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STEADY STATE SPURIOUS ERRORS IN SHOCK-CAPTURING NUMERICAL SCHEMES

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SUMMARY

The behaviour of the steady state spurious error modes of the MacCormack scheme and the upwind scheme of Warming and Beam is obtained from a linearized difference equation for the steady state error. It is shown that the spurious errors can exist either as an eigensolution of the homogeneous part of this difference equation or because of excitation from large discretization errors near oblique shocks. It is found that the upwind scheme does not permit spurious oscillations on the upstream side of shocks. Examples are given for the inviscid Burgers' equation and for one- and two-dimensional gasdynamic flows.

This report contains 24 pages including 6 figures.

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CONTENTS

1. INTRODUCTION

One of the major difficulties in numerical computation of gasdynamic flows is caused by the occurrence of shock waves. The most straightforward way of dealing with shocks is based on the concept of weak solutions of conservation laws introduced by Lax [1]. By a conservative formulation of the difference equations the shocks are captured automatically and no special treatment is required. The price to be paid for this simplicity is generally large errors in the vicinity of the shocks, most commonly in the form of pre- and post-shock oscillations. Efficient use of these so called shock-capturing methods therefore requires som understanding of the nature of these errors.

The existing work on this question is mostly based on the time-dependent equations. One standard procedure is to investigate the truncation error of simple linear model equations [2]. The results obtained are limited to the amplification and phase errors of the Fourier components of the solution and do not give any direct information on the effects of shocks. The case of an unsteady travelling shock has been treated by Kreiss and Lundqvist [3] for the simple linear wave equation $\partial u/\partial t - \partial u/\partial x = 0$ and by Lerat and Peyret [4] for the nonlinear, inviscid Burgers' equation. Both these works show that oscillating errors are generally to be expected near the shock.

Time-dependent numerical methods are also a useful tool for many steady flows of aerodynamic interest. In this paper the errors in the final steady state of such computations will be considered. Since none of the above methods of analysis are particularly well suited for the steady case, we shall describe a procedure by which it is possible to study the steady state errors more directly [7], [14]. Consider the system of conservation laws in one space dimension

$$\frac{\partial F}{\partial t} + \frac{\partial H}{\partial x} = 0 \tag{1}$$

where for inviscid, compressible flow $F = \{\rho, m, e\}$ is the field vector of mass, x-momentum, and total energy densities. We solve this system by the stable time--dependent numerical scheme

$$F_j^{n+1} = D_j\,(F_j^n) \qquad j = 1,\ 2, \ldots,\ N \tag{2}$$

where F_j^n is the computed field vector at grid point j at time step n, and D_j is the difference operator replacing the partial differential problem, i.e. eq. (1) with appropriate boundary conditions. The procedure (2) has converged to a steady state if $F_j^{n+1} = F_j^n = F_j^s$ to a specified accuracy in all the N grid points. Our purpose is to study the error in this result, particularly when shocks appear in the field. The error is defined by:

$$\varepsilon_j^n = F_j^n - F_{0j}^n \tag{3}$$

where $F_{0j}^n = F(n\,\Delta t,\ j\,\Delta x)$ is the exact solution of the differential problem with initial conditions F_{0j}^0. Substitution of F_j^n from eq. (3) into the difference eq. (2) gives an equation for the error expressed in the exact solution F_{0j}^n. Such an equation is of course just as complicated as the original difference problem and furthermore requires a knowledge of the unknown exact solution F_0. The discussion is therefore limited to small errors, and the nonlinear effects will be neglected. Substitution of (3) into (2) gives after linearization:

$$\varepsilon_j^{n+1} = L_j(\varepsilon_j^n) + T_j^n \tag{4}$$

where L_j is the linearized operator and

$$T_j^n = D_j(F_{0j}^n) - F_{0j}^{n+1} \tag{5}$$

is the truncation error. From (4) the usual requirements for convergence of the linearized problem is obtained. If the error shall become smaller as the mesh is refined, the operator D_j must be consistent so that $T_j^n \to 0$. This is particularly important if shocks appear in the field. We must also require the operator L_j to be stable [2]. When a steady state is reached, eqs. (4) and (5) reduce to:

$$(I - L_j)\ \varepsilon_j^s = T_j^s \tag{6}$$

$$T_j^s = D_j(F_{0j}^s) - F_{0j}^s \tag{7}$$

If we assume that the exact solution F_{0j}^s is known, then T_j^s and L_j are determined, and eq. (6) is a linear algebraic system for the error at every grid point. The scheme is consistent with p-th order of accuracy if $T_j^s = O(\Delta x^p)$, where Δx is the grid spacing. From eq. (7) it follows that the scheme must be consistent everywhere if the error shall vanish as $\Delta x \to 0$. In particular eq. (7) implies that the difference scheme must be a consistent approximation of the jump relations when shocks or other discontinuities appear in the field. Finally we must also require that the coefficient matrix obtained from the operator $I - L_j$ remains non-singular as $\Delta x \to 0$. If this is not the case, there can be an error in the final steady state (of indetermined amplitude in the linear approximation) determined by eq. (6) which is a singular homogeneous system in this limit. It is interesting to note that in this case an eigenvalue of L_j approaches 1, so that the time--dependent scheme ceases to converge when $T_j^n \to 0$. Below we shall give simple examples of such behaviour for a model equation and for steady one-dimensional flow with a shock.

Eqs. (6) and (7) will be used below to study the behaviour of small errors for some simple steady cases with known piecewise constant exact solutions F_0. The analysis for more general F_0 would be prohibitively difficult even if such a solution was known. For a slowly varying field these simple results could be used to judge the errors locally. The analysis will be applied to the two-step scheme suggested by MacCormack [5], and also with the upwind corrector of Warming and Beam [6], although some of the results are applicable to a wider class of schemes.

We shall first discuss the homogeneous error problem which arises from a simple nonlinear scalar equation. The properties of the operator $I - L_j$ of eq. (6) will be discussed and an example given which does not converge in the limit $\Delta x \to 0$, although the computation is stable. An analysis of the initial value problem for this scalar equation has been given by Harten et al [14], for the Lax-Wendroff scheme. Their analysis shows that the steady state is weakly unstable in the L_2 norm. It can be shown, however, that the initial-boundary value problem is stable when the number of grid points N is bounded which is also indicated by the computational results in [14].

Similar results will be derived for the one-dimensional gasdynamic case with a stationary shock. For the two-dimensional case we shall finally discuss the magnitude of the discretization error for steady, oblique shocks.

