JOURNAL OF COMPUTATIONAL PHYSICS 8, 214–229 (1971)

Contour Dynamics for Numerical Fluid-Flow Calculations

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Received December 15, 1970

The numerical solution of problems in fluid dynamics is discussed in terms of a Dynamics-of-Contours (DOC) methodology. Elements of the flow are represented by contour points (or lines or surfaces) that move relative to the fluid in a manner that rigorously conserves mass, momentum and energy, and also represents the transient dynamics. The principal advantage of this technique is that it automatically gives fine resolution of flow features in regions of detailed structure, and coarse resolution where not much is occurring. Several examples are presented to illustrate the results of test problems.

INTRODUCTION

The numerical calculation of high-speed fluid dynamics is especially difficult for problems that require local regions of fine resolution in a fluid that is strongly distorting. Classical Lagrangian techniques are excellent for achieving resolution of details moving with the fluid, but accuracy decreases rapidly as the configuration distorts; in addition, it is difficult to assure that the fine resolution is always present only where required. Pure Eulerian methods, on the other hand, are excellent for studying strong distortions, but exhibit considerable difficulty in the achievement of resolution. A variety of modified or combined techniques have therefore been developed and used with varying degrees of success; a bibliography of some of these is given in Ref. [1].

The purpose of this report is to describe a new type of technique that is neither Lagrangian nor Eulerian, but nevertheless possesses some of the best features of both. The coordinates are contour lines of the basic quantities to be conserved, namely, the densities of mass, momentum and energy. The calculation method consists of moving these contours in such a way as to represent solutions of the full nonlinear, time-dependent equations of motion. We refer to the technique as a Dynamics-of-Contours (DOC) method.

* This work was performed under the auspices of the United States Atomic Energy Commission.

Several novel features and properties are introduced by this type of numerical solution technique.

1. The fluid configuration is represented by several overlapping sets of coordinates. Each of these refers to a particular quantity, and the discrete entities used in the representation are marker particles, called f-trons, which show the locality at which the fluid has the specific field-variable value appropriate to the fixed magnitudes carried by each f-tron. The letter f may refer to mass density ρ to momentum density $m_j(\equiv \rho u_j)$ or to energy density $e(\equiv \rho E)$. For example, a ρ-tron corresponding to $\rho = 1.4$ gm/cm^3 marks at all times the position within the fluid at which the density is equal to 1.4 gm/cm^3.

2. The f-trons usually move relative to the fluid, the various kinds often moving in several different directions. In addition, there will arise circumstances in which f-trons must either be created or destroyed.

3. Appropriate equations of motion will require the interaction of each f-tron with others of its own or different kinds, so that the calculations will require a process for determining which f-trons are the neighbors of each other.

4. To accurately represent the behavior of a true fluid, the f-tron motions will have to be governed by the rigorous principles of mass, momentum and energy conservation.

5. Representation of the fluid configuration by f-trons automatically maximizes efficiency in the attainment of resolution. This is because the greatest density of f-trons always occurs exactly where needed, namely, in regions of greatest detail in flow structure. Where the fluid properties vary slowly in space, the f-trons are widely dispersed and accordingly not wasted.

6. In contrast to Eulerian calculation methods, the DOC technique possesses rotational and Galilean invariance, since there is no tie to a laboratory reference frame.

7. Although the DOC method is especially suitable for one-dimensional problems (in plane, cylindrical or spherical coordinates), the extension to several space dimensions appears possible, even though difficulties are introduced, as discussed below.

8. Despite the unaccustomed nature of the f-tron coordinate system, it is easy to generate all of the usual visual display features that have proved useful in previous representations of calculational results. Contour plots emerge in straightforward fashion from the configurations of f-trons. Fluid streaklines are easily generated by embedded marker particles that move with the actual local fluid speed.

The full development of the DOC method requires the assembly of a number of elements, most of which are discussed in detail in this report. They include

1. Formulation of the *f*-tron equations of motion,
2. Proof of their conservation properties,
3. Efficient neighbor-search routines,
4. Interpolation routines,
5. Creation and destruction criteria for *f*-trons,
6. Boundary conditions derived from flux expressions in order to assure conservation,
7. Techniques for assuring numerical stability.

