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MEMORANDUM REPORT BRL-MR-3400

A VAN LEER SHOCK CAPTURING ALGORITHM FOR THE EULER EQUATIONS

Charlie H. Cooke

October 1984



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Van Leer's second-order accurate sequel to the first-order method of Godunov, originally formulated in the framework of Lagrangean fluid dynamics, is revised so as to apply to numerical calculation of solutions to the one-dimensional Euler equations of compressible flow. Comparisons of performance between the first and second order method are shown for the linear shock tube problem. Use of artificial viscosity, as opposed to oscillation limiting, is discussed.

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I. INTRODUCTION

A current focus of interest in the U.S. Army ballistic research program involves the numerical calculation of compressible flow about muzzle brake devices. By absorbing a portion of the recoil impulse, the muzzle brake permits design of large caliber weapons characterized by increased range without increased weight. Near field calculations are helpful in studying fatigue life and structural integrity of blast-loaded surfaces. Far-field calculations, which often can be performed with less complex flow models, can determine if safe maximum overpressures exist in the gun crew area.

Near-to-intermediate range muzzle brake calculations have recently been obtained using a popular, locally one-dimensional, first-order accurate method of Godunov. Model results afford predictions of peak over-pressure levels in the proximity of the brake and provide initial data for continuing far-field calculations by independent means.

In the interest of economizing computer resources, for far-field calculations, it is desirable to employ simple one-dimensional flow models. Mach contours for the early stages of a typical blast are exhibited in Figure 1. Already, local spherical symmetry is suggested, and evidence from spark photography confirms that the trend is characteristic of later evolution. Under this hypothesis, some exploratory far-field calculations are underway, which utilize spherically symmetric flow models and the numerical method of characteristics. 3,4

^{1.} G. E. Widhopf, J. C. Buell, and E. M. Schmidt, "Time Dependent Near-Field Muzzle Brake Simulations," AIAA-82-0973, AIAA/ASME 3rd Joint Thermophysics, Fluids and Heat Transfer Conference, St. Louis, Missouri, June 1982.

^{2.} A. M. Godunov, A. V. Zabrodin, and G. P. Prokopov, "Difference Schemes for Two-Dimensional, Unsteady Problems in Gas Dynamics and Calculation of Flows With a Detached Shock Wave," Journal of Computing Mathematics and Mathematical Physics, USSR Academy of Sciences, Vol. 1, No. 6, November - December 1961. (Translation)

^{3.} M. L. Bundy, "A Nonsimilar Solution for Blast Waves Driven by an Asymptotic Piston Expansion," AIAA-83-0496, AIAA 21st Aerospace Sciences Meeting, January 1983, Reno, Nevada and U. S. Army Ballistic Research Laboratory, Aberdeen Proving Ground, MD, BRL Technical Report ARBRL-TR-02497, June 1983. (AD A130012)

^{4.} M. L. Bundy, C. H. Cooke, and E. M. Schmidt, "Reshaping an Artificially Diffused Shock Solution," BRL Report, to be published.

The objective of the present research is to investigate an alternative numerical method, which might complement, or perhaps supplant, the method of characteristics approach. Our intent is to revise Van Leer's second-order accurate, Godunov method, 5 originally formulated in the framework of Lagrangean fluid dynamics, for application to the one-dimensional Euler equations. A similar effort, as yet unpublished, and which differs somewhat in philosophy, has been carried out by Colella. 6

The desirability of investigating second-order accurate methods for shock capturing is illustrated by Figure 2. Here, the first-order Godunov method, implemented by personnel of Aerospace Corporation for numerical solution of the two-dimensional axis-symmetric Euler equations, has been applied to calculate a conical flow which simulates some of the more dominant characteristics of a muzzle blast. Assuming there is provided some heuristic model of contact surface history, as well as initial data between the outer shock and its driving contact surface, this calculation could be continued into the far-field by the method of characteristics. However, shock smearing due to the artificial viscosity of the numerical method in this case makes troublesome the question of precise shock location and strength. A reshaping of initial data near the shock, or else a more accurate calculation which provides crisper shock structure, appears to be called for.

In the past few years, a variety of new methods for numerical calculation of flows with embedded shocks has evolved, of which references 5-9 are perhaps a representative sample. Van Leer's second-order sequel to the original Godunov method appears among the more promising. The method is alledged⁵ to give

^{5.} B. Van Leer, "Towards The Ultimate Conservative Difference Scheme. V. A Second-Order Sequel to Godunov's Method," <u>Journal of Computational Physics</u>, Vol. 32, pp. 101-136, 1979.

