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Gasdynamic Modeling and Computational Accuracy

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The study of the behavior of computational solutions of Burgers' equation at large mesh Reynolds numbers $Re\Delta x$ is extended to a one-dimensional steady-state model gasdynamic system with downstream extrapolation conditions. The oscillations generally present in computed results at large $Re\Delta x$ can be minimized by choosing a particular formally second-order accurate, conservative discretization of the nonlinear terms $(\rho u)_x$ and $(\rho u^2)_x$ in the continuity and momentum equations. This minimally oscillatory solution has small pointwise error even at large $Re\Delta x$. It is seen that smoothness by itself may not guarantee computational accuracy, and that overly refined spatial meshes may lead to large errors. Results from a realistic two-dimensional computation showing some qualitative agreement with the present conclusions are given.

1. INTRODUCTION

This paper extends the analysis of Ref. [1] for Burgers' equation to a one-dimensional steady-state model which is more representative of the gasdynamics equations system. The results of [1] show that for the Burgers finite difference model with fixed boundary values, the oscillations usually observed in computed results at large values of the mesh Reynolds number $Re\Delta x$ [3, 4, 6] can be minimized by choosing an appropriate second-order accurate discretization of the nonlinear term uu_x. This minimally oscillatory solution has very small pointwise error even at large $Re\Delta x$. These results for the fixed boundary value case were extended in [2] to cases with a downstream extrapolation condition. In [2] it was shown additionally how incorrect Hugoniot jumps and large pointwise error can occur if the mesh is overly refined in attempting to obtain "smooth" solutions. This paper generalizes the above results to a system of equations which includes the mass continuity relation and which contains nonlinear terms more complicated than uu_x. Results showing the occurrence of a minimization of oscillations in a two-dimensional computation with the full Navier-Stokes equations are given.

It is stressed that the present model results are essentially nonlinear and deal with the system of difference equations in the practical case of large $Re\Delta x$; the equations are not linearized and the limit $Re\Delta x \to 0$ is not taken. It is also emphasized that this study deals only with a class of difference algorithms that are strictly conservative or

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"summable" in difference form, and is concerned only with solutions in the steady-state (as the large time limit). In this context, time dependence is viewed only as an expedient to proceed from some initial guess to a solution of the steady-state equations.

2. Model Problem

A. *Differential Model*

The one-dimensional steady-state model gasdynamic system considered here is

$$\text{Continuity:} \qquad (\rho u)_x = 0 \tag{1a}$$

$$\text{Momentum:} \qquad (\rho u^2)_x = -p_x + \frac{1}{RE} u_{xx} \tag{1b}$$

$$\text{Energy (and state):} \qquad p = A\rho^r \tag{1c}$$

Here ρ is the density, u the velocity, and p the pressure. All variables have already been suitably nondimensionalized by upstream reference values (indicated by subscript "ref"). The last equation (1c) represents an "integrated" energy equation where $A = (p/\rho u^2)_{\text{ref}}$ is a thermodynamic constant specifying the reference or initial state, and r is the polytropic index representing the thermodynamic processes. Except for this simplified treatment of the energy equation, Eqs. (1) strongly resemble the full system of gasdynamic equations. The fluid flow represented by (1c) is isothermal when $r = 1$, whereas the flow is isentropic or reversible if r equals the ratio of specific heats c_p/c_v. Other values of r allow the model to take approximate account of nonisentropic effects. When the flow is isentropic and the fluid is a perfect gas, A can be identified as $(1/rM^2)$, where M is the flow Mach number. The parameter $RE = (\rho u)_{\text{ref}} L/\mu$ is a Reynolds number based upon the (dimensional) reference density and velocity, a length L equal to half the computational field size, and the coefficient of fluid viscosity μ. The change in notation from "*Re*" in [1] to "*RE*" here emphasizes that the Reynolds number is now based upon the upstream reference velocity, rather than on the velocity jump as for the Burgers' model. The nondimensional computational field is taken to be $-1 \leqslant x \leqslant 1$, and the upstream boundary conditions are taken to be the given nondimensional values

$$u(x = -1) = 1, \rho(x = -1) = 1 \tag{2}$$

The downstream conditions at $x = 1$ remain to be specified.

Within the differential framework, the system (1) can be readily reduced to the single model differential equation

$$u_x + \left[\frac{A}{u^r}\right]_x = \frac{1}{RE} u_{xx} \tag{3}$$

If $r = 1$, the exact solution of (3) is given implicitly as

$$RE(x - x_0) = \ln\left[\frac{(u-1)}{(u-A)^A}\right]^{1/(1-A)} \tag{4}$$

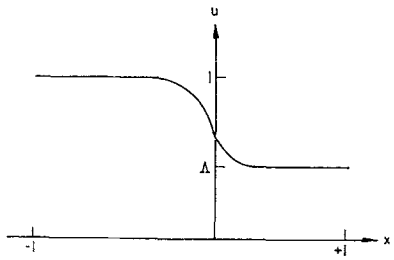

FIG. 1. Differential solution of model problem for $r = 1$.

Assuming that the Reynolds number RE is large, Eq. (4) represents a steep, non-symmetric transition from $u = 1$ to $u = \Lambda$ (Figure 1). Except for the asymmetry, solution (4) behaves very much the same as does the steady solution of Burgers' equation [1].

