Finite-Difference Method-of-Characteristics Scheme for the Equations of Gasdynamics

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A finite-difference method for the characteristic equations of gasdynamics is developed. The method is based on a directed discretization of the characteristic compatibility conditions. The choice of wave propagation directions is arbitrary, and there is no need to fit interpolating functions to the initial data. The proposed method is not conservative and therefore must be used with a shock-fitting procedure in regions wherever the flow is discontinuous. Numerical results are presented for sample two-dimensional problems.

Introduction

I UMERICAL schemes based on the method of characteristics have been applied successfully to a large number of problems in multidimensional gasdynamics. Schemes of this type are attractive because they are typically robust, in no small part because of their direct relationship to the physics of nonlinear wave propagation. The review paper by Roe¹ outlines a number of characteristics-based methods, including algorithms for both the conservative and nonconservative forms of the governing equations. In this paper, we present a nonconservative discretization for the characteristic compatibility conditions. It is important to keep in mind that algorithms of this type must, in general, incorporate a capability to track discontinuities in the flowfield explicitly to ensure that the Rankine-Hugoniot jump conditions are satisfied in these regions.

A number of conservative and nonconservative schemes for multidimensional flow are constructed under the assumption that the multidimensional problem can be split into quasi-onedimensional pieces in which waves travel normal to the mesh lines (this is true of approximate Riemann solvers, 2,3 flux vector splitting schemes, 4,5 and also of the nonconservative SCM scheme⁶). How this assumption affects the quality of the numerical results is not entirely clear, especially if the comparison is made keeping the total computational effort fixed. Nevertheless, there is evidence that numerical methods that account for the multidimensional nature of the problem can produce high-resolution solutions. One family of methods of this type has evolved from Colella's conservative unsplit Godunov method:7 multidimensional characteristics information is propagated to the faces of the computational cell to compute the numerical fluxes required in the solution of the integral form of the conservation equations. Perhaps even more sophisticated is Roe's model, 8 for which, unfortunately, little data is available. Several recent papers report research and opinions on this subject.8,9,10

Many nonconservative, truly multidimensional schemes, based on the method of characteristics for multidimensional flow, have evolved from the method of Butler. 11 According to this method, a number of characteristic compatibility conditions are combined to yield a set of equations in which the spatial derivatives of the dependent variables are evaluated along the projections onto space of the stream- and wave-type characteristic rays. The advantage in this approach is clear: the "upwind" directions are defined by the characteristic rays.

We note here that such a set of equations, although obtained from the characteristic equations, are not, in general, characteristic compatibility conditions.

We now loosely define full-characteristics schemes as those in which the characteristic rays are actually traced in the solution procedure, and finite-difference characteristics-based schemes as those that simply use the characteristic information to form upwind differences. In the first approach, the data, which is available only at mesh points, must be interpolated to form the initial values of the Riemann variables. 11,12,13 This is expensive to do, especially in three space dimensions, and furthermore, the resulting conditioning (smoothing) of the data can be quite arbitrary. The second approach is exemplified in the technique developed by Moretti and Zanetti, 14 in which combinations of the characteristic compatibility conditions are simply finite differenced.

In this paper, we propose a nonconservative finite-difference scheme to directly integrate the characteristic compatibility conditions for arbitrary wave orientation. The new scheme is in some ways related in approach to the method of Ref. 14, differing in the choice of equations that are discretized. One important consequence of the differencing of the true characteristic compatibility conditions is that the resulting scheme is upwind biased, not fully upwind.

The extension of the scheme to discontinuous initial data might follow the lines of the the arguments in Ref. 15. This raises the exciting possibility of computing strong waves of arbitrary orientation, which is the subject of our ongoing research.

We begin with an outline of the method of characteristics for the equations of gasdynamics. The numerical scheme is then developed and tested for two-dimensional flowfields.