2. A SCALAR MODEL EQUATION

As an illustration we shall study the nonlinear, inviscid Burgers' equation

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) = 0$$

subject to the following initial and boundary conditions:

$$u(x,0) = \begin{cases} 1 & x=0 \\ 0 & 0<x<1 \\ -1 & x=1 \end{cases} \qquad \begin{aligned} u(0,t) &= 1 \\ u(1,t) &= -1 \end{aligned}$$

The exact solution of this problem is

$$u_0(x,t) = \begin{cases} 1 - S(x-\frac{1}{2}t) - S(x-1+\frac{1}{2}t); & t<1 \\ 1-2S(x-\frac{1}{2}); & t \geq 1 \end{cases}$$

where $S(x)$ is the unit step function. This solution represents two discontinuities (shocks) travelling away from the boundaries with velocities $\frac{1}{2}$ and $-\frac{1}{2}$. When they meet at $x=\frac{1}{2}$, they form a stationary discontinuity with the jump 2.

For the one-dimensional case given by eq. (1) with $F=u$ and $H=\frac{1}{2}u^2$ the MacCormack (MC) scheme is:

$$\overline{F_j^{n+1}} = F_j^n - \sigma h\,(H_j^n - H_{j-\sigma}^n) \tag{8a}$$

$$F_j^{n+1} = \tfrac{1}{2}\,(F_j^n + \overline{F_j^{n+1}} - \sigma h\,(\overline{H_{j+\sigma}^{n+1}} - \overline{H_j^{n+1}})) \tag{8b}$$

where $h=\Delta t/\Delta x$, $\overline{H_j^{n+1}} = H(\overline{F_j^{n+1}})$, and $\sigma=1$ gives backward predictor - forward corrector differencing, and the converse for $\sigma=-1$. When u is positive, the predictor with $\sigma=1$ is upwind, and the second-order upwind scheme of Warming and Beam (WB) is obtained if (8b) is replaced by the corrector:

$$F_j^{n+1} = \tfrac{1}{2}\,(F_j^n + \overline{F_j^{n+1}} - h\,(H_j^n - 2H_{j-1}^n + H_{j-2}^n) - h\,(\overline{H_j^{n+1}} - \overline{H_{j-1}^{n+1}})) \tag{8c}$$

In a steady state $F_j^{n+1} = F_j^n$ we get from eq. (8) for the MC (with $\sigma = 1$) and WB schemes respectively:

$$H_j - H_{j-1} + \bar{H}_{j+1} - \bar{H}_j = 0 \tag{9a}$$

$$2H_j - 3H_{j-1} + H_{j-2} + \bar{H}_j - \bar{H}_{j-1} = 0 \tag{9b}$$

where the superscripts have been dropped for simplicity.

The only possible exact steady solution in the one-dimensional case is $H_0 = H(F_0) = \text{const.}$ Since this solution exactly satisfies the difference eqs. (8), the steady state truncation error T_j^s of eq. (7) is exactly zero. The eq. (6) for small errors on the steady state is therefore homogeneous. For the present scalar problem we substitute $u_j = u_{0j} + \varepsilon_j$ into the difference eq. (9 a) :

$$\begin{aligned} &(1 - hu_{0j+1})\, u_{0j+1}\, \varepsilon_{j+1} + h\,(u_{0j+1} + u_{0j})\, u_{0j}\, \varepsilon_j \\ &- (1 + hu_{0j})\, u_{0j-1}\, \varepsilon_{j-1} = 0 \end{aligned} \tag{10}$$

This equation, together with the boundary conditions $u_1^n = \overline{u_1^{n+1}} = 1$, $u_N^n = \overline{u_N^{n+1}} = -1$, i.e. $\varepsilon_1 = \varepsilon_N = 0$, leads to a system of linear algebraic equations corresponding to eq. (6). If we substitute the exact steady solution u_0 into these, we could investigate under which circumstances the coefficient matrix becomes singular. This method, however, is not very practical for more complicated situations and a different approach is therefore taken. Let us assume that the shock is located between mesh points m and $m+1$, and hence separates two regions of constant u_0. With $u_{0j} = u_0 = \text{const.} \neq 0$ eq. (10) gives:

$$(1 - \nu)\, \varepsilon_{j+1} + 2\nu\, \varepsilon_j - (1 + \nu)\, \varepsilon_{j-1} = 0 \tag{11}$$

where $\nu = hu_0$ is the Courant number. Eq. (11) is a linear difference equation with constant coefficients and has solutions of the form $\varepsilon_j = \text{const.} \cdot \lambda^j$. Eq. (11) gives two solutions $\lambda_1 = 1$ and $\lambda_2 = \frac{\nu+1}{\nu-1}$, and the general solution is:

$$\varepsilon_j = k_1 + k_2(\lambda_2)^j \tag{12}$$

The mode $\lambda_1 = 1$ is necessary for consistency and is termed the correct mode. The other mode is an additional solution of the difference scheme and is therefore called a spurious mode. Since the variation of the error is exponential in space, we shall refer to this second mode as the exponential mode. For stability of the scheme it is required that $|\nu| \leq 1$. λ_2 is hence always negative, and the exponential mode is therefore oscillating. For $j \leq m$ u_0 is positive, $\lambda_2 \leq -1$ and the exponential mode is increasing towards the shock. For $j \geq m+1$ u_0 is negative and we therefore define the Courant number by $\nu = -h u_0$ to make it positive. In this region the eigenvalue λ_2 is $\frac{\nu-1}{\nu+1}$ which means that the errors decay with the same rate away from the shock on both sides. If we use the notation $\lambda_2 = \frac{\nu+1}{\nu-1}$ the general solution in this region is:

$$\varepsilon_j = k_3 + k_4 \left(\frac{1}{\lambda_2}\right)^j \tag{13}$$

To study the errors through the shock discontinuity it is more suitable to consider the error δ_j in the flux $H = \frac{1}{2}u^2$. In the linear approximation $\delta_j = u_{0j}\,\varepsilon_j$ which makes eq. (10) an equation for δ_j, and eqs. (12) and (13) remain valid with ε_j replaced by δ_j. From eq. (10) it can be seen that (12) is valid for $j \leq m-1$ and (13) for $j \geq m+1$. With $j=m$ and $u_{0m} = -u_{0m+1}$ (the jump relation) eq. (10) gives a relation for the error across the shock:

$$\delta_{m+1} - \delta_{m-1} = 0 \tag{14}$$

With the boundary conditions $\delta_1 = \delta_N = 0$ we also obtain from (12) and (13):

$$k_1 = -k_2 \lambda_2 \tag{15}$$

$$k_3 = -k_4 \left(\frac{1}{\lambda_2}\right)^N \tag{16}$$

From (12) and (13) we obtain with (15) and (16):

$$\delta_m = \frac{1 - \left(\frac{1}{\lambda_2}\right)^{m-1}}{1 - \left(\frac{1}{\lambda_2}\right)^{m-2}} \lambda_2 \, \delta_{m-1} = \frac{1 - \left(\frac{1}{\lambda_2}\right)^{N-m}}{1 - \left(\frac{1}{\lambda_2}\right)^{N-m-1}} \lambda_2 \, \delta_{m+1} \tag{17}$$