To obtain the differential "Hugoniot" relation, (3) is integrated once to give

$$u + \frac{\Lambda}{u^r} = \text{constant} = 1 + \Lambda, \tag{5}$$

where the term $(1/RE)\, u_{xx}$ is neglected on the assumption that it is small sufficiently far upstream and downstream of the discontinuity. The constant is evaluated using (2). For the case $r = 1$, one obtains

$$\left(u + \frac{\Lambda}{u}\right)_{x=1} = \left(u + \frac{\Lambda}{u}\right)_{x=-1} = 1 + \Lambda \tag{6}$$

from which it follows that the downstream value is either

$$(u)_{x=1} = 1 \tag{7a}$$

or

$$(u)_{x=1} = \Lambda \tag{7b}$$

Equation (7a) represents the uniform flow solution (which is of no interest here), and (7b) is the specific allowable jump discontinuity. When $r > 1$, the Hugoniot (5) will lead to

$$(u)_{x=1} = 1 \tag{7c}$$

or

$$(u)_{x=1} = \Lambda' > \Lambda \tag{7d}$$

with Λ' being the positive real solution of (5) giving the downstream value after the jump.

B. *Difference Model*

To obtain the model difference equation, the x-coordinate is discretized as $x = j\Delta x\, (j = 0, \pm 1, \pm 2, \ldots, \pm J)$ so that $J\Delta x = 1$, and the mesh functions are taken as

$U_j = U(j\Delta x)$ and $\rho_j = \rho(j\Delta x)$. Employing a second-order accurate conservative difference algorithm analogous to the one used in [1], the difference equations representing system (1) are

$$\left(\frac{2}{2+\gamma_1}\right)\left[\frac{(\rho U)_{j+1} - (\rho U)_{j-1}}{2\,\Delta x}\right] + \left(\frac{\gamma_1}{2+\gamma_1}\right)\left[\frac{\rho_j(U_{j+1} - U_{j-1}) + U_j(\rho_{j+1} - \rho_{j-1})}{2\,\Delta x}\right] = 0 \tag{8}$$

$$\left(\frac{2}{2+\gamma_2}\right)\left[\frac{(\rho U^2)_{j+1} - (\rho U^2)_{j-1}}{2\,\Delta x}\right] + \left(\frac{\gamma_2}{2+\gamma_2}\right)\left[\frac{U_j((\rho U)_{j+1} - (\rho U)_{j-1}) + (\rho U)_j(U_{j+1} - U_{j-1})}{2\,\Delta x}\right] + A\left[\frac{\rho^r_{j+1} - \rho^r_{j-1}}{2\,\Delta x}\right] = \frac{1}{RE}\left[\frac{U_{j+1} - 2U_j + U_{j-1}}{\Delta x^2}\right] \tag{9}$$

Equations (8) and (9) hold for $j = -J+1, -J+2, \ldots, J-2, J-1$. The first two terms in each equation represent weighted averages of centered difference approximations of the (differentially equivalent) divergence and convective forms of the nonlinear terms. (The physical and mathematical implications of conservative differencing are explained in detail in [5], where such differencing of the "convective form", e.g., $\rho u_x + u\rho_x$, is illustrated.) The parameters γ_1 and γ_2 are independent and arbitrary, and difference system (8, 9) is formally second-order accurate and conservative (in the sense of summability without residue) for any choice of these parameters. The choice $\gamma_i = 0$ represents pure divergence form differencing, whereas $\gamma_i = \infty$ represents pure convective form differencing.

The boundary conditions for the present model are

$$U_{-J} = 1,\ \rho_{-J} = 1 \tag{10a,b}$$

$$U_J = U_{J-1},\ \rho_J = \rho_{J-1} \tag{10c,d}$$

where (10c,d) are simple extrapolation conditions employed at the downstream boundary $j = J$. The motivation for (and philosophy of) using such conditions is discussed briefly in section 2C and more thoroughly in [2].

Unlike the differential system, difference system (8, 9) can only be reduced to a single difference equation under special circumstances. This reduction occurs when $\gamma_1 = 0$. Equation (8) then gives

$$(\rho U)_{j+1} = (\rho U)_{j-1} \tag{11}$$

which together with (10) yields

$$(\rho U)_j = \text{constant} = 1. \tag{12}$$

Difference system (8, 9) then becomes

$$(U_{j+1} - U_{j-1}) + \Lambda\left(\frac{1}{U_{j+1}^r} - \frac{1}{U_{j-1}^r}\right) = \frac{2}{RE\,\Delta x}(U_{j+1} - 2U_j + U_{j-1}) \tag{13}$$

which is the appropriate discretized version of the simplified model differential equation (3). It is emphasized that (13) is differencely equivalent to system (8, 9) only when $\gamma_1 = 0$. The parameter $RE\Delta x = [(\rho u)_{\text{ref}} L\Delta x/\mu]$ is a mesh Reynolds number which is based on the upstream reference velocity u_{ref}. It will later be shown that a mesh Reynolds number $Re\Delta x$ based on the physical jump magnitude (as for the Burgers' model) is a more representative computational parameter. In practical computation, $Re\Delta x$ is $O(10)$ or larger.

The difference Hugoniot relation is obtained by summing Eqs. (8) and (9) from $j = -J + 1$ to $j = J - 1$, giving

$$\begin{aligned} &2[(\rho U)_J + (\rho U)_{J-1}] + \gamma_1[\rho_{J-1}U_J + \rho_J U_{J-1}] \\ &\quad = 2[(\rho U)_{-J} + (\rho U)_{-J+1}] + \gamma_1[\rho_{-J+1}U_{-J} + \rho_{-J}U_{-J+1}] \end{aligned} \tag{14}$$

and

$$\begin{aligned} &2[(\rho U^2)_J + (\rho U^2)_{J-1}] + \gamma_2[(\rho_{J-1} + \rho_J)\,U_{J-1}U_J] \\ &\quad + \Lambda(2 + \gamma_2)[\rho_J^r + \rho_{J-1}^r] - \frac{2(2 + \gamma_2)}{RE\,\Delta x}[U_J - U_{J-1}] \\ &= 2[(\rho U^2)_{-J} + (\rho U^2)_{-J+1}] + \gamma_2[(\rho_{-J+1} + \rho_{-J})\,U_{-J+1}U_{-J}] \\ &\quad + \Lambda(2 + \gamma_2)[\rho_{-J}^r + \rho_{-J+1}^r] - \frac{2(2 + \gamma_2)}{RE\,\Delta x}[U_{-J+1} - U_{-J}] \end{aligned} \tag{15}$$