Method of Characteristics

In this section, the theory of characteristics for multidimensional flow is outlined, following the detailed treatment of Rusanov.¹⁶

The Euler equations, which govern the flow of an inviscid, nonconducting gas, are

$$\mathfrak{L}_1 = \rho_t + \boldsymbol{u} \cdot \nabla \rho + \rho \nabla \cdot \boldsymbol{u} = 0 \tag{1a}$$

$$\mathcal{L}_{2,3,4} = \boldsymbol{u}_t + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \frac{1}{\rho}\nabla p = 0$$
 (1b)

$$\mathcal{L}_5 = p_t + \boldsymbol{u} \cdot \nabla p + \rho a^2 \nabla \cdot \boldsymbol{u} = 0 \tag{1c}$$

where the dependent variables ρ , u, and p are the density, particle velocity, and pressure, respectively, and $a(p, \rho)$ is the speed of sound. We seek combinations of Eqs. (1)

$$\mathfrak{L} = \alpha_1 \mathfrak{L}_1 + \alpha_2 \mathfrak{L}_2 + \ldots + \alpha_5 \mathfrak{L}_5 \tag{2}$$

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such that all derivatives are taken in directions that lie in the characteristic plane, defined by its normal $N = (n_t, n) = (n_b, n_x, n_y, n_z)$. From Eq. (2), we see that the dependent variables are differentiated in the directions

$$\tau^{\rho} = (\alpha_1 + a^2 \alpha_5)(1, u) \equiv (\alpha_1 + a^2 \alpha_5)U$$

$$\tau^{u} = (\alpha_2, \alpha_1 \rho + \alpha_2 u + \alpha_5 \rho a^2, \alpha_2 v, \alpha_2 w)$$

$$\tau^{v} = (\alpha_3, \alpha_3 u, \alpha_1 \rho + \alpha_3 v + \alpha_5 \rho a^2, \alpha_3 w)$$

$$\tau^{w} = (\alpha_4, \alpha_4 u, \alpha_4 v, \alpha_1 \rho + \alpha_4 w, \alpha_5 \rho a^2)$$

$$\tau^{\rho} = \left(\alpha_5, \frac{\alpha_2}{\rho} + \alpha_5 u, \frac{\alpha_3}{\rho} + \alpha_5 v, \frac{\alpha_4}{\rho} + \alpha_5 w\right)$$

where U=(1, u)=(1, u, v, w) is the four-dimensional velocity vector. Setting $N \cdot \tau^{\rho} = \ldots = N \cdot \tau^{p} = 0$ gives the characteristic condition:

$$\begin{bmatrix}
N \cdot U & 0 & 0 & 0 & 0 \\
\rho n_{x} & N \cdot U & 0 & 0 & \rho a^{2} n_{x} \\
\rho n_{y} & 0 & N \cdot U & 0 & \rho a^{2} n_{y} \\
\rho n_{z} & 0 & 0 & N \cdot U & \rho a^{2} n_{z} \\
0 & n_{x}/\rho & n_{y}/\rho & n_{z}/\rho & N \cdot U
\end{bmatrix}
\begin{pmatrix}
\alpha_{1} \\
\alpha_{2} \\
\alpha_{3} \\
\alpha_{4} \\
\alpha_{5}
\end{pmatrix} = 0 \quad (3)$$

If a nontrivial solution for the multipliers α_1 exists, then the determinant of the coefficient matrix must vanish. This gives the characteristic polynomial:

$$(N \cdot U)^3 \{ (N \cdot U)^2 - a^2 n \cdot n \} = 0$$
 (4)

from which the time component n_t of the characteristic normal vector can be determined for a specified space component n. To the triple root there corresponds

$$n_t = -\mathbf{u} \cdot \mathbf{n}$$

and to the quadratic factor of the characteristic polynomial

$$n_t = -(u \cdot n + a \mid n \mid)$$

where we have adopted a sign convention for the characteristic normal. We are at liberty to impose a normalizing condition, and we choose

$$|n| = 1$$

As the space component of the characteristic normal vector is rotated on the unit sphere, the characteristic normal N will sweep out a cone in space time. Now each characteristic normal defines a characteristic plane, and the envelope of characteristic planes is also a cone in space time. From the theory of envelopes, it can be shown that the generator of the (degenerate) cone corresponding to the repeated root is the four-dimensional velocity vector U. The generator of the cone corresponding to the quadratic factor is V = (1, u + an). The generators of the characteristic cones are called characteristic rays, and the preceding results justify the labels stream-type and wave-type associated with the characteristic rays corresponding to the repeated root and quadratic factor, respectively.

