LA-2806

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

THEORY OF CORRESPONDENCE BETWEEN FLUID DYNAMICS AND PARTICLE-AND-FORCE MODELS

Printed in USA. Price $ .75. Available from the

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

LA-2806
PHYSICS
TID-4500, 18th Ed.

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

REPORT WRITTEN: November 1962

REPORT DISTRIBUTED: January 17, 1963

THEORY OF CORRESPONDENCE BETWEEN FLUID DYNAMICS AND PARTICLE-AND-FORCE MODELS

by

Francis H. Harlow

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

ABSTRACT

Particle-and-Force models for high-speed-computer calculations of fluid dynamics problems have several conceptual advantages over most presently used techniques; in addition, test calculations with several versions have indicated considerable promise for wide application. For these reasons, the analysis presented here was undertaken to demonstrate the basis for expecting success in one class of such models (the completely statistical class) and in addition to show how to choose the interparticle force function to correspond to a given material equation of state. The method of analysis employs a many-particle distribution function equation whose reduction is accomplished through the assumption of two-body forces and of strong correlations with the mean. Primary results include correspondence equations between conservative force function and equation of state, and between dissipative force function and viscous stress. Solutions are given for the first type of correspondence equation, and comparisons are made with previous heuristic studies.

Introduction

In the pioneering work of Pasta and Ulam (1), it was shown that many features of the dynamics of fluids can be represented by a calculation of the trajectories of interacting particles, each representing a macroscopic fluid element. They studied in particular the problem of the instability at the interface between a heavy fluid falling into a lighter one, with the entire configuration resolved by only 256 points. The fluids were forced to move adiabatically, representing an unspecified equation of state; nevertheless, the results are surprisingly realistic and suggest that an extremely useful computing method could be derived as a generalization of their techniques.

One such generalization that has received considerable application is the Particle-in-Cell (PIC) method (2) in which the particle dynamics are controlled by calculations that refer to an Eulerian mesh of cells through which the particles move. Another is the Nearest-Neighbor method of Kolsky (3), an elaborate and promising technique for which actual computations are yet to be performed. Finally, there is the Particle-and-Force (PAF) method (4,5) for which preliminary tests have indicated potential usefulness.

Of these modified approaches, the PAF method is most like the original

procedure of Pasta and Ulam. More conservative is Kolsky's technique which, in effect, employs many-body forces among the particles, and for which he is able to give a direct, mechanical derivation of the relationship between the representation and the true fluid dynamics. The PIC method is likewise conservative, resembling the well-known Eulerian methods more closely than any other particle method. It is, however, intermediate between the Kolsky and PAF methods in that the accuracy of results depends to some extent upon the proper statistical averaging of some of its local variables (6); convergence and accuracy analysis is only partly mechanical and requires certain statistical assumptions. At the other extreme, the PAF method and its ancestral forms are in a certain sense completely statistical. This has the effect of rendering them capable of analysis, however, and the main purpose of this paper is to show how the methods of kinetic theory can be applied as a first step.

Dynamics of the Particles

Consider a set of particles labeled with indices i,j = 1 ... N, and characterized by coordinates $\vec{r}_j$ and velocities $\vec{u}_j$. For this discussion, they all have the same mass, m. The force exerted by particle #i onto particle #j is $\vec{F}_{ij}$, and is assumed to be a function only of the variables describing those two particles. It is further assumed that the appropriate dynamics of the model is described simply by the usual law of mechanics,

$$m \frac{d\vec{u}_j}{dt} = \sum_i^* \vec{F}_{ij}, \qquad (1)$$

where the * excludes the term i = j and may also restrict the sum to

certain neighbors of #j. The dynamics cannot follow completely the classical laws of particle mechanics, however, since the elements of fluid that the particles represent must have another degree of freedom to allow dissipative effects. It is not necessary to specify at this stage the precise form of this extra variable, except that we shall require it to be a function of the entropy of the element, only; it is here designated by φ_j. We shall, however, be required to derive a precise form for the equation of variation of φ_j, and in preparation, it is assumed that the force function can be separated into two parts,

$$\vec{F}_{ij} \equiv \vec{s}_{ij} f(r_{ij}, \varphi_{ij}) + \vec{g}_{ij} \equiv \vec{s}_{ij} f_{ij} + \vec{g}_{ij}, \tag{2}$$

where

$$r_{ij} \equiv \left| \vec{r}_i - \vec{r}_j \right|,$$

$$\vec{s}_{ij} \equiv \frac{(\vec{r}_j - \vec{r}_i)}{r_{ij}},$$

and φ_{ij} is the average of φ_i and φ_j.

The $\vec{g}_{ij}$ force is introduced only to produce dissipation, so that the φ_j values will change only in circumstances in which $\vec{g}_{ij}$ is nonzero. The dissipative force must therefore be velocity-dependent, must vanish if there are no velocity gradients, and indeed for translational invariance must depend upon velocity as a function of $\vec{u}_i - \vec{u}_j$ only.