The conservative property of the difference algorithm allows such a summation to be conveniently carried out (the sum is "telescopic"). In the event that the computed upstream and downstream solution is smooth so that

$$\begin{aligned} \rho_{-J} = \rho_{-J+1} = U_{-J} = U_{-J+1} = 1 \\ \rho_J = \rho_{J-1}\,,\ U_J = U_{J-1} \end{aligned} \tag{16}$$

the summed difference relations (14, 15) reduce to

$$U_J + \frac{\Lambda}{U_J^r} = 1 + \Lambda \tag{17}$$

for all choices of γ_1 and γ_2, so that the difference Hugoniot relation (17) is *identical* to the differential Hugoniot (5). Hugoniot relation (17) is, of course, also valid for the simplified difference equation (13) obtained when $\gamma_1 = 0$. Equations (14) and (15) indicate that the correctness of the Hugoniot jump computationally obtained using boundary conditions (10) depends on the smoothness of the computed inlet flow (i.e., on $|\,U_{-J+1} - U_{-J}\,|$ and $|\,\rho_{-J+1} - \rho_{-J}\,|$).

C. *Comments on the Models*

The parameter γ_1 plays an important role in the present difference model. The choice $\gamma_1 = 0$ will enforce strict pointwise equality of mass flow rates, whereas for $\gamma_1 \neq 0$ this pointwise equality is not guaranteed since the conservative differencing serves only to prevent *accumulation* of the local errors, not to eliminate the local error itself. It is noted that the parameter γ_2 disappears when $\gamma_1 = 0$, since the convective term becomes linear. Now the disappearance of the differencing parameter γ_2 may seem unfortunate, since it is precisely the presence of such an arbitrary parameter in the Burgers' model investigated in [1] which allows one to vary the optimal $Re\,\Delta x$ of computation. However, the case $\gamma_1 = 0$ is interesting for other reasons and, as shown later in Section 5, γ_1 and γ_2 can indeed be chosen to obtain such an optimal $Re\,\Delta x$ for coarse mesh computation with the present model.

It is noted that strict divergence form discretization of the mass conservation equation in related two-dimensional models will not result in a similar effective linearization of the nonlinear terms in the momentum equations, so that discretization parameters in those equations will not become ineffective. Moreover, the differencing of the nonlinear term $(\rho u^2)_x$ in the present one-dimensional model can be further generalized by including, in addition to $(\rho u^2)_x = (\rho u)\, u_x + u(\rho u)_x$, the other differentially equivalent form $\rho(u^2)_x + u^2\rho_x$. It is also possible (though awkward) to generalized even further by noting that for any function $f(x), f_x = [(f^{1/2})^2]_x = 2f^{1/2}f_x^{1/2}$ so that the corresponding conservative difference form is

$$f_x \sim \left(\frac{2}{2+\gamma}\right)\left[\frac{f_{j+1} - f_{j-1}}{2\,\Delta x}\right] + \left(\frac{\gamma}{2+\gamma}\right)\left[\frac{2f_j^{1/2}(f_{j+1}^{1/2} - f_{j-1}^{1/2})}{2\,\Delta x}\right] \tag{18}$$

Such differencing could be used for the term $(\rho^r)_x$ in the present model; however, these generalizations are not considered here.

The mesh Reynolds number $RE\,\Delta x$ is a composite parameter which reflects the physical characteristics of the flow $((\rho u)_{\text{ref}}, \mu)$, the computational field size L, and the mesh size Δx. This parameter measures mesh fineness relative to the steepness of the gradient one wishes to compute. Small values of $RE\,\Delta x$ indicate a fine mesh, while large values mean that the mesh is coarse. Note that $RE\,\Delta x$, and not Δx alone, stands as a parameter in the difference equations. Despite this, the value $J = (1/\Delta x)$ still plays a role because difference equations (8, 9) must be satisfied at precisely $2J - 1$ mesh points. However, the computational results as indicated in Ref. [1] become essentially a function of $RE\,\Delta x$ alone for J sufficiently large, and this sufficient value of J ($\sim$10) is ordinarily achieved in practical coarse mesh computations (Ref. [2]).

Some comments on the downstream extrapolation condition (10c, d) are in order. Analogous extrapolation conditions are often used in practical computations, ordinarily when there is reason to believe that some derivative should be "small" when the boundary of the computational field is "sufficiently far away" from the flow features of interest. Using this kind of extrapolation condition involves two approximations; namely, replacing the small derivative with a finite difference set equal to zero, and imposing the approximate boundary specification at a finite (rather

than infinite) distance "downstream." Nevertheless, this procedure is assumed to yield physically reasonable approximate solutions, even if setting the derivative equal to zero at some finite field location in the differential formulation is questionable [2]. The difficulty inherent in such a boundary specification cannot be conveniently avoided by specifying the downstream function value, since this is often an unknown to be determined by the computation. Nor is the problem alleviated by matching the downstream "derivative" to a known asymptotic solution, since the computed values downstream are dominated by the effects of computational oscillations at large $Re\,\Delta x$. Moreover, with downstream extrapolation, the differential formulation could be poorly-posed. In this case, convergence of the difference solution to the solution of the analogous differential problem should *not* be assumed to occur in the limit of vanishingly small mesh size. However, the difference formulation may yield physically reasonable approximations for small but finite (*not* vanishingly small) mesh sizes; it is demonstrated that this can happen.

