

**PROPOSAL AND ANALYSIS OF A NEW
NUMERICAL METHOD FOR THE TREATMENT OF
HYDRODYNAMICAL SHOCK PROBLEMS**

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Summary

A. The differential equations of (compressible, non-viscous, nonconductive) hydrodynamics are of a not too complicated type as long as the motion is continuous and isentropic. It is known, however, that almost all hydrodynamical setups cause a development of discontinuities, so-called **shocks**, sooner or later. These shocks almost never remain "straight", and as soon as they are "curved" or intersect each other, isentropy ceases. The mathematical problem then becomes one of a most unusual and altogether intractable type: A differential equation in a domain with an unknown, "free", boundary along which "supernumerary" boundary conditions hold, and in many cases the coefficients of the differential equation will themselves depend on the (unknown) boundary.

A rigorous treatment of such a problem is only possible in a few exceptional cases. The direct computational procedures for its treatment are very complicated and lengthy.

B This report suggests a computational treatment which corresponds to the original differential equations, completely ignoring the possibility of shocks. Arguments are brought forth to support the view that this computational treatment will always produce (arbitrarily) good approximations of the rigorous theory which allows for shocks. That is, even when shocks are formed, and the motion ceases to be isentropic.

It is shown that the suggested treatment corresponds to a return from the continuum (hydrodynamical) theory to a kinetic (molecular) theory, using, however, a very simplified quasi-molecular model. The essential simplifications are these:

- a)** The number of molecules N ("Loschmidt's number" for a mol of substance) is "scaled down" from its actual value $\sim 10^{24}$ to sizes of 10 to 100.
- b)** The intramolecular forces are correspondingly "scaled up" so as to approximate the correct hydrodynamical situation.
- c)** The intramolecular forces are essentially simplified in various other respects.

C. The envisaged computations appear to be well suited to be efficiently carried out on punch-card equipment. The use of such equipment was made available for the exploration of certain problems of this type by the Ballistic Research Laboratory of the Ordnance Research Center, Aberdeen, Maryland. A number of these problems have already been solved, under the direction of

Mr. L. E. Cunningham of that laboratory. Among these three "experimental" problems are discussed in this report. They lead to very encouraging results.

Specifically: In one-dimensional shock problems values of $N \sim 14$ or 29 (that is, 14 to 29 "molecules") and a Δt about one-half of its maximum allowable value (for details cf. section 18) produced results of highly satisfactory precision. The duration of the computations, including their setting up, was very reasonable.

D. The report contains an analysis of these computations, and of the main viewpoints in connection with further computations of this type. Physical aspects of the problems, like the hydrodynamical theory of the propagation of disturbances (sound) and the conservation of the total energy as well as its partial "degradation" by shocks, play an important role in discovering errors and keeping the equipment under control.

The possibilities of extending this method to spherically symmetric problems, and to "truly" many-dimensional problems, are discussed.

It is proposed to treat in the future various problems concerning the development, interaction, reflection, refraction and decay of shocks by this method and its extensions.

§1. The considerations which follow apply to any gas or liquid in which compressibility is taken into account, but viscosity and heat conduction are neglected.

From the point of view of gas dynamics such a substance is conveniently characterized by its **caloric equation of state**, which specifies the **internal energy** U as a function of two characteristic parameters, preferably of the **specific volume** v and the **specific entropy** S :

$$(1) \quad U = U(v, S)$$

Then the density ρ is

$$(2) \quad \rho = \frac{1}{v},$$

and the **pressure** p and **temperature** T are given by the equations

$$(3) \quad p = -\frac{\partial U}{\partial v}, \quad T = \frac{\partial U}{\partial S}.$$

The **equations of motion** will be stated in the **Lagrange-ian form**, for the main part of this discussion one-dimensionally. Then each **elementary volume** of the substance is characterized by a **label** a , its **position** being x at the **time** t . The purpose of the equations of motion, is to determine x as a function of a, t .

$$(4) \quad x = x(a, t).$$

It is convenient to choose the label a . in such a manner that the substance contained in the interval $a, a + da$ has the mass da , i.e., that the "density in the label space" is identically 1. This being understood, it is immaterial whether the label a is also the position x at some "initial instant" t_0 (which is frequently the case) or not.

With the above convention concerning the label, the specific volume v is simply given by

$$(5) \quad v = \frac{\partial x}{\partial a}.$$

The **conservation of momentum** states that

$$(6) \quad \frac{\partial^2 x}{\partial t^2} = -v \left(\frac{\partial p}{\partial x} \right)_{t=const}$$

i.e., by (3) and (5)

$$(7) \quad \frac{\partial^2 x}{\partial t^2} = -\frac{\partial}{\partial a} p \left(\frac{\partial x}{\partial a}, S \right).$$

The **conservation of energy**, on the other hand, gives a relation which is easily transformed with the help of (3) and (7) into

$$(8) \quad \frac{\partial S}{\partial t} = 0.$$

In all these equations a, t are **independent variables**.

§2. The conservation of energy and the principle of isentropy

Equation (8) implies that if S is constant at some initial instant $t = t_0$, then it stays constant at all times, and so (8) can be replaced by

$$(9) \quad S = S_0 = \text{constant}.$$

This **principle of isentropy** then makes (7) the sole equation governing the motions, and renders the problem amenable to analytical or numerical treatment.

It is essential to realize that the decisive equation (8) expresses the conservation of energy, and nothing else. Thus, although it involves the specific entropy alone, it expresses nevertheless the first, and **not the second law of thermodynamics**. Furthermore, since (8) secures the constancy of specific entropy along the world line of each elementary volume, the second law, which requires that specific entropy should never decrease along that line, does not now impose any additional restriction.