To complete the dynamical description of the model, it is convenient to invoke the basic conservation laws from the viewpoint of fluid

dynamics. Conservation of mass is automatic; the particle masses are constant in time, and in addition the change of mass in any fixed volume exactly equals the amount flowing over the bounding surface. For conservation of momentum it can be shown that it is sufficient that $\vec{F}_{ij} \equiv -\vec{F}_{ji}$, from which it follows from Eq. (2) that $\varphi_{ij} \equiv \varphi_{ji}$ and $\vec{g}_{ij} \equiv -\vec{g}_{ji}$.

The energy conservation equation marks the point of departure from ordinary particle mechanics and furnishes the required equation for the changes of φ_j. Let $K_j \equiv (m/2)\vec{u}_j \cdot \vec{u}_j$ be the kinetic energy of particle #j, while J_j is its internal energy. The basis for the energy discussion is that the rate of change of energy of a particle should be given by the rate that the other particles do work on it. This work rate is in turn given by the product of force by velocity. Overall conservation will require antisymmetry of this work flux, so that the velocity which carries it must be the average from the two particles. Thus we write

$$\frac{d}{dt}\left(K_j + J_j\right) = \sum_i{}^{*} \vec{F}_{ij} \cdot \left(\frac{\vec{u}_i + \vec{u}_j}{2}\right). \tag{3}$$

It follows, as required, that the energy of any subset of particles changes only through work done on it by external particles.

Now, by definition

$$\frac{dK_j}{dt} = m\vec{u}_j \cdot \frac{d\vec{u}_j}{dt} = \vec{u}_j \cdot \sum_i{}^{*} \vec{F}_{ij},$$

which, in combination with Eqs. (2) and (3), can be put into the form

$$\frac{dJ_j}{dt} = -\frac{1}{2}\sum_i^* f_{ij}\frac{dr_{ij}}{dt} + \frac{1}{2}\sum_i^* \vec{g}_{ij}\cdot(\vec{u}_i - \vec{u}_j). \tag{4}$$

This in turn may be compared with the identity

$$\frac{dJ_j}{dt} \equiv \sum_i^* \frac{1}{2}\frac{dJ_{ij}}{dt}$$

$$\equiv \sum_i^* \frac{1}{2}\left[\frac{\partial J_{ij}}{\partial r_{ij}}\frac{dr_{ij}}{dt} + \frac{\partial J_{ij}}{\partial \varphi_{ij}}\frac{d\varphi_{ij}}{dt}\right],$$

in which J_{ij} is the total internal energy of the ij pair, half of which is assigned to each particle.

This comparison shows that the internal energy of a particle changes according to two processes, one having to do with coordinate variations and the other with φ variations. The first change is of the potential energy relative to surrounding particles, while the second, referring to entropy changes, suggests that φ_j can now be set equal to the entropy itself. Using the first law of thermodynamics, we are led to the result

$$mT_j\frac{d\varphi_j}{dt} = \frac{1}{2}\sum_i^* \vec{g}_{ij}\cdot(\vec{u}_i - \vec{u}_j). \tag{5}$$

The temperature, T_j, is considered to be a function of φ_j and of the mean interparticle spacing, which dependence need not be further discussed here. We see as a consequent restriction that because φ_j must increase monotonically in time, the dissipative part of the force must be such that $\vec{g}_{ij}\cdot(\vec{u}_i - \vec{u}_j)$ is positive definite.

To proceed, now, to describe an actual computing method, it would be

necessary to prescribe in detail the forms of f_{ij} and $\vec{g}_{ij}$, to set up a technique for finite-difference time advancement consistent with stability and accuracy requirements, and to determine the appropriate manner by which initial and boundary conditions could be incorporated. An example of these, together with discussions of results and interpretations, is given in reference 4. There, however, choice of the force function, f_{ij}, was made on a very loose basis, whereas here it will be seen that the nature of this function can be related to expressions for the continuum equation of state in a more satisfactory manner by the statistical analysis. The choice of $\vec{g}_{ij}$ in reference 4 was likewise not based on rigorous arguments, but again the statistical treatment shows how the force can be related to viscous forces (real or "artificial").

Statistical Analysis of Particle Representations

It is known from the start that a particle calculation with only two-body forces cannot exactly represent the dynamics of a fluid. In reality, the force exerted by one element onto another must depend upon the relationship of the first element to all of its neighbors; the more it is compressed by closeness of those neighbors, the greater will be the force it exerts. In a PAF-like method, however, there is no provision for this effect to be accurately represented at every instant. (In contrast, the Kolsky method with its many-body forces can properly represent the effect.) The only hope, then, for PAF-like methods is that the representation is good in some statistical sense. If this can be demonstrated, the numerous advantages of a PAF-like method can then be exploited.