3. Influence of Thermodynamic Parameters Λ and r

In order to investigate the influence of the thermodynamic parameters Λ and r on the difference solutions, it is assumed that $\gamma_1 = 0$ so that the greatly simplified difference system

$$\begin{cases} (U_{j+1} - U_{j-1}) + \Lambda\left(\dfrac{1}{U_{j+1}^r} - \dfrac{1}{U_{j-1}^r}\right) = \dfrac{2}{RE\,\Delta x}(U_{j+1} - 2U_j + U_{j-1}) \\ \qquad\qquad j = -J+1, -J+2, \ldots, J-2, J-1 \quad (19a) \\ U_{-J} = 1 \quad (19b) \\ U_J = U_{J-1} \quad (19c) \end{cases}$$

can be studied in place of (8, 9). The effect of the parameters γ_1 and γ_2, not present in this simplified model, is discussed in Section 5.

Two families of solutions of system (19) for special values of the mesh Reynolds number $RE\,\Delta x$ are now displayed. They are:

$$\begin{aligned} U_j &= 1 && j = -J, -J+1, \ldots, k-1 \\ &= \frac{U_J + 1}{2} && j = k \\ &= U_J && j = k+1, k+2, \ldots, J-1, J \end{aligned}$$

$$\text{for} \quad RE\,\Delta x = RE^*\,\Delta x = \frac{U_J - 1}{((U_J - 1)/2) - \Lambda\left[1 - \dfrac{1}{((U_J + 1)/2)^r}\right]}$$

$$k = -J+1, -J+2, \ldots, J-2 \quad (20)$$

and

$$\begin{aligned} U_j &= 1 \quad j = -J, -J+1, \ldots, k \\ &= U_J \quad j = k+1, k+2, \ldots, J-1, J \\ &\quad \text{for} \quad RE\,\Delta x = R\hat{E}\,\Delta x = \infty \\ &\quad k = -J, -J+1, \ldots, J-2 \end{aligned} \tag{21}$$

Here U_J is the correct Hugoniot value which is the proper real solution of Hugoniot relation (17) for given values of r and Λ. Solutions (20) and (21) are remarkable in that they accomplish an abrupt jump from the upstream value $U = 1$ to the downstream value $U = U_J$ (in 2 Δx and 1 Δx respectively) without generating any computational oscillations. In this simple model problem, the computed abrupt jump can occur almost anywhere in the computational field, according to the choice of k. Such arbitrariness is essentially due to the translational invariance of the physical problem [2]. Solutions (20) and (21) are shown in Figure 2 for the case $k = J - 2$. It is noted that

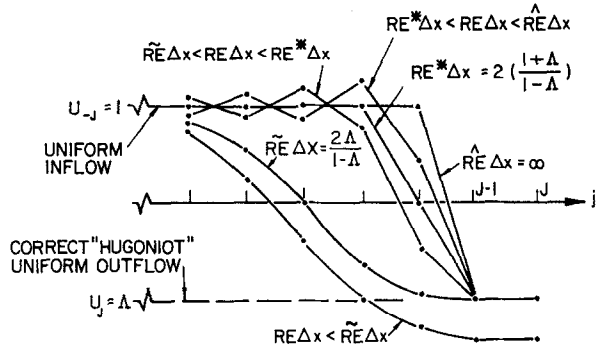

FIG. 2. Difference solutions, $r = 1$.

this abrupt jump solution would also be obtained if the downstream boundary condition at $x = 1$ was the specification of the correct downstream value; thus the existence of an abrupt jump solution is not dependent upon the precise boundary specification.

The difference Hugoniot relation (17) provides a real solution (in addition to the uniform flow value $U_J = 1$) for all positive values of r and Λ in the physical range. Even though not explicitly specified by the extrapolation boundary condition (19c), this computed value is the same as that given by the Hugoniot relation (5) of the differential problem. It thus appears that the detailed thermodynamic processes may not significantly affect the difference behavior provided that the correct values of the parameters r and Λ are adopted. Since the analysis of difference system (19) becomes greatly simplified for $r = 1$, it is desirable to approximate the difference behavior for

$r \neq 1$ by using the $r = 1$ results with some appropriate change in Λ. This is done by rewriting the pressure gradient term in Eq. (19a) as

$$\Lambda\left(\frac{1}{U_{j+1}^r} - \frac{1}{U_{j-1}^r}\right) = \left\{\Lambda \cdot \frac{U_{j+1}^r - U_{j-1}^r}{(U_{j+1} - U_{j-1})\, U_{j+1}^{r-1} U_{j-1}^{r-1}}\right\}\left(\frac{1}{U_{j+1}} - \frac{1}{U_{j-1}}\right) \tag{22}$$

so that some estimate of $\{\ \}$ can be recognized as the equivalent $\bar{\Lambda}$ when r is taken to be unity. This $\bar{\Lambda}$ will vary only slightly since r is only a little larger than unity.

4. Typical Difference Behavior

The behavior of difference solutions of system (19) is now demonstrated. These solutions are approximately representative of those for $r \neq 1$ if Λ is altered to $\bar{\Lambda}$ in the manner previously described. With $r = 1$, relation (17) and (20) governing U_J and $RE^* \Delta x$ become

$$U_J = \Lambda \tag{23}$$

and

$$RE^* \Delta x = 2\left(\frac{1 + \Lambda}{1 - \Lambda}\right) \tag{24}$$

Thus for a given value of the thermodynamic parameter $\Lambda (0 < \Lambda < 1)$, the magnitude of the Hugoniot jump of U is $1 - \Lambda$.