Eqs. (14) and (17) are two equations for δ_{m-1} and δ_{m+1}. It can clearly be seen that these equations become identical, and hence the operator $I - L_j$ singular, when the factors $(1/\lambda_2)^i$ in (17) vanish. This happens when either $\nu \to 1$ or $N, m \to \infty$. The last possibility corresponds to $\Delta x \to 0$. From eq. (17) it is also seen that when such errors are possible, they are dominated by the exponential modes, and the constants k_1 and k_3 vanish in the above limits. The decay of the error away from the shock made possible by the exponential modes are therefore the important factor. This is of importance in more complicated problems where it would be difficult to study the coefficient matrix from $I - L_j$.

Fig. 1 shows the result of a numerical computation of the present problem with $N = 20$ and $\nu = .4$ after 100 time-steps. The oscillating steady state error can clearly be seen, although the decay of the exponential modes is relatively slow for this low Courant number. Because of the singular nature of the error in the steady state, the amplitude is mainly determined by the errors introduced in the computation of the discontinuous unsteady transient. To illustrate this effect we have also made a computation with initial conditions given by the exact solution of the differential problem at the time when the discontinuities have travelled two mesh intervals from the boundaries. This leads to a more well behaved transient in the subsequent numerical computation. Fig. 2 shows the final steady state, and the error is now about 1.5 %. The ratio of the errors on both sides of the shock $\delta_{m+1} / \delta_{m-1}$ is 1.04 in this result which is in good agreement with the value predicted from eq. (14).

In [7] we have shown that the error equations can be made nonsingular simply by switching from $\sigma = 1$ for $u_0 > 0$ to $\sigma = -1$ for $u_0 < 0$ in the MC scheme. Computation with this switching gives the exact steady solution to machine accuracy as expected. Since the equations for constant u_0 (12) and (13) are the same as before, the error equations are nonsingular because of the special relation across the shock which does not permit the oscillating exponential modes. This type of switching is not very effective for more complicated systems of conservation laws, because we then have several coexisting exponential modes as will be seen below for the gasdynamic case.

A much more efficient way to make the operator $I - L_j$ nonsingular is to use a scheme with a different behaviour in the exponential modes. We therefore consider the scheme with the WB upwind corrector (8c). Proceeding in the same way as for the MC scheme on the steady state equation (9b) it is easily shown that the eigenvalue of the exponential mode for $u_0 > 0$ is given by:

$$\lambda_2 = \frac{\nu - 1}{\nu - 3}$$

This scheme is stable for $\nu \leq 2$ [6]. The exponential mode is oscillating for $\nu > 1$ and monotonic for $\nu < 1$. The interesting fact is, however, that the error always decays with increasing j towards the shock. If the MC scheme is used as before for $u_0 \leq 0$, the exponential mode is everywhere decaying with increasing j. Since the error is zero at $j = 1$, it must remain so at every point towards the shock. To keep the scheme fully conservative the switching operator of [6] must be used. When the MC scheme is used for $u < 0$, a steady oscillation is still possible on this side of the shock [9]. If the upwind scheme is used on both sides, the exact steady state is obtained as expected.

3. ONE-DIMENSIONAL INVISCID, COMPRESSIBLE FLOW

For this case we have $F = \{\rho, m, e\}$ and $H = \{m, \frac{m^2}{\rho} + p, (e+p)\frac{m}{\rho}\}$ where the pressure for a perfect gas is given by the equation of state $p = (\gamma - 1)(e - \frac{1}{2}\frac{m^2}{\rho})$, γ being the ratio of specific heats. The only possible exact steady solution is $H_0 = \text{const.}$, $T_j^s = 0$ and the error equations are homogeneous as for the previous case. $H_0 = \text{const.}$ is the Rankine-Hugoniot relation, giving a possible supersonic state F_{01} and a subsonic state F_{02} such that $H(F_{01}) = H(F_{02}) = H_0$.

A small error ε_j on the steady state F_0 gives an error in H_j which is $\delta_j = A_j \varepsilon_j$, provided that the Jacobian A_j of H with respect to F is given by $A_j = A(F_{0j})$, i.e. we neglect its variation with ε_j. A_j must also be nonsingular which rules out the special cases $M = 0, \pm 1$, where $M = \frac{u}{a}$ is the Mach number, u is the velocity and a the speed of sound. Substitution of this into eq. (9a) and using (8a) for the error in the predictor, we get the following equation for the steady state errors of the MC scheme:

$$(I - hA_{j+1})A_{j+1}\varepsilon_{j+1} + h(A_{j+1} + A_j)A_j\varepsilon_j - (I + hA_j)A_{j-1}\varepsilon_{j-1} = 0 \qquad (18)$$

We shall investigate the simple case consisting of a constant upstream supersonic flow F_{01} ($j \leq m$), a normal shock between $j = m$ and $j = m+1$, and downstream subsonic flow F_{02} ($j \geq m+1$). Since A_j is constant except for the jump across the shock, we first study the behaviour of the error on both sides of the shock by solving eq. (18) for A_j = const. = A. The solutions are of the form $\varepsilon_j = \varepsilon_0 \lambda^j$, which leads to the eigenvalue problem:

$$((\lambda^2 - 1) I - (\lambda^2 - 2\lambda + 1) hA) \varepsilon_0 = 0$$

There are obviously 3 eigenvalues $\lambda = 1$ which represent the constant correct mode. The problem for the remaining 3 eigenvalues for the exponential modes is:

$$(A - \frac{1}{h} \frac{\lambda + 1}{\lambda - 1} I) \varepsilon_0 = 0$$

so that

$$\frac{1}{h} \frac{\lambda_i + 1}{\lambda_i - 1} = \omega_i$$

where ω_i are the eigenvalues of A given by $\omega_1 = a(M+1)$, $\omega_2 = aM$, and $\omega_3 = a(M-1)$. In the following it will be assumed that $M > 0$. The von Neumann condition for stability is then for the MC scheme:

$$\nu = h a(M+1) \leq 1$$

The eigenvalues λ_i can therefore be written

$$\lambda_1 = \frac{\nu + 1}{\nu - 1}$$

$$\lambda_2 = \frac{M(\nu+1) + 1}{M(\nu-1) - 1}$$

$$\lambda_3 = \frac{M(\nu+1) - (\nu-1)}{M(\nu-1) - (\nu+1)}$$

For $\nu < 1$ the eigenvalues are always negative which corresponds to oscillatory increasing or decaying modes. The λ_1 mode is always decaying in the upstream direction and does so more rapidly as $\nu \to 1$. Fig. 3 shows λ_2 and λ_3 as functions of the Mach number for different ν. The λ_2 mode also decays in the upstream direction, whereas the λ_3 mode decays upstream for $M > 1$ and downstream for $M < 1$. The λ_3 mode is very significant since it allows errors produced at the shock to decay in both directions away from it. The decay rates grow towards the λ_1 mode as $M \to \infty$. As $M \to 0$ the decay rate of the λ_2 mode vanishes since $\lambda_2 \to -1$, and the downstream decay of the λ_3 mode becomes increasingly more rapid, $\lambda_3 \to 0$.

