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1

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AUTHOR(S): Weh Hc Lee and Paul P. Whalen

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Los Alamos National Laboratory
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CALCULATION OF SHOCK PROBLEMS BY USING FOUR DIFFERENT SCHEMES

by

Wen Ho Lee and Paul P. Whalen†

Summary

Results are shown of the use of several different shock treatments in one- and two-dimensional Lagrangian code calculations of strong shock problems with known solutions. The shock treatments are (A) von Neumann-Richtmyer artificial viscosity (B) Fixed length artificial viscosity; (C) Artificial energy diffusivity combined with artificial viscosity and (D) Modified Godunov. The similarity test problems are plane and spherical implosions followed through a reflection. The problems are generated in the codes by imposing an inward directed velocity at one boundary of an initially, quiescent, gamma law gas with the other boundary fixed. Results are shown for calculations on uniform and non-uniform meshes. On non-uniform meshes, no method gives good results although method D is probably superior. Method B produces good appearing results with much shock smearing for the initial shock transit but the worst results after shock reflection. On uniform meshes, method C does the best job of handling the effects of shock initiation at boundaries while method A produces the worst results. Method D results in the smoothest flow field with less over-or-under-shooting, Gibbs phenomena.

†Computational Physics Group
Applied Theoretical Physics Division
Los Alamos National Laboratory
Los Alamos, New Mexico, U.S.A.

INTRODUCTION

In 1950, von Neumann and Richtmyer [1] proposed the use of the artificial viscosity q for calculating shock wave propagaton in one-dimensional inviscid flow. It is well known that using the artificial viscosity introduces errors for shock wave propagation through material interfaces or non-uniform meshes [2]. At material interfaces, impedence matching reduces the errors. Other errors arise at shock start up and reflection boundaries. The q method was orginally derived for steady shock propagation in plane geometry so in taking the method over to curvilinear systems there is a question of whether to use grad u or div u (where u is the particle velocity). In non-tensor codes grad u should be used.

For shock propagation in variable zoning, Noh [3] proposed the use of the fixed length q. This method results in spreading a shock over a fixed physical length rather than a fixed number of zones. A linear term similar to Landshoff's [4] is added in this q. This technique computes the thermodynamic properties (e.g., density or pressure) very accurately for a particular direction of shock propagation but very badly for the other direction.

Use of an artificial energy diffusivity with the artificial viscosity improves solutions at reflective or non-flow moving boundaries. The other methods tend to give too high internal energy and too low density at boundaries.

The modified Godunov scheme, computes interface velocity and pressure through a Riemann solver. In uniform zoning and a single material, the formulation reduces to that of the regular Godunov scheme. In a varieble mesh or multi-material problem, the method has second order features.

I. BASIC GOVERNING EQUATIONS

The mass, momentum, and energy equations for one-dimensional flow in planes, cylinders and spheres are [5]:

$$V = R^{\alpha-1} \frac{\partial R}{\partial M} , \tag{1}$$

$$\frac{du}{dt} = -R^{\alpha-1} \frac{\partial P}{\partial M} , \text{ and} \tag{2}$$

$$\frac{dE}{dt} = - \frac{\partial P u R^{\alpha-1}}{\partial M} . \tag{3}$$

In Eqs. (1), (2), and (3), V is the specific volume, R the Eulerian radius, M the mass per unit length or unit of solid angle, u the particle velocity, t the time, α (= 1 for plane, = 2 for cylinder, = 3 for sphere), P the pressure, and E the total energy, Also,

$$E = I + \frac{1}{2} u^2 \quad , \tag{4}$$

$$\frac{dR}{dt} = u \quad , \quad \text{and} \tag{5}$$

$$dM = \rho R^{\alpha-1} dR \quad , \tag{6}$$

where I is the internal energy, ρ the density (= 1/V), and dM the element of mass per unit solid angle (for cylinder or sphere) or of surface (for plane). The two-dimensional Lagrangian calculations, are done in cylindrical coordinates. Define an area Jacobian J as:

$$J = R\,(R_\xi Z_\eta - R_\eta Z_\xi) \quad , \quad \text{where} \tag{7}$$

R: Eulerian coordinate in radial direction, $R = R(\xi,\eta,t)$
Z: Eulerian coordinate in axial direction, $Z = Z(\xi,\eta,t)$
ξ: Lagrangian coordinate, at t = 0, $\xi = R(\xi,\eta,0)$,
η: Lagrangian coordiante, at t = 0, $\eta = Z(\xi,\eta,0)$,
and $R_\xi = \frac{\partial R}{\partial \xi}$ etc.

