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LAGRANGIAN HYDRODYNAMIC COMPUTATIONS AND MOLECULAR MODELS OF MATTER

(1) Hydrodynamic Computations

(2) Molecular Models of Matter

(3) Models for flow problems

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LAGRANGIAN HYDRODYNAMIC COMPUTATIONS AND MOLECULAR MODELS OF MATTER

by

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ABSTRACT

An analysis is made of the analogy between schemes for integrating the equations of motion of a compressible fluid, in Lagrangian coordinates, and molecular models of matter. Computation schemes involving one and two independent variables are considered, for flows with and without shocks.

CONTENTS

I. FLOWS IN ONE SPACE DIMENSION

1. Introduction. In his pioneer paper [9] on the numerical solution of time-dependent compressible flow problems, von Neumann suggested using Lagrangian independent variables. That is, he suggested computing the vector position $\underline{x}$ of a moving fluid particle with material coordinate $\underline{a}$, as a function $\underline{x}(\underline{a},t)$ of time t. For homentropic flow in one space dimension (see § 2), this amounts to integrating the hyperbolic equation

$$(1) \qquad x_{tt} = - p_a = F'(\sigma)\, x_{aa}, \qquad \text{where } \sigma = x_a;$$

and

$$(2) \qquad p = p_o - F(\sigma)$$

is a homentropic equation of state. Here subscripts denote partial derivatives (thus $x_{tt} = \partial^2 x/\partial t^2$), $\sigma = \rho^{-1}$ is the specific volume, and $F'(\sigma) > 0$.

Von Neumann observed* that the natural spatial discretization of (1) yielded a system of ordinary differential equations of the form

$$(3) \qquad m\, d^2x_i/dt^2 = f(x_i - x_{i-1}) - f(x_{i+1} - x_i),$$

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*Though [9] is not easily available, it has been summarized in [6].

where we set $f(\delta) = -F(\delta/\Delta a)$. These are the equations of motion of a system of identical particles of mass $m = \Delta a$, joined by springs — i.e., of a mass-spring system.

Von Neumann also suggested that the trajectories $x_i(t)$ of these particles were analogous to those of gas molecules in the kinetic theory of gases. Essentially because of this analogy, he "expected that the approximation (3) would prove itself better than its original (1), and give adequate approximate descriptions of shocks".

Since 1944, von Neumann's computational ideas have been extensively explored. Von Neumann himself [11] decided to introduce "artificial viscosity" (dashpots) into the mass-spring system (3) to simulate shocks, as being more efficient computationally than statistical averaging of the type used in the kinetic of gases. But no systematic exploration has been made of the analogy which seemed so interesting to von Neumann.

The present paper* represents such an exploration; it analyzes the relation between Lagrangian hydrodynamical computation schemes and molecular models of matter.

First, it notes that the force-laws of the system (3) correspond to molecular models of crystals and liquids ("dense" gases) more closely than to the models of "rare" gases used in the kinetic theory of gases. It then shows how various physical concepts, familiar in theories of the

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*It was begun jointly with S. Ulam in 1953, in informal collaboration with von Neumann. The collaboration of Mr. Lynch started in 1958. The work has been done largely at the Los Alamos Scientific Laboratory, and under Contract AT(30-1)-1987.

liquid and solid state, are applicable to hydrodynamical computation schemes. It continues with applications of ideas from statistical mechanics to such computation schemes.

Finally, it explores the mechanical properties which are possessed by the synthetic materials defined by such computation schemes. Such materials* may well simulate the behavior of real solids under large deformations, and that of real solids and liquids under extremely high rates of strain, as well as or better than the classical models of continuum mechanics.** In addition, their properties can be effectively investigated on high-speed computing machines, and a number of specific investigations of this type are proposed.

2. Elastic fluids. The simplest model of continuum mechanics is defined by the following two assumptions: (i) the stress at any point $\underline{x}$ and time t is a scalar pressure $p(\underline{x},t)$, and (ii) the stress is a single-valued function of the density, $p = p(\rho)$. These assumptions may be said to define a homogeneous elastic fluid, since they hold in any homogeneous isotropic elastic medium incapable of sustaining a static shear stress.

In fluid mechanics, flows with these properties are called homentropic. They arise in the isentropic (e.g., adiabatic) flow of a homogeneous fluid. We omit the proof, and also the derivation of

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*In the limiting case $\Delta t \to 0$ of zero time-step, they constitute molecular models of matter in the classical sense.

**To simulate quantum-mechanical phenomena, however, one must use techniques very different from those discussed below.

Eqs. (1)-(2) of § 1, as a convenient mathematical expression of these hypotheses.

In the adiabatic flow of a perfect gas, we have $p_0 = 0$ and

$$(4) \quad p = -F(\sigma) = k\sigma^{-\gamma}, \qquad F'(\sigma) = k\gamma\sigma^{-\gamma-1},$$

the so-called "polytropic" equation of state. (See the discussion in § 4.) The approximation (4) seems physically adequate for atmospheric air, with $\gamma = 1.4$. A wide variety of other gases can also be fitted quite closely by (4), over fairly wide temperature ranges, under adiabatic conditions, with values of γ between 1.3 and 2 (see [4]).

For small deformations, one can fit (2) adequately by the linearization ($\gamma = -1$)

$$(4') \quad p = p_0 - b^2\sigma, \qquad F'(\sigma) = b^2 > 0, \text{a constant.}$$

This approximation (Hooke's Law) is used in linear elasticity theory; $b = \rho c = c/\sigma$ is the rate at which material is passed by a sound wave, c being the sound speed. In fluid mechanics, it is called the Chaplygin-Karman-Tsien approximation. Note that it reduces (1) to

$$(1') \quad x_{tt} = b^2 x_{aa},$$

the ordinary wave equation. Alone among equations of state, (4') permits plane waves of finite amplitude to travel without change of form. Correspondingly, it avoids the formation of shocks [22, §§ 12, 13]. Unfortunately, it is not satisfied by any known real fluid.

In classical continuum mechanics, equations (1)-(2) are assumed to be applicable also to "slab" motions of solids; we shall discuss this assumption in Part II.

Radial cylindrical and spherical motion leads to analogous equations.* By using appropriate conditions of interfacial continuity in velocity $u = x_t$ and pressure p, one can treat problems involving several homogeneous layers (slabs) or shells in contact with each other. And by letting $F(\sigma) = F(a,\sigma)$, one can also treat problems of non-homentropic isentropic flow.

3. Spatial discretization. In order to solve initial value (Cauchy) problems for (1)-(2) on a digital computing machine, one must use a finite set of values $a_o, \ldots, a_N$ of the Lagrangian mass-variable a, and a finite set of times $t_o < t_1 < t_2 < \cdots$. One can then think of $x(a_i, t_j)$ as representing the position of the i-th particle at time t_j. In this way, each finite difference approximation to (1)-(2) can be regarded as defining a law of motion for a discrete system of particles, movements being in discrete jumps.

It is very suggestive to fix the number of particles, and to let $\Delta t_j = t_j - t_{j-1}$ tend to zero. In the limit, one obtains a system of ordinary DE's from the given system of partial DE's, of exactly the type (3) considered in molecular models of matter. This gives a spatial discretization, sometimes also called semi-discrete. Such spatial discretizations have been considered since the time of Lagrange by many

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*[5, § 18]; the first exponent 2 in the last formula there should be deleted.

authors, who have had four distinct purposes in mind.

First, the system (3) and its generalizations have been considered as defining molecular models of solid crystals by Cauchy, Kelvin, Born, L. Brillouin, and others ([1], [2], [3], [24]). These authors have generally considered the small deformations typical of the theory of elasticity; for such small deformations, linear stress-strain relations like (4') are adequate.

Second, three-dimensional analogs of (2) have been applied to the kinetic theory of dilute gases, by Maxwell, Boltzmann, and their successors ([4], [8], [17]). The force-laws assumed here have been highly non-linear, the forces being negligible except occasionally, during binary encounters corresponding to near-collisions. These encounters are then studied statistically.

Third, analogs of (3) have been applied to simulate equations of state, and especially the change of phase from dense gases to liquids. A resume of the status of such applications may be found in [17, Ch. 4].

Finally, there is the tradition stemming from von Neumann [9], in which the numerical integration of (3) is used to compute approximate solutions to the non-linear wave equation (1)-(2). Since a characteristic feature of this work consists in the use of non-linear force-laws which are almost never negligible, it corresponds mathematically most closely to molecular models of dense gases and liquids.*

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*Such models were first studied by Newton, who speculated that "the phenomena of Nature ... may all depend on certain forces by which the particles of bodies ... are either mutually impelled towards one another, and cohere in regular figures, or are repelled" (Principia, preface to the first edition). See also ibid., Book II, Prop. 23, where "near neighbor" force-laws are considered.

4. Shocks; equation of state. It is well-known that the homentropic equation of state (2) breaks down physically across (strong) shock fronts in gases and liquids. When such shocks occur, one must replace (2) by a thermodynamic equation of state of the form

$$(5) \qquad p = p(\sigma, T), \qquad T = \text{temperature}.$$

The essential feature of (5) is its use of two variables in place of one to specify the local state of matter.

When heat conduction k and viscosity μ are negligible (adiabatic flow), so that the entropy S is constant, one can deduce (2) by combining appropriate assumptions about the internal energy

$$(5') \qquad I = I(\sigma, T)$$

with energy conservation principles. Thus, for a perfect gas, $I = c_v T$ by definition and (4) follows with $\gamma = c_p/c_v$; see [5].