At the present time, most of the developmental difficulties have been overcome for the specification of the DOC method in one space dimension, and several features for multidimensional problems have also been determined. Most of the discussion, however, is limited to the one-dimensional version.

Equations of Motion

In usual Eulerian form, the equations of motion for a compressible fluid are

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}(m + q_1), \tag{1}$$

$$\frac{\partial m}{\partial t} = -\frac{\partial}{\partial x}(um + p + q_2), \tag{2}$$

$$\frac{\partial e}{\partial t} = -\frac{\partial}{\partial x}[u(e + p) + q_3], \tag{3}$$

where, ρ, m, and e are, respectively, the densities of mass, momentum, and energy; p is the pressure; and q_1, q_2, q_3 are added terms required for numerical stability, as described below. In addition, there is an equation of state $p = p(\rho, I)$ in which I is the specific internal energy. To complete the equations we have the relations

$$m \equiv \rho u, \tag{4}$$

$$e \equiv \rho(\tfrac{1}{2}u^2 + I). \tag{5}$$

Equations (1)–(3) are all of the conservative form

$$\frac{\partial f}{\partial t} = -\frac{\partial F_f}{\partial x} \tag{6}$$

and we shall see that this is necessary for the achievement of conservation in the f-tron dynamics equations.

To derive an expression for the velocity of an f-tron, it is sufficient to observe that along the path of its motion, the value of f remains constant. Thus

$$\frac{df}{dt} \equiv \frac{\partial f}{\partial x}\frac{dx}{dt} + \frac{\partial f}{\partial t} = 0$$

along the path such that $dx/dt = u_f$, the f-tron velocity. Accordingly,

$$u_f = -\left(\frac{\partial f}{\partial t}\right)\Big/\left(\frac{\partial f}{\partial x}\right). \tag{7}$$

Combination of this with Eq. (6) gives the result

$$u_f = \left(\frac{\partial F_f}{\partial x}\right)\Big/\left(\frac{\partial f}{\partial x}\right). \tag{8}$$

In particular,

$$u_\rho = \frac{\partial}{\partial x}(\rho u + q_1)\Big/\frac{\partial \rho}{\partial x}, \tag{9}$$

$$u_m = \left(\frac{\partial}{\partial x}(um + p + q_2)\right)\Big/\left(\frac{\partial m}{\partial x}\right), \tag{10}$$

$$u_e = \left(\frac{\partial}{\partial x}[u(e + p) + q_3]\right)\Big/\left(\frac{\partial e}{\partial x}\right), \tag{11}$$

are the velocities, respectively, of ρ-trons, m-trons, and e-trons. If x_f is the coordinate of an f-tron, then the equations of motion are completed by the kinematical relationship

$$\frac{dx_f}{dt} = u_f. \tag{12}$$

Conservation

Derivation of the approximation equations appropriate for resolution with a finite number of f-trons requires a careful consideration of the nature of the conservation that must be achieved. It is reasonable to assume that the total amount of f associated with the j-th f-tron is given by the product of the value of f carried by that f-tron and the fluid volume surrounding it. The fluid volume

in one space dimension is the sum of distances from the f-tron to the mid-points of its two adjacent neighbors:

$$\begin{aligned}\text{Volume}_j &= \tfrac{1}{2}(x_{j+1} - x_j) + \tfrac{1}{2}(x_j - x_{j-1}) \\ &\equiv \tfrac{1}{2}(x_{j+1} - x_{j-1}).\end{aligned}$$

Thus, summing over a set of f-trons, we see that the quantity to be conserved is

$$G \equiv \frac{1}{2}\sum_{j=1}^{N} f_j(x_{j+1} - x_{j-1}). \tag{13}$$

By conservation, we mean that changes in G can occur only from processes taking place at the ends of the summation set, so that no changes in G are attributed to interior gains or losses. This stringent requirement almost uniquely specifies the way in which the gradients in Eqs. (9)–(11) are to be approximated, leaving freedom only in the manner of expressing inter-f-tron fluxes.

