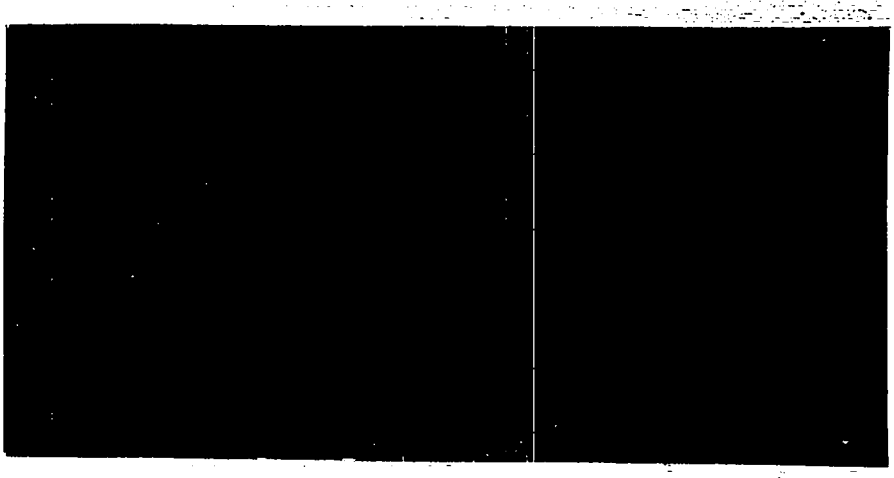
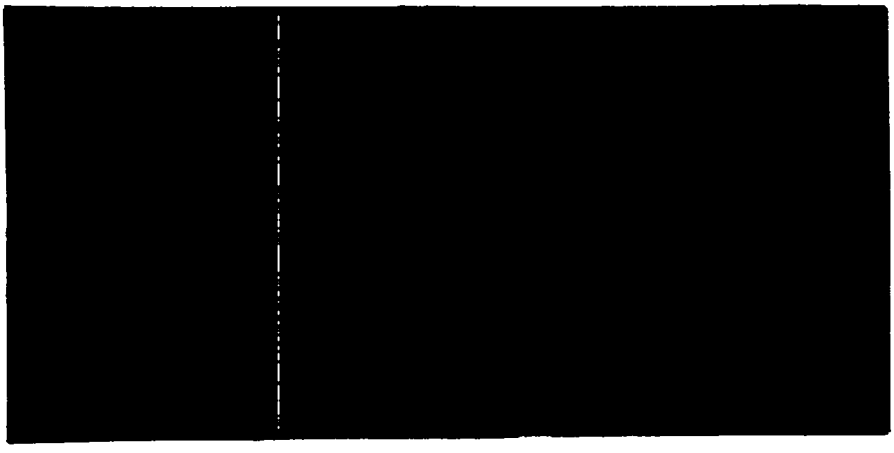
LOS ALAMOS SCIENTIFIC LABORATORY

OF THE UNIVERSITY OF CALIFORNIA

LOS ALAMOS, NEW MEXICO



CONTRACT W-7405-ENG.36 WITH THE
U.S. ATOMIC ENERGY COMMISSION



Copy # 19

LOS ALAMOS SCIENTIFIC LABORATORY
of the
UNIVERSITY OF CALIFORNIA

Report written:
September 27, 1954
Report distributed: MAR 2 8 1955

LA-1867

A METHOD FOR THE NUMERICAL SOLUTION OF TRANSIENT HYDRODYNAMIC SHOCK PROBLEMS IN TWO SPACE DIMENSIONS

by
Harwood G. Kolsky

PHYSICS

ABSTRACT

A method for numerically solving hydrodynamic problems involving two space dimensions and time is developed based on the von Neumann-Richtmyer method of treating shocks. Finite difference equations for the system are constructed from the basic differential equations of hydrodynamics. Difference formulas are also given for checking the stability of the space-time mesh, and for checking the total energy of the system. The results of four sample shock problems are presented. The requirements imposed on electronic computers by problems of this type, and possible extensions of the method to other types of physical problems, are discussed briefly.

ACKNOWLEDGMENTS

I wish to thank Dr. George N. White, Jr., of Los Alamos for many stimulating discussions which we have had concerning these and other calculations. I also wish to thank Prof. George F. Carrier of Harvard University and Prof. Otto Laporte of the University of Michigan, who while consultants at Los Alamos expressed interest in these calculations and offered a number of very helpful suggestions concerning possible applications and improvements of the method.

CONTENTS

I. INTRODUCTION

During the past five years there have been two major developments which have made the detailed numerical step-wise solution of transient hydrodynamic problems involving shocks feasible. One was the theoretical development by von Neumann and Richtmyer (Ref. 1) of a method for greatly simplifying the computation of hydrodynamic shocks. The other was the engineering development of high speed electronic computers, which have made truly astonishing progress in speed and capability during this period. (Ref. 2)

Although it has always been possible in principle to calculate numerically the motion of shocks in transient problems by solving the Rankine-Hugoniot conservation equations step-wise in time, in practice this becomes extremely difficult if more than one shock is present or if there are complicated boundaries in the problem. The von Neumann-Richtmyer method uses a pseudo-viscosity term added to the pressure which has the effect of broadening a shock in space and time so that it need no longer be treated as a discontinuity. Yet the final values of volume, pressure, velocity, etc., of the fluid after the passage of the artificially broadened shock are those which satisfy the Rankine-Hugoniot conditions for a true sharp shock. It is hard to overemphasize the importance for computing, particularly on automatic machines, of not having to worry ahead of time about all cases of shocks interacting with boundaries, rarefactions and other shocks which may arise in a given problem and to make special allowances for each.

Concerning electronic computers, not much need be said here except that without the existence of machines such as the IBM 701, one would never attempt calculations of the type described here except under real emergency conditions. The future of the numerical solution of partial differential equations in general, which require the error-free execution of millions of arithmetic steps, is very closely tied to the future development of faster and larger computers. (See Sect. V)

From time to time, a number of people have worked on different phases of the problem of extending the von Neumann-Richtmyer method to transient problems and to more dimensions. (Ref. 3) Roughly speaking the method described in this paper is more specialized than those sought by others; however, for problems to which it can be applied, it has a considerable advantage in simplicity and speed over more general procedures.

II. THE BASIC EQUATIONS OF HYDRODYNAMICS

A. The Equation of Continuity (Ref. 4)

Considering fluid motion in three dimensions, one may represent the original Lagrangian coordinates of a fluid element as (x,y,z) and the Eulerian coordinates as (X,Y,Z). The Eulerian coordinates which may be considered as functions, $X = X(x,y,z,t)$, give the positions at time t of fluid elements which were originally at (x,y,z). (Ref. 5) The law of conservation of mass in such a system becomes

$$\frac{V}{V_o} = \frac{\partial(X,Y,Z)}{\partial(x,y,z)} \quad \text{independent of time} \tag{1}$$

where $V = 1/\rho$ is the specific volume of the fluid element (volume/unit mass), V_o is the original specific volume in the Lagrangian system, and the right hand term is the Jacobian of the transformation from the original coordinate system to the one given by (X,Y,Z).