The eigenvectors ε_0 corresponding to the eigenvalues of the exponential modes are given by the column vector matrix:

$$E = \begin{pmatrix} 1 & 1 & 1 \\ a(M+1) & aM & a(M-1) \\ a^2(\frac{1}{2}M^2 + M + \frac{1}{\gamma-1}) & a^2\frac{M^2}{2} & a^2(\frac{1}{2}M^2 - M + \frac{1}{\gamma-1}) \end{pmatrix}$$

which are the eigenvectors of the Jacobian A. They are always linearly independent for $\gamma \neq 1$.

Since we have taken A to be constant and linearized, these results are valid for any Lax - Wendroff type scheme using 3 points in the spatial coordinate. It can also be expected that the results should be locally valid if A is slowly varying, such as for example in a slowly diverging one-dimensional duct flow.

In the constant flow on both sides of the shock the exponential part of the error can be written:

$$\varepsilon_j = E\,\Lambda^j\,K \tag{19}$$

where Λ is a diagonal matrix with $\lambda_{1,2,3}$ as elements and K is an amplitude vector. A more suitable form of eq. (19) is:

$$\varepsilon_{j+1} = C\,\varepsilon_j \tag{20}$$

where $C = E\,\Lambda\,E^{-1}$

As before it is better to consider the error in H for the equations valid through the shock. From eq. (20) we get for the upstream and downstream sides respectively:

$$\delta_m = C_1\,\delta_{m-1} \tag{21}$$

$$\delta_{m+1} = C_2\,\delta_m \tag{22}$$

A relation for the error across the shock is obtained from eq. (18) with $j = m$:

$$(I - hA_2)\,\delta_{m+1} + h\,(A_2 + A_1)\,\delta_m - (I - hA_1)\,\delta_{m-1} = 0$$

which can be identically written as

$$(I - hA_2)\,\delta_{m+1} + (I + hA_2)\,\delta_m = (I - hA_1)\,\delta_m + (I + hA_1)\,\delta_{m-1} \tag{23}$$

It is easily shown that the two sides of eq. (23) are identically zero by eq. (21) and eq. (22) respectively. The three eqs. (21) - (23) for the errors δ_{m-1}, δ_m, and δ_{m+1} are hence not linearly independent, and a non-zero solution can exist for the error through the shock. On the subsonic side of the shock there is only one mode which decays in the downstream direction, given by the eigenvalue λ_3. The other two modes cannot exist because they would produce an increasingly large error at the downstream boundary where the boundary conditions must be satisfied. The error δ_{m+1} therefore has the form given by the eigenvector of the λ_3 mode. Because of the exponential decay with j, the remaining error at the downstream boundary rapidly approaches zero as the mesh is refined, thus satisfying the exact downstream boundary conditions. From eq. (22) the error δ_m in the last point upstream of the shock must have the same form as δ_{m+1}, only larger by the factor $(1/\lambda_3)_2$. In the supersonic part all the exponential modes decay upstream, and the error therefore vanishes at the upstream bondary as the mesh is refined, thus satisfying the given inlet conditions. Since the eigenvectors of the modes are linearly independent, any error δ_m can decay in this manner.

To illustrate this error behaviour a simple numerical experiment has been made. The mesh consisted of 50 grid points, and the initial conditions were taken as the exact steady solution with the shock at $m = 25$, except for a 10 % increase in the pressure at the first downstream point $j = 26$. At $j = 1$ the inlet conditions were kept fixed during the computation with $\rho_1 = 1$ kg/m^3, $m_1 = 600$ kg/m^2 s, $e_1 = 4.3 \cdot 10^5$ J/m^3, which gives an upstream Mach number $M_1 = 1.60$. The exact values were also kept at the downstream boundary. The computation was run for 2000 time-steps with upstream Courant number $\nu_1 = .9$. The relative change in density per time-step was then less than 10^{-5}. The resulting steady state relative error in the flux vector near the shock is shown in Fig. 4. Table I shows this computed relative error together with the errors calculated from the linear theory above. To determine the amplitude of the theoretical modes the error in the mass flux was chosen to have the same value at the first downstream point $j = m+1$. As can be seen the agreement is very good. Although the maximum relative error in the flux vector is only about .6 %, corresponding errors in density and pressure is 2 and 4 % respectively.

By similar calculations it is easily shown that the exponential modes of the WB scheme (8 c) are given by:

$$\lambda_1' = \frac{\nu - 1}{\nu - 3}$$

$$\lambda_2' = \frac{M(\nu-1) - 1}{M(\nu-3) - 3}$$

$$\lambda_3' = \frac{M(\nu-1) - (\nu+1)}{M(\nu-3) - (\nu+3)}$$

This scheme is stable for $M > 1$ and $\nu \leq 2$. For $\nu < 1$ the error is monotonic since $\lambda_i' > 0$. The λ_1' mode is oscillating for $\nu > 1$, and the other two for sufficiently high Mach number. The behaviour of λ_2' and λ_3' is shown in Fig. 5. As for previous scalar case all the eigenvalues have the interesting property $|\lambda_i'| < 1$ which means that the error always decays in the streamwise direction. Since the error upstream in the supersonic part is cancelled by the specified inlet conditions, the exponential modes are absent down to the shock. If the switching operator of [6] is used with the MC scheme downstream, the λ_3 mode can still remain on the downstream side [9]. An interesting proposal to remedy this situation is the splitting technique of Warming and Beam [15], which treats the waves going upstream in subsonic parts by downstream differencing similar to the WB scheme.

