates obviously also apply for Eulerian coordinates, but the convective term may add some complexities that should be considered with care.

3. Finite Difference Scheme and Test Boundary Conditions

The basic finite difference scheme used in the interior of the domain in all tests is the two-step Lax–Wendroff scheme [4]. Rewriting (2) as

$$\mathbf{F}_t + \mathbf{G}_\xi = 0, \tag{3}$$

where $\mathbf{F}$ is the column vector (ρ^{-1}, u), and $\mathbf{G}$ the column vector $(-u, p)$, the scheme is just

$$\begin{aligned} \frac{\mathbf{F}_{j+1/2}^{n+1/2} - (1/2)(\mathbf{F}_{j+1}^n + \mathbf{F}_j^{\,n})}{\Delta t/2} + \frac{G_{j+1}^n - G_j^{\,n}}{\Delta\xi} &= 0, \\ \frac{\mathbf{F}_j^{n+1} - \mathbf{F}_j^{\,n}}{\Delta t} + \frac{\mathbf{G}_{j+1/2}^{n+1/2} - \mathbf{G}_{j-1/2}^{n+1/2}}{\Delta\xi} &= 0, \end{aligned} \tag{4}$$

i.e., the first half step is a Lax–Friedrichs dissipative scheme, and the second half-step is leap-frog scheme. Here, as is customary, $t = n\Delta t$, $\xi = j\Delta\xi$, $\mathbf{F}_j^{\,n} = \mathbf{F}(j\Delta\xi, n\Delta t)$, etc., $n = 0, 1, 2, \ldots j = 0, 1, 2, \ldots$.

For constant coefficients, this scheme is identical to the more familiar form

$$\frac{\mathbf{F}_j^{n+1} - \mathbf{F}_j^{\,n}}{\Delta t} + \frac{\mathbf{G}_{j+1}^n - \mathbf{G}_{j-1}^n}{2\Delta\xi} - \frac{\Delta t}{2}\,\frac{\mathbf{G}_{j+1}^n + \mathbf{G}_{j-1}^n - 2\mathbf{G}_j^{\,n}}{(\Delta\xi)^2} = 0. \tag{5}$$

The reason for selecting the two-step Lax–Wendroff scheme for all the tests is that (1) it is second order accurate, and relatively low in dissipation; (2) it is single-leveled and easy to apply; and (3) it is widely used by fluid dynamicists and hence would be desirable to understand more fully.

The boundary conditions to be tested here will be given in Table I. The description is made for a solid wall at $\xi = 0$, where $u = 0$ is prescribed and ρ is treated by the various schemes. Analogous prescriptions at the piston, and at a constant pressure end (problem B) where ρ is given and u is treated by the various schemes, are obvious, and need not be detailed here.

We comment on these boundary conditions. Condition (**1**) was first proposed by Parter [15], in one of the earliest mathematical papers to deal with the question of overspecification at a boundary, in which he studied the Lax–Wendroff and Lax–Friedrichs schemes for the model equation $u_t + u_x = 0$. He concluded that if the overposed boundary value is uniformly bounded, the method would be stable and the solution will converge to the correct solution, except for a thin boundary layer at the boundary. However, for systems of equations, this boundary layer will propagate along the backward characteristics everywhere and destroy the accuracy of the solution [6]. This indeed occurs in all our calculations.

TABLE I

Boundary Conditions

(1) Overspecification $\rho_0 = \text{constant}$.

(2) First-order extrapolation $\rho_0 = \rho_1$.

(3) Second-order extrapolation $\rho_0 = 2\rho_1 - \rho_2$.