^{6.} P. Colella, "A Direct Eulerian MUSCL Scheme for Gas Dynamics," Lawrence Berkeley Laboratory Report LBL-14104, February 1982.

^{7.} J. L. Steger and W. F. Warming, "Flux Vector Splitting of the Inviscid Gas Dynamics Equations with Application To Finite Difference Methods," Journal of Computational Physics, Vol. 40, No. 2, April 1981.

^{8.} G. Moretti, "The λ Scheme," <u>Computers and Fluids</u>, Vol. 7, pp. 191-205, Pergamon Press, 1979.

^{9.} H. C. Yee and R. J. Warming, "Implicit Total Variation Diminishing Schemes For Steady Flow Calculations," AIAA-83-1902, AIAA 6th Computational Fluid Dynamics Conference, Danvers, Massachusetts, July 1983.

superior resolution of shocks and flow discontinuities, compared, say, to the methods surveyed by Sod¹⁰ and Miner and Skop.¹¹ However, remapping from the Lagrangean to Euler variables requires, perhaps significant, extended computing time per cycle.⁵ Hence, it appears an unnecessary encumbrance.

The purpose, then, of this research is to reformulate Van Leer's algorithm in Eulerian fluid dynamics framework, revising as it becomes necessary, in order to achieve a more accurate, one-dimensional shock capturing algorithm, which could also be employed in two-dimensional calculations through fractional splitting of the equations of flow.

II. GOVERNING EQUATIONS

In strong conservation law form, the Euler equations for one-dimensional ideal compressible flow can be written

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial R} + G = 0 . \tag{1}$$

Here

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho E \end{bmatrix} \qquad F = \begin{bmatrix} \rho u \\ P + \rho u^{2} \\ (P + \rho E)u \end{bmatrix} \qquad G = \frac{\sigma}{R} \begin{bmatrix} \rho u \\ \rho u^{2} \\ (P + \rho E)u \end{bmatrix}$$
(2)

where σ = 0,1, or 2, in turn for cartesian, cylindrical, or spherical coordinates. R is the respective distance coordinate.

The fluid dynamic variables are:

- c = local speed of sound in fluid
- ρ = density
- u = velocity

^{10.} G. A. Sod, "A Survey of Several Finite Difference Methods For Systems of Hyperbolic Conservation Laws," <u>Journal of Computational Physics</u>, Vol. 27, pp. 1-31, 1978.

^{11.} E. W. Miner and R. A. Skop, "Explicit Time Integration For The Finite Element Shock Wave Equations," AIAA-82-0994, ASME/AIAA 3rd Joint Thermophysics, Fluids, Plasma and Heat Transfer Conference, St. Louis, Missouri, June 1982.

p = pressure

E = specific total energy

e = specific internal energy.

Here cp, c, are specific heats, and

$$\gamma = c_p/c_v$$

$$c^2 = \gamma P/\rho$$

$$P = (\gamma - 1) \rho e$$

$$E = e + \frac{u^2}{2}$$

III. GODUNOV METHODS

We shall derive the Godunov algorithm for the case of a uniform grid; however, the method is readily adaptable to encompass non-uniformity. By integrating Equation (1) over a typical space-time cell $R_i \leq R \leq R_{i+1}$; $t_n < t < t_{n+1}$ and applying Green's theorem for the plane, we arrive at the exact equation

$$\overline{U}^{i + \frac{1}{2}} = \overline{U}_{i + \frac{1}{2}} - \frac{\Delta t}{\Delta R} < F > \begin{bmatrix} i + 1 \\ -\frac{1}{\Delta R} \end{bmatrix} \int_{t_{n}}^{t_{n} + 1} \int_{R_{i}}^{R_{i} + 1} G dR dt.$$
 (3)

Here, superscript usage of a space index denotes advanced time level, while corresponding subscript usage denotes present time level: i.e.,

$$()^{i} = ()_{i,n+1}$$
 (4)
 $()_{i} = ()_{i,n}$

The space average over a cell, space-centered at R_{i} + $\frac{1}{2}$, is

$$\overline{U}_{i+\frac{1}{2}} = \frac{1}{\Delta R} \int_{R_{i}} U(R,t_{n}) dR, \quad \Delta R = R_{i+1} - R_{i};$$
(5)

while the time average flux on interface R = R; is

$$\langle F \rangle_{i} = \frac{1}{\Delta t} \int_{t_{n}}^{t_{n}+1} F(U(R_{i},t))dt, \quad \Delta t = t_{n+1} - t_{n}.$$
 (6)

Godunov's method can be made first-or second-order accurate, depending upon how the flux integrals, Equation (6) and the cell integral of G in Equation (3) are approximated.