4. TWO - DIMENSIONAL FLOW

The basic difficulty in the two-dimensional case is due to the large discretization error arising from an inconsistent treatment of shocks and other discontinuities. This error will remain large as the mesh is refined except in a few special cases which are discussed below in a simplified manner. For this case the system of conservation laws is

$$\frac{\partial F}{\partial t} + \frac{\partial H}{\partial x} + \frac{\partial G}{\partial y} = 0 \tag{24}$$

where $F = \{\rho, m, n, e\}$, $H = \{m, \frac{m^2}{\rho} + p, \frac{mn}{\rho}, (e+p)\frac{m}{\rho}\}$,
$G = \{n, \frac{mn}{\rho}, \frac{n^2}{\rho} + p, (e+p)\frac{n}{\rho}\}$, n is the y-momentum, and
$p = (\gamma - 1)(e - \frac{1}{2}(m^2 + n^2)/\rho)$.

If shocks appear, they satisfy the steady state jump condition

$$\frac{dy_s}{dx}[H]_x + [G]_y = 0 \tag{25}$$

where dy_s/dx is the local shock inclination and $[\cdot]_x$, $[\cdot]_y$ are the jumps in the x, y - directions.

The MC scheme for eq. (24) is:

$$\overline{F^{n+1}_{j,k}} = F^n_{j,k} - \sigma_x h_x (H^n_{j,k} - H_{j-\sigma_x,k}) - \sigma_y h_y (G^n_{j,k} - G^n_{j,k-\sigma_y}) \tag{26a}$$

$$F^{n+1}_{j,k} = \frac{1}{2}(F^n_{j,k} + \overline{F^{n+1}_{j,k}} - \sigma_x h_x (\overline{H^{n+1}_{j+\sigma_x,k}} - \overline{H^{n+1}_{j,k}})$$

$$- \sigma_y h_y (\overline{G^{n+1}_{j,k+\sigma_y}} - \overline{G^{n+1}_{j,k}})) \tag{26b}$$

where $h_x = \Delta t/\Delta x$, $h_y = \Delta t/\Delta y$, and σ_x, $\sigma_y = \pm 1$ determines the differencing sequence in the two directions.

The error modes are excited by the discretization errors $T_{j,k}$ (eqs. (6) and (7)) which act as local source terms. In the scheme considered the magnitude of these errors are $0(\Delta x^2, \Delta y^2)$ and can thus be made arbitrarily small in smooth regions of the field be refining the mesh. This is, however, not the case for grid points close to discontinuities, and in the following we shall only consider the part of $T_{j,k}$ which is not necessarily $0(\Delta x^2, \Delta y^2)$. For the MC scheme this part is

$$T_{j,k} = - [H_{0j+1,k} - H_{0j-1,k} + h_{xy}(G_{0j,k+1} - G_{0j,k-1})]$$

$$- \sigma_x (\overline{\Delta H}_{0j,k} - \overline{\Delta H}_{0j-\sigma_x,k}) - h_{xy}\sigma_y (\overline{\Delta G}_{0j,k} - \overline{\Delta G}_{0j,k-\sigma_y}) \tag{27}$$

where $h_{xy} = \Delta x/\Delta y$, subscript 0 means the exact steady solution as before, and $\overline{\Delta H_0}$, $\overline{\Delta G_0}$ is the change in H, G after application of the predictor step on the exact solution. If the change in the Jacobians $A_{j,k}$ and $B_{j,k}$ caused by the predictor step is neglected, we have:

$$\overline{\Delta H}_{0j,k} = A_{0j,k}\,\bar{\varepsilon}_{j,k}$$
$$\overline{\Delta G}_{0j,k} = B_{0j,k}\,\bar{\varepsilon}_{j,k} \tag{28}$$
$$\bar{\varepsilon}_{j,k} = -\sigma_x h_x (H_{0j,k} - H_{0j-\sigma_x,k}) - \sigma_y h_y (G_{0j,k} - G_{0j,k-\sigma_y})$$

For simplicity the case of two constant parallel flow regions separated by a straight shock will be considered. The local difference between this case and a smoothly varying field is only due to terms which vanish as the mesh is refined. The term in square brackets in eq. (27) for $T_{j,k}$ can only vanish in two special cases. If the mesh is aligned with the shock, the jumps in H and G across the shock are zero. For this case the remaining terms also vanish, and the previous one-dimensional results are applicable.

Secondly the first term of eq. (27) is also consistent with the shock jump relation (25) if the local inclination of the shock dy_s/dx is equal to $1/h_{xy}$, in which case the shock is parallel to the mesh diagonals. To make the remaining terms in eq. (27) vanish the differencing sequence cannot be arbitrarily chosen, i.e. σ_x, σ_y. From eq. (28) it follows that differences should be taken across the shock in both directions in either the predictor or the corrector step, and not in one direction in each step.

If neither of these two conditions are satisfied, the discretization error is always $0(1)$ regardless of mesh refinements. The largest errors are produced when the scheme captures the jump in only one direction. This will occur at regular intervals along a straight, oblique shock in a rectangular mesh.

A good example of these effects is seen in the computations of Kutler et. al. [10] for the reflection of an incoming shock on a wedge in supersonic flow. The errors are large along all shocks except for the reflection from the wedge surface, where the above conditions seem to be at least approximately satisfied. The results given here are easily extended to self-similar problems such as [10]. Another example for a self-similar case is also given in [11] for the reflection of a strong shock from a wedge. The mesh and differencing sequence was chosen to minimize the errors along the discontinuities and the result is shown in Fig. 6.

For the MC scheme with permuted differencing [5], the time-split scheme [8] and the upwind WB scheme the square bracketed term of eq. (27) is the same as for the regular MC scheme. The remaining terms are, however, always $0(1)$ for these schemes. It is therefore possible that the advantage of these schemes resulting from better stability and faster convergence towards the steady state, may be largely offset by the better shock-capturing properties of the regular MC scheme when properly applied.

5. CONCLUDING REMARKS

It has been explained in the previous sections how the discretization errors near steady shocks can excite the spurious exponential error modes of a shock-capturing scheme, and also why these errors can exist even in the special cases when the discretization errors are small. We feel that proper understanding of the behaviour of the spurious modes is important to improve the quality of the steady state results obtained from such schemes.

In the arguments above it has been assumed that the shock is correctly located in the mesh. A wrong shock location can be interpreted as a large discretization error locally and will hence lead to large errors in the vicinity of the shock. To minimize this possibility a fully conservative scheme should be used. It is worth noting, however, that a conservative scheme does not guarantee correct shock locations. According to the theory above a wrong shock location in the steady state is also possible with the use of a shock-fitting technique, provided that the error introduced can decay sufficiently fast towards the boundaries. The reason why the present two-dimensional shock-fitting techniques [12] work so well is probably because the special numerical schemes used along the shock boundary tend to suppress the oscillating exponential error modes [13]. The applicability of such schemes is unfortunately severely limited for three-dimensional cases. The shock-capturing approach with conservative schemes can be applied without difficulty in problems of arbitrary dimension. The results given here are also easily extended to multi-dimensional cases.