By combining the preceding considerations with mass and momentum conservation, and allowing heat conduction across shocks, one can then deduce the Rankine-Hugoniot shock relations [5, §§ 54-62]. These are independent of the specific conductivity k assumed, which merely affects the thickness of the shock layer.

It is generally believed that the inviscid compressible flow equations of § 1, when taken with the Rankine-Hugoniot equations across shocks, give rise to a system of partial differential equations and interface conditions which define a well-set initial value problem. Moreover, it is believed that the resulting system, if integrated, adequately simulates real fluid motions under many conditions. However, this has never been rigorously proved.

It is further believed that the preceding model is adequate for the treatment of strong shocks in solids.* If supplemented by chemical kinetics considerations, it can be used to treat inviscid hypersonic fluid motions. And if supplemented by realistic fluid friction and heat transfer relations, it can be used to treat fluid flow in a heated channel.

5. Viscous compressible flow; shock thickness. However, the preceding hybrid model is not logically satisfactory. It is more logical, and more consistent with physical reality generally, to treat explicitly the effects of viscosity μ and thermal conductivity k. It is generally believed that the model of § 4 can be obtained rigorously from the resulting system of partial differential equations as the limit $\mu \downarrow 0$, $k \downarrow 0$.

This being assumed, it seems likely that the limit $\mu \downarrow 0$ with $k = 0$ will do as well and be simpler. It is primarily this limit which will be discussed below.** Only for a quantitative analysis of shock wave thickness is k important.

We therefore treat now the one-dimensional viscous compressible

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*See [19]; shear strength is perhaps negligible.

**See [5,(63.04)], where however bulk viscosity is neglected.

flow of a perfect gas in the limiting case $k = 0$; this is the only case for which computations are available.

In a perfect gas, the entropy $S = c_v \ln (p\,\sigma^{\gamma})$. One can define the "viscous" stress $q = 4\,\mu\, u_x/3$ [18,(5)], where $\mu = \mu(T)$ is a material constant* depending on the temperature. The one-dimensional Euler-Lagrange equation of motion (1) is then replaced by the one-dimensional Navier-Stokes equation

$$(6) \qquad x_{tt} = u_t = -(p - q)_a, \qquad q = \mu\, u_x = \rho\mu\, u_a = \mu x_{ta}/x_a.$$

At the same time, the polytropic equation of state (4) is replaced by the thermodynamic equation of state of a perfect gas [18,(4)]

$$(7) \qquad p = c_V(\gamma - 1)T/\sigma = e^{S/c_V}\,\sigma^{-\gamma}, \qquad \sigma = x_a.$$

The rate of change of entropy is [18,(3)]

$$(8) \qquad S_t = qx_{at}/T = qu_a/T.$$

Shock thickness. In a viscous compressible fluid, shock waves have a finite thickness. The shock thickness can be estimated by assuming time-independent flow in (6)-(8). Given the upstream state (S_1,σ_1) and associated sound velocity, there exists** for each $u_1 > c_1$ a time-independent flow (unique up to translation) for which $\lim_{x \to -\infty} u(x) = u_1$,

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*Both [18] and [5,§ 63] ignore the difficult problem of treating "bulk viscosity" correctly; for this problem, see [22, § 33].

**H. Weyl, Comm. pure appl. math. 2 (1949), 103-22; D. Gilbarg, Am. J. Math. 73 (1951), 256-74.

$\lim_{x \to +\infty} \sigma(x) = \sigma_1$. For this flow, $u_2 = \lim_{x \to +\infty} u(x)$, $\sigma_2 = \lim_{x \to +\infty} \sigma(x)$, and $S_2 = \lim_{x \to \infty} S(x)$ exist and are given by the Rankine-Hugoniot equations. For shocks of finite amplitude (with $\sigma_1/\sigma_2 > 1.01$, say), most of the flow is nearly uniform, the "shock thickness" δ over which 99% of the change in $\sigma(x)$ takes place being very small. The shock thickness δ decreases with the strength, being of the order of the molecular mean free path* if $\sigma_1/\sigma_2 > 2$.

6. <u>Real and artificial viscosity</u>. If a physically real viscosity is used in Eqs. (6)-(8), the effect is negligible except in shock layers. Moreover these are so thin in comparison with mesh-lengths of interest that real viscosity effects cannot be computed effectively on digital computing machines, in typical high-speed flows (large Reynold numbers).

For somewhat the same reason, it is also awkward to treat the model of § 4 on computing machines with a rectangular space-time mesh. The shocks go between mesh-points and "shock-fitting" must be done by inverse interpolation.** To indicate what is done in practice, we write down the spatial discretization of the partial differential equations (6)-(8). This is (since $p_t = ([\gamma - 1]\, q - \gamma p)\, x_{at}/x_a$ by these equations):

$$(9) \qquad m\ddot{x}_n = -\,(p_{n+\frac{1}{2}} - p_{n-\frac{1}{2}}) + (q_{n+\frac{1}{2}} - q_{n-\frac{1}{2}}), \qquad m = a_n - a_{n-1},$$

$$(10) \qquad \dot{p}_{n+\frac{1}{2}} = [(\gamma - 1)q_{n+\frac{1}{2}} - \gamma p_{n+\frac{1}{2}}]\,(\dot{x}_{n+1} - \dot{x}_n)/(x_{n+1} - x_n),$$

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*D. Gilbarg and A. Paolucci, J. nat. mech. anal. 2 (1953), 617-42. See also R. Becker, Z. Phys. 8 (1922), 321-62; L. H. Thomas, J. Chem. Phys. 12 (1944), 449-53; H. Grad, Comm. pure appl. math. 5(1952), 257-300.

**See L. H. Thomas, Comm. pure appl. math. 7 (1954),195-206.

(11) $$q_{n+\frac{1}{2}} = \frac{4}{3}\,\mu(\dot{x}_{n+1} - \dot{x}_n)/(x_{n+1} - x_n).$$

The pressure relation corresponds to the equation of state (7):

(12) $$p_{n+\frac{1}{2}} = e^{S/c_V}[(x_{n+1} - x_n)/m]^{-\gamma}.$$

Since (9)-(12) define a system of ordinary differential equations, it is easy to integrate the system numerically with high accuracy by any of various methods.

The spatial discretization (9)-(12) reduces, in the limit $\mu = 0$ $(q = 0)$, to von Neumann's mass-spring system (3). The viscous or damping term q is equivalent to inserting a dashpot in parallel with each spring. This model was proposed for solids by Kelvin and Voigt; it is the simplest model of rheology.

To achieve smooth velocity profiles with a finite mesh-length, one must introduce an artificial viscosity large enough to make the thickness of the shock layer two or three mesh-lengths, but not much larger than this. To achieve this, one postulates that q in (6) and (11) shall depend on the velocity gradient according to some arbitrary law $q(u_x,T)$ (see [6, Part IX], [11], [18], [20]); it may even be non-linear* in u_x.

7. Molecular and continuum models of matter. The idea that continuum models of matter can be derived from molecular models, as the limiting case $N \to \infty$ of N particles of equal mass $m = \Delta a = a_{k+1} - a_k$, is

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*See [12, Ch. X, § 9]; R. Landshoff, Report LA-1930. Lax [20] advocates using a linear viscosity. One can postulate a wave-front, and then deduce the associated viscosity "law" (inverse method).

very old. It can be justified for elastic fluids as follows.

If the molecules attract each other according to a force-law $F([x_{k+1} - x_k]/m)$, the equations of motion are

$$(13) \qquad m\ddot{x}_i = F([x_{i+1} - x_i]/m) - F([x_i - x_{i-1}]/m), \qquad i = 1,2,\cdots,N.$$

Let $y = y(a,t)$ be a function with two continuous derivatives with respect to a such that $y(a_i,t) = x_i(t)$, $i = 1,2,\cdots,N$. Then, expanding F in Taylor series about $\partial y/\partial a$ for $a = a_i$, substituting into (13), and dividing by m, we obtain

$$(14) \qquad \partial y(a_i,t)/\partial t = F'(\partial y[a_i,t]/2a)\partial^2 y(a_i,t)/\partial a^2 + O(\Delta a).$$

In the limit $\Delta a = m \rightarrow 0$ $(N \rightarrow \infty)$, tends to (1) <u>if</u> $y \in \mathcal{C}^2$ varies sufficiently smoothly in position and time, and $F \in \mathcal{C}^1$.

The mass-spring model (13) and its generalizations have been considered for many hypothetical force-laws, and it is interesting to consider some peculiarities of these laws. We begin with the force-law $f(r) = kr^{\gamma}$ corresponding to the <u>polytropic</u> equation of state (4).

In this case, the particle model defined by (10) admits the <u>energy integral</u>, constant in time,

$$(15) \qquad E = \frac{1}{2} m \sum \dot{x}_i^2 + \frac{km}{1-\gamma} \sum |(x_i - x_{i-1})/m|^{1-\gamma}, \qquad \gamma \neq 1.$$

(A similar integral holds for any $F(\sigma)$.)

If $\gamma \geq 1$ (a logarithmic analog of (15) exists for $\gamma = 1$), then it takes infinite energy to make two particles collide. As a corollary, the order of particles cannot change: each particle always has the same two "nearest neighbors". On the other hand, if $\gamma < 1$, it only takes finite energy to make $x_i = x_{i-1}$, and particles can collide or pass "through" each other. (For $\gamma = -1$ and for particles of equal mass, such interpenetration is mathematically equivalent to elastic collision.)