In one space dimension this reduces to

$$\frac{V}{V_o} = \frac{\partial X}{\partial x} \tag{2}$$

In two space dimensions, in rectangular coordinates, it is

$$\frac{V}{V_o} = \frac{\partial X}{\partial x}\frac{\partial Y}{\partial y} - \frac{\partial X}{\partial y}\frac{\partial Y}{\partial x} \tag{3}$$

B. The Equation of Motion

Using the von Neumann-Richtmyer method, the equation of motion for a fluid may be written

$$\frac{\partial^2 \vec{R}}{\partial t^2} = - V \text{ Grad}(p + q) = - V \text{ Grad } P \tag{4}$$

where $\vec{R}$ is the position vector of point (X,Y,Z), t is time, p is the fluid pressure due to its state equation, and q is the pseudo-viscosity pressure term. For convenience, capital P will be used for the sum of p and q for the remainder of this report.

In one space dimension, this equation becomes

$$\frac{\partial^2 X}{\partial t^2} = - V \frac{\partial P}{\partial X} \tag{5}$$

If one uses the equation of continuity, Eq. 2, it may be written

$$\frac{\partial^2 X}{\partial t^2} = - V_o \frac{\partial P}{\partial x} \tag{6}$$

This form is usually preferable for numerical work because the quantities V_o and ∂x are independent of time.

In two space dimensions, the equations of motion may be written as

$$\frac{\partial^2 X}{\partial t^2} = - V \frac{\partial P}{\partial X}$$
$$\frac{\partial^2 Y}{\partial t^2} = - V \frac{\partial P}{\partial Y} \tag{7}$$

In this case, using the equation of continuity (Eq. 3) results in equations

$$\frac{\partial^2 X}{\partial t^2} = - V_o \left(\frac{\partial P}{\partial x} \frac{\partial Y}{\partial y} - \frac{\partial P}{\partial y} \frac{\partial Y}{\partial x} \right)$$

$$\frac{\partial^2 Y}{\partial t^2} = - V_o \left(\frac{\partial P}{\partial y} \frac{\partial X}{\partial x} - \frac{\partial P}{\partial x} \frac{\partial X}{\partial y} \right) \qquad (8)$$

Although the quantities ∂x, ∂y, and V_o are independent of time as in the one dimensional case, the equations have become considerably more complicated by the transformation. In the present calculations it was found to be easier to work with the original equations (7) directly.

C. The Equation of Energy Conservation

Assuming no heat source terms in the fluid, the von Neumann-Richtmyer form of the energy conservation equation is

$$dE = - (p + q)\, dV = - P\, dV \qquad (9)$$

where E is the specific internal energy of the fluid (energy/unit mass)

Since the energy is a point function, not depending on space gradients, this equation has the same form regardless of the number of dimensions considered.

D. The Equation of State

In addition to the above three fundamental conservation equations, one needs the state equation for the fluid being used, preferably in the form

$p = p(V,E)$ since E occurs directly in Eq. 9 . For a gamma law gas, this form is quite simple.

$$p = (\gamma - 1)\frac{E}{V} \tag{10}$$

E. The Conservation or Increase of Entropy

The law of conservation or increase of entropy is automatically satisfied by the energy equation (Eq. 9), provided the equation of state for p satisfies certain physically realistic conditions (Ref. 4), which are certainly satisfied by the gamma law gas assumed here. Note that the term $-q\,dV$ corresponds to the usual $T\,dS$ in Eq. 9. This helps emphasize the fact that entropy increases occur only in shocks where q is significant and is constant elsewhere.

F. Definition of the Pseudo-viscosity Term

One would expect the pseudo-viscosity pressure to be a point function like the energy and true pressure, and thus independent of the number of dimensions being considered. However, it may or may not be, depending on the definition used in the problem. The usual definition is

$$q = \frac{b(\rho_o\, l)^2}{V}\left(\frac{\partial V}{\partial t}\right)^2 \qquad \text{for } \frac{\partial V}{\partial t} < 0$$

$$q = 0 \qquad \text{for } \frac{\partial V}{\partial t} \geqslant 0 \tag{11}$$

The latter equation is to prevent unnecessary smearing of rarefaction waves.

For some calculations it is more convenient to use a definition based on material velocity.

$$q = \frac{b\,l^2}{V} \quad (\text{div } \vec{v})^2 \qquad \text{for div } \vec{v} < 0$$

$$q = 0 \qquad \text{for div } \vec{v} \geqslant 0 \tag{12}$$

where $\vec{v}$ is the velocity of the fluid, l is a characteristic length for the finite difference scheme being used--usually the mesh size, and b is called the "shock width constant" since it determines the number of lengths l the broadened shock will cover in the calculation.

Although the two definitions are equivalent differentially, in finite differences Eq. 11 is the same in one or two dimensions, whereas Eq. 12 changes form since the div $\vec{v}$ term involves spacial derivatives. Equation 12 is usually more convenient when the Eulerian form of the equation of continuity is used in the calculation, since the term div $\vec{v}$ is then already available; otherwise, Eq. 11 is the easier to compute.

G. The Total Energy Check

When accompanied by proper initial conditions, the above equations are sufficient to describe the behavior of a compressible fluid system as a function of time. It is often convenient to calculate other quantities which are not necessary to the calculation, but which are very useful in interpreting results or in guarding against numerical errors. The total

energy check has been particularly useful in this connection.

$$T = \int_{vol} (\tfrac{1}{2} v^2 + E)\rho \, d\tau \tag{13}$$

If the total energy of the system is changing because of work being done on it from the outside (e.g. the piston in Prob. A described below), this work done may be computed and compared with the change in T as a check.

$$W = -\int_0^t \int_{surf} P \vec{v} \cdot d\vec{\sigma} \, dt$$

$$\delta T = T(t) - T(0) - W(t) \tag{14}$$

where δT is the error due to the inexactness of the numerical calculation.

As long as δT remains small and does not change rapidly from one time step to the next, one may be fairly confident that no random machine error has occurred, although there are certainly types of errors which will not be caught in this manner.

H. The Stability Condition Check

Another quantity of particular interest to the numerical solution of hyperbolic differential equations is the criterion for stability of a finite difference mesh. (Ref. 6) In the present calculations a stability criterion derived by George N. White, Jr., (Ref. 7) especially for the

von Neumann-Richtmyer equations was used.

$$w = \left\{ \left(\frac{c\Delta t}{\Delta \vec{R}} \right)^2 + 4b \frac{|\Delta V|}{V} \right\}^{\frac{1}{2}} \leq 1 \quad \text{for stability} \tag{15}$$

where c is the sound speed in the fluid, $\Delta \vec{R}$ and Δt are space and time mesh spacings respectively, and ΔV is the change in volume from one time cycle to the next.

The second term in the expression will ordinarily dominate in the vicinity of a shock, while the first term will dominate elsewhere.

III. THE DIFFERENCE EQUATIONS

Although most workers involved in computing problems of this type can agree on the differential equations to be solved, there is considerable divergence of opinion as soon as one begins to discuss difference equation formulations. In the absence of any reliable theoretical norm by which one can predict the accuracy and convenience of a finite difference method, the best criterion still seems to be experimentation.

