D3
D-3

LAMS-2567

LOS ALAMOS SCIENTIFIC LABORATORY

OF THE UNIVERSITY OF CALIFORNIA o LOS ALAMOS NEW MEXICO

THE PARTICLE-AND-FORCE COMPUTING METHOD FOR FLUID DYNAMICS

LA/124 (duplicate)

LEGAL NOTICE

Printed in USA. Price $ 1.25. Available from the

Office of Technical Services
U. S. Department of Commerce
Washington 25, D. C.

LAMS-2567
PHYSICS
TID-4500 (16th Ed.)

LOS ALAMOS SCIENTIFIC LABORATORY
OF THE UNIVERSITY OF CALIFORNIA LOS ALAMOS NEW MEXICO

REPORT WRITTEN: June 1961

REPORT DISTRIBUTED: October 3, 1961

THE PARTICLE-AND-FORCE COMPUTING METHOD FOR FLUID DYNAMICS

by

Francis H. Harlow
Billy D. Meixner

Contract W-7405-ENG. 36 with the U. S. Atomic Energy Commission

ABSTRACT

A fluid-dynamic computing method is proposed in which the materials are represented by discrete particles interacting with one another by means of pair forces. Details of technique, accuracy, and stability are discussed in preliminary form. Results are presented of some simple tests of the method, and it is shown that even though considerable development effort is yet required, the method appears to have some desirable properties not present in any other.

CONTENTS

I. INTRODUCTION

The perfection of high-speed electronic computers has opened the way for solving a wide variety of complicated problems for which no solutions previously were possible. Among these are the problems of compressible fluid dynamics, for which numerous techniques have been developed, mostly using finite-difference approximations to the appropriate partial differential equations. In many applications, particularly those involving one space dimension, the results have been very satisfactory. Sufficient precision has been obtainable so that direct use could be made with confidence in experimental design work. In situations depending upon two space dimensions, there are likewise successful techniques, but at present they all are limited in applicability. One method may be successful in a situation in which another would fail. In some cases, problems have been solved by using one method for part of the flow and another for the rest. This has been quite successful for cases when a period of validity exists for both methods, but has led to frustration when circumstances would force use of this procedure for a problem in which both methods would give questionable results at the time of change-over.

We are here proposing a computing technique for solving problems in

multidimensional compressible-fluid dynamics that avoids some of the troublesome features of other existing methods. It is based on a representation of the fluid by a set of mass points which are accelerated by mutual forces and whose consequent motions represent that of a fluid. For reference, the technique is referred to as the "Particle and Force" (PAF) method.

We illustrate the need for a new computing method by reviewing briefly some of the existing multidimensional techniques which have been used at the Los Alamos Scientific Laboratory. This review will also serve as a basis for demonstrating some of the properties of the new method.

1. Eulerian finite-difference methods

Every numerical technique for solving fluid-dynamics problems has as its basis the differential equations of motion, or equivalently the conservation laws from which the equations are derived. A principal difference among techniques comes from the nature of the coordinate system used in the study. In Eulerian techniques the coordinate system is at rest relative to an external observer, and fluid flows by the lines of constant coordinate. In devising a finite-difference approximation to the partial differential equations of motion, one constructs a grid of coordinate lines which divides space into a set of finite zones or cells. The fluid at any given instant is then described by specifying a set of values for each cell of such quantities as velocity, temperature, and density. The cell-wise values are interpreted as some sort of cell-wise averages.

Space derivatives in the equations of motion are written as the ratio of intercell difference to cell size. In addition, the passage of time occurs in finite steps of interval δt each, so that the time derivatives are represented by the ratio of the difference from end to beginning of a cycle, to δt. Thus the differential equations become algebraic equations by which new values for each cell (i.e., those at the end of the nth time cycle) can be determined from the known values at the beginning of the cycle. Starting of a problem requires specification of appropriate initial conditions, and progress through time requires boundary conditions, translated into appropriate finite-difference form. With proper care in the formulation, and with small enough space and time intervals, the calculation may be both stable and sufficiently accurate (see reference 1). The qualification is expressed because for some situations the proper formulation is not at present known, while for others the achievement of accuracy would be only at the expense of intolerable amounts of computing time. The most vexing difficulties with the Eulerian methods are of three types. First, moving regions with structure which is small compared to the over-all dimensions of the system are difficult to resolve properly. It is wasteful to have fine zones throughout the entire space through which the small structure will move, and it is very difficult to devise a good means for creating and destroying zones, so that a region of fine resolution follows the structure. A second difficulty concerns the boundaries between materials, which must have a special explicit treatment or else be subject to an unrealistic smearing diffusion.[2,3]

Third, there is an inherent lack of Galilean invariance and isotropy.

One of the overwhelming advantages of the Eulerian approach is that there is no difficulty in treating problems in which there are large distortions or slips in the fluid.

2. Lagrangian finite-difference methods

The approach is similar to the Eulerian described above, in that the space containing the fluid is divided into finite zones, and the configuration advances through time in finite steps. The fundamental difference is that the Lagrangian coordinate system follows the motion of the fluid.[4,5] As a result, two of the principal difficulties of the Eulerian methods are avoided. Those regions in which fine resolution is necessary retain their fine zoning because the coordinate system moves right along. Material interfaces are easily treated because coordinate lines can be placed along them and will forever follow them. The difficulties in the Lagrangian approach arise when the fluid develops internal slips or large distortions. Special techniques have been developed to allow slip lines to be handled; when it is initially known, for example, where the slip will occur, then a coordinate line can be placed there with special treatment given. But when the slip-line position is not initially known the matter is considerably complicated. Distortions are even more serious in limiting applicability. When, for example, initially rectangular cells have become distorted into arbitrarily shaped quadrilaterals, the initially-appropriate form of the difference equations may be quite inapplicable, although, here again, special techniques have been

proposed[6] which hold promise for solving the difficulty somewhat. The Lagrangian method also has trouble with collapsing free surfaces (as in the shaped-charge problem); some attempts to solve this difficulty are also discussed in reference 6.

3. Combination Eulerian-Lagrangian techniques

Some unpublished work has been done[7] on a technique in which the coordinate system is Lagrangian in one direction and Eulerian in another (in two space dimensions). Another alternative would be to have a Lagrangian coordinate system for part of the fluid which moves through an Eulerian system in which the dynamics of the rest of the fluid is calculated. Both approaches are nicely suited to some situations which are not well treated in a homogeneous coordinate system of either pure type.

Another combination form which has been extensively applied is called the Particle-in-cell (PIC) method.[8] The entire space occupied by the fluid is covered by an Eulerian mesh of cells, and the fluid is represented by a set of particles (essentially a Lagrangian mesh) which move through the cells. The finite-difference equations are written relative to the Eulerian mesh; the particles are moved with velocities determined from adjacent cells. The method has the Eulerian advantage of calculating distortions with ease and the Lagrangian advantage of giving information about motions of fluid elements, especially of material interfaces which are automatically handled well. PIC-method disadvantages include the Eulerian difficulties in lacking fine resolution

and invariance, together with an additional disadvantage of requiring the storage of information for both the Lagrangian and Eulerian systems.

4. Series methods

The dependent variables are expressed as infinite series in functions of position with time-dependent coefficients. The approximation comes in truncation of the series so that only a finite number of coefficients remain. Their changes through time proceed in a sequence of finite intervals, governed by equations obtained from substitution of the series into the appropriate partial-differential equations. Very little work on this method has been done at Los Alamos, but Thomas[9] has reported success in application to calculations of stability of plane-parallel flow. A variety of difficulties concerning computational stability, conservation, running time on computer, and interpretation are forseeable.

5. Particle methods

The PAF method, which we are proposing in this report, was inspired by the heuristic studies of Pasta and Ulam[10] on the dynamics of a set of particles with mutual forces. With forces dependent on separation only, their calculations represented adiabatic motion with no dissipation. Nevertheless, their results on a pair of Taylor-instability calculations were quite encouraging, and strongly suggested that a real fluid-dynamic computing method could be obtained from a generalization of their ideas. Presentation of the resulting techniques is the main purpose of this report.