It is curious that the condition $\gamma > 1$ should also coincide with the condition that $c^2 = dp/d\rho = k\gamma\, \rho^{\gamma-1}$ should increase with the density — i.e., that the fluid should be normal.* (H. Weyl (op. cit. supra, p. 105) postulates the related but weaker condition that $\rho^2 c^2$ should increase with the density.) Note that $k\gamma > 0$ since $F'(\sigma) > 0$ in (2).

8. Wave transmission. A fundamental description of real and synthetic homogeneous materials concerns their mode of transmission of plane waves of given frequency and amplitude. For acoustic or small-amplitude waves, all elastic fluid continua are characterized by their sound velocity $c_o = b/\rho_o$; the general wave form is $x = f(a - bt) + g(a + bt)$ in Lagrangian coordinates, where $b^2 = F'(\sigma_o)$. In Eulerian (space-time) coordinates, the general wave form $\delta x = f(x - c_o t) + g(x + c_o t)$ is the same, because of the small amplitude approximation.

Dispersion. Using Fourier analysis, one can attribute the preceding result to the fact that sinusoidal acoustic waves travel in elastic fluid continua without attentuation or dispersion. This is however not

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*See [5,p. 5]; also the footnote on p. 5 of G. Birkhoff and J. M. Walsh, Riabouchinsky Jubilee Volume, Paris, 1954. Glass may be "abnormal": $d\rho/\rho^2 dp$ seems to increase with p up to 10 kilobars.

true in molecular models: though there is no attenuation (in pass-bands), there is always dispersion. The wave velocity c of a sinusoidal acoustic wave of length λ, in a one-dimensional mass-spring system with particles spaced $h = 1/N$ apart, satisfies [3, p. 4]

$$(16) \qquad c = c_\infty \sin(\pi h/\lambda)/(\pi h/\lambda),$$

where c_∞ is the velocity of long waves ($\lambda \to \infty$). That is, there is dispersion: c varies with λ, between the limits c_∞ and $2c_\infty/\pi \simeq 0.6335c_\infty$.

Though the preceding phenomenon of dispersion is not observed physically in gases, it does simulate (with molecular particle spacing) some characteristic features of the behavior of solid crystals. For example, many crystals have a frequency cutoff. Other models consisting of two kinds of masses, alternatively spaced, will transmit waves only in certain frequency bands. In this respect, such models simulate the optical behavior of many crystals and the behavior of electric band-pass networks; see [3].

For large-amplitude waves in elastic fluid continua, the wave form is still given in Lagrangian coordinates by $x = f(a - c_0t) + g(a + c_0t)$ in the case $\gamma = -1$ of linear elasticity theory (Hooke's Law), with which most of the relevant literature has been concerned. In molecular models, (16) still holds.

Shocks. It is well-known that shocks arise in polytropic elastic fluids if $\gamma > -1$. Moreover simple shocks (with uniform flow on each side of the shock) are transmitted without change of form for any (normal) equation of state in any continuous elastic fluid. (For simple shocks in viscoelastic media, see § 5.)

As a result of dispersion, this feature is not reproduced in the spatial discretization discussed above, even when $\gamma = -1$. This was first observed by von Neumann [9], for $\gamma = 1.4$ (approximately).

When $\gamma = -1$, the analog for molecular models of Kelvin's Principle of Stationary Phase* is applicable to simple shocks and other pulses of short duration. This principle asserts that each Fourier component travels with its own wave velocity, so that the appearance of a pulse of short duration after being transmitted through a long distance should be as follows. The "head" of the pulse (which travels most rapidly) should largely conserve its initial form; but the "tail" should be wavy with wavelength diminishing continuously to the shortest observable wavelength 2/N. It would be interesting to test, by numerical calculation, whether this was also true in the non-linear case, with $\gamma > -1$.

One can speculate that dispersion will also make shock wave thickness in molecular models greater than in continuum models (see § 5). It would be interesting to study this question for the viscoelastic molecular model of § 6, looking for solutions <u>periodic</u> in time. If the equations were linear ($\gamma = -1$), the shock thickness would increase indefinitely with time.

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*[3, p.77]; [23, § 241]; J. J. Stoker, "Water waves", Interscience (1957), p. 163.

9. Finite time-steps. In § 1-8, we have discussed systems of particles whose positions were continuously defined in time, of a type familiar in the kinetic theory of gases and in the molecular theory of crystals. In digital computations one uses finite time-steps Δt.

It is important to choose these Δt so as to minimize the computational (truncation and roundoff) errors. In the special case $\gamma = -1$, both truncation and dispersion can be eliminated by using $\Delta t = \Delta x/c$, i.e., by integrating along characteristics. The accuracy of the approximation depends solely upon roundoff and the accuracy of determining $x_i(0)$ and $x_i(\Delta t)$.

Convergence theorems. The discussion at the beginning of § 7 suggests that, as Δa_i tends to zero, the solutions of suitable difference approximations to (1)-(2) should converge to the solution of the differential equations, for the same initial conditions. The natural conjecture is that this is true provided no shock waves occur and that the time-steps Δt_i satisfy the stability condition $\Delta t_i \leqq \Delta x/c$, the local sound speed.

For the differential equations describing the motion of an elastic fluid in Eulerian coordinates,

$$u_t + uu_x = - c^2(\rho)\, \rho^{-1}\, \rho_x, \qquad \rho_t + (\rho u)_x = 0,$$

convergence follows from a general theorem of Courant, Isaacson and Rees.* It also follows for the coupled first-order hyperbolic equations

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*R. Courant, E. Isaacson, and M. Rees, Comm. pure appl. math. 5 (1952), 243-55.

$$u_t = b^2(\sigma)\sigma_a, \qquad u_a = \sigma_t, \qquad b(\sigma) = \sqrt{F'(\sigma)},$$

equivalent to (1)-(2), from the same general theorem. To obtain x(a,t) from the approximate solution, one must then integrate the equation $x_a = \sigma$.

The natural difference approximation to the second-order hyperbolic equation (1), is

$$(17) \qquad x_j^{n+1} - 2x_j^n + x_j^{n-1} = \frac{\Delta t^2}{\Delta a}\left\{F([x_{j+1} - x_j]/\Delta a) - F([x_j - x_{j-1}]/\Delta a)\right\},$$

where

$$x_j^n = x(j\Delta a, n\Delta t).$$

The solution of this set of difference equations converges* to the solution of (1) as Δt and Δa go to zero, subject to the stability requirement $\Delta t^2 F'/\Delta a^2 < 1$; this requirement is met if $\Delta t/\Delta a$ is chosen small enough so that $\Delta x_j^n/\Delta t$ is greater than the local speed of sound $c = \sigma|\partial p/\partial \sigma|^{\frac{1}{2}} = \sigma|F'(\sigma)|^{\frac{1}{2}}$.

As a corollary, letting first $\Delta t \downarrow 0$ for fixed Δa and then letting $\Delta a \downarrow 0$, one obtains a rigorous proof for the convergence of the spatial discretization (1)-(2) to the exact solution of the corresponding continuum problem, provided there are no shocks.

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*Provided $F \in \mathcal{C}^2$, $x(a,0) \in \mathcal{C}^2$, and $x_t(a,0) \in \mathcal{C}^1$, and that the derivatives $F_{\sigma\sigma}, x_{aa}(a,0)$ and $x_{at}(a,0)$ satisfy Lipschitz' conditions. The proof will be given in the thesis of Robert E. Lynch.

Unfortunately, no similar results have been proved for the one-dimensional Navier-Stokes equations (6)-(8). Even the convergence of solutions of (9)-(11) to solutions of (6)-(8) as $m \to 0$ $(N \to \infty)$ has not been established. Neither has any convergence theorem been proved in the limit $\Delta a \to 0$, $\mu \to 0$ to the motion of an elastic fluid with shocks.

Synthetic materials. Referring back to § 1, it is interesting to speculate as to what kind of synthetic materials are defined by computation schemes like (17) with finite time-steps Δt. This question can be asked also for difference approximations to the equations of a visco-elastic fluid. For some computing processes (such as forward-difference methods), the use of discrete time-steps can be regarded as introducing a finite delay time into reactions. Such delay times or relaxation times have also been suggested as being responsible for various physical phenomena, such as ultrasonic attenuation.* In the theory of viscoelastic solids, similar delay times characterize Maxwell solids. Their characteristic property is to cause high attenuation in narrow resonance bands — as contrasted with monotonically varying viscous attenuation. Such resonance bands are observed physically.

Further study may reveal other qualitative phenomena associated with the use of finite time-steps, also observable physically. By studying such phenomena in one space dimension, one can hope to gain insight into the three-dimensional case.

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*See, for example, M. Brillouin, "La viscosité des liquides et des gaz," Paris, 1907, vol. 2, pp. 93-5; K. F. Herzfeld in Part H of "Thermodynamics and physics of matter," F. D. Rossini, editor, Princeton, 1955.

II. STATISTICAL MECHANICS

10. Kinetic theory of gases. In the kinetic theory of gases, it is assumed that gases are composed of very many moving particles,* interacting with each other according to appropriate molecular force-laws. In the semi-discrete model (§ 3) of a shock advancing into a uniform gas, irregular particle motion occurs behind the shock; von Neumann suggested [9] that this motion was analogous to the molecular motion in the kinetic theory of gases. We will now analyze this suggestive idea critically.