(4) Local characteristic

$$R_-(t + \Delta t, 0) = R_-(t, \alpha\Delta\xi) = (1 - \alpha)R_-(t, 0) + \alpha R_-(t, \Delta\xi)$$

$$\alpha = a\rho(t, \alpha\Delta\xi) \cdot \Delta t/\Delta\xi.$$

(5) One-sided difference, first order space and time

$$\frac{V_0^{n+1} - V_0^{n}}{\Delta t} - \frac{u_1^{n} - u_0^{n}}{\Delta\xi} = 0.$$

(6) One-sided difference, second order space

$$\frac{V_0^{n+1} - V_0^{n}}{\Delta t} - 2\frac{u_1^{n} - u_0^{n}}{\Delta\xi} + \frac{u_2^{n} - u_0^{n}}{2\Delta\xi} = 0.$$

(7) Box scheme

$$\frac{V_0^{n+1} - V_0^{n}}{\Delta t} + \frac{V_1^{n+1} - V_1^{n}}{\Delta t} - \frac{u_1^{n+1} - u_0^{n+1}}{\Delta\xi} - \frac{u_1^{n} - u_0^{n}}{\Delta\xi} = 0.$$

Condition (2) is standard extrapolation, and is very much similar to the more common reflection (in which an addition row of points is added beyond the boundary, denoted by say $(\ )_{-1}$, and ρ_{-1} is set equal to ρ_1). It is equivalent to setting $\partial\rho/\partial x = 0$ at the boundary. Condition (3) is higher order extrapolation, and ρ_0 is obtained by a straight-line extrapolation from ρ_2 and ρ_1. Condition (4) is integration along the characteristic at the boundary. In this sample problem, because of the existence of the Riemann invariants, this procedure is very simple; in general, some algebric manipulations are required, but unlike the regular method of characteristics, these manipulations only occur at the boundary.

Conditions (5), (6) and (7) are all one-sided difference equations for the unspecified quantity, in this case ρ or V. Condition (5) is first order accurate in space and time, (6) is first order accurate in time and second-order accurate in space, (7) is second-order accurate in both space and time. Condition (7) is also similar to the box scheme used for the neutron transport equation.

One would have expected (2) to be rather poor, (3) to be better, (4) and (5) to be rather good, and (6) and (7) to be even better. Rather surprisingly, the calculated results as given in the next section show that this is not the case in general. All these schemes are stable when used in conjunction with the Lax–Wendroff scheme. When Eqs. (2) are first cast into diagonal (or characteristic) form, then Gustafsson *et al.* [6] have proved the stability for schemes (2), (3), (5) and (7).

For problem B of the constant pressure atmosphere, we prescribe p and thus ρ at the end $\xi = L$, and apply these various boundary treatments to u.

For problem C of the nonreflecting end, we apply (2)–(7) for both ρ and u. In this case, the fact that we have a simple wave and thus straight characteristics at the nonreflecting boundary is used when we apply scheme (4).

4. Results

The three test problems A, B and C are run under these seven different boundary conditions. The parameters chosen are as follows.

Initial density, $\rho = 1$.

Initial velocity, $u = 0$.

Initial sound speed, $a = 1$.

Piston speed (A and C), $U = 1$.

Atmospheric pressure, (B), $p = 1/1.4$.

Adiabatic exponent, $\gamma = 1.4$.

$\Delta t = 0.5$, $\Delta x = 1$ for regular calculations.

$\Delta t = 0.25$, $\Delta x = 0.5$ for finer calculations.

Tube length $L = 10$.

Figures 2 and 3 show the velocity distribution at two different instants of time for problem A (piston–wall); only the portion near the piston is shown, since the end near the wall is rather uneventful and all schemes give the same results. The solid line is the exact solution. Figure 4 and 5 show the velocity distribution at the same two instants of time for problem B (atmosphere–wall).

We can conclude quite clearly from those results that: (1) the higher order schemes, i.e., (3), (6) and (7), all have large oscillations, and are rather disappointing; (2) the characteristic method (4) is the best overall; (3) the first-order one-sided derivative (5) is usable, though not as accurate as (4); (4) simple extrapolation (2) is amazingly good; this may be fortuitous, since the exact solution does indeed give a vanishing derivative on ρ or on u in these special cases. Condition (1) is indeed not even convergent, though stable as expected, so the results will not be shown.

