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PSEUDO-CHARACTERISTIC METHOD OF LINES SOLUTION OF FIRST-ORDER HYPERBOLIC EQUATION SYSTEMS *

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SUMMARY

First-order hyperbolic partial differential equations are difficult to solve numerically because of their ability to transmit steep waves. It is well known that the method of characteristics is the natural method for such equations, as it precisely follows wave interactions. However, a characteristic solution is expensive, as it requires repeated solution of non-linear algebraic equations. This gives considerable motivation to the development of fixed grid numerical schemes.

Unfortunately any attempt to use a finite fixed grid generates spurious numerical oscillation and dispersion, which must be minimized by artificial damping or directional differentiation. For sets of hyperbolic equations, the appropriate assignment of damping or direction is difficult to determine, as variables are coupled in non-linear form. However, a clear definition of directionality is given in the characteristic form of the equations, and may be used to develop a pseudo characteristic fixed grid statement of the equations, which is readily solved by the method of lines, is simple to implement, and produces stable accurate solutions.

Applications are illustrated for the solution of equations describing shallow water flow, and compressible gaseous flow.

INTRODUCTION

First-order hyperbolic partial differential equations (PDEs) are an extremely important class, as they arise inevitably in the modelling of any transient flow situation, and are deceptively difficult to solve numerically. This difficulty is principally due to their inherent ability to transmit spatial discontinuities without dissipation. The method of characteristics is recognized as the natural procedure for solving such equations as it is formulated to precisely follow wave interactions[6]. This requires repeated expensive nonlinear algebraic equation solutions or iterations, but does permit the propagation of steep fronted waves.

In contrast, fixed grid schemes are inexpensive and simple to implement. However, symmetric fixed grid finite difference and finite element schemes develop spurious numerical oscillations in the neighbourhood of steep fronted waves[12], and may be used successfully only for systems in which response is slow and spatial gradients are not severe[6]. Numerical oscillation may be reduced either by using directional differentiation, or adding artificial damping terms to the equations, in fact these alternatives are equivalent, as directional differentiation is dissipative. A multitude of such schemes have been proposed, and the more popular are summarized in references 3 and 11.

A single first order hyperbolic equation, such as the advective equation discussed in reference 3, or loosely coupled equation sets such as those describing flow in linear heat exchangers[8], may be solved efficiently by directionally weighted methods. In fact the correct, or upwind direction is dictated by the method of characteristics[7], but is normally obvious from the physical situation.

However, in conservation equations, variables are usually coupled in a nonlinear fashion, and waves may propagate in both directions, thus directional strategy is not made obvious by physics, or by the appearance of the equations in conservation law form. Furthermore, non-rigourous application of upwind techniques is known to give poor results[11]. In contrast, the characteristic form of stating the same equations explicitly defines the governing directions, and it has only recently been pointed out that these may be utilized to guide the rational formulation of a directional finite difference scheme[4,8]. Such a characteristic finite difference scheme has been successfully incorporated in a production code for transient two-phase flow simulation[1].

On further investigation it becomes apparent that the characteristic form may be used in a similar manner to formulate a characteristic method of lines scheme which eliminates the necessity of the matrix inversion required by the characteristic finite difference scheme, and also introduces the possibility of using higher-order methods in time and space[2].

The method of lines is used collectively to refer to a class of methods in which piecewise approximation functions are used to represent spatial variation and to transform partial differential equations, PDEs into coupled sets of ordinary differential equations, ODEs.

A general one-dimensional PDE set may be written

$$\phi_i(x,t,u,u_t,u_x,u_{tt},u_{xx},u_{xt},\ldots,v,v_t,\ldots) = 0 \qquad (1)$$

$i=1,NPDE$

Conversion to ODE form is accomplished by representing the spatial variation of u, v, etc., in terms of spatial basis functions B(x) and discrete values of u_i at nx points:

$$u_a(x,t) = \sum_{i=m}^{n} B_i(x)u_i(t) \qquad (2)$$

where $1 \leq m \leq n \leq nx$ and (n-m) is the order of coupling in space. The approximation (2) is substituted in (1), and algebraic manipulation produces a set of k=nx*NPDE coupled ODEs.

$$[A][U_t] = [B][U] + [C] \qquad (3)$$

where A, B and C are k square matrices and u, u_t and k column vectors containing the values of the spatial variable and its time derivative at each point.