Kolsky[11] recently has also described a generalized particle-like method which differs considerably from the one here proposed.

II. DESCRIPTION OF THE METHOD

A. Differential Theory

The particles whose dynamics we follow are to represent a fluid. Insofar as we may be aided in formulating the method by referring to classical particle-dynamic theory, we may proceed with that guidance. We know, however, that at some point a divergence will be necessary so that the dissipative effects in a real fluid can be represented. Our particles are not molecules whose internal energy is carried by velocity fluctuations; indeed, we expect that the velocity of a particle is to represent the mean velocity of the finite mass of fluid it represents. The macroscopic kinetic energy of the fluid is exactly the kinetic energy of all the particles. The internal energy is represented by an additional variable. If this latter is expressed as a function of particle positions only, then only adiabatic motion can be represented. Compression and subsequent expansion can return the set of particles to exactly their initial configuration with no dissipation. Thus a special prescription is needed to describe variations of particle internal energy.

We start by considering the dynamics of a set of particles described by the following nomenclature.

$i,j \equiv$ indices describing the particle number

$m_j \equiv$ mass of particle #j

$\vec{r}_j \equiv$ space coordinate of particle #j

$\vec{u}_j \equiv$ velocity of particle #j

$\vec{F}_{ij} \equiv$ force exerted by particle i onto particle j

$\vec{r}_{ij} \equiv \vec{r}_j - \vec{r}_i$

$r_{ij} \equiv |\vec{r}_{ij}|$

$\vec{s}_{ij} \equiv \vec{r}_{ij}/r_{ij}$ (a unit vector pointing from particle #i to particle #j)

$\vec{M}_j \equiv m_j \vec{u}_j \equiv$ momentum of particle #j

$K_j \equiv \frac{1}{2} m_j \vec{u}_j \cdot \vec{u}_j \equiv$ kinetic energy of particle #j

$J_j \equiv$ internal energy of particle #j

Additional nomenclature will be introduced as required by developments of the theory.

We commence by assuming that the particles are governed by the equations of motion

$$m_j \frac{d\vec{u}_j}{dt} = \sum_i^* \vec{F}_{ij} \tag{1}$$

$$\frac{d\vec{r}_j}{dt} = \vec{u}_j \tag{2}$$

The summation over i, modified by the presence of *, does not include the term i = j, and is further restricted to include only certain neighbors of j as discussed further ahead. Summation without * includes all

particles in the system.

Next, we assume that the force function can be divided into two parts

$$\vec{F}_{ij} = \vec{s}_{ij} f_{ij} + \vec{g}_{ij} \tag{3}$$

where

$$f_{ij} \equiv f(r_{ij}, J_i, J_j)$$

The first term in the force is associated in form with the equation of state of the fluid; the second term is introduced to achieve dissipation in the same manner as the "artificial viscosity" of von Neumann and Richtmyer,[12] or for the purpose of including real viscous effects.

The correspondence with fluid mechanics comes through an examination of the conservation laws in forms appropriate to the nature of the continuum to be represented.

1. Conservation of mass. This is automatic. Each particle has constant mass, m_j, so that the total does not change with time. Likewise the change of mass in any fixed volume exactly equals the amount flowing over the bounding surface.

2. Conservation of momentum. To satisfy this requirement, the restriction is the same as in classical particle dynamics, namely $\vec{F}_{ij} \equiv -\vec{F}_{ji}$. Proof of this is demonstrated as follows. Consider the momentum change rate of a particular subset of all the particles

$$\frac{d\vec{M}}{dt} = \sum_{j(\text{subset})} m_j \frac{d\vec{u}_j}{dt} = \sum_{j(\text{subset})} \sum_{i}^{*} \vec{F}_{ij}$$

We break the sum over i into two parts and write

$$\frac{d\vec{M}}{dt} = \sum_{i(\text{inside})}^{*} \sum_{j(\text{subset})} \vec{F}_{ij} + \sum_{i(\text{outside})} \sum_{j(\text{subset})} \vec{F}_{ij}$$

where "inside" and "outside" refer to inclusion or exclusion from the subset. In the first double sum, each pair of particles enters twice, so that the total contribution to the sum from a particular pair is $\vec{F}_{ij} + \vec{F}_{ji}$. Since there must be no contribution to momentum change from particles <u>within</u> the subset, the sum of the two terms must vanish. The second double sum does not thereby vanish, since each pair enters only <u>once</u>. Thus with $\vec{F}_{ij} = -\vec{F}_{ij}$, the momentum change of any subset of particles arises only through external forces, as required.

The restriction also means that

$$\left.\begin{aligned} f_{ij} &\equiv f_{ji} \\ \vec{g}_{ij} &\equiv -\vec{g}_{ji} \end{aligned}\right\} \qquad (4)$$

3. <u>Conservation of energy</u>. Here we must make a break from the usual procedure in particle mechanics. In devising a reasonable approach we will thereby be able to establish some of the crucial parts of the technique. The basis for the energy discussion is that the rate of change of energy of a particle should be given by the rate that the other particles do work on it. This work rate is in turn given by the product of force by velocity. (To be properly symmetric, the velocity through which the work flux is carried from one particle to another must be the mean value of the two velocities.) Thus we write

$$\frac{d}{dt}(K_j + J_j) = \sum_i^* \vec{F}_{ij} \cdot \left(\frac{\vec{u}_i + \vec{u}_j}{2}\right) \tag{5}$$

It follows that the total energy of an isolated system is conserved

$$\frac{dE}{dt} \equiv \frac{d}{dt}\sum_j (K_j + J_j) = \frac{1}{2}\sum_j \sum_i^* \vec{F}_{ij} \cdot (\vec{u}_i + \vec{u}_j) = 0$$

where equality to zero follows from separate vanishing of the sum of contributions from each pair. Likewise the energy of any subset of particles changes only through work done on them by external particles.

Now, we already know that

$$\frac{dK_j}{dt} = m_j \vec{u}_j \cdot \frac{d\vec{u}_j}{dt}$$

$$= \vec{u}_j \cdot \sum_i^* \vec{F}_{ij}$$

Combination of this with (5) can be arranged to give

$$\frac{dJ_j}{dt} = \frac{1}{2}\sum_i^* \vec{F}_{ij} \cdot (\vec{u}_i - \vec{u}_j) \tag{6}$$

or

$$\frac{dJ_j}{dt} = -\frac{1}{2}\sum_i^* f_{ij} \frac{d\, r_{ij}}{dt} + \frac{1}{2}\sum_i^* \vec{g}_{ij} \cdot (\vec{u}_i - \vec{u}_j) \tag{7}$$

B. Finite Time Intervals

In practice, the numerical computations must proceed through a sequence of finite time advancements, whose steps are of duration δt.

This is accomplished through a replacement of (1), (2), and (6) by

$$m_j \frac{\vec{u}_j^{n+1} - \vec{u}_j^{n}}{\delta t} = \sum_i^* \vec{F}_{ij}^{\,n} \tag{8}$$

$$\frac{\vec{r}_j^{n+1} - \vec{r}_j^{n}}{\delta t} = \vec{u}_j^{n+1} \tag{9}$$

$$\frac{J_j^{n+1} - J_j^{n}}{\delta t} = \frac{1}{2} \sum_i^* \vec{F}_{ij}^{\,n} \left(< \vec{u}_i > - < \vec{u}_j > \right) \tag{10}$$

where

$$< \vec{u} > \equiv \tfrac{1}{2} (\vec{u}^{\,n} + \vec{u}^{\,n+1})$$

This shows how the variables for the beginning of cycle #n+1 are obtained algebraicly from those at the beginning of cycle #n. The choice of time-centering of the equations is justified as follows:

Eq. (8) — At the beginning of the calculations for the advancement through a cycle, the only information available for the force calculation is that which pertains to the beginning of cycle #n. The force is thus labeled with index n.