Fig. 1 shows a schematic of the two dimensional space mesh used here. Fig. 1a is the original Lagrangian mesh, which may be taken rectangular as shown or may be some other quadrilateral, such as combinations of parallelograms or trapezoids, if these are more convenient. Fig. 1b shows the same mesh as it might appear at a later time in the problem.

Quantities denoting spacial positions and velocities are calculated as belonging to mass points located at the intersections of the mesh lines. The mass associated with the mass point is taken to be one-quarter of the mass of fluid enclosed by its four neighboring quadrilaterals. The mass points and the quantities associated with them are labeled by subscripts (i,j), which refer respectively to the column and row of the mesh where the point is found.

Quantities such as volumes, pressures, and energies are considered as being situated at the centroids of the areas between the mesh lines. These locations are denoted by subscripts $(i+\frac{1}{2}, j+\frac{1}{2})$. The time steps at which the above quantities are calculated are denoted by superscripts n, $n+1$, etc., where $n+1$ means $n+\Delta n$.

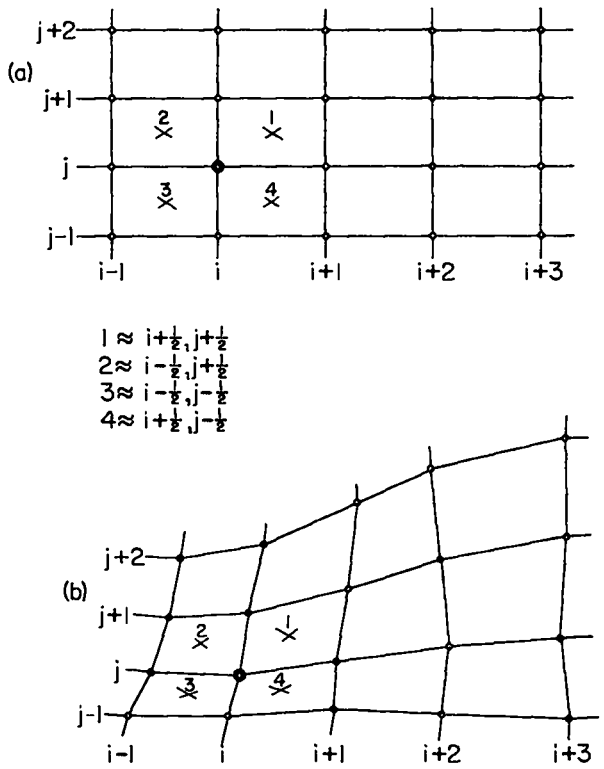


Figure 1

Schematic of the finite difference space mesh, where (a) shows the original Lagrangian mesh at time $t = 0$ and (b) shows the same mesh as it might appear at a later time (Eulerian). The mass points are located at the intersections of the mesh lines and are labeled i, j. Quantities related to volumes, pressures, and energies are located at the centroids of the quadrilaterals and are labeled $i+\frac{1}{2}$, $j+\frac{1}{2}$, marked with X's above.

All the difference equations are designed to be correct to first order approximations only. For example, note in Fig. 1b that the curves connecting the mass points are taken as straight lines. Using the true curves given by the Jacobian of the transformation (assuming it were known) instead of the straight lines would result in second order changes in the volumes calculated. These and all other second order effects are assumed to be negligible, provided the fluid is reasonably continuous over distances the order of two or three mesh spacings. Since the shock width constant b in Eq. 11 is chosen such that a true discontinuous shock is spread over about three mesh spaces, this gives a sort of "limit of resolution" of the method consistent with using only first order terms in the difference equations.

A. The Equation of Continuity

The relative specific volumes (V/V_o) are taken as being the ratios of the areas of the distorted quadrilaterals of Fig. 1b to their original areas, Fig. 1a. This is done in preference to devising an approximate difference equation for the Jacobian of Eq. 3 directly because the exact formula for the area of a quadrilateral whose corners are known turns out to be easier to compute, particularly if the original areas, $A^{o}_{i+\frac{1}{2},j+\frac{1}{2}}$, of each of the quadrilaterals are carried as problem constants. The equation of continuity then becomes in the notation described above:

$$V^{n}_{i+\frac{1}{2},j+\frac{1}{2}} = \left\{\left(X^{n}_{i+1,j}-X^{n}_{i,j+1}\right)\left(Y^{n}_{i+1,j+1}-Y^{n}_{i,j}\right)-\left(Y^{n}_{i+1,j}-Y^{n}_{i,j+1}\right)\left(X^{n}_{i+1,j+1}-X^{n}_{i,j}\right)\right\}\Big/2A^{o}_{i+\frac{1}{2},j+\frac{1}{2}} \tag{16}$$

where the X's and Y's are the coordinates of the mass points on the four corners of the quadrilateral.

For convenience from here on, V with subscripts and superscripts will be understood to mean V/V_o.

B. The Equation of Motion

Evaluating the pressure gradients in two space dimensions has been one of the more difficult questions of technique to be answered. The difficulty becomes apparent when one tries to extend the simple but very successful method usually used in one dimension directly to two dimensions.

In one dimension we can consider the mass points as lying on a line with the pressures situated at the centroids between them. For a given point, i, at time n, there are two neighboring pressures, $P^n_{i+\frac{1}{2}}$ and $P^n_{i-\frac{1}{2}}$. If the pressure profile is continuous, as has been assumed, we can get a first order approximation to the gradient by taking the difference of the pressures divided by the difference in their locations. More exactly, we can express the value of the pressure at $x_{i+\frac{1}{2}}$ in terms of a Taylor's series

$$P_{i+\frac{1}{2}} = P_i + \left.\frac{\partial P}{\partial x}\right|_i (x_{i+\frac{1}{2}} - x_i) + \tfrac{1}{2}\left.\frac{\partial^2 P}{\partial x^2}\right|_i (x_{i+\frac{1}{2}} - x_i)^2 + \ldots \qquad (17)$$

This and a similar expression for $x_{i-\frac{1}{2}}$ may be considered as two equations from which one may solve for the two unknowns, P_i and $\left.\frac{\partial P}{\partial x}\right|_i$. The result for the latter may be written

$$\frac{\partial P}{\partial x}_i = \frac{(P_{i+\frac{1}{2}} - P_{i-\frac{1}{2}})}{(x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}})} - \left.\frac{\partial^2 P}{\partial x^2}\right|_i \delta - \left.\frac{\partial^3 P}{\partial x^3}\right|_i \left\{\frac{(x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}})^2}{24} + \delta^2\right\} - \ldots \qquad (18)$$

where δ, a measure of the asymmetry of the mesh, is defined as

$$\delta = \tfrac{1}{2}(x_{i-\frac{1}{2}} + x_{i+\frac{1}{2}}) - x_i \tag{19}$$

The second derivative term is thus zero if the mass points are equally spaced. The third derivative term represents the error inherent in taking only a linear average for the gradient.