With the time component of the characteristic normal specified in terms of its space component, we are now able to find the multipliers α_i that give characteristic combinations of the original system of Eqs. (1). These characteristic combinations are scaled characteristic compatibility conditions. With $N \cdot U = 0$, the nullspace of the coefficient matrix is spanned by the three vectors

$$\alpha^1 = (a^2, 0, 0, 0, -1) \tag{5}$$

$$\alpha^2 = (0, s^{(1)}, 0) \tag{6}$$

$$\alpha^3 = (0, s^{(2)}, 0) \tag{7}$$

where $s^{(1)}$ and $s^{(2)}$ are linearly independent, and $s^{(1)} \cdot n = s^{(2)} \cdot n = 0$. Thus there exist three independent compatibility conditions of the stream type for a given choice of n. For α specified by Eq. (5), we have

$$a^{2}(\rho_{t} + \boldsymbol{u} \cdot \nabla \boldsymbol{\rho}) - (p_{t} + \boldsymbol{u} \cdot \nabla \boldsymbol{p}) = 0$$
 (8)

which expresses the constancy of particle entropy along a particle path in continuous flow. The compatibility conditions for the choices Eqs. (6) and (7) are projections of the momentum equation onto the vector s:

$$s \cdot \left(u_t + (u \cdot \nabla)u + \frac{1}{\rho} \nabla p \right) = 0 \tag{9}$$

With $n_t = -(\mathbf{u} \cdot \mathbf{n} + a \mid \mathbf{n} \mid)$, the rank of the coefficient matrix is 4, and there is only one independent vector α :

$$\alpha = (0, \rho a n_{x}, \rho a n_{y}, \rho a n_{z}, 1) \tag{10}$$

to which corresponds the wave-type characteristic compatibility condition

$$\rho a \boldsymbol{n} \cdot \left(\boldsymbol{u}_t + (\boldsymbol{u} \cdot \nabla \boldsymbol{u}) + \frac{1}{\rho} \nabla \boldsymbol{p} \right) + (\boldsymbol{p}_t + \rho \boldsymbol{a}^2 \nabla \cdot \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{p}) = 0$$
(11)

Our intention at the outset was to replace the original system of governing equations, Eqs. (1), by a characteristic system of equations in which all of the dependent variables were differentiated in a common plane. We have shown that there exist an infinite number of characteristic compatibility conditions, corresponding to the infinite number of choices for the spatial component n of the characteristic normal. However, because each of the characteristic equations is formed by a combination of the original equations, only five can be independent.

Corresponding to a given choice of n, there exist a maximum of three independent compatibility conditions of the stream type and only one of the wave type. It is apparent, therefore, that a characteristic system that is to serve as a replacement for the Euler equations is obtained by choosing from among the characteristic relations obtained for more than one choice of n. The condition that a given choice of five compatibility conditions is correct is that the determinant of the multipliers be different from zero:

$$\det \alpha^{(j)} = \begin{vmatrix} a^2 & 0 & 0 & 0 & -1 \\ 0 & s_x^{(s)} & s_y^{(s)} & s_z^{(s)} & 0 \\ \vdots & & & \vdots \\ 0 & \rho a n_x^{(1)} & \rho a n_y^{(1)} & \rho a n_z^{(1)} & 1 \\ \vdots & & & \vdots \\ 0 & \rho a n_x^{(r)} & \rho a n_y^{(r)} & \rho a n_z^{(r)} & 1 \end{vmatrix} \neq 0 \quad (12)$$

The preceding considerations require that in Eq. (12) we must have $0 \le s \le 3$, $1 \le r \le 4$, r + s = 4, and the set of multipliers must contain the first vector because it cannot be obtained from any combination of the remaining vectors.

Finite-Difference Method of Characteristics

Equations (8-11), written for a number of choices of the space component n of the characteristic normal and subject to the restriction expressed by Eq. (12), provide a set of linearly independent characteristic compatibility conditions. The characteristic compatibility conditions now serve to replace the original system of Eqs. (1). Strictly speaking, the characteristic equations must be integrated together with a system of equations that describe the evolution of the characteristic normals along the rays that are specified in the initial data plane (see Varley and Cumberbatch¹⁷). In many full method-of-characteristics algorithms, the additional work is avoided by "freezing" the characteristic normal, which implies that the frozen rays deviate from the true rays by an amount that is dependent on the time step. 12,13 In the present approach, we shall treat the vectors n as frozen.

