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ON THE APPLICATION AND EXTENSION OF HARTEN'S HIGH-RESOLUTION SCHEME

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ABSTRACT

Most first-order upstream conservative differencing methods can capture shocks quite well for one-dimensional problems. A direct application of these first-order methods to two-dimensional problems does not necessarily produce the same type of accuracy unless the shocks are locally aligned with the mesh. Harten has recently developed a second-order high-resolution explicit method for the numerical computation of weak solutions of one-dimensional hyperbolic conservation laws. The main objectives of this paper are (a) to examine the shock resolution of Harten's method for a two-dimensional shock reflection problem, (b) to study the use of a high-resolution scheme as a post-processor to an approximate steady-state solution, and (c) to construct an implicit method in the delta-form using Harten's scheme for the explicit operator and a simplified iteration matrix for the implicit operator.

I. INTRODUCTION

The stability, accuracy and efficiency of a numerical scheme should have a symbiotic relationship with the types of equations that one intends to solve numerically and the methods for treating shocks, contact discontinuities, and numerical boundary conditions. A typical complaint about the application of a scheme that is developed under the guideline of linear theory for the compressible Euler or Navier-Stokes equations is that the resulting scheme is not robust and or not accurate enough. Often the root of the instability and inaccuracy lies in the improper treatment of nonlinear effects [1,2] (shocks and contact discontinuities) and numerical boundary condition procedures [3].

In problems with shocks where conventional second or higher-order accurate central spatial difference methods are used, the resulting numerical solution exhibits overshoots and undershoots in the vicinity of discontinuities [4]. The oscillations not only degrade the accuracy but can cause nonlinear instabilities. One remedy is to add numerical dissipation. Unfortunately, ad hoc methods of adding dissipation generally smear the discontinuities.

This work was motivated by Harten's [5] recent success in developing a high-resolution second-order explicit method for one-dimensional hyperbolic conservation laws which has the following properties:

(a) The scheme is developed in conservation form to ensure that the limit is a weak solution.

(b) The scheme satisfies a proper entropy inequality [1-2] to ensure that the limit solution will have only physically-relevant discontinuities.

(c) The scheme is designed such that the amount of numerical dissipation used produces highly accurate weak solutions.

The goal of this paper is to examine the shock resolution of Harten's method for a two-dimensional gas-dynamic problem, and to investigate other applications of his method including the possible extension to a high-resolution implicit method for both one- and two-dimension problems.

We have applied Harten's method to shock tube [5] and quasi-one-dimensional nozzle problems. Also, we have made a direct application of his method to two-dimensional transient [5] and steady-state gas-dynamic problems. In both one and two dimensions, accurate weak solutions were obtained.

A brief description of a particular version of Harten's method and its extension is given in sections II and III. In section IV, we will describe the two-dimensional implementation of Harten's method by a fractional step method and a modified implicit method. Numerical experiments for quasi-one dimensional nozzle problems and a two-dimensional shock reflection problem are given in sections V and VI.

II. HARTEN'S SCHEME

To aid the development and motivation of the next section, we briefly describe a particular version of Harten's second-order explicit scheme for a one-dimensional system of conservation laws. The reader should refer to the original paper [5] for a more detailed description.

Consider a system of conservation laws of the form

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0 \qquad (1)$$

where U is the vector of m conserved variables and F is the flux vector. The Jacobian matrix $A(U) = \partial F(U)/\partial U$ has real eigenvalues $(\lambda^1, \lambda^2, \ldots, \lambda^m)$ and a complete set of (right) eigenvectors. Let $R = (R^1, R^2, \ldots, R^m)$ be a matrix whose columns are the right eigenvectors of A and let L be a matrix whose rows are the left eigenvectors of A normalized such that $LR = I$.

Let $U_{j+1/2} = V(U_j, U_{j+1})$ denote an average of U_j and U_{j+1}. A simple example is the arithmetic average $U_{j+1/2} = (U_{j+1} + U_j)/2$ (see Roe [6] for a more sophisticated formula for $U_{j+1/2}$ for inviscid gas-dynamic problems). Also let $L_{j+1/2}$ be the matrix L evaluated at $U_{j+1/2}$ i.e.,

$$L_{j+1/2} = L(U_{j+1/2})$$

and

$$\Delta_{j+1/2} U = U_{j+1} - U_j \qquad (2)$$

$$\alpha_{j+1/2} = \begin{pmatrix} \alpha^1_{j+1/2} \\ \alpha^2_{j+1/2} \\ \vdots \\ \alpha^m_{j+1/2} \end{pmatrix} = L_{j+1/2} \cdot (\Delta_{j+1/2} U) \qquad (3)$$

Then Harten's explicit conservative difference scheme can be written as follows:

$$U_j^{n+1} - U_j^n = -\frac{\Delta t}{\Delta x}\left(\hat{F}^n_{j+1/2} - \hat{F}^n_{j-1/2}\right) \tag{4a}$$

with

$$\hat{F}_{j+1/2} = \frac{1}{2}\left[F(U_j) + F(U_{j+1})\right] + \frac{\Delta x}{2\Delta t}\sum_{l=1}^{m}\left[\beta^l_{j+1/2}(g^l_j + g^l_{j+1}) - Q^l\left(\nu^l_{j+1/2} + \beta^l_{j+1/2}\gamma^l_{j+1/2}\right)\alpha^l_{j+1/2}\right] R^l_{j+1/2} \tag{4b}$$

where Δt is the time increment, Δx is the spatial increment, with

$$\beta^l_{j+1/2} = (1 + 2\,\theta^l_{j+1/2}) \tag{4c}$$

and

$$\theta^l_{j+1/2} = \max\left(\theta^l_j, \theta^l_{j+1}\right) \tag{4d}$$

$$\theta^l_j = \left(\left||\alpha^l_{j+1/2}| - |\alpha^l_{j-1/2}|\right|\right) / \left(|\alpha^l_{j+1/2}| + |\alpha^l_{j-1/2}|\right)$$

$$\nu^l_{j+1/2} = \frac{\Delta t}{\Delta x}\lambda^l(U_{j+1/2}) \tag{4e}$$

$$g^l_j = S^l_{j+1/2}\cdot \max\left[0, \min\left(|\tilde{g}^l_{j+1/2}|, \tilde{g}^l_{j-1/2}\cdot S^l_{j+1/2}\right)\right] \tag{4f}$$

$$S^l_{j+1/2} = \mathrm{sign}\left(\tilde{g}^l_{j+1/2}\right) \tag{4g}$$

$$\tilde{g}^l_{j+1/2} = \frac{1}{2}\left[Q^l(\nu^l_{j+1/2}) - (\nu^l_{j+1/2})^2\right]\alpha^l_{j+1/2} \tag{4h}$$

$Q^l(\nu^l_{j+1/2})$ is a function of $\nu^l_{j+1/2}$

$$\gamma^l_{j+1/2} = \begin{cases} (g^l_{j+1} - g^l_j)/\alpha^l_{j+1/2} & \text{if } \alpha^l_{j+1/2} \neq 0 \\ 0 & \text{if } \alpha^l_{j+1/2} = 0 \end{cases} \tag{4i}$$

For a discussion of the choice and properties of the function $Q(\nu)$, the reader should refer to Harten's original paper. Two choices of Q that we have investigated are:

(a) $$Q(\nu) = \nu^2 + 1/4 \tag{4j}$$

(b) $$Q(\nu) = \begin{cases} \frac{\nu^2}{4\epsilon} + \epsilon & \nu < 2\epsilon \\ |\nu| & \nu \geq 2\epsilon \end{cases} \tag{4k}$$

ϵ a fixed constant

The last term in equation (4b) is designed in such a way that the approximation satisfies the guidelines listed in the previous section; that is, these are terms which ensure that a true physical weak solution can be obtained with high accuracy.