§3. The formation of shocks

It is well known that a motion satisfying (7), (8), develops sooner or later a discontinuity of the first derivatives $\frac{\partial x}{\partial a}$, $\frac{\partial x}{\partial t}$. More precisely: apart from exceptional and degenerate cases, no solution can be continued beyond some finite $t = t_s$, and the singularity at this t_s sets in by $\frac{\partial^2 x}{\partial a^2}$, $\frac{\partial^2 x}{\partial a \partial t}$ becoming infinite. At the next instant x can only be kept one-valued by permitting first-order discontinuities in $\frac{\partial x}{\partial a}$, $\frac{\partial x}{\partial t}$.

It has been established experimentally that this strange behavior of the solutions corresponds to a certain extent to the facts: In typical situations like those referred to above, real substances do indeed develop "discontinuities", -

i.e., rapid changes of the specific volume $v = \frac{\partial x}{\partial a}$ and of the velocity

$V = \frac{\partial x}{\partial t}$, which are discontinuities in the same approximation in which

viscosity and heat conduction can be neglected, and are called **shocks**. These shocks appear even if the state of the substance at the initial instant $t = t_0$ was perfectly continuous, they develop as far as can be observed at the times $t = t_s$ at which the solution of (7), (8) becomes discontinuous, and as far as the motion stays continuous (7), (8) seem to be satisfied.

§4. The shock equations of Rankine and Hugoniot. Shocks and entropy

After shocks have formed, the motion is still governed by the same conservation principles (of momentum and energy) on which (7), (8) are based. Hence (7), (8) still hold in the regions of space which contain no shocks, but beyond this it is necessary to apply those same conservation principles to the shocks themselves.

Let a shock at $a = \bar{a}(t)$ be formed by the states

$$\frac{\partial x}{\partial a} = v = v_1, \quad \frac{\partial x}{\partial t} = V = V_1, \quad p_1, \quad S_1, \quad U_1 \quad \text{at} \quad a = \bar{a} - 0,$$

and

$$\frac{\partial x}{\partial a} = v = v_2, \quad \frac{\partial x}{\partial t} = V = V_2, \quad p_2, \quad S_2, \quad U_2 \quad \text{at} \quad a = \bar{a} + 0.$$

The position of the shock is $\bar{x} = x(\bar{a}(t), t)$, its velocity $D = \frac{d\bar{x}}{dt}$; $\frac{d\bar{a}}{dt} = M$

is the **flow mass across the shock**. Then the conservation theorem of mass (which is an identity in the Lagrange-ian form, and was therefore not referred

to explicitly in §1, but which is better made use of now), momentum and energy give successively

$$(10) \quad \frac{D-V_1}{v_1} = \frac{D-V_2}{v_2} = M = \pm \sqrt{\frac{p_2 - p_1}{v_1 - v_2}},$$

$$(11) \quad \frac{p_1 + p_2}{2} = \frac{U_2 - U_1}{v_1 - v_2}.$$

Equations (10) are based on the conservation of mass and of momentum alone, (11) expresses (with the help of (10)) the conservation of energy. These are familiar **equations of Rankine and Hugoniot**.

It is well known that (11) (together with (1), (3) for p_1, v_1, S_1, U_1 and p_2, v_2, S_2, U_2) necessitates in general that $S_1 \neq S_2$. As was shown by C. Duhem, H. Bethe, and H. Wyle, for the most important equations of state (1),

$$(12) \quad \text{sign}(S_2 - S_1) = \text{sign}(p_2 - p_1) \cdot \text{sign}(\pm in(10)).$$

Now the second law of thermodynamics forbids a decrease of the specific entropy S along the world line of each elementary volume; i.e., it requires

$$(13) \quad \text{sign}(S_2 - S_1) = \text{sign} M, \text{ (for } S_1 \neq S_2, M \neq 0 \text{)}$$

hence by (13)

$$(14) \quad \text{sign}(\pm in(10)) = \text{sign}(p_2 - p_1).$$

Summing up: When a world line crosses a shock, the specific entropy S changes, and the second law imposes the additional restrictions (24).

§5. Mathematical complications caused by the presence of shocks

The general motion is thus described by (7), (8) in the regions where derivatives are continuous, and by (10), (11) with (14) on the discontinuity surfaces. Accordingly the specific entropy S is constant along each world line while it moves in the regions of continuity, but it undergoes a discontinuous increase each time a surface of discontinuity is crossed. The second law of thermodynamics is automatically fulfilled in the former regions, but it excludes 50 per cent of the solutions at the latter surfaces.

This is a most remarkable, and at first sight rather paradoxical violation of Hanckel's principle of the "conservation of formal laws", but the investigations of W. Rayleigh, G. I. Taylor, and R. Becker on one hand, and extensive experimental material on the other, make it impossible to question these conclusions.

From a mathematical point of view the emergency of shocks, and the addition of (10), (11), (14) to (7), (8) represent an extreme complication. Without shocks there is usually isentropy, i.e., (8) implies (9), and (7) can be

written as

$$(15) \quad \frac{\partial^2 x}{\partial t^2} = -\frac{\partial}{\partial a} p_0 \left(\frac{\partial x}{\partial a} \right),$$

where

$$(16) \quad p_0(v) \equiv p(v, S_0)$$

may be considered a known function. Then (15) is a hyperbolic differential equation of a familiar type, and can be treated adequately by Riemann's classical method of integration. If shocks are present, however, the situation changes radically. They act as unknown boundaries for the regions in which (7), (8) hold, and along these boundaries (10), (11), (14) must be fulfilled. The latter are easily seen to contain twice as many equations as a natural boundary condition (on a known boundary) for such a differential equation should, and this overdetermination along the unknown boundary should lead to its determination. Such problems with a "free boundary" are difficult at best, but in the present case an additional difficulty intervenes. The change of specific entropy S at the shock $a = \bar{a}(t)$ depends by (11) on the trajectory of the shock, i.e., on the unknown boundary $a = \bar{a}(t)$.