The choice of the spatial approximation polynomial B and its subsequent handling defines the particular method. If (2) is applied in an explicit sense a

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finite difference method of lines evolves with [A]=[I], otherwise, if (2) is applied in an implicit weighted residual sense, a finite element method of lines evolves, and [A] is banded and symmetric except for the particular case of upwind weighting[3].

In either case, the resulting ODEs may be integrated by an efficient digital algorithm which will normally vary the time step as integration progresses to obtain optimal compliance with an imposed tolerable error limit.

The method of lines is extremely flexible as it comprises an infinite number of combinations of spatial approximation functions and integrators, any of which may be applied to the same equation system. The equations are programmed in general form, and the appropriate combinations are selected to operate on the equations to produce the solution.

In particular, for hyperbolic equations, a number of directionally weighted schemes may be developed. Several of these, including upwind Lagrangian, Hermite, spline, and weighted residual are reviewed for use with the advective equation in reference 3.

This paper extends the same approach to coupled PDE systems by identifying the characteristic directions and transforming the resulting matrix equations into an explicit form.

THE PSEUDO-CHARACTERISTIC METHOD OF LINES

(a) Incompressible Fluid Flow

For simplicity, the method is first illustrated for two equations describing the flow of fluid over an isolated ridge[10]. If m is the mass flux, h, the depth, and y_x is the local slope of the ridge, these equations may be written in conservation law form as

$$\frac{\partial}{\partial t}[\phi] + \frac{\partial}{\partial x}[F(\phi)] = D(\phi) \tag{4}$$

where

$$\phi = \begin{bmatrix} m \\ h \end{bmatrix}, \quad F = \begin{bmatrix} \frac{m^2}{h} + \frac{gh^2}{2} \\ m \end{bmatrix}, \quad D = \begin{bmatrix} -ghy_x \\ 0 \end{bmatrix}$$

the primitive form follows directly,

$$\begin{aligned} &\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + g\frac{\partial h}{\partial y} = -g\frac{\partial y}{\partial x} \\ &\frac{\partial h}{\partial t} + h\frac{\partial u}{\partial x} + u\frac{\partial h}{\partial x} = 0 \end{aligned} \tag{5}$$

Using both symmetric and assymmetric differentiation formulae, Heydweiler and Sincovec[9] were unable to obtain stable solutions to equations (5) until they added an arbitrarily large second derivative artificial dissipation term to each of the equations (5). Principally this is because it is impossible to develop a rationale for assigning a directional bias to any spatial derivative term in the primitive form of equation (5). In fact, waves propagate in both directions and the obvious upwind difference scheme used for single equations, the simplest form of which expresses terms such as

$$u\frac{\partial \rho}{\partial x} \text{ as } u_i(\rho_i - \rho_{i-si})/\Delta x \tag{6}$$

where s_i is the sign of u_i, also gives unstable results[11].

However, by transformation, equations (5) may be written in a form to which the application of (6) gives entirely stable results.

It is convenient to change variables to s = gh and $c = \sqrt{s}$ such that the matrices now become

$$\phi = \begin{bmatrix} u \\ s \end{bmatrix}, \quad A_1 = \begin{bmatrix} u & 1 \\ s & u \end{bmatrix}, \quad G_1 = \begin{bmatrix} -gy_x \\ 0 \end{bmatrix} \tag{7}$$

Performing a similarity transform $BA^{-1}B$ to extract the diagonal eigenvectors gives:

$$\begin{aligned} &B\frac{\partial}{\partial t}\phi_1 + \Lambda B\frac{\partial}{\partial x}\phi_1 = G_2 \\ &B = \begin{bmatrix} c & 1 \\ c & -1 \end{bmatrix}, \quad \Lambda = \begin{bmatrix} u+c & 0 \\ 0 & u-c \end{bmatrix}, \quad G_2 = \begin{bmatrix} -gcy_x \\ -gcy_x \end{bmatrix} \end{aligned} \tag{8}$$