We can view this conservative differencing as a form of the second-order accurate Lax-Wendroff scheme plus an additional term. The global accuracy of this scheme is second-order and it is a nonlinear differencing scheme even if the Jacobian A is a constant matrix. In addition, Harten's method, like Lax-Wendroff, has a steady-state dependence on Δt.

III. EXTENSIONS

It is well-known that the time step of conventional explicit schemes are limited by a CFL number of order one and result in long computation times for "stiff" problems or for steady-state calculations. For stiff problems we would like to retain Harten's high resolution feature but modify the scheme to be implicit. For steady-state calculations, we consider the following ways of incorporating high-resolution schemes:

(a) Compute an approximate steady-state solution by some efficient scheme (explicit, implicit or a mixture of the two) and then apply an explicit high-resolution scheme like Harten's as a post-processor.

(b) Modify an implicit scheme in delta form [7], where the iteration matrix on the left-hand side is a simple modification of the original implicit operator, while the right-hand side is the appropriate representation of the explicit high-resolution scheme.

(c) Develop a fully implicit version of the high-resolution method with a proper linearization for the implicit operator.

One-Dimensional Problem:

Preliminary numerical experiments with techniques (a) and (b) for the quasi-one-dimensional nozzle problems showed encouraging results (see section V for details). However, preliminary analysis of technique (c) shows that Harten's scheme is highly nonlinear and special techniques need to be developed for a fully implicit efficient implementation; therefore, technique (c) will not be discussed further in this paper. Here we will describe technique (b) for the one-dimensional problems.

For simplicity, consider the class of implicit linear one-step time differencing in a noniterative delta-form [8] for the system of conservative laws(1)

$$\left(I + \theta\Delta t \frac{\partial}{\partial x} A^n\right)\Delta U^n = -\Delta t\left(\frac{\partial F}{\partial x}\right)^n \tag{5}$$

where $\Delta U^n = U^{n+1} - U^n$ and should not be confused with $\Delta_{j+1/2} U$ defined in equation (2). If $\theta = 1/2$, the time differencing method is the trapezoidal formula and if $\theta = 1$, the time differencing method is backward Euler. There is no connection between the "θ" in equation (5) with the "θ_j" in equation (4d). For the spatial differencing, three-point central differencing or upstream differencing is commonly used. The simplest implicit extension of Harten's method is to replace the right-hand side of (5) by the right-hand side of equation (4a). Some modification of the left-hand side of (5) can also be made. For comparison, this differencing of the spatial derivative can be viewed as three-point central differencing plus some "appropriate" numerical dissipation, implicit on the left-hand side, explicit on the right-hand side. This method will be called the "modified implicit method".

For a steady-state calculation, the right-hand side differencing determines the solution. We can keep the left-hand side the way it is or (to improve convergence) add a scalar dissipation term [9] to the left-hand side; e.g.,

$$\frac{\partial(A^n\Delta U^n)}{\partial x} = \frac{A^n_{j+1}\Delta U^n_{j+1} - A^n_{j-1}\Delta U^n_{j-1}}{2\Delta x} + \frac{\xi^n_{j+1}\Delta U^n_{j+1} - 2\xi^n_j\Delta U^n_j + \xi^n_{j-1}\Delta U^n_{j-1}}{2\Delta x} \tag{6}$$

with $\xi_j^n = \max\left\{|\lambda_j^1|, |\lambda_j^2|, \cdots, |\lambda_j^m|\right\}$. A constant version of the scalar dissipation term of equation (6) is obtained by setting ξ_j^n = constant for all j and n. This form of dissipation is sometimes called second-order implicit numerical dissipation.

Two-Dimensional Problem:

Although, Harten's scheme was developed for one-dimensional problems, the scheme can be implemented in two spatial dimensions by applying a Strang type sequence of fractional step (time splitting) [10]. Again, numerical experiments for the two dimensional shock reflection problem show that the technique described in (a) is applicable.

The extension of technique (b) in two dimensions is not straightforward. It is well-known that fractional step methods have the property that the steady-state (if one exists) depends on Δt even if the original one-dimensional version of the scheme does not depend on Δt. For explicit methods, a fractional step procedure does not introduce a serious error. However, if one could take a large time-step by making the method implicit, then the steady-state accuracy will be degraded. In general, the steady-state dependence on Δt for implicit methods can be avoided by using an alternating direction implicit method. Recall that Harten's one-dimensional scheme has an inherent dependence on Δt in the steady-state. Consequently, technique (b) will also have a steady-state dependence on Δt even if we use the alternating direction implicit method. This dilemma is the subject of further investigation. For the purpose of this paper, a preliminary version of technique (b) in two space dimensions is called the "modified implicit method. In the next section, we will describe the implementation of Harten's method and the modified implicit method for the two-dimensional inviscid compressible (Euler) equations of gas dynamics.

IV. APPLICATION OF HARTEN'S METHOD TO TWO-DIMENSIONAL EQUATIONS OF GAS DYNAMICS

In two spatial dimensions, the inviscid compressible equations of gas dynamics can be written in conservative form as

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = 0 \qquad (7)$$

where

$$U = \begin{pmatrix} \rho \\ m \\ n \\ e \end{pmatrix}, \quad F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ u(e+p) \end{pmatrix}, \quad G(U) = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ v(e+p) \end{pmatrix} \qquad (8)$$

with $m = \rho u$ and $n = \rho v$. The primitive variables of (8) are density ρ, velocity components u and v, and the pressure p. The total energy per unit volume e is related to p by the equation of state for perfect gas as

$$p = (\gamma - 1)\left[e - \frac{(m^2 + n^2)}{2\rho}\right] \qquad (6)$$

where γ is the ratio of specific heats.

Let A denote the Jacobian matrix $\partial F(U)/\partial U$ whose eigenvalues are $(\lambda^1,\lambda^2,\lambda^3,\lambda^4) = (u-c,u,u+c,u)$, where c is the local speed of sound. The right eigenvectors form the matrix $R_x = (R_x^1, R_x^2, R_x^3, R_x^4)$ given by

$$R_x = \begin{pmatrix} 1 & 1 & 1 & 0 \\ u-c & u & u+c & 0 \\ v & v & v & 1 \\ H-uc & \frac{u^2+v^2}{2} & H+uc & v \end{pmatrix} \tag{10}$$

$$H = \frac{c^2}{\gamma+1} + \frac{u^2+v^2}{2} \tag{11}$$

Let the grid spacing be denoted by Δx and Δy such that $x = j\Delta x$ and $y = k\Delta y$. Using the same notation as in section II, the vector α of equation (3) for the x-direction (omitting the k index) is

$$\begin{Bmatrix} \alpha^1_{j+1/2} \\ \alpha^2_{j+1/2} \\ \alpha^3_{j+1/2} \\ \alpha^4_{j+1/2} \end{Bmatrix} = \begin{Bmatrix} (aa-bb)/2 \\ (\Delta_{j+1/2}\rho) - aa \\ (aa+bb)/2 \\ (\Delta_{j+1/2}n) - v_{j+1/2}(\Delta_{j+1/2}\rho) \end{Bmatrix} \tag{12}$$

where
$$aa = \frac{(\gamma-1)}{c^2_{j+1/2}}\left[(\Delta_{j+1/2}e) + \frac{(u^2_{j+1/2}+v^2_{j+1/2})}{2}(\Delta_{j+1/2}\rho) - u_{j+1/2}(\Delta_{j+1/2}m) - v_{j+1/2}(\Delta_{j+1/2}n)\right]$$

$$bb = \left[(\Delta_{j+1/2}m) - u_{j+1/2}(\Delta_{j+1/2}\rho)\right]/c_{j+1/2}$$