Choice of Equations

We now make the specific choice for the characteristic system

$$a^{2}(\rho_{t} + u \cdot \nabla \rho) - (p_{t} + u \cdot \nabla p) = 0$$

$$p_{t} + \left[u + an^{(i)} \right] \cdot \nabla p + \rho an^{(i)} \cdot \left[u_{t} + (u \cdot \nabla)u \right]$$

$$+ \rho a^{2} \nabla \cdot u = 0, \qquad i = 1, \dots, r$$

$$(14)$$

In three-dimensional problems, the wave-type equation, Eq. (14), is written for four vectors $n^{(i)}$, (that is, r=4), and Eq. (12) requires that the endpoints of the unit normals laid off from a common origin not lie in a plane. In two dimensions, r=3, and the three unit normals must simply be distinct. In continuous flowfields, one would expect the dependence of the solution on the particular choice of normals to be of the order of the truncation error (and one might choose the normals to minimize some measure of the error). For two-dimensional problems, we choose the normals to be uniformly distributed over the unit circle, as shown in Fig. 1. In three dimensions, we would choose the unit normals to be uniformly distributed over the unit sphere.

Upwinding is accomplished by identifying the direction along which each of the dependent variables is differentiated.

and

In Eq. (13), both the density and pressure are differentiated along the velocity vector U. Thus the upwind directions for the x, y, and z-derivatives are determined by examining the signs of the velocity components u, v, and w, respectively.

The wave-type compatibility condition, Eq. (14), involves derivatives of the pressure and the velocity. The directions along which each of the dependent variables is differentiated are obtained immediately by inspection. For example, the pressure is differentiated along the characteristic ray $V = [1, u + an^{(i)}]$, and the upwind direction is therefore determined by the sign of $u + an^{(i)}$. Similarly, the x component of the velocity is differentiated in the direction

$$dt:dx:dy:dz = n_x:un_x + a:vn_x:wn_x$$

the upwind direction for the x derivative is identified according to the sign of

$$\frac{\mathrm{d}x}{\mathrm{d}t} = u + \frac{a}{n_x}$$

and so on.

Coordinate Transformation

Consider a transformation of corrdinates according to

$$\xi = \xi(x, y, z, t), \quad \eta = \eta(x, y, z, t), \quad \zeta = \zeta(x, y, z, t), \quad \tau = t$$

The characteristic system can be rewritten in ξ , η , ζ , and τ coordinates as

$$Aq_x + B^{(\xi)}q_x + B^{(\eta)}q_y + B^{(\xi)}q_z = 0$$
 (15)

where $q = (\rho, u, p)$, and the subscripts denote partial derivatives. The coefficient matrices are of the form

$$A = \begin{pmatrix} a^{2} & 0 & 0 & 0 & -1 \\ 0 & \rho a n_{x}^{(1)} & \rho a n_{y}^{(1)} & \rho a n_{z}^{(1)} & 1 \\ 0 & \rho a n_{x}^{(2)} & \rho a n_{y}^{(2)} & \rho a n_{z}^{(2)} & 1 \\ 0 & \rho a n_{x}^{(3)} & \rho a n_{y}^{(3)} & \rho a n_{z}^{(3)} & 1 \\ 0 & \rho a n_{x}^{(4)} & \rho a n_{y}^{(4)} & \rho a n_{z}^{(4)} & 1 \end{pmatrix}$$
(16)

$$B^{(k)} = \begin{cases} a^{2}V^{(k)} & 0 & 0 & -V^{(k)} \\ 0 & \rho a \left(V^{(k)} n_{x}^{(1)} + a k_{x}\right) & \rho a \left(V^{(k)} n_{y}^{(1)} + a k_{y}\right) & \rho a \left(V^{(k)} n_{z}^{(1)} + a k_{z}\right) & V^{(k)} + a \left(n^{(1)} \cdot \nabla k\right) \\ 0 & \rho a \left(V^{(k)} n_{x}^{(2)} + a k_{x}\right) & \rho a \left(V^{(k)} n_{y}^{(2)} + a k_{y}\right) & \rho a \left(V^{(k)} n_{z}^{(2)} + a k_{z}\right) & V^{(k)} + a \left(n^{(2)} \cdot \nabla k\right) \\ 0 & \rho a \left(V^{(k)} n_{x}^{(3)} + a k_{x}\right) & \rho a \left(V^{(k)} n_{y}^{(3)} + a k_{y}\right) & \rho a \left(V^{(k)} n_{z}^{(3)} + a k_{z}\right) & V^{(k)} + a \left(n^{(3)} \cdot \nabla k\right) \\ 0 & \rho a \left(V^{(k)} n_{x}^{(4)} + a k_{x}\right) & \rho a \left(V^{(k)} n_{y}^{(4)} + a k_{y}\right) & \rho a \left(V^{(k)} n_{z}^{(4)} + a k_{z}\right) & V^{(k)} + a \left(n^{(4)} \cdot \nabla k\right) \end{cases}$$