For other values of $RE\, \Delta x$, the construction of the difference solutions follows that of [2]. The difference equation (19a) is first considered at $j = J - 1$, then $J - 2$, etc., and at each step j the appropriate root U_{j-1} of the quadratic is chosen. To begin, Eq. (19a) at $j = J - 1$ together with the extrapolation condition (19c) gives

$$(U_{J-1} - U_{J-2})\left(1 + \frac{2}{RE\, \Delta x} - \frac{\Lambda}{U_{J-1} U_{J-2}}\right) = 0 \tag{25}$$

Thus either

$$U_{J-2} = U_{J-1} \tag{26a}$$

or

$$U_{J-1} U_{J-2} = \frac{\Lambda}{1 + 2/RE\, \Delta x} \tag{26b}$$

Root (26b) is chosen, which fixes the "location" of the jump at $j = J - 2$ and eliminates the translational arbitrariness of the present model. It is assumed that the correct Hugoniot value $U_J = \Lambda$ is computed (as can be verified a posteriori [2]), so that (26b) gives

$$U_{J-2} = \frac{\Lambda}{(1 + 2/RE\, \Delta x)\, U_{J-1}} = \frac{1}{1 + 2/RE\, \Delta x} \tag{27}$$

The general behavior of the difference solutions can then be determined from Eq. (27),

and from relation (19a) at $j = J - 2$, $J - 3$, etc. The results, which are depicted in Figure 2, have been verified by direct digital computation with time-dependent equations which reduce to (19) in the steady-state.

It is observed that if $RE\,\Delta x$ equals the special value $R\tilde{E}\,\Delta x = 2\Lambda/(1 - \Lambda)$, then $U_{J-2} = \Lambda$. As shown in [2], this solution is that special smooth solution separating the oscillatory solutions at $RE\,\Delta x > R\tilde{E}\,\Delta x$ with correct computed jump values from those smooth solutions at $RE\,\Delta x < R\tilde{E}\,\Delta x$ with Hugoniot jump values that are too large (see Fig. 2). This incorrect Hugoniot jump for $RE\,\Delta x < R\tilde{E}\,\Delta x$ occurs because the computed solution is such that $| U_{-J} - U_{-J+1} |$ is not small, so that the summed relations (14, 15) will not yield the same downstream values of U_J as does the differential Hugoniot, Eq. (5). The difference problem (19) becomes ill-posed (for the physically interesting solution) in the limit $RE\,\Delta x \to 0$, possibly because there does not exist a non-constant *differential* solution satisfying $u_x(x = 1) = 0$. Note that, for the sake of clarity, Fig. 2 does not show that as $RE\,\Delta x$ is decreased from $RE^*\,\Delta x$ to $R\tilde{E}\,\Delta x$, the behavior of the difference solution changes "continuously" to the smooth $R\tilde{E}\,\Delta x$ solution by having more and more mesh points (first U_{J-4}, then U_{J-5}, etc.) within a smooth jump profile before the first overshoot of $U = 1$ occurs.

The present method of constructing the difference solutions by starting at the downstream location $j = J$ is particularly appropriate when the downstream extrapolation condition (10c, d) is imposed. The exact satisfaction of this extrapolation condition is the feature which prevents oscillations from occuring downstream of the jump transition in this simple model problem. Should the extrapolation condition be only approximately satisfied. other construction methods are attractive and they can yield solutions with oscillations both upstream and downstream of the jump.

5. Use of Discretization Parameters γ_1, γ_2 to Obtain Large $RE^*\Delta x$

If $\gamma_1 \neq 0$, pointwise (local) mass conservation is secured only to the order of the (non-accumulating) local truncation error $O(\Delta x^2)$, and there is little apparent simplification of difference system (8, 9). Despite the complexities, for particular choices of γ_1 and γ_2 there exists "exact" solutions giving an abrupt jump across $2\,\Delta x$ without oscillations at fairly large values of $RE\,\Delta x$. Such solutions provide guidance for achieving "optimal" coarse mesh computation. No exact solutions giving an abrupt jump in $1\,\Delta x$ exist for $\gamma_1 \neq 0$.

The exact solutions which do exist are of the form

$$\begin{aligned} &U_j = 1, \quad \rho_j = 1 && j = -J, -J+1, \ldots, k-1 \\ &U_k, \quad \rho_k && j = k \\ &U_j = U_J, \quad \rho_j = \rho_J = \frac{1}{U_J} && j = k+1, k+2, \ldots, J-1, J \end{aligned} \tag{28}$$

where the values ρ_k, U_k at the "midpoint" of the jump (Fig. 3) are given in the

Appendix, as is the analytic method for obtaining such abrupt jump solutions. The values ρ_J and U_J are the *correct* downstream Hugoniot values. Difference solution (28) is obtained only for the combinations of values $\gamma_1 = \gamma_1^*, \gamma_2 = \gamma_2^*$, and $Re\,\Delta x = Re^*\,\Delta x$ shown in Figures 4, 5, and 6. There is one degree of freedom which is here used to select γ_1^*. Then Figure 4 displays the appropriate choice of γ_2^* as a function of γ_1^* for two reasonable choices of r and Λ. Other physically reasonable choices $0 < \Lambda < 1$ and $1 \leqslant r \leqslant 1.4$ yield results which are very nearly the same, so that γ_2^* is essentially dependent only on γ_1^* as given by Figure 4.

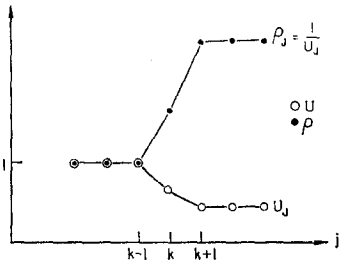

FIG. 3. Abrupt jump ("exact") difference solutions for $RE\Delta x = RE^*\Delta x$.