Now S enters explicitly into the differential equation (7). Hence we are dealing here with a "free boundary" problem where the coefficients of the differential equation themselves depend explicitly on the unknown, "free", boundary.

Problems of this type have never been treated in any generality, and appropriate analytical methods to deal with them are entirely unknown. Rigorous solutions have only been determined in very special cases, where the trajectories of the shocks could be guessed by other means, up to a few numerical parameters. Analytical approximative methods (e.g., expansions) or numerical ones are also very difficult and restricted to very few special cases. Furthermore the approximative numerical procedures do not seem to lend themselves for problems of this type to efficient mechanization.

§6. The idea of a simplified numerical approximative procedure

The idea which will be discussed here is to treat the continuous case (7), (8) with an approximative, numerical method, and to ignore the possibility of shocks, (10), (11), (14).

In order to diagnose the character and the implications of this idea, let us consider a special case of the equations of state (1), (3), which is itself of not inconsiderable practical importance.

Assume that there exists an absolute relation of the form

$$(17) \quad p = p_0(v),$$

where $p_0(v)$ is a known, fixed function. That is that the source of (17) is not (16) and (9) — that the differential equation (7) assumes the form (15) without (9), i.e., without isentropy. Owing to (3), (17) can hold only if the caloric equation of state has the form

$$(18) \quad U = U(v, S) \equiv U_*(v) + U_{**}(S),$$

in which case (3) gives

$$(19) \quad \begin{cases} p = -\frac{\partial U}{\partial v} \equiv -\frac{dU_*(v)}{dv} \equiv p_0(v) \\ T = \frac{\partial U}{\partial S} \equiv \frac{dU_{**}(S)}{dS} \equiv T_0(S) \end{cases}.$$

I.e.: In order that the pressure p be determined by the specific volume v alone, the same need not be true for the internal energy U , but U must be the sum of two terms U_* , U_{**} , of which U_* depends on the specific volume v alone and U_{**} on the specific entropy S alone — and there can be no "interaction energy" involving v, S together.

In many compression and shock problems involving solids and liquids those can be treated as such "interactionless" substances.

In this case the specific entropy S disappears from the differential equation of the continuous case, which assumes the form (15), and also from the shock conditions (10), (14). These equations are sufficient to determine the variation of x, v, p, V , i.e., the visible motion of matter and the mechanical forces acting upon it. They depend only on the U_* term of the inner energy U (cf. (18)). U_{**} and S, T come in only in (11), which becomes

$$(20) \quad \begin{aligned} U_{**2} - U_{**1} &= \frac{(p_1 + p_2)(v_1 - v_2)}{2} - (U_{*2} - U_{*1}) \\ &= \frac{(p_1 + p_2)(v_1 - v_2)}{2} - \int_{v_2}^{v_1} p dv \end{aligned}.$$

Thus (8) is not needed in the case of continuous motion, and (11) is not needed in the case of shocks. However (8) and (11) express the conservation of energy, so we see: For an "interactionless" inner energy (18) the visible motion and the mechanical forces can be determined by themselves, without using the conservation of energy.

The latter then determines S, T by (8) and by (11), i.e., (20), respectively.

§7. Expressions for the degradation of energy

$U_n = U_n(v)$ is the **potential energy**, $U_{**} = U_{**}(S)$ is the **thermic energy**. The total energy is made up of the **kinetic**, the **potential**, and the

thermic energies. Since the total energy of the entire substance is conserved, and since in the case of continuous motion the thermic energy is conserved in each element by (8), so in this case the kinetic plus potential energy of the entire substance is conserved too. In the case of shocks proceed like this: Let the shock be oriented in the direction of the flow of substance, i.e., $M > 0$. Then $S_1 < S_2$ by (13); hence $U_{**1} < U_{**2}$. All sides of (20) are hence positive, and so the last expression in (20) necessitates $v_1 > v_2$ ($p = p_0(v)$ is usually convex from below as a function of v). (10) now necessitates $p_1 < p_2$. Since the thermic energy increases in each element by the above, the kinetic plus potential energy for the entire substance decreases.

So we see: If the thermic energy is left out of account, then the **conservation of energy** is still valid for the continuous motion, but it is replaced by a **loss of energy** for shocks.

This explains the apparent conflict between the mechanical conservation of energy and the principles of thermodynamics in the earlier forms of the theory of shocks.

According to the above, this loss of energy is better described as a **degradation of energy**. The **specific degradation** of energy (i.e., per unit mass) is

$$(21) \quad \Delta_s = U_{**2} - U_{**1},$$

the **rate of degradation** of energy (i.e., per unit time) is

$$(22) \quad \Delta_r = M \Delta_s.$$

(21), (22) must be evaluated with the help of (10), (20).

§8. Physical interpretation of the proposed numerical approximative procedure

In carrying out numerical approximations of the hyperbolic differential equation (15), the continuous independent variables a, t must be replaced by discrete ones. For various reasons it is advantageous to carry this out in **two successive steps**, and to begin by making a alone discrete. One of these reasons is that a is really a discrete quantity, which was made artificially continuous by the classical transition from the kinetic theory to the continuous, hydrodynamical one: the elementary volumes of the substance, for which a is a label, should be naturally discrete entities. Thus the label a is "naturally" discrete, while the coordinates x, t are "naturally" continuous. (Note that in this setup the Lagrange-ian form is preferable to the Euler-ian, since the latter deals with x, t only, without a .) Making a discrete, and leaving x, t continuous, has therefore a certain physical meaning, and this will turn

out to be very helpful presently.