The procedure for determining whether or not the statistical averaging does give a proper representation can be outlined as follows. The starting point is a generalized Liouville equation appropriate to the study of the probable distribution of a set of dissipative particles. This is then reduced by the well-known integration method to the one-particle distribution-function equation which involves integrals of the two-particle function. (This complete reduction can be carried through only as a result of the two-body force assumption.) The resulting equation is exact, but a study of its moments, from which the fluid-dynamic analogy is observed, requires some simplifying assumptions. In essence, these assumptions are, first, that there are strong interparticle correlations and, second, that there are strong correlations between individual characteristics and those of the local mean. Surely if the particles are to represent macroscopic elements of fluid, then these assumptions must be good. Our results then show that the use of these assumptions allows the force-function conditions to be derived such that the particle representation of the fluid dynamics is indeed statistically valid. Stated in other words, this means that if a choice of technique can be found such that each particle follows closely the local mean of motion (with no interpenetrations, strong oscillations, etc.), and if the force functions are properly chosen, the results should statistically represent the fluid dynamics as desired. The remainder of this section shows how this analysis can be accomplished in detail.

The basic entity for the discussion is the distribution function for

the N particles, $z_N(\vec{r}_1 \cdots \vec{r}_N, \vec{u}_1 \cdots \vec{u}_N, \varphi_1 \cdots \varphi_N, t)$, which is the joint probability density at time t for finding the particles in a configuration characterized by the specified variables. Normalization is such that integration over the allowed ranges of all the particle variables gives N!, independent of time. (Normalization was chosen to be N! rather than N or unity in order to conveniently count the permutations of the identical particles.) From z_N there can be derived subset distribution functions

$$z_n\left(\vec{r}_1 \cdots \vec{r}_n, \vec{u}_1 \cdots \vec{u}_n, \varphi_1 \cdots \varphi_n, t\right)$$

$$= \frac{1}{(N-n)!} \int d\vec{r}_{n+1} \cdots \int d\vec{r}_N \int d\vec{u}_{n+1} \cdots \int d\vec{u}_N \int d\varphi_{n+1} \cdots \int d\varphi_N z_N,$$

and in particular we shall be concerned with z_1 and z_2.

In the generalized $\vec{r}$, $\vec{u}$, φ space through which the particles move, one can imagine a closed surface defined to move in such a way that every point follows a particle trajectory allowable by the dynamics. Such a surface must then contain a fixed number of particles, so that the time derivative of the integral of z_N over all particle variables within the ranges contained by such a surface must vanish. Since this must be true for any arbitrary initial choice of surface, it follows that the integrand obtained from the time differentation must vanish, leading to the generalized Liouville equation

$$\frac{\partial z_N}{\partial t} + \sum_{j=1}^{N} \left[\nabla_{\vec{r}_j} \cdot \left(z_N \frac{d\vec{r}_j}{dt} \right) + \nabla_{\vec{u}_j} \cdot \left(z_N \frac{d\vec{u}_j}{dt} \right) + \frac{\partial}{\partial \varphi_j} \left(z_N \frac{d\varphi_j}{dt} \right) \right] = 0,$$

where the subscripts of the divergence operators give the coordinates of variation, and the total time derivatives are constrained to refer to trajectories allowed by the dynamics. These trajectory constraints are just those derived in the preceding section, Eqs. (1) and (5), plus the velocity definition, $\vec{u}_j \equiv d\vec{r}_j/dt$. With these, the Liouville equation becomes

$$\frac{\partial z_N}{\partial t} + \sum_{j=1}^{N} \vec{u}_j \cdot \nabla_{\vec{r}_j} z_N$$

$$+ \sum_{j=1}^{N} \sum_{i}^{*} \left\{ \nabla_{\vec{u}_j} \cdot \left[\frac{z_N}{m} \left(\vec{s}_{ij} f_{ij} + \vec{g}_{ij} \right) \right] + \frac{\partial}{\partial \varphi_j} \left[\frac{z_N}{2mT_j} \vec{g}_{ij} \cdot \left(\vec{u}_i - \vec{u}_j \right) \right] \right\} = 0.$$

To reduce this equation to a usable form, integrate over the complete ranges of the variables of all the particles except #1 and impose the condition that there must be no flux of probability across the extremities of those ranges. Then, after some manipulation, there is obtained the reduced Liouville equation for the one-particle distribution function,

$$\frac{\partial z_1}{\partial t} + \vec{u}_1 \cdot \nabla_{\vec{r}_1} z_1$$

$$+ \int d\vec{r}_2 \int d\vec{u}_2 \int d\varphi_2 \left\{ \nabla_{\vec{u}_1} \cdot \left[\frac{z_2}{m} \left(\vec{s}_{21} f_{21} + \vec{g}_{21} \right) \right] + \frac{\partial}{\partial \varphi_1} \left[\frac{z_2}{2mT_1} \vec{g}_{21} \cdot \left(\vec{u}_2 - \vec{u}_1 \right) \right] \right\} = 0. \tag{6}$$