Similarly, let B denote the Jacobian matrix $\partial G(U)/\partial U$ whose eigenvalues are $(\lambda^1,\lambda^2,\lambda^3,\lambda^4) = (v-c, v, v+c, v)$. The right eigenvectors form the matrix $R_y = (R_y^1, R_y^2, R_y^3, R_y^4)$ given by

$$R_y = \begin{pmatrix} 1 & 1 & 1 & 0 \\ u & u & u & 1 \\ v-c & v & v+c & 0 \\ H-vc & \frac{u^2+v^2}{2} & H+vc & u \end{pmatrix} \tag{13}$$

The vector α for the y-direction (omitting j index) is

$$\begin{Bmatrix} \alpha^1_{k+1/2} \\ \alpha^2_{k+1/2} \\ \alpha^3_{k+1/2} \\ \alpha^4_{k+1/2} \end{Bmatrix} = \begin{Bmatrix} (cc-dd)/2 \\ (\Delta_{k+1/2}\rho) - cc \\ (cc+dd)/2 \\ (\Delta_{k+1/2}m) - u_{k+1/2}(\Delta_{k+1/2}\rho) \end{Bmatrix} \tag{14}$$

where

$$cc = \frac{(\gamma-1)}{C^2_{k+1/2}}\left[(\Delta_{k+1/2}e) + \frac{(u^2_{k+1/2}+v^2_{k+1/2})}{2}(\Delta_{k+1/2}\rho) - u_{k+1/2}(\Delta_{k+1/2}m) - v_{k+1/2}(\Delta_{k+1/2}n)\right]$$

$$dd = \left[(\Delta_{k+1/2}n) - v_{k+1/2}(\Delta_{k+1/2}\rho)\right] / C_{k+1/2}$$

As mentioned previously, the simpliest form of $U_{j+1/2,k}$ is

$$U_{j+1/2,k} = \left(U_{j+1,k} + U_{j,k} \right)/2 \tag{15}$$

Roe in [6] uses a special form of averaging that has the computational advantage of perfectly resolving stationary discontinuities (for one-dimension). Roe's averaging takes the following form:

$$\left.\begin{aligned}
u_{j+1/2,k} &= \left(D\, u_{j+1,k} + u_{j,k} \right) / (D+1) \\
H_{j+1/2,k} &= \left(D\, H_{j+1,k} + H_{j,k} \right) / (D+1) \\
c^2_{j+1/2,k} &= (\gamma - 1)\left[H_{j+1/2,k} - \left(u^2_{j+1/2,k} + v^2_{j+1/2,k} \right)/2 \right] \\
D &= \sqrt{\rho_{j+1,k}/\rho_{j,k}} \\
H &= \frac{\gamma p}{(\gamma-1)\rho} + \frac{1}{2}\left(u^2 + v^2 \right)
\end{aligned}\right\} \tag{16}$$

In all the computational results presented in this paper, we used Roe's averaging.

Fractional Step Method:

Harten's explicit method can be conveniently implemented in two space dimensions by the method of fractional steps with h = Δt as follows:

$$U^*_{j,k} = U^n_{j,k} - \frac{h/2}{\Delta x}\left(\hat{F}^n_{j+1/2,k} - \hat{F}^n_{j-1/2,k} \right) = \mathcal{L}^{h/2}_x U^n_{j,k} \tag{17}$$

$$U^{n+1}_{j,k} = U^*_{j,k} - \frac{h/2}{\Delta y}\left(\hat{G}^*_{j,k+1/2} - \hat{G}^*_{j,k-1/2} \right) = \mathcal{L}^{h/2}_y U^*_{j,k} \tag{18}$$

that is

$$U^{n+1}_{j,k} = \mathcal{L}^{\Delta t/2}_{y}\,\mathcal{L}^{\Delta t/2}_{x}\,U^{n}_{j,k}$$

where

$$\hat{F}_{j+1/2,k} = \frac{1}{2}\left[F(U_{j,k}) + F(U_{j+1,k})\right] + \frac{\Delta x}{\Delta t}\sum_{l=1}^{4}\left[\beta^{l}_{j+1/2}(g^{l}_{j}+g^{l}_{j+1}) - Q^{l}(\nu^{l}_{j+1/2}+\beta^{l}_{j+1/2}\gamma^{l}_{j+1/2})\alpha^{l}_{j+1/2}\right]R^{l}_{j+1/2} \tag{19}$$

$$\hat{G}_{j,k+1/2} = \frac{1}{2}\left[G(U_{j,k}) + G(U_{j,k+1})\right] + \frac{\Delta y}{\Delta t}\sum_{l=1}^{4}\left[\beta^{l}_{k+1/2}(g^{l}_{k}+g^{l}_{k+1}) - Q^{l}(\nu^{l}_{k+1/2}+\beta^{l}_{k+1/2}\gamma^{l}_{k+1/2})\alpha^{l}_{k+1/2}\right]R^{l}_{k+1/2} \tag{20}$$

Here, it is understood that the scalar values and the vector R^{l} in the summations in equations (19) and (20) are values of (4c-4k) evaluated at the corresponding x-coordinate by using equations (10-12) and at the y-coordinate by using equations (11,13,14). We use the subscripts j for x and k for y for the indexing of the computational mesh. Recall, for simplicity, that we omitted the k index in equation (12) and omitted the j index in equation (14).

In order to retain the original second-order time accuracy of the method, we use a Strang type of fractional step operators, namely

$$U^{n+2}_{j,k} = \mathcal{L}^{\Delta t/2}_{x}\,\mathcal{L}^{\Delta t/2}_{y}\,\mathcal{L}^{\Delta t/2}_{y}\,\mathcal{L}^{\Delta t/2}_{x}\,U^{n}_{j,k} \tag{21}$$

or

$$U_{j,k}^{n+2} = (\mathcal{L}_x^{1/2}\mathcal{L}_y^{1/2}\mathcal{L}_y^{1/2}\mathcal{L}_x^{1/2})(\mathcal{L}_x^{1/2}\mathcal{L}_y^{1/2}\mathcal{L}_y^{1/2}\mathcal{L}_x^{1/2}) \cdots (\mathcal{L}_x^{1/2}\mathcal{L}_y^{1/2}\mathcal{L}_y^{1/2}\mathcal{L}_x^{1/2}) U_{j,k}^{0} \tag{22}$$

We will call equation (21) the half-step fractional step method. For steady-state calculations, the intermediate steps of equation (22) are just a part of the iteration procedure. Therefore if we handle the boundary data for the intermediate steps correctly, we can combine the adjacent $\mathcal{L}_x^{1/2}\mathcal{L}_x^{1/2}$ operators into $\mathcal{L}_x^{1}$ and the adjacent $\mathcal{L}_y^{1/2}\mathcal{L}_y^{1/2}$ operators into $\mathcal{L}_y^{1}$. The half-step operators need only be applied at the first and last iterations, i.e.

$$U_{j,k}^{n+2} = \mathcal{L}_x^{1/2}\mathcal{L}_y^{1}\mathcal{L}_x^{1}\mathcal{L}_y^{1} \cdots \mathcal{L}_y^{1}\mathcal{L}_x^{1/2} U_{j,k}^{0} \tag{23}$$

We will call equation (23) the full-step fractional step method. Numerical experiments on the shock reflection problem show that equation (22) and (23) give almost identical numerical results and the amount of CPU time required for equation (23) is half that required for equation (22).

