THE PARTICLE-IN-CELL METHOD

FOR NUMERICAL SOLUTION OF PROBLEMS IN FLUID DYNAMICS

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ABSTRACT

The Particle-in-Cell method is a procedure to be used on high-speed computer for studies of the dynamics of compressible fluids undergoing large distortions. The technique is described in detail for calculation of the dynamics of two fluids confined to move in a two-dimensional rectangular box, and techniques are discussed for the extension to numerous other types of problems. Discussion is also given of many properties, limitations and uses of the method, which have been learned through the application to a wide variety of problems.

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I. INTRODUCTION

In response to several needs at the Los Alamos Scientific Laboratory, the Particle-in-Cell method, abbreviated PIC method, was developed for the numerical solution of problems involving the dynamics of compressible fluids. At the time that the need became apparent there already were in existence several numerical methods, and in many cases the results from them had been spectacular, especially for one-dimensional problems. For calculation in two space dimensions, however, the applicability of existing methods was more limited, as explained below.

In most numerical techniques for solving fluid dynamics problems the fluid is imagined to be subdivided into a number of small zones or cells. Partial differential equations are then written in finite difference form as an approximation procedure. There are two basic viewpoints that may be adopted in the writing of the equations; these are termed Lagrangian and Eulerian. In the Lagrangian viewpoint, the coordinate system is fixed in the fluid. The finite difference analogy thereto has the zones following the fluid as it moves. Associated with each corner in the mesh is a certain fixed mass and a velocity which varies with time. The center of each cell has associated with it

pressure, density, and energy which likewise vary with time. The Lagrangian approach has proved particularly useful for treating systems involving several fluids because each mesh point retains identity with its initial portion of the fluid. The internal fluid boundaries are therefore clearly delineated. A large number of strikingly successful calculations have been performed by several groups of workers. The Lagrangian methods are usually limited, however, to systems in which no large distortions of the fluid occur. Rather serious doubt is cast upon the accuracy of representing the true solution when, for example, a system whose equations are based on an orthogonal mesh becomes distorted significantly away from orthogonality. Problems involving oblique collision of two free surfaces are likewise difficult to solve by the Lagrangian method.

In the Eulerian viewpoint, the coordinate system is fixed relative to the laboratory and the fluid moves through the mesh of cells. In the strict application of this approach, each cell of the mesh is characterized by uniform density, pressure, velocity and material kind. Eulerian methods have the tremendous advantage of applicability to problems with arbitrary distortions or slippages of the fluid. They also, however, suffer from several disadvantages. One of these is the introduction of a false diffusion, especially noticeable with material boundaries. This arises from the fact that each cell is forced to be homogenous. When material enters a cell, its properties are uniformly mixed with those of all the other materials in the cell. Also, in Eulerian methods, it is difficult to resolve very fine structures which move with the fluid. In this last respect the Lagrangian viewpoint has an advantage. Many fine zones can be constructed

across the small structure, and as it moves with the fluid the fine zoning follows along. Finally, an Eulerian calculation is not invariant to uniform translation.

Numerous special procedures have been invented to overcome the difficulties of the Lagrangian and the Eulerian methods. In some cases, features of the methods can be combined and some of the disadvantages thereby eliminated. The Particle-In-Cell method that we shall discuss here is the result of one particular type of combination. The two features especially desired during the development of the PIC method were those of allowing large distortions to occur in the fluid without reducing the calculations to nonsense, and of being able to calculate the history of each element of the fluid, particularly when several fluids are present.

The general features of the PIC method can be described as follows: There are two computing meshes; one is Eulerian, the other Lagrangian. The domain through which the fluid is to move is divided into a finite number of computational cells which are fixed relative to the observer. This is the Eulerian mesh. In addition the fluid itself is represented by particles or mass points which move through the Eulerian mesh, representing the motion of fluid. This is the Lagrangian mesh. Associated with the mesh points of each system are certain variables whose history the calculation develops. Thus for each Eulerian cell there is kept the velocity, the internal energy, and the total mass of each kind of material. For the Lagrangian mesh of particles, individual masses and positions are kept.

To perform the calculations it is necessary to arrange the equations of motion in such a way as to be appropriate to this special representation of the fluid. A fairly general example of how this is done has been

given in Part II, while in Part III it is shown how other situations can be handled by relatively simple extension. It is likely that the reader will think of a variety of modifications to the techniques as presented, which could be tried. Indeed the history of development of the PIC method is filled with experimentation with alternatives. These are discussed in detail in several Los Alamos Scientific Laboratory reports,[1,2] which in turn contain references to older reports, mostly not now available. Discussions of earlier-used alternatives have also been given in several papers,[3,4,5] which in addition demonstrate some applications.

On the basis of this brief description it can already be seen in what manner the PIC method will share the advantages or disadvantages of the more strictly interpreted Lagrangian and Eulerian methods. Compared with the Lagrangian method, the PIC method shares the ability to follow the detailed history of every element of fluid, and to keep separated the boundaries between fluids. The Lagrangian disadvantage of breakdown during large distortions is not shared by the PIC method. As in the Eulerian method, large distortions are automatically taken care of. On the other hand, the PIC method shares the disadvantage of the Eulerian method in the inability to resolve fine detail moving with the fluid. Also, since the properties of the fluid are related to a coordinate system which is fixed relative to the observer, there results a fictitious difference between a fluid which is stagnated and a fluid which is moving. The extent of this difficulty and procedures which have been used to overcome it are discussed in Part IV.

Performance of a calculation by the PIC method resembles the performance of an experiment. The finite-difference equations in suitable form, together with the initial and boundary conditions for a specific situation,

are given to an electronic computer which in turn develops the solution at a sequence of later times separated by small time increments. There is no a priori assumption of a model for the flow configurations. The development of a shock, for example, occurs automatically where required. The result is always an approximate solution, and the purpose of empirical and theoretical studies of the methodology is directed towards improving the goodness of the approximation. In Part II of this paper, we have shown how the method can be applied to a rather simple type of situation, that is, to finding the motion of two fluids in a Cartesian two-dimensional coordinate system, bounded by rigid walls. Part III shows how the method can be used in various other coordinate systems and for fluids in which viscosity, heat conduction and external forces are important. Various other boundary conditions are also discussed. In Part IV are presented the results of some empirical and theoretical studies which have shown the advantages and weaknesses of the method.

II. AN EXAMPLE OF THE METHOD

Most of the features of the PIC method can be demonstrated by showing its application to a relatively simple problem. Consider the dynamics of two materials which are confined to move in a two-dimensional rectangular box whose walls are rigid and allow perfect slippage. The materials are nonviscous and nonconducting of heat; each has an equation of state which relates pressure, p, to density, ρ, and specific internal energy, I. The appearance of the box at some instant of time can be imagined to be as in Fig. 1.

Fig. 1

The box is oriented with one corner at the origin and with the edges along the x and y axes. It is subdivided into a number of equal rectangular cells to which the finite-difference equations are to be related. The cells have dimensions δx and δy.

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Each fluid is represented by a number of mass points called "particles," each with a constant mass. As shown in the figure, these are represented by dots and x's; we shall call the materials "dot material" and "x material," respectively. In this example, all dot particles have the same mass, $m_\bullet$, and all the x particles have the same mass, m_x. (For calculations in cylindrical coordinates or for certain situations in cartesian coordinates, it is more convenient to have a different mass for every particle.) For each particle there are stored in the computing-machine memory its x and y coordinates. These are changed in time, by the method described below, to give a representation of the motion of the fluids through the mesh of cells.