The first of the two strong-correlation assumptions, which asserts that two neighboring particles must not differ by much in their variables,

can be expressed in the form

$$z_2(\vec{r}_1,\vec{r}_2,\vec{u}_1,\vec{u}_2,\varphi_1,\varphi_2,t)$$
$$\equiv z_1(\vec{r}_1,\vec{u}_1,\varphi_1,t)\rho(\vec{r}_2,t)\sigma(\rho_{12},\varphi_{12},r_{12})\delta(\vec{u}_2 - \vec{u}_1 - \vec{\alpha}_{12})\delta(\varphi_2 - \varphi_1 - \beta_{12})$$
$$+ z_2' \tag{7}$$

In this expression, $\rho(\vec{r},t)$ is the local number density of particles, defined by

$$\rho(\vec{r},t) \equiv \int d\vec{u} \int d\varphi \; z_1(\vec{r},\vec{u},\varphi,t), \tag{8}$$

while $\sigma(\rho_{12},\varphi_{12},r_{12})$ is a radial function, yet to be specified, which vanishes outside of the range of interparticle forces; ρ_{12} denotes the average density between the particles. z_2', on the other hand, is that part of the two-particle function which is important only outside the range of interparticle forces; indeed, we shall assume that its product with the force function vanishes everywhere. The δ-functions are the usual Dirac entities, while $\vec{\alpha}_{12}$ and β_{12} are small quantities representing the expected mean differences in velocity and entropy between the particles. The first approximations for them would be

$$\vec{\alpha}_{12} = \left[(\vec{r}_2 - \vec{r}_1)\cdot\nabla_{\vec{r}_1}\right]\bar{\vec{u}}, \tag{9}$$

$$\beta_{12} = \left[(\vec{r}_2 - \vec{r}_1)\cdot\nabla_{\vec{r}_1}\right]\bar{\varphi}, \tag{10}$$

where $\bar{\vec{u}}$ and $\bar{\varphi}$ are the local means of these quantities, that is,

$$\rho\bar{\vec{u}} \equiv \int d\vec{u} \int d\varphi \; \vec{u}\, z_1(\vec{r},\vec{u},\varphi,t), \tag{11}$$

$$\rho\bar{\varphi} \equiv \int d\vec{u} \int d\varphi\ \varphi\ z_1(\vec{r},\vec{u},\varphi,t), \tag{12}$$

so that they both are functions of $\vec{r}$ and t. This first approximation will turn out to be adequate for β_{12} but not for $\vec{\alpha}_{12}$; the reason for this is explained in the text following Eq. (23). Apparent lack of interchange symmetry in Eq. (7) will be resolved by restrictions on the form of z_1.

Substitution of Eq. (7) into Eq. (6) results in the equation

$$\frac{\partial z}{\partial t} + \vec{u}\cdot\nabla_{\vec{r}} z + \nabla_{\vec{u}}\cdot(\vec{P}z) + \frac{\partial Q z}{\partial \varphi} = 0, \tag{13}$$

in which the subscripts have been dropped from z_1, $\vec{u}_1$, $\vec{\varphi}_1$, and $\vec{r}_1$, and

$$P \equiv \frac{1}{m}\int d\vec{r}_2 \int d\vec{u}_2 \int d\varphi_2 (\vec{s}_{21} f_{21} + \vec{g}_{21})\rho(\vec{r}_2)\sigma(\rho_{12},\varphi_{12},r_{12}) \tag{14}$$
$$\times\ \delta(\vec{u}_2 - \vec{u}_1 - \vec{\alpha}_{12})\delta(\varphi_2 - \varphi_1 - \beta_{12}),$$

$$Q \equiv \frac{1}{2mT_1}\int d\vec{r}_2 \int d\vec{u}_2 \int d\varphi_2\ \vec{g}_{21}\cdot(\vec{u}_2 - \vec{u}_1)\rho(\vec{r}_2)\sigma(\rho_{12},\varphi_{12},r_{12}) \tag{15}$$
$$\times\ \delta(\vec{u}_2 - \vec{u}_1 - \vec{\alpha}_{12})\delta(\varphi_2 - \varphi_1 - \beta_{12}).$$

Note that z_2' does not appear.

The second of the two strong-correlation assumptions states that the instantaneous velocity and entropy of any particle differ inappreciably from their local means; mathematically,

$$z_1(\vec{r},\vec{u},\varphi,t) = \rho(\vec{r},t)\delta(\vec{u} - \bar{\vec{u}})\delta(\varphi - \bar{\varphi}). \tag{16}$$

It can be shown that this choice for z_1 makes z_2 symmetric as required.