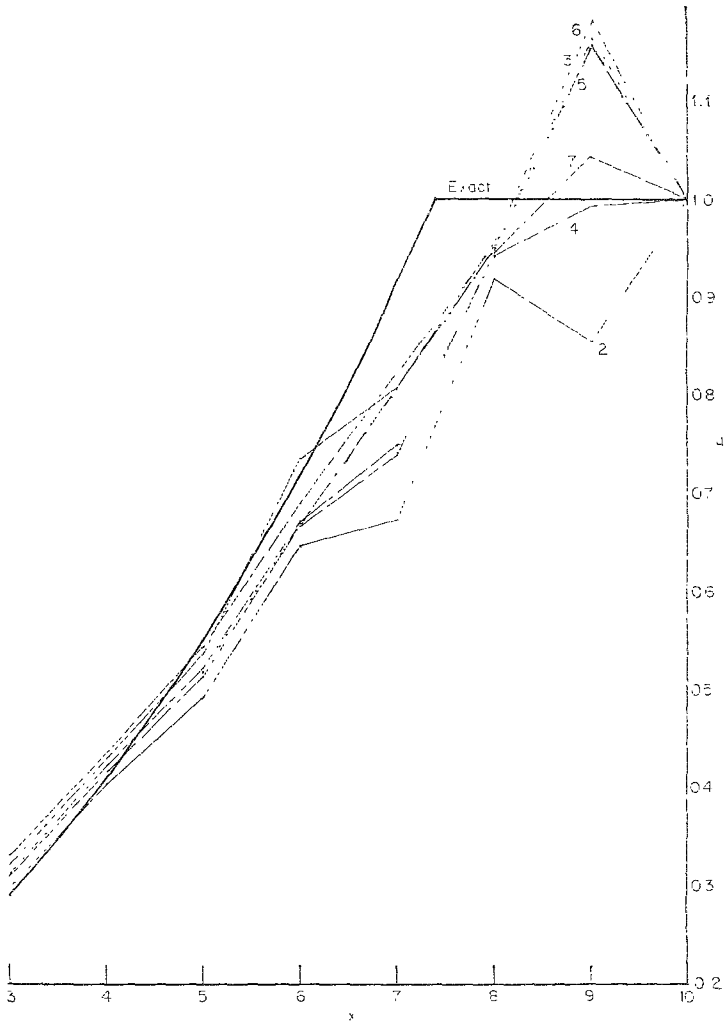

FIG. 2. Velocity near the piston, at $t = 10$. (Solid line represents the exact solution, numbers 2–7 correspond to different boundary conditions in the Table.)

These facts are seen even better in Figs. 6 and 7. Figure 6 gives the velocity at the point next to the piston in problem A plotted as a function of time, and Figure 7 gives the velocity at the open end in problem B plotted as a function of time. The oscillations of the higher order schemes (3), (6), and (7) are very apparent. The characteristic scheme (4) is still seen to be the best, while simple extrapolation (2) is much more sluggish than all the other schemes, suggesting a high degree of dissipation at the boundary.

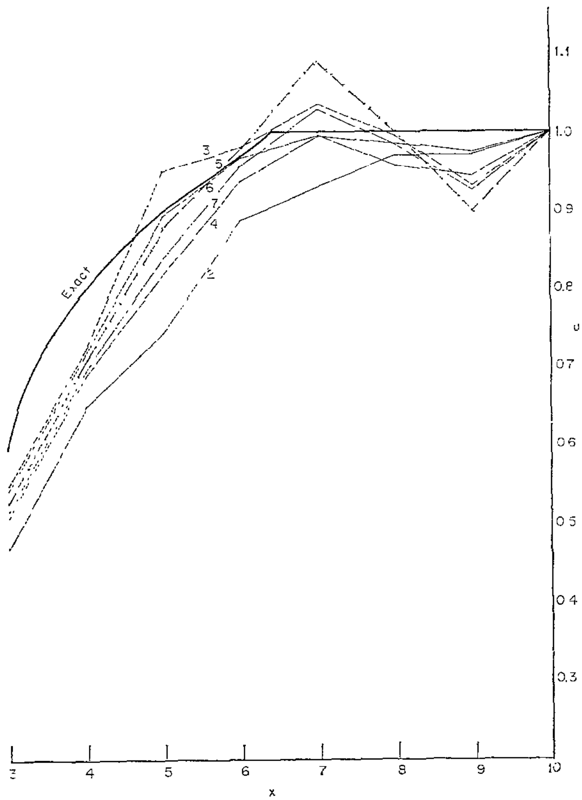

FIG. 3. Velocity near the piston at $t = 25$ (Problem A).