Accordingly, let a . run over a sequence of equidistant values, which may as well be normalized so as to be the integers:

$$(25) \quad a = \dots, -2, -1, 0, 1, 2, \dots$$

It is also advantageous to write for x

$$(24) \quad x = x(a, t) \equiv x_a(t).$$

The hyperbolic (partial) differential equation (15) can now be replaced by the approximative system of (total) differential equations

$$(25) \quad \frac{d^2 x_a}{dt^2} = p_0(x_a - x_{a-1}) - p_0(x_{a+1} - x_a).$$

§9. (Continuation)

It is an essential circumstance concerning the equations (25) that they are not only mathematical approximations of the rigorous equation (15), but also the rigorous equations of another physical system, which is a physical approximation of that one underlying (15). Indeed, the system (25) is that one of the equations of motion of an ordinary (point) mechanical system with the coordinates $\dots, x_{-2}, x_{-1}, x_0, x_1, x_2, \dots$ and with the total energy

$$(26) \quad \frac{1}{2} \sum_a \left(\frac{dx_a}{dt} \right)^2 + \sum_a U_*(x_a - x_{a-1}).$$

This is a system of mass points Nos. $\dots, -2, -1, 0, 1, 2, \dots$, the point No. a having the coordinate x_a , the mass 1, and any two neighbors x_{a-1} and x_a being connected by a "**spring**" which has the potential energy $U_* = U_*(v)$ when its length is $v = v_a = x_a - x_{a-1}$.

Now this system of "**beads on a line, connected by springs**" is clearly a reasonable physical approximation of the substance which the hydrodynamical equation (15) describes. It corresponds to a quasi-molecular description of this substance, where the mass ascribed to one "**bead**" (i.e., the one elementary volume) is the mass of a "molecule". We chose to treat this as the unit mass, but it may nevertheless correspond to any desired real mass. Clearly this is not the "true" molecular description of the substance: For any workable computing scheme the number of these "molecules", i.e., of elementary volumes, will be much smaller than the actual number of molecules. Thus if a gram-mol of a real substance is considered, the true number of molecules in it is **Loschmidt's number** $N \sim 6 \times 10^{23}$, while for a practical computing scheme some number of "molecules" N between 10 and 100 will be appropriate. However, the actual value of Loschmidt's number N never figures in hydrodynamics; all that is required for the validity of (15) is

Avogadro Number

that N should be a great number. The actual $N \sim 6 \times 10^{23}$ is certainly great, but much smaller numbers N may already be sufficiently great. Thus there is a chance that $N \sim 10^2$ will suffice.

So the replacement of (15) by (25) amounts to the introduction of a quasi-molecular description with a Loschmidt number N chosen for computing purposes, and therefore much too low. Reality is not (15) either; it is molecular with the correct $N \sim 6 \times 10^{23}$. Hence (25) is an acceptable approximation if this "scaling down" of N from 6×10^{23} to the value used, say 10^2 , is acceptable. At this point two more remarks are in order:

First: This "scaling down" of N requires a corresponding "scaling up" of the "intramolecular forces", to produce the correct hydrodynamical forces. This has indeed been done: The potentials in (26), i.e., the forces in (25), were chosen so as to approximate just the correct forces in (15).

Second: The actual intramolecular forces are of course much more complicated than those of the simple "beads and springs" model used in (25), (26). However, the classical derivations of hydrodynamics from molecular kinetic models have established that these more subtle details of the intramolecular forces are immaterial for this part of hydrodynamics: It can be derived from the "beads and springs" model just as well as from one where those details are taken into consideration.

§10. The behavior of energy

The above considerations make it plausible that the system (25) is a good approximation of the hydrodynamical equation (15), even for moderate values of the number of elementary volumes N . The minimum size of N which will give acceptable approximations must, of course, be determined by effective computation, and it may vary from problem to problem. We expressed above the surmise that values between 10 and 100 will usually suffice.

All these considerations are, however, only plausible as long as (15) describes reality without any further complications, i.e., in a continuous motion. When shocks appear, the situation seems considerably less favorable. These two remarks suggest themselves immediately:

First: In the presence of shocks the real motion is not described by (15) alone, but by (15) together with (10), (14). Now while (25) is clearly an approximation of (15), it is not at all clear whether it is also one of (10), (14).

Second: Actually there are reasons to expect that something must go wrong with this latter approximation. Indeed, we saw in §7 that the total

kinetic plus potential energy is not conserved in hydrodynamics when shocks are present, but that it is continuously degraded (i.e., decreasing) according to (22). On the other hand the expression (26) represents precisely the total kinetic plus potential energy — no thermic energy makes its appearance in this expression, and there is indeed no room for a separate thermic energy in such a quasi-molecular model. And since (25) is the system of the ordinary (point) mechanical equations of motion belonging to the total energy (26), therefore (25) must conserve this energy.

Thus (25) must conserve (26), while (15) with (10), (14) does not conserve the analogue of (26). How then can (25) be an approximation of (15) with (10), (14)?

§11. Discussion of an example

Nevertheless it is hard to see how (25) can fail to describe the equivalents of shocks in certain situations. E.g., let the "**beads and springs**" model of §9 collide with a rigid wall; in this situation the wall would send a shock into a compressible substance (in hydrodynamical theory), and something similar must happen to the "beads and springs" model. The boundary conditions which describe this are easy to specify: For $t = 0$ the substance is in its normal state (i.e., each $v_a = x_a - x_{a-1} = 1$, hence $x_a = a + \text{const}$, e.g., $x_a = a$) and is moving uniformly to the left:

$$(27) \quad \text{For } t = 0 \text{ all } x_a = a, \quad \frac{dx_a}{dt} = -\alpha, \text{ with a given } \alpha > 0.$$

For $t > 0$ the wall stops the molecule $a = 0$ at $x = 0$:

$$(28) \quad \text{For all } t \geq 0 \quad x_0 = 0.$$

Clearly (27) should only apply to the right half, i.e., to $a = 1, 2, \dots$

Now (25) conserves the energy (26), i.e., the total kinetic plus potential energy, while (11) i.e., (20), excludes such a conservation. And the laws of Rankine and Hugoniot, on which (11) is based, are merely applications of the basic conservation principles, which hold for (25) too. How then can (25) still conserve the energy (26)?