<u>Modified Implicit Method for Two Spatial Dimensions</u>:

The two dimensional alternating direction implicit version of (5) is

$$\left(I + \theta\Delta t \frac{\partial}{\partial x} A^n\right)\Delta U^{*} = -\Delta t\left(\frac{\partial F^n}{\partial x} + \frac{\partial G^n}{\partial y}\right) \tag{24}$$

$$\left(I + \theta\Delta t \frac{\partial}{\partial y} B^n\right)\Delta U^{n} = \Delta U^{*} \tag{25}$$

$$U^{n+1} = U^n + \Delta U^n \tag{26}$$

The modified implicit method is obtained by replacing $F_x^n + G_y^n$ on the right-hand side of (24) by

$$\frac{1}{\Delta x}\left(\hat{F}^n_{j+1/2,k} - \hat{F}^n_{j-1/2,k}\right) + \frac{1}{\Delta y}\left(\hat{G}^n_{j,k+1/2} - \hat{G}^n_{j,k-1/2}\right) \tag{27}$$

where $\hat{F}$ and $\hat{G}$ are given by (19) and (20), and the left-hand sides of (24) and (25) are replaced by the appropriate analogues of (6).

V. NUMERICAL RESULTS FOR QUASI-ONE-DIMENSIONAL NOZZLE PROBLEM

A detailed implementation of Harten's method for the one-dimensional inviscid compressible equations of gas dynamics can be found in Harten's original paper [5]. Here, we will only describe some of our numerical results. For the numerical experiments, we chose the quasi-one-dimensional nozzle problem with two nozzle shapes (divergent and convergent-divergent). In all of the calculations the computational domain was $0 \leqslant x \leqslant 10$. Two mesh spacing were considered for the divergent nozzle; $\Delta x = 0.5$ and $\Delta x = 0.2$. The mesh spacing for the convergent-divergent nozzle was $\Delta x = 0.2$.

<u>Analytical Boundary Conditions</u>:

We specified all three primitive variables ρ, u and p for the supersonic inflow case, the two primitive variables ρ and p for the subsonic inflow case, and the variable p for the subsonic outflow case.

Numerical Boundary conditions:

We use first-order space extrapolation for the outgoing characteristic variables [11] to obtain the numerical boundary conditions for the unknown flow variables at the boundaries. Since Harten's scheme is a five-point scheme in space, we also need the values of g_j and θ_j on both boundaries. For convenience, we will use zeroth-order space extrapolation for these values.

The Form of Q and $U_{j+1/2}$:

In all of the numerical experiments for the one-dimensional test problems, we use equations (4j) or (4k) for the representation of the Q function and Roe's formula for the evaluation of $U_{j+1/2}$. Numerical experiments show that the two forms of the Q function have little effect on the steady-state numerical results of these test problems.

Initial Conditions:

We use linear interpolation between the exact steady-state boundary values as initial conditions.

Discussion of Results:

To illustrate the shock-capturing capabilities of Harten's method and the modified implicit method, we compare in figures (1) and (2) the computed results with the first-order flux-vector splitting scheme [9], and a conventional implicit method (5) using three-point central spatial differencing with an added fourth-order explicit numerical dissipation [8]. From the results, we can see a definite improvement in shock resolution by Harten's scheme and the modified implicit method, especially for the coarse mesh spacing.

To demonstrate the advantage of using Harten's method as a fine tuning process for the conventional implicit scheme, we plot in figure (3a) a more difficult flow solution with the conventional implicit scheme as a pre-processor to obtain the steady-state solution. The undershoot and overshoot near the shock are typical of the three-point central spatial scheme. Figure (3b) shows the improvement of the solution after we applied Harten's scheme as the post-processor. Figure (4) also shows the solution improvement after we applied Harten's scheme as the post-processor for the solution illustrated in figure (1d). Note that it took approximately 700 steps for Harten's method alone as opposed to 50 steps of the implicit flux-vector splitting method plus 40 steps of Harten's method to converge to the steady-state solution. Figures (3-4) illustrate how well the method can capture the shock, especially for the more sensitive subsonic inflow, subsonic outflow case. In all of the above test problems (except for Harten's method), we used the backward Euler method as the time differencing.

VI. NUMERICAL COMPUTATION OF TWO-DIMENSIONAL SHOCK REFLECTION PROBLEM

Various first-order upstream conservative differencing methods have been developed for systems of one-dimensional hyperbolic conservation laws [6,9,12-14]. When these methods are applied to the one-dimensional inviscid equations of gas dynamics, most of the methods capture shocks very well. However, a direct application of these methods to problems in two-dimensions does not necessarily produce the same type of high resolution near shocks unless the shocks are aligned with one of the computational coordinates. This is due to the fact that first-order methods are generally not adequate to solve a complicated flow field accurately except on a very fine mesh. On the other hand higher-order extensions of these first-order upstream methods are usually rather complicated to use (see for example, van Leer [15]). Harten's method is less complicated than other recently proposed second-order high-resolution methods; however, it was developed for one-dimensional problems.

In order to see how well Harten's method and the modified implicit method can capture shocks for two-dimensional inviscid gas-dynamic problems, we consider a simple inviscid flow field developed by a shock wave reflecting from a rigid surface (fig. 5). The steady-state solution can be calculated exactly and thus can aid us in evaluating the quality of the numerical method. Figure 5 shows the indexing of the computational mesh.

Analytical Boundary Conditions:

The boundary conditions are given as follows: (a) supersonic inflow at $j = 1$, $k = 1,\ldots,K$ which allows the values $U_{1,k}$ to be fixed at freestream conditions; (b) prescribed fixed values of $U_{j,k}$ at $k = K$, $j = 1,\ldots,J$ which produce the desired shock strength and shock angle; (c) supersonic outflow at $j = J$, $k = 1,\ldots,K$; (d) a rigid flat surface at $k = 1$, $j = 1,\ldots,J$ which can be shown to be properly represented by the condition $v = 0$, with the additional condition $\partial p/\partial y = 0$ at $k = 1$ from the normal y-momentum equation.

Initial Conditions:

Initially, the entire flow field is set equal to the freestream supersonic inflow values plus the analytical boundary conditions as described above.

Numerical Boundary Conditions [11]:

The supersonic outflow values $U_{J,k}$, $k = 1,\ldots,K-1$ are obtained by zeroth-order extrapolations, i.e.,

$$U_{J,k} = U_{J-1,k}, \qquad k = 1,\ldots,K-1 \qquad (28)$$

The values of $\rho_{j,1}$, $m_{j,1}$ on the rigid surface with $j = 1,\ldots,J$ are also obtained by zeroth-order extrapolations, i.e.

$$\left.\begin{array}{l} \rho_{j,1} = \rho_{j,2} \\ m_{j,1} = m_{j,2} \end{array}\right. \qquad j = 1,\ldots,J \qquad (29)$$

Three different methods were used in approximating $\partial p/\partial y = 0$ to get $e_{j,1}$, $j = 1,\ldots,J$

(a) normal derivative of e equal to zero (first-order)

$$e_{j,1} = e_{j,2} \tag{30a}$$

(b) normal derivative of e equal to zero (second-order)

$$e_{j,1} = (4e_{j,2} - e_{j,3})/3 \tag{30b}$$

(c) normal derivative of p equal to zero (second-order)

$$p_{j,1} = (4p_{j,2} - p_{j,3})/3 \tag{30c}$$

$$e_{j,1} = p_{j,1}/(\gamma - 1) + m_{j,1}/(2\rho_{j,1}) \tag{30d}$$

Equation (30a) together with equation (29) is an approximation to $p_{j,1} = p_{j,2}$; i.e., a first-order approximation for the normal derivative of p equal to zero. Equation (30b) together with equation (29) is an approximation to equation (30c). We use equations (30a) or (30b) for the implicit methods mainly because of their ease of application with implicit numerical boundary conditions. From the numerical experiments, we found that equation (30b) or (30d) produce better numerical solutions near the wall than equation (30a).