In the kinetic theory of gases, pressure p and temperature T are independent variables, as in the continuum model of § 4. Moreover, the temperature has a purely mechanical significance, as the mean translational energy of molecular motion. Thus, by analogy with the three-dimensional case, we can write**

$$RT = \frac{1}{2} m\overline{(\dot{x} - \bar{\dot{x}})^2} = \frac{1}{2N} \sum_i m_i(\dot{x}_i - \frac{1}{N} \sum_k \dot{x}_k)^2, \tag{18}$$

allowing for the possibility of variable mass m_i. Here x_i is the

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*About $N = 2.7 \times 10^{19}$ per cc (Avogadro's number) under standard atmospheric conditions [8, p. 8]; the incorrect value 6×10^{23} (Loschmidt's number) is frequently quoted.

**See [8, § 146, p. 311], and compare with § 141, p. 299 and § 26, p. 32.

position of the i-th mass point in the semi-discrete model of § 1; the summations are over N gas molecules. (Note that, by Maxwell's Principle of the Equipartition of Energy [8, p. 81], the statistical expectation of $E_i = m_i(\dot{x}_i - \dot{\bar{x}})^2/2$ is independent of i.) Whereas in mass-spring models of elastic fluids, which reproduce the adiabatic equation of state under quasi-static conditions (i.e., very gradual compression), the pressure p determines the nominal temperature T.

As $N \to \infty$, the convergence theorems of § 9 show that motions of most individual molecules in the mass-spring model (3) will deviate less and less from the mean motion, <u>except</u> behind shocks. That is, the effective local temperature (in the sense of kinetic theory) is zero. In particular, the intermolecular forces f(r) between adjacent particles in Lagrangian hydrodynamical computations act continuously and normally vary by a factor of at most ten, whereas the intermolecular forces treated in the kinetic theory of dilute gases are negligible most of the time, being appreciable only during brief near-collisions (encounters).

<u>Specific heat</u>. The proportionality of temperature to the kinetic energy of relative motion (relative to the local mean motion) is clearly illustrated by a study of specific heats. In monatomic gases, the specific heat is about 3 cal/mole °C [4, p. 42] above the critical point; in diatomic gases, it is about 5 cal/mole °C. In solids, where the potential energy of vibration and the kinetic energy of vibration are about equal, it is often* about 6 cal/mole °C. The number 3 is equal to the

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*This is the Dulong and Petit Law [3, p. 166], approximately valid if the "Debye temperature" is one or greater.

number of degrees of freedom of motion, due to a lucky coincidence: that H_2O, with molecular weight 18, has the abnormally large specific heat of 18 cal/mole $^\circ C$ at $20^\circ C$.

At low temperatures, the specific heats of solids are considerably less than 6 cal/mole $^\circ C$. For various force-laws $f(r)$, it would be interesting to study the mean energy in thermal equilibrium of a "solid" consisting of n particles of mass m, bombarded at random times by particles of mass m having a Maxwell velocity distribution and mean energy $mv^2/2$. From this one could infer the ratio of specific heats and the Debye temperature curve for various one-dimensional "solids".

11. Equation of state. In the mass-spring model of § 3, the pressure is attributed to static molecular repulsion; in the kinetic theory of gases, it is attributed to molecular motion. The first model simulates liquids and solids, to a first rough approximation, while the second simulates dilute gases very well, especially monatomic gases. That is, pressure in gases is dominantly kinetic, whereas in liquids and solids it is dominantly static.

In general, the virial of Clausius[*] allows one to decompose the pressure into a kinetic component proportional to RNT, and a static component proportional to $N\overline{rf(r)}$, where N is the number of particles per unit volume. In n dimensions,

$$(19) \qquad p\sigma' = \frac{1}{n}\,[RNT + N\overline{rf(r)}] = \frac{N}{n}\,[RT + \overline{rf(r)}].$$

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[*] See [8, §§ 163-73], where the three-dimensional case is treated.

Here T is defined as the mean kinetic energy of translation per particle.

One of the oldest problems in the molecular theory of matter is to simulate the equations of state of real material by molecular models, postulating an appropriate intermolecular force-law. Among the force-laws which have been studied ([4], [8], [17]), the hardsphere, power laws $f(r) = Ar^{-\alpha}$, and the Lennard-Jones formula $f(r) = Ar^{-\alpha} - Br^{-\beta}$ have received the most attention.* The problem is to deduce the observed pressure $p(\sigma,T)$, internal energy $E(\sigma,T)$, and phase transitions as functions of the specific volume σ and temperature T.

Because such studies ignore the fact that real matter is made up of positively charged atomic nuclei and negatively charged electrons of much smaller mass, their conclusions cannot be taken as having a direct physical significance. Rather, they must be considered as suggestive. In particular, they may suggest computation schemes for simulating the behavior of real materials in (say) atomic explosions more realistically than would be possible with an idealized elastic or inelastic fluid.

For such purposes, studies in one space dimension have much to recommend them. Moreover in one dimension, it is easy to supplement analytical studies by numerical studies of the motions of sample systems of particles.** We hope that such studies will be made. Because of

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*The Lennard-Jones formula is also assumed by Grüneisen, in an attempt to correlate the Debye temperatures of solids with their compressibilities; see Born and Huang [2, p. 52].

**Such a study has recently been made, for the rigid-sphere model in three dimensions, by Alder and Wainwright. See "Transport processes in statistical mechanics," I. Prigogine, editor, Interscience, 1958, 97-140.

similarity (see § 14), one should be able to compute some quantities with $N < 100$. In [9], von Neumann suggested (in another context) that $N = 14^n$ might be adequate in n dimensions.

In anticipation of such studies, we make a few elementary remarks about statistical mechanics in one space dimension.

In the rigid-sphere model, it is evident that the equation of state will be $p(\sigma - \sigma_o) = NT$, where $T = \overline{mc^2}/2$ and $\sigma_o = Nr_o$ is the one-dimensional "volume" occupied by molecules.

In general, one must distinguish between forces assumed to act only between <u>nearest neighbors</u>, as in mass-spring systems, and <u>universal</u> forces (like gravitation) assumed to be defined for all particle-pairs. We will here consider only forces of the first kind. These were originally postulated by Newton (loc. cit. in § 3), and they are better suited to numerical computation.

In general, letting $f_k(t) = p_{k-\frac{1}{2}}(t)$ be the force exerted on the k-th particle by the (k-1)-st particle, it is easily seen that $\bar{f}_k = \bar{f}_{k+1}$, averaged over a long period of time. Otherwise, the k-th particle would undergo a net acceleration. Hence, $\bar{f}_k$ must be independent of k in the one-dimensional case.

Now consider the case $\gamma = -1$ of Hooke's Law. In this case, if $f(r) = p_o - Br$ is the repulsive force, then $\bar{f}_k = p_o - B(\bar{x}_k - \bar{x}_{k-1})$. Since $\bar{f}_k = \bar{f}$ is independent of k, it follows that $N\bar{f} = Np_o - B(\bar{x}_N - \bar{x}_1)$. Solving for $\bar{f} = p_o - B(\bar{x}_N - \bar{x}_1)/N$, we see that the pressure $p = f$ satisfies

(20) $$p = p_0 - Bm\sigma, \qquad \sigma = (x_N - x_1)/Nm.$$

This shows that the pressure is independent of the temperature (kinetic energy). In (19), the term in $\overline{rf(r)}$ is decreased by molecular motion just enough to compensate for the increase in RNT; the Clausius decomposition (19) is completely misleading.

Similar considerations suggest that, in the synthetic gas defined by the mass-spring model of § 3, the total pressure will increase with the temperature (we will have $(\partial \rho/\partial T)_\sigma > 0$) if $\gamma > -1$, so that repulsion increases more than linearly with approach (case of "stiff" springs). In the opposite case, $\gamma < -1$ of "soft" springs, $(\partial p/\partial T)_\sigma$ will be negative in (3). The simplest model of elastic collision is the extreme case of a "stiff" spring; water below 4°C corresponds to the hypothesis of a "soft" spring; $\gamma = 2$ corresponds to an inverse square repulsion law.

It would be desirable to study the dependence of $p(\sigma,T)$ on $f(r)$ quantitatively by the method described above. Using larger computing machines such as STRETCH and LARC, one could try to simulate more generally the statistical mechanics of polar molecules and the elusive phenomena of condensation and evaporation.*

Monte Carlo methods. Monte Carlo methods have also been used to calculate the equation of state for various intermolecular force-laws

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*See [17, Ch. 5]; H. N. Temperley, "Changes of state," London, 1956, pp. 2-3; O. K. Rice, Part E of "Thermodynamics and physics of matter," Princeton, 1955; C. N. Yang, Phys. Rev.

— and especially for rigid elastic spherical molecules.[*] This approach is related to that discussed in this report only in its objective and its use of high-speed computing machines.

12. Ergodic theory. Though the conditions of statistical equilibrium assumed in kinetic theories of matter are not attained during times typical of hydrodynamical interest, it is interesting to speculate what these conditions are, and what is the order of magnitude of the time scale required to attain them. High-speed computing machines may be expected to provide useful information regarding these questions, and hence indirectly regarding molecular models of matter based on equations of the form (3) and statistical mechanics.

In using computing machines to perform such research, it is important to realize that some of the fundamental concepts of statistical mechanics have themselves never been rigorously established. For instance, it has never been proved that, as $t \to \infty$, the only statistical invariants of an assembly of molecules in a rigid container with elastic walls are temperature and density. Stated more abstractly, one of the gaps in the theory is the lack of proof of the assumption of "metric transitivity" (also called the ergodic hypothesis): that all time-histories having given energy and density have equivalent statistical averages, with probability one.