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Table I. Comparison of relative errors.

j	Mass flux error $\cdot 10^3$		Momentum flux error $\cdot 10^3$		Energy flux error $\cdot 10^3$	
	Theory	Computed	Theory	Computed	Theory	Computed
23	-4.485	-4.440	-1.111	-1.079	-2.701	-2.647
24	6.003	5.898	-1.003	1.045	3.814	3.740
25	-5.912	-5.927	1.132	1.098	-4.463	-4.449
26	4.505	4.505	-0.862	-0.886	3.401	3.417
27	-3.433	-3.433	0.657	0.639	-2.592	-2.577
28	2.616	2.598	-0.501	-0.514	1.975	1.976

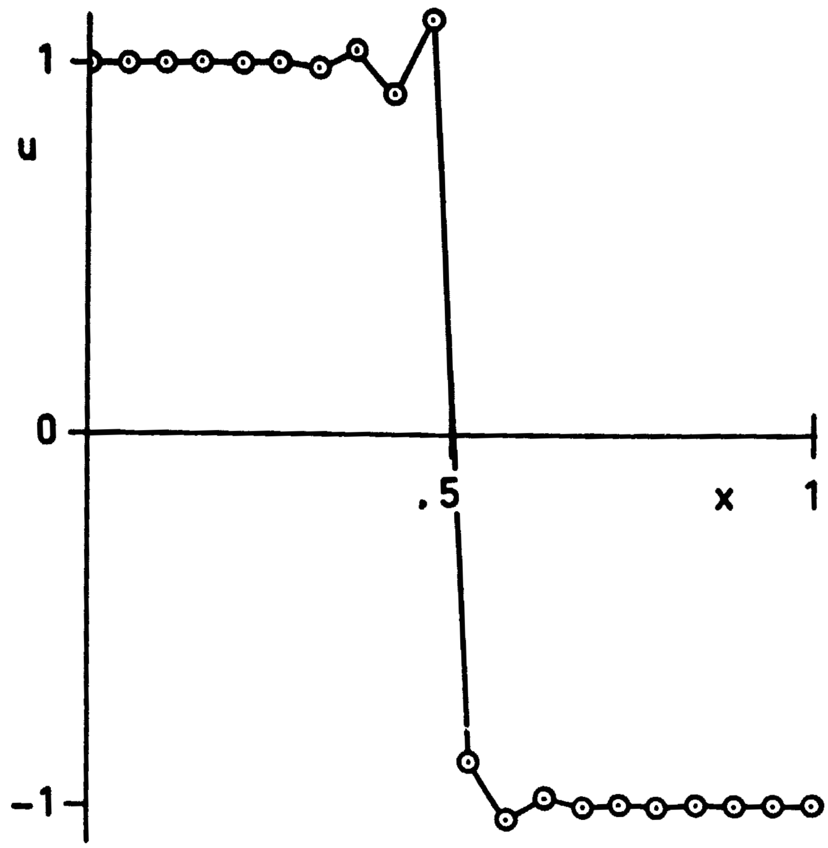


Fig. 1 Steady state solution of model scalar problem, $n = 100$, $\nu = .4$

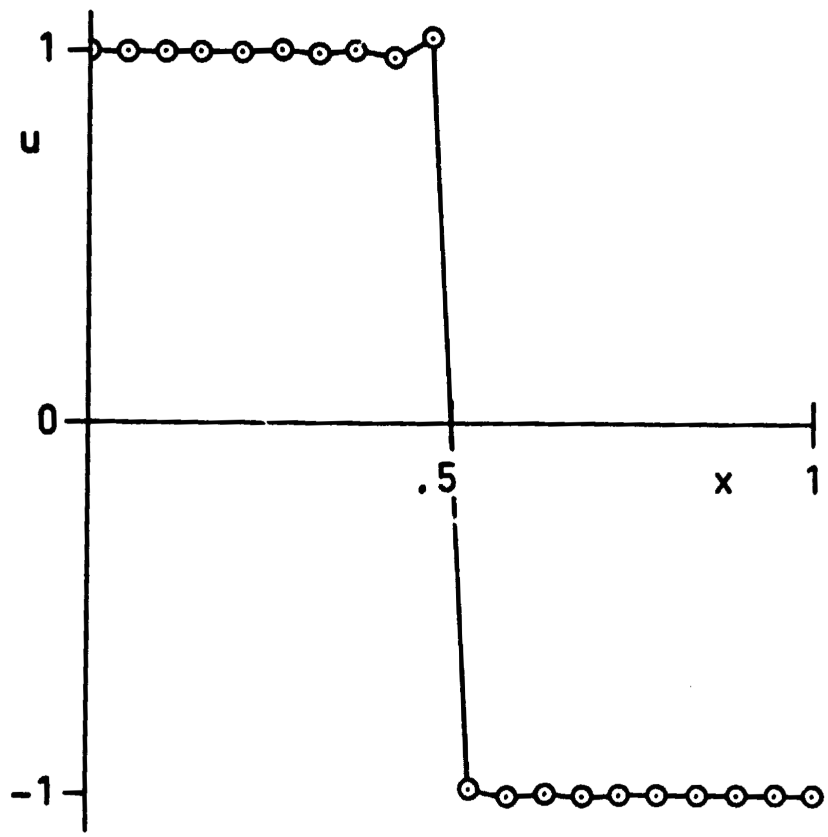


Fig. 2 Steady state solution of model scalar problem with modified initial conditions.