Eq. (9) — After calculation of the new velocity by (8), there is some arbitrariness as to what velocity should be used to determine the new coordinate. To show that the newly calculated velocity is preferred over that which the particle had at the beginning of the cycle, we appeal to a simple example of stability properties. Suppose that, in one dimension, a particle is subjected to an external potential which is a function

of the particle position only. Then

$$\frac{du}{dt} = - \omega_o^2 \, x$$

$$\frac{dx}{dt} = u$$

are the appropriate equations for small oscillations about a potential minimum centered at x = 0. The solution can be written

$$u = u_o \, e^{i\omega_o t}$$

$$x = x_o \, e^{i\omega_o t}$$

In finite-difference form, analogous to (8) and (9), we write

$$u^{n+1} - u^n = - \omega_o^2 \, \delta t \, x^n$$

$$x^{n+1} - x^n = u^{n+\epsilon} \, \delta t$$

where if $\epsilon = 1$ we have the proposed procedure, and if $\epsilon = 0$ we have the alternative whereby the particle is moved with its beginning-of-cycle velocity. We try the solution

$$u^n = u_o \, e^{i\omega n \delta t}$$

$$x^n = x_o \, e^{i\omega n \delta t}$$

and find the condition for solution to be

$$(r - 1)^2 = - r^{\epsilon} (\omega_o \delta t)^2$$

where $r \equiv e^{i\omega\delta t}$. Instability of the difference approximation is indicated by the presence in ω of a negative imaginary part, or equivalently by a magnitude of r which exceeds unity. For $\epsilon = 0$, $r = 1 \pm i\omega_o\delta t$ and $|r| = \sqrt{1 + \omega_o^2 \delta t^2}$, indicating unconditional instability. For $\epsilon = 1$, however, $r = 1 - (\omega_o\delta t)^2 \pm \sqrt{(\omega_o\delta t)^4 - 2(\omega_o\delta t)^2}$. If $\omega_o\delta t > 2$, then r is real and one of the solutions has magnitude exceeding unity. If $\omega_o\delta t < 2$, then $|r| \equiv 1$, indicating the achievement of stability for sufficiently small values of δt. (The time interval per cycle must be less than π^{-1} times the period of oscillation.)

Eq. (10) — The right side contains the average of the old and new velocities, which combination is introduced to assure rigorous energy conservation in the time-difference form of the equations. (Mass and momentum have likewise been conserved; proof of this is the same as for the differential equations.) To demonstrate energy conservation we start from the identity

$$\frac{1}{2}\left[\left(\vec{u}_j^{\,n+1}\right)^2 - \left(\vec{u}_j^{\,n}\right)^2\right] \equiv \langle \vec{u}_j \rangle \cdot \left(\vec{u}_j^{\,n+1} - \vec{u}_j^{\,n}\right)$$

Thus, from (8), the change in kinetic energy of a particle is

$$K_j^{n+1} - K_j^{\,n} = \delta t \sum_i^* \vec{F}_{ij}^{\,n} \cdot \langle \vec{u}_j \rangle$$

Combination of this with (10) gives for the change in total particle energy, E_j,

$$E_j^{n+1} - E_j^{\,n} = \frac{1}{2}\sum_i^* \vec{F}_{ij} \cdot \left(\langle \vec{u}_i \rangle + \langle \vec{u}_j \rangle\right) \qquad (11)$$

Since $\vec{F}_{ij} \equiv - \vec{F}_{ij}$, this result shows that the energy transferred from particle #i to particle #j is equal in magnitude but opposite in sign from that transferred from #j to #i, thus proving the contention of conservation.

C. Dissipation

There is at least one other form alternative to (10) which could be considered for the internal energy calculation. The total energy difference could be calculated in a form analogous to (11), but with any time centering of the right side. The result would still be conservative as long as the proper reciprocal symmetries were preserved. From the new total energy of the cell, the new kinetic energy could then be subtracted giving the new internal energy.

The reason for the specific choice of the form (10), however, follows from the requirement of monotonic dissipation. With (10), proper choice of the $\vec{g}_{ij}$ forces can always result (at least to lowest order in δt) in increasing entropy, while in most of the alternative forms there can be circumstances leading to significant decreases in entropy.

D. Neighbors

Two kinds of particle-wise sums have been introduced so far. The unmodified summation is over all particles of the system, while a summation modified by superscript * means a neighbor sum. Thus $\sum_i^* \vec{F}_{ij}$ denotes a sum over the neighbors, i, of particle #j. Such a modified summation is required in order to achieve a proper fluid-dynamic representation, in which elements of fluid do, indeed, interact only with

those adjacent. There are several methods by which the neighbors of a particle could be chosen, so that some criteria must be evolved for deciding among them. Important among these criteria is the requirement of reciprocity: for rigorous conservation of momentum and energy it is necessary that particle #i be a neighbor of particle #j <u>if and only if</u> #j is a neighbor of #i. This is satisfied by the neighbor-choosing method in which all those particles lying closer than some given distance to #j are considered to be neighbors of #j. The distinguishing distance must be the same for all particles, with the result that in regions of high compression each particle will have many neighbors, in violation of the requirement of interaction only with adjacent elements. We have therefore used a somewhat different means for finding neighbors.

The neighbor-choosing procedure we have used involves two steps. First, for each particle we find the N other particles lying closest to it. (In Cartesian coordinates, N is twice the number of space dimensions.) Since the reciprocity condition is not automatically satisfied by this, we proceed in the second step to <u>add</u> to the neighbors of each particle just those necessary to give complete reciprocity. As a result, each particle can have more neighbors than the ideal number, N, but we do not therefore modify the nature of the interparticle forces or any of the procedures so far described. An argument justifying this, and a demonstration of its validity, are given in Part III.

The following table shows how many neighbors a particle would have under various circumstances, in Cartesian coordinates.

Number of Dimensions	$\mathcal{N}$ ≡ Number of Neighbors			
	N	Ordinary Total	Maximum Possible Total	Usual Extreme Total
1	2	~ 2	4	3
2	4	~ 5	9(?)	8
3	6	~ 8	15(?)	12

The numbers are not meant to have any absolute significance, only to indicate approximately the magnitudes to be expected. The numbers for three dimensions were guessed as extrapolations from one- and two-dimensional observations.

A combination of the above two procedures also might be appropriate. The search for N nearest neighbors could be conducted only among those which lie closer than a prescribed distance. This would mean that a small number of particles far from the rest could actually become completely detached, and no longer influence the rest.

E. Boundary Conditions

The boundary adjacent to a vacuum is simply a point, line, or surface separating a region with particles from one without any. One might speculate that no special consideration would be necessary for obtaining properly the surface motion, and in Part III it is shown that such is indeed the case.

A rigid wall can be produced by an image method in which the neighbors of a particle near the wall include the images of itself and of its neighbors. Each image particle has the reflected properties of the corresponding one in the system. This is easily accomplished if the wall

is straight (or flat), but becomes more complicated if the wall is curved. In this latter case one might, for simplicity, be content to allow a given particle to be influenced by its own image only (or images, if the wall forms a small pocket).

So far our studies have been limited to examples with only the simplest boundary conditions; much thought and experimentation will be required to perfect general techniques.

F. Fluid-Dynamics Equivalence, Choice of Force Functions

The most difficult, but most important, question to be answered is: How well will results from the proposed computing method represent the solution of a fluid-dynamics problem? At this time only a partial answer can be given, and most of the rest of this report will show that which so far has been learned.

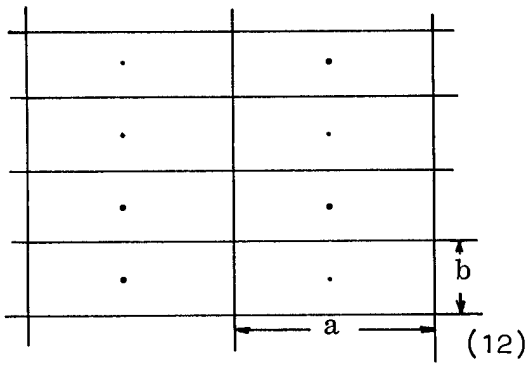
Up to this point, no specification has been made of the force function, except as implied by the dependence of the $\vec{s}_{ij} f_{ij}$ part upon the mutual distance, the internal energies, and an ordering variable (such that the force vanishes between two particles if they are not neighbors), together with the statement that the $\vec{g}_{ij}$ part is included only to produce dissipation. Already it follows that goodness of the method will depend upon some statistical properties of the particle behavior. An ideal particle-and-force treatment might base the force between two particles upon particle-wise volumes and interparticle area. (Both of these depend in complicated fashion upon the positions of all the other surrounding particles, and would therefore require very large amounts of computing

time.[13]) In the PAF technique, however, the force between two particles is completely independent of the other surrounding particles, with the important exception that the two particles must be neighbors.