It is useful to consider the normalization properties of z_2 and z_1

in the forms given by the strong correlation assumption. Thus, we must have

$$\iiint z_2 \, d\vec{r}_2 \, d\vec{u}_2 \, d\varphi_2 \equiv (N - 1) z_1,$$

$$\iiint z_1 \, d\vec{r}_1 \, d\vec{u}_1 \, d\varphi_1 \equiv N.$$

From Eq. (16) it is seen that the second normalization requirement becomes

$$\int \rho(\vec{r}) \, d\vec{r} = N,$$

which only demonstrates consistency and gives no added information. With Eq. (7), the first normalization condition becomes

$$\frac{1}{z_1} \iiint z_2' \, d\vec{r}_2 \, d\vec{u}_2 \, d\varphi_2 + \int \rho(\vec{r}_2) \, \sigma(\rho_{12}, \varphi_1 + \frac{1}{2} \beta_{12}, r_{12}) \, d\vec{r}_2 = N - 1.$$

Now z_2' is considered to vanish within some region about particle #1, while σ vanishes outside that region. Furthermore, in the region in which z_2' does not vanish, we may suppose that the two-particle correlation is weak, so that $z_2' = z_1(1) \, z_1(2)$, which nomenclature signifies the product of the separate one-particle functions. Thus the normalization on z_2 becomes

$$\int \rho(\vec{r}_2) \, d\vec{r}_2 + \int \rho(\vec{r}_2) \, \sigma(\rho_{12}, \varphi_1 + \frac{1}{2} \beta_{12}, r_{12}) d\vec{r}_2 = N - 1.$$

The primed integration is over the exterior region, and thus equals $N - (N^* + 1)$, where N^* is the number of neighbors of particle #1 implied by the * sum of Eq. (1). It therefore follows that

$$\int \rho(\vec{r}_2) \, \sigma(\rho_{12}, \varphi_1 + \frac{1}{2} \beta_{12}, r_{12}) \, d\vec{r}_2 = N^*.$$

To lowest order, then

$$4\pi \int_0^\infty r^2 \rho\sigma(\rho,\varphi,r)\, dr = N^*,$$

which implies that σ is a function of $r^3\rho$ only, together with the condition

$$\frac{4\pi}{3} \int_0^\nu \sigma(\xi)\, d\xi = N^*.$$

Here ν is the cutoff value of ρr^3 beyond which σ vanishes. Since the corresponding radius must include $N^* + 1$ particles, we obtain for ν the value

$$\nu = \frac{3}{4\pi}(N^* + 1).$$

This completes the preparation for the transition from particle dynamics to fluid dynamics. The treatment resembles that used in the kinetic theory of gases, but differs in several essential respects. In particular, the two strong-correlation assumptions, both of which are appropriate to the present situation (and indeed are essential properties of the particle dynamics if the fluid-dynamics analogy is to be valid), will be seen to remove from the statistics those fluctuations which in gas dynamics produce internal energy, heat transport, viscosity, diffusion, etc. These have, instead, been replaced by force functions which return the missing gas properties, but in a manner appropriate to the correlated motions of macroscopic fluid elements. Still missing from the present treatment are the phenomena of heat conduction and diffusion. At least the former (and perhaps the latter) could be included in the present model by addition of

appropriate interparticle fluxes.

The next step, now, is to make the actual transition to fluid dynamics. This is accomplished by taking appropriate moments of Eq. (13), in which z_1 is of the form given in Eq. (16). The simplest moment is obtained by integration of Eq. (13) over $\vec{u}$ and φ. The result is the fluid-dynamics mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla_{\vec{r}} \cdot (\rho \bar{\vec{u}}) = 0. \tag{17}$$

This result, which could as well have been obtained from Eq. (6), does not depend upon the strong-correlation assumptions.

Next is the velocity moment which, after some manipulation, reduces to

$$\frac{\partial \rho \bar{\vec{u}}}{\partial t} + \nabla_{\vec{r}} \cdot (\rho \bar{\vec{u}} \bar{\vec{u}}) = \rho \bar{\vec{P}}, \tag{18}$$

in which $\bar{\vec{P}}$ means $\vec{P}$ evaluated at $\vec{u} = \bar{\vec{u}}$ and $\varphi = \bar{\varphi}$. Here the consequences of the strong-correlation assumptions are clearly manifested in the absence of the gas-dynamics fluctuation pressure.

Finally, the φ moment of Eq. (13) can be put into the form

$$\frac{\partial \rho \bar{\varphi}}{\partial t} + \nabla_{\vec{r}} \cdot (\rho \bar{\vec{u}} \bar{\varphi}) = \rho \bar{Q}, \tag{19}$$

where $\bar{Q}$ means Q evaluated at $\vec{u} = \bar{\vec{u}}$ and $\varphi = \bar{\varphi}$. As expected, this shows that the entropy will change along the motion of a fluid element if and only if the dissipative force, $\vec{g}_{ij}$, is nonzero.

The next step is the reduction of $\rho \bar{\vec{P}}$ and $\rho \bar{Q}$ to more meaningful forms.

from which, for example, the relationship between equation of state and force function can be derived. To proceed, it is necessary to examine the force functions in somewhat more detail. The nondissipative force has already been specified to be of the form $f_{ij} = f(r_{ij},\varphi_{ij})$; in addition the dissipative force is now specified to be of the form $\vec{g}_{ij} \equiv \vec{g}(r_{ij},\vec{s}_{ij},\varphi_{ij},\vec{u}_i - \vec{u}_j)$, which is the most general form consistent with symmetry and invariance requirements.