A. First-Order Accurate Method

In Godunov's original derivation, 2 the function $U(R,t_n)$ is approximated with a piecewise constant function which on cell $R_i \le R \le R_{i+1}$ assumes the average value $\overline{U_{i+\frac{1}{2}}}$. Cell averages are updated to the next time level through approximating the integrals in Equation (3), by solving a Riemann problem at each cell interface. The Riemann problem entails the solution of Equation (1) for t>t, with $\sigma=0$ and with initial conditions at t = t given by:

$$V = \begin{cases} \overline{V}_{i+\frac{1}{2}}, & R > R_{i} \\ \overline{V}_{i-\frac{1}{2}}, & R < R_{i} \end{cases}$$
 (7)

where $V^T = (P, \rho, u)$. However, only the resulting values of V on the interface R_i are of interest. The primary mechanism for interaction of the discontinuity, Equation (7), is the propagation of expansion or compression waves away from the interface. The nonlinear equations which afford an iterative solution of the Riemann problem are well-documented in references 5, 10, and 12.

For purposes of numerical stability, the time step Δt is chosen to be such that propagation times are insufficient to allow waves from adjacent discontinuities to have influence on interface $R=R_1$. Then values

$$V_{i}^{\dagger} = \lim V(R_{i}, t)$$

$$t \rightarrow t_{n}^{\dagger}, \qquad (8)$$

^{12.} M. Holt, <u>Numerical Fluid Dynamics</u>, Springer-Verlag, Berlin, Heidelburg, New York, 1977.

obtained from solving the Riemann problem at each interface, together with cell average values, are used to approximate the integrals in Equation (3). Godunov's first-order accurate method results:

$$\overline{U}^{i+\frac{1}{2}} = \overline{U}_{i+\frac{1}{2}} - \frac{\Delta t}{\Delta R} \left[F(U_{i+1}^*) - F(U_{i}^*) \right] - \Delta t G(\overline{U}_{i+\frac{1}{2}}). \tag{9}$$

B. Second Order Method

For the second-order accurate Godunov method, primitive quantities stored at each time level are cell average $\overline{U}_i + \frac{1}{2}$ and interface differences $[V]_{i+\frac{1}{2}} = V_{i+1} - V_i$. The calculation of the average derivative is now possible:

$$(\overline{V}_{R})_{i+\frac{1}{2}} = \frac{\overline{\partial V}}{\overline{\partial R}_{i+\frac{1}{2}}} = \frac{1}{\Delta R} \qquad \int_{R_{i}}^{R_{i}+1} \frac{\partial V}{\partial R} dR = \frac{[V]_{i+\frac{1}{2}}}{\Delta R}.$$
 (10)

This affords a more accurate, piecewise linear function approximation: On a cell $R_i \leq R \leq R_{i+1}$,

$$V = \overline{V}_{i+\frac{1}{2}} + (\overline{V}_{R})_{i+\frac{1}{2}} (R - R_{i+\frac{1}{2}}) . \tag{11}$$

Corresponding inputs for the Riemann problem at interface R_i are, from Equation (11),

$$V_{i \pm} = \overline{V}_{i \pm \frac{1}{2}} + \frac{1}{2} [V]_{i \pm \frac{1}{2}}.$$
 (12)

The output from the Riemann problem, solved as previously, is the value

$$V_{i}^{\star} = \lim_{n \to t_{n}^{+}} V(R_{i}, t),$$

$$t \to t_{n}^{+}$$
(13)

which results immediately after the interface discontinuity is resolved. In addition, a value

$$V_{t}^{*} = \lim_{t \to t_{n}^{+}} \frac{\partial V}{\partial t} (R_{i}, t)$$
 (14)

for the corresponding resolved time derivative is to be obtained by auxiliary

means (see next section). As established by Van Leer, the interface approximation

$$V = V_{i}^{*} + (V_{t})_{i}^{*} (t - t_{n}) + 0 (\Delta t)^{2}$$
 (15)

can be applied to evaluate, with a higher order of accuracy, the flux integrals in Equation (3). The cell integral can be approximated, employing the trapezoidal rule, with

$$\int_{t_n}^{t_n+1} \int_{R_i}^{R_i+1} G dR dt =$$
 (16)

$$\frac{\Delta R}{2} \int_{t_n}^{t_{n+1}} [G(R_{i+1},t) + G(R_{i},t)] dt + 0 (\Delta R)^3$$

which now involves interface values. For a typical interface integral

$$\int_{t_n}^{t_n+1} G(U,R_i)dt = \frac{\Delta t}{2} [G(U^i,R_i) + G(U_i,R_i)] + O(\Delta t)^3.$$
 (17)