The plausible answer is that (25) will produce something like a shock under the conditions specified, but that the motion of the x_a beyond the shock will not be the smooth hydrodynamical one, but rather one with a superposed oscillation. This oscillation should contain, as a kinetic energy, that degraded energy which can only be accounted for in the hydrodynamical case ((15) with (10), (14)) by introducing a separate thermic energy U_{**} . Indeed, (25) describes a quasi-molecular model, and in such a model the

thermic energy appears necessarily as a part of the kinetic energy.

§12. The oscillations caused by shocks

These considerations suggest the surmise that (25) is always a valid approximation of the hydrodynamical motion, i.e., of (15) with (10), (14), but with this qualification: It is not the $x_a = x_a(t)$ of (25) which approximates the $x = x(a, t)$ of (15), but the average of the x'_a over an interval (of sufficient length) of continuous a 's. The x_a themselves perform oscillations around these averages, and these oscillations do not tend to zero, but they make finite contributions to the total energy (26). Indeed, these contributions are continuously increasing when shocks are present, and they account for the degradation of energy according to (21), (22).

The velocities produced by these oscillations are easy to estimate. Denoting such a velocity by V_{osc} , amplitudes (maxima) by V^{am} and averages by \bar{V} , clearly

$$\frac{1}{2} \overline{(V_{osc})^2} = \Delta_s = \frac{(p_1 + p_2)(v_1 - v_2)}{2} - \int_{v_2}^{v_1} p dv,$$

(use (21), (20)), and assuming that the oscillations are essentially harmonic;

$$\frac{1}{2} \overline{(V_{osc})^2} = \Delta_s = \frac{1}{2} \overline{(V_{osc}^{am})^2}.$$

From these

$$(29) \quad \overline{(V_{osc}^{am})^2} = 4 \left\{ \frac{(p_1 + p_2)(v_1 - v_2)}{2} - \int_{v_2}^{v_1} p dv \right\}.$$

Actually (29) should be corrected inasmuch as Δ_s may not be entirely kinetic energy: If the oscillations are of finite size, the nonlinearity of the potential energy $U_* = U_*(v)$ will cause $U_*(\overline{x_a - x_{a-1}})$ to be different from $\overline{U_*(x_a - x_{a-1})}$, and while the hydrodynamical energy contains the first expression, (26) contains the second one. Thus $\overline{U_*(x_a - x_{a-1})} - U_*(\overline{x_a - x_{a-1}})$ too contributes to the specific dissipation Δ_s . If the oscillation of $v_a = x_a - x_{a-1}$ is v_{osc} , then this term is approximately

$$\frac{1}{2} \frac{d^2 U_*}{dv^2} (v_{osc})^2 = -\frac{1}{2} \frac{dp}{dv} (v_{osc})^2 = \frac{1}{2} \frac{c^2 (v_{osc})^2}{v^2},$$

where

$$(30) \quad c = \sqrt{\frac{dp}{d(1/v)}} = v \sqrt{-\frac{dp}{dv}}$$

is the **local sound velocity**. The average is

$$\frac{1}{2} \frac{c^2 \overline{(v_{osc})^2}}{v^2}.$$

Assuming harmonicity

$$\overline{(v_{osc})^2} = \frac{1}{2}(v_{osc}^{am})^2.$$

so the left-hand side (29) should be replaced by

$$(31) \quad (V_{osc}^{am})^2 + \frac{c^2 (v_{osc}^{am})^2}{v^2}.$$

§13. Mathematical interpretation. Weak convergence

In the mathematical terminology the surmise of §12 means that the quasi-molecular kinetic solution ((25)) converges to the hydrodynamical one ((15) with (10), (14)), but in the **weak** sense. I.e., that only the averages converge numerically. (Even this requires a slight qualification due to what was observed above concerning the U_* -averages, but there is no need to consider such details already here.)

A mathematical proof of this surmise would be most important, but it seems to be very difficult, even in the simplest special cases. The procedure to be followed here will therefore be a different one: We shall test the surmise experimentally by carrying out the necessary computations for certain moderate values of N (cf. §§9, 10), on problems where the rigorous hydrodynamical solution ((15) with (10), (14)) is known, and produces shocks. The comparison of the computed, approximate motion with the rigorous, hydrodynamical one will then be the test.

§14. Statement of the program. Choice of Δa and Δt

It is worth while to state once more what we propose to do: The system (25) is a computational approximation of (15). (15) describes continuous hydrodynamical motions, but not shocks. It is nevertheless expected that the approximation (25) will prove itself better than its original (15), and give adequate approximate descriptions of shocks.

In order to evaluate the system (25) by effective computation it is now necessary to carry out the second step mentioned at the beginning of §8, i.e., to make the remaining independent variable t discrete too. Choosing for t a sequence of equidistant values

$$(32) \quad t = s \cdot \tau, \quad \tau \text{ fixed and } > 0, s = \dots, -2, -1, 0, 1, 2, \dots$$

a certain care in choosing τ is necessary.

First, we amplify (24) by writing

$$(33) \quad x = x(a, t) \equiv x_a(t) \equiv x_a^s.$$

Second, the system of total differential equations (25) must now be replaced

by the system of difference equations

$$(34) \quad \frac{x_a^{s+1} - 2x_a^s + x_a^{s-1}}{\tau^2} = p_0(x_a^s - x_{a-1}^s) - p_0(x_{a+1}^s - x_a^s).$$

Third, it is clear that in the recursion of (34) x_a^{s+1} is determined by

$$x_{a-1}^s, x_a^s, x_{a+1}^s, x_a^{s-1},$$

i.e., x_a^s by

$$x_{a-1}^{s-1}, x_a^{s-1}, x_{a+1}^{s-1}, x_a^{s-2}.$$

So x_a^s is determined by a family of $x_a^{s'}$'s with

$$|a' - a| \leq |s' - s|.$$

I.e., $x(a, t)$ is determined by a family of $x(a', t')$'s with

$$(35) \quad |a' - a| \leq \frac{1}{\tau} |t' - t|.$$

On the other hand the underlying hyperbolic partial differential equation (15) has a definite way to propagate influences: along the **characteristic lines**.