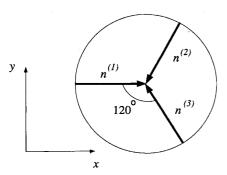


Fig. 1 Choice of normals.

where $V^{(k)}$ is the k-contravariant velocity: $V^{(k)} = k_t + \mathbf{u} \cdot \nabla k$, and k is ξ, η , or ζ .

In transformed coordinates, the upwind directions follow directly by inspection of the coefficient matrices in Eq. (15). In the stream-type equation, both the pressure and density are differentiated along

$$\left[1, V^{(\xi)}, V^{(\eta)}, V^{(\zeta)}\right]$$

In the wave-type equations, the pressure is differentiated along the vector

$$\left[1,V^{(\xi)}+an\cdot\nabla\xi,V^{(\eta)}+an\cdot\nabla\eta,V^{(\zeta)}an\cdot\nabla\zeta\right]$$

and the u, v, and w components of the velocity along the directions

$$\begin{split} \mathrm{d}\tau : & \mathrm{d}\xi : \mathrm{d}\eta : \mathrm{d}\zeta = n_x \colon V^{(\xi)} n_x + a \, \xi_x \colon V^{(\eta)} n_x + a \, \eta_x \colon V^{(\xi)} n_x + a \, \zeta_x \\ \mathrm{d}\tau : & \mathrm{d}\xi : \mathrm{d}\eta : \mathrm{d}\zeta = n_y \colon V^{(\xi)} n_y + a \, \xi_y \colon V^{(\eta)} n_y + a \, \eta_y \colon V^{(\xi)} n_y + a \, \zeta_y \\ \mathrm{d}\tau : & \mathrm{d}\xi : & \mathrm{d}\eta : & \mathrm{d}\zeta = n_z \colon V^{(\xi)} n_z + a \, \xi_z \colon V^{(\eta)} n_z + a \, \eta_z \colon V^{(\zeta)} n_z + a \, \zeta_z \end{split}$$

respectively.

Boundary Conditions

Enforcement of the boundary conditions in a method-of-characteristics algorithm is fairly straightforward. At a boundary, each boundary condition is supposed to replace a characteristic compatibility condition carrying information from the region outside the computational domain. At physical boundaries (for example, at a wall), the boundary conditions to be enforced are quite well defined. This might not be the case at an artificial boundary (such as at the exit of an unchoked nozzle), where one must resort to some plausible and simple model for the way in which the flow outside the boundary influences the solution in the computational domain. Some successful procedures for the far-field boundary in external flows have recently been suggested by Roe. 18

To show how a boundary point treatment is formulated, we shall consider an $\eta=$ const wall boundary calculation. At such a point, one wave-type equation is replaced by the boundary condition. If the remaining two wave-type equations are retained and chosen to be oriented arbitrarily towards the wall, then we are not guaranteed that the upwind directions for the η derivatives will be toward the interior of the computational domain. We have therefore developed a procedure in which one wave-type equation is written for $n=\pm \nabla \eta/|\nabla \eta|$ (oriented towards the wall), and the second wave-type equation is replaced by a combination of stream-type equations: the sum of Eqs. (8) and (9). The combined relation is formed with $s=\tau^w$, where τ^w is the unit vector pointing upstream, parallel to the local velocity vector. Note that such a combination is characteristic.

Numerical scheme

The development of a numerical scheme to integrate the characteristic system, Eq. (15), is straightforward, namely, the partial derivatives are replaced by the appropriate one-sided finite-difference expressions. For illustration of the method, we consider explicit first- and second-order accurate implementations.

In the first-order accurate algorithm, we use a simple forward time difference. If we denote the forward and backward finite-difference approximation for the spatial derivative of a variable f by $\delta^+ f$ and $\delta^- f$, respectively, then for first-order accuracy,

$$\delta^{\pm} f = \mp f_i \pm f_{i+1} \tag{18}$$

where the mesh spacing in the transformed coordinates is assumed to be unity. The fixed indices have been omitted in this expression.