The $\vec{s}_{ij} f_{ij}$ part of the force function has been chosen in such a way as to represent the equation of state in a rectangular array of particles. Consider the case of two dimensions, with the particles all having the same mass, m. For a polytropic gas, for which the equation of state is $p = (\gamma - 1)\rho I$ (in which p, ρ and I are respectively pressure, density, and specific internal energy), the force between two particles in a horizontal direction is thus

$$\begin{aligned} f_{ij} &= (\text{pressure}) \text{ times } (\text{area}) \\ &= (\gamma - 1)\left(\frac{m}{ab}\right)\left(\frac{J}{m}\right) \text{ times } (b) \\ &= \frac{(\gamma - 1)J}{a} \end{aligned}$$

$$f_{ij} \rightarrow \frac{(\gamma - 1)\,(J_i + J_j)}{2\, r_{ij}} \qquad (12)$$



The same form results for the vertical direction, and (12) is thus the force function (actually appropriate to use in one, two, or three dimensions).

More difficult to derive is the form which should statistically represent a more general equation of state. For $p = p(\rho, I)$, the recipe corresponding to the polytropic gas treatment would lead to

$$\text{horizontal:} \quad f_{ij} = b\, p\left(\frac{m}{ab}, \frac{J}{m}\right)$$

$$\text{vertical:} \quad f_{ij} = a\, p\left(\frac{m}{ab}, \frac{J}{m}\right)$$

The result cannot, therefore, be directly related to the requirement which states, in effect, that the horizontal force should not depend upon b, while the vertical force should not depend upon a. (If, however, the motion is purely horizontal, then b is constant and the requirement is satisfied.)

Actually, a rectangular array is configurationally unstable, as has been pointed out by Birkhoff and Lynch,[14] and the particles will most usually be distributed "randomly." (A discussion of configuration instability is given in Appendix I.) In addition, the randomness of spacing will probably be maintained at least at a rate comparable to the rate of the over-all dynamics. Thus the area between particles should, statistically, be proportional to the mean interparticle distance, while the volume used to calculate the density should be proportional to the square thereof. This leads, therefore, to the proposal for general equation of state

$$f_{ij} = r_{ij}^{\alpha-1}\, p\left[\frac{m}{(r_{ij})^{\alpha}}, \frac{J_i + J_j}{2m}\right] \tag{13}$$

to be appropriate for α space dimensions. (The constants of proportionality are chosen to give agreement with the polytropic equation of state, and the density formula for a square array.)

Incidentally, Beyer has pointed out[15] that, at least with a

rectangular array of particles, an infinite line at any angle through them will have the proper force acting across it when the fluid is a polytropic gas. It would be useful to have a generalization of his observation to the determination of the probability of finding a specified force across a finite line segment through a random distribution of particles with generalized force function.

The $\vec{g}_{ij}$ forces are much more easily specified in general. Indeed, we have chosen

$$\vec{g}_{ij} \equiv m\omega\,(\vec{u}_i - \vec{u}_j) \tag{14}$$

for a region of compression and $\vec{g}_{ij} = 0$ for a region of expansion; ω is a constant with dimensions of reciprocal time. (An alternative form is discussed in Appendix II.) The analogy to viscosity is easily demonstrated and the contribution that the $\vec{g}_{ij}$ force makes to stability is discussed in Part III. The dynamic effect can be seen as follows. Consider a group of particles for which the f_{ij} forces vanish. Then (1) becomes

$$m\frac{d\vec{u}_j}{dt} = m\omega \sum_i^* (\vec{u}_i - \vec{u}_j)$$

$$\equiv \mathcal{N}\, m\omega(\vec{u}_j' - \vec{u}_j)$$

where $\vec{u}_j' \equiv \frac{1}{\mathcal{N}} \sum_i^* \vec{u}_i$ is the average velocity of the $\mathcal{N}$ neighbors. If this average is constant in time then particle #j, starting from $\vec{u}_{jo}$ at $t = 0$, will change velocity according to

$$\vec{u}_j = \vec{u}_j' + (\vec{u}_{jo} - \vec{u}_j')\, e^{-\mathcal{N}\omega t}$$

The velocity will decay to the mean velocity of its neighbors, with a decay time of $(\eta\omega)^{-1}$.

Thus, the crudeness of our proposed method is now laid bare. If it can be made to work as proposed, or with relatively minor variations, then it will have tremendous advantages of generality without requiring the great computing time of most proposals of this generality. The proof of applicability must come through considerable analytical study of the statistics of such a system, together with an analysis of numerous computing experiments. These projects are in progress in Group T-3 of the Los Alamos Scientific Laboratory, and contributions or suggestions will be enthusiastically welcomed.

III. PAF IN ONE SPACE DIMENSION

The one-dimensional form of PAF differs little from the usual techniques of one-dimensional Lagrangian finite difference methods. The principal difference for which concern was felt is the fact that a PAF particle can have either one or two neighbors on each side, as a result of the reciprocity requirement. Thus, for example, as a compression wave moving to the right approaches a particle, there will come a time when that particle will have two neighbors to the left and one to the right. Briefly, its rightward acceleration will be too great. Soon, however, the situation is reversed — after the front of the compression wave has passed, the particle will have for another brief time two neighbors to the right and only one to the left. As a result, the effects of previous over-acceleration can be expected to be removed; the computations discussed below show that the expectation is indeed realized.

The one-dimensional calculations were performed for the additional purposes of studying the behavior of internal energy and certain matters concerning stability.

A. Negative Internal Energy

With the neighbor-search procedure which gives each particle at

least N neighbors, even when it has flown off from the rest of the system, it is possible to obtain negative values for the specific internal energy. This can be seen by considering the motion of a particle which is at a distance x from its two neighbors (both of which are on the same side of the particle). If the particle has internal energy J, and its neighbors have internal energy J_o (assumed constant), then, for J small,

$$\frac{dJ}{dt} \approx - \frac{(\gamma - 1)\, J_o u}{2x} = - \frac{(\gamma - 1) J_o}{2} \frac{1}{x} \frac{dx}{dt}$$

$$J \approx \text{const} - \frac{(\gamma - 1) J_o}{2} \ln x$$

and since x continues to increase (since the force does not become attractive until somewhat after J = 0), it is seen that J could become negative. This situation could probably be remedied by the combination neighbor-searching procedure described at the end of Part II-D.

B. Stability of the PAF Procedure

Consider a one-dimensional region which is only slightly perturbed from a constant state. For simplicity, we use a polytropic-gas equation of state, but the results are more generally applicable. The equations of motion are

$$\frac{m}{\delta t}\left(u_j^{n+1} - u_j^n\right) = \frac{\gamma - 1}{2}\left(\frac{J_{j-1}^n + J_j^n}{x_j^n - x_{j-1}^n} - \frac{J_j^n + J_{j+1}^n}{x_{j+1}^n - x_j^n}\right)$$

$$+ \left[\zeta_-\left(u_{j-1}^n - u_j^n\right) + \zeta_+\left(u_{j+1}^n - u_j^n\right)\right]$$

$$x_j^{n+1} - x_j^n = u_j^{n+1}\,\delta t$$

The values of $\zeta_\pm$ are zero and one, for expansion and compression respectively. Into these equations we introduce the linearizations

$$x_j - x_{j-1} \equiv \delta x(1 + \epsilon_{j-\frac{1}{2}})$$

$$J_j \equiv J(1 + 2\sigma_j)$$

and drop higher than first order terms in u_j, $\epsilon_{j-\frac{1}{2}}$ and σ_j; J and δx are constants. The resulting linearized equations of motion, plus energy equation, are

$$\frac{m}{\delta t}\left(u_j^{n+1} - u_j^n\right) = \frac{(\gamma - 1)J}{\delta x}\left(\sigma_{j-1}^n - \sigma_{j+1}^n + \epsilon_{j+\frac{1}{2}}^n - \epsilon_{j-\frac{1}{2}}^n\right)$$

$$+ m\omega\left[\zeta_-\left(u_{j-1}^n - u_j^n\right) + \zeta_+\left(u_{j+1}^n - u_j^n\right)\right]$$

$$\epsilon_{j-\frac{1}{2}}^{n+1} - \epsilon_{j-\frac{1}{2}}^n = \frac{\delta t}{\delta x}\left(u_j^{n+1} - u_{j-1}^{n+1}\right)$$

$$\sigma_j^{n+1} - \sigma_j^n = \frac{(\gamma - 1)\,\delta t}{8\,\delta x}\left(u_{j-1}^n + u_{j-1}^{n+1} - u_{j+1}^n - u_{j+1}^{n+1}\right)$$