The equation of those lines is

$$(da)^2 = -\left(\frac{dp}{dv}\right) \cdot (dt)^2,$$

i.e., the area in which a change made at a, t makes itself felt is given by

$$|da| \leq \sqrt{-\frac{dp}{dv}} \cdot |dt|,$$

or, using (50), by

$$(36) \quad |c'a| \leq \frac{c}{v} |dt|.$$

Note that c was the **velocity of sound** in the **physical space** x, t , while c/v is the velocity of sound in the **label space** a, t . Equivalently, c/v is the **flow of mass across the sound wave**.

Now as R. Courant pointed out first for a more general class of problems, the computation cannot give significant results unless the dependences (35) which it permits contain the dependences (36) which the underlying problem demands. Consequently it is necessary that

$$\frac{1}{\tau} \geq \frac{c}{v},$$

i.e., that

$$(37) \quad \tau \leq \frac{v}{c}.$$

Practically even a certain "factor of safety" in (37) will be advisable.

§15. Procedure

The system of difference equations (34) is well suited to mechanization. Specifically, it can be solved with **punch-card equipment**, with s being the number of each one of the successive stacks of cards produced, and a the current number of each card within its stack. However, the following points must be emphasized:

First: We expect that after crossing the equivalent of a shock, a "molecule" a will develop an oscillation of x_a^s , which represents thermic agitation. The period of this oscillation will be of the order 1 in a , i.e., of the "grain size" introduced by the numerical approximation, by the operation of making the continuous a discrete.

Now by the usual standards of numerical computing, the appearance of such oscillations (of a period which is imposed by the "grain size" of the approximation, and not by some quantity derived from the underlying differential equation (15)) is a symptom of some inadequacy of the computing setup. It is therefore important to visualize that in the proposed setup this criterion must be abandoned: As soon as a shock has been crossed such oscillations must develop, and they have a perfectly good physical significance. They represent the thermic agitation caused by the degradation of energy through the shock.

Second: Since this important criterion for spotting errors or inadequacy of the computing setup is lost, we must see what other criteria remain. For errors there is always effective numerical checking, but it is practically difficult to get along without additional criteria of a more intrinsic significance, and they are also necessary in order to judge the adequacy of the entire setup.

The following criteria suggest themselves:

(A) Any conspicuous feature which appears in the initial conditions or anywhere later in the solution, will be propagated by the computation according to (35), while hydrodynamics cause propagation according to (36). The signal of (35) is the **numerical** or **false signal**, while the signal of (36) is the **hydrodynamical** or **true signal**. According to (37) the false signal must always be ahead of the true signal. Hence an actual computation can only be significant if the false signal is very weak (it should become weaker than any specified amount for a sufficiently small "grain size"), and if the essential changes arrive with the true signal.

(B) Since (25) conserves the total energy (26), therefore (34) should approximately conserve the equivalent of (26), i.e.,

$$(38) \quad \frac{1}{8\tau^2} \sum_a (x_a^{s+1} - x_a^{s-1})^2 + \sum_a U_*(x_a^s - x_{a-1}^s).$$

Of course (38) will oscillate, since this conservation is only an approximate one. But after its average statistical behavior has been determined, any excessive deviation is an indication of some error of computation. Any clear trend of (38) with s is an indication of an inadequacy of the computing setup, particularly if it is in the direction (decrease) and of the order of magnitude of the shock degradation of energy according to (21), (22). Here the **numerical rate of degradation** is the significant quantity, i.e., the degradation of energy while s increases by 1, i.e., during τ units of time. By (21), (22) this is

$$(39) \quad \Delta_{nr} = \tau \Delta_r = \tau M \Delta_s.$$

Hence oscillations and trends of (38) must be judged by comparing them in size with this Δ_{nr} .

(C) It is advisable to acquire some general routine regarding the adequacy of computing setups, by dealing first with some selected experimental problems, i.e., simple problems in which the hydrodynamical solution is known. The comparison of the approximate, numerical solution with the (known) rigorous, hydrodynamical one will clearly be of considerable orienting value. The problems should be chosen in such a manner as to make it sure that shocks will develop, and preferably also other characteristic features of continuum hydrodynamics, such as Riemann rarefaction waves, wave reflections and intersections, etc.

§16. The three problems

The Ballistic Research Laboratory of the Ordnance Research Center, Aberdeen, Maryland, is carrying out explorations of the suitability of its punch-card equipment for certain computations of the type described. This work began in early March 1944 and is continuing at the present time, under the direction and following the setups of Mr. L. E. Cunningham of the laboratory. The author wishes to take this opportunity to express his thanks to the laboratory and to Mr. Cunningham, whose active interest made the decisive tests possible.

Three experimental tests of the kind described above, which were made at Aberdeen, will be discussed in §§16-20 which follow.