Similar conclusions can be drawn from problem C, the nonreflecting end. Figure 8 shows the velocity and density at the nonreflecting end plotted as a function of time. We again can conclude the following.

1. The characteristic method (4) is the best.

2. Pure extrapolation (2) is still surprisingly good. This is all the more unexpected since in this problem, the exact solution does not give zero ρ or u derivatives at this end, although they are indeed not large.

3. The schemes (3) and (5), i.e., linear extrapolation and first-order one-sided derivative, are both usable schemes, though not as good as the two schemes above.

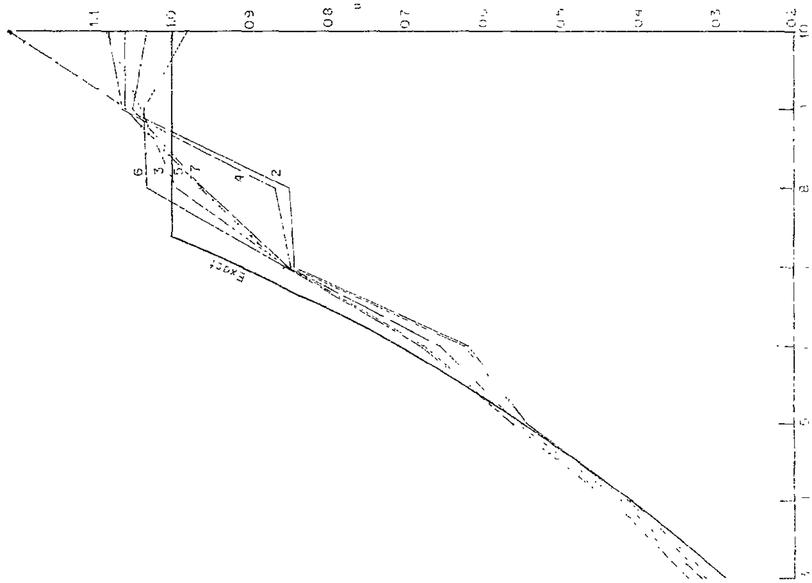

FIG. 4. Velocity near the open atmosphere at $t = 10$ (Problem B).

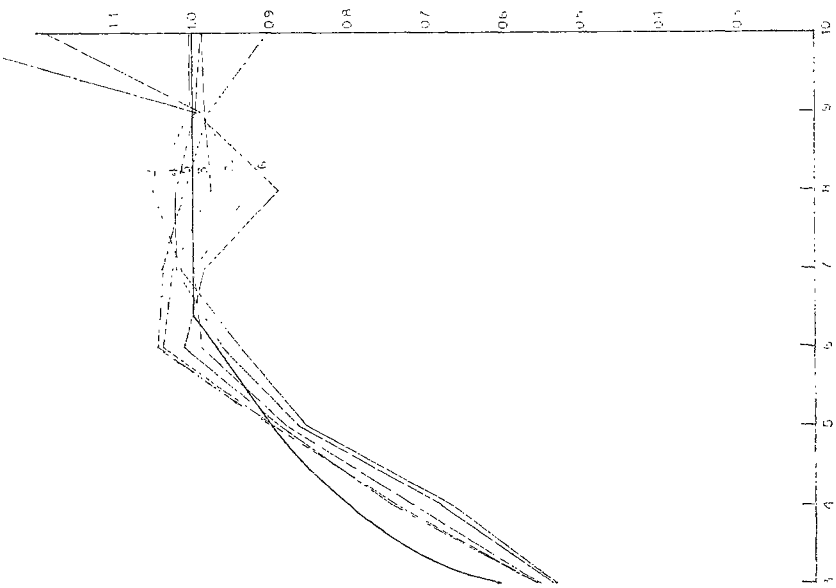

FIG. 5 Velocity near the open atmosphere at $t = 25$ (Problem B).