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[*] The pioneer study (for a two-dimensional "gas") was by N. Metropolis, A. W. and M. N. Rosenbluth, and A. H. and E. Teller, J. chem. phys. 21 (1953), 1087-92. For subsequent work, see W. W. Wood et al., Nuovo Cimento 9 (1958), 133-43; Z. W. Salsburg et al., J. chem. phys. 30 (1959), 67-72, and refs. given there.

Though various theoretical arguments tending to confirm this hypothesis have been given,* it still rests on an essentially experimental basis, and the generality of the conditions under which it may be expected to hold is not clear. Without it, special arguments are needed to show that the function $p(\sigma,T)$ is well defined (i.e., single-valued).

And yet it is easy to show that the ergodic hypothesis stated above does not always hold. For instance the power spectrum (energy density as a function of wavelength) is an invariant in a Chaplygin fluid with $\gamma = -1$. In a three-dimensional cube, the energy density as a function of the wave-vector $(|k_1|,|k_2|,|k_3|)$ is invariant.

Turning to one-dimensional molecular models, it is classic that for N rigid elastic spheres in one dimension, the entire set of velocities is conserved. Hence, again, density and temperature are not a complete set of invariants, even though $p(\sigma,T) = NRT/(\sigma - \sigma_o)$ is a single-valued function.

In the discrete analog of a Chaplygin fluid, defined by a mass-spring system with Hooke's Law, there is no energy interchange of energy between different wavelength (i.e., different portions of the spectrum). Hence the motion is not metrically transitive. However, since the frequencies $\omega_j = 2 \sin (j\pi/2N)$ of the normal modes are ordinarily

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*The most important is that of Oxtoby and Ulam, Annals of Math. 40 (1939), 560-66. J. Moser has recently proved a complementary unpublished result on the existence of invariants. For a physical discussion, see G. Uhlenbeck in Appendix I of Mark Kac, "Probability in the physical sciences," Interscience, 1959.

incommensurable* (i.e., rationally independent), one may expect phase randomization by dispersion in discrete models.

One can surmise that, in the non-linear case $\gamma \neq -1$, both frequency and phase will tend to distribute themselves statistically in a uniform way, so that time-averages will again be independent of initial conditions. This is suggested by the Theorem of Oxtoby and Ulam; some interesting experiments bearing on it have been performed by Fermi, Pasta, and Ulam [16].** Some further experiments along similar lines for a single "ping-pong ball" have been reported and analyzed at the Fourth Berkeley Symposium by S. Ulam and J. M. Hammersley.

One can also surmise that, in two or more dimensions, molecular models of fluids will be ergodic for arbitrary force-laws with probability one (i.e., for almost all initial velocities and distributions). This is because of the great variety of possible angles of scattering. (We exclude cases like that of closely packed rigid spheres, where the neighbors of a fixed "particle" cannot change.)

13. Diffusivities; correlation functions. From statistical studies of time-histories of assemblies of particles subjected to various assumed force-laws f(r), one can also try to estimate the viscosity

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* This is especially likely if N is a prime, because the cyclotomic equation is then irreducible (Eisenstein's Theorem).

**These experiments apparently indicate that equipartition of energy does not occur. Joseph Ford, J. Math. Physics 2 (1961), 387-93, has suggested an explanation of this. His suggestion is that, for the number of mass-points used in the experiments, there is no appreciable energy sharing between the weakly coupled oscillators.

(momentum diffusion), thermal conductivity k (heat diffusion), and material diffusivity D associated with molecular models (3) of fluids. If the ergodic hypothesis is fulfilled, time-averages should be independent of the initial conditions.

For dilute gases (i.e., at high temperatures), such studies will probably not be immediately rewarding. Classical methods of estimating binary deflection probabilities seem more powerful as mathematical techniques. Moreover physically, the ratio of the three diffusivities (for momentum, heat, and matter) seems to be nearly independent of the force-law assumed. Thus the Prandtl number $\mu C_v/k$ is about 0.4 [4, Ch. 10], while $D\rho/\mu$ is between 1.0 and 1.5 [8, Ch. 13] for spherically symmetric molecules. Deviations of real gases from these laws seem to be due largely to the fact that real gas molecules have energy of rotation as well as energy of translation, unless they are monatomic.

However, for dense gases and liquids, one can probably best estimate the dependence of diffusivities on the force-law assumed from numerical experiments. Such experiments might also reveal interesting relations between the shear viscosity μ and the bulk viscosity μ', which is zero in a dilute monatomic gas.

To get the most information out of such (necessarily elaborate) numerical experiments, a great deal of ingenuity will certainly be required. This is especially true of dynamical studies: The statistical mechanics of non-uniform gases is very difficult.

For example, let the kinetic temperature $T(x_i)$ of a mass-spring system ("gas") with a temperature gradient be defined in statistical equilibrium as the mean kinetic energy $m_i u_i^2/2$ of the particle with mean position $x_i = \bar{x}(a_i)$. If one defines the kinetic temperature $T(x,t)$ by an average over phase-space, how can one compute this effectively from a small sample of a few nearby particles? What is the probable error?

To obtain some information on this question, in the case of stationary "gases" containing just one kind of molecule of mass m, one can define a closely related <u>correlation function</u>

$$\phi(k) = \overline{u_i u_{i+k}} \;/\; \overline{u_i^2}, \qquad u_i = \dot{x}_i. \tag{21}$$

This will provide a measure of the smoothness of a computation, and is also a fundamental statistical entity.* The evolution of $\phi(k,t)$ with time would be especially interesting to study.

The study of such correlation functions should help in separating out local mean motions (those which one would obtain in the limit $N \to \infty$) from random molecular motions. Hence, indirectly, it would help in the effective definition and computation of conductivities and viscosities.** By analogy with the theory of turbulence, it would also lead to the interesting concept of an energy <u>spectrum</u> of molecular motion, which could

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*To avoid difficulties associated with $\overline{u_i u_{i+k}}$ being undefined, it is inconvenient to use a periodic gas with $u_N(t) = x_o(t) + X$.

**For some other ambiguities in the kinetic theory of viscosity, see C. Truesdell, Zeits. fur Physik 131 (1952), 273-89.

be studied as a function of the force-laws being considered.

14. Springs with dashpots. The preceding discussion referred to mass-spring models, with emphasis on nearest neighbor force-laws in one space dimension. It follows from the discussion of § 13 that such models will have a molecular viscosity μ. Offhand, one would expect μ to be of the order of magnitude of $\rho\bar{v}h/3$, where $\bar{v}$ is the mean molecular velocity and h (the particle spacing) is the analog of the mean free path. It would follow that $\mu \propto \sqrt{T}$, as in elementary kinetic theory.*

Of great interest are, also, molecular models constructed by formulas (9)-(12) from the Navier-Stokes equations. These provide molecular models for viscoelastic fluids and for viscoelastic solids of various kinds.** These models also describe some computation schemes using an artificial viscosity $\mu^* \gg \mu$ to smooth out the computed flow behind shocks. In such computation schemes, where the pressure depends on an internal energy (temperature) T for given σ, one can introduce an energy conservation law (and prove that the entropy increases monotonically). The temperatures may be attributed to the masses or the springs; we omit the formulas.

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* [8, Ch. XI]. For real gases, $\mu \propto T^n$, where $0.65 < n < 1$.

**[21, Part II]; W. P. Mason, "Physical acoustics and properties of solids," Van Nostrand, 1958, Ch. VII; D. R. Bland, "Linear viscoelasticity," Pergamon Press, 1960. In their models of solids, some rheologists would also include a block on a rough surface to reproduce the transition to plastic flow at the yield point. Springs, dashpots, and blocks, in various series and parallel combinations (Bingham, Prandtl, Kelvin, Maxwell bodies, etc.) have been found useful in reproducing characteristics of dough and other substances.

For each choice of γ, artificial viscosity μ^*, and spacing h, one can thus define a synthetic gas, whose effective viscosity is a combination of the molecular viscosity and the artificial viscosity postulated. (This is analogous to combining molecular viscosity with turbulent "eddy viscosity".)

Similarity. One can reduce the number of parameters required to define such synthetic gases by identifying systems of particles whose behavior is similar up to change in scale. For linear viscosities, one can thus define a natural Reynolds number $Re = \rho\, \bar{c}h/\mu^*$, where $\bar{c} \propto T^{\frac{1}{2}}$. Synthetic "dilute" gases having the same γ and Re should be completely similar.

Analogous remarks apply to thermal conductivity, which is given quite well in dilute gases by the formula $Pr = \mu\, C_V/k = 4/(9\gamma - 5)$ for the Prandtl number [8,§ 301].

Even in dense gases, the addition of a constant p_0 to the equation of state has no effect on the particle dynamics defined by (3), or on the continuum problem defined by (1)-(2). For example, with the polytropic equation of state $p = p_0 + k\rho^{\gamma}$, a measure of the diluteness of a gas (in the sense of kinetic theory) is provided by $h[\overline{u^2}/k(\gamma - 1)]^{1/\gamma-1}$, which estimates the average ratio of the distance of closest approach of two adjacent molecules, to the mesh-length.*

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*For a related similarity law involving mass-spring models without dashpots, see Rayleigh, Proc. roy. soc. A66, p. 68 (ref. in [8, p. 283]).

III. PLANE FLOWS

15. Elastic fluids. The concept of an elastic fluid was defined in § 2. It can also be defined as an elastic continuum (see § 18) in which the stress tensor has no shear component in any direction, and the pressure at any material point is determined by the specific volume. In fluid dynamics, these correspond to the assumptions of homentropic flow. We will treat below only the case of a homogeneous elastic fluid, for simplicity.