The precise formulation of these problems is this:

The equations of state which correspond to (19) are assumed to be as simple as possible without impairing the significance of the results, in order to facilitate the computations. Specifically

$$(40) \quad p = p_0(v)$$

is assumed to be a polynomial. It is well known from hydrodynamics that in order to be realistic, the curve (40) must be convex from below. Accordingly

$$(41) \quad p = p_0(v) \equiv 1 - v + \frac{1}{4}v^2$$

was chosen. This "substance" "collapses" (i.e., $v = 0$) for $p = 1$, and it "cavitates" (i.e., $p = 0$) for $v = 2$; however it behaves reasonably in the intervals

$$(42) \quad 0 < v < 2, \quad 1 > p > 0,$$

and

$$(43) \quad v = v_1 = 1; \quad p = p_1 = 0.25$$

was used as the "normal", initial state of the substance. By (30) the sound velocity is

$$(44) \quad c = v \sqrt{1 - \frac{1}{2}v},$$

hence the "normal", initial value is

$$(45) \quad c_1 = \sqrt{\frac{1}{2}} = 0.707.$$

The boundary conditions correspond to the collision of this substance with a wall, as described at the beginning of §11. It is preferable, however, to have a definite finite number of particles, i.e., of values of a ,

$$(46) \quad a = 0, 1, 2, \dots, a_0 - 2, a_0 - 1, a_0,$$

and to place rigid wall at the two ends:

$$(47) \quad \text{For all } t \geq 0, \quad v_0 = 0, \quad v_{a_0} = a_0.$$

This corresponds to (28). The initial state of the substance is as in (27), i.e., "normal" specific volume $v = 1$ and uniform motion to the left:

$$(48) \quad \text{For } t = 0, \quad x_a = a, \quad \frac{dx_a}{dt} = -a, \quad \text{for all } a = 1, 2, \dots, a_0 - 2, a_0 - 1,$$

with a given $\alpha > 0$.

As the system of total differential equations (25) is replaced by the system of difference equations (34), the boundary conditions (47), (48) are to be replaced by

$$(49) \quad \text{For all } s = 0, 1, 2, \dots, \quad x_0^s = 0, \quad x_{a_0}^s = a_0.$$

$$(50) \quad \text{For all } a = 1, 2, \dots, a_0 - 2, a_0 - 1, \quad x_a^0 = a, \quad x_a^1 = a - \sigma\tau.$$

The following remarks are now in order:

First: Of the $a_0 + 1$ "molecules" $a = 0, 1, 2, \dots, a_0 - 2, a_0 - 1, a_0$ the first and the last, $a = 0, a_0$, represent the two walls. Hence the substance

proper consists of the $a_0 - 1$ molecules $a = 1, 2, \dots, a_0 - 2, a_0 - 1$.

Second: The initial velocity α points to the left (towards $a = 0$, away from $a = a_0$), hence there will be a compression wave originating at the wall $a = 0$, and an expansion wave at the wall $a = a_0$. I.e., the former will be a shock, and the latter a Riemann rarefaction wave.

Third: In order to have a way to estimate the significance of a given initial velocity α on an absolute scale, it is best to compare it with the "normal" sound velocity c_1 of (45). This gives as a measure

$$(51) \quad \mu = \frac{\alpha}{c_1} = \sqrt{2}\alpha = 1.414\alpha,$$

the **Mach number** of the initial motion.

§17. (Continuation)

The three problems which were solved

The problems considered correspond to the choices

$$(52) \quad \alpha = 0.2, 0.4 \text{ i.e., } \mu = 0.283, 0.566.$$

With these initial conditions (and the equation of state (41)) simple hydrodynamical considerations allow determination of the rigorous, hydrodynamical solutions. The results are these:

(A) At the wall $a = 0$ a shock originates. The velocity of this shock is $D = 0.555, 0.400$; the state behind it is given by $v = 0.735, 0.500$ and $p = 0.400, 0.625$ mass velocity 0.

(B) At the wall $a = a_0$ a Riemann rarefaction wave originates. The velocity of the front of this wave is $D' = 0.907, 1.107$; the velocity of its back is $D'' = 0.770, 0.646$; the state behind it is given by $v = 1.310, 1.718$ and $p = 0.119, 0.020$ and mass velocity 0.

(C) The waves of (A) and (B) meet at the time $t = \frac{a_0}{D' + D''}$. At this instant the rarefaction wave begins to undergo a refraction on the shock, and its front continues behind the shock with the velocity $D^* = 0.584, 0.433$.

(D) The shock of (A) has the specific dissipation of energy $\Delta_s = 0.00077, 0.00521$, and the rate of dissipation of energy $\Delta_r = 0.00058, 0.00417$.

§18. (Continuation)

The choice of τ in each problem is governed by (37). The upper limit of (37) is the smallest v/c which occurs in the problem, i.e., by (44) the smallest

$\frac{1}{\sqrt{1-v/2}}$. I.e., the $\frac{1}{\sqrt{1-v/2}}$ belonging to the smallest v . This is clearly

the v behind the shock, hence by (A) above $v = 0.735, 0.500$, and so

$$\frac{1}{\sqrt{1-v/2}} = 1.26, 1.15. \text{ Thus the requirement of (37) is } \tau \leq 1.26, 1.15 \text{ and}$$

therefore $\tau = 0.5$ would seem to be a safe value.

We can now state the three problems for which the solutions were computed:

Problem 1: $\alpha = 0.2$, i.e., the first choice of §17. $a_0 = 15$, i.e., $N = a_0 - 1 = 14$ "molecules". $\tau = 0.5$. Calculation carried until $s = 31$, i.e., $t = 15.5$.

Problem 2: Same as Problem 1, but $\tau = 0.25$ (as a check), calculation carried until $s = 51$, i.e., $\tau = 12.75$.

Problem 3: $\alpha = 0.4$, i.e., the second choice of §17. $a_0 = 30$, i.e., $N = a_0 - 1 = 29$ "molecules". $\tau = 0.5$, calculation carried until $s = 61$, i.e., $t = 30.5$.

As pointed out at the beginning of §§15 and 16, the computations were carried out on the punch-card equipment of the Ballistic Research Laboratory at Aberdeen, Maryland. They produced very encouraging results. Such difficulties as presented themselves were all overcome by the very complete and efficient punch-card equipment of the Ballistic Research Laboratory under the direction of Mr. Cunningham. The actual computations on each problem required 6-12 working hours net, and the entire program (setting up, etc.), insofar as these three problems were concerned, took less than ten days.

A detailed analysis of the numerical material obtained was undertaken, and it gave very valuable pointers for the further development of this method. It will not be attempted to give here a detailed account of this analysis. We shall, however, point out some of the main features, and attach some graphical representations.