Advanced time level interface values are predicted by means of

$$V^{i} = V_{i}^{*} + (V_{i})_{i}^{*} \Delta t + 0 (\Delta t)^{2},$$
 (18)

and initial interface differences with

$$[V]^{i + \frac{1}{2}} = V^{i + 1} - V^{i}. \tag{19}$$

At the cost of additional storage and altered processing stream, after solution of the Riemann problem adjusted interface differences

$$[V]_{i+\frac{1}{2}}^{*} = V_{i+1}^{*} - V_{i}^{*}$$
 (20)

could be computed, to be used for more accurate evaluation of the interface time derivatives, described below. However, Van Leer does not appear to have used this device, and we have not verified whether the additional cost is justified.

C. Resolved Interface Initial Time Derivatives

For the compressible flow equations, Equations (1-2), compatibility relations along characteristics are,

$$\frac{dP}{dt} = c^2 \frac{d\rho}{dt} \tag{21}$$

on
$$\frac{dR}{dt} = u$$

$$\frac{du}{dt} \pm \frac{1}{\rho c} \frac{dP}{dt} = \pm \frac{\sigma uc}{R}$$
on $\frac{dR}{dt} = u \pm c$. (22)

To better insure correct transmission of signals, these Equations are differenced (spatially) as in Moretti's λ - scheme, 8 in order to obtain relations which can be solved for initial interface time derivatives. This differencing is given by the equations

$$\frac{\partial u}{\partial t_i}^* + \left(\frac{1}{\rho c}\right)_i^* \left(\frac{\partial P}{\partial t}\right)_i^* = -\left(u + c\right)_{i+} \left\{\frac{\partial u}{\partial R} + \frac{1}{\rho c} \frac{\partial P}{\partial R}\right\}_{i+} + \left(\frac{\sigma uc}{R}\right)_i^*$$
(23)

$$\frac{\partial u}{\partial t}^* - (\frac{1}{\rho c})_i (\frac{\partial P}{\partial t})_i = -(u - c)_{i-} \{\frac{\partial u}{\partial R} - \frac{1}{\rho c} \frac{\partial P}{\partial R}\}_{i-} - (\frac{\sigma uc}{R})_i^*$$
 (24)

$$\frac{\partial \rho}{\partial t_{i}}^{*} = \frac{1}{(c_{i}^{*})^{2}} \left\{ \frac{\partial \rho}{\partial t_{i}}^{*} + \left(u_{i}^{*} \frac{\partial \rho}{\partial R} \right)_{i \pm} \right\} - \left(u_{i}^{*} \frac{\partial \rho}{\partial R} \right)_{i \pm}$$
(25)

Where space derivative occur in Equations (23-29), average space derivatives are used, on the (\pm) side of an interface. Depending upon whether or not u is positive, up- or down-wind differencing is employed in Equation (25).

IV. COMPUTATIONAL RESULTS

The first and second-order Godunov methods previously discussed have been applied to the linear shock tube calculation reported by Miner and Skop. 11 Here, an infinite tube contains gas in two compartments initially separated by a diaphragm. Table I shows the respective initial conditions.

TABLE 1. LINEAR SHOCK TUBE DATA

$$P_0 = 1.$$
 $P_1 = .1$ $P_0 = 1.$ $P_1 = .125$ $P_0 = 0.$ $P_1 = .125$

The Godunov calculation is programmed to choose its own time step, in accordance with stepwise stability restrictions. The results after one hundred cycles, for the first-order accurate calculation, are displayed in Figures 3-6. Figures 4-5, in particular, show the smearing of shock structure due to the inherent numerical dissipation of the method, present even on this very fine grid.

The second-order accurate method is activated by a program switch. Figures 7-10 show the results after another one hundred cycles of calculation. An immediate sharpening of the shock is to be observed.

It seems to be a consensus of opinion that higher order methods for shock capturing are likely to be characterized by overshoot and oscillations behind the shock. Our results appear to be no exception. Van Leer's oscillation limiting techniques were attempted, as well as sparse use of numerical viscosity in the vicinity of the shock. For our code, the second approach seemed to give as good results as the first. Here, the Riemann solver provides a shock Mach number, which is a maximum at the point of inflection occurring within the structure of the physical shock. This provided a means for limiting application of artificial viscosity, to a few points either side, but concentrated more to the upstream side of the shock. For density and velocity, the artificial viscosity was chosen as

$$V = 10^{-3} \begin{cases} \frac{P_{i+1} - 2P_{i} + P_{i-1}}{P_{i+1} + 2P_{i} + P_{i-1}} \{V_{i+1}^{2} - 2V_{i} + V_{i-1}^{2}\}; \end{cases} (26)$$

^{13.} J. L. Steger, private communication.