Since Harten's scheme is a 5-point scheme (in each spatial direction), we also need the values of $g_{1,k}$, $g_{J,k}$, $g_{j,1}$, $g_{j,K}$, $\theta_{1,k}$, $\theta_{J,k}$, $\theta_{j,1}$, $\theta_{j,K}$, for j = 1,...,J or k = 1,...,K. For convenience, we will set

$$\begin{aligned} g_{1,k} &= g_{2,k}, & \theta_{1,k} &= \theta_{2,k} \\ g_{J,k} &= g_{J-1,k}, & \theta_{J,k} &= \theta_{J-1,k} \\ g_{j,1} &= g_{j,2}, & \theta_{j,1} &= \theta_{j,2} \\ g_{j,K} &= g_{j,K-1}, & \theta_{j,K} &= \theta_{j,K-1} \end{aligned} \tag{31}$$

The Form of Q and $U_{j+1/2,k}$:

In all of the numerical experiments for the shock reflection problem, we use equation (4j) for the representation of the Q function and equation (16), (Roe's formula) for the evaluation of $U_{j+1/2,k}$.

Boundary Data for the Intermediate Steps:

When fractional steps are used for the two-dimensional problems, there are intermediate boundary data which are not required for non-fractional step and alternating direction implicit methods. For example, in order to advance from equation (17) (the $\mathcal{L}_x^{1/2}$ operator) to equation (18) (the $\mathcal{L}_y^{1/2}$ operator), we need values of $U^*_{j,1}$ for j = 1,...,J. Since we are solving for steady-state solutions, we set $v^*_{j,1} = 0 = v^n_{j,1}$ at the rigid surface, and $U^*_{j,K}$ j = 1,...,J equal to the precribed boundary values. For the remaining intermediate boundary data $\rho^*_{j,1}$, $m^*_{j,1}$ and $e^*_{j,1}$, we use equation (17) to solve for the values. The reason is that we know the values of the entire flow field at level n. Therefore we can advance to the next step by equation (18), and update the numerical boundary conditions by equations (28-30). We can repeat the process by using the sequence indicated in equation (22).

For the full-step fractional step method, every step is an intermediate step. The process is as follows:

step 1: the $\mathcal{L}_x^{1/2}$ operator

$$U^*_{j,k} = U^n_{j,k} - \frac{\Delta t}{2\Delta x}\left(\hat{F}^o_{j+1/2,k} - \hat{F}^o_{j-1/2,k}\right) \tag{32}$$

where $\hat{F}^{o}_{j+1/2,k}$ is the value of F evaluated at the initial value of $U_{j+1/2,k}$.

step 2: the $\mathcal{L}_y^h$ operator

$$U^{**}_{j,k} = U^{*}_{j,k} - \frac{\Delta t}{\Delta y}\left(\hat{G}^{*}_{j,k+1/2} - \hat{G}^{*}_{j,k-1/2}\right) \qquad (33)$$

step 3: the $\mathcal{L}_x^h$ operator

$$U^{***}_{j,k} = U^{**}_{j,k} - \frac{\Delta t}{\Delta x}\left(\hat{F}^{**}_{j+1/2,k} - \hat{F}^{**}_{j-1/2,k}\right) \qquad (34)$$

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Thus, we can start out by setting the intermediate values of $v^{*}_{j,1}$, $\rho^{*}_{j,1}$, $m^{*}_{j,1}$, $e^{*}_{j,1}$, $U^{*}_{j,K}$, $j = 1,\ldots,J$ the same way as the half-step method at step 1 ($\mathcal{L}_x^{1/2}$ operator). The reason is that we know the values of the entire flow field by the initial conditions and the analytical boundary conditions. Therefore we can advance to the next step by equation (33). After the values of $U^{**}_{j,k}$, $k = 1,\ldots,K$ and $j = 2,\ldots,J$ are calculated, we use the precribed values at the inflow as $U^{*}_{1,k}$ and equation (28) as $U^{*}_{J,k}$ in equation (33) to solve for $U^{**}_{1,k}$ and $U^{**}_{J,k}$. At this stage step 2 ($\mathcal{L}_y^h$ operator) is finished and we can apply similar process to step 3 ($\mathcal{L}_x^h$ operator). We can repeat the process by using the sequence shown in equation (23).

<u>Modified Implicit Method:</u>

Recall we use of the term "modified implicit method" to denote the algorithm obtained by applying technique (b) of section III to equation (7) (i.e., by the alternating direction method as described at the end of section IV). A fully implicit form of the Harten's method results in a more complicated solution inversion procedure. Work is underway to develop a proper linearization procedure. Here we only study the applicability of the less complicated iteration matrix as the implicit operator.

Other Numerical Methods:

We choose four methods for comparison with Harten's method and the modified implicit method: (a) a first-order explicit method of Roe [6], (b) the first- and second-order flux-vector splitting method [9], (c) the explicit-implicit MacCormack's method (finite volume) [16], and (d) a conventional implicit method with three-point central differencing in space and a fourth-order explicit numerical dissipation term [8]. In the calculations with the implicit methods (except MacCormack's method), we use the backward Euler for the time differencing.

Discussion of Results:

The main purpose of the two-dimensional numerical experiments is to evaluate the shock resolution of Harten's method and the modified implicit method. Convergence rate and computational efficiency will be investigated and reported elsewhere. We expect that techniques (b) and (c) proposed in section III will speed up convergence for subsonic (dominated) steady-state problems.

In all of the numerical experiments, the incident shock angle ψ was 29° and the freestream Mach number M_{∞} was 2.9. The computational domain was $0 \leqslant x \leqslant 4.1$, and $0 \leqslant y \leqslant 1$, and the grid size was 61X21. The appropriate analytical boundary conditions are applied along the boundaries of the domain. Only pressure contour and pressure coefficients will be illustrated. Here, the pressure coefficient is defined as $c_p = \frac{2}{\gamma M_{\infty}^2}\left(\frac{p}{p_{\infty}} - 1\right)$ with p_{∞} the freestream pressure. The exact minimum pressure corresponding to $\psi = 29^{\circ}$ and $M_{\infty} = 2.9$ is 0.714286 and the exact maximum pressure is 2.93398 (see Fig. 6). Forty-one pressure contour levels between the values of 0 and 4 with uniform increment 0.1 were used for the contour plots. The pressure coefficient was evaluated at $y = 0.5$ for $0 \leqslant x \leqslant 4.1$.

The exact pressure solution is shown in figure 6. Pressure contours and the pressure coefficient evaluated at $y = 0.5$ are shown in figure 7 for seven different methods. Both the first-order explicit method of Roe and the implicit first-order flux-vector splitting method yield smeared discontinuities as shown in figures (7a) and (7b). The second-order (in space) flux-vector splitting method, the second-order (in space) conventional implicit method, and MacCormack's explicit-implicit method are shown in figures (7c)-(7e). (The results for MacCormack's method were provided by W. Kordulla, National Research Council resident research associate at NASA Ames Research Center.) Harten's method with full-step fractional steps and the modified implicit method are shown in figures (7f) and (7g). These methods show a definite improvement in shock resolution. There are practically no oscillations over the entire flow field. Figure 8 shows the pressure contours of Harten's method by using the half-step fractional step method. The solution is nearly identical to figure (7f) but required half the number of iterations (i.e., half of the step size, double the CPU time). Figure (9a) shows the results after 30 steps of the conventional implicit method. Figure (9b) shows the improvement after we applied 200 steps of Harten's method as post processor. All of the above methods required 15^-600 iterations to converge with CFL numbers ranging from 0.5 to 0.8 (except figure (9a)).