Such quantities as velocity, density, and pressure are kept in the machine memory by cell, so that, for example, the pressure of a cell is meant to represent a certain average of the pressure throughout the volume of fluid contained in the cell. (Further discussion of this point is given by Bromberg in Appendix II of Ref. 1, where there is an enlightening alternative derivation of the PIC-method equations.) The cells are labeled with index $\binom{j}{i}$, with i and j increasing in the x and y directions, respectively; the lower left cell in the figure is cell number $\binom{1}{1}$. Thus, for example, the pressure for cell $\binom{j}{i}$ is p_i^j, while the average pressure along the boundary between cells $\binom{j}{i}$ and $\binom{j}{i+1}$ is $p_{i+\frac{1}{2}}^j$, and analogous symbols are used for the other boundary pressures.

The nomenclature for various cellwise quantities is shown in Table 1.

The Pressures. The two equations of state are given in the form

$$p = f_{\cdot}(\rho, I)$$

$$p = f_{x}(\rho, I)$$

where $f_{\cdot}$ and f_{x} are appropriate functions for the dot and x materials, respectively. The density in a cell is defined to be the quotient of the masses in the cell divided by its area. Thus, for a cell containing only dot material or x material, the pressure equations become

$$p_i^j = f_{\cdot}\left[\frac{M_{.i}^{j}}{\delta x \delta y}\ ,\ I_{.i}^{j}\right]$$

$$p_i^j = f_{x}\left[\frac{M_{xi}^{j}}{\delta x \delta y}\ ,\ I_{xi}^{j}\right]$$

Various procedures are possible for the determination of total pressure in a mixed cell. One of these is based on the requirement of pressure continuity across a material interface. Assuming that the fraction of a cell occupied by dot material is σ, one writes the two equations, from which σ is to be eliminated,

$$p_i^j = f_{\cdot}\left[\frac{M_{.i}^{j}}{\sigma \delta x \delta y}\ ,\ I_{.i}^{j}\right] = f_{x}\left[\frac{M_{xi}^{j}}{(1-\sigma)\delta x \delta y}\ ,\ I_{xi}^{j}\right]$$

If the pressure is strictly proportional to the density for both materials, then the result is the same as that from adding partial pressures:

$$p_i^j = f_{\cdot}\left[\frac{M_{.i}^{j}}{\delta x \delta y}\ ,\ I_{.i}^{j}\right] + f_{x}\left[\frac{M_{xi}^{j}}{\delta x \delta y}\ ,\ I_{xi}^{j}\right]$$

If the equations of state are complicated, it may be convenient, as well as sufficiently accurate, to still calculate the pressure in a mixed cell by adding the partial pressures in this manner. In some cases, however, the result of this is far from reasonable and a different approach has been found useful on several occasions. A value σ_o, is assumed for σ and the pressure is taken to be

$$p_i^j = \frac{1}{2}\left\{ f_{\cdot}\left[\frac{M_{\cdot i}^{j}}{\sigma_o \delta x \delta y}\,,\ I_{\cdot i}^{j}\right] + f_x\left[\frac{M_{xi}^{j}}{(1-\sigma_o)\delta x \delta y}\,,\ I_{xi}^{j}\right]\right\}$$

The choice of

$$\sigma_o = \frac{M_{\cdot i}^{j}}{M_{\cdot i}^{j} + RM_{xi}^{j}}$$

has sometimes yielded reasonable results, where R is the ratio of the initial density of the dot material to that of the x material. In this case, the value of σ_o is based on the assumption that the compression of each of the two materials is in the same ratio as their initial compressions. Various iterative procedures are also possible for solving for the mixed-cell pressure;

Often it is useful to add an "artificial viscosity" pressure, q, to the equation of state pressure. Further discussion of this is given in Part IV. We shall use $P = p + q$ for the sum of the two pressures.

Phase I of a Calculation Cycle. In the computer memory there are stored all the results of the previous-cycle calculations or else the initial conditions

for the problem. These are to be advanced in time according to a finite-difference approximation to the differential equations

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} + \rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = 0$$

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} + \frac{\partial P}{\partial x} = 0$$

$$\rho \frac{\partial v}{\partial t} + \rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} + \frac{\partial P}{\partial y} = 0$$

$$\rho \frac{\partial I}{\partial t} + \rho u \frac{\partial I}{\partial x} + \rho v \frac{\partial I}{\partial y} + P\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = 0$$

The first of these equations, that of mass conservation, is automatically satisfied by the particle model. The momentum equations are treated as follows: In Phase I, the contributions to the time derivatives which arise from the terms involving pressure are calculated. The particles are not moved at this step; thus the transport terms are dropped, and the equations, in finite space-difference form, become

$$\rho_i^j \left(\frac{\partial u}{\partial t}\right)_i^j = - \frac{1}{\delta x}\left[P_{i+\frac{1}{2}}^j - P_{i-\frac{1}{2}}^j\right]$$

$$\rho_i^j \left(\frac{\partial v}{\partial t}\right)_i^j = - \frac{1}{\delta y}\left[P_i^{j+\frac{1}{2}} - P_i^{j-\frac{1}{2}}\right]$$

Cell-boundary pressures are averaged from adjacent cells.

Experience has shown that the energy equation can best be treated by considering the separate effects of p and q. The transport terms are again dropped, and the differential form is rearranged to

$$\rho \frac{\partial I}{\partial t} + p\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + \frac{\partial qu}{\partial x} + \frac{\partial qv}{\partial y} - u \frac{\partial q}{\partial x} - v \frac{\partial q}{\partial y} = 0$$

which becomes, in difference form,

$$\rho_i^j \left(\frac{\partial I}{\partial t}\right)_i^j = - p_i^j \left(\frac{u_{i+\frac{1}{2}}^j - u_{j-\frac{1}{2}}^j}{\delta x} + \frac{v_i^{j+\frac{1}{2}} - v_i^{j-\frac{1}{2}}}{\delta y}\right)$$

$$- \frac{(qu)_{i+\frac{1}{2}}^j - (qu)_{i-\frac{1}{2}}^j}{\delta x} - \frac{(qv)_i^{j+\frac{1}{2}} - (qv)_i^{j-\frac{1}{2}}}{\delta y}$$

$$+ u_i^j \left(\frac{q_{i+\frac{1}{2}}^j - q_{i-\frac{1}{2}}^j}{\delta x}\right) + v_i^j \left(\frac{q_i^{j+\frac{1}{2}} - q_i^{j-\frac{1}{2}}}{\delta y}\right)$$

Cell-boundary velocities are averaged from adjacent cells.

The reason for treating the p and q terms in different fashion is that whereas the equation-of-state pressure, p, is basically a cell-centered quantity, the viscous pressure, which will be shown to depend upon velocity differences, is basically a cell-boundary quantity. In addition, the form for the p terms is based upon the desirability of their conserving entropy in difference form. The q terms in that form, however, (with cell-centered q values obtained from boundary averages) contribute to instability of the equations. Only in the form shown are the q terms really effective for their purpose. Further discussion of this matter is given in Part IV.