Applying this method directly to the rectangular case in two dimensions, the Taylor's series will give <u>four</u> equations of the form

$$P_{i+\frac{1}{2},j+\frac{1}{2}} = P_{i,j} + \frac{\partial P}{\partial x}\Delta x + \frac{\partial P}{\partial y}\Delta y + \tfrac{1}{2}\frac{\partial^2 P}{\partial x^2}\Delta x^2 + \tfrac{1}{2}\frac{\partial^2 P}{\partial y^2}\Delta y^2 + \tfrac{1}{2}\frac{\partial^2 P}{\partial x \partial y}\Delta x \Delta y \quad \ldots \tag{20}$$

Considering first derivatives only, there are but <u>three</u> unknowns, $P_{i,j}$ $\frac{\partial P}{\partial x}$, $\frac{\partial P}{\partial y}$, to be found. This overdeterminacy seems to be fundamental for the rectangular mesh. Trying to take more neighboring points and solve for higher derivatives always results in an unsymmetrical mesh. A considerable amount of effort has gone into devising schemes to avoid this problem. (Ref. 3) The solutions usually suggested are: (1) use some type of least squares calculation, based on from 4 to 10 neighboring pressures, or (2) use a mesh based on triangles or hexagons which will give three neighbors naturally. Methods based on (1) have the disadvantage of being very time-consuming and difficult logically, as well as being susceptible to instability. Meshes based on triangular symmetry have the

disadvantage of not fitting together nor to the boundaries easily. Usually one needs a number of alternative difference schemes which make the code complicated and the interpretation of results difficult, although the calculational speed is much better than using least squares.

The method proposed here is an attempt to salvage the best features of both the above. The overdeterminacy is removed by first solving for two gradients diagonally across the mass point, then solving these together to get $\frac{\partial P}{\partial x}$ and $\frac{\partial P}{\partial y}$.

The pressure differences across the diagonals are of the form

$$(P_1 - P_3) = \frac{\partial P}{\partial x}(x_1 - x_3) + \frac{\partial P}{\partial y}(y_1 - y_3) + \frac{\partial^2 P}{\partial x^2}(x_1 - x_3)\,\delta x_{13} + \frac{\partial^2 P}{\partial y^2}(y_1 - y_3)\,\delta y_{13} + \frac{\partial^2 P}{\partial x \partial y}\tfrac{1}{2}\left[(x_1 - x_3)\,\delta y_{13} + (y_1 - y_3)\,\delta x_{13}\right] + \cdots \tag{21}$$

where for convenience we substitute the quadrant numbers about i,j for the subscripts: 1 for $i+\frac{1}{2}, j+\frac{1}{2}$, 2 for $i-\frac{1}{2}, j+\frac{1}{2}$, etc. The asymmetry terms are defined as in Eq. 19.

Solving Eq. 21 with the similar one for $P_2 - P_4$, the gradients become

$$\left.\frac{\partial P}{\partial x}\right|_{ij} = \left\{(P_1 - P_3)(y_2 - y_4) - (P_2 - P_4)(y_1 - y_3)\right\}/d + Rx$$

$$\left.\frac{\partial P}{\partial y}\right|_{ij} = \left\{-(P_1 - P_3)(x_2 - x_4) + (P_2 - P_4)(x_1 - x_3)\right\}/d + Ry \tag{22}$$

$$d = (x_1 - x_3)(y_2 - y_4) + (x_4 - x_2)(y_1 - y_3)$$

The error terms represented by Rx and Ry are lengthy expressions involving second and higher derivatives, however, they can easily be shown to have the same order as the error terms in the one dimensional case, that is, Rx = (2nd derivs.) δ + (3rd derivs.) $\triangle x^2$ + ...

These formulas for the gradients are the same either for the original Lagrangian mesh or for the Eulerian mesh at a later time. If the spacing of the original mesh is uniform, they become considerably simpler, however this simplicity is bought at the price of having to evaluate numerically the other terms of the Jacobian in Eq. 8. If one wishes to retain the generality of being able to use somewhat non-uniform spacing in the original mesh, then it appears to be simpler to work with Eulerian gradients in Eq. 7 directly.

The specific volume at point i,j needed in Eq. 7 is taken as the average of the volumes of the four neighboring quadrilaterals. The exact formula for the centroid of a quadrilateral was deemed too lengthy, so the average of the locations of the four corners was substituted as a good first order approximation. Finally, the time derivative in the equation of motion was evaluated, using ordinary centered differences to yield the coordinates of point i,j at time n+1 in terms of quantities known at time n or n-1. The equations of motion as calculated then become

$$X^{n+1}_{i,j} = X^{n}_{i,j} + \Delta X^{n-\frac{1}{2}}_{i,j} + B^{n}_{xi,j}$$

$$Y^{n+1}_{i,j} = Y^{n}_{i,j} + \Delta Y^{n-\frac{1}{2}}_{i,j} + B^{n}_{yi,j}$$

$$\Delta X^{n-\frac{1}{2}}_{i,j} = X^{n}_{i,j} - X^{n-1}_{i,j}$$

$$\Delta Y^{n-\frac{1}{2}}_{i,j} = Y^{n}_{i,j} - Y^{n-1}_{i,j} \qquad P_1 (Y_2 - Y_4) \qquad (23)$$

$$B^{n}_{xi,j} = \frac{-(\Delta t)^2}{4 \rho_o d} \left\{ V_1 + V_2 + V_3 + V_4 \right\} \left\{ (P_1 - P_3)(Y_2 - Y_4) - (P_2 - P_4)(Y_1 - Y_3) \right\}$$

$$B^{n}_{yi,j} = \frac{-(\Delta t)^2}{4 \rho_o d} \left\{ V_1 + V_2 + V_3 + V_4 \right\} \left\{ -(P_1 - P_3)(X_2 - X_4) + (P_2 - P_4)(X_1 - X_3) \right\}$$

$$d = (X_1 - X_3)(Y_2 - Y_4) + (X_4 - X_2)(Y_1 - Y_3)$$

C. The Equation of Energy Conservation and the Equation of State

Since the energy equation contains only simple time derivatives, it may be written in centered difference form as

$$E^{n} = E^{n-1} - \tfrac{1}{2}(p^{n-1} + q^{n-1} + p^{n} + q^{n})(V^{n} - V^{n-1}) \qquad (24)$$

All the quantities are for $i+\frac{1}{2}, j+\frac{1}{2}$. In keeping with the convention that V with subscripts and superscripts actually means V/V_o, E with subscripts and superscripts will mean E/V_o, i.e., energy per original unit volume.

Since p^n depends on E^n as well as V^n, the above equation must be solved simultaneously with the equation of state. For the ideal gas, Eq. 10, the difference equations for P^n and E^n become (all quantities at $i+\frac{1}{2}, j+\frac{1}{2}$)

$$E^n = \frac{2E^{n-1} - \Delta V(P^{n-1} + q^n)}{2 + (\gamma - 1)\Delta V/V^n}$$

$$P^n = q^n + (\gamma - 1)\, E^n/V^n \qquad (25)$$

$$\Delta V = V^n - V^{n-1}$$

D. Definition of the Pseudo-viscosity Term

The definition based on $\frac{\partial V}{\partial t}$, Eq. 11, is used in the form

$$q^n = \frac{\rho_o\, bA^o}{V^n}\left(\frac{\Delta V}{\Delta t}\right)^2 \qquad \text{for } \Delta V < 0$$

$$q^n = 0 \qquad \text{for } \Delta V \geqslant 0 \qquad (26)$$

Again all quantities are for $i+\frac{1}{2}, j+\frac{1}{2}$. The term l^2 has been replaced, rather arbitrarily, by $A^o_{i+\frac{1}{2}, j+\frac{1}{2}}$. A value of b which works well with this choice of l^2 is 1.44.