Substitution into Eqs. (14) and (15) and insertion of mean values for $\vec{u}$ and φ result in the equations

$$\vec{\vec{P}} = \frac{1}{m}\int d\vec{r}_2 \left[\vec{s}_{21} f(r_{12},\bar{\varphi} + \frac{1}{2}\beta_{12}) + \vec{g}(r_{12},\vec{s}_{21},\bar{\varphi} + \frac{1}{2}\beta_{12},\alpha_{12})\right] \times \rho(\vec{r}_2)\ \sigma(\rho_{12},\bar{\varphi} + \frac{1}{2}\beta_{12},r_{12}), \tag{20}$$

$$\bar{Q} = \frac{1}{2mT_1}\int d\vec{r}_2 \vec{g}(r_{12},\vec{s}_{21},\bar{\varphi} + \frac{1}{2}\beta_{12},\vec{\alpha}_{12})\cdot\vec{\alpha}_{12}\rho(\vec{r}_2)\ \sigma(\rho_{12},\varphi + \frac{1}{2}\beta_{12},r_{12}). \tag{21}$$

In the integrand, those quantities not depending on the position of particle #2 are no longer subscripted, consistent with the dropping of subscripts in the moment equations.

Consider, further, the integral in Eq. (20). It can be reduced through the expansions

$$f(r_{12},\bar{\varphi} + \frac{1}{2}\beta_{12}) = f + \frac{1}{2}\beta_{12}\frac{\partial f}{\partial \bar{\varphi}},$$

$$\vec{g}(r_{12},\vec{s}_{21},\bar{\varphi} + \frac{1}{2}\beta_{12},\vec{\alpha}_{12}) = \vec{g} + \frac{1}{2}\beta_{12}\frac{\partial \vec{g}}{\partial \bar{\varphi}} + \vec{\alpha}_{12}\cdot\left(\nabla_{\vec{\alpha}}\vec{g}\right),$$

$$\rho(\vec{r}_2) = \rho + r_{12}\vec{s}_{12}\cdot\left(\nabla_{\vec{r}}\rho\right),$$

$$\sigma(\rho_{12},\bar{\varphi} + \frac{1}{2}\beta_{12},r_{12}) = \sigma + \frac{1}{2} r_{12}\vec{s}_{12}\cdot\left(\nabla_{\vec{r}}\rho\right)\left(\frac{\partial\sigma}{\partial\rho}\right) + \frac{1}{2}\beta_{12}\frac{\partial\sigma}{\partial\bar{\varphi}},$$

in which the functions $f,\vec{g}$, and σ on the right are evaluated at $\beta_{12} = 0$, $\vec{\alpha}_{12} = 0$, and $\vec{r}_2 = \vec{r}_1$ (except that they remain functions of r_{12} in their explicit dependence on that variable). The subsequent lengthy manipulation consists of evaluating the angular parts of the integrations and the collecting of terms, all leading to the result

$$\rho\vec{\bar{P}} = -\nabla_{\vec{r}}\left\{\frac{2\pi\rho^2(\vec{r})}{3m}\int_0^\infty r^3\sigma[\rho(\vec{r}),\bar{\varphi}(\vec{r}),r]\ f[r,\bar{\varphi}(\vec{r})]\ dr\right\}$$

$$+\frac{\rho^2(\vec{r})}{m}\int\sigma[\rho(\vec{r}),\bar{\varphi}(\vec{r}),r]\ \vec{\alpha}_{12}\cdot\left(\nabla_{\vec{\alpha}}\vec{g}\right)\ d\vec{r}_2.$$

The second integral can be further reduced through the assumption that

$$\vec{g} = \vec{\alpha}_{12}\ G(r_{12},\bar{\varphi}) + \vec{s}_{21}(\vec{s}_{21}\cdot\vec{\alpha}_{12})\ H(r_{12},\bar{\varphi}). \qquad (22)$$

The first term is directed along the line of velocity difference while the second is along the interparticle line. The first term does not necessarily conserve angular momentum microscopically while the second one does. This expression for $\vec{g}$ is the most general reasonable combination to first order in velocity differences. We now let

$$\vec{\alpha} = \left(r_{12}\vec{s}_{12}\cdot\nabla_{\vec{r}}\right)\vec{\bar{u}} + \frac{1}{2}\left(r_{12}\vec{s}_{12}\cdot\nabla_{\vec{r}}\right)^2\vec{\bar{u}}\ , \qquad (23)$$

which contains the next step in the expansion beyond that in Eq. (9), retained because all integrals vanish identically when only the first step is included. A further lengthy but straightforward set of angular integrations reduces the expression for $\rho\vec{\bar{P}}$ to its final form

$$\rho\vec{P} = -\nabla_{\vec{r}}\left\{\frac{2\pi\rho^2(\vec{r})}{3m}\int_0^\infty x^3\sigma[x^3\rho(\vec{r})]\ f[x,\bar{\varphi}(\vec{r})]\ dx\right\}$$
$$+ (\lambda+\mu)\ \nabla_{\vec{r}}\left(\nabla_{\vec{r}}\cdot\vec{u}\right) + \mu\ \nabla^2_{\vec{r}}\ \vec{u}, \tag{24}$$

in which

$$\mu \equiv \frac{2\pi\rho^2(\vec{r})}{15\ m}\int_0^\infty x^4\sigma[x^3\rho(\vec{r})]\ (5G + H)\ dx, \tag{25}$$

$$\lambda + \mu \equiv \frac{4\pi\rho^2(\vec{r})}{15\ m}\int_0^\infty x^4\sigma[x^3\rho(\vec{r})]\ H\ dx. \tag{26}$$