At the present stage of development, the prliminary version of the modified implicit method for two-dimensional problems has several deficiencies. In particular, the implicit operators (left-hand sides of (24) and (25)) are not proper linearizations of the right-hand side. In fact, the linearizations are crude at best, and one would expect that this would have a serious effect on the stability of the method. In addition, Harten's method, like Lax-Wendroff, has a steady-state dependence on Δt. For explicit methods, this does not introduce a serious error. However, if one could take a large time-step by making the method implicit, then the steady-state accuracy is expected to be degraded. Figure 10 shows the pressure contour for the shock reflection problem at a CFL number of 1.2. Even at this modest CFL value, the accuracy is degraded as compared to the same problem run at a CFL number of 0.5 shown in figure 7g.

VII. CONCLUSION

The application of Harten's explicit method to quasi-one-dimensional nozzle problems and to a two-dimensional shock reflection problem resulted in high shock-resolution steady-state numerical solutions. By combining the adjacent half-step operators into full-step operators of the fractional step method, one can cut the computation time in half. Applications of the post-processor method and the modified implicit method for steady-state calculations show encouraging results for one-dimensional problems; however, testing in two dimensions is not complete and further investigation is needed for efficient implementation of the implicit method.

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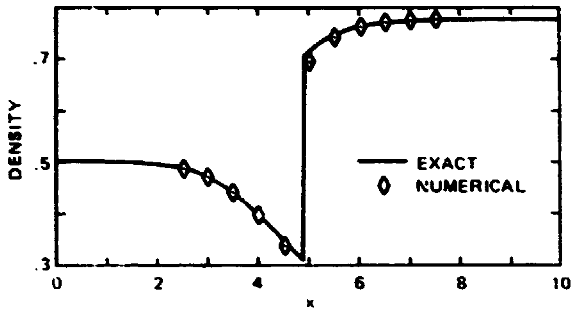
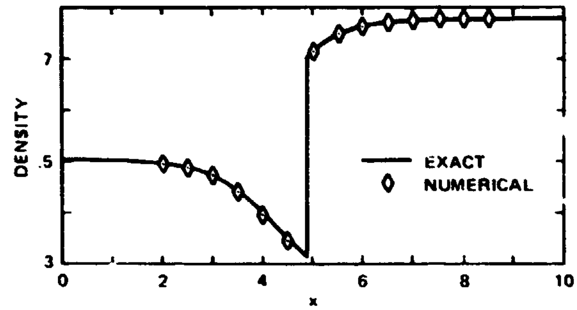
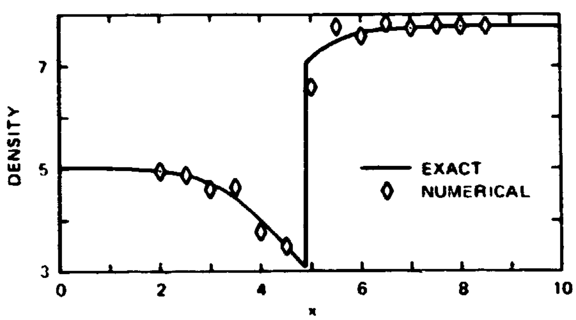


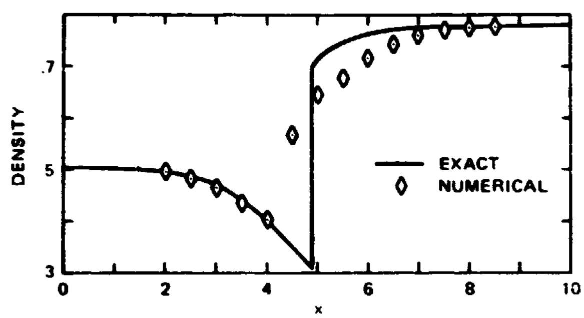
(a) Harten's method (explicit).



(b) Modified implicit method.



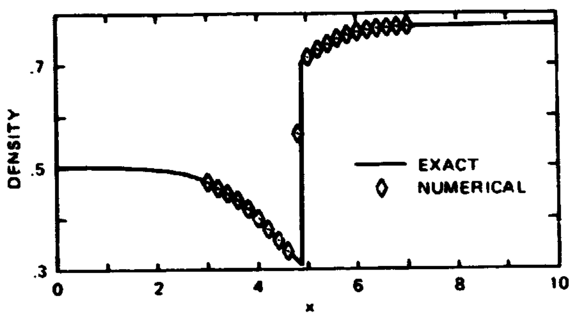
(c) Conventional implicit method.



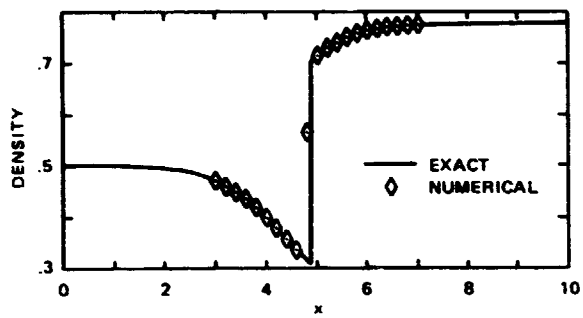
(d) First-order implicit flux-vector splitting method.

Fig. 1 Density distribution: supersonic inflow, subsonic outflow.

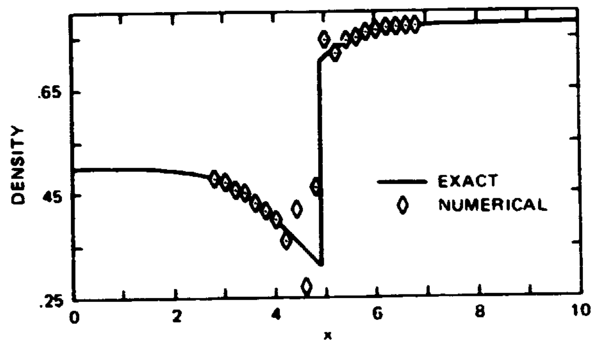
Nozzle shape: ; 20 spatial intervals.



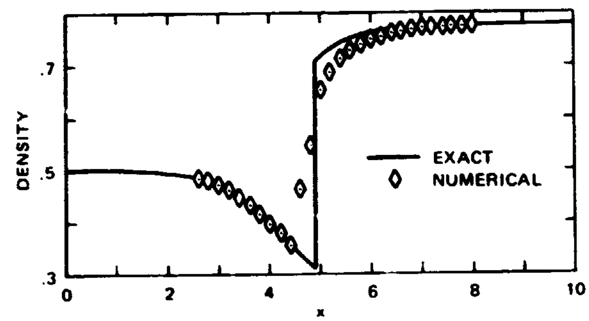
(a) Harten's method (explicit).



(b) Modified implicit method.

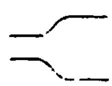


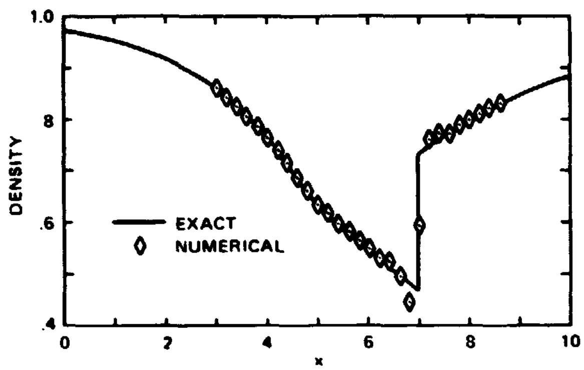
(c) Conventional implicit method.