E. The Total Energy Check

The total energy of the fluid contained in one quadrilateral may be written in finite difference form as

$$T^{n-\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2}} = \tfrac{1}{2} A^{o} \left\{ \rho_{o} \left(v^{n-\frac{1}{2}}\right)^{2} + E^{n-1} + E^{n} \right\}$$

$$\left(v^{n-\frac{1}{2}}\right)^{2} = \frac{1}{4(\Delta t)^{2}} \sum \left\{ \left(\Delta X^{n-\frac{1}{2}}_{i,j}\right)^{2} + \left(\Delta Y^{n-\frac{1}{2}}_{i,j}\right)^{2} \right\} \qquad (27)$$

The latter is summed over the four corners of the quadrilateral. The total energy is taken centered at time $n-\frac{1}{2}$ for convenience since the ΔX, ΔY terms are centered at that time.

If one is interested in the energy balance in only one region which is bounded by a mesh line $i = I$, the above expression for T is summed for quadrilaterals $I \leq i \leq i_L - 1$, $j_o \leq j \leq j_L - 1$, where the subscripts o and L refer to the first and last mesh lines respectively. Similarly the work-done expression will then have to be computed only for the points on the mesh line $i = I$. This allows one to use much simpler expressions for the P and $\vec{v}.d\vec{\sigma}$ of Eq. 14 than would otherwise be possible. In particular

$$\Delta W^{n-\frac{1}{2}}_{I} = - \sum_{j_o}^{j_{L-1}} P^{n-\frac{1}{2}}_{I,j+\frac{1}{2}} \Delta V^{n-\frac{1}{2}}_{I,j+\frac{1}{2}}$$

where
$$P^{n-\frac{1}{2}}_{I,j+\frac{1}{2}} = \frac{\left(P^{n-1} + P^{n}\right)_{I+\frac{1}{2},j+\frac{1}{2}}}{2 + 2r} + \frac{\left(P^{n-1} + P^{n}\right)_{I-\frac{1}{2},j+\frac{1}{2}}}{2 + 2/r} \qquad (28)$$

$$r = A^{o}_{I+\frac{1}{2},j+\frac{1}{2}} \,/\, A^{o}_{I-\frac{1}{2},j+\frac{1}{2}}$$

$$\Delta V^{n-\frac{1}{2}}_{I,j+\frac{1}{2}} = \tfrac{1}{2} \left\{ \left(X^{n}_{Ij} - X^{n-1}_{I,j+1}\right)\left(Y^{n}_{I,j+1} - Y^{n-1}_{I,j}\right) - \left(Y^{n}_{I,j} - Y^{n-1}_{I,j+1}\right)\left(X^{n}_{I,j+1} - X^{n-1}_{I,j}\right) \right\}$$

The discrepancy between the total energy in the region being checked and the work which has been done on it through surface $i = I$, is then

$$\delta = \sum_{i=I}^{i_{L-1}} \sum_{j=j_o}^{j_{L-1}} \left(T^{n-\frac{1}{2}}_{i+\frac{1}{2},j+\frac{1}{2}} \right) + \tfrac{1}{2} \Delta W_I^{n-\frac{1}{2}} + \sum_{n=0}^{n-1} \Delta W_I^{n-\frac{1}{2}} - T^o \qquad (29)$$

Note that only one-half the second term is added in since the total energy is centered at $n-\frac{1}{2}$, whereas the ΔW term represents the work done from cycle $n-1$ to n.

Extending the above formulas to two or more surfaces, or to surfaces which fall on more than one mesh line, presents no difficulty in principle although the coding can become rather involved.

F. The Stability Condition Check

The calculation of w, Eq. 15, is made quite simple if one is willing to use an approximate value for the sound speed c based on the pressure from one cycle to the next, that is

$$c^2 = \frac{\partial p}{\partial \rho}\bigg|_s = - \frac{V^2}{\rho_o} \frac{\partial p}{\partial V}\bigg|_s \doteq - \frac{V^2}{\rho_o} \frac{\Delta p}{\Delta V} \qquad (30)$$

where Δp and ΔV now represent changes from one time step to the next. This is a good approximation if the q terms are not dominating in Eq. 24.

If one assumes $(\Delta \vec{R})^2 \doteq V^2 A^o$ in Eq. 15, and agrees to compute the stability condition only when the fluid is compressing, $\Delta V < 0$, the sound speed term may be written

$$c\left(\frac{\Delta t}{\vec{\Delta R}}\right)^2 \doteq -\left(\frac{\Delta p}{q}\right)\left(\frac{\Delta V}{V}\right) b \tag{31}$$

which gives a formula for w independent of the form of the equation of state or any of the space dimensions:

$$w^n_{i+\frac{1}{2},j+\frac{1}{2}} = \left\{- b\left(\frac{\Delta V}{V}\right)\left(4 + \frac{\Delta p}{q}\right)\right\}^{\frac{1}{2}} \tag{32}$$

In the calculations, w was used to give an automatic indication of when the size of the time step, Δt, should be changed. The criterion used was that if two mesh volumes had w's greater than 0.9 on a given cycle, Δt would be cut automatically.

G. Boundary Conditions

Each problem usually has its own peculiar boundary conditions which must be specially coded, so only a few generalities can be mentioned here.

The boundary conditions are included in the calculation by having special equations for the B terms in Eq. 23 for boundary points. If the points are immobile, as the corners in Prob. D below, the B's are set to zero. If the points can slide along a wall but not leave it (e.g., the bottom points in Prob. D) then B_y is zero and B_x is calculated by a simplified formula. Points which remain on a slanting line, as in Prob. B, have B's which are related by the tangent of the angle of the slope, etc.

IV. SAMPLE PROBLEMS

The following problems were done using the difference equations of Sect. III coded for the IBM 701 Electronic Computer. An interpretive sub-routine known as "Dual Coding" (Ref. 8) was used, which is very useful for exploratory calculations. This routine performs all arithmetic steps in "floating point" (i.e., numbers are in the form $A \times 10^B$), so that most questions of scaling and precision of intermediate steps in the calculation are handled automatically. One pays for this convenience by increased calculation time; however, if the total computing time for the problem is not excessive, the convenience still results in a net gain in total time from inception to completion of the problem.

A. A One-dimensional Shock Problem

The first problem tried was that of a plane steady shock formed by a constant velocity piston (Ref. 4) in a tube of finite length. This proved to be quite a good problem for testing the method on known ground for which exact solutions were available.