The normalization result has been incorporated into the form of σ, and x is a dummy integration variable. The brace factor in Eq. (24) is the pressure given by the equation of state as $p(\rho,\bar{\varphi})$, while μ is the first viscosity coefficient and $\lambda + 2\mu/3$ is the second.

We have seen that $\sigma(\xi) = 0$ for $\xi > \nu = (3/4\pi)(N^* + 1)$; presumably $\sigma(\xi) \to 0$ as $\xi \to 0$. We thus take, as a first approximation,

$$\sigma(\xi) = \sigma \equiv \text{const for } \zeta < \xi < \nu,$$

$$= 0 \quad \text{otherwise,}$$

where σ and ζ are determined by

$$\frac{4\pi}{3}\int_0^\zeta \sigma d\xi = 1,$$

$$\frac{4\pi}{3}\int_\zeta^\nu \sigma d\xi = N^*.$$

This, then, gives $\sigma = 1$, $\zeta = 3/4\pi$.

We thus have the integral equation to solve:

$$\frac{2\pi\rho^2}{3m}\int_{x_1}^{x_2} x^3 f(x,\varphi)\,dx = p(\rho,\varphi), \tag{27}$$

where $x_1 \equiv (3/4\pi\rho)^{1/3}$ and $x_2 = [3(N^* + 1)/4\pi\rho]^{1/3}$; the result is the correspondence between force function and equation of state. Note that this equation applies to calculations in three space dimensions. An analogous derivation for two space dimensions results in a similar correspondence equation

$$\frac{\pi\rho^2}{2m}\int_{x_1}^{x_2} x^2 f(x,\varphi)\,dx = p(\rho,\varphi), \tag{28}$$

in which we now have $x_1 = (1/\rho\pi)^{1/2}$ and $x_2 = [(N^* + 1)/\rho\pi]^{1/2}$.

Before discussing the solution of these integral equations, it is useful to consider two aspects of their derivation. The first concerns interpretation of N^*, the number of neighbors of a particle. If these neighbors were chosen to include all within a certain <u>fixed</u> prescribed radius, then our assumption of two-body forces in the Liouville equation reduction would indeed be valid. In that case, however, N^* would be a function of density, and the subsequent analysis would not be strictly correct. On the other hand, if N^* were to include a <u>fixed</u> number of <u>nearest</u> neighbors, then the two-body force assumption would no longer be strictly valid, and the reduction itself would give only an approximation. In either interpretation, however, the inaccuracies must be small since the results as applied to polytropic gases have proved to be good, both

in conceptual form and in accuracy of application.

The second aspect of the derivation concerns the meaning of φ, to which a correspondence with entropy has been assumed. A review of the derivations shows that this correspondence is required only in the analysis of the dissipative part of the interparticle forces. Insofar as the equation-of-state correspondence is concerned, as given in Eq. (27) or Eq. (28), φ could be <u>any</u> appropriate second variable in the equation of state. In particular, we shall find it convenient (and in some respects even <u>necessary</u>) to interpret φ as the specific internal energy, the reason being that only with that association can energy be rigorously conserved in the finite-time-interval solution of the particle-dynamics equations.

Consider, now, the solution of Eq. (27) for a polytropic gas. First, with $\varphi \equiv$ entropy, we have

$$p = A\rho^{\gamma} e^{\varphi/c_v},$$

in which c_v is the specific heat and A is a constant. The solution for f is then

$$f(x,\varphi) = Kx^{2-3\gamma} e^{\varphi/c_v},$$

in which

$$K = \frac{9mA(2-\gamma)}{2\pi\left\{\left[\frac{3(N^*+1)}{4\pi}\right]^{2-\gamma} - \left[\frac{3}{4\pi}\right]^{2-\gamma}\right\}}.$$

This is a generalization of a result given previously (reference 7,

page 37), which had been derived from simple energy considerations. If, however, $\varphi \equiv$ specific internal energy, then

$$p = (\gamma - 1)\, \rho\varphi,$$

and the solution for f is

$$f = \frac{2\eta m}{N^*} (\gamma - 1)\, \frac{\varphi}{x}\,, \tag{29}$$

in which η is the number of dimensions. [This is, in other words, the solution of both Eq. (27) for which $\eta = 3$ and Eq. (28) for which $\eta = 2$.] Comparison with other previous results (reference 4, page 25) shows exact agreement if one chooses $N^* = 2\eta$ (as was indeed specified in that reference, page 23, for the primary number of neighbors).