The results of Figures 7-10 are calculated with this dissipation, which is of the order

$$V = 0 \ (10^{-6} \ \frac{\partial^2 V}{\partial R^2}) \ . \tag{27}$$

The effects seem to be a dampening of oscillations behind the shock, with no apparent degradation in crispness. However, the overshoot appears to persist, about 3% in error.

In order to see that the shock is propagating properly, the calculation with the second-order method has been allowed to continue to time t=.14. As reported by Miner and Skop, 11 at this time the shock front should have progressed to R=.75. Figures 11-12 verify that the shock front is approximately at this location.

V. SUMMARY AND CONCLUSIONS

First and second-order accurate Godunov methods for the numerical solution of ideal compressible flows with embedded shock waves have been formulated, programmed, and tested by means of a linear shock tube calculation. Results show an immediate improvement of the crispness in shock structure, for the higher order accurate method. The higher order method appears to have inherent overshoot at the shock, together with oscillations behind the shock. It appears mandatory to dampen these oscillations, by means of Van Leer-type oscillation limiting schemes, or else through addition of artificial viscosity restricted to a small region behind the shock. Surprisingly enough, for the present problem both schemes were found to give comparable results in this respect.

Perhaps we should mention how the present method differs from Van Leer's original version, 5 aside from the conversion to Eulerian fluid dynamics. Major differences are:

- a. Omission of some near-shock terms from Equations (23-24), heuristically added, perhaps to insure entropy increase at the shock.
- b. Use of Godunov's original nonlinear iteration scheme (References 2, 12) for the Riemann problem, versus Van Leer's more elaborate accelerated version. Although slower computationally, this scheme does distinguish between shock and compression waves; hence, it should be more accurate, as evidenced by the omission of (a).
- c. For the Lagrangean formulation, the contact surface in the Riemann problem lies along the cell interface. Hence, it is reasonable for Van Leer to employ separate left and right density $\rho_{i\pm}$ in calculating $\overline{\rho}_R$. However,

for the Euler version this practice does not appear as logical, since the contact surface can lie on either side of the cell interface. The result, and possibly the biggest drawback of the Euler version, is that contact surface resolution does not much improve, when going over to second-order accuracy.

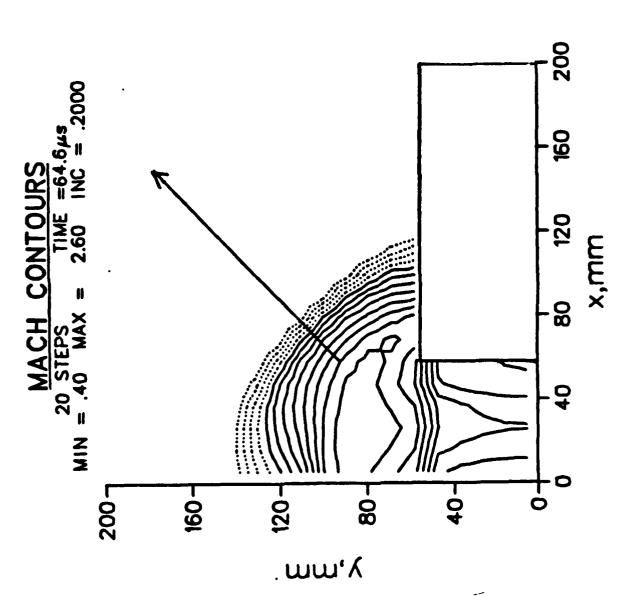
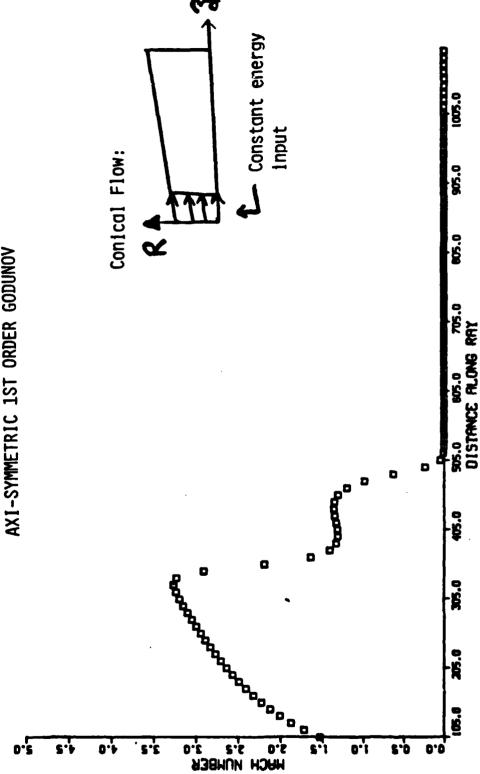