The mass, momentum and energy equation in two-dimensional Lagrangian form can be written as;

$$\rho J = M \quad , \tag{8}$$

$$\frac{du_R}{dt} = -V\frac{\partial P}{\partial R} \quad , \tag{9}$$

$$\frac{du_Z}{dt} = -V\frac{\partial P}{\partial Z} \quad , \quad \text{and} \tag{10}$$

$$\frac{dI}{dt} = -P\frac{dV}{dt} \quad . \tag{11}$$

In Eqs. (9) and (10), u_R and u_Z are the material velocities in the R and Z directions.

In general the artificial viscosity, q, can be described as combinations of terms linear and quadratic in Δu. The quadratic term concentrates the artificial viscosity near the shock front while the effect of the linear term is more diffuse. A purely linear form of q will result in a large overshoot in energy behind a shock followed by rapid damping. A purely quadratic form will result in a smaller overshoot followed by undamped oscillations. Some of the q's used for one-dimensional problems are:

1. RICHTYMER -VON NEUMANN (1950) [1]

$$q = -a^2 \rho \Delta u |\Delta u| , \qquad (12)$$

2. ROSENBLUTH (1950) [6]

$$q = a^2 \rho (\Delta u)^2 , \qquad \partial u/\partial x < 0 , \qquad (13)$$

3. LANDSHOFF (1955) [4]

$$q = a^2 \rho (\Delta u)^2 - 0.5 \rho C_s \Delta u [b + (1 - b) C_s \Delta t/\Delta x] , \qquad \partial u/\partial x < 0 , \qquad (14)$$

where $0 < b < 1$ and C_s is the sound speed

4. PIC (1957) [7]

$$q = -a \rho \Delta u |\bar{u}| , \qquad \partial u/\partial x < 0 , \qquad (15)$$

5. SCHULZ (1963) [8]

$$q = -b \rho \Delta u |0.5(\Delta u_{i+1} - \Delta u_{i-1})| , \qquad \partial u/\partial x < 0 , \qquad (16)$$

6. KUROPATENKO (1967) [9]

$$q = 0.5(\gamma + 1) \rho (\Delta u)^2 - \rho C_s \Delta u , \qquad \partial u/\partial x < 0 , \qquad (17)$$

7. AFWL-PUFF (1968) [10]

$$q = a^2 \rho (\Delta u)^2 - b \rho C_T \Delta u , \qquad \partial u/\partial x < 0 , \qquad (18)$$

where C_T is the isothermal sound speed

8. QLQ (1970) [11]

$$q = a^2 \rho (\Delta u)^2 + 50. b^2 \rho (\Delta u)^2/(1 + 50. |\Delta u|) , \qquad \partial u/\partial x < 0 , \qquad (19)$$

9. WHITE (1973) [12]

$$q = a^2 \rho (\Delta u)^2 (|\Delta P/(\rho C_s \Delta u)|)^{0.5} - b \rho C_s \Delta u (|\Delta P/(\rho C_s \Delta u)|)^{0.25} , \qquad \partial u/\partial x < 0 , \qquad (20)$$

10. WINKLER (1978) [13]

$$\vec{q} = a^2 \rho \nabla . \vec{u} [\nabla u - \nabla \cdot \vec{u}/3] , \qquad \nabla \cdot \vec{u} < 0 , \qquad (21)$$

11. AND NOH FIXED LENGTH (1980) [3]

$$q = a^2 \rho (\Delta x_{max})^2 (\Delta u/\Delta x)^2 - b \rho C_s \Delta x_{max} \Delta u/\Delta x , \qquad \partial u/\partial x < 0 , \qquad (22)$$