Expanding (8) gives the characteristic form

$$c\frac{\partial u}{\partial t} + \frac{\partial s}{\partial t} + (u+c)\left(c\frac{\partial u}{\partial x} + \frac{\partial s}{\partial x}\right) + gcy_x = 0 \tag{9a}$$

$$c\frac{\partial u}{\partial t} - \frac{\partial s}{\partial t} + (u-c)\left(c\frac{\partial u}{\partial x} - \frac{\partial s}{\partial x}\right) + gcy_x = 0 \tag{9b}$$

The requisite directional weighting for equations (9a) and (9b) is now dictated by the sign of (u+c) and (u-c) respectively. Following Hancox et al[7] one can assign a directional difference scheme for the spatial derivatives of each equation, invert the B matrix and integrate the equations

$$\phi_t = -B^{-1}\{\Lambda B\phi_x - G\} \tag{10}$$

It is a simple matter, however, to obtain an explicit definition of ϕ_t which is fully equivalent to (10) by performing the matrix inversion analytically. When derivatives originating from (9a) and (9b) are designated + and -, to show differentiation will be in the direction dictated by the component along (u+c) or (u-c) respectively, this gives

$$\begin{aligned} &\frac{\partial u}{\partial t} + \frac{u}{2}\left(\frac{\partial u}{\partial x_+} + \frac{\partial u}{\partial x_-}\right) + \frac{1}{2}\left(\frac{\partial s}{\partial x_+} + \frac{\partial s}{\partial x_-}\right) + \\ &+ \frac{c}{2}\left(\frac{\partial u}{\partial x_-} - \frac{\partial u}{\partial x_-}\right) + \frac{u}{2c}\left(\frac{\partial s}{\partial x_+} - \frac{\partial s}{\partial x_-}\right) + ghy_x = 0 \\ &\frac{\partial s}{\partial t} + \frac{c^2}{2}\left(\frac{\partial u}{\partial x_+} + \frac{\partial u}{\partial x_-}\right) + \frac{u}{2}\left(\frac{\partial s}{\partial x_+} + \frac{\partial s}{\partial x_-}\right) \\ &+ \frac{uc}{2}\left(\frac{\partial u}{\partial x_+} - \frac{\partial u}{\partial x_-}\right) + \frac{c}{2}\left(\frac{\partial s}{\partial x_+} - \frac{\partial s}{\partial x_-}\right) = 0 \end{aligned} \tag{11}$$

Note that only terms involving (u+c) and (u-c) have been directionally differentiated, y_x is not a dependent variable.

One may now solve equations (11) directly by the method of lines, incorporating any suitable directional approximation to the derivatives, such as (6) or the higher order methods reviewed by Carver and Hinds[3].

It is instructive first to apply the simplest first-order formula (6) to equations (11). Thus if

$$\frac{\partial \omega}{\partial x_+} = \frac{(\omega_i - \omega_{i-1})}{\Delta x} \text{ and } \frac{\partial \omega}{\partial x_-} = \frac{(\omega_{i+1} - \omega_i)}{\Delta x} \tag{12}$$

$$\left(\frac{\partial\omega}{\partial x_+} + \frac{\partial\omega}{\partial x_-}\right) = \frac{\omega_{i+1}-\omega_{i-1}}{\Delta x} = 2\left(\frac{\partial\omega}{\partial x}\right)_c \tag{13}$$

$$\left(\frac{\partial\omega}{\partial x_+} - \frac{\partial\omega}{\partial x_-}\right) = -\frac{\omega_{i+1}-2\omega_i+\omega_{i-1}}{\Delta x} = -2\Delta x\left(\frac{\partial^2\omega}{\partial x^2}\right)_c$$

where $(\partial\omega/\partial x)_c$ and $(\partial^2\omega/\partial x^2)_c$ are three-point symmetric first and second derivative formulae.