Figure 1. Two-Dimensional, Axis-Symmetric Muzzle Blast Calculation

AXI-SYMMETRIC 1ST ORDER GODUNOV MACH NUMBER ON RAY



Shock Smearing Typical of a First Order Accurate Godunov Calculation Figure 2.





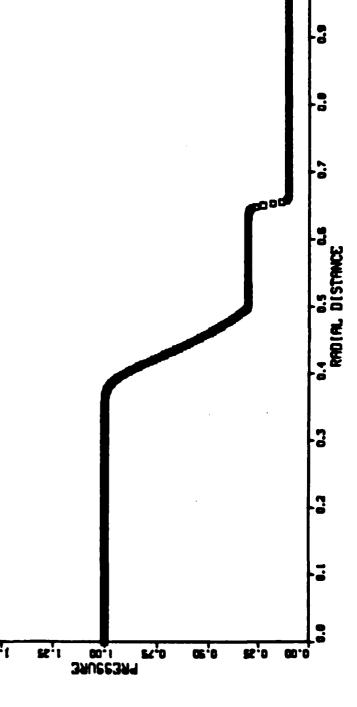


Figure 3. First Order Godunov Calculation

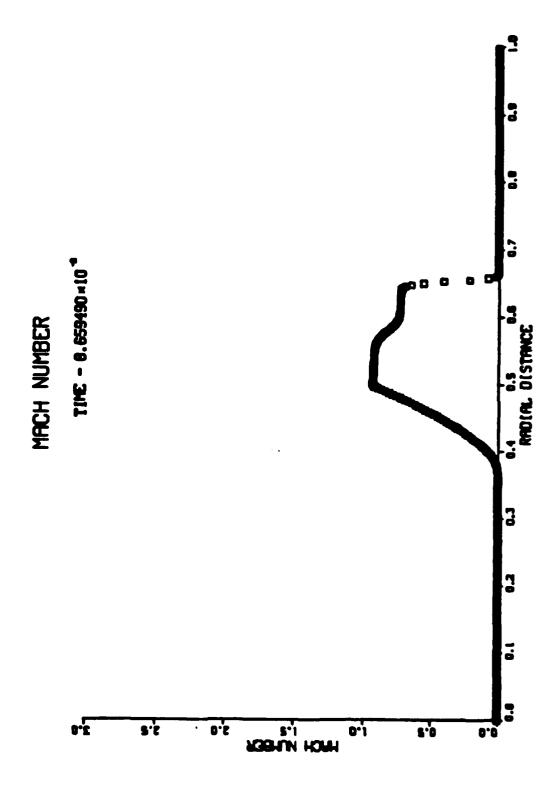


Figure 4. First Order Godunov Calculation



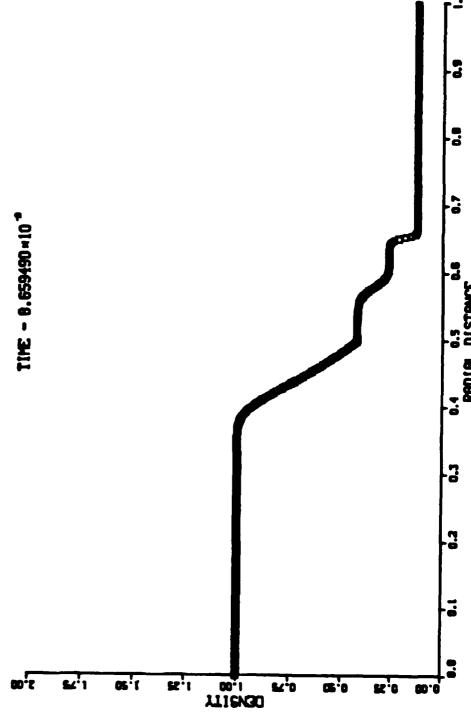
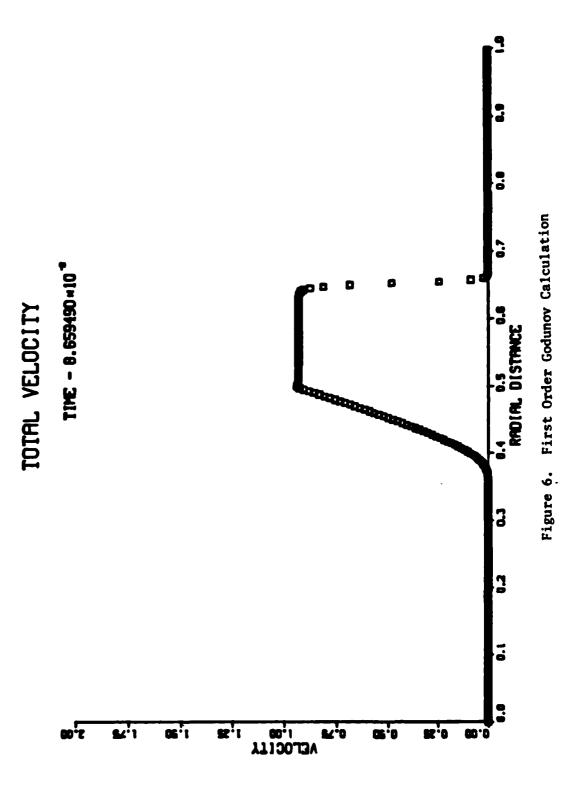