To compute the tentative new velocities for the end of a computational cycle, in terms of those from the beginning of the cycle, we use the lowest order terms of the expansion

$$\tilde{u}_i^j = u_i^j + \delta t\left(\frac{\partial u}{\partial t}\right)_i^j + \cdots$$

$$\tilde{u}_i^j = v_i^j + \delta t\left(\frac{\partial v}{\partial t}\right)_i^j + \cdots$$

or

$$\tilde{u}_i^j = u_i^j - \frac{\delta y \delta t}{M_i^j}\left[p_{i+\frac{1}{2}}^j - p_{i-\frac{1}{2}}^j\right]$$

$$\tilde{v}_i^j = v_i^j - \frac{\delta x \delta t}{M_i^j}\left[p_i^{j+\frac{1}{2}} - p_i^{j-\frac{1}{2}}\right]$$

Analogous treatment of the energy equation is made complicated by two difficulties. The first is that the specific internal energy, I_i^j, is not defined for a mixed cell. For this reason we write

$$\rho_i^j\left(\frac{\partial I}{\partial t}\right)_i^j \rightarrow \frac{1}{\delta x \delta y}\left(\frac{\partial Q}{\partial t}\right)_i^j$$

where Q_i^j is the total internal energy of the cell. Division into the separate changes of internal energy for the various materials in the cell is thereby deferred to a later step in the calculation cycle. The second difficulty is that the use of only the first terms of the expansion

$$\tilde{Q}_i^j = Q_i^j + \delta t\left(\frac{\partial Q}{\partial t}\right)_i^j + \cdots$$

does not result in rigorous energy conservation unless some careful adjustment is made in the calculation of $\partial Q/\partial t$. It is assumed that the new velocities have already been calculated so that, for example, both u_i^j and $\tilde{u}_i^j$ are available in memory for the internal energy calculation. Then, with

$$\bar{u} \equiv \tfrac{1}{2}(u + \tilde{u})$$

$$\bar{v} \equiv \tfrac{1}{2}(v + \tilde{v})$$

the proper form is

$$\left(\frac{\partial Q}{\partial t}\right)_i^j = - p_i^j\left[\delta y\left(\bar{u}_{i+\frac{1}{2}}^j - \bar{u}_{i-\frac{1}{2}}^j\right) + \delta x\left(\bar{v}_i^{j+\frac{1}{2}} - \bar{v}_i^{j-\frac{1}{2}}\right)\right]$$

$$- \delta y\left[(q\bar{u})_{i+\frac{1}{2}}^j - (q\bar{u})_{i-\frac{1}{2}}^j - \bar{u}_i^j(q_{i+\frac{1}{2}}^j - q_{i-\frac{1}{2}}^j)\right]$$

$$- \delta x\left[(q\bar{v})_i^{j+\frac{1}{2}} - (q\bar{v})_i^{j-\frac{1}{2}} - \bar{v}_i^j(q_i^{j+\frac{1}{2}} - q_i^{j-\frac{1}{2}})\right]$$

The total energy in a cell is

$$E_i^j = Q_i^j + \frac{1}{2} M_i^j\left[(u_i^j)^2 + (v_i^j)^2\right]$$

With this and the equations of change, it is possible to show that $\tilde{E}_i^j - E_i^j$ can be expressed as a pair of cell-boundary differences, so that in a summation of the energy changes over the whole mesh of cells, all internal contributions cancel in pairs, leaving only boundary fluxes from the edges of the computing region. It is by this procedure that finite-difference forms of common boundary conditions are derived in Part III.

From the result for δQ_i^j, the values of $\tilde{I}_{.i}^{\ j}$ and $\tilde{I}_{xi}^{\ j}$ are to be determined. For an unmixed cell with, say, dot material only,

$$\tilde{I}_{.i}^{\ j} = I_{.i}^{\ j} + \frac{\delta Q_i^j}{M_{.i}^{\ j}}$$

If the cell is mixed, then various procedures for distributing internal energy changes to the several materials may be used.

(1) The materials could be heated as though each had been compressed or expanded adiabatically through the same pressure change.

(2) Each could be given the same change in total internal energy.

(3) Each could be given the same change in specific internal energy.

The first and second of these procedures have proved satisfactory in several trials, while the third inhibited the flow of energy across an interface in a test problem.

Phase II, The Transport of Material. By the end of Phase I, there are stored in memory ten quantities for every cell. Table 2 shows these, together with the quantities which replace them during the sequence of Phase II calculations.

Step 1. The results of the Phase I calculations are transformed into total cellwise energies and momenta:

$$\tilde{E}_{\cdot} \equiv M_{\cdot}\left[\tilde{I}_{\cdot} + \frac{1}{2}\left(\tilde{u}^2 + \tilde{v}^2\right)\right]$$

$$\tilde{E}_{x} \equiv M_{x}\left[\tilde{I}_{x} + \frac{1}{2}\left(\tilde{u}^2 + \tilde{v}^2\right)\right]$$

$$\tilde{X} \equiv \left(M_{\cdot} + M_{x}\right)\tilde{u}$$

$$\tilde{Y} \equiv \left(M_{\cdot} + M_{x}\right)\tilde{v}$$

Step 2. The particles are moved. The coordinates of each mass point change according to

$$x' = x + u_{eff}\delta t$$

$$y' = y + v_{eff}\delta t$$

In some calculations (see, for example, Ref. 5), the values of u_{eff} and v_{eff} were simply the values of $\tilde{u}$ and $\tilde{v}$ of the cell containing the particle, no

matter where in the cell the particle originated its motion for the cycle. The results can almost always be improved, however, by using the time-consuming process called "velocity weighting;" indeed, tests have indicated that the increase in accuracy thereby realized could not be achieved by that increase in mesh fineness which would consume equal extra computer time.

In the velocity weighting procedure, a rectangle of cell size is imagined to be located about each particle, the particle being at the center. Such a rectangle then overlaps four adjacent cells, and the effective velocity for moving the particle is taken as a weighted average of the four cellwise tilde velocities, the weightings being proportional to the overlap areas. If the surrounding rectangle lies partly in an empty cell, then that cell may be assumed to have the same velocity as does the cell with the particle. If the surrounding rectangle lies partly outside the walls of the computation region (these being assumed rigid), then the fictitious outside cells may be given either reflected velocities or the same velocities as in the adjacent interior cells. In the former case, it can be shown that for properly-small values of δt, no particle will be lost from the system. The procedure is less desirable, however, as it can lead to the "boundary catastrophe" discussed in Ref. 1, page 17. In the latter case, it is necessary to reflect the particle back in; the particle then carries a change in momentum as though entering from a cell with reflected velocity, and the boundary catastrophe is avoided.

When a particle is thus moved, it may be found to remain in the same cell from which it started. In this case, there is no modification to any

of the cellwise quantities. Some of the particles, however, will end up in new cells; in these cases, cellwise changes are necessary. From the cell which was left, the particle mass, momentum, and energy are subtracted and these are added to the new cell. Thus, through step 2, the cellwise values of mass, momentum, and energy cumulate to their final values for the cycle.

Step 3. The final velocities for the cycle are computed

$$u' = \frac{X'}{M'_{\cdot\cdot} + M'_x}$$

$$v' = \frac{Y'}{M'_{\cdot} + M'_x}$$

where $M'_{\cdot}$ and M'_x are the new masses for the cell.