Inserting these formulae into (11) gives:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{\partial s}{\partial x_c} + c\Delta x\frac{\partial^2 u}{\partial x_c^2} + \frac{u\Delta x}{c}\frac{\partial^2 s}{\partial x_c^2} = ghy_x$$

$$\frac{\partial s}{\partial t} + c^2\frac{\partial u}{\partial x_c} + u\frac{\partial s}{\partial x_c} + uc\Delta x\frac{\partial^2 u}{\partial x^2} + c\Delta x\frac{\partial^2 s}{\partial x_c^2} = 0 \tag{14}$$

Note that equations (14) are now the primitive form of the equations (5) plus explicitly defined dissipative terms, all expressed to second-order accuracy. Similar expressions may be derived starting with higher-order expressions in place of equations (13). In particular, the two most accurate explicit formulations reviewed in reference 3 may be used readily with equations (14). They are the four-point upwind Lagrange form

$$\frac{\partial}{\partial x}(U(I)) = S_I(U(I-2S_I) - 6U(I-S_I) + 3U(I) + 2U(I+S_I))/6\Delta x \tag{15}$$

and the three-point upwind Hermite expression

$$\frac{\partial}{\partial x}(U(I)) = S_I(U(I+S_I) + 4U(I) - 5U(I-S_I))/4\Delta x - \frac{1}{2}\frac{\partial}{\partial x}(U(I-S_I)) \tag{16}$$

The example used by Houghton and Kasahara, and Heydweiler and Sincovec will be used. This is equations (5) with

$y(x) = \max[0, 10-10(x/40)^2]$

$u(0,x) = 60,\ h(0,x) = 20-y(x),$

$u(t,-400) = u(t,+400) = 60,$

$h(t-400) = h(t,+400) = 20.$

The solution develops a major stationary shock downstream of the ridge, and smaller fronts move both upstream and downstream.

Figure 1 shows the solution at t=2, obtained using the formulae (12), (15) and (16) respectively in equations (14), and clearly illustrates the discontinuities developed. Figure 2 shows a typical unstable solution obtained by using symmetric differencing of the primitive equations and progressive stabilization by the addition of arbitrary dissipative terms.

(b) Equations of Compressible Flow

Following similar principles, the Eulerian equations governing one-dimensional compressible flow may be expressed in conservation law form similar to equation (4), where now

$$\phi = \begin{bmatrix}\rho\\ m\\ E\end{bmatrix},\quad F = u\phi + \begin{bmatrix}0\\ \rho\\ pu\end{bmatrix},\quad D = \begin{bmatrix}0\\ -\rho(f+gX_x)\\ \alpha Q\end{bmatrix} \tag{17}$$

and E is volumetric energy, ρ pressure and Q,f represent heat transfer and friction and X_x is the elevation gradient.

Introducing the speed of sound and the equation of state produces the primitive formulation:

$$\frac{\partial}{\partial t}\psi + A\frac{\partial}{\partial z}\psi = D$$

$$\psi = \begin{bmatrix}\rho\\ u\\ p\end{bmatrix},\quad A = \begin{bmatrix}u & \rho & 0\\ 0 & u & 1/\rho\\ 0 & c^2 & p\end{bmatrix},\quad D = 0 \tag{18}$$

The similarity transform again produces the characteristic form. D=0 is now used merely for brevity.

$$B\frac{\partial}{\partial t}\psi + \Lambda B\frac{\partial}{\partial x}\psi = BD$$

$$B = \begin{bmatrix}\rho c & 0 & 1\\ 0 & c^2 & -1\\ -\rho c & 0 & 1\end{bmatrix},\quad \Lambda = \begin{bmatrix}u+c & 0 & 0\\ 0 & u & 0\\ 0 & 0 & u-c\end{bmatrix} \tag{19}$$

or

$$\rho c\frac{\partial u}{\partial t} + \frac{\partial P}{\partial t} + (u+c)\left(\rho c\frac{\partial u}{\partial x} + \frac{\partial P}{\partial x}\right) = 0$$

$$c^2\frac{\partial\rho}{\partial t} - \frac{\partial P}{\partial t} + u\left(c^2\frac{\partial\rho}{\partial x} - \frac{\partial P}{\partial x}\right) = 0 \tag{20}$$

$$-\rho c\frac{\partial u}{\partial t} + \frac{\partial P}{\partial t} + (u-c)\left(-\rho c\frac{\partial u}{\partial x} + \frac{\partial P}{\partial x}\right) = 0$$

Explicit equations for $\partial u/\partial t$, etc. may now be obtained by inverting the B matrix and assigning the subscripts +, ., − to derivatives to be computed according to the directions dictated by the (u+c), u, (u−c) vectors respectively.

$$\frac{\partial P}{\partial t} + \frac{u}{2}\left(\frac{\partial P}{\partial x_+} + \frac{\partial P}{\partial x_-}\right) + \frac{\rho c^2}{2}\left(\frac{\partial u}{\partial x_+} + \frac{\partial u}{\partial x_-}\right) + \frac{c}{2}\left(\frac{\partial P}{\partial x_+} - \frac{\partial P}{\partial x_-}\right) + \frac{u\rho c}{2}\left(\frac{\partial u}{\partial x_+} - \frac{\partial u}{\partial x_-}\right) = 0$$

$$\frac{\partial u}{\partial t} + \frac{u}{2}\left(\frac{\partial u}{\partial x_+} + \frac{\partial u}{\partial x_-}\right) + \frac{1}{2\rho}\left(\frac{\partial P}{\partial x_+} + \frac{\partial P}{\partial x_-}\right) + \frac{c}{x}\left(\frac{\partial u}{\partial x_+} - \frac{\partial u}{\partial x_-}\right) + \frac{u}{2\rho c}\left(\frac{\partial P}{\partial x_+} - \frac{\partial P}{\partial x_-}\right) = 0 \tag{21}$$

$$\frac{\partial\rho}{\partial t} + u\frac{\partial\rho}{\partial x.} + \frac{\rho}{2}\left(\frac{\partial u}{\partial x_+} + \frac{\partial u}{\partial x_-}\right) = -\frac{u}{2c}\left(\frac{\partial u}{\partial x_+} - \frac{\partial u}{\partial x_-}\right) - \frac{1}{2c^2}\left[(u+c)\frac{\partial P}{\partial x_+} - 2u\frac{\partial P}{\partial x.} + (u-c)\frac{\partial P}{\partial x_-}\right]$$

Once again, having chosen any suitable formula to compute the directional derivatives, it may be shown that equations transform into a higher-order symmetric approximation to the primitive form (18) with specifically defined second derivative dissipative terms added. Reference 2 develops this, and shows tests illustrating that the pseudo characteristic formulation (21) caters for flow reversals and choking flow, as these automatically influence the difference scheme through the characteristic directions. Here we quote only one example, the standard shock tube problem discussed by Sod[11], who considers a tube of unit length with initial conditions:

$0 \le x < 0.5$: $p = \rho = 1.0,\ u = 0$
$0.5 < x \le 1.0$: $p = 0.1,\ \rho = 0.125,\ u = 0$

Fig. 1. HYDRAULIC JUMP PROBLEM
Pseudo Characteristic Methods

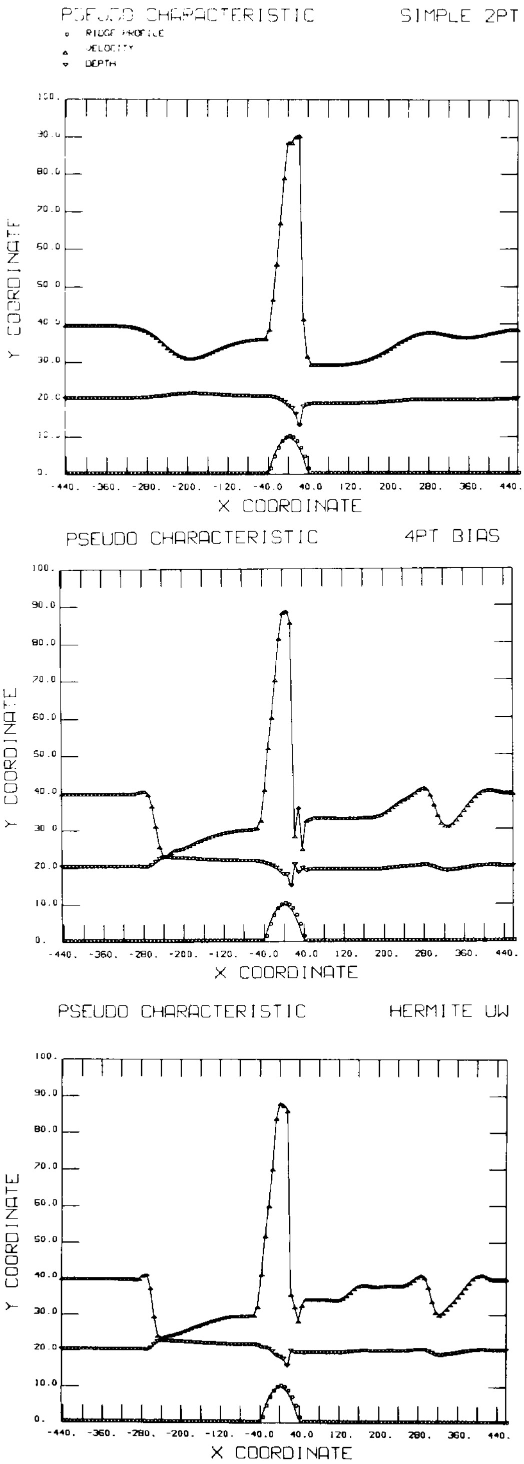


Fig. 2. HYDRAULIC JUMP PROBLEM
Central Difference Methods