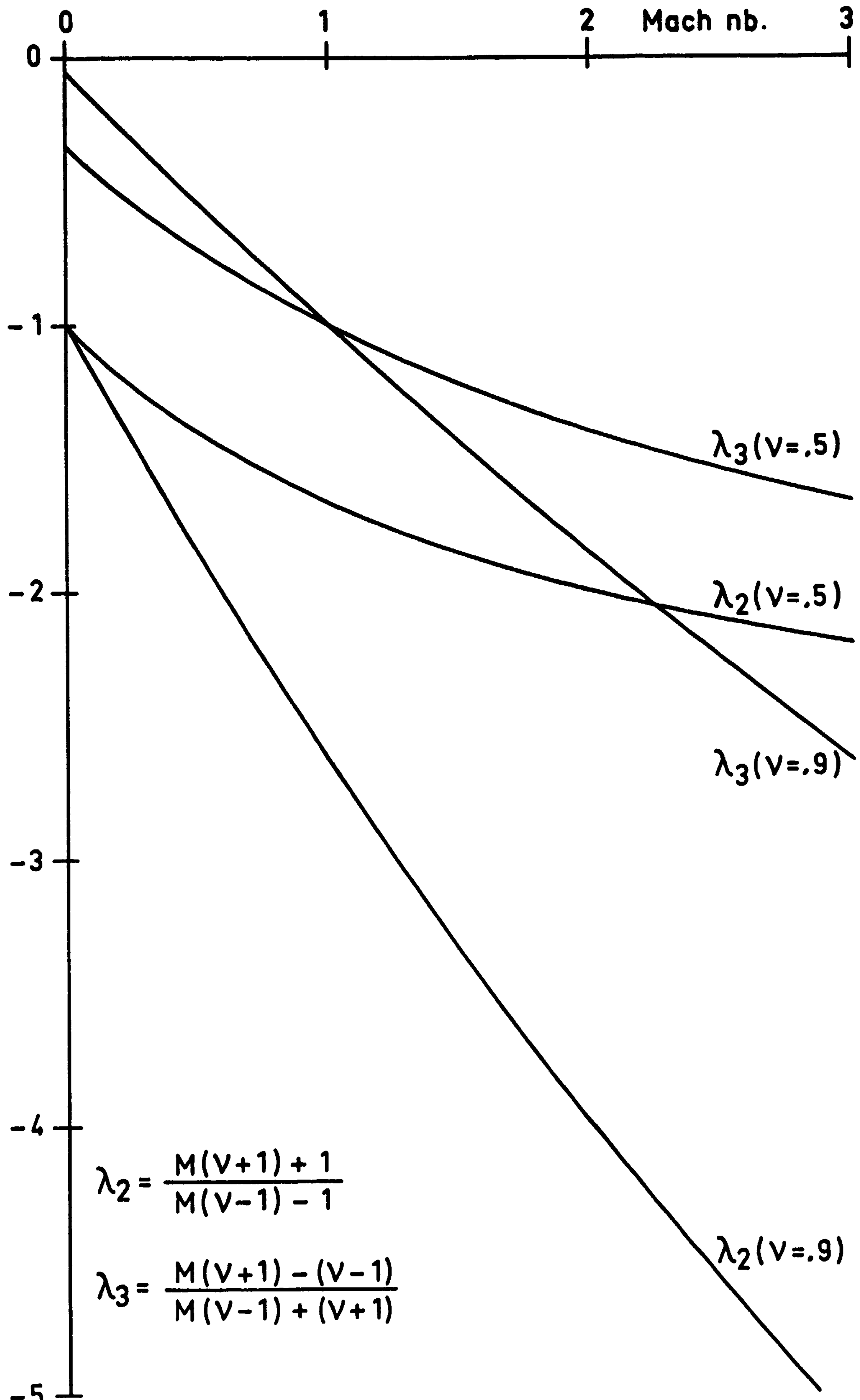


Fig. 3 Eigenvalues λ_2 and λ_3 for the exponential modes of MacCormack's scheme.

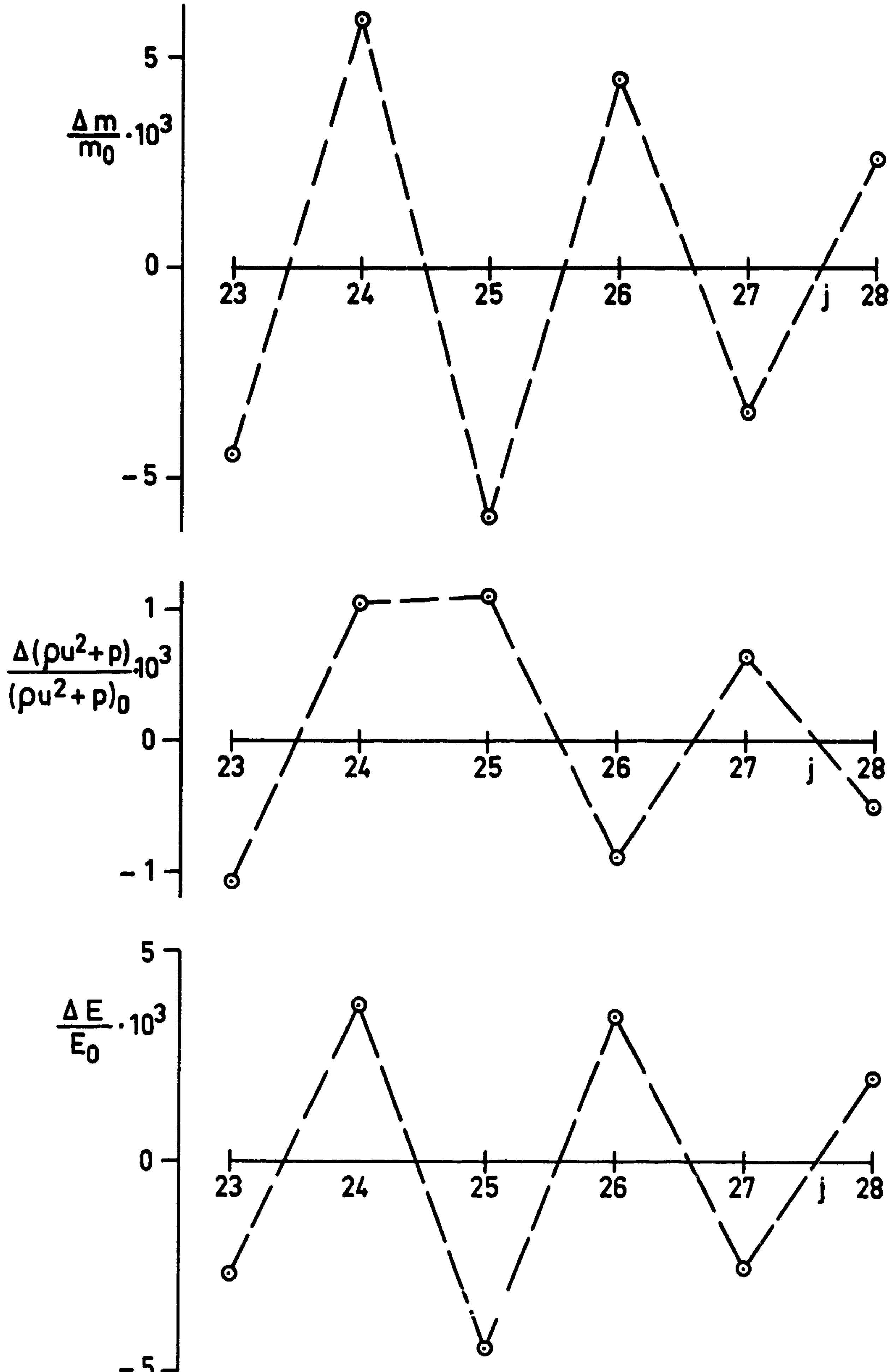


Fig. 4 Relative errors near one-dimensional steady shock.