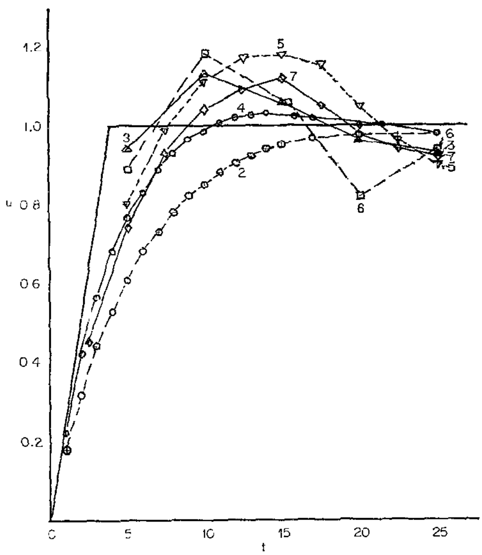

FIG. 6. Velocity at one grid point from piston as a function of time, Problem A.

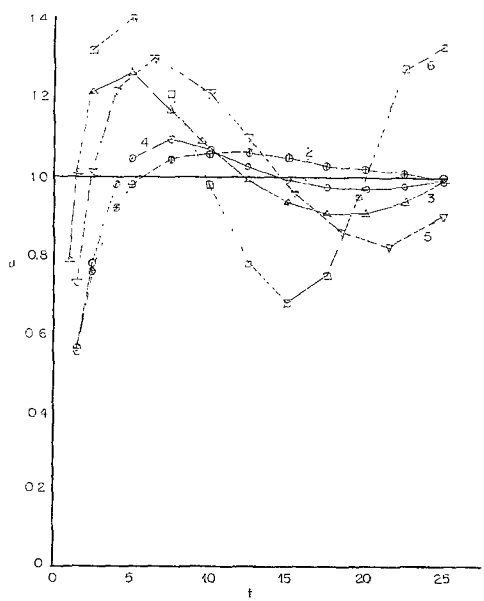

FIG. 7. Velocity at open end as a function of time, Problem B.

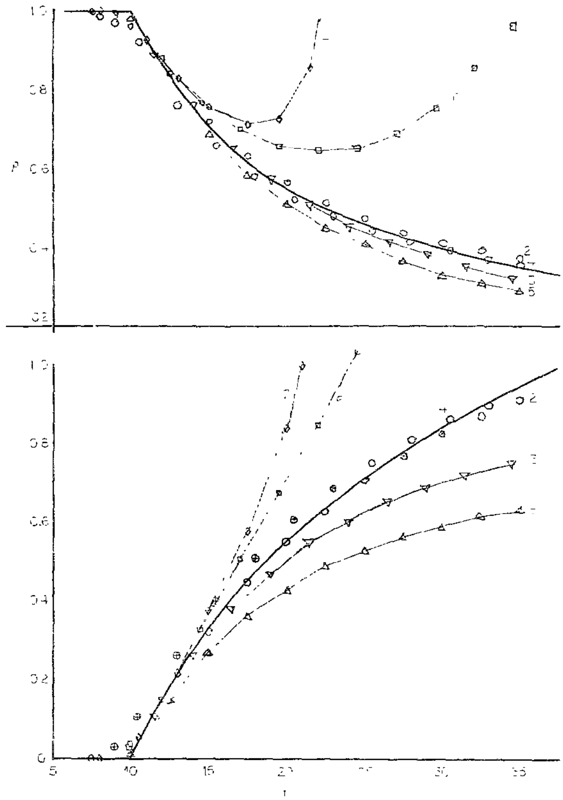

FIG. 8. Density (upper figure) and velocity (lower figure) at the nonreflecting end as functions of time, Problem C.