Figure 5. First Order Godunov Calculation





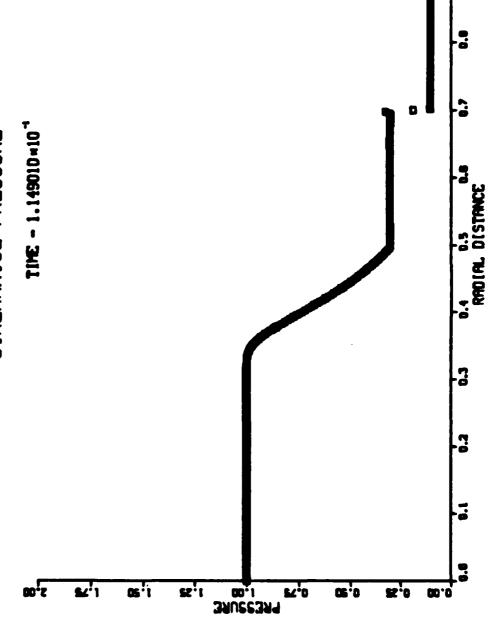


Figure 7. Second Order Godunov Calculation

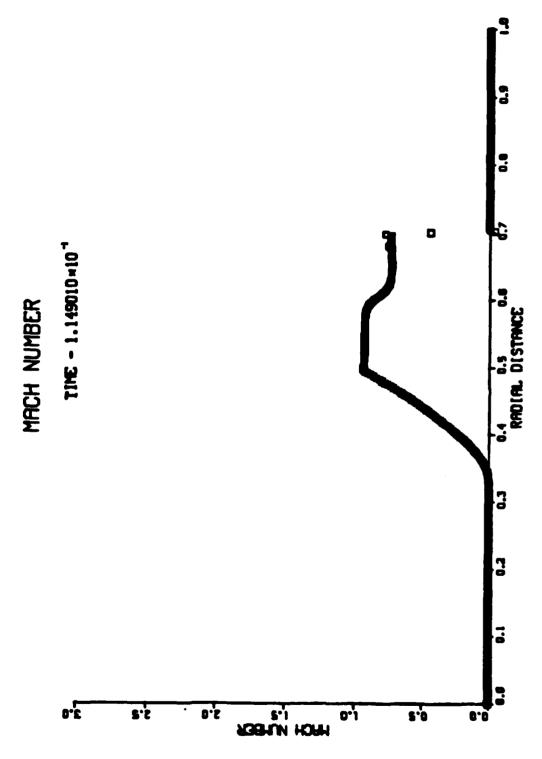


Figure 8. Second Order Godunov Calculation



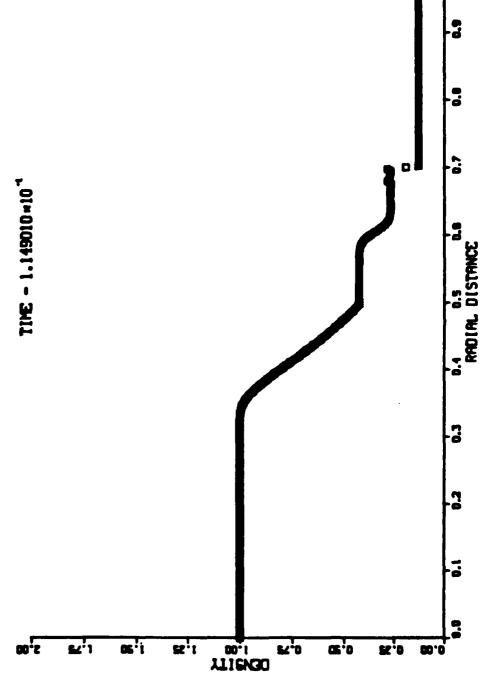


Figure 9. Second Order Godunov Calculation