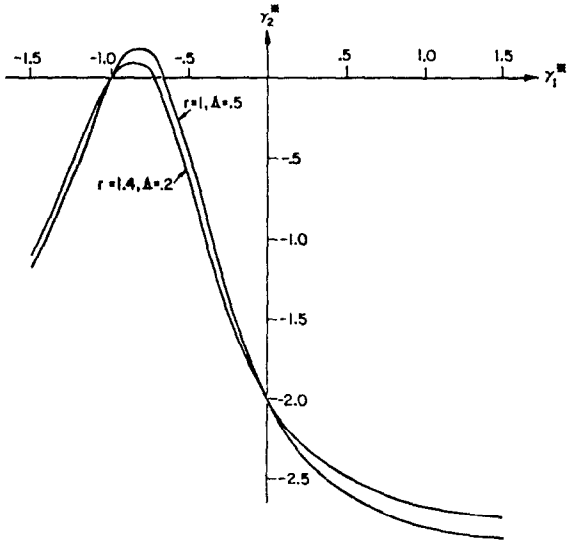

FIG. 4. Choice of γ_2 as a function of γ_1 for "exact" solution (essentially the same for other $0 < \Lambda < 1$, $1 \leqslant r \leqslant 1.4$).

Figure 5 shows $Re^*\,\Delta x \equiv ((1 - U_J)/2)\,RE^*\,\Delta x$ as a function of γ_1^* for $r = 1$; Fig. 6 does the same for $r = 1.4$. The change from the mesh Reynolds number $RE\,\Delta x$ based on the upstream reference velocity to $Re\,\Delta x$ based on half of the computed velocity jump causes the results for all choices of Λ to nearly coincide, and thus

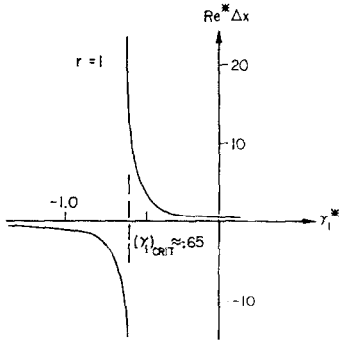

FIG. 5. $\mathrm{Re}^*\Delta x = ((1 - U_J)/2)\, RE^*\Delta x$ as a function of γ_1^*, $r = 1$ (essentially the same for all $0 < A < 1$).

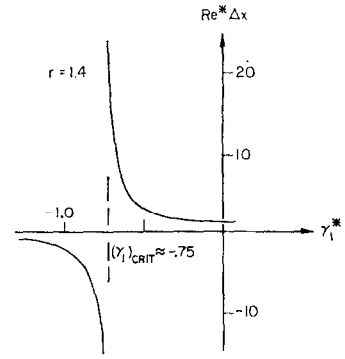

FIG. 6. $\mathrm{Re}^*\Delta x = ((1 - U_J)/2)\, RE^*\Delta x$ as a function of γ_1^*, $r = 1.4$ (essentially the same for all $0 < A < 1$).

suggests that the mesh Reynolds number defined in this way is the most representative computational parameter for such problems. It is apparent from Figures 5 and 6 that there is a critical value $(\gamma_1)_{\text{crit}}$ at which $Re^*\ \Delta x$ becomes arbitrarily large; this critical value depends slightly on r and is about $-.65$ and $-.75$ for $r = 1$ and $r = 1.4$ respectively. Since practical computation is generally carried out at large $Re\ \Delta x$, the choice $\gamma_1 \approx \gamma_2 \approx -.6 \gtrsim (\gamma_1)_{\text{crit}}$ is nearly optimal in the sense that it provides the minimally oscillatory abrupt jump solution (28) despite the coarse computational mesh. It is noted that these choices of γ_1 and γ_2 do not represent divergence form differencing. In particular the choice $\gamma_1 = 0$, which is certainly desirable for analytic simplicity, need not be computationally optimal at large mesh Reynolds numbers.

It is now desirable to determine the errors in the difference solutions as such solutions depart from the abrupt-jump solution (28) when γ_1 and γ_2 are *not* optimally chosen for computation at a given large $RE\ \Delta x$. Difference equations (8) and (9) at $j = J - 1$ and $j = J - 2$ are used, along with boundary conditions (10c, d) to obtain the values U_{J-2}, ρ_{J-2}, U_{J-3}, and ρ_{J-3}. A reference abrupt jump solution from $U = \rho = 1$ to $U = U_J$, $\rho = \rho_J$ may be assumed to pass through the computed mesh

point values U_{J-2} and ρ_{J-2} at $j = J - 2$. The values of U_{J-3} and ρ_{J-3} will generally differ from the correct values $U = \rho = 1$ when γ_1 and γ_2 are arbitrarily chosen. The error in U at $j = J - 3$

$$e_{J-3} = | 1 - U_{J-3} | \tag{29}$$

is a measure of the "error" in the computed difference solution, and is shown in Figure 7 for the specific values $r = 1.4$, $\Lambda = .305$, $U_J = .5$; the results are similar for other values if the variation of $(\gamma_1)_{\text{crit}}$ is accounted for. The abscissa in Figure 7 is the

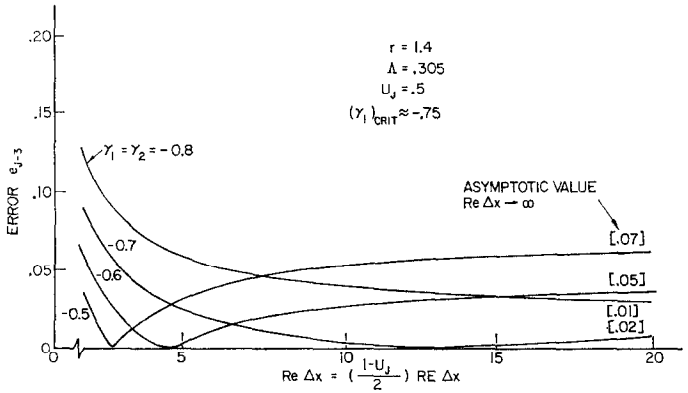

FIG. 7. Error in difference solution for $r = 1.4$ and the non-optimal choice $\gamma_1 = \gamma_2 \approx (\gamma_1)_{\text{crit}}$.