The piston was started in a gradual manner so that the von Neumann-Richtmyer shock would be formed with only small initial transient effects. The graphs in Fig. 2 show some of the results of this problem. The upper curve shows the pressures of some of the mesh points as functions of time. The lower shows the relative specific volumes of the same points. The agreement with the theoretical curves is typical for the von Neumann-Richtmyer method. The small oscillations after the shock could be damped out by taking a larger value of b. However, this would result in a loss

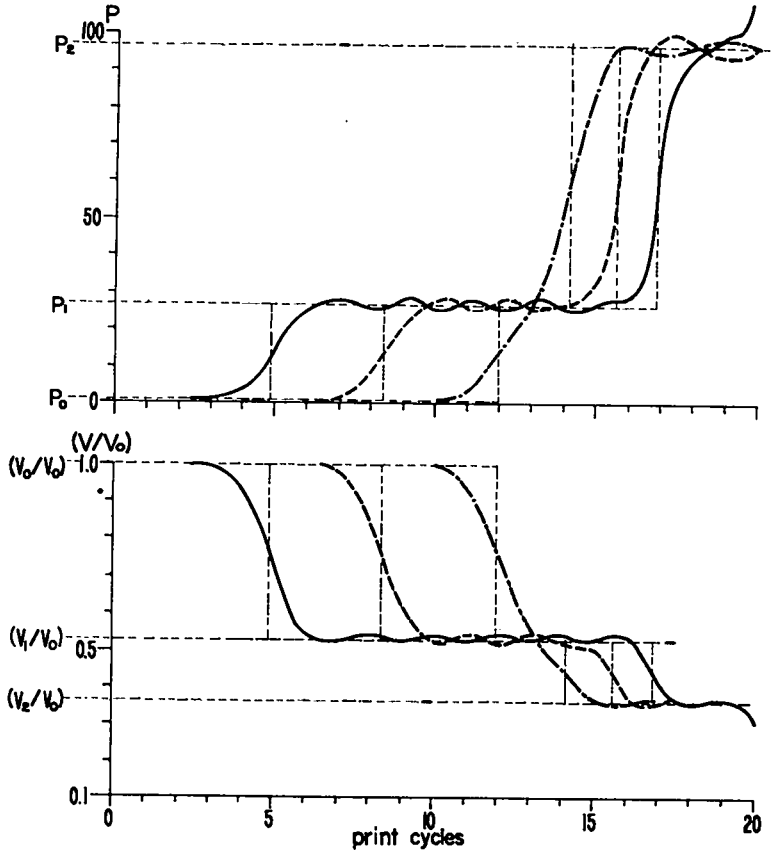


Figure 2

Figure 2

Problem A. A one dimensional shock reflected from a rigid wall. The upper curve gives the total pressure, p+q , versus time for three of the mesh points. The lower gives the relative specific volumes of the points versus time. The dotted curves give the theoretical values from the Rankine-Hugoniot equations.

of resolution since the whole shock would be widened.

The problem was stopped when the reflected shock from the fixed end of the tube collided with the piston.

B. An Oblique Shock Problem

For the second problem, it was desired to try a case which had true two dimensional character, yet which also possessed an exact solution in reasonably simple form. The case of steady supersonic flow past a wedge seemed ideal for the purpose. (Ref. 9)

Values of material velocity, etc., were chosen to give the theoretical pattern shown in Fig. 3a. The angle of the wedge was approximately 10°, chosen to give an angle of the shock of 30°. The exact solution is time independent. However, since the present numerical method must solve transient problems, one can expect the time independent solution to be reached only in some average sense. The method chosen for mocking-up the steady boundary conditions was to hold the right and left boundaries of the region on their theoretical paths as a function of time and allow the rest of the points to be computed by the difference equations.

Fig. 3a and 3b show "snapshots" of the positions of the mass points and the values of the pressures at two times in the problem. Note that all the quantities show evidences of the typical oscillations mentioned in Prob. A. The upper numbers give the total pressure, P, of the mesh volume, the lower numbers give the viscosity term, q, only. The positions of the viscosity terms do indeed cluster about the theoretical shock position. The scattered small terms elsewhere indicate oscillations, and are

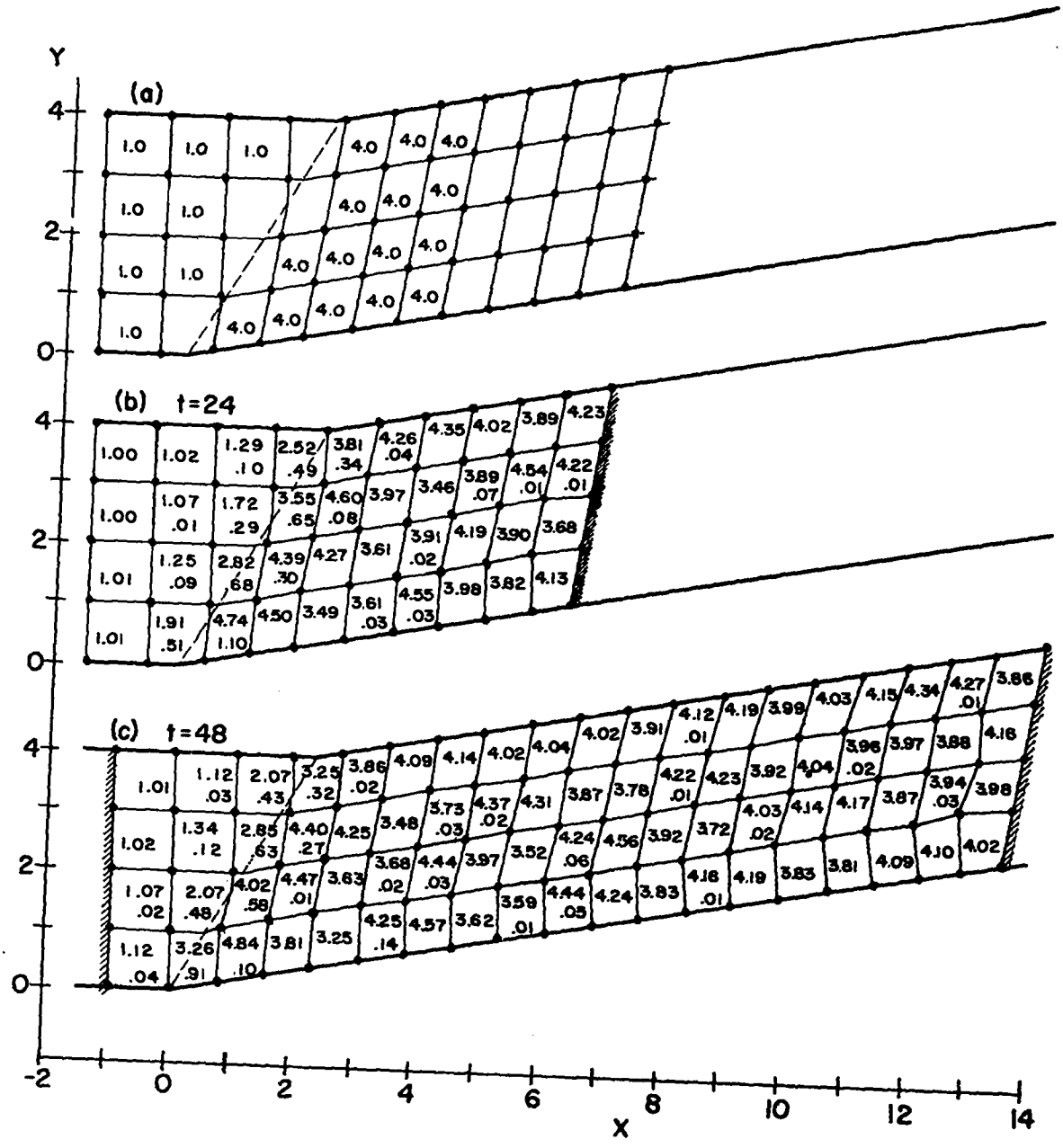


Figure 3

Problem B. An oblique shock problem where (a) gives the theoretical configuration of typical mass points and pressures. The initial velocity is from left to right at Mach 2. The initial pressure is 1.0 in arbitrary units, the final pressure to the right of the shock is 4.0. Parts (b) and (c) give the mass point positions and pressures at different times during the problem. The upper numbers are the total pressure, p + q, the lower are the dissipative pressures, q , only.

negligible for the most part. The shape of the flow pattern is also considered quite gratifying.