4. For the higher-order schemes (6) and (7), a completely unexpected phenomenon occurs. Both the density and the velocity increase without bound. It is tempting to classify this behavior as a numerical instability, but it is not a usual instability. In a numerical instability, the solution becomes unbounded at a fixed t as we refine Δt. In our case, fixing t and refining Δt increases the accuracy and retards the blowing up of the solution. The solution blows up only as t increases. It is a typical exponential growth caused by the accumulation of errors from multiple boundary reflections (i.e., between $\xi = 0$ and $\xi = L$). Gustafsson *et al.* [6] have discussed this type of behavior.

It may be questioned why we had not compared our extrapolation (2) with the more popular reflection procedure, already alluded to earlier. In fact, we had done the calculations for the reflection case, but the results cannot be considered conclusive. This is due to the fact that our difference scheme (the Lax–Wendroff scheme) requires three points at the old time level, hence when a row of points are introduced beyond the boundary, extrapolation must be carried out not only for the unspecified variable (say ρ at the piston), but also for the specified variable (u at the piston) to the added row. The latter is not a unique process, and thus may cloud the issue. If we reflect the density and straight-line extrapolate the velocity u (naturally through the given boundary value), then the reflection scheme gives results similar to (5).

It has also been suggested that we compare our results with the staggered leap-frog scheme, which indeed avoids the boundary condition over-specification problem. Such a comparison, however, would not be fair. First of all, the finite-difference schemes are already different, and it is difficult, if at all possible, to attribute whatever differences in the results to either the finite-difference scheme or to the boundary condition. Second, the leap-frog scheme requires some manipulation to generate another row of initial data, so that the problems we discuss for the boundary conditions are encountered in the initial conditions. While the latter are indeed better known, we nevertheless feel a fair comparison cannot be made.

5. Theoretical Analysis of Some Boundary Conditions

We make some theoretical explanation of the performance characteristics of some of the boundary conditions. As it stands, this analysis is still relatively rudimentary, but it does give us some insight into the nature of these various boundary conditions. Our analysis is in spirit akin to an investigation of the dissipation and dispersion properties of a finite difference scheme for a pure initial value problem.

To be definite, we consider an ordinary one-dimensional wave equation with wave speed 1 (instead of, say, linearizing the Eqs. (2)), rewritten as a first order system:

$$\begin{pmatrix} u \\ v \end{pmatrix}_t + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}_x = 0.$$

The characteristics are $x - t = \text{const}$, and $x + t = \text{const}$, with the corresponding Riemann invariants $r = u + v$ and $s = u - v$. Let a wave be incident on a solid wall (which is the only case we shall consider) from the right, and let the wall be at $x = 0$:

$$s = -Ae^{i[k(x+t)+\varphi]},$$

where k is the frequency or wave number (here equal since $c = 1$) and φ is the phase of the incident wave. Assume that up till $t = 0$, a correctly reflected wave has been emitting from the wall toward the right:

$$r = Ae^{i[k(x-t)+\varphi]}.$$

These two waves give the standard standing wave pattern satisfying $v = 0$ at the boundary:

$$u = A \sin (kt + \varphi) \sin kx,$$

$$v = A \cos (kt + \varphi) \cos kx.$$

Obviously, we could equally well treat other boundary conditions and less special initial conditions, but this problem as specified is easier than most to handle.

We then ask: What is the strength of the reflected wave $r(0, \Delta t) = r_0^1$ at the wall at time Δt, as given by the various schemes in Table I before, for various values of k and φ? Again for simplicity, we consider only schemes (4), (5), and (6), i.e., characteristic scheme, first-order and second-order one sided derivatives. We find the following expressions, when the schemes are applied to v ($u = 0$ always):

Exact solution:

$$r_0^1 = A (\cos \varphi \cos k\Delta t - \sin \varphi \sin k\Delta t).$$

Characteristic method (4):

$$r_0^1 = A[(1 - \lambda) \cos \varphi + \lambda \cos (k\Delta x + \varphi)], \ \lambda = \Delta t/\Delta x.$$