In the two-dimensional calculations q is computed only when the cell is compressing. Eq. (1) in the two-dimensional calculations is

$$q = 1.4\ \rho A \left[\frac{V^n - V^{n-1}}{V^n \Delta t} \right]^2 \text{ where A is the area.} \qquad (23)$$

For methods A, B, and C, the artificial viscosity calculations, the pressure P in Eqs. (2), (3), (9), (10), and (11) is replaced by P + q. (Note that in tensor hydrodynamics, Schultz [8] and Winkler [13], the equations change in curvilinear coordinates.)

Because it was noticed that the standard artificial viscosity methods produced poor answers when following a shock through a variable mesh, Gee, Kramer, and Noh [3] suggested the use of the fixed length q, method B, which spreads a shock over a fixed length rather than a fixed number of zones. The coefficients a and b in Eq. (22) are empirically related to the zone ratio Z.

$$Z = \frac{\Delta X^{\circ}_{i-1/2}}{\Delta X^{\circ}_{i+1/2}} \qquad (24)$$

where i is the grid number defined at cell edge and Z is defined at t = 0.

The Richtmyer-von Newmann q was orginally derived from considerations of a plane shock running in a mesh where both sides of a cell could respond to the shock. As this condition is not satisfied at a programmed boundary, the entropy production in boundary cells is too large, Landshoff [4]. To correct this, Noh [14] suggests the use of an artificial heat diffusivity, method C. An artificial heat flux H is added to the right hand sides of the energy equations, Eqs. (3) and (1.). For the two-dimensional calculations,

$$H = C_H \left(\frac{\partial I}{\partial R^2} + \frac{\partial I}{\partial Z^2} \right) \qquad (25)$$

The C_H should be at least dependent on coefficient a e.g., see Eq. (12) and zone ratio Z (in case of non-uniform zoning).

For one-dimensional problems, Noh [14] suggests that

$$H = h_o^2 \rho\ \Delta u\ \Delta I + h_1 \rho C_s \Delta I \quad \text{when } \partial u/\partial x < 0 \qquad (26)$$

and h_o and h_1 are constants.

In the q-free modified Godunov method D discussed here, the one-dimensional Lagrangian equation is solved

$$\frac{\rho d(\vec{W})}{dt} + \frac{\partial[\vec{F}(\vec{W})]}{\partial x} = \vec{S} \quad , \tag{27}$$

where $\vec{W}$ represents specific volume V, velocity u, and the total energy E in the cell (i-1/2). The flux term $\vec{F}$ represents -u P and Pu at the cell boundary (i). $\vec{S}$ is a vector of possible source terms. With initial conditions $\vec{W}^n_{i-1/2}$ at cell center a Riemann problem is solved to get the flux at the cell boundary $\vec{F}_i^{n+1/2}(\vec{W})$. Then

$$\vec{W}^{n+1}_{i-1/2} = \vec{W}^{n}_{i-1/2} - \left(\vec{F}_i^{n+1/2} - \vec{F}_{i-1}^{n+1/2}\right)\frac{\delta t}{\Delta x} \quad . \tag{28}$$

At t = n+1/2, in compression the pressure P* and velocity u* at the interface are related by two Hugoniot relations to the adjacent cells:

$$P_i^* = P^n_{i\pm 1/2} + 0.25\, \rho^n_{i\pm 1/2}(\gamma + 1)(u_i^* - \bar{u}^n_{i\pm 1/2})^2$$

$$\pm \Big[(u_i^* - \bar{u}^n_{i\pm 1/2})^2\, \gamma P^n_{i\pm 1/2}\, \rho^n_{i\pm 1/2}$$

$$+ \rho^{n^2}_{i\pm 1/2}(u_i^* - \bar{u}^n_{i\pm 1/2})^4(\gamma + 1)^2/16\Big]^{1/2} \tag{29}$$

The two unknowns, P_i^* and u_i^*, in these two equations can be solved in any desired manner. We do a three step iteration. The $\bar{u}^n$ defined at the cell center, is a cell average velocity which we take as a free parameter to partition total energy between the kinetic energy and internal energy. The P_i^* and u_i^* depend on the density, the local velocity and γ. For a nonideal fluid, γ must be the effective γ.