In terms of Lagrangian independent variables, elastic fluids are defined by a plane analog of Eqs. (1)-(2). This analog involves a vector function $\underline{x}(\underline{a};t)$, whose components are $x(a,b;t)$ and $y(a,b;t)$. The analog of (1) in this notation is

$$(22) \qquad x_{tt} = -\sigma\nabla p, \qquad \text{where } \sigma = \begin{vmatrix} x_a & x_b \\ y_a & y_b \end{vmatrix}.$$

This is combined with a homentropic equation of state (2):

$$(23) \qquad p = p_o - F(\sigma).$$

The function $F(\sigma)$ is chosen to agree with experimental values measured under quasi-static adiabatic conditions. Typically, one supposes that

$\underline{x}(\underline{a};0)$ is given inside a domain of interest, and the normal component u_n of $\underline{x}_t = \underline{u}$ on the boundary. (Alternatively, one can suppose p given on a "free" boundary.)

Though mathematical existence and uniqueness theorems seem not to be available, physical and numerical experience suggests that such problems are usually well-set, except for the development of shock waves. Shock waves must be treated by special techniques, involving the Rankine-Hugoniot equations. These techniques will be discussed in § 17.

We will analyze below various schemes for solving Eqs. (22)-(23) and related systems of equations on digital computing machines. Only a few of these schemes define <u>molecular</u> models of matter in the classical sense. But they can all be regarded as defining "synthetic materials," or models of matter which may simulate highly stressed real materials to a greater or less extent.

16. <u>Spatial discretizations</u>. It is easy to think of spatial discretizations of the system (22)-(23). For example, one can select* a square or rectangular network of particles ("molecules") (a_i, b_j) in (a,b)-space, and consider the particle paths $x_{ij}(t) = x(a_i,b_j;t)$. By (22)-(23), these should satisfy the <u>ordinary</u> DE's.

$$\text{(24)} \qquad \ddot{x}_{ij} = \sigma_{ij}\, F'(\sigma_{ij})\, \partial\sigma/\partial x, \qquad y_{ij} = \sigma_{ij} F'(\sigma_{ij}) \partial\sigma/\partial y,$$

the partial derivatives being evaluated at (a_i,b_j).

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*One can also use triangular or hexagonal networks in place of rectangular ones.

There are many ways of evaluating

$$\sigma = \begin{vmatrix} x_a & x_b \\ y_a & y_b \end{vmatrix}$$

approximately. For instance, one can use the central difference scheme

$$(25) \qquad \sigma_{ij} \simeq \begin{vmatrix} (x_{i+1,j} - x_{i-1,j}) & (x_{i,j+1} - x_{i,j-1}) \\ (y_{i+1,j} - y_{i-1,j}) & (y_{i,j+1} - y_{i,j-1}) \end{vmatrix} (4\Delta a\Delta b)^{-1}.$$

A logical scheme for evaluating $\partial\sigma/\partial x$ and $\partial\sigma/\partial y$ is less easy to select, because of the many options for taking differences in (x,y)-space and (a,b)-space. Unless care is exercised, one may find that the final formulas involve $x_{i\pm2,j}$ and $x_{i,j\pm2}$, which is undesirable.

To avoid this, one can define a nominal specific volume at each <u>half</u>-integer mesh-point by

$$(26) \qquad \sigma_{i-\frac{1}{2},\, j-\frac{1}{2}} = \begin{vmatrix} (x_{i,j} - x_{i-1,j}) & (x_{i,j} - x_{i,j-1}) \\ (y_{i,j} - y_{i-1,j}) & (y_{i,j} - y_{i,j-1}) \end{vmatrix} (\Delta a\Delta b)^{-1}.$$

One can then (for example) use <u>bilinear interpolations</u>* between the four members $\sigma_{i\pm\frac{1}{2},j\pm\frac{1}{2}}$, in (x,y)-space or (a,b)-space, to evaluate $\nabla\sigma_{ij}$. Substitution back into (24) gives a system of second-order ordinary DE's in the vectors (x_{ij},y_{ij}), in which the right-hand side involves all eight neighboring mesh-points.

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*Bilinear interpolation uses bilinear functions $\alpha + \beta x + \gamma y + \delta xy$ with undetermined coefficients.

Mechanical models. One can also derive a spatial discretization by mechanical analogy, placing a particle of mass m at each mesh-point, joining adjacent particles by impermeable but weightless straight rods free to lengthen or shorten longitudinally, and letting the "gas" in each quadrilateral area bounded by these rods expand and contract adiabatically. That is, if $N_{i',j'}$ $(i' = i-\frac{1}{2},\ j' = j-\frac{1}{2})$ is the area of the quadrilateral with vertices at $\underline{x}(a_{i'\pm\frac{1}{2}}, b_{j'\pm\frac{1}{2}}, t)$, then $p_{i',j'}(t) = p_o - F(N_{i',j'}/m)$ as in (23). One easily obtains formulas for the kinetic energy $T = \Sigma\, m_{ij}(\dot{x}_{ij}^2 + \dot{y}_{ij}^2)/2$ and the potential energy $V = \Sigma\, V_{i',j'} = -\Sigma \int p_{i',j'}\, dA_{i',j'}$ of such a system. If $p = k\rho^\gamma = p_o(A_o/A)^\gamma$ $(\gamma \neq 1)$, then $\int p dA = kA^{1-\gamma}/(1-\gamma)$ with $k = p_o A_o^\gamma$, for example. As in Lagrangian dynamical systems without external forces generally,* the equations of motion are then given variationally, by setting $d(\partial L/\partial \dot{q}_j)/dt = \partial L/\partial q_j$, where $L = T - V$. This model was suggested by one of the authors (Garrett Birkhoff, unpublished note, 1959).

A program for computing the motion of the preceding "synthetic fluid," with finite time-steps, has been devised by Walter Goad [25]. His method differs in several respects from an approximate method for a slightly different model suggested earlier by Harwood Kolsky [14]. It is not clear that, in the limit $\Delta t \downarrow 0$, Kolsky's model corresponds to a Lagrangian system. Lagrangian systems are not only esthetically satisfying, they have the advantage that they make $L(\underline{q},\dot{\underline{q}})$ constant in time,

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*For the continuum problem of § 14, similar variational formulations have been given by H. Bateman, "Partial differential equations," p. 164; Lamb, p. 188; P. Lush and T. Cherry QJMAM 9 (1956), 6-21.

thus providing a useful check on computations.

17. Shocks and viscosity. The primary aim of the computation schemes devised by Kolsky and Goad was to calculate approximately the motion of an elastic fluid, allowing for shock discontinuities. Much as in § 6, one does this by introducing a large so-called artificial viscosity, chosen so as to smooth out irregularities behind the shock while permitting a step shock front to propagate without change of form. We will now try to correlate such schemes with the concept of a viscous elastic fluid.

A viscous elastic fluid may be defined as a continuum in which the stress tensor (matrix) $||p_{ij}||$ is a single-valued linear function of the rate-of-strain tensor $||\partial u_i/\partial x_j||$ at any point. We consider below only homogeneous and isotropic viscous elastic fluids, which necessarily satisfy the Navier-Stokes equations.

Viscous effects in such fluids are known to be characterized by their shear viscosity μ and their bulk viscosity μ', material constants which depend on the temperature T and pressure p (the "state" (p,T)) of the fluid. To determine exactly the motion of a viscous elastic fluid, one must know its conductivity $k = k(p,T)$ as well as μ and μ'. In practice, one is satisfied with approximate results, and makes simplifying assumptions such as $\mu = \text{const.}$, $\mu' = 0$.

In compressible flow computations, one seldom attempts to simulate real physical viscosity at all. Instead, since the assumption $\mu > 0$ would give rise to the complication of no slip on solid boundaries, one tends rather to set $\mu = 0$ and to introduce a large artificial[*] bulk viscosity $\mu^* \gg \mu$ in calculating plane flows. Bulk viscosity also has the advantage over shear viscosity of introducing a scalar pressure stress, and not a symmetric tensor shear stress with three components, in plane flows. The whole purpose of μ^* is to smooth out "random" fluctuations behind shocks, and to make the calculated "shock thickness" a few mesh-lengths.

As stated, the real aim is thus to simulate an elastic fluid with shocks, in which the shocks satisfy Rankine-Hugoniot relations determined by a function $p(I,\sigma)$, expressing the pressure at any point as a function of the internal energy per unit mass of the fluid, I, and the local specific volume. In a perfect gas, $I = c_v T$ and $p = RT/\sigma = RI/c_v\sigma$.

In practice, this simulation has been successfully achieved in many cases, using finite time-steps Δt governed by variants of the Courant stability condition [14, p. 13]. It has the advantage over "shock fitting" that it treats all points alike. It has the disadvantage of requiring a second dependent variable (internal energy I or entropy S) to define the local "state" of the fluid.

18. The Kolsky-Goad fluid. To apply the computational methods of Kolsky and Goad to real materials, one must know both the pressure $p(\sigma,T)$ and the internal energy $I(\sigma,T)$ as functions of the variables σ,T. Especially, one must know $p(\sigma,I)$ across a single shock (the Hugoniot

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[*] Real bulk viscosity is subject to many anomalies; only in monatomic gas is Stokes' assumption $\mu' = 0$ justified.

curve of [26, p. 152]). For solids, this will depend on the effective Poisson ratio, which may be unknown under the conditions considered; see § 19. This uncertainty suggests a number of interesting questions.

It is also interesting to consider the "Kolsky-Goad fluid" defined by the mechanical model of § 16 as a synthetic material. For it to be stable, $p(\sigma)$ must be a decreasing function.