To proceed, we employ a summation by parts, whereby the expression for G can be transformed algebraically to the form

$$G = \frac{1}{2}(f_1x_0 + f_0x_1) - \frac{1}{2}(f_{N+1}x_N + f_Nx_{N+1}) - \frac{1}{2}\sum_{j=1}^{N} x_j(f_{j+1} - f_{j-1}). \tag{14}$$

(The identical equivalence of Eqs. (13) and (14) can be proved by rewriting the summations in either equation with the indices offset by ± 1, where appropriate.)

A formulation of the conservation criterion can be stated as follows: The time rate of change of G in Eq. (14) must receive no contributions from the interior parts of the summation term. Thus, we write

$$\begin{aligned}\frac{dG}{dt} = &\frac{1}{2}\left(f_1\frac{dx_0}{dt} + f_0\frac{dx_1}{dt}\right) - \frac{1}{2}\left(f_{N+1}\frac{dx_N}{dt} + f_N\frac{dx_{N+1}}{dt}\right) \\ &- \frac{1}{2}\sum_{j=1}^{N}\frac{dx_j}{dt}(f_{j+1} - f_{j-1}),\end{aligned} \tag{15}$$

and inquire as to the circumstances in which the interior parts of the summation term in Eq. (15) identically vanish. Once those circumstances have been found, then the remaining parts of Eq. (15) consist only of flux terms for each end of the summation set. It is these flux terms that lie at the heart of the boundary-condition derivations.

Insertion of Eqs. (8) and (12) into the summation term in Eq. (15) transforms that term to the following:

$$-\frac{1}{2}\sum_{j=1}^{N}(f_{j+1} - f_{j-1})\left(\frac{\partial F_f}{\partial x}\right)_j \Big/ \left(\frac{\partial f}{\partial x}\right)_j.$$

Accordingly, we conclude that the quantity

$$(f_{j+1} - f_{j-1}) \Big/ \left(\frac{\partial f}{\partial x}\right)_j$$

must be independent of the f-tron value interval, which is to say that

$$\left(\frac{\partial f}{\partial x}\right)_j \to \frac{f_{j+1} - f_{j-1}}{2\delta x_j}, \tag{16}$$

in which $\delta x_j \equiv \frac{1}{2}(x_{j+1} - x_{j-1})$. In addition, it follows that we must require

$$\left(\frac{\partial F_f}{\partial x}\right)_j \to \frac{(F_f)_{j\to j+1} - (F_f)_{j-1\to j}}{\delta x_j}, \tag{17}$$

in which $(F_f)_{j\to j+1}$ is the flux from f-tron number j to f-tron number $j+1$. These requirements assure that the interior parts of the summation vanish, since the terms in that sum cancel in pairs, leaving

$$-\sum_{j=1}^{N} [(F_f)_{j\to j+1} - (F_f)_{j-1\to j}] \equiv (F_f)_{0\to 1} - (F_f)_{N\to N+1}.$$

Our conclusion, putting $u_f \equiv dx/dt$, is, therefore,

$$\frac{dG}{dt} = \{\tfrac{1}{2}[f_1(u_f)_0 + f_0(u_f)_1] + (F_f)_{0\to 1}\} - \{\tfrac{1}{2}[f_{N+1}(u_f)_N + f_N(u_f)_{N-1}] + (F_f)_{N\to N+1}\}. \tag{18}$$

This, together with Eqs. (16) and (17), are the principal conclusions from the conservation analysis. In summary, they show how the gradient terms must be approximated, and the nature of the flux terms at each end of any summation set. These flux terms are each composed of two parts. The first is a pseudo-convective flux, which occurs in a ZIP-like form [2], while the second accounts for inter-f-tron fluxes that arise from the fact that f-trons actually do not move with fluid speed (so that the pseudo-convective fluxes do not describe true fluid convection effects), and that there are force and work fluxes of momentum and energy.

The Difference Equations

Reference to Eqs. (1)–(3) shows that the flux expressions are

$$F_\rho = m + q_1, \tag{19}$$

$$F_m = