# Pseudo Characteristic Method of Lines Solution of the Conservation Equations 

Michael B. Carver<br>Mathematics and Computation Branch, Chalk River Nuclear Laboratories, Atomic Energy of Canada Limited, Chalk River, Ontario K0J 1.J0, Canada

Received September 18, 1978; revised May 10, 1979


#### Abstract

A method which combines the natural directional properties of the method of characteristics with the computational efficiency of the method of lines is proposed for solving the conservation equations of compressible fluid flow. Although the equations are expressed initially in implicit characteristic form, neither iteration nor matrix inversion is required as the equations are transformed analytically to an equivalent set in which time derivatives are explicitly defined. Reduced to its simplest form, the method is shown to be equivalent to adding optimal dissipation to the primitive form of the conservation equations, but a more accurate implementation is recommended.


## Introduction

The method of characteristics has long been recognized as a natural procedure for solving the equations governing transient compressible flow, as it is formulated in a way which precisely follows wave interactions. Unfortunately the overhead required to perform a characteristics solution becomes prohibitively expensive to follow long term transients involving shock waves. There has, therefore, been considerable interest in developing finite difference methods designed to solve the problem more economically. Centered difference schemes generate spurious numerical oscillation in the neighbourhood of propagating waves, particularly shock waves. Such oscillation may be reduced either by using a dissipative difference scheme or by adding artificial dissipative terms to the equations. These alternatives may be shown to be equivalent. Some methods are reviewed in [1, 2].

For systems of implicitly coupled equations, however, it is difficult to determine a satisfactory rationale for assigning the form and magnitude of dissipative forms or assigning direction to the differentiation scheme, and inappropriate choices may degrade rather than improve the solution. A procedure first introduced by Courant, Isaacson and Rees [3] shows that this difficulty can be minimized by utilizing the method of cheracteristics to properly assign a directional differentiation scheme. This paper shows further, that although the resulting implicitly defined equations can be solved by standard finite difference methods, they can be transformed to an explicit statement which may be solved directly by the computationally efficient method of
lines. In the latter technique, the partial differential equations are converted, by means of piecewise functions approximating spatial variation, into coupled ordinary differential equations. These are then integrated by an efficient, variable order, error controlled optimal step size algorithm.

The method of lines solution is readily formulated to use, both in time and space, approximations of higher orders than are normally practical in finite difference solutions. The advantages of using higher order directional pseudo characteristic derivative formulae for numerically solving the advective equation have been discussed by Carver and Hinds [2]. These formulae have also been used successfully to solve the Burger's nonlinear equation shock problem, and the coupled linear equations describing counter current heat exchange, for which theoretical solutions are available. These comparisons are briefly summarized in the appendix, but the main object of this paper is to show that the higher order pseudo characteristic method of lines also yield accurate, stable and easily implemented solutions to nonlinear coupled systems such as the conservation equations.

## Formulation of the Equations

The Eulerian equations governing transient one-dimensional flow of a compressible fluid can be expressed in conservation law form as

$$
\begin{equation*}
\frac{\partial}{\partial t} \boldsymbol{\phi}+\frac{\partial}{\partial z} \mathbf{F}(\phi)=\mathbf{D}(\phi) \tag{1}
\end{equation*}
$$

where $\phi$ is a vector of dependent variables, $\mathbf{F}$ is a matrix nonlinear in $\phi$, and $\mathbf{D}$ is a vector accounting for irreversibility. In terms of the quantites to be conserved, mass density $\rho$, momentum $m$, and volumetric energy $E$, the vector components are

$$
\boldsymbol{\phi}=\left[\begin{array}{c}
\rho  \tag{2}\\
m \\
E
\end{array}\right], \quad \mathbf{F}=u \boldsymbol{\phi}+\left[\begin{array}{c}
0 \\
p \\
p u
\end{array}\right], \quad \mathbf{D}=\left[\begin{array}{c}
0 \\
-\rho\left(f+g \frac{d Z}{d z}\right) \\
\rho Q
\end{array}\right]
$$

where $u$ is velocity, $p$ is pressure and $Q$ and $f$ represent heat transfer and friction. The latter are normally computed by empirical relationships, and their omission from the subsequent discussion is merely for clarity and does not detract from the generality of the method proposed.

As (2) comprises three equations and four variables, a fourth relationship is required in the form of the equation of state. Using the internal energy per unit mass

$$
\begin{equation*}
e=\frac{1}{\rho}\left(E-\frac{1}{2} \rho u^{2}\right) \tag{3}
\end{equation*}
$$

the equation of state may be written

$$
\begin{equation*}
e=\psi(p, \rho) \tag{4}
\end{equation*}
$$

It is convenient to introduce the local speed of sound

$$
\begin{equation*}
c=(d p / d \rho)^{1 / 2} \tag{5}
\end{equation*}
$$

along an adiabat. For locally isentropic variations, we have

$$
\begin{equation*}
d e+p d\left(\frac{1}{\rho}\right)=0 \tag{6}
\end{equation*}
$$

so combining (3), (4), and (5) gives

$$
\begin{equation*}
c^{2}=\frac{p / \rho^{2}-\partial \psi / \partial \rho}{\partial \psi / \partial p} \tag{7}
\end{equation*}
$$

This may be used to arrive at the so-called primitive form of the Eulerian equations

$$
\begin{equation*}
\frac{\partial}{\partial t} \psi+A(\psi) \frac{\partial}{\partial z} \psi=0 \tag{8}
\end{equation*}
$$

where

$$
\psi=\left[\begin{array}{l}
u \\
\rho \\
p
\end{array}\right], \quad A=\left[\begin{array}{ccc}
u & 0 & 1 / \rho \\
\rho & u & 0 \\
\rho c^{2} & 0 & u
\end{array}\right]
$$

Finally, the matrix $A$ can be reduced to diagonal form $A$ by a similarity transform, where $\Lambda$ is the matrix of eigenvalues and the eigenvectors are columns of $B^{-1}$. Multiplying through by $B$ gives the equations in characteristic form:

$$
\begin{gather*}
\mathbf{B} \frac{\partial}{\partial t} \psi+\mathbf{B} \frac{\partial}{\partial z} \psi=0 \\
\psi=\left[\begin{array}{c}
u \\
\rho \\
p
\end{array}\right], \quad \boldsymbol{\Lambda}=\left[\begin{array}{ccc}
u+c & 0 & 0 \\
0 & u & 0 \\
0 & 0 & u-c
\end{array}\right], \quad \mathbf{B}=\left[\begin{array}{ccc}
\rho c & 0 & 1 \\
0 & c^{2} & -1 \\
-\rho c & 0 & 1
\end{array}\right] \tag{9}
\end{gather*}
$$

Solution Procedures
For the method of characteristics, the equalities to be maintained along each characteristic, follow directly from (9). They are

$$
\begin{align*}
\text { along } \frac{d z}{d t} & =u+c: & \rho c \frac{\partial u}{\partial t}+\frac{\partial P}{\partial t}+(u+c)\left(\rho c \frac{\partial u}{\partial z}+\frac{\partial P}{\partial z}\right) & =0  \tag{10a}\\
\text { along } \frac{d z}{d t} & =u: & c^{2} \frac{\partial \rho}{\partial t}-\frac{\partial P}{\partial t}+u\left(c^{2} \frac{\partial \rho}{\partial z}-\frac{\partial P}{\hat{c} z}\right) & =0 \\
\text { along } \frac{d z}{d t} & =u-c: & -\rho c \frac{\partial u}{\partial t}+\frac{\partial P}{\partial t}+(u-c)\left(-\rho c \frac{\partial u}{\partial z}+\frac{\partial P}{\partial z}\right) & =0 \tag{10c}
\end{align*}
$$

These are resolved into the associated compatibility relations, ordinary differential equations obtained, for example by writing (10a) as

$$
\text { along } \frac{d z}{d t}=u+a, \quad \frac{\partial P}{\partial t}+(u+a) \frac{\partial P}{\partial z}+\rho c\left(\frac{\partial u}{\partial t}+(u+a) \frac{c u}{\partial z}\right)=0
$$

i.e.,

$$
\begin{equation*}
\frac{d P}{d t}+\rho c \frac{d u}{d t}=0 \tag{11}
\end{equation*}
$$

The method of characteristics procedure computes values, from finite difference approximations to the three compatibility equations thus obtained. Unlike fixed grid methods, this allows discontinuities to propagate without diffusion and as the procedure traces the wave motion, the results are regarded as the most accurate readily attainable [4]. However, the solution involves linear interpolation and iterative solution of the resulting algebraic equations and is more time consuming than fixed grid methods [4]. Thus a fixed grid method which minimizes diffusion is sought.

Finite difference formulations are normally based on some form of Eq. (1) or Eq. (8). All such schemes tend to generate spurious numerical oscillation in the neighbourhood of propagating waves, unless this is damped by one of the equivalent techniques of building in some form of dissipative difference scheme or adding artificial viscosity terms. Reported examples of such schemes are legion; a recent paper by Sod [1] reviews many of them.

The use of the method of lines reduces the problem of developing a difference scheme, as progression in the time variable may be taken care of by a reliable highorder error controlled predictor-corrector integration algorithm, such as those reported by Gear [5] or Hindmarsh [6]. The problem of spurious oscillation must still be reduced by dissipative techniques.

The difficulties in both the method of lines and the finite difference approach are compounded by the implicit coupling of the variables in systems such as the conservation equations. This makes it difficult to assign a direction to an upwind derivative or a magnitude and form to an artificial viscosity. Further complexities arise in the need to cater for possible flow reversals and to determine the number and nature of boundary conditions applicable in a given situation.

Attempts to overcome these dilemmas using the method of lines have been only partially successful. Heydweiler and Sincovec [7] use a sliding formula which combines central and directional differentiation, Hyman [8] obtains a stable solution by introducing artificial dissipation to the conservation form (2) but avoids the need to apply an energy boundary condition by using reflective boundaries.

Neither of these approaches takes advantage of the information that can be gleaned from the characteristic structure, and this has been done only occasionally in finite difference schemes. Courant, Isaacson and Rees [3] proposed that in a fixed grid method, expressions should be differentiated and boundary restraints applied in the direction dictated by the characteristics, but this method has apparently not been greatly exploited until recently. A series of papers by Walkden and coauthors report successful use of the method in conjunction with pseudo viscous smoothing terms for
modelling two-dimensional supersonic flow fields [9]. Beam and Warming [10] also report a scheme in which the local eigenvalues are used to assign directionality in a block tridiagonal implicit scheme, but do not quote the exact formulation.

Recent investigations by Hancox and Banerjee [4] have extended the applications of the characteristic finite difference technique, and the procedure has been used to develop an implicit finite difference scheme using sparse techniques to handle the matrices which result from (9) once the derivatives have been evaluated in the appropriate sense. This method has been implemented in a versatile program package for simulating transient two-phase flow, and numerical predictions compare very favourably with experimental results [11]. Below we show that these equations may be formulated in an equivalent manner which retains the same useful features but uses high-order formulae to attain better accuracy. The resulting block matrix is inverted analytically to obtain an explicit expression for the time derivative at each point, so these equations may be readily solved by finite difference means or by the method of lines. The latter course also uses higher order formulae in time and guarantees an optimal time step size for numerical stability.

## Pseudo Characteristic Form

Consider now the expanded form of Eqs. (9) in which spatial derivatives have been subscripted,+- , and 0 , to denote differentiation according to the $u+c, u-c$ and $u$ characteristic directions:

$$
\begin{align*}
\rho c \frac{\partial u}{\partial t}+\frac{\partial P}{\partial t}+(u+c)\left(\rho c \frac{\partial u}{\partial z_{+}}+\frac{\partial P}{\partial z_{+}}\right) & =0 \\
c^{2} \frac{\partial \rho}{\partial t}-\frac{\partial P}{\partial t}+u\left(c^{2} \frac{\partial \rho}{\partial z_{0}}-\frac{\partial P}{\partial z_{0}}\right) & =0  \tag{12}\\
-\rho c \frac{\partial u}{\partial t}+\frac{\partial P}{\partial t}+(u-c)\left(-\rho c \frac{\partial u}{\partial z_{-}}+\frac{\partial P}{\partial z_{-}}\right) & =0
\end{align*}
$$

Explicit equations for $\partial u / \partial t, \partial \rho / \partial t$ and $\partial P / \partial t$ may now be obtained by elimination. They are:

$$
\begin{align*}
-\frac{\partial P}{\partial t}= & \frac{u}{2}\left(\frac{\partial P}{\partial z_{+}}+\frac{\partial P}{\partial z_{-}}\right)+\frac{\rho c^{2}}{2}\left(\frac{\partial u}{\partial z_{+}}+\frac{\partial u}{\partial z_{-}}\right) \\
& +\frac{c}{2}\left(\frac{\partial P}{\partial z_{+}}-\frac{\partial P}{\partial z_{-}}\right)+\frac{u \rho c}{2}\left(\frac{\partial u}{\partial z_{+}}-\frac{\partial u}{\partial z_{--}}\right) \\
-\frac{\partial u}{\partial t}= & \frac{u}{2}\left(\frac{\partial u}{\partial z_{+}}+\frac{\partial u}{\partial z_{-}}\right)+\frac{1}{2 \rho}\left(\frac{\partial P}{\partial z_{+}}+\frac{\partial P}{\partial z_{--}}\right)  \tag{13}\\
& +\frac{c}{2}\left(\frac{\partial u}{\partial z_{+}}-\frac{\partial u}{\partial z_{-}}\right)+\frac{u}{2 \rho c}\left(\frac{\partial P}{\partial z_{+}}-\frac{\partial P}{\partial z_{--}}\right) \\
-\frac{\partial \rho}{\partial t}= & u \frac{\partial \rho}{\partial z_{0}}+\frac{\rho}{2}\left(\frac{\partial u}{\partial z_{+}}+\frac{\partial u}{\partial z_{-}}\right)+\frac{u \rho}{2 c}\left(\frac{\partial u}{\partial z_{+}}-\frac{\partial u}{\partial z_{-}}\right) \\
& +\frac{1}{2 c^{2}}\left[(u+c) \frac{\partial P}{\partial z_{-}}+2 u \frac{\partial P}{\partial z_{0}}+(u-c) \frac{\partial P}{\partial z_{-}}\right]
\end{align*}
$$

Note that for the case in which identical formulae are used for the,+- , and 0 subscripted derivatives, these equations reduce to the primitive form (8).

Equations (13) are obviously more complicated to assemble in finite difference form than equations (9). but this is no deterrent to applying the method of lines, as all differentiation is done automatically by directional formulae of any suitable accuracy. The computation will also proceed more efficiently than an attempted solution of (9), as numerical matrix inversion is no longer necessary.

## The Simplest Case

Although any order or type of formula may be used to compute the directional derivatives in (13), it is instructive to further investigate the simplest case, that in which first order formulae are used for subsonic flow and equally spaced coordinates. For any variable $q$, this gives:

$$
\begin{equation*}
\frac{\partial q}{\partial z_{+}}=\frac{q_{i}-q_{i-1}}{\Delta z}, \quad \frac{\partial q}{\partial z_{-}}=\frac{q_{i+1}-q_{i}}{\Delta z} \tag{14}
\end{equation*}
$$

Note that now

$$
\begin{equation*}
\left(\frac{\partial q}{\partial z_{+}}+\frac{\partial q}{\partial z_{-}}\right)=\frac{q_{i+1}-q_{i-1}}{\Delta z}=2 \frac{\partial q}{\partial z_{*}} \tag{15}
\end{equation*}
$$

and

$$
\begin{equation*}
\left(\frac{\partial q}{\partial z_{+}}-\frac{\partial q}{\partial z_{-}}\right)=-\frac{q_{i+1}-2 q_{i}+q_{i-1}}{\Delta z}=-\Delta z \frac{\hat{\partial}^{2} q}{\partial z_{*}^{2}} \tag{16}
\end{equation*}
$$

where $\partial q / \partial z_{*}$ and $\partial^{2} q / \partial z_{*}$ are the second-order central difference formulae for first and second derivatives.

The equations, therefore, reduce to

$$
\begin{align*}
& -\frac{\partial P}{\partial t}=u \frac{\partial P}{\partial z_{*}}+c^{2} \frac{\partial u}{\partial z_{*}}-c \frac{\Delta z}{2}\left(\frac{\partial^{2} P}{\partial z_{*}^{2}}+\rho u \frac{\partial^{2} u}{\partial z_{*}^{2}}\right) \\
& -\frac{\partial u}{\partial t}=u \frac{\partial u}{\partial z_{*}}+\frac{1}{\rho} \frac{\partial P}{\partial z_{*}}-\frac{\Delta z}{2}\left(\frac{u}{\rho c} \frac{\partial^{2} P}{\partial z_{*}^{2}}+c \frac{\partial^{2} u}{\partial z_{*}^{2}}\right)  \tag{17}\\
& -\frac{\partial \rho}{\partial t}=u \frac{\partial \rho}{\partial z_{0}}+\rho \frac{\partial u}{\partial z_{*}}-\frac{\Delta z}{2 c}\left(\left(1+\frac{u}{c}\right) \frac{\partial^{2} P}{\partial z_{*}^{2}}+\rho u \frac{\partial^{2} u}{\partial z_{*}^{2}}\right)
\end{align*}
$$

which can be regarded as the primitive form of the equations expressed in secondorder accuracy, with explicitly defined dissipative terms added. These dissipative terms are not arbitrary, as their magnitude depends on local properties and on the coordinate spacing, thus correctly linking the dissipation to convection as discussed
in [2]. In fact any dissipative finite difference scheme derives its dissipative properties from the fact that it can be rearranged to reveal some sort of approximation to a second derivative term [12].

Equations (17) result from taking the simplest expression for the directional derivatives. It is, however, computationally more effective to program the equations in the general form (12) as this permits the use of higher-order upwind difference formulae such as those available in the FORSIM method of lines package [14]. In particular, we will here consider two third-order formulae recommended by Carver and Hinds [2]. They are the four-point Lagrangian upwind bias formula

$$
\begin{equation*}
\frac{\hat{c}}{\partial z}(U(I))=S_{I}\left(U\left(I-2 S_{I}\right)-6 U\left(I-S_{I}\right)+3 U(I)+2 U\left(I+S_{I}\right)\right) / 6 \Delta Z \tag{18}
\end{equation*}
$$

and the three-point upwind Hermite formula
$\frac{\partial}{\partial z}(U(I))=S_{I}\left(U\left(I+S_{I}\right)+4 U(I)-5 U\left(I-S_{I}\right)\right) / 4 \Delta Z-\frac{1}{2} \frac{\partial}{\partial z}\left(U\left(I-S_{I}\right)\right)$
In each case the direction is assigned by $S_{I}=U(I) /|U(I)|$. These formulae were developed and discussed in [2], other possibilities, such as the three-point upwind Lagrangian, and two-point upwind Hermite, were found to give excessive phase error when applied to the advective equation, while higher-order methods were too time consuming for general use. Equations (18) and (19) may also be rearranged to revela dissipative terms. The only problem in applying these formulae occurs at the boundaries, where, if necessary, order is maintained at the expense of directionality as this has been shown to be more accurate [2].

A choice of integrator is also possible in the method of lines. For all the applications quoted, a version of the Hindmarsh-Gear integrator [6] was used. Because the transients are rapid, there is, however, little advantage in using the high-order Adams formulation available in this algorithm, so maximum order was restricted to four, and no Jacobian estimates were used to accelerate the predictor corrector. A much simpler algorithm, retaining efficient step size control, would suffice.

## Test Problems

Vichnevetsky [15] has shown that all finite difference, finite element and method of lines schemes generate spurious numerical oscillations in the neighbourhood of travelling waves, and that these oscillations are compounded by each reflection until the spurious oscillations overwhelm the signal wave.

The following test problems illustrate that the pseudo characteristic method minimizes this instability in contrast to the primitive method of lines, standard finite difference methods, and the linear finite element method.

## Test Problem A

Sod [1] compares a number of finite difference methods with reference to a simple shock tube problem. In this case, initial conditions are

$$
\begin{gather*}
0<x<0.5, \quad P=\rho=1.0, \quad u=0, \quad \Delta x=0.01 \\
0.5<x<1.0, \quad p=0.1, \quad \rho=0.125, \quad u=0 \tag{20}
\end{gather*}
$$

This problem does not involve flow reversal or changing boundary conditions. It does, however, have a large pressure ratio which generates shock and rarefaction waves resulting in a pressure discontinuity and three discontinuities in the spatial derivative of density.

Comparing results of the simple pseudo characteristic (PC) method shown in Fig. 1 with those of methods illustrated by Sod, it is apparent that the PC method


Fig. 1. Shock tube problem, test problem A. Simple (two-point) pseudo characteristic method.
does not exhibit the erroneous steep fronted rarefaction wave developed by the rudimentary upwind method discussed by Sod. The simple PC method also is superior in accuracy to the Lax-Wendroff method [16], the MacCormack method [17], and Rusanov methods [18], as all of these require additional dissipation to produce stable results. The MacCormack second-order method with dissipation appears to give the
best results of this group [1], and is used here as a basis for comparison. In brief this method for Eq. (1) is in two-step predictor-corrector form,

$$
\begin{align*}
& \phi_{i}^{\overline{n+1}}=\phi_{i}{ }^{n}-\frac{\Delta t}{\Delta x}\left(F_{i+1}^{n}-F_{i}^{n}\right) \\
& \left.\phi_{i}^{n+1}=\frac{1}{2}\left(\phi_{i}^{n}+\phi_{i}^{\overline{n+1}}\right)-\frac{\Delta t}{\Delta x}\left(\overline{F_{i}^{n+1}}-\overline{F_{i-1}^{n+1}}\right)\right) \tag{21}
\end{align*}
$$

An artificial damping term defined as

$$
\begin{align*}
& \phi_{i}^{n+1}=\phi_{i}^{n+1}+\alpha \frac{\Delta t}{\Delta x} \Delta^{\prime}\left(\left|\Delta^{\prime} \phi_{i}^{n+1}\right| \cdot \Delta^{\prime} \phi_{i}^{n+1}\right) \\
& \Delta^{\prime} \phi_{i}=\phi_{i}-\phi_{i-1} \tag{22}
\end{align*}
$$

must be used as a third step to obtain stable results, and the choice of $\alpha$ is entirely arbitrary. Figure 2 shows results obtained for two choices of $\alpha$.

Results from the pseudo characteristic method using the higher order formulae (18) and (19) are shown in Fig. 3. Small spurious peaks are evident in the neighbourhood of discontinuities, but it will be shown in Test Problem $B$ that these do not become unstable on reflection, and the addition of further dissipation, at least for these conditions, appears unnecessary.
The accuracy of the higher-order PC methods also appear to compare very favourably to the more complicated methods reviewed by Sod, but the PC method is easier to implement and computationally efficient. The rationale of the PC method is also naturally founded on the characteristics, and does not rely on arbitrary numerical stabilization.

## Test Problem B

In order to assess the performance of the PC method during wave reflections and flow reversals, the scheme has also been tested on the classic shock tube problem discussed by Rudinger [19]. A long closed cylinder, initially containing quiescent gas at pressure $P_{0}$ is suddenly exposed to an ambient pressure $P_{A}$ at one end. If the pressure ratio $P_{R}=P_{0} / P_{A}$ is less than 1 , a compression wave enters the duct; if greater, gas flows out and a rarefaction wave enters. In either case the incident wave reflects at the closed end and then reflects negatively on returning to the open end. If $P_{R}$ is large enough, the outlet becomes choked at sonic velocity. This very simple test problem, therefore, incorporates compression and rarefaction waves, reflection, flow reversal and possibly, choked flow, all of which cause problems in most numerical schemes.
It is difficult to obtain independent solutions to this problem as few schemes will handle the flow reversal, as efficiently as the pseudo characteristic method, so it is more convenient to invent a Utopian situation in which the entire process, including in-flow and out-flow, is reversible. Under such conditions, the wave action is uniform and cyclic, and a good test of the numerical scheme is how well the waves can be reproduced during several cycles of propagation and reflection.


Fig. 2. Test problem A. MacCormack method. (a) $\alpha=0.25$, (b) $\alpha=0.5$.


Fig. 3. Test problem A. Higher-order Pseudo characteristic methods. (a) Four-point bias, (b) upwind Hermite.

If several cycles of reflection are depicted, graphs of spatial profile at different times are difficult to assimilate, so in the following figures, the performances of the pseudo characteristic schemes and others are illustrated by the transient response of normalized pressure at points $x=0,0.25,0.5,0.75,1.0$ in a 101 -point grid.
Figure 4 shows that all the pseudo characteristic schemes remain stable through several cycles of reflection. The simple PC method permits attenuation after several cycles due to numerical dissipation losses, but the higher-order methods are conservative, retaining the wave form well.
The primitive form, Eqs. (8) with artificial dissipation added:

$$
\begin{equation*}
\frac{\partial}{\partial t} \psi+\mathbf{A}(\psi) \frac{\partial}{\partial z} \psi=\alpha \frac{\partial^{2}}{\partial z^{2}} \psi \tag{23}
\end{equation*}
$$

may also be programmed easily to account for flow reversals, and is used as a basis for comparison.
Figure 5 shows results from the primitive form, using central differences and various magnitudes of dissipation. As for the MacCormack method, these may be stabilized by sufficient dissipation but this attenuates the waves. Finally, Fig. 6 shows that results from the linear finite element solution of the primitive equations are subject to similar failings in stability and conservation.


Fig. 4. Test problem B. Pseudo characteristic methods cyclical response of pressure at various axial stations. (a) Simple (two-point) PC method, (b) four-point upwind bias PC method; (c) upwind Hermite PC method.


Fig. 4-Continued.


Fig. 5. Test problem B. Primitive form with central derivatives. (a) $\alpha=0$, (b) $\alpha=0.001$, (c) $\alpha=0.01$.


Fig. 5-Continued.


Fig. 6. Test problem B. Primitive linear finite element form with dissipation. (a) $\alpha=0,(b) \alpha=$ 0.001 , (c) $\alpha=0.01$.


Fig. 6-Continued.

## Conclusions

The pseudo characteristic method follows naturally from the characteristic formulation of the conservation equations, and may be shown to contain explicitly defined dissipative terms. Even in its simplest formulation it is more stable and more accurate than conventional finite difference and method of lines formulations. Higher order formulations increase accuracy without detracting from stability. The computational overhead is no greater than that for the primitive method with artificial dissipation, as six first derivatives in space must be evaluated instead of three first and three second derivatives. It is planned to use the method for comparison to applications benchmarks. such as those described in [4], and to investigate the applicability to other hyperbolic systems such as those mentioned in [7].

## Appendix <br> Application of Higher-Order Pseudo Characteristics Methods to Simple Hyperbolic Equations

The use of higher-order directional derivative formulae in method of lines solution to the advective equation is discussed in detail in reference [2], which recommends two third-order formulae, the four-point upwind biased Lagrangian, and a three-point upwind biased Hermite. They are respectively:
$\frac{\partial}{\partial Z}(U(I))=S_{I}\left(U\left(I-2 S_{I}\right)-6 U\left(I-S_{I}\right)+3 U(I)+2 U\left(I+S_{I}\right)\right) / 6 \Delta Z$
$\frac{\partial}{\partial Z}(U(I))=S_{I}\left(U\left(I+S_{I}\right)+4 U(I)-5 U\left(I-S_{I}\right)\right) / 4 \Delta Z-\frac{1}{2} \frac{\partial}{\partial x}\left(U\left(I-S_{I}\right)\right)$
In support of their use in the numerical solution of the conservation equations of compressible flow, their application to simpler hyperbolic equations is considered here, Two test examples are used, in each case integration is by the Hindmarsh-Gear integration algorithm [6] in which a relative accuracy of $10^{-1}$ was imposed such that the dominant error is spatial in origin. Errors quoted are the average absolute error over the range of $t$ and $x$ quoted.

## Case 1. Burger's Equation

The equation

$$
\begin{equation*}
\frac{\partial u}{\partial t}+u \frac{\partial u}{\partial x}=\alpha \frac{\partial^{2} u}{\partial x^{2}} \tag{A3}
\end{equation*}
$$

can be regarded as the nonlinear advective equation with the addition of an arbitrary dissipation term, but this interpretation can be misleading; unless $\alpha$ is made a function
of coordinate spacing, the dominance of the dissipation term increases with the number of solution points chosen; we will, however, test a fixed number of points.

The particular application investigated here is that in which initial and boundary conditions are extracted from the analytical solution.

$$
\begin{gather*}
u(x, t)=\frac{0.1 e^{-a}+0.5 e^{-b}+e^{-c}}{e^{-a}+e^{-b}+e^{-c}}  \tag{A4}\\
a=0.05(x-0.5+4.95 t) / \alpha \\
b=0.25(x-0.5+0.75 t) / \alpha \\
c=0.50(x-0.375) / \alpha
\end{gather*}
$$

This establishes two shock waves travelling at different speeds and merging at $t=.5$. The problem is well documented in [8,20] so the table A.1, showing average errors is sufficient evidence here. Note that as $\alpha$ decreases, convection dominates diffusion, and the higher-order, five-point symmetric differencing begins to produce less accurate results than the reference three-point difference method, whereas the directional methods are considerably superior at low values of $\alpha$.

TABLE A1
Burger's Equation-Travelling Waves ${ }^{a}$

|  | Normalized Errors |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\alpha$ | 0.01 | 0.005 | 0.002 | 0.001 | 0.0005 |
| Ref. error | $\left(1.1 \times 10^{-4}\right)\left(1.8 \times 10^{-3}\right)\left(1.0 \times 10^{-3}\right)\left(2.1 \times 10^{-2}\right)\left(3.7 \times 10^{-2}\right)$ |  |  |  |  |
| 3-pt. Central | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| 5-pt. Central | 0.41 | 0.32 | 0.65 | 0.89 | 1.13 |
| 2-pt. Upwind | 8.5 | 4.6 | 1.4 | 0.72 | 0.47 |
| 4-pt. Upwind bias | 0.39 | 0.36 | 0.44 | 0.40 | 0.33 |
| 3-pt. Upwind Hermite | 0.35 | 0.26 | 0.26 | 0.29 | 0.26 |

${ }^{a}$ Average absolute error over time and space expressed with reference to the three-point central difference formula results ( $x \in(0,1), \Delta x=0.02, t \rightarrow 1.0$ ).

## Case 2. Counter Current Heat Exchange

The hot and cold side temperatures $u_{1}$ and $u_{2}$ of fluids travelling with velocities $v_{1}$ and $v_{2}$ in a single pass counter current heat exchanger are given by the equations

$$
\begin{align*}
& \frac{\partial u_{1}}{\partial t}=-y_{1}\left(u_{1}-u_{2}\right)-v_{1} \frac{\partial u_{1}}{\partial z}  \tag{A5}\\
& \frac{\partial u_{2}}{\partial t}=+y_{2}\left(u_{1}-u_{2}\right)+v_{2} \frac{\partial u_{2}}{\partial z}
\end{align*}
$$

and the inner fluid temperature above steady state after an inlet step change $v_{0}$ at $x=0$ is given in Ref. [21] as:

$$
\begin{aligned}
u & =u_{0} e^{-\alpha x} \int_{\beta x}^{t-\gamma x} e^{-\rho \tau} \frac{\sigma \beta x}{\left[\tau^{2}-(\beta x)^{2}\right]^{1 / 2}} \cdot I_{1}\left(\sigma\left[\tau^{2}-(\beta x)^{2}\right]^{1 / 2}\right) \delta \tau+e^{-\rho \beta x} \\
\alpha & =\left(v_{2} y_{1}-v_{1} y_{2}\right) / 2 v_{1} v_{2}, \quad \beta=\left(v_{1}+v_{2}\right) / 2 v_{1} v_{2} \\
\rho & =\left(v_{2} y_{1}-y_{1} y_{2}\right) /\left(v_{1}+v_{2}\right), \quad \gamma=\left(v_{2}-v_{1}\right) / 2 v_{1} v_{2} \\
\sigma^{2} & =4 v_{1} v_{2} y_{1} y_{2} /\left(v_{1}+v_{2}\right)^{2},
\end{aligned}
$$

$I_{1}=$ modified Bessel function of the first kind, order 1.
$v_{1}=v_{2}=1, \quad y_{1}=0.1, \quad y_{2}=0.001, \quad u_{0}=1, \quad x \in(0,10), \quad t \rightarrow 10$.

The resulting transient is a travelling discontinuity in $u_{1}$ and $u_{2}$. The discontinuity is not as severe as is the previous equation for low $\alpha$, but the directional difference formulae are again markedly superior, as shown in Table A2.

TABLE A2
Counter Current Heat Exchanger ${ }^{a}$

|  | 21 points | 41 points | Normalized CPU time |
| :---: | :---: | :---: | :---: |
| $\Delta x$ <br> Ref. error | 0.5 | 0.25 |  |
|  | 0.0465 | 0.0358 | ( 21 \& 41 pts.$)$ |
|  | Normalized errors |  |  |
| 3-pt. Central | 1.00 | 1.00 | 1.00 |
| 5-pt. Central | 0.98 | 0.97 | 1.03 |
| 2-pt. Upwind | 1.30 | 1.37 | 1.02 |
| 4-pt. Upwind bias | 0.66 | 0.52 | 1.06 |
| 3-pt. Upwind Hermite | 0.60 | 0.45 | 1.06 |

${ }^{a}$ Average absolute error over time and space expressed with respect to the three-point central difference formula result $\left(x \in(0,10), t \rightarrow 10.0, u_{0}=1.0\right)$.

## References

1. G. A. Sod, J. Comput. Phys. 24 (1978), 402.
2. M. B. Carver and H. W. Winds, Simulation 11, No. 2 (August 1978), 59-69.
3. R. Courant, E. Isaacson, and M. Rees, Comm. Pure Appl. Math. 5 (1952), 243.
4. W. T. Hancox and S. Banerjee, Nucl. Sci. Eng. 64 (1977), 106.
5. C. W. Gear, Commun. ACM 3 (1971), 176.
6. A. C. Hindmarsch, "Gear Ordinary Differential Equation Solver," Lawrence Livermore Laboratory Report UCID-30001-R3, 1974.
7. J. C. Heydweiler and R. F. Sincovec, J. Comput. Phys. 22 (1976), 377.
8. J. M. Hyman, "Method of Lines Solution of Partial Differential Equations," Courant Institute Report COO-3077-139, New York, 1976.
9. F. Walkden and J. E. Sellars, Aeronaut. Quart. (1966) 285; F. Walkden and P. Caine, Int. J. Numer. Meth. Eng. 5 (1972), 151; F. Walkden, P. Caine, and G. T. Laws, J. Comput. Phys. 27 (1978), 103.
10. R. M. Beam and R. F. Warming, J. Comput. Phys. 22 (1976), 87.
11. F. W. Barclay, D. Bean, and R. W. Neimann, in "Proceedings of Iasted Symposium on Simulation and Modelling in Energy Systems" (M. B. Carver, Ed.), Acta Press, Calgary, 1978.
12. W. F. Ames, "Nonlinear Partial Differential Equations in Engineering," Academic Press, New York, 1965.
13. R. D. Richtmyer and K. W. Morton, "Difference Methods for Initial Value Problems," Interscience, New York, 1967.
14. M. B. CARVER, AAICA 3 (1975), 195.
15. R. Vichnevetsky and B. Peiffer, in "Advances in Computer Methods for Partial Differential Equations" (R. Vichnevetsky, Ed.), p. 52, AAICA Press, Rutgers University, New Brunswick, N.J., 1975.
16. P. Lax and B. Wendroff, Comm. Pure Appl. Math. 13 (1960), 217.
17. R. MacCormack, "Proceedings of the Second International Conference on Numerical Methods in Fluid Dynamics," Lecture Notes in Physics, No. 8 (M. Holt, Ed.), Springer-Verlag, New York, 1971.
18. V. V. Rusanov, USSR Comput. Math. Math. Phys. 2 (1962).
19. G. Rudinger, "Wave Diagrams for Non Steady Flow in Ducts," Van Nostrand, New York, 1955.
20. N. K. Madsen and R. F. Sincovec, in "Numerical Methods for Differential Systems" (L. Lapidus and W. E. Schiesser, Eds.) p. 229, Academic Press, New York, 1975.
21. D. H. Herron and D. U. Von Rosenburg, Chem. Eng. Sci. 21 (1966), 337.