Step 4. The final specific internal energies for the cycle are computed

$$I'_{\cdot} = \frac{E'_{\cdot}}{M'_{\cdot}} - \frac{1}{2}\left[(u')^2 + (v')^2\right]$$

$$I'_x = \frac{E'_x}{M'_x} - \frac{1}{2}\left[(u')^2 + (v')^2\right]$$

Phase III, Functionals of Motion. The final arrangement of storage after the sequence of calculations is such as to allow immediate re-entry into Phase I of the next cycle. Ordinarily, however, before proceeding to the next cycle, it is useful to compute various functionals of the motion such as total kinetic and internal energy for each material, components of total momentum, positions of centers of mass, entropy, and numerous other quantities. In some cases, it is possible to compare changes of these quantities with the changes calculated by summing boundary fluxes. Thus, in the

example at hand, the total energy of the system should be rigorously conserved. (Actually, machine roundoff will introduce some change in total energy, but the relative change per cycle should be bounded by a number which is predictable from a knowledge of the number of significant figures retained by the calculation.) Likewise, changes in the momentum components should be exactly predictable in terms of the sum of the boundary forces. Computed by machine, such checks serve to indicate machine or coding errors and have proved extremely valuable on many occasions.

III. BOUNDARY CONDITIONS AND GENERALIZATIONS

The relatively simple procedure discussed in Part II is easily extended to more complicated problems involving a variety of other boundary conditions or coordinate systems. In addition, extensions can be made to problems involving viscosity, heat conduction, or external forces. As a basis for discussing the generalization to more complicated boundary conditions, we here examine the conservative properties of the equations. No discussion is required concerning the conservation of mass; the model of the particles insures that mass is rigorously conserved. Conservation of momentum is easily demonstrated as follows: We refer to the finite difference momentum equations presented in Part II

$$\left.\begin{aligned} M_i^j\left(\tilde{u}_i^j - u_i^j\right) &= -\delta y \delta t\left(P_{i+\frac{1}{2}}^j - P_{i-\frac{1}{2}}^j\right) \\ M_i^j\left(\tilde{v}_i^j - v_i^j\right) &= -\delta x \delta t\left(P_i^{j+\frac{1}{2}} - P_i^{j-\frac{1}{2}}\right) \end{aligned}\right\}$$

These equations represent the Phase I change in momentum of a cell. Changes which occur in Phase II are automatically conservative of momentum. To show

that this is likewise true in Phase I it is merely necessary to sum the equations given above over all the cells of the system. In the summation the pressures cancel in pairs; that is, for example, $P^j_{i-\frac{1}{2}}$ for cell number i is the same as $P^j_{i+\frac{1}{2}}$ for cell number i - 1 and these two pressures cancel from two successive terms in the summation. Thus all that is left are the boundary pressures, showing that changes in momentum of the system arise only through forces which appear on the surface. This also shows that the pressure must vanish on the boundary between a cell with material and one which is empty.

Some slight additional manipulation is required to show that the energy equation is also conservative. If one adds the change in kinetic energy resulting from the momentum equation to the change in internal energy resulting from the energy equation, then it is again found that terms will cancel in pairs in a sum over the entire system. The result shows that the flux of energy across a boundary is typically given in the form

$$(\text{Flux})^j_{i+\frac{1}{2}} = \frac{1}{2}\left(p^j_{i+1}\,\bar{u}^j_i + p^j_i\,\bar{u}^j_{i+1}\right) + (q\bar{u})^j_{i+\frac{1}{2}}$$

Thus, for example, if this boundary is adjacent to an empty cell, which we here consider to be number i+1, then the properties of that empty cell for use in computing with cell number i are determined by the requirement that the flux vanish. This is reasonably accomplished in the following way.

$$p^j_{i+1} = -\,p^j_i$$

$$\bar{u}^j_{i+1} = \bar{u}^j_i$$

$$q^j_{i+\frac{1}{2}} = 0$$

In contrast, if the boundary had been a perfectly rigid wall, then the fictitious cell beyond the wall, number i+1, must possess the following properties during computation for cell number i,

$$p^j_{i+1} = p^j_i$$

$$\bar{u}^j_{i+1} = - \bar{u}^j_i$$

$$\bar{u}^j_{i+\frac{1}{2}} = 0$$

These conditions have the effect that the interpolated velocity of the wall is zero. Calculation of the boundary value of $q^j_{i+\frac{1}{2}}$ uses the appropriately reflected quantities — see Part IV. Other types of boundaries and related modifications are described as follows:

1. Periodic channel. The rectangular computation region can be considered to be one section of an infinite channel with walls parallel to say, the x axis. It is assumed that all properties of the entire flow field are periodic along the channel, the period being the width of the computation region. The change in computing procedure is slight. For example, along the right-hand boundary the cells are treated just like interior cells with their right-hand neighbors being the cells along the left-hand boundary. Particles leaving the system across the boundary re-enter from the left while those which go out the left-hand boundary are inserted from the right. Such a system is completely conservative of particles, energy and horizontal momentum.

2. Prescribed input. Along one or several of the boundaries a prescribed input of fluid can be inserted. This could, for example, be used to represent the flow conditions behind a shock which has entered across one of the boundaries at the beginning of the problem. Consider the example of input

along the left boundary. The left-hand cells of the computation region can be treated as interior cells with their left-hand neighbors being considered to possess the prescribed conditions of the input flow. Particles are periodically created for insertion across the left boundary. There is thus a slight additional bookkeeping difficulty with regard to the storage of particle coordinates because the number of particles is not constant.

3. Continuative output. Whenever the input condition is used, a provision for output at some other boundary is usually required. If the flow out of that boundary is supersonic, then the exact manner by which it is treated is of little importance. We have always used a continuative boundary treatment for such an output line. Accordingly, the boundary cells are treated as interior, being bounded on the outside by cells with identically the same properties at any instant as their adjacent interior neighbors. The machine-memory locations for storage of the coordinates of lost particles can then be made available for incoming particles so that the total required machine storage is bounded and the calculation can be continued indefinitely.

4. Moving Mesh. In all previous discussions the computation region has been considered to be at rest and the fluid streams by. Alternately, it might be desirable to study some feature of the flow moving with fluid speed or some other speed and this could be followed by a traveling region of computation. Suppose, for example, one wished to follow the motion of a shock wave during its passage down a channel in say, the x direction. This could be accomplished as follows. A zone of several cells would always be present ahead of the shock. Whenever the shock had advanced a cell width, a new column of cells would be created to their right with conditions representing

the initial state ahead of the shock. At the same time a column of cells downstream would be destroyed. Conditions ahead of the shock could be constant or could vary with space. Boundary conditions of the downstream boundary could be continuative. No calculations have been performed using such a moving computation region.

5. Rigid obstacles. A rigid obstacle can be placed within the computation region. This is most easily accomplished if the boundaries of the obstacle follow cell boundaries. Then the treatment is exactly the same as at the rigid walls of the computation region. Such a calculation was reported in Ref. 4. If the obstacle boundary is curved or oblique relative to the cell orientation, then the procedure is somewhat more complicated. Numerous partial cells are created. The finite difference equations for such cells can be derived from the integral form of the equations of motion by a procedure like that used by Bromberg[1] for deriving the equations under ordinary circumstances. The results of calculations for flow past a circular object, for example, were reported in Ref. 5.

Alternatively, the rigid obstacle can be represented by a material whose density is very great. No modification to the computing procedure is required, provided that for the obstacle material an equation of state is used which does not give too-high pressures.

6. An externally applied pressure. We have often encountered problems in which the fluid is driven by an externally applied pressure prescribed as a function of space and time. This can be accomplished by a variation of the empty cell treatment, using flagged empty cells to signal the presence of an applied pressure. The boundary of every fluid cell adjacent to a flagged cell is given the appropriate applied pressure, and it is assumed that the

velocity of that boundary is that of the fluid cell. The pressure within a cell next to a flagged one is calculated using normal density in the equation of state if the cell would otherwise have subnormal density. In all other respects these edge cells are treated as ordinary interior cells. This procedure has been used with success in a variety of calculations.