We assume that the time average of $\zeta_\pm$ is $\frac{1}{2}$ and put this value in. To analyze the stability of these equations we substitute the trial functions

$$u_j^n \equiv u_o\, e^{ikj}\, r^n$$

$$\epsilon_j^n \equiv \epsilon_o\, e^{ikj}\, r^n$$

$$\sigma_j^n \equiv \sigma_o \, e^{ikj} \, r^n$$

and find them to be a solution provided that r satisfies the equation

$$(r - 1)\,[r - 1 + \xi(1 - \cos k)] + \frac{\mu^2}{\gamma}\,[4r \sin^2 \frac{k}{2} + \frac{\gamma - 1}{2}\,(1 + r) \sin^2 k] = 0$$

in which

$$\xi \equiv \omega \delta t$$

$$\mu \equiv \frac{c \delta t}{\delta x}$$

and the sound speed is $c \equiv \sqrt{\gamma(\gamma - 1)J/m}$. The equations are not stable for those circumstances in which the magnitude of r exceeds unity. Consider first the case in which the roots of r are real. At $r = 1$ we find that except for certain peculiar values of k, it is necessary that $\mu = 0$, while for $\mu > 0$, $r < 1$, and no restriction therefore results. At $r = -1$,

$$\xi + \frac{\mu^2}{\gamma} = \frac{2}{1 - \cos k}$$

If $\xi + \mu^2/\gamma$ exceeds the right side, then $r < -1$. The most restrictive case comes from the smallest right side, and can be expressed in the stability requirement

$$\xi + \frac{\mu^2}{\gamma} < 1 \qquad (15)$$

Finally, we must examine the complex roots of r, which can be shown to have magnitude

$$|r| = \sqrt{1 - \xi(1 - \cos k) + \frac{\gamma - 1}{2\gamma}\,\mu^2 \sin^2 k}$$

so that, at $|r| = 1$,

$$\xi = \frac{\gamma - 1}{2\gamma} \mu^2 (1 + \cos k)$$

In this case, if ξ is less than the right side, then $|r| > 1$. As a function of k, the right side has maximum value at $\cos k = 1$. We thus obtain the additional restriction for stability

$$\xi > \frac{\gamma - 1}{\gamma} \mu^2 \tag{16}$$

In more familiar nomenclature, the two stability conditions can be summarized

$$\left.\begin{aligned} \omega \delta t + \frac{1}{\gamma} \left(\frac{c\ \delta t}{\delta x}\right)^2 < 1 \\ \delta t < \left(\frac{\gamma}{\gamma - 1}\right) \left(\frac{\delta x}{c}\right)^2 \omega \end{aligned}\right\} \tag{17}$$

The result may be compared to that for Example 3, p. 18 of Ref. 1, in which a similar stability analysis is made. Finally, with

$$\mu \equiv \frac{c \delta t}{\delta x}$$

$$\eta = \frac{\omega \delta x}{c}$$

being dimensionless measures of δt and ω, we may write the stability conditions

$$\left.\begin{aligned} \eta\mu + \frac{1}{\gamma} \mu^2 < 1 \\ \mu - \frac{\gamma}{\gamma - 1} \eta < 0 \end{aligned}\right\} \tag{18}$$

As an example, Fig. 1 shows a plot of the stable region for $\gamma = 5/3$.

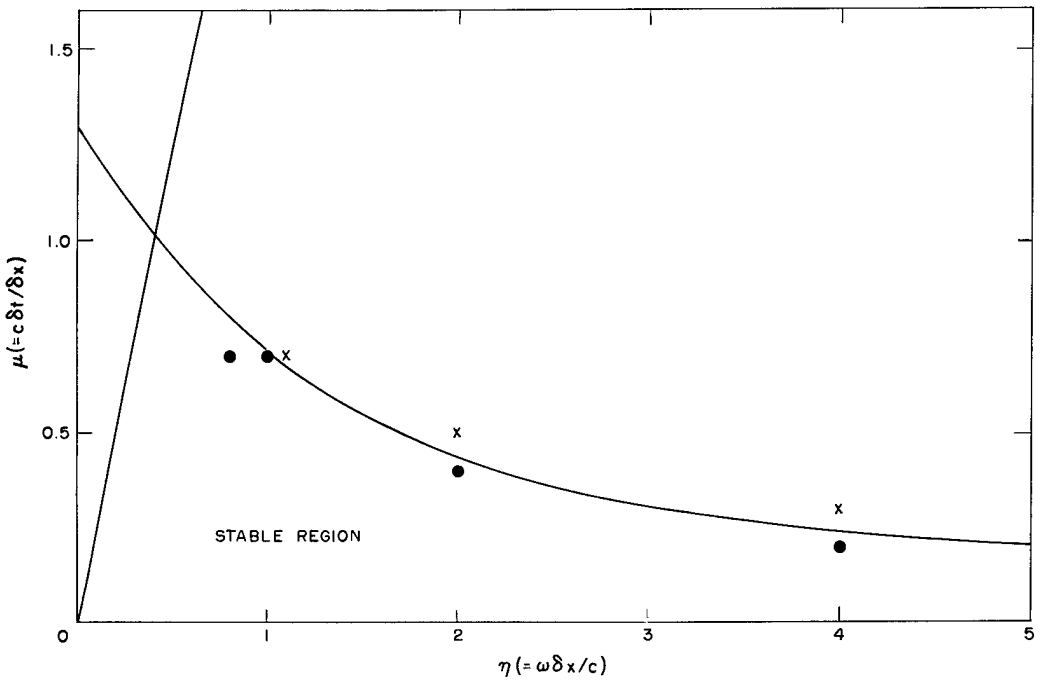


FIG. 1

The points were tested by machine calculations; those marked ● were found to be stable while those marked x were found to be unstable.

The results of this stability analysis are similar to those which would result for a much more general class of equations with both wave-like and diffusion-like properties. In general, the conditions for stability can be violated in either of two ways (corresponding to leaving the stability region either to the right or to the left, in Fig. 1). In one case, there is too much diffusion for the given sizes of δt and δx. A perturbation to an otherwise smooth profile is over-corrected, and the result is oscillation with increasing amplitude. Such instability is

easily observed, and is the nature of all the unstable points marked in Fig. 1. The other type of instability corresponds to too little diffusion. Since the equations without the diffusion properties, and with $\delta x \to 0$, $\delta t \to 0$, have solutions with constant amplitude, the truncation resulting from finite differences can easily be expected to add slowly-growing influences. Such is the case with the unstable region to the left in Fig. 1; and while two attempts were made to observe the instability in that region, the rate of growth was so small as to leave doubt concerning confirmation of instability. Actually these results are not unreasonable since the equation for r, giving the rate of growth, shows that the examples tried (both chosen for large growth rate) correspond to two too small rates to be observed with the computing code used.

C. Some Results of the Tests

1. The rarefaction wave. Gas adjacent to a wall at x = 0 is initially at rest. Beyond the gas to the right is vacuum. Initial data for the PAF calculation are

Number of particles	= 30
Internal energy per particle	= 1.0
Specific heat ratio, γ	= 2.0
Mass per particle	= 1.0
δx	= 1.0
δt	= 0.1
ω	= 1.0

The initial sound speed is thus 1.414 and the escape speed of the free surface is 2.818. The configuration of particles together with their internal energy, velocity, and specific volume (i.e., δx) are shown as functions of position for time t = 20 in Fig. 2. The datum points are from the machine calculation, while the solid lines show the true solution.