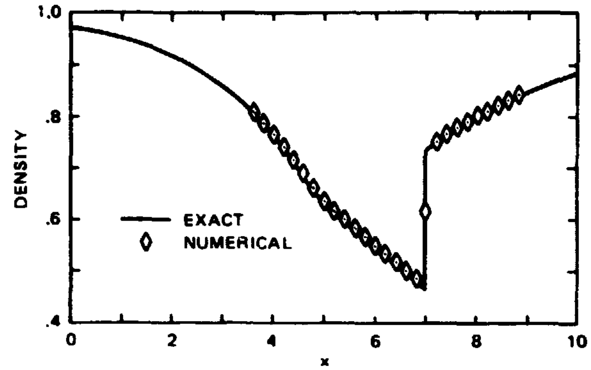
(d) First-order implicit flux-vector splitting method.

Fig. 2 Density distribution: supersonic inflow, subsonic outflow.

Nozzle shape:  ; 50 spatial intervals.



(a) Conventional implicit method.



(b) Harten's method as post-processor.

Fig. 3 Density distribution: subsonic inflow, subsonic outflow.

Nozzle shape:  ; 50 spatial intervals.

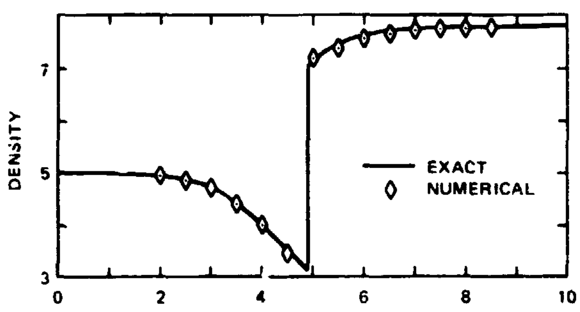


Fig. 4 Density distribution: supersonic inflow, subsonic outflow. Harten's method as post-processor (use the result of fig. (1d) as initial conditions).

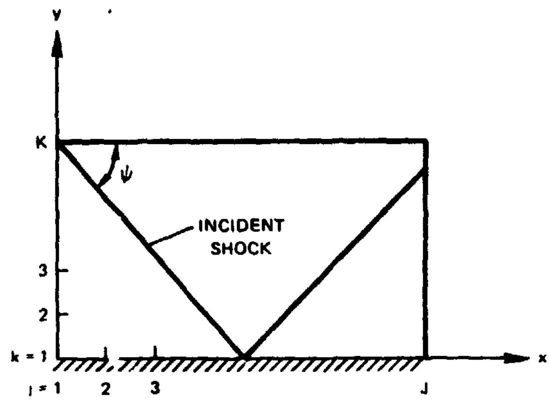


Fig. 5 Indexing of computational mesh for shock reflection problem.

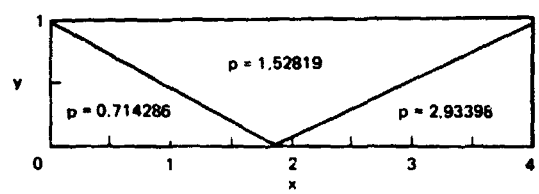
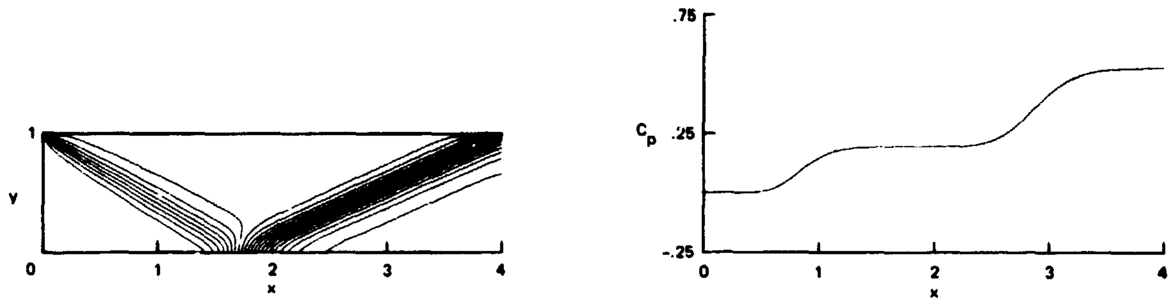
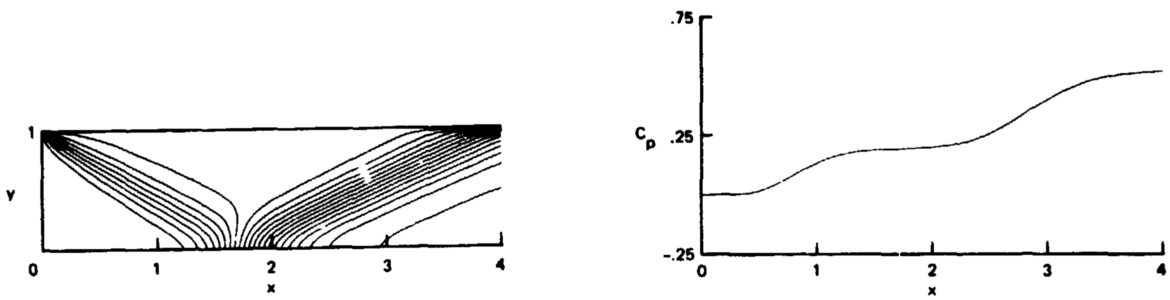


Fig. 6 The exact pressure solution for the shock reflection problem.

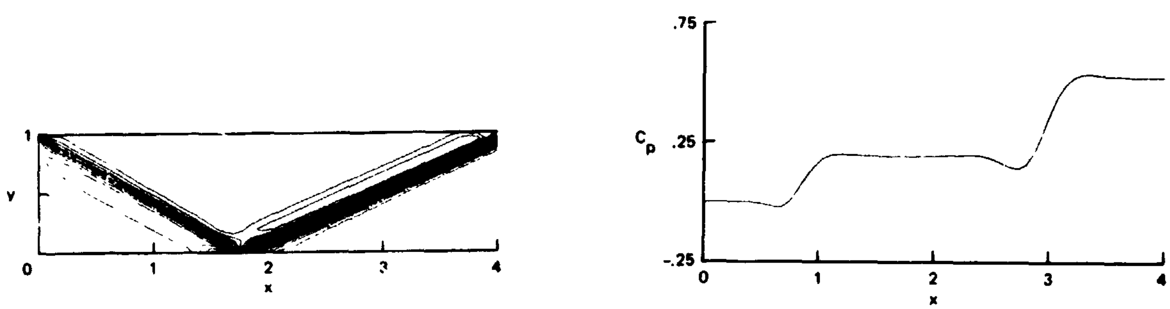
PRESSURE CONTOURS **PRESSURE COEFFICIENT**



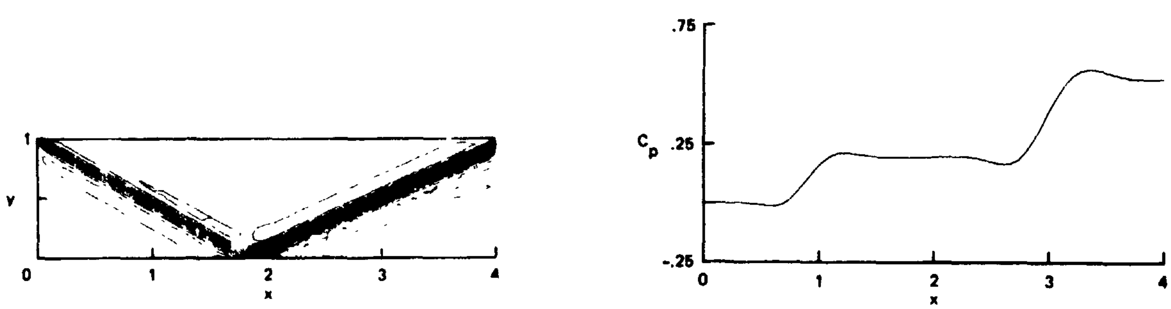
(a) First-order explicit method of Roe.