C. An Oblique Shock and Rarefaction Problem

Making a relative minor change in the right-hand boundary condition of Prob. B made it possible to try a true transient problem--a sort of idealized collapsing cone problem. The right boundary was allowed to be a free surface which could be accelerated by the pressure differences appearing across it.

An exact solution of this problem was not available. However qualitatively one would expect (a) the pressures and particle velocities to approach the theoretical values of Prob. B near the wedge as time advanced, and (b) a material jet (Ref. 10) to form along the lower edge. The latter was not expected to be very well represented since the resolution of the space mesh is rather coarse.

Fig. 4 shows the results of this calculation at various times. The qualitative behavior expected was indeed observed. The rarefaction from the free surface managed to keep the stationary shock from attaining its final value by the time the problem was stopped, although the pressures near the wedge were rising steadily in time. The formation of the jet was clearer than expected. Figs. 4c and 4b show the maximum mesh distortion seen in any of the problems. The position of the points on the upper boundary are not realistic since they were constrained in the problem to remain on the 10^{o} line. A relatively minor change in the code could permit them to separate and flow down into the jet.

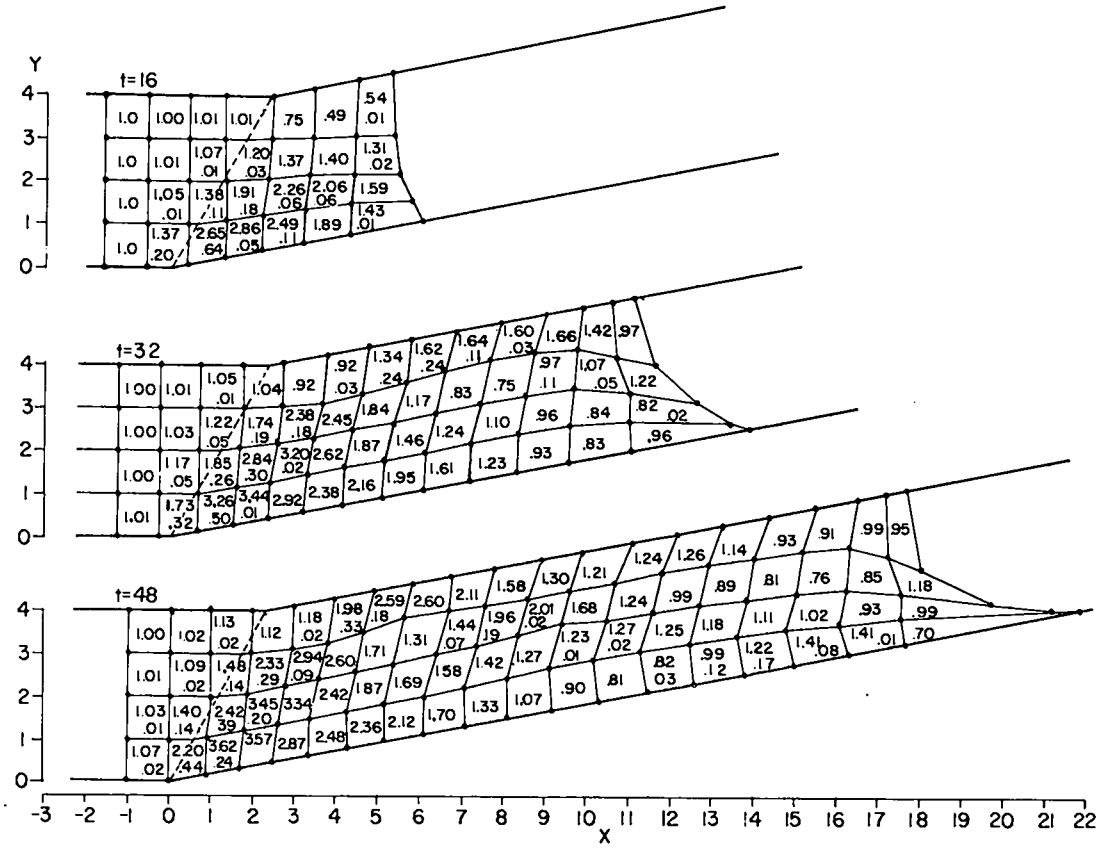


Figure 4

Problem C. An oblique shock with a rarefaction from a free surface. Mass point positions and pressures are plotted at different times during the problem. The formation of a material jet is indicated.

D. An Explosion Problem

Another two dimensional problem about which much qualitative information is known is the interaction of a diverging shock from a point explosion with the ground. (Ref. 11) The pressure profile is in the form of a peak followed by a trough which usually exhibits a negative phase, i.e., pressure below the original atmospheric pressure. When a shock strikes the ground the pressure is approximately doubled in a reflected shock. As the intersection of the first shock and the ground becomes more oblique, a Mach stem is eventually formed. (Ref. 4)

One question which this calculation was expected to answer concerning the method was, will the calculated shock travel with the same speed at an angle with respect to the mesh as it does parallel to it?

For convenience the problem was started with all the mass points at rest but with high pressures in the four rectangles in the upper left corner. These pressures were chosen so as to approximate the distribution expected a short time after a point explosion at the corner. Fig. 5 shows the positions and pressures at later times. The shaded regions are bounded by the 5% pressure disturbance line and the peak pressure line for each shock. The actual shock position is about midway between them.

Again the qualitative results were most gratifying, even though the present problem represents an explosion along an infinite line rather than at a point. The shock does travel with uniform speed at all angles with respect to the mesh, and the reflected shock behaves much as it should. Because of the coarse resolution, one cannot state with any certainty that a Mach stem is being formed in the last picture, although the results are at least not inconsistent with there being one.