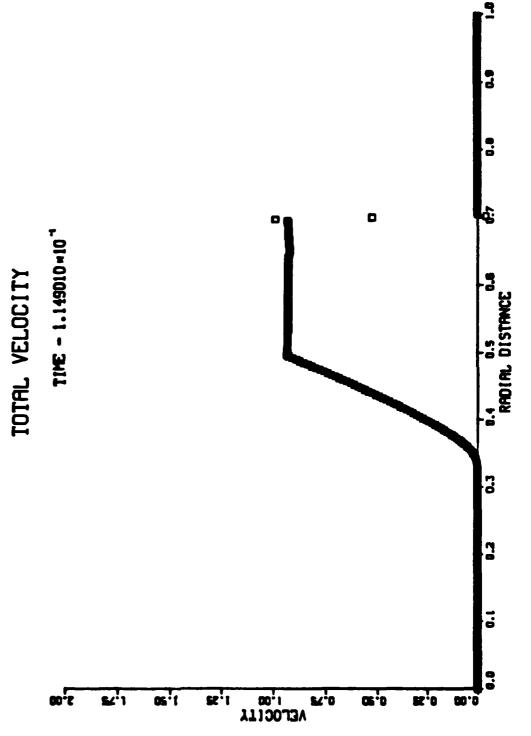


Figure 10. Second Order Godunov Calculation



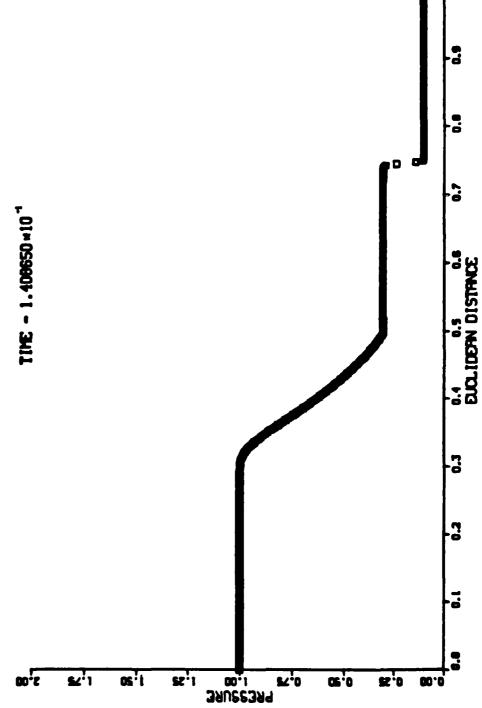
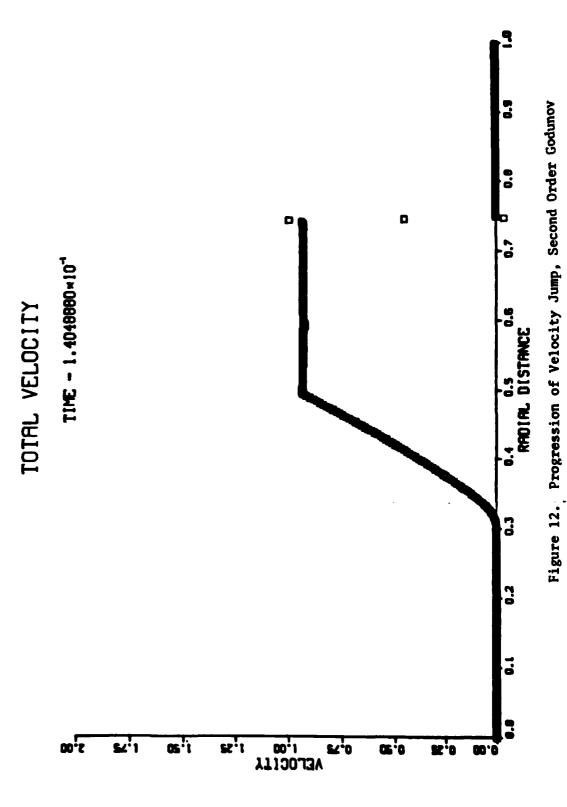


Figure 11. Progression of Pressure Jump, Second Order Godunov



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