An interpretation of the applied pressure boundary condition can be given as follows. The empty applied-pressure cells behave as though they were filled with a gas whose density is very small compared to that of the adjacent material but whose temperature is very high in such a way that the pressure is finite, the prescribed value. As a result, the sound speed is very high and the pressure remains homogeneous.

7. Three-dimensional Cartesian problems. It should be remarked that the boundary conditions and method as discussed here are quite applicable to three-dimensional situations with essentially no modification except those which are obvious. The difficulty with three-dimensional problems is that the storage space available in present machines is so limited as to restrict considerably the available resolution. Nevertheless we have attempted some three dimensional calculations and found that no additional difficulties existed, excepting perhaps that of representation of the results. No simple print-out of results for three-dimensional problems has yet been devised in such a way as to give easy visualization.

8. The addition of viscosity, heat conduction or body forces. We have found that the effects of viscosity and heat conduction as well as of body forces are easily added by a simple generalization of the equations.

The differencing follows in a very straightforward manner and while the equations are rather lengthy, there is no difficulty in applying them. They are written out in full in Ref. 2 and are not repeated here.

9. Cylindrical coordinates. Problems with symmetry of motion about a fixed axis are easily treated by the PIC method with almost no modification of the procedure already outlined. The particles are now replaced by circles about the axis and the cells are toroids of revolution of the rectangles. In such problems it has been found convenient to assign different masses to ~~each~~ each particle, the values being proportional to the original radius of the particle from the axis so that the particle density is initially proportional to the true density. The difference equations for Phase I must be written in perfectly conservative form. The particle motion in Phase II is accomplished by an areawise weighting to find the effective velocity.

10. Polar coordinates. We have not yet performed any calculations in polar coordinates although at the present time some are in preparation. It is expected that a variety of modifications will be necessary in order to accomplish the calculations properly. The effects of centrifugal and Coriolis accelerations must be properly taken care of and can be accomplished by a careful modification of the Phase II procedure.

IV. PROPERTIES OF THE COMPUTING METHOD

Through the running of numerous calculations, many chosen for comparisons with known solutions, it has been possible to learn some of the properties of the PIC method. It has also been possible to demonstrate analytically the origin of many of them, and thereby to correct for some which were undesirable. In this section we discuss several of these.

1. An example of application

Figure 2 shows a typical situation to which the PIC method has been applied. A cylindrical object strikes a laminated plate, and the problem is to find the strength of the transmitted shock, the amount of material splashed away, the deformation of the projectile, and various other features of the interaction. In (a) the downward-moving projectile is just about to hit; in (b) is shown the configuration at an intermediate time; (c) shows it at a time twice as late as in (b). The Eulerian cells are not shown; the particles only are present in the pictures; the grid of lines is a reference coordinate system. Note how the transmitted shock is shown by deflections of the particle lines. Comparisons of results of some similar calculations with actual experiments have shown that for problems of this type, the PIC method results are surprisingly accurate.

2. The density fluctuations

The feature of the method which at first seems most peculiar is the stepwise representation of density. Typically, the numberof particles per cell averages from four to sixteen. Thus the loss or gain of a particle makes a relatively large jump in cell-wise density and pressure. Success or failure of the method was known from the start to depend upon proper behavior in some average sense, and only through considerable experimentation was it discovered just how well the averaging takes place.

Actually, the fluctuation averaging is not completely automatic; it must be assisted in one respect. Consider, for example, a region of space in which the fluid is supposed to be completely uniform at density ρ_o and specific internal energy I_o. (We here neglect fluctuations in the latter.) The pressure in that region, as given by the equation of state, should then be $p_o = f(\rho_o, I_o)$. In the PIC-method calculation, however, some of the

cells in the region will have density greater than ρ_o, while others will have less than ρ_o. Indeed, there will be some distribution function giving the probability that a cell has N particles in a region where the mean number of particles per cell is N_o. It can be seen that even though the mean number of particles per cell is N_o, corresponding to the proper mean density, the mean pressure of such a region will not necessarily be p_o. If, for example, $\frac{\partial p}{\partial \rho} > 0$, then the mean pressure of the region will be greater than p_o. This is because each cell with $N > N_o$ will have an increase in pressure which is greater than the decrease for the corresponding cell for which $N < N_o$. If the distribution function for particle numbers is known, then a correction can be added to the equation of state to give more nearly the true mean pressure. We have found that such a correction is feasible to lowest order; that it is usually small; and that its use improves results where comparisons could be made.

Thus a knowledge of the particle-number distribution function is useful. Experimentally, we have determined the function for regions either at rest or in uniform translation relative to the Eulerian mesh. The distribution is, of course, always sharper than the Poisson function for random particle placement, but in a region of perturbed stagnation the Poisson distribution is approached as the time interval per cycle is increased. A variety of small changes in the method have been tried for sharpening the function. Recently, some success has been obtained through a modification of the energy calculation; the modified form has been given in this paper.

In discussing the pressure-fluctuation example, the dependence of pressure on internal energy was neglected. Actually, in circumstances in which

the pressure depends quite weakly on the internal energy (as in solids when the motions are slow compared with sound speed) the PIC method becomes difficult to apply. Fluctuations are particularly strong, with velocity deviations of the order of sound speed. We have found that at least sometimes useful results can be obtained by replacing the true equation of state by that for a polytropic gas with high specific heat ratio.

3. The "Artificial viscosity."

Most finite difference computing methods for compressible fluid dynamics have employed "artificial viscosity" of one sort or another, mainly for the purpose of allowing automatic shock calculation, but also for adding stability to the difference equations. Forms for these added terms and discussions of their usefulness have been given by von Neumann and Richtmyer,[6] Landshoff,[7] Longley,[8] Goad,[9] Fromm,[10] and others. The most common method is to add to the equations terms which resemble those of true viscosity, with coefficients adjusted in such a way as to smear any shocks over the width of several finite-difference zones. With proper choice of form for the terms (in particular they must not destroy the conservative properties of the method) the shock jump conditions will still be satisfied, and many desirable functionals of the motion will be accurately obtained without any additional special shock treatment.

The fictitious viscosities may also serve a stabilizing purpose. The terms in the difference equations, which refer to values of quantities separated by finite intervals of space and time, can be expanded in Taylor's series about some particular space-time point. The result will be the original differential equations plus terms which depend upon δx, δy and δt. (One requirement of any method is that the additional terms go to zero as the

values of δx, δy and δt are made to vanish in an appropriate manner.) These extra terms beyond those of the desired differential equations usually involve higher derivatives, and may be positive or negative. Usually some of them introduce diffusive properties, thus being effectively like viscosities themselves, and if negative they tend to reduce the stability of the equations. The artificial viscosities, which likewise introduce diffusive effects, can therefore be constructed so as to tend to counteract the inherent negative diffusions otherwise present.