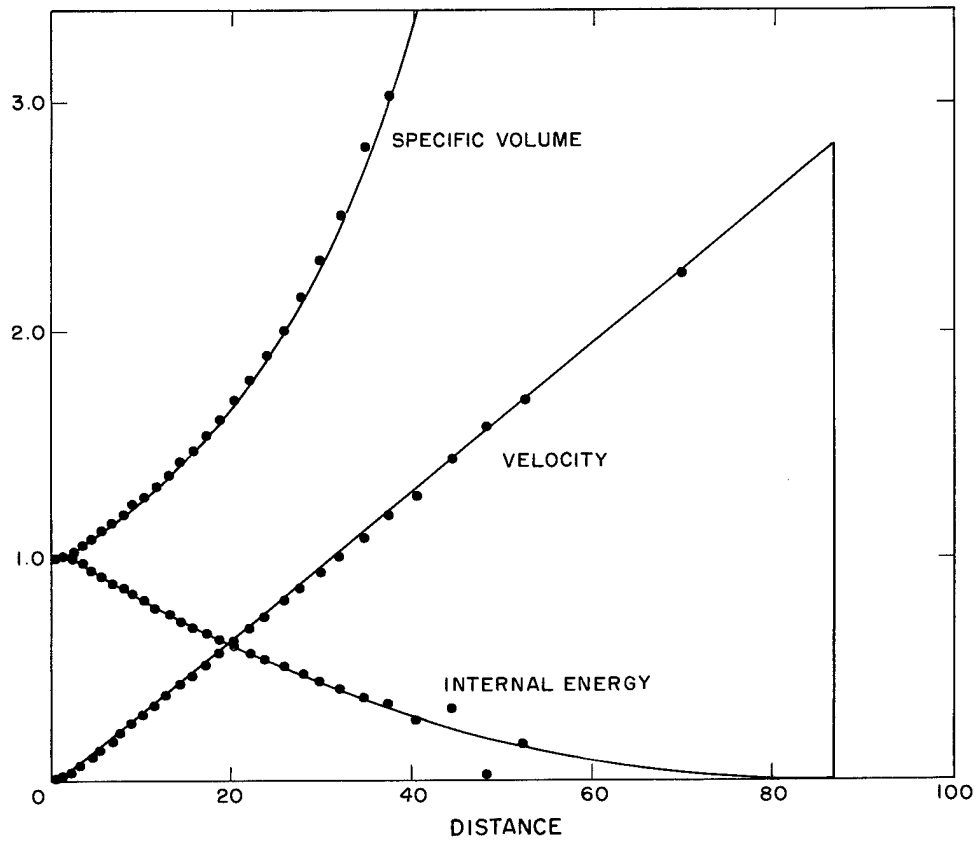


FIG. 2

2. The shock wave. Gas adjacent to a wall at x = 0 is initially cold and moving towards the wall. Initial data for the PAF calculation are

Number of particles	= 51	δx	= 1.0
Velocity of particles	= - 2.0	δt	= 0.1
Specific heat ratio, γ	= 2.0	ω	= 1.0
Mass per particle	= 1.0		

The configuration of particles, together with their internal energy, are shown for time t = 15 in Fig. 3. Datum points are from the machine calculation, while the solid line shows the true solution. Note the usual Lagrangian difficulty of overproduction of internal energy at the wall.

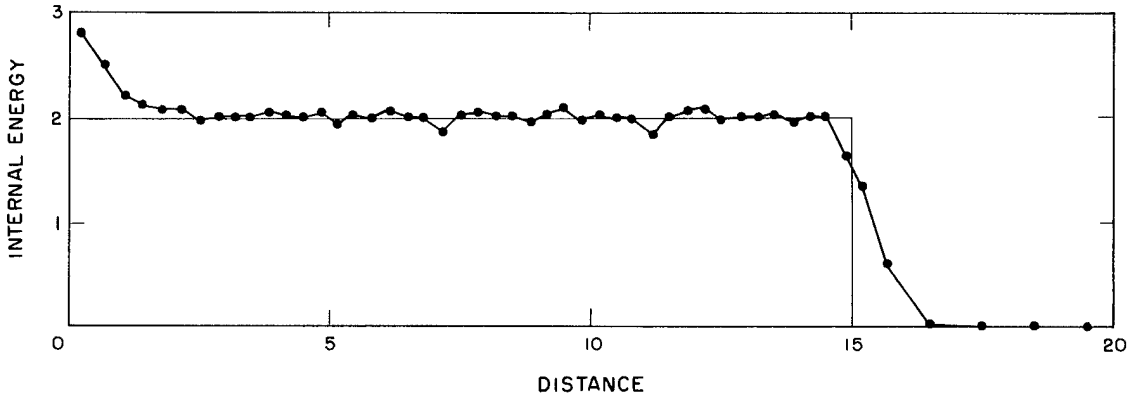


FIG. 3

For contrast, the calculation was also performed with $\omega = 5.0$, and the results are shown in Fig. 4.

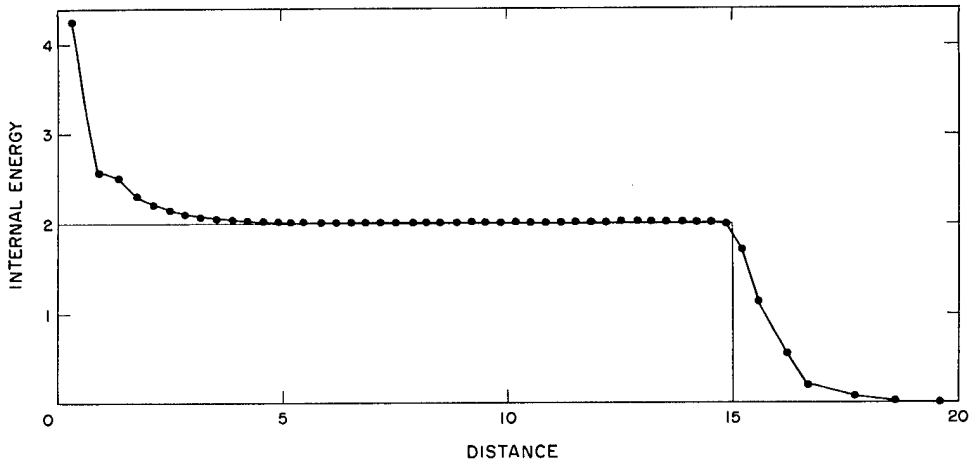


FIG. 4

The results from the first shock calculation are also shown as a function of time in Fig. 5. The graph shows the total energy of the system together with the negative of the total momentum. Datum points are from the calculation while solid lines show the true solution.

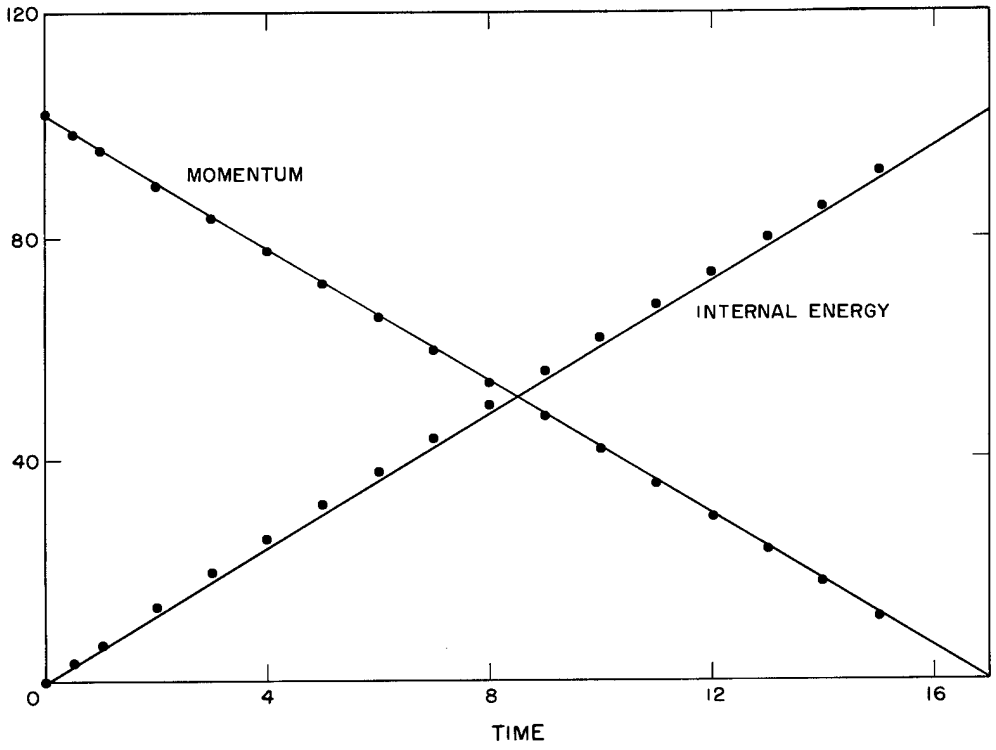


FIG. 5

Finally, in Fig. 6 is shown as a function of time the difference between calculated and true histories of internal energy for various values of ω.