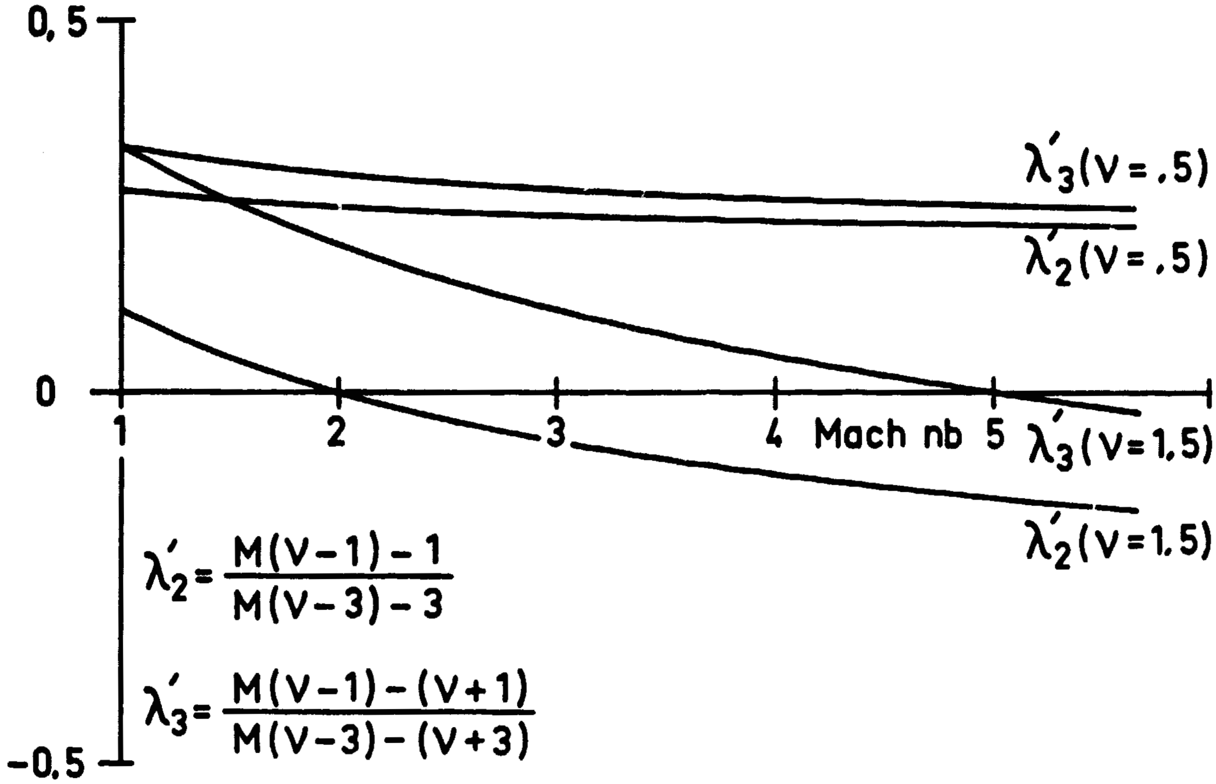
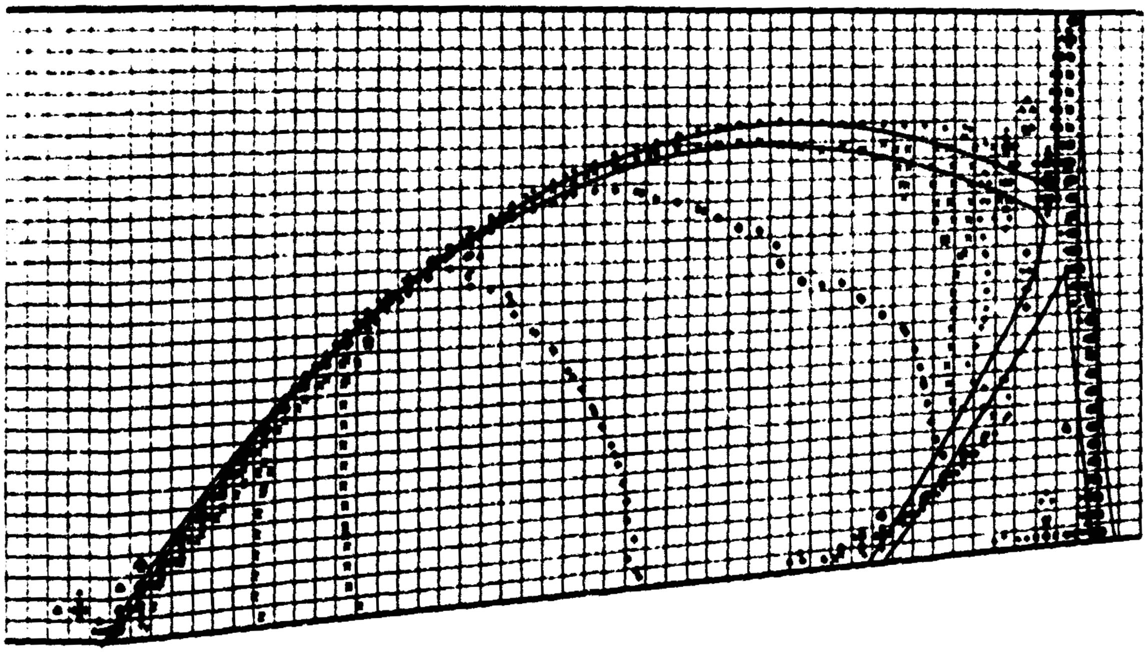


Fig. 5 Eigenvalues λ_2' and λ_3' for the exponential modes of the Warming and Beam scheme.



ρ_1 = upstream (left) density

ρ/ρ_1 : 0.8 □ , 0.9 ○ , 0.95 △ , 1.03 + , 1.05 x , 1.07 ◇ , 1.10 ↑ , 1.15 ⌘
1.20 z , 1.25 Y , 1.30 ● , 1.35 ✱ , 1.40 ⌛

═══ Experiment

Fig. 6 Reflection of shock wave from a wedge. Density contours. Full lines are drawn from a Schlieren photograph of the corresponding shock tube experiment.