§19. Analysis and interpretation of the results

First: The results obtained in Problems 1 and 3 are represented by Figures 1 and 2, respectively. The results in Problem 2 agree so well with those in Problem 1 that a graphical representation of the former would not have been distinguishable from one of the latter, i.e., from Figure 1 (except for the halving of τ , i.e., the doubling of s).

In each figure the abscissae are the a , and the ordinates are the s . The full lines, originating at $s = 0$ and $a = 1, 2, \dots, a_0 - 2, a_0 - 1$ are the **world lines** of the corresponding "molecules". The dash-dash lines represent the main hydrodynamical features, that is, the loci where the rigorous,

hydrodynamical solution places them according to (A)-(C) in §17: the line originating at the lower left corner is the **shock**, the two lines originating at the lower right corner are the **front** and the **back** of the **Riemann rarefaction wave**, and the **refracted front** of the rarefaction wave on the shock is also indicated.

Second: Both figures show that the initial motion, which is a family of parallel straight lines in the a, s -plane, is significantly modified only when the shock or the front of the rarefaction are reached. These are the true signals in the sense of (A) in §15; the false signals are at the lines $s = a$ or $s = a_0 - a'$, i.e., well ahead of the true ones, and at the false signals nothing visible happens. (The numerical material shows this in more precise quantitative detail.) Also, the change of direction at the shock is rather sudden, while that at the rarefaction is gradual and continuous. Summing up, the criterion of (A) in §15 is satisfied, and even the details of the compression and the expansion caused by the two walls are those which the rigorous, hydrodynamical solution leads one to expect.

Third: The numerical material shows that in all three problems the shocks are followed by oscillations of a more lasting nature than those which accompany the rarefaction. In Problems 1, 2 these are too small to show on Figure 1, but in Problem 3 they are considerably greater and Figure 2 shows them accordingly. That figure makes it quite clear that the shock, but not the rarefaction, is followed by strong "thermic agitation" due to the degradation of energy which is caused by the shock alone.

Fourth: The values of v obtained in (A), (B) in §17 for the regions behind the shock and the rarefaction can be compared with the compression and the expansion shown on Figures 1, 2. The quantitative agreement is excellent. The world lines of individual "molecules" are also in good agreement with those obtained from the rigorous, hydrodynamical solution, if allowance is made for the post-shock oscillations.

Fifth: The numerical rate of degradation of energy is, by (39) in (B) in §15 together with (D) in §17 and the τ -values of §18, found to be

$$(53) \quad \Delta_{nr} = \tau \Delta_r = 0.00029, 0.00015, 0.00208$$

for Problem 1, 2, 3, respectively.

As discussed in (B) in §15, this is the quantity which provides the significant standard of size for the oscillations and trends of the approximate energy (38).

Computations of (38) show that its total oscillations never exceed the quadruple of (53) in either problem, and that the overall trend of (38) is less

per unit of s than one-twentieth of (53). This makes the significance of our computing procedure very plausible, and permits an easy spotting of computing errors with the help of the oscillations of the approximate energy (38).

§20. Conclusions

A more detailed inspection of the numerical results in Problem 3 allows also locating the course of the shock across the rarefaction. This is shown by the dash-dot line on Figure 2. It should be noted that this represents already a result which cannot be obtained by classical methods in the rigorous, hydrodynamical theory: the "collision" of a shock and a rarefaction.

It is proposed to extend this method to more problems of this latter type, involving more complicated one-dimensional interactions of shocks and rarefactions. The experience with Problems 1, 2, 3 shows that a "substance" with 14 or 29 "molecules" is fully adequate to describe the finer nuances of hydrodynamic motion. We believe therefore that the possibilities which are opened up by this method are considerable.

The equation of state (41)

$$p = 1 - v + \frac{1}{4}v^2$$

must of course be replaced by more realistic ones. Actually non-polynomial equations, e.g., the "adiabatic"

$$(54) \quad p = v^{-\gamma}$$

can be handled by the punch-card equipment through appropriate arrangements quite simply and efficiently.

All these problems, as well as the extension from the special equation of state (18), (19) to the general one (1), (3), will be dealt with in subsequent reports.

§21. The spherically symmetric case

Among more-than-one-dimensional problems, those of spherical symmetry suggest themselves first. Here x and a may be viewed as the distances from the center of symmetry of the physical space or the label space. This replaces the hydrodynamical partial differential equation (15) by

$$(55) \quad \frac{\partial^2 x}{\partial t^2} = -\frac{x^2}{a^2} \frac{\partial}{\partial a} p_0 \left(\frac{x^2}{a^2} \frac{\partial x}{\partial a} \right),$$

which is of a very similar nature. Our approximative, numerical procedure applies to (55) in essentially the same way as to (15) in the one-dimensional

case.

Numerical investigations of (55) are very desirable, since such problems as the decay of a spherical shock belong in this class. This subject will also be considered in subsequent reports.

§22. Two- and three-dimensional problems

Truly two- or three-dimensional problems without the symmetries used in §21 are more difficult to handle. Our general approximative procedure still applies, but there seem to be reasons to fear that here the necessary number of "molecules" becomes inconveniently large. As pointed out in §20, 14 or slightly more "molecules" may suffice in one dimension, but this suggests that $10^2 \sim 200$ and $14^3 \sim 3000$ may be needed in truly two- or three-dimensional problems. These numbers seem too high for the existing machines, although 200 "molecules" are perhaps not altogether beyond capacity. The subject will be investigated further, particularly in view of the great importance of the hydrodynamical problems which a success in this direction would make accessible.

In the truly many-dimensional cases the possibility of using other types of machines will also have to be investigated. In this respect the relay-selector type machines seem very promising among the "digital" ones. The exploration of the "non-digital", "physical analogy" type machines is also being undertaken; some of these seem to be quite promising, although of lower precision than the "digital" machines.