More particularly for the PIC method, such expansions show that the statistical effect of the lowest order terms in δx and δy are such as to give for the momentum equation

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho(\vec{u}\cdot\nabla)\vec{u} = -\nabla p + \frac{\partial}{\partial x}\left[\left(\tfrac{1}{2}\rho|u|\delta x\right)\frac{\partial \vec{u}}{\partial x}\right] + \frac{\partial}{\partial y}\left[\left(\tfrac{1}{2}\rho|v|\delta y\right)\frac{\partial \vec{u}}{\partial y}\right]$$

For the energy equation there is likewise introduced an artificial heat conduction. The derivations are straightforward — details are presented in Reference 1. The effective viscosity is thus not isotropic; it does, however, usually have a beneficial effect in the PIC method in that the diffusive effect is positive, hence stabilizing. Thus, PIC-method calculations would seem not to require additional artificial viscosity terms, and indeed many calculations have been performed without their inclusion. In some cases, however, the effective viscosity has not been desirable. An example is given in Ref. 5, in which it is shown that in calculation of a gas moving away from a rigid wall, the adverse effect came through

a spurious decrease of pressure in the rarefaction, resulting in cavitation where none should have occurred. Another situation in which the effective viscosity of the PIC method caused trouble was seen in an attempted calculation of spherical motion in cylindrical coordinates. The radial component of the viscous effect was very strong near the axis and tended to destroy the spherical symmetry. Finally, when $|u|$ and $|v|$ are small, these diffusive effects are small and fluctuations in velocity produced by the stepwise pressures are not damped sufficiently rapidly.

Thus, we have experimented with a double viscosity procedure, in which to the equation-of-state pressure, p, we may add both q_1 and q_2. The purpose of q_1 is to subtract the effects of the automatic viscosity, while that of q_2 is to add a more satisfactory form, such, for example, as that proposed by von Neumann and Richtmyer.[6] In two dimensions, q_1 must be different for the two directions. (In cylindrical geometry the motion of q_1 is purely symbolic; that is, the radial-direction treatment is not simply accomplished by a pressure modification. The equations themselves must be altered to remove the effects.)

There is another approach to removing the first order diffusive effects of the difference equations in the PIC method. They arise from the manner of particle movement; for example, when a particle goes from one cell to another, it carries with it an amount of energy given by the product of its mass and the specific energy of the cell it left. Alternately it could carry energy derived from the interpolated specific energy analogous to the effective velocity with which it was moved. This would remove part of the lowest order effective viscosity, but would introduce a substitute difficulty in that it

then would become possible for more energy to be removed from a cell that it possessed. Tests of this procedure did indeed show failure related to this explanation.

Thus, the procedure for removing the effective viscosity must be selective and subject to automatic appropriate modification. Fortunately, in most situations it does little harm; where it is undesirable as in the rarefaction, its removal can be limited to a specific region, or to a specific type of motion (i.e., expansive in this case). In most cases we have simply left it alone.

4. Restrictions and applicability

The PIC method has been applied with considerable success to a variety of problems. Its strongest advantage is applicability to flows with large distortions or in which voids may open or close. No special procedures are necessary for such occurrences. Its disadvantages can be listed as follows.

1. Lack of rotational and translational invariance — not a serious disadvantage in most cases.

2. Lack of resolution of the fine detail of a large system.

3. Relatively great consumption of computer storage space — both the Lagrangian and the Eulerian meshes require storage.

4. Somewhat greater computing time — since computations must be made for both meshes, the computing time is nearly double that required for a Lagrangian or Eulerian mesh alone.

5. Inappropriateness for far-subsonic flow — this disadvantage, shared with other methods of solution for compressible flow problems, arises from the necessity of having sound signals travel less than a cell width in one time cycle (the Courant condition).

It seems likely that whatever success the PIC method may enjoy is closely connected to the fact that mass, momentum and energy are rigorously conserved by the method. It is probably always true that any method for numerical treatment of partial differential equations will most likely enjoy success if the approximation method preserves the physical features upon which the original equations were based.

The overall results of considerable experimentation have been that the PIC method is most accurately applicable to problems in fluid dynamics in which no physically interesting part of the configuration is very small compared with the whole, in which the equation of state is not too internal-energy-insensitive, and in which the fluid speeds are comparable to the sound speeds, or greater. Several materials are easily handled, and large distortions cause no difficulties. The experimentation has also shown that in many cases in which there are deviations from ideal circumstances the results can still be quite useful. Often only slight changes in procedure have changed hopelessly nonsensical results into calculations which make sense. Anyone attempting to apply the method should keep that in mind, and not fear to experiment.

The development of the PIC method has been made possible through the efforts of a large number of people. Eleazer Bromberg, Daniel Butler, Bart Daly, Donald Dickman, David Harris, Robert Martin, and many others have all made important contributions, but most especially valuable has been the work of Martha Evans and Billy Meixner. All work has been performed under the auspices of the United States Atomic Energy Commission.

FIGURE CAPTIONS

Fig. 1: Example of a configuration of particles in a coarse mesh of cells.

Fig. 2: Configuration of particles at several times representing a cylinder of fluid striking a laminated plate. This shows a cross section of the process.

(a) The moment of impact

(b) Some time later

(c) Twice as late as in (b)

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*Los Alamos Scientific Laboratory Publications are available through the Office of Technical Services, U. S. Department of Commerce, Washington 25, D. C.

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TABLE 1

IDENTITY OF NOMENCLATURE FOR CELL $\binom{j}{i}$

u_i^j ≡ x-direction component of velocity

v_i^j ≡ y-direction component of velocity

$M_{.i}^{\ j}$ ≡ mass of dot material

$M_{xi}^{\ j}$ ≡ mass of x material

$M_i^j \equiv M_{xi}^{\ j} + M_{.i}^{\ j}$

$I_{.i}^{\ j}$ ≡ specific internal energy of dot material

$I_{xi}^{\ j}$ ≡ specific internal energy of x material

p_i^j ≡ pressure

δQ_i^j ≡ the Phase I change in total internal energy

$E_{.i}^{\ j}$ ≡ total energy of dot material

$E_{xi}^{\ j}$ ≡ total energy of x material

X_i^j ≡ total x-direction momentum

Y_i^j ≡ total y-direction momentum

$(\tilde{\ })$ ≡ result of Phase I calculation for ( )

$(\ )'$ ≡ result of Phase II calculation for ( )

TABLE 2

SEQUENCE OF STORAGE CHANGES FOR CELL $\binom{j}{i}$ DURING PHASE II

	$M_{\cdot}$	M_x	$I_{\cdot}$	I_x	$\tilde{I}_{\cdot}$	$\tilde{I}_x$	u	v	$\tilde{u}$	$\tilde{v}$
Step 1 >	"	"	$\tilde{E}_{\cdot}$	$\tilde{E}_x$	"	"	$\tilde{X}$	$\tilde{Y}$	"	"
Step 2 >	$M'_{\cdot}$	M'_x	$E'_{\cdot}$	E'_x	"	"	X'	Y'	"	"
Step 3 >	"	"	"	"	"	"	u'	v'	"	"
Step 4 >	"	"	$I'_{\cdot}$	I'_x	"	"	"	"	"	"