mesh Reynolds number $Re\,\Delta x$ based upon half of the computed jump magnitude, and each curve represents one specific choice of $\gamma_1 = \gamma_2 \approx (\gamma_1)_{\text{crit}}$. It is noted that $\gamma_1 = \gamma_2$ is not necessarily the combination (γ_1^*, γ_2^*) suggested by Figure 4. It is therefore surprising that the error e_{J-3} shows a conspicuous dip (i.e., the difference solution is very nearly (28)) for $Re\,\Delta x$ near the value of $Re^*\,\Delta x$ corresponding to the chosen value of $\gamma_1 \gtrsim (\gamma_1)_{\text{crit}}$. Furthermore, even if $\gamma_1 < (\gamma_1)_{\text{crit}}$ where no minimal point of the error curve may be expected and the negative value of $Re^*\,\Delta x$ might be disturbing, the values of e_{J-3} are still small. Generally speaking, then, the accuracy of the difference solution depends somewhat more sensitively on γ_1 than on γ_2, and the error values are well within practical accuracy requirements ($\lesssim$ 10-20% of the jump) if $\gamma_1 \approx (\gamma_1)_{\text{crit}}$. It is also important that the error curves are quite flat for $Re\,\Delta x \gtrsim 10$, since in practice the value of $Re\,\Delta x$ will vary over the field of computation so that a precise value of $Re^*\,\Delta x$ cannot be defined.

The question of difference solution behavior during the process of mesh refinement for a fixed discretization method (choice of γ_1 and γ_2) is now briefly discussed. Reference is made to Figure 2 for $\gamma_1 = 0$ and to Figure 7 for $\gamma_1 = \gamma_2 \approx (\gamma_1)_{\text{crit}}$.

Refining the computational mesh means reducing Δx for a fixed RE (or Re), so that $RE\,\Delta x$ (or $Re\,\Delta x$) is correspondingly reduced. As demonstrated in Figure 2, the difference solution is non-oscillatory at $RE\,\Delta x = R\hat{E}\,\Delta x = \infty$. As $RE\,\Delta x$ is reduced, the solution becomes oscillatory at finite $RE\,\Delta x > RE^*\,\Delta x$, is again nonoscillatory

at $RE^* \Delta x$, and then switches oscillatory behavior many times as the computed profile spreads out before smooth (nonoscillatory) solutions are again obtained as $RE \Delta x$ approaches $R\tilde{E} \Delta x$. If $RE \Delta x$ is reduced below $R\tilde{E} \Delta x$, an incorrect Hugoniot jump is obtained, despite the smooth computational results. It is thus wrong to pursue smooth solutions without regard to the error of the computed results. If the desired computational result is a nonoscillatory solution with minimal error at fairly large $RE \Delta x$, the abrupt-jump solution is clearly optimal, and it is quite possible that further mesh refinements will give worse approximations. Analogously, in Figure 7 for $\gamma_1 = \gamma_2 \approx (\gamma_1)_{\text{crit}}$, moving to the left on a given curve is equivalent to mesh refinement. The mesh should not be refined to a value of $RE \Delta x$ significantly below that corresponding to the minimum point of the error curve.

6. Two-Dimensional Example

A brief example is now given which shows the existence of an error minimum in a realistic two-dimensional computation with the full Navier-Stokes equations. These results were obtained by Neale Messina for an oblique shock with incident Mach number 2 and pressure ratio 1.910, and are thoroughly explained in [7]. The computation employed the Cheng-Allen algorithm with discretization parameter $\gamma = 0$ for all nonlinear terms to obtain a steady solution on a mesh of $28 \Delta y$ by $60 \Delta x$ ($\Delta y = \Delta x$). Figure 8 displays the L_∞ and L_1 errors in velocity and density as functions of the mesh Reynolds number $Re \Delta x$ based on half of the computed velocity jump. The vertical bars represent the range of errors computed along $I \Delta y$ ($I = 1, 2, \ldots, 28$) and the cross shows the average over I. These results are in qualitative agreement with our simple one-dimensional model; a more complete exposition on multi-dimensional results is forthcoming [8].

7. Conclusions

The present analytical study of steady-state difference approximations to gas-dynamic model system (1) leads to the following conclusions pertinent to practical computation:

(i) The mesh Reynolds number $Re \Delta x$ is a useful parameter reflecting computational resolution and accuracy. For problems involving discontinuities, $Re \Delta x$ should be based on the velocity jump across the discontinuity, and not on the upstream reference value or the local value.

(ii) When downstream extrapolation conditions are used, a difference formulation which is conservative can yield good approximations to the physical problem (correctly computed Hugoniot jumps) in the practical range of large $Re \Delta x$ ($\gtrsim 0(10)$),