For second-order accuracy, we use Gabutti's three-step scheme¹⁹: first-order one-sided finite differences, Eq. (18), in the predictor and final steps, and the first-order difference formula

$$\delta^{\pm} f = \mp 2f_i \pm 3f_{i\pm 1} \mp f_{i\pm 2}$$

in the intermediate step.

Results

Supersonic Expansion

Results using the second-order accurate version of the new scheme are shown for a supersonic expansion around a 15 deg

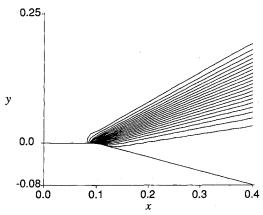


Fig. 2 Pressure contours for the supersonic expansion test case.

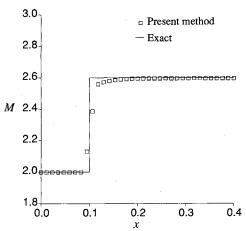
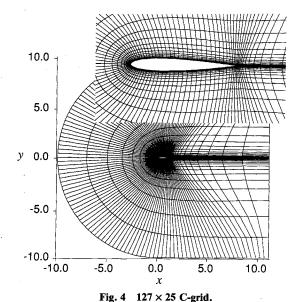


Fig. 3 Mach number distribution along the lower wall.



corner. A uniform 35×35 grid was used, and the upstream Mach number was taken to be 2.0. The pressure contours are shown in Fig. 2, and the Mach number distribution along the wall is shown in Fig. 3.

Airfoil Flow

Figure 4 shows a typical C-grid used in the calculation of the flow about a NACA 0012 section. Two cases were computed: 1) $M_{\infty} = 0.63$, $\alpha = 2$ deg: The predicted pressure distribution on a 127×25 grid, with the far-field boundary at a

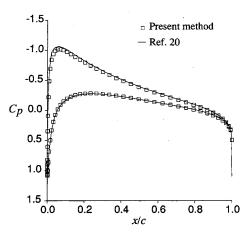


Fig. 5 Pressure distribution over the NACA 0012 section, $M_{\infty} = 0.63$, $\alpha = 2$ deg.

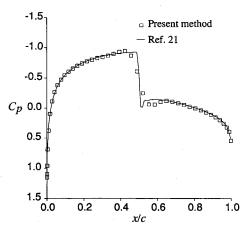


Fig. 6 Pressure distribution over the NACA 0012 section, $M_{\infty} = 0.80$, $\alpha = 0$.

distance of ten chord lengths from the airfoil, is compared to the benchmark calculation of Lock ²⁰ in Fig. 5.

2) $M_{\infty} = 0.80$, $\alpha = 0$: This flowfield is discontinuous and, strictly speaking, the proposed method is not applicable to problems of this type. The errors are, of course, dependent on the strength of the discontinuity. We note here that the averaging procedure detailed in Ref. 15 may be used to construct the entries in the coefficient matrices $B^{(k)}$ in Eq. (17) to produce a scheme that can more accurately capture shocks of weak to moderate strength (but the scheme modified in this way is still not strictly conservative). We show in Fig. 6 that there is fairly good agreement between the pressure prediction according to the present method (on a 127×21 mesh with the far-field boundary at five chord lengths from the airfoil) and the results reported by Pulliam et al. using a conservative scheme (on a 181×33 mesh).²¹

Concluding Remarks

A large number of numerical algorithms for aerodynamic calculations are given a "physical" basis using arguments from the theory of characteristics. It has been our intention to develop a characteristics-based scheme in which the underlying physics is modeled rigorously, while keeping the scheme simple to implement. Toward this goal, we have proposed a scheme in which the characteristic compatibility conditions for arbitrary wave orientations are discretized directly. This leads to an algorithm in which upwinding is accomplished easily and elegantly. We have shown that the method performs well in smooth two-dimensional flows and also gives fairly good results for flows with weak shock waves. The method is, however, nonconservative and therefore cannot be relied upon,

without modification, to "capture" discontinuities accurately. Our present research is aimed toward the removal of this limitation. We note in closing that the proposed method is applicable to any hyperbolic system of equations, and it is uniformly valid for linear wave propagation problems of current interest.

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