For non-uniform meshes, a zone ratio Z is defined depending on the direction of wave motion in the mesh.

$$Z_{i-1/2} = \begin{cases} \rho\Delta X_{i-1/2}/\rho\Delta X_{i-3/2} & \text{grad } P < 0 \\ \rho\Delta X_{i-1/2}/\rho\Delta X_{i+1/2} & \text{grad } P > 0 \end{cases} \tag{30}$$

The momentum equation is solved for $\delta u = u^{n+1} - u^{n}$

$$\delta \overline{u}_{i-1/2} = - \frac{\delta t (P^*_{i-1} - P^*_{i})}{(\rho \Delta X)_{i-1/2}} \quad Z^{\alpha}_{i-1/2} \tag{31}$$

$$I^{n+1}_{i-1/2} = I^{n}_{i-1/2} - \mathrm{div}(P^* u^*)/M_{i-1/2}$$

$$- \left[\left(\frac{\overline{u}^{n+1} + \overline{u}^{n}}{2} \right) \delta \overline{u} \; Z^{\beta - \alpha} \right]_{i-1/2} \tag{32}$$

For the result shown, $\alpha = o$, $\beta = 1/2$.

III. SAMPLE PROBLEM CALCULATIONS

First, we show comparisons of this q-free Godunov method with the Richtmyer von Neumann scheme. The calculation is for a plane piston moving from right to left with a velocity of $u = -1.0$ against an initially cold ideal gas of density $\rho^{\circ} = 100$. The left boundary is rigid.

Figure 1a shows the piston calculation before shock reflection. The initial density of 100 has quadrupled behind the shock. The Richtmyer and Von Neumann method with $a = 2$ and no linear term has oscillations behind the shock which are much reduced in the Godunov scheme.

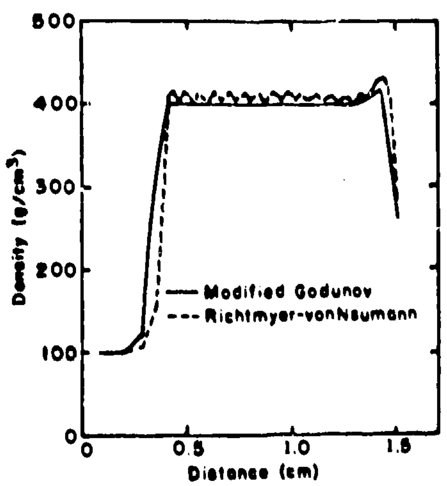

Fig. 1-a Density Profile before Reflection

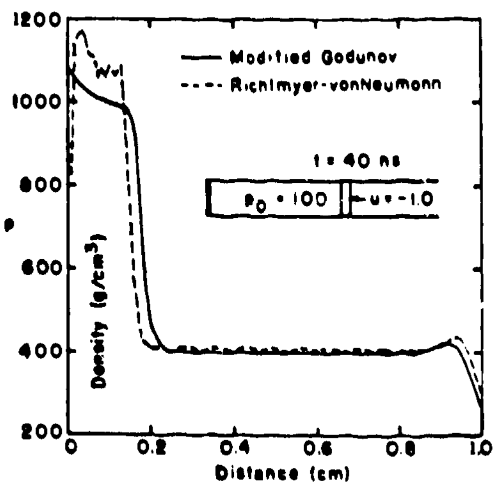

Fig. 1-b Density Profile after Reflection

Figure 1b shows the density profile after shock reflection. The figure shows again that the modified Godunov scheme calculates a smoother density, closer to the analytic solution of 1000. The Richtmyer-von Neumann front is a little behind. In general, the various methods calculate pressure well, therefore the errors in density are reflected in the calculated energy.