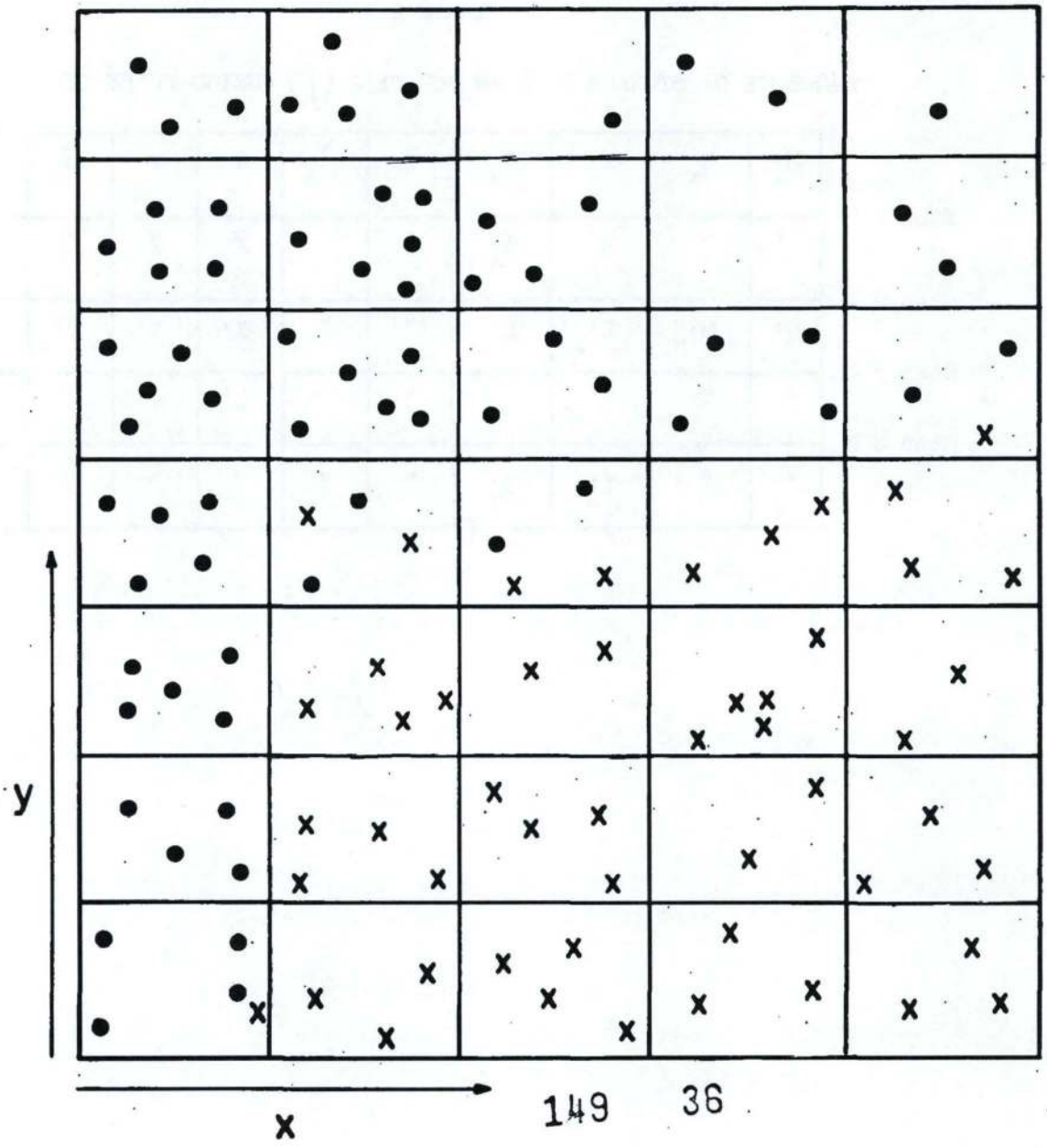
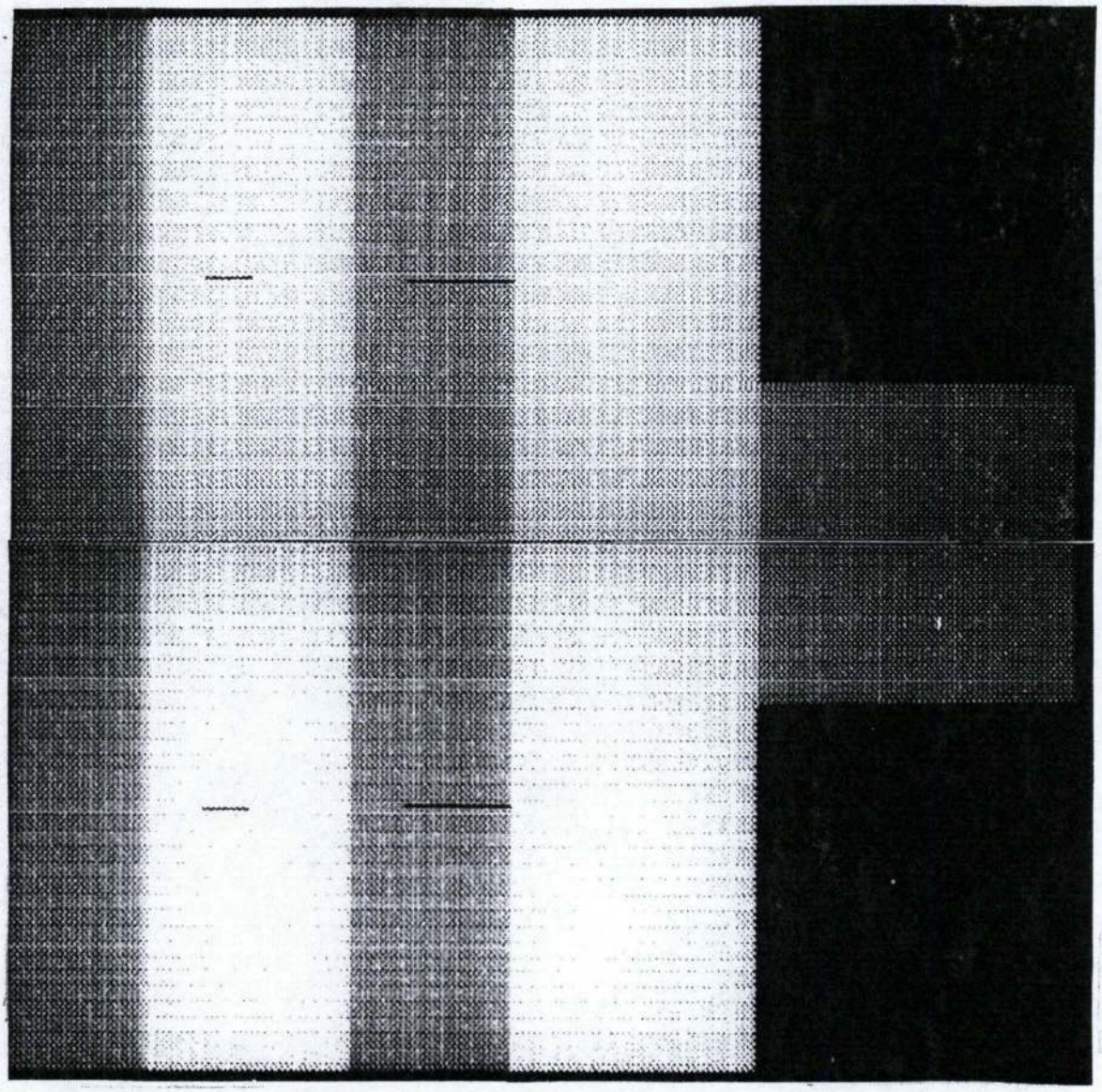
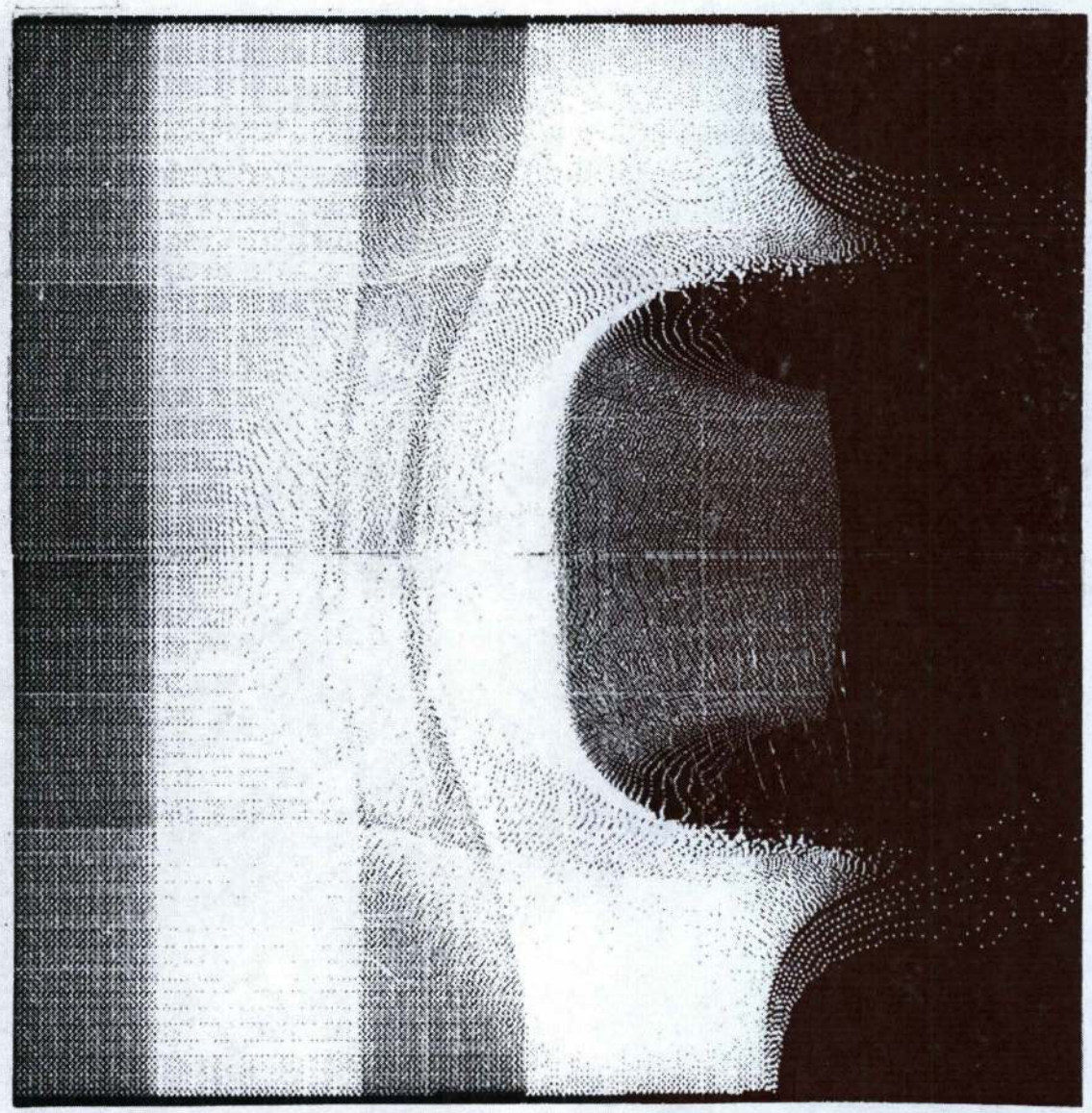