Though the microscopic appearance of this spatial discretization of (22)-(23) is quite unlike that of real liquids and gases, its macroscopic behavior is that of an elastic fluid. One wonders whether it might not be used, for example, to simulate real equations of state for gases and liquids, including phase-transition. For instance, if one defines the temperature T as the mean kinetic energy $m\overline{v^2}/2$ of translation of the particles, one can ask for $p(\sigma,T)$.

Due to the complications which arise when the quadrilateral areas A_{ij} become extremely distorted (which are also inconvenient in ordinary calculations), this may not be easy. But one wonders whether some modified scheme, perhaps using triangular or hexagonal areas and allowing unwanted rods to disappear and new rods to subdivide irregular areas, might not be successful in simulating the behavior of real gases and liquids. It must be confessed that other models for liquids* also fail to simulate real molecular physics in any detail.

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*E.g., the "free volume" and "hole" theories [17, § 4.4, § 4.8]. See also J. Frenkel, "Kinetic theory of liquids," Oxford, 1946; M. Born and H. S. Green, "A general kinetic theory of liquids," Cambridge Univ. Press, 1946.

19. Elastic solids. In continuum mechanics, one defines an elastic solid as a continuum in which the stress tensor $||p_{ij}||$ is a single-valued function of the strain tensor $||\partial x_i/\partial a_j||$. The theory of elastic solids is highly developed only for infinitesimal deformations from static equilibrium of homogeneous, isotropic media which have not been prestressed. One then assumes $||p_{ij}|| = 0$ if $\partial x_i/\partial a_j = \delta_{ij}$, and makes $||p_{ij}||$ depend linearly on the difference $||\partial x_i/\partial a_j|| - ||\delta_{ij}||$.

Under these assumptions, the elastic characteristics of a three-dimensional medium can be shown [21] to be characterized by a rigidity or shear modulus μ and a bulk modulus $\mu' = \lambda + (2\mu/3)$; the analogy with the viscosity coefficients is obvious. In the plane, one has $\mu' = \lambda + \mu$ instead.

It is frequently suggested that the equations of an elastic fluid can be substituted for those of elastic solids, in two cases: (i) in one-dimensional motion [5, §§ 3-5 and §§ 97-101], and (ii) in violent explosions, when stresses far exceed the yield point of the solid considered. However, this substitution must be employed with caution, because of ambiguity as to the relevant modulus of elasticity.

Thus, across a slab, the velocity of compressive acoustic waves is $[(\lambda + 2\mu)/\rho]^{\frac{1}{2}}$; along a bar, it is $[E/\rho]^{\frac{1}{2}}$ according to the simple theory, where [21, p. 42] $E = \mu\,[(3\lambda + 2\mu)/(\lambda + \mu)]$. For accurate results, edge corrections are needed [26, p. 33]. Likewise the triaxial stress required to produce a uniaxial strain $(\epsilon,0,0)$ is $(\lambda + 2\mu, \lambda, \lambda)\epsilon$, and this is very different from the hydrostatic pressure $(\lambda + 2\mu/3)\epsilon$ required to produce the same bulk compression. Thus for steel, in which $\mu/\lambda = 11/14$ because the Poisson ratio $\nu = \lambda/2(\lambda + \mu) = 0.28$ [26, p.154], the x-component of pressure, σ_{xx}, is nearly twice as great in the first case as in the second.

All this shows that elastic solids are much more complicated than fluids in their reactions to one-dimensional stresses.

As regards waves of finite amplitude, consider a shock front. Lateral contraction over the short transition-time would produce unbelievably large acceleration stresses; hence the compression-jump is almost surely uniaxial. In view of Bridgman's data* on the increase in shear strength under hydrostatic pressure and under rate of strain, how can one be sure that shear stresses (proportional to μ in the elastic range) are negligible?

Because of all these uncertainties, it seems desirable to explore the many kinds of matter which have been found in Nature, and molecular models for these kinds of matter. Besides elastic fluids and solids, we have already mentioned viscoelastic fluids and Maxwell solids. Viscoelastic and plastic solids should certainly also be considered. Perhaps one should also consider glasslike, rubberlike, and doughlike substances.** What about sand and sintered metals?

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*P. J. Bridgman, "Studies in large plastic flow and fracture," McGraw-Hill, 1952, esp. Ch. 16 (see also Ch. 12, where various complicated phenomena affecting volume changes are described).

**We follow the classification of R. Houwink, "Elasticity, plasticity, and structure of matter," 2d ed., Harren press, 1953. Houwink also points out distinctive mechanical properties of casein, starch, and clay. Sols, gels, paints, etc., have other peculiarities.

Against the background of this general philosophy, we will now explore a few very simple mass-spring models, which seem especially promising as possible substitutes for pure fluids in computation schemes which purport to approximate the motion of violently stressed solids.

20. Mass-spring networks. Mass-spring networks in the plane and in space have been studied since the time of Cauchy, as providing molecular models of elastic solids. In accordance with the terminology introduced earlier, one can think of them as defining synthetic crystals.

It is interesting to consider the mechanical properties of such synthetic crystals for their own sake, especially when one really wishes to simulate a solid. Following Cauchy and Kelvin, Brillouin [3] has investigated the propagation of waves through such systems connected by linear springs ($\gamma = -1$); however, for hydrodynamical computations, it seems more appropriate to choose $F(\sigma)$ to match p in (23) for uniform (hydrostatic) compression. For example, for $F(\sigma) = k\sigma^{-\gamma}$, one might consider the non-linear force-law $f(r) = -\alpha r^{-\delta}$. A simple dimensional analysis shows that this makes $\delta = 2\gamma - 1$; the relation between k and α depends on the type of crystal.

Simple networks. The simplest plane crystals have polygonal cells; the cases of squares, equilateral triangles, and regular hexagons are the most interesting. If, in a square (or hexagonal) network, each particle acts only on its 4 (or 3) immediate neighbors as indicated in Fig. 1, then the network is obviously unstable in compression,

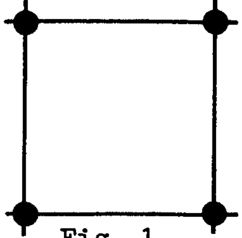

Fig. 1

because the area enclosed can be flattened without shortening the springs. Moreover, the equation of state for this model is not a function of specific volume — if the area of a cell goes to zero without shortening the springs, the pressure does not change.

Though unstable in compression, the square network defined above is stable in tension. This shows that the dynamic behavior of plane mass-spring systems may change when p_0 is changed in the equation of state simulated — even though this is not true of continuous fluids or for networks in one space dimension.

Braced square networks. Another synthetic crystal is defined by the diagonally braced square cell of Fig. 2. Each net point is connected with its 8 nearest neighbors. Though not necessarily isotropic, such crystals have two orthogonal "principal planes" of reflection symmetry. To compute the elastic constants of this model,* we suppose that the spring constants for the horizontal and vertical springs are a, while those for the diagonal springs are b. The associated stiffness constants are then a and $b/\sqrt{2}$, respectively.

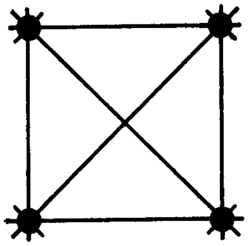

Fig. 2

The elastic moduli can be easily computed. We obtain $c_{11} = a + b$, $c_{12} = b$, and $c_{66} = b$. The stress-strain relation is given by

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*We use the notation of I. Sokolnikoff, "Theory of elasticity," second edition, McGraw-Hill, 1956.

$$(27)\qquad \begin{pmatrix}\tau_{11}\\ \tau_{22}\\ \tau_{12}\end{pmatrix} = \begin{pmatrix} a+b & b & 0\\ b & a+b & 0\\ 0 & 0 & b\end{pmatrix}\begin{pmatrix}\epsilon_{11}\\ \epsilon_{22}\\ \epsilon_{12}\end{pmatrix},$$

where τ_{ij} and ϵ_{ij} are components of stress and strain. The condition for isotropy is $c_{11} = c_{12} + 2c_{66}$; a mass-spring system of this type, in which $a = 2b$, is elastically isotropic. The Poisson ratio $\nu = b/(a + b)$ is 1/3 in the isotropic case as it should be, for reasons which will now be explained.

21. <u>Networks as spatial discretizations</u>. In one dimension, mass-spring systems define useful spatial discretizations of elastic solids (and fluids). It is natural to ask if this is also true in the plane (and in space).

As far as infinitesimal deformations of homogeneous isotropic solids are concerned, this question was partly answered by Cauchy. He assumed implicitly what may be called Cauchy's Hypothesis: that the mass-spring system remained in static equilibrium under any affine deformation. This is true, with central forces, for any crystal having central symmetry in all its mass-points — hence for all the models of § 20.

Under Cauchy's hypothesis, $\mu = \lambda$, which implies $\nu = 1/3$ in the plane (as above), and $\nu = 1/4$ in space. But experimentally, ν is far from 1/4 in many solids; thus for lead, $\nu = 0.45$ [26, p. 154].

It follows that one cannot approximate the behavior of most elastic solids by simple mass-spring networks centrally symmetric in every mass-point, even as far as plane waves of infinitesimal amplitude are concerned. In particular, the bulk modulus and shear (rigidity) modulus are proportional, so that one cannot easily simulate an elastic fluid. This is also true of the ionic crystals (with oppositely charged particles) used to simulate the alkali halides ([1], [2], [3]) — though various interesting properties of real crystals (e.g., "Brillouin zones") are simulated qualitatively.