Figures 2a and 2b show the piston problem in a non-uniform mesh. The initial zoning was coarse at the boundaries decreasing uniformly (R = 1.15) to the center. This is Noh's problem [3]. In Figure 2a, the shock has just passed through the minimum zone area. Neither method A or D does well (the density behind the shock should be 400), although the modified Godunov scheme does a little better. The shock velocity calculated with the modified Godunov scheme agrees with the anlaytic solution, but the shock calculated with the Richtmyer-von Neumann scheme is a little behind again.

The calculation using Noh's fixed length q agrees very well with the analytic solution at this time. Figure 2b shows the density profile after shock reflection. The fixed length q method has become a diffusion solution for u and has lost all relation to the analytic solution $\rho/\rho^{\circ} = 10$.

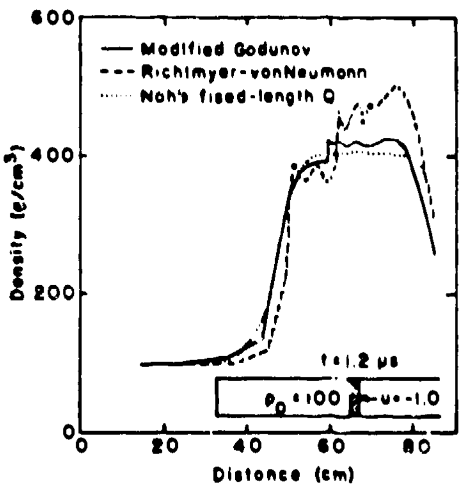

Fig. 2-a Density Profile with Variable Mesh before Reflection

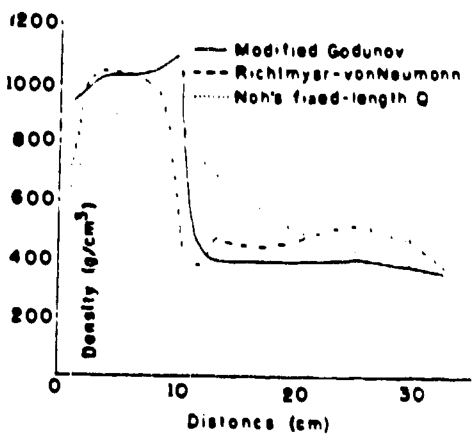

Fig. 2-b Density Profile with Variable Mesh after Reflection

The next problem shown is a spherical convergent shock reflecting from the origin; initial conditions are, $\rho^\circ = 1$, $E^\circ = 0$, $P^\circ = 0$, and $u^\circ = 0$. Material is ideal gas with $\gamma = 5/3$. Boundary conditions in the form $R_T(t)$ and $\dot{R}_B(t)$ are given in Table I. Shock collapse occurs at t = 440 μsec. The analytic solutions are obtained by the similarity method.

Figure 4 shows the pressure profiles at time t = 420 μsec calculated by the two-dimensional code before shock collapse. The calculation with heat conduction is much better. Both over-calculate pressure in the shocked region.

TABLE I

SIMILARITY BOUNDARY CONDITIONS

Time(μsec)	Radius(cm)	Velocity(cm/μsec)
0.	6.0000	-.00705
20.	5.8585	-.00708
40.	5.7167	-.00711
60.	5.5743	-.00714
80.	5.4308	-.00717
100.	5.2869	-.00721
120.	5.1423	-.00724
140.	4.9972	-.00727
160.	4.8515	-.00730
180.	4.7055	-.00732
200.	4.5589	-.00734
220.	4.4121	-.00735
240.	4.2649	-.00736
260.	4.1177	-.00736
280.	3.9707	-.00735
300.	3.8238	-.00733
320.	3.6775	-.00730
340.	3.5319	-.00726
360.	3.3874	-.00720
380.	3.2438	-.00712
400.	3.1024	-.00702
420.	2.9633	-.00689
440.	2.8273	-.00672
460.	2.6951	-.00650
480.	2.5677	-.00622
500.	2.4471	-.00578
520.	2.3329	-.00544
540.	2.2278	-.00492
560.	2.1344	-.00430
580.	2.0560	-.00350