(b) First-order implicit flux-vector splitting method.



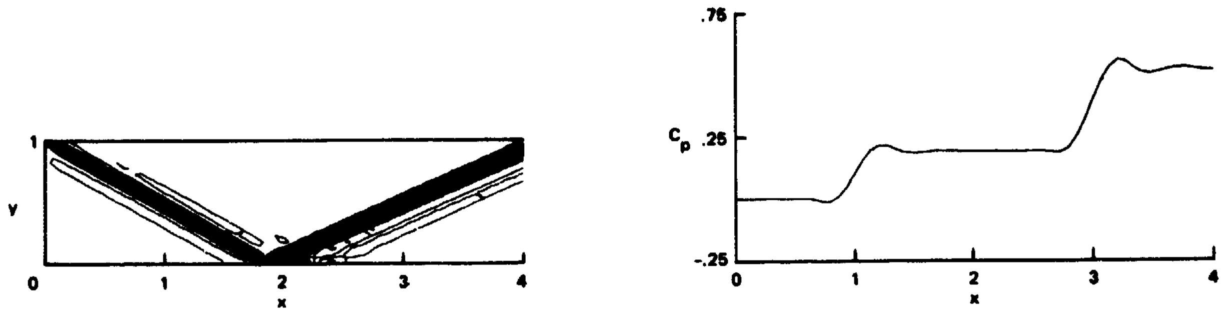
(c) Second-order implicit flux-vector splitting method.



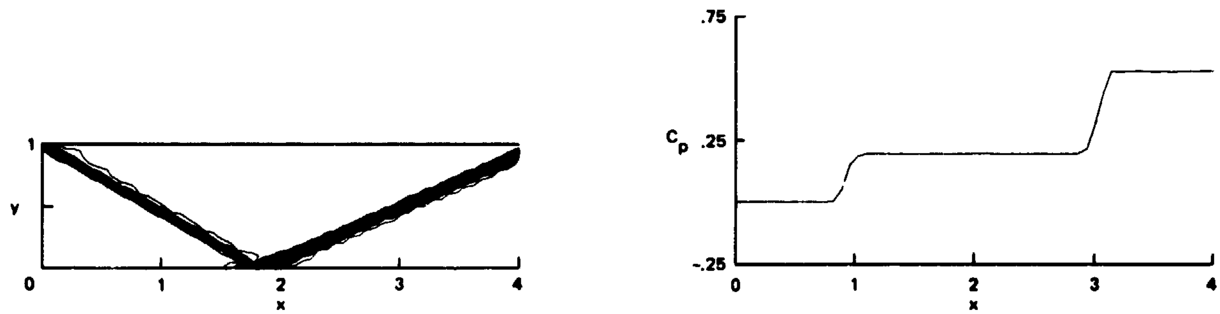
(d) Conventional implicit method.

Fig. 7 Pressure contours and pressure coefficients for the shock reflection problem.

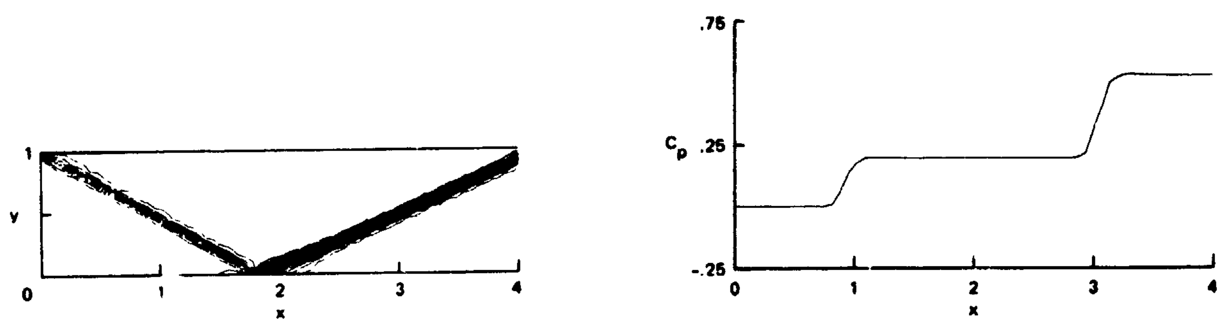
PRESSURE CONTOURS PRESSURE COEFFICIENT



(e) MacCormack's explicit-implicit method.



(f) Harten's method (explicit).



(g) Modified implicit method.

Fig. 7 (continued).

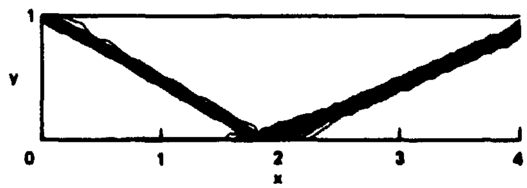
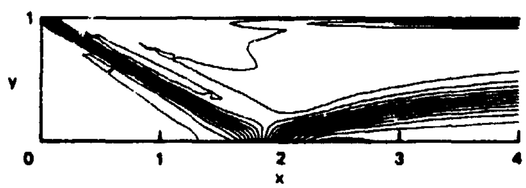
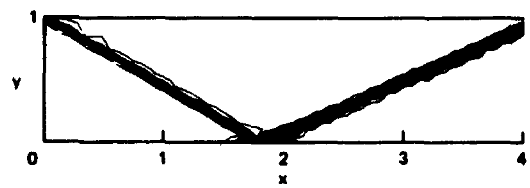


Fig. 8 Pressure Contours: Harten's method (half-step fractional steps).



(a) 30 steps of the conventional implicit method.



(b) 200 steps of Harten's method (use the result of fig. (9a) as initial conditions).

Fig. 9 Pressure Contours: Harten's method as post-processor.

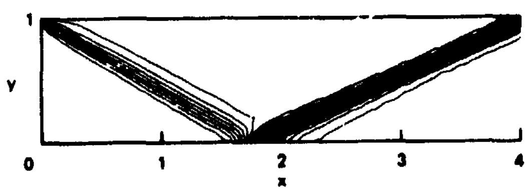


Fig. 10 Pressure Contours: Modified implicit method at CFL = 1.2.

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16. Abstract

Most first-order upstream conservative differencing methods can capture shocks quite well for one-dimensional problems. A direct application of these first-order methods to two-dimensional problems does not necessarily produce the same type of accuracy unless the shocks are locally aligned with the mesh. Harten has recently developed a second-order high-resolution explicit method for the numerical computation of weak solutions of one-dimensional hyperbolic conservation laws. The main objectives of this paper are (a) to examine the shock resolution of Harten's method for a two-dimensional shock reflection problem, (b) to study the use of a high-resolut resolution scheme as a post-processor to an approximate steady-state solution, and (c) to construct an implicit method in the delta-form using Harten's scheme for the explicit operator (right-hand side) and a simplified iteration matrix for the implicit operator (left-hand side).

17. Key Words (Suggested by Author(s))	18. Distribution Statement
Numerical method, Computational fluid dynamics, System of hyperbolic conservation laws, Numerical accuracy, Weak solutions, Shock capturing, Conservative differencing.	Unlimited Subject Category - 64

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