Anisotropy. The mechanical behavior of synthetic crystals under small deformations is determined by their moduli of elasticity. Hence, the braced square network discussed earlier is elastically isotropic, even though no molecular model can be isotropic in all its physical properties. However, even elastic isotropy is lost under large deformations, a fact which makes it difficult to use synthetic crystals to simulate isotropic polycrystalline solids (like steel) with ν near 1/4.

Consider for example a simple synthetic crystal corresponding to a mass-spring network of equilateral triangles. Let the springs satisfy the force-law $f(r) = \alpha r^{-\delta}$. The pressure will then be $p = k \sigma^{-\gamma}$ if $\delta = 2\gamma - 1$ and if $\alpha = k(\sqrt{3}/4m)^{-\gamma}/\sqrt{3}$, where m is the mass of a "molecule."

Then, under large uniaxial compressions, one obtains the configuration of Fig. 3. It is easily verified that the horizontal stress τ_{11} and the vertical stress τ_{22} satisfy

$$\tau_{11} = \alpha \frac{2 + (1/2 \sec \beta)^{1-\delta}}{\csc \beta}$$

$$\tau_{22} = \alpha \frac{2(1/2 \sec \beta)^{-\delta} \sin \beta}{1}$$

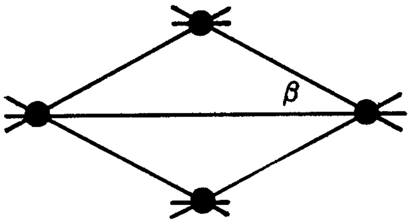

Fig. 3

Also this crystal is isotropic for infinitesimal deformations; it is highly non-isotropic (and unsuitable for hydrodynamical computations) as regards finite deformations.

Kinetic theory. As in the one-dimensional case, it would be interesting to compute equations of state for synthetic crystals subject to various force-laws, expressing the specific volume $\sigma = \sigma(p,T)$ as a function of the temperature. As in § 10, one would have to define T in terms of statistical equilibrium with a perfect gas at the stated temperature, and *not* in terms of the mean energy per particle. Expansion anisotropy could also be computed.

22. *Universal force-laws.* In the computation schemes and synthetic crystals discussed so far, forces have been assumed to act only between *preassigned* "near neighbors". It is, of course, more reasonable to let forces be determined entirely by the *distances* between the particle-pairs involved, irrespective of their initial locations. (For the small deformations of classical elasticity theory, to be sure, the distinction is largely academic.)

The artificial restriction of molecular forces to preassigned pairs of neighbors has been avoided by Born ([1], [2]) using Madelung's constants. However, he makes the equally artificial assumption of perfectly *periodic* displacements in calculating the mechanical properties of crystals. (Somewhat similarly, Cauchy and others have made calculations assuming that all particles except the one under consideration remained stationary.)

Only recently have genuine "kinetic theory" calculations been made, in which forces were allowed to act between arbitrary pairs of sufficiently near particles, by F. Harlow* and (for the model discussed in § 16) by Harwood Kolsky.**

However, Harlow's model uses central forces and a simple initial configuration; it seems likely that it has shear rigidity if it is isotropic. Moreover it retains the artificiality of not having a universal force-law, applicable to all sufficiently close particle-pairs. It would seem to us that the device of having a cutoff radius (depending on the entropies S or temperatures T of the particle-pairs involved) would be more logical and perhaps as effective computationally as restricting forces to a preassigned number of neighbors of each particle. This could be combined with an artificial conductivity, acting between "nearby" particle-pairs with $f_{ij} > 0$, so as to smooth out both shocks and irregularities due to particle diffusion.

Postulating forces with such a cutoff radius was originally suggested by Newton (loc. cit. in § 3). It avoids the possible paradox of infinite potential energy associated with distant particles, implicit in some universal force-laws. For instance, if $f(r) = kr^{-p}$ with $p \leqq 4$, then the volume integral $C\int r^{p-1}\, r^2 dr (C = 4\pi k/[p - 1])$ of probable potential energy of randomly distributed particles is infinite. This paradox

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*F. H. Harlow and B. D. Meixner, "The particle-and-force computing method for fluid dynamics," Report LAMS-2567, Los Alamos, 1961.

**H. Kolsky, "The nearest neighbor hydrodynamics calculation," Memo, dated July 1, 1961.

has been discussed by Maxwell (see [8, § 165]).

In the computation schemes of Harlow and Kolsky mentioned above, an artificial viscosity is introduced, and a time-dependent entropy is attributed to particles (or cells). It would be interesting to study the synthetic materials defined by the same models without viscosity, and to compute the equations of state $p(\sigma,T)$ and internal energy functions $I(\sigma,T)$ for the synthetic materials which they define. This can be regarded as an extension to the plane and to universal force-laws of the ideas introduced in § 11, for one-dimensional mass-spring systems.

Plastic solids. Under increasing shear strains, particle-and-force systems with universal force-laws behave somewhat like plastic solids. Consider for example the square network of § 20 with molecular spacing h and, for simplicity, a universal force-law with cutoff distance $d = 2h$. For small deformations from equilibrium, the system will behave like a braced square network. But if a shear strain is imposed which slides each m-th row through a distance $mh/2$, then symmetry shows that there will be static equilibrium (zero stress).

It would be interesting to try to simulate other features of plastic behavior by quasi-molecular particle-and-force systems. Especially, it would be interesting to determine the relations to large strains of ideal simple crystals corresponding to the fourteen Bravais lattices.*

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*C. K. Hel, "Introduction to solid state physics," Wiley, 1956, Ch. I. To simulate the effect of dislocations in imperfect crystals would clearly be harder. See R. Hill, "The mathematical theory of plasticity," Oxford, 1956, Ch. I.

23. PIC models. Perhaps the most novel scheme which has been used successfully to simulate an elastic fluid with shocks is the particle-in-cell or PIC computation scheme developed at Los Alamos by Harlow and his co-workers. As the usefulness of this scheme as a computational tool has been discussed in some detail in other reports,* we will consider here primarily the synthetic materials which its variants define. (The scheme now used in hydrodynamical computations evolved after extensive trial-and-error experiments with such variants.**)

To represent a homogeneous material, a box is supposed divided into square (or rectangular) cells, each of which contains a number $N_c(t)$ of identical particles. Each cell C has density $\rho_c = N_c$ (in suitable units) and pressure $p_c = f(N_c, I_c)$, where I_c is an internal energy depending on the past history of particles which have been in the cell. In the simple adiabatic case, we would have $p_c = f(N_c)$, but the various averaging processes used in actual PIC codes (KAREN, SUNBEAM, etc.) act like artificial viscosity in converting mechanical energy into heat.

An obvious peculiarity of the synthetic material defined by some such schemes is the instability of static equilibrium unless N_c is a half-integer. Unless the cells neighboring a given cell on each side contain the same number of particles, the cell will be accelerated. It follows that in any stable static array of particles, all "red" squares

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*See [13], [24], and F. H. Harlow, J. assoc. comp. mach. 4 (1957), 137-42.

**Described in earlier Los Alamos Reports LAMS-1956 and LAMS-2082.

of a checkerboard must contain the same number of particles, and so must all "black" squares. The converse is also true, which shows that static stability is possible if and only if the average density $\rho = \bar{N}_c$ is an integer or half-integer.

Obviously, the "diophantine" static instability described above becomes less serious as $\bar{N}_c$ increases. It is interesting to consider the behavior of PIC material in the limit $N_c \to \infty$. In one dimension this can be treated semi-analytically, taking the density $\rho(x,t)$ as dependent variable. Possibly convergence to the behavior of an elastic fluid can be proved in this way, taking the iterated limit as $N_c \to \infty$ and cell size tends to zero.

It has been shown [13, p. 16] that, in one dimension, the PIC material has an effective (bulk) viscosity $\mu' = \rho|\mu|s/2$ (s = cell length); the analogy with the formula $\mu = \rho c\bar{u}/3$ of the kinetic theory is obvious. On the other hand,* the natural shear viscosity is zero: the drag layer along slip boundaries is at most one cell wide, even if averaging is used.

The PIC material is highly non-linear (because of its "diophantine" behavior, remotely suggestive of quantum mechanics). Hence it would be interesting to compare the formula for bulk viscosity quoted above with <u>attenuation rates</u> for sinusoidal waves of variable frequency and amplitude, in directions parallel to cell boundaries and at a 45° angle with them.

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*F. Harlow, J. assoc. comp. mach. 4 (1957), p. 139.

24. <u>Synthetic materials testing</u>. As the number of "synthetic materials" proposed for hydrodynamic computations increases, the need for objective standards of comparison clearly grows. It seems to us that standard <u>materials testing</u> procedures used in mechanical engineering provide good precedents in this connection. (Only dynamic tests would ordinarily be of interest.)

Thus, in the linear range, one can derive moduli of elasticity and viscosity by studying the velocity of propagation and the rate of attenuation of plane waves in various directions. Explosions of highly compressed spheres, cubes (squares), etc., give some useful comparisons in the non-linear range. So do simple plane shocks, of varying intensity and moving with varying velocity.* Impact tests (say of high-speed rigid missiles), somewhat analogous to drop tests, could also be used.

But just as in the case of ordinary materials testing, the standardization of such a series of tests can probably best be decided by a committee. Therefore we will not elaborate further on the subject.

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*Though the problems which they attempt to solve are invariant under transformation to moving axes, the same is not true of digital Eulerian or quasi-Eulerian schemes, such as PIC.

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