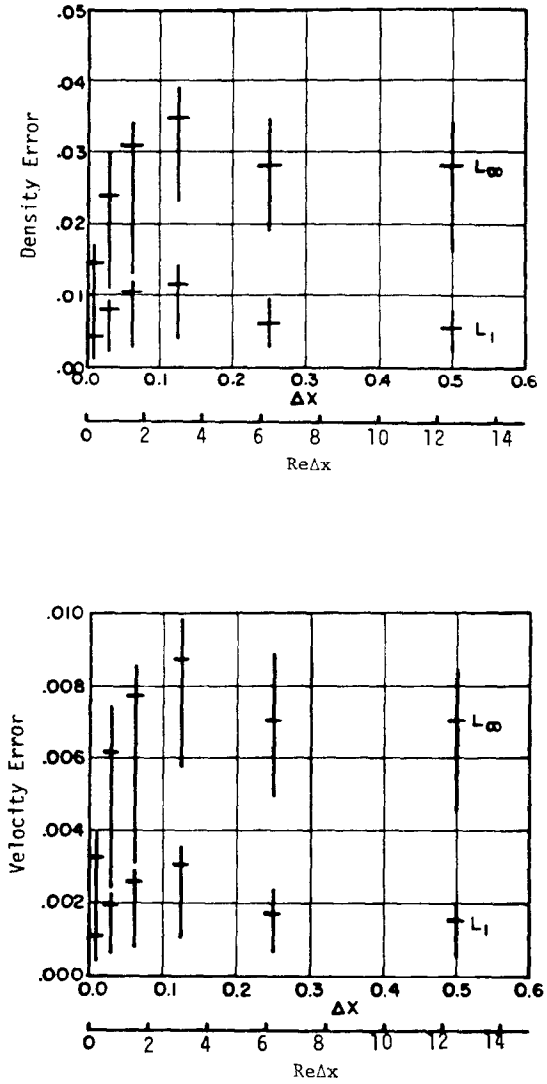

FIG. 8. L_1 and L_∞ errors for velocity and density in the Navier-Stokes solution of an oblique shock wave, as a function of mesh Reynolds number ReΔx.

despite computational oscillations. If the formulation is not conservative, little can be determined by the present method.

(iii) The magnitude of computational oscillations and the pointwise error at such large $Re\,\Delta x$ can be significantly reduced by correctly choosing the discretization parameters γ_1 and γ_2 which select specific conservative discretizations of the nonlinear terms $(\rho u)_x$ and $(\rho u^2)_x$ in the continuity and momentum equations. In obtaining the optimal computational solution, the choices of these parameters are interdependent. The discretization of the continuity equation is especially crucial. The extension of this type of weighted average conservative differencing to other terms in similar equations is straightforward.

(iv) The specific choice $\gamma_1 = \gamma_2 \approx (\gamma)_{\text{crit}}$ is recommended for problems similar to the present model.

(v) For a given discretization (choice of γ_i), it is possible to refine the computational mesh (decrease $Re\,\Delta x$) and obtain a more oscillatory solution. Furthermore, the mesh should not be overly refined in attempting to approach the small mesh limit, since for $Re\,\Delta x \lesssim 0(1)$, the difference solution obtained with downstream extrapolation, although smooth, will have large error due to an incorrectly computed Huguniot jump and excessive extension of the jump region.

APPENDIX: Derivation of Abrupt Jump Solution (28)

Solution (28) must satisfy the two difference equations (8), (9) at points $j = k - 1$, k, $k + 1$, or a total of six nonlinear relations. However, due to summability (difference form conservation), one of the continuity relations (8) and one of the momentum relations (9) are redundant. This is because "exact" solution (28) automatically satisfies the summed difference relation (17), so that if (say) solution (28) satisfies continuity and momentum at $j = k - 1$ and $j = k$, the two difference relations at $j = k + 1$ will be identically satisfied. Thus the exact solution (28) is obtained by solving for four of the five unknowns $(U_k, \rho_k, \gamma_1 = \gamma_1^*, \gamma_2 = \gamma_2^*, RE\,\Delta x = RE^*\,\Delta x)$ from four equations. Here the extra degree of freedom is used to select γ_1.

Specifically, continuity equation (8) at $j = k$ gives

$$\rho_k = U_k/U_j \tag{A.1}$$

and at $j = k - 1$ gives (using (A.1))

$$U_k^2 + \frac{\gamma_1^*(U_J + 1)}{2} U_k - U_J(1 + \gamma_1^*) = 0 \tag{A.2}$$

Now the downstream value U_J is given by Hugoniot relation (17) for any specified physical problem (i.e., given r, A). Thus the "midpoint" values U_k, ρ_k, are completely

determined by the choice of γ_1^*. The momentum equation (9) at $j = k$ and $j = k - 1$ then yield respectively

$$\frac{2}{2+\gamma_2^*}[U_J - 1] + \frac{\gamma_2^*}{2+\gamma_2^*}\left[\frac{U_k^2}{U_J}(U_J - 1)\right] + A\left[\frac{1}{U_J{}^r} - 1\right] = \frac{2}{RE^*\,\Delta x}[U_J - 2U_k + 1] \tag{A.3}$$

$$\frac{2}{2+\gamma_2^*}\left[\frac{U_k^3}{U_J} - 1\right] + \frac{\gamma_2^*}{2+\gamma_2^*}\left[\frac{U_k^2}{U_J} + U_k - 2\right] + A\left[\left(\frac{U_k}{U_J}\right)^r - 1\right] = \frac{2}{RE^*\,\Delta x}[U_k - 1] \tag{A.4}$$

which determine $RE^*\,\Delta x$ and γ_2 uniquely.

The above method of generating exact solutions of the difference system can be generalized straightforwardly to jumps over more mesh points.

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REFERENCES

1. S. I. CHENG AND G. SHUBIN, *J. Computational Physics*, in press.
2. G. SHUBIN, Ph.D. thesis, Princeton University, 1977.
3. P. ROACHE, "Computational Fluid Dynamics," Hermosa, Albuquerque, N.M., 1972.
4. L. CROCCO, *AIAA J.*, **3** (1965), 1824.
5. S. I. CHENG, *in* "Progress in Numerical Fluid Dynamics" (H. J. Wirz, Ed.), Lecture Notes in Physics No. 41, Springer-Verlag, New York, 1975.
6. S. I. CHENG, *Phys. Fluids*, **12**, Suppl. II (1969), II-34.
7. N. MESSINA, Ph.D. thesis, Princeton University, 1977.
8. S. I. CHENG, Sixth International Conference on Computational Methods, Tbilisi, USSR, June 1978.