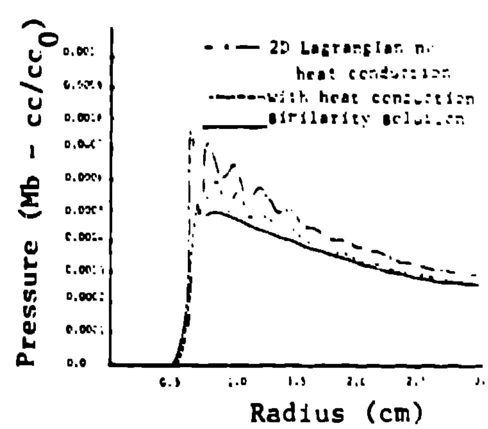

Fig. 4 Pressure profile in sphere at time t = 420 μsec.

Figures 5 and 6 show the pressure profiles at time t = 460 μsec after the shock has reflected from the center in the two-dimensional Lagrangian calculations. Without artificial heat diffusivity, the maximum pressure may be off by more than 133 percent; with the artificial heat diffusivity, it is in error by 20 percent. In addition, the shock front position is much closer to the similarity solution.

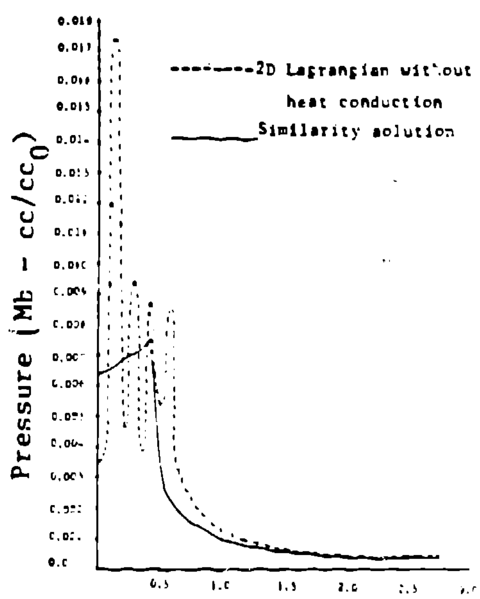

Fig. 5 Pressure profile at time t = 460 μsec for 2D Lagrangian code.

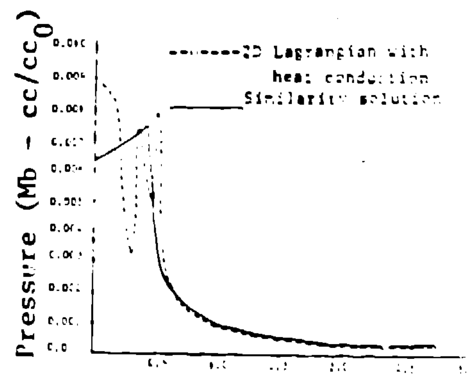

Fig. 6. Pressure profile at time t = 460 μsec for 2D Lagrangian code with heat conduction.

IV. CONCLUSION AND DISCUSSION

In solving problems of shock generation and propagation by numerical integration, the most popular method has been to add artificial iscosity to smear the shock front (or any discontinuity). For 30 years many researchers have tried to invent new forms of q with magical properties for their problems. Others have tried to solve shock problems without an entropy generation mechanism. Tests of the myriad forms of q with claimed magical properties are not shown. No magical properties will overcome the basic first order in space nature of the prevailing codes. As shown in the previous section, the modified Godunov scheme gives better calculations. For non-uniformly zoned problems, a clever choice of coefficients a and b of Eq. (22) may produce good results for the first shock passage but not for multiple shocks or reflected shocks. However, since artificial viscosity is still very popular, we recommend the artificial heat flux mechanism to couple with the q term. The appropriate relation between q and the flux can be taken from statistical mechanics.

Recently developed methods such as adaptive grid, moving finite element, Glimm's Riemann method, piecewise-parabolic method, and local mesh refinement are all of q-free type methods. Most of these methods show good results for one-dimensional shock problems and some of them may have a practical application for two-dimensional geometry especially when solving problems with multiple materials. We recommend pursuing techniques such as the fully second order Godunov scheme.

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