To find the general solution for Eq. (27) or Eq. (28), consider the problem of solving for $\Phi(x,\varphi)$ the equation

$$\int_{\Omega}^{k\Omega} \Phi(y,\varphi)\, dy = \psi(\Omega,\varphi).$$

The two equations of interest are both special cases of this, and can be identified with it by the proper choices of Φ, ψ, Ω, and k. Note in particular that for Eq. (27), $k = (N^* + 1)^{1/3}$, while for Eq. (28), $k = (N^* + 1)^{1/2}$. In both cases, therefore, $k > 1$. By differentiation, the equation becomes

$$k\Phi(k\Omega) - \Phi(\Omega) = \frac{d\psi}{d\Omega}\,,$$

from which it follows that

$$\Phi(\Omega) = \frac{1}{k^n}\,\Phi\left(\frac{\Omega}{k^n}\right) + \sum_{j=1}^{n} \frac{d\psi(\Omega k^{-j})}{d\Omega},$$

where n is any positive integer. In many circumstances, the equation of state will be such that we may let $\eta \to \infty$ and arrive at the solution

$$\Phi(\Omega,\varphi) = \frac{d}{d\Omega}\sum_{j=1}^{\infty} \psi(\Omega k^{-j},\varphi). \tag{30}$$

As an example, consider Eq. (28) with a polytropic gas in which φ is specific internal energy. This leads to the identities

$$\Omega \equiv (1/\rho\pi)^{1/2},$$

$$\psi(\Omega) \equiv 2m(\gamma - 1)\,\Omega^2,$$

$$\Phi(y,\varphi) \equiv y^2 f(y,\varphi),$$

$$k \equiv (N^* + 1)^{1/2},$$

and the solution

$$f(\Omega,\varphi) = \frac{4m(\gamma - 1)\varphi}{\Omega}\sum_{j=1}^{\infty} \frac{1}{k^{2j}}\,.$$

The sum converges to the value $1/N^*$ so that the result agrees exactly with that of Eq. (29).

In general, for two dimensions

$$\Omega \equiv (1/\rho\pi)^{1/2},$$

$$\psi(\Omega,\varphi) \equiv 2m\pi\,\Omega^4 p\left(\frac{1}{\pi\Omega^2},\varphi\right),$$

$$\Phi(y,\varphi) \equiv y^2 f(y,\varphi),$$

$$k \equiv (N^* + 1)^{1/2} ,$$

while for three dimensions,

$$\Omega = (3/4\pi\rho)^{1/3},$$

$$\psi(\Omega,\varphi) = \frac{8}{3}\, \pi m\, \Omega^6\, p\left(\frac{3}{4\pi\Omega^3},\varphi\right) ,$$

$$\Phi(y,\varphi) = y^3 f(y,\varphi),$$

$$k = (N^* + 1)^{1/3}.$$

Note that in both cases, a requirement for convergence of the sum in Eq. (30) is that $p/\rho^2 \to 0$ as $\rho \to \infty$, a requirement satisfied by all gases under ordinary circumstances. Materials whose equations of state do not satisfy this criterion will require alternative methods for solution of the correspondence equation.

Conclusions

It has been shown that if a Particle-and-Force computing method with two-body forces can accomplish strong correlations between particles and of each particle with the local mean, then the use of a force function given by the correspondence equation can result in statistical representation of the true dynamics of a fluid. In addition, if some prescribed dissipative force is required to accomplish the correlations, then the analysis shows the relation of this to viscous stress (true or "artificial"); or conversely, if a certain viscous effect is desired, the

corresponding dissipative force can be derived.

Derivation of an actual working method requires considerably more than the statistical analysis presented here; some preliminary efforts have been described in the references, and at present Group T-3 of this Laboratory is engaged in a program of development which will be reported later.

REFERENCES

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

2. F. H. Harlow, D. O. Dickman, D. E. Harris, Jr., and R. E. Martin, "Two-Dimensional Hydrodynamic Calculations," Los Alamos Scientific Laboratory Report LA-2301 (April, 1959). Contains complete references to earlier reports on the Particle-in-Cell method.

3. H. G. Kolsky, "The Nearest Neighbor Hydrodynamics Calculation." Internal manuscript, Los Alamos Scientific Laboratory (July, 1961).

4. F. H. Harlow and B. D. Meixner, "The Particle-and-Force Computing Method for Fluid Dynamics," Los Alamos Scientific Laboratory Report LAMS-2567 (June, 1961).

5. W. A. Beyer. Unpublished studies performed at the Los Alamos Scientific Laboratory.

6. S. Ulam, "Stability of Many-Body Computations," in Proceedings of Symposia in Applied Mathematics, vol. 13, Hydrodynamic Instability, pp. 247-258, American Mathematical Society, Providence, Rhode Island, 1962.

7. M. W. Evans and F. H. Harlow, "The Particle-in-Cell Method for Hydrodynamic Calculations," Los Alamos Scientific Laboratory Report LA-2139 (June, 1957).