First-order one-sided (5):

$$r_0^1 = A (\cos \varphi - \lambda \sin \varphi \sin k\Delta x).$$

Second order one-sided (6):

$$r_0^1 = A [\cos \varphi - \lambda \sin \varphi \sin k\Delta x (2 - \cos k\Delta x)].$$

We plot these quantities r_0^1 versus $k\Delta x$ for various values of φ in Figs. 9a and 9b. Four values of φ are represented 0°, 45°, 90°, 135°. (180°, 225°, etc. behave symmetrically). Figure 9b corresponds to $\lambda = 1/2$, and Fig. 9a to $\lambda = 1/4$.

In all these cases, it is quite evident that the reflected wave in the characteristic scheme (4) is generally weaker than that in the exact solution, that in the first-order one-sided scheme (5) is somewhat stronger than the exact solution, and that in the second-order scheme (6) is much stronger. This explains to a large extent the oscillatory versus damped behavior of the solutions obtained by the use of the various boundary conditions.

It would be desirable to further extend and develop this type of analysis to more general boundary schemes.

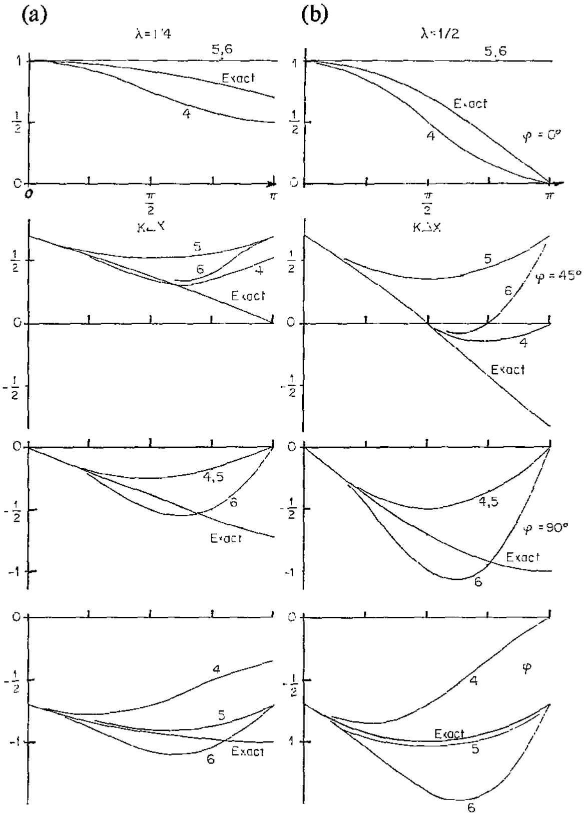

FIG. 9. Amplitudes of reflected waves: r_0^1 vs $k\Delta x$ for different φ.

6. CONCLUSIONS

It would have been desirable at the end of such a study to conclude which of the boundary conditions is optimal for practical use. This is unfortunately virtually impossible to do, any more than it is to conclude which is the optimal difference scheme to use for a given differential equation; the particular application determines the choice of the boundary condition, as does the difference scheme. It would also have been desirable to conclude which type of boundary conditions lead to failure of the numerical solution. This can largely be answered by investigating the stability of the boundary condition with the difference scheme (see, e.g., [6]), and it is quite an involved process. All the schemes we considered in this study are stable and do not result in failure of the numerical solution, but their accuracy can still differ by a large amount.

What we can conclude is that boundaries reflect the solutions with amplification or with damping. The latter kind gives in general better solutions in that they are less oscillatory, and that they do not blow up in problems such as Problem C, but they are invariably more sluggish in response. The situation is again analogous to dissipation in finite-difference schemes, where as here the precise application determines the choice of the scheme.

Moreover, this study has suggested a procedure to predetermine this amplification or damping in a given boundary scheme. As expected, the procedure is quite a bit clumsier than just looking at dissipation or dispersion in a pure initial-value scheme. This is to be expected, as all treatment of mixed initial-boundary questions tend to be much more complicated than treatment of corresponding purely initial value questions.

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