Fig 1

Harlow Fig 1





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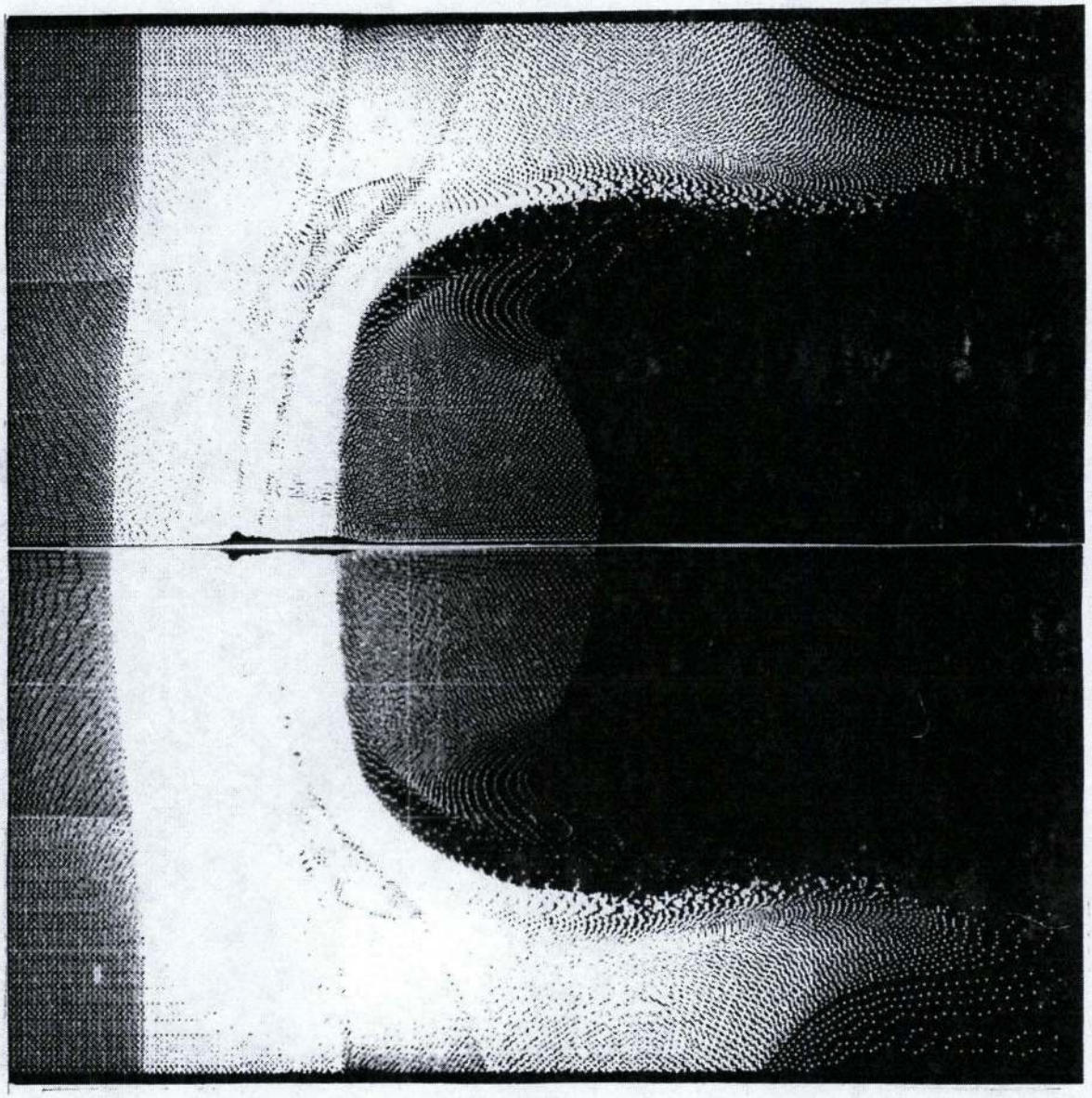

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