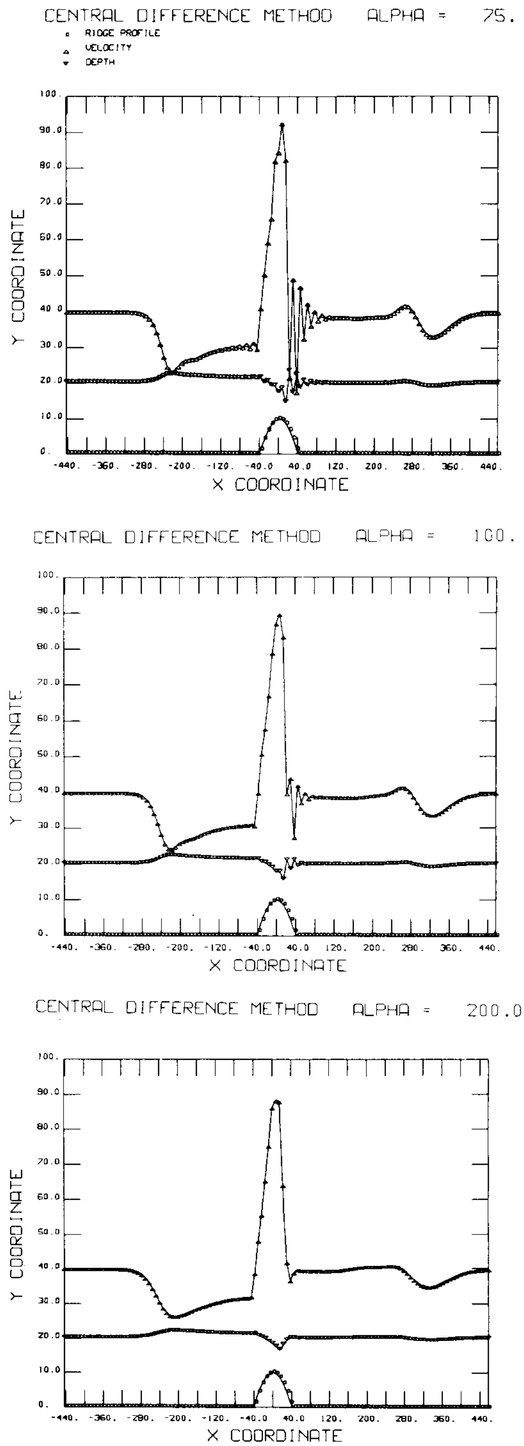


Fig. 3. SHOCK TUBE PROBLEM

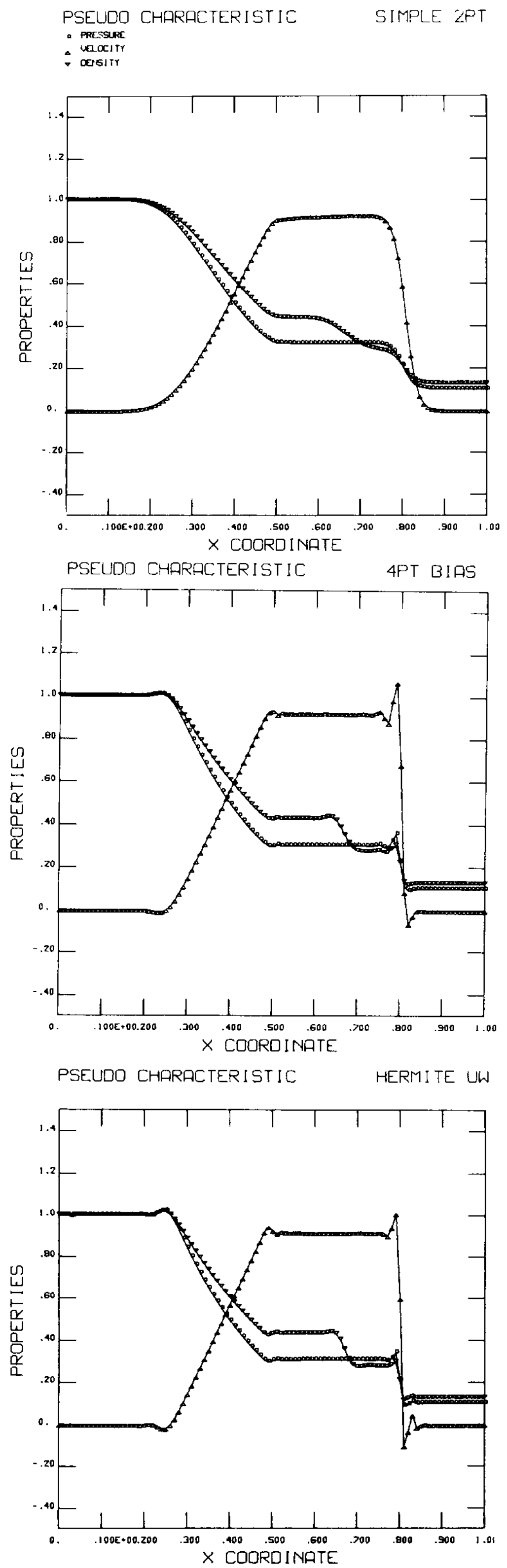
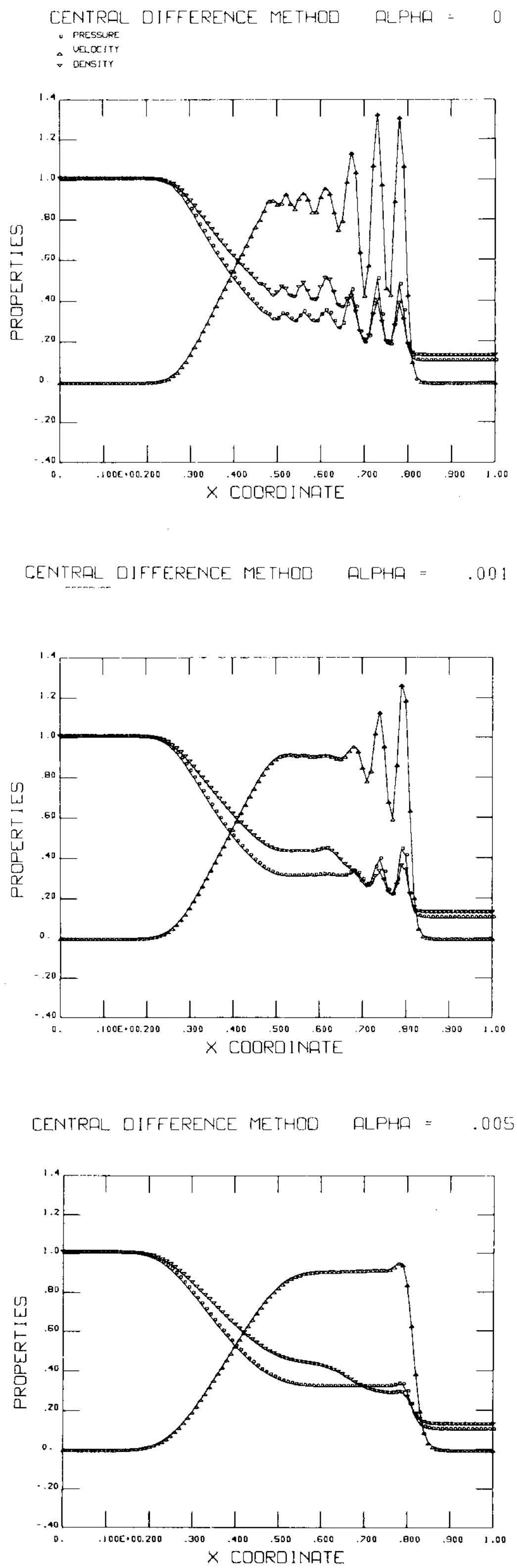