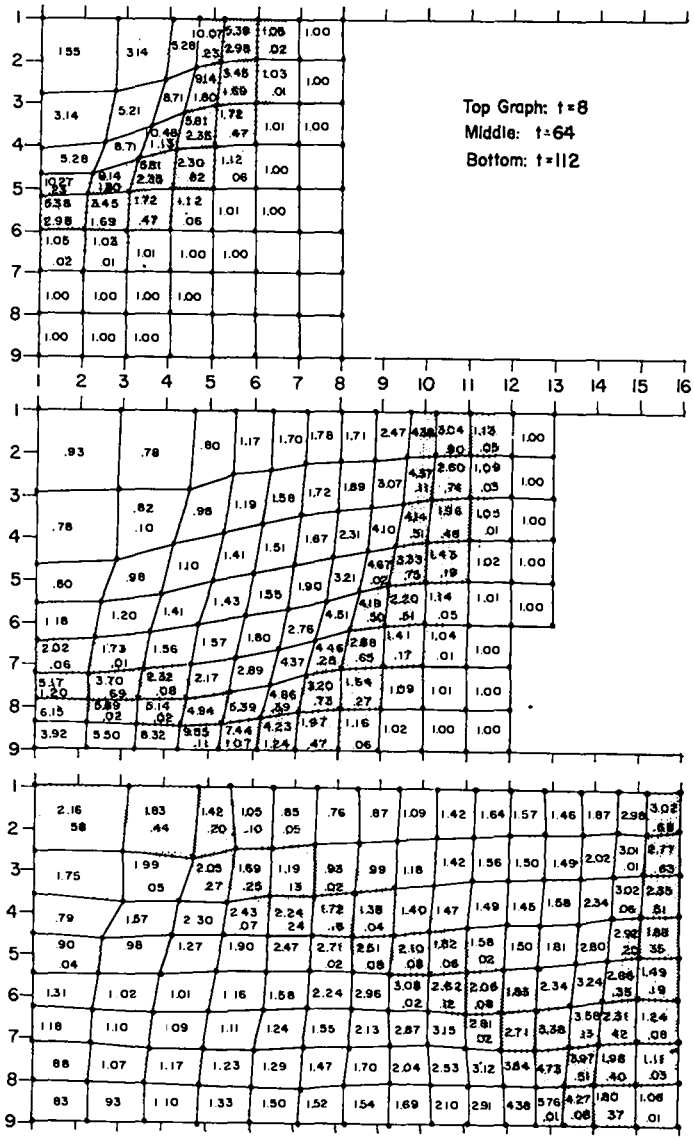


Figure 5

Problem D. The shock wave from an infinite line explosion is shown interacting with rigid ground. The mass point positions and pressures are plotted at three different times during the problem. The shaded regions are bounded by the 5% pressure disturbance and the peak pressure lines for each shock.

V. DISCUSSION OF RESULTS AND FUTURE POSSIBILITIES

One fact is apparent throughout all the above problems: the mesh size determining the space and time resolution of the quantities calculated is too coarse for detailed study of any but large-scale results. This was in part intentional in the present problems, but for the most part the limitation is one of computer speed and storage capacity.

The difference equations of Sect. III assume that seven quantities are stored for each mass point from one time step to the next: X, ΔX, Y, ΔY, P, E, and A°. The last quantity, A°, the original area of the quadrilateral, need not be stored separately for each point if the mesh is regular. However, one sacrifices much flexibility by making this stipulation. The storage block needed for the above seven quantities is called "permanent storage" and will be equal to $3(R-1)(C-1) + 4RC$ words of storage, where R is the number of rows and C is the number of columns in the mesh.

One also always needs the additional quantities $(V,X,Y,P)_{i+\frac{1}{2},j+\frac{1}{2}}$ for the points in the column next to the one being computed at a given time. This block is called "intermediate storage" and is equal to $8(R-1)$ words. Finally one needs space for the problem code itself and the temporary storage which it uses during the calculation. The size of this "code storage" is not a sensitive function of the size of the mesh being used, although the code will tend to be longer and more involved as the mesh gets larger.

The total storage required in the computer may thus be expressed as

$$S = S_c + 3(R-1)(C-1) + 4RC + 8(R-1)$$

The total time necessary to do a calculation may be given approximately by

$$T = NRC(t_c + rt_p)$$

where N is the total number of time cycles in the problem, t_c is the time required to calculate all the difference equations for one mass point for one time step, t_p is the time needed to print the quantities for one mass point, and r is the ratio of the number of time cycles for which quantities are printed to the total number of cycles calculated.

In Prob. D, the numbers were approximately: $R = 9$ rows, $C = 16$ columns, $N = 112$ cycles, $S_c = 1168$ words (including "Dual"), $t_c = 0.3$ sec, $t_p = 1.2$ sec, and $r = 0.25$. This yields the total storage $S = 2048$ words (the capacity of the 701 memory), and the total time = 9677 sec or about $2\frac{1}{2}$ hours.

Experience has shown that to do a problem with good resolution in one dimension requires at least 50 to 100 mass points. If one takes this many rows and columns in a two dimensional problem, the total number of points will be 2,500 to 10,000! Also, from stability arguments, if one cuts the size of the space mesh by 10, he will also have to cut the size of the time mesh by at least as much, so the number of time cycles in this hypothetical case will be in the vicinity of 500. On the other hand, by giving up the luxury of floating point Dual operations one can cut t_c from 0.3 sec to about 0.06 sec. Similarly, by using more specialized printing procedures (fewer significant figures, etc.), one can easily cut

t_p from 1.2 sec to 0.4 sec. The finer time steps in the calculation mean that one need not print as often, so r can be made 0.03 or less.

Using these numbers, one arrives at figures for the total storage of 20,000 to 70,000 words, and for times of calculation, 25 to 100 hours per problem! On machines which are presently available it is probably foolish to consider problems of this magnitude, although there are certainly a great many useful two dimensional problems which one can do with one-tenth the above storage and time, which is practical on existing machines.

There are a number of ways in which the present method may be generalized to other physical cases. For example, it could be altered to include: (a) two or more different materials, (b) other equations of state (c) coordinate systems other than rectangular, (d) energy release terms, (e) shear viscosity and rigidity terms, and also (f) more elaborate boundary conditions which can allow for movement of the boundary walls, slippage along moving boundaries, separation and intersection of moving boundaries, etc. It is hoped to be able to report on some such extensions at a later time.

The main limitation of the method is expressed in the stipulation made in the introduction to Sect. III, that the fluid must be continuous over distances the order of the mesh size. This certainly will limit its usefulness in fluid problems involving turbulence and mixing, or extensive shearing and slipping.

REFERENCES

1. J. von Neumann and R. D. Richtmyer, J. Appl. Phys., 21, 232 (1950).
2. "Computer Issue", Proc. IRE 41, Oct. (1953).
3. Private communications: R. D. Richtmyer and P. Lax of N.Y.U.; R. LeLevier, R. Jastrow, J. Griffith, and T. Kishi of Livermore Lab.; D. Carter, A. Carson, R. Landshoff, J. Pasta, and G. N. White, Jr., of Los Alamos; and Prof. J. von Neumann.
4. R. Courant and K. O. Friedrichs, Supersonic Flow and Shock Waves, pp. 13, 121, 141, 150, 334, Interscience Publishers, Inc., New York, 1948.
5. H. Lamb, Hydrodynamics, 6th ed., p. 12, Dover Publications, New York, 1945.
6. Courant, Friedrichs, and Lewy, Math. Ann., 100, 32 (1928).
7. G. N. White, Jr., (Presently being submitted to J. Appl. Phys. as a letter to the Editor).
8. S. Schlesinger, Los Alamos Report LA-1573 (1953).
9. H. W. Leipmann and A. E. Puckett, Aerodynamics of a Compressible Fluid, p. 51, John Wiley & Sons, Inc., New York, 1947.
10. J. M. Walsh, R. G. Shreffler, and F. J. Willig, J. Appl. Phys., 24, No. 3, 349 (1953).
11. Los Alamos Scientific Laboratory, The Effects of Atomic Weapons, p. 45 ff., U. S. Government Printing Office, Washington, 1950.