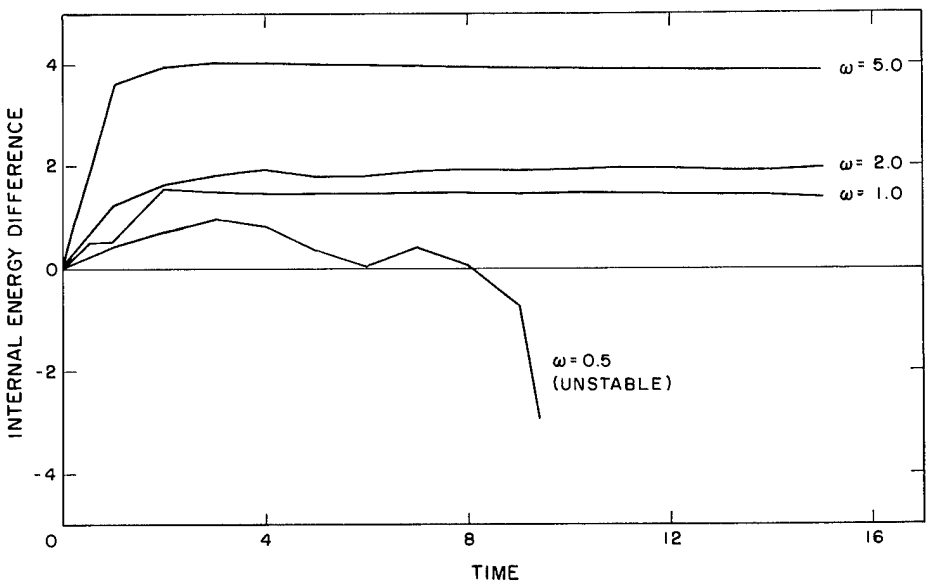


FIG. 6

It is apparent that the overproduction arises at early times when the shape of the smeared shock is adjusting itself. Once this is completed, subsequent internal energy production proceeds at very nearly the proper rate.

IV. PAF IN TWO SPACE DIMENSIONS

The only two-dimensional tests so far performed have been of a relatively simple nature, for the purpose of revealing whether or not some basic difficuty exists. The test results have been encouraging, however, and we are therefore developing a much more elaborate computing code which will allow the interaction of several materials with several boundaries.

In the simple tests, a region of gas was allowed to interact with one rigid wall. In the first calculation, the gas region was rectangular, with one side initially along the wall, and the gas was cold but possessed a velocity towards the wall. Initial conditions were much like those in the one-dimensional shock problem.

Number of particle rows (parallel to wall)	= 8	Velocity of particles (normal to wall)	= -2.0
Number of particle columns (normal to wall)	= 15	Mass per particle	= 1.0
Internal energy per particle	= 0	Specific heat ratio, γ	= 2.0
Velocity of particles (parallel to wall)	= 0	$\delta x = \delta y$	= 1.0
		δt	= 0.1
		ω	= 1.0

The problem is one dimensional along the center line until signals from the side arrive. The two-dimensional effects come from lateral splashing of the rectangle of gas. While exact comparison solutions for the two-dimensional effects were not obtained, it was possible to approximate the effects using simple elements of shock and rarefaction theory.[16] Thus, Fig. 7 shows the time history of the normal momentum of the gas. The solid line is the theoretical one-dimensional history (that is, the history without splash effects), while the dashed line shows the lowest order solution with splash effects included. Datum points are from the calculation.

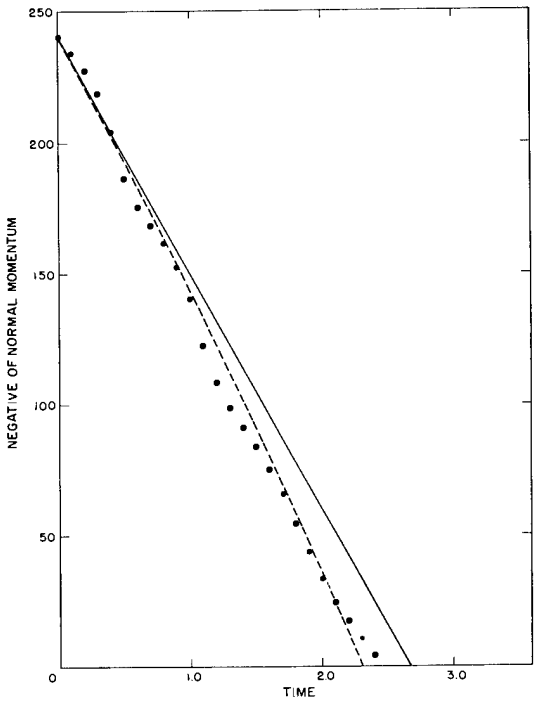


FIG. 7

Considering the crudeness of the computational resolution, the agreement appears quite good. Figure 8 shows the tangential momentum of one side of the gas.

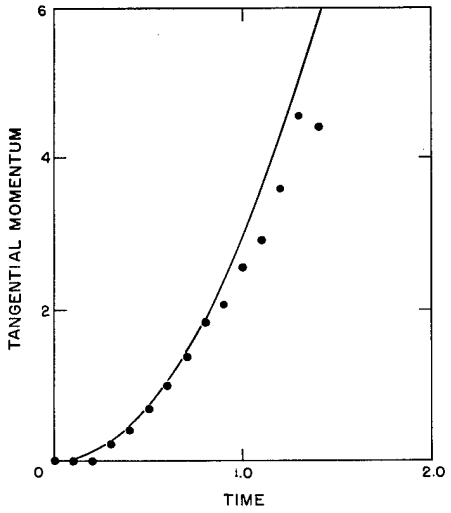


FIG. 8

Here the effect is entirely two-dimensional, associated with the splash. The theoretical curve (solid line) is based upon the lowest order effects. Later times were not shown because the configurational instability (see Appendix I) mentioned earlier made determination of the computed momentum difficult. Agreement is again considered good.

Additional calculations were performed in which a circular bubble of gas was collapsed by the passage of a shock over it. (The physical conditions were, of course, only crudely simulated, since two materials were not possible for the calculation to handle.) The results showed no particular surprises, and since no quantitative comparisons could be made, the results are not shown here.

V. DIRECTION FOR FURTHER DEVELOPMENT

Besides those problems which have already been brought up in Parts I to IV, there are several others which come to mind.

1. The method should be adapted to cylindrical coordinates. Particles might become rings around the central axis (assuming dependence of the flow on r and z only), and the appropriate force law between particles would have to be found. If a ring were to have constant mass, then its approach to the axis would cause difficulties; thus it may be necessary for ring mass to be time-dependent. Boundary conditions will be required.

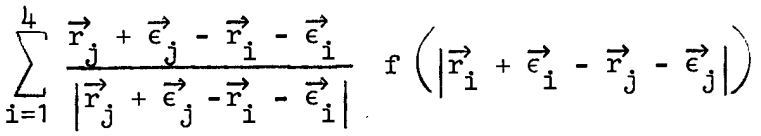
2. Most problems of interest involve several materials with different state equations. A method must be evolved for treating properly their interaction.

3. The effects of heat conduction and true viscosity will have to be considered; it is not expected that their inclusion will be difficult.

Our program calls for an exploration of these and other matters relative to eventual development of a useful computing method. Comments and suggestions will be very much welcome from whomever may be interested.

APPENDIX I. CONFIGURATIONAL INSTABILITY

Birkhoff and Lynch[14] have remarked that a rectangular array of particles can be deformed with no change of interparticle distances, suggesting, therefore, that such a configuration must not be stable. To see in more detail the nature of configurational instability, we consider the simple use of a square array of particles. A typical particle, #j, with four neighbors numbered as shown, will have zero net force on it. We now suppose that all five particles of this subset be displaced by small distances without change of internal energy, and examine the resulting force. The initial coordinates $\vec{r}_j$ and $\vec{r}_i$ ($i = 1, 2, 3, 4$) become $\vec{r}_j + \vec{\epsilon}_j$ and $\vec{r}_i + \vec{\epsilon}_i$ and the resulting force is



$$\vec{F}_j = \sum_{i=1}^{4} \frac{\vec{r}_j + \vec{\epsilon}_j - \vec{r}_i - \vec{\epsilon}_i}{\left|\vec{r}_j + \vec{\epsilon}_j - \vec{r}_i - \vec{\epsilon}_i\right|} f\left(\left|\vec{r}_i + \vec{\epsilon}_i - \vec{r}_j - \vec{\epsilon}_j\right|\right)$$

This can be expanded in powers of $\vec{\epsilon}$ and, with use made of the equilibrium conditions, the result is

$$\vec{F}_j = \frac{f_o}{\delta x_o}\left(4\vec{\epsilon}_j - \sum_{i=1}^{4} \vec{\epsilon}_i\right) + \left(f_o' - \frac{f_o}{\delta x_o}\right)\left\{2\vec{\epsilon}_j - \sum_{i=1}^{4} (\vec{S}_{ij})_o\left[(\vec{S}_{ij})_o \cdot \vec{\epsilon}_i\right]\right\}$$

where prime means derivative with respect to argument; δx_o is the unperturbed interparticle distance; and $f_o = f(\delta x_o)$. The displacement mentioned by Birkhoff and Lynch is (to lowest order, consistent with our expansions) accomplished by taking $\vec{\epsilon}_j = \vec{\epsilon}_1 = \vec{\epsilon}_3 = 0$ and $\vec{\epsilon}_2 = -\vec{\epsilon}_4$ parallel to a line from #1 to #3. The result leaves $\vec{F}_j = 0$. Various other displacements are likewise possible with $\vec{F}_j = 0$.

From another point of view, we may examine the question of configurational instability as follows. As a result of the displacements, if the forces on all the particles are directed towards returning them to their initial positions, then the system can be considered stable. We have already seen that such a tendency to return cannot in general result from arbitrary displacement. There is one special case of interest, however, that is easily analyzed. If the only non-vanishing displacement is that of particle #j, then the resulting force on #j is

$$\vec{F}_j = 2\vec{\epsilon}_j\left(f_o' + \frac{f_o}{\delta x_o}\right)$$

and the condition of stability is thus

$$f_o' + \frac{f_o}{\delta x_o} < 0$$

This, then, is a necessary (but not sufficient) condition upon the force function for configurational stability. If, for example, f(r) is proportional to $r^{-\zeta}$ then the stability condition is $\zeta > 1$. For a polytropic

gas in adiabatic motion, this will be satisfied, while in isothermal motion the satisfaction is borderline.

APPENDIX II. ANGULAR MOMENTUM

After the main body of this report was written, it was discovered that the form of the $\vec{g}_{ij}$ force would not allow angular momentum conservation, and a review of the situation both clarifies the angular momentum question and leads to an alternative expression for $\vec{g}_{ij}$. No qualitative changes would result in the discussions of this report from the use of the alternative form of $\vec{g}_{ij}$, since the two forms become the same in one dimension and differ only slightly in two.

The angular momentum of particle #j at the beginning of time cycle #n is

$$\vec{\Omega}_j^n \equiv \vec{r}_j^n \times m_j \vec{u}_j^n$$

so that

$$\vec{\Omega}_j^{n+1} - \vec{\Omega}_j^n \equiv \frac{1}{2}(\vec{r}_j^n + \vec{r}_j^{n+1}) \times m_j(\vec{u}_j^{n+1} - \vec{u}_j^n) + (\vec{r}_j^{n+1} - \vec{r}_j^n) \times \frac{1}{2} m_j(\vec{u}_j^n + \vec{u}_j^{n+1}) \qquad \text{(II-1)}$$

Now if, in Eq. (9) of the text, we had used the form

$$\frac{\vec{r}_j^{n+1} - \vec{r}_j^n}{\delta t} = \frac{1}{2}(\vec{u}_j^n + \vec{u}_j^{n+1}) \qquad \text{(II-2)}$$

for advancing the particle coordinates, then the second term on the right of (II-1) would vanish and angular momentum would change only as a result of the moment of forces. The form (II-2) is not allowed, however, because of its undesirable property of instability, which may be proved by analysis such as used in Part II-B. Thus there must be a discrepancy in angular-momentum conservation, with cumulative effect proportional to δt.

We may also examine the change of angular momentum of any subset of particles, and find for conservation (to lowest order in δt) that the interparticle forces must lie along the lines of centers. This leads to the alternative form for the dissipative force

$$\vec{g}_{ij} = m\omega \vec{s}_{ij} \left[\vec{s}_{ij} \cdot (\vec{u}_i - \vec{u}_j) \right]$$

REFERENCES

1. Harlow, F. H., "Stability of Difference Equations, — Selected Topics," Los Alamos Scientific Laboratory Report LAMS-2452 (September 1960).

2. Blair, A., et al., "A Study of a Numerical Solution to a Two-Dimensional Hydrodynamical Problem," Los Alamos Scientific Laboratory Report LA-2165 (October 1958).

3. Longley, H. J., "Methods of Differencing in Eulerian Hydrodynamics," Los Alamos Scientific Laboratory Report LAMS-2379 (April, 1960).

4. Kolsky, H. G., "A Method for the Numerical Solution of Transient Hydrodynamic Shock Problems in Two Space Dimensions," Los Alamos Scientific Laboratory Report LA-1867 (March, 1955).

5. Fromm, J. E., "Lagrangian Difference Approximations for Fluid Dynamics," Los Alamos Scientific Laboratory Report LA-2535 (June, 1961).

6. Goad, W. B., "Wat: A Numerical Method for Two-Dimensional Unsteady Fluid Flow," Los Alamos Scientific Laboratory Report LAMS-2365 (November, 1960).

7. Frank, R. M., and R. B. Lazarus, private communication.

8. Harlow, F. H., et al., "Two-Dimensional Hydrodynamic Calculations," Los Alamos Scientific Laboratory Report LA-2301 (September, 1959). This report contains a complete list of earlier published PIC-method work.

9. Thomas, L. H., private communication.

10. Pasta, J. R., and S. Ulam, "Heuristic Numerical Work in Some Problems of Hydrodynamics," Mathematical Tables and Other Aids to Computation," Vol. 13, pp. 1-12 (January, 1959).

11. Kolsky, H. G., "The Nearest Neighbor Hydrodynamics Calculation," Unpublished Memorandum, July, 1961, distributed by Group T-5, Los Alamos Scientific Laboratory.

12. Von Neumann, J., and R. D. Richtmyer, "A Method for the Numerical Calculation of Hydrodynamic Shocks," J. Appl. Phys., 21, 232 (March, 1950).

13. Peaslee, A. T., Personal communication based on experience by Peaslee with such a computing method.

14. Birkhoff, G., and R. E. Lynch, Los Alamos Scientific Laboratory Report (to be issued).

15. Beyer, W. A., Personal communication.

16. Harlow, F. H., "Dynamics of Compressible Fluids," Los Alamos Scientific Laboratory Report LA-2412 (November, 1960).