Fig. 4. SHOCK TUBE PROBLEM



This problem does not involve flow reversals or the associated change in boundary conditions, but the large pressure ratio generates shock and rarefaction waves resulting in four slope discontinuities in the pressure profile. Figure 3 shows the pressure profiles obtained from the three pseudo characteristic methods (12, 15, and 16) and results obtained by symmetric differentiation. These may be compared to a number of popular schemes for the conservation equations reviewed by Sod[11], and it will be noted that the simple PC method appears more accurate than the popular Lax-Wendroff, MacCormack and Rusanov methods, and that the higher-order PC methods compare very favourably to the more complicated methods reviewed. The PC method achieves comparable accuracy, is considerably easier to implement, even simpler to switch from one form to another, and has its foundation squarely in the physics, not relying on numerical stabilization artifacts.

Finally, it is of interest to review what happens to the example problem when symmetric differencing with arbitrary artificial dissipation terms are added. Figure 4 shows results obtained for the same problem from the conservation statement of the equations with an artificial dissipation term $\alpha(\partial^2/\partial x^2)\phi$ added. It becomes obvious that the dissipation required to stabilize causes excessive attenuation.

BOUNDARY CONDITIONS

The correct formulation of boundary conditions in systems of conservation equations causes considerable concern, as the number, location, and form of boundary restraint is not always apparent from the physics or the mathematics, and an incorrect formulation will obviously destroy the solution. One recourse is to avoid the problem altogether by banishing the boundaries to infinity, and while this has been done in references 9 and 11 for the two examples quoted here, such an approach is not helpful for applied problems.

Although the presence of three first-order equations in three variables suggests that three boundary restraints are required, in fact this is not so. The number and nature of the boundary conditions is dictated by the flow configuration at any given instant, or more particularly the number and direction of the characteristics at each boundary. Thus, a straight flow through situation in a pipe requires two boundary conditions at the inlet, and one at the outlet, a closed pipe with outflow requires one at each end, and a pipe experiencing inflow through both ends at any given instant requires four conditions, these numbers being the number of outward pointing characteristics at each boundary for each situation, or equally the number of simple directional difference analogs(12) which are not satisfied within the pipe. It is thus obvious that any scheme which is to cater for possible flow reversal must not only represent this adequately in the differencing scheme, but must also permit dynamic change in the number and type of boundary conditions. The pseudo characteristic method permits both these operations to be performed automatically.

CONCLUSION

The pseudo-characteristic method of lines is one of the few available methods which completely automates integration time step selection, spatial differentiation weighting and the handling of flow reversal and choking flow. It is easy to implement in a general fashion which permits selection between alternative approximation functions, and derives its stability directly from physical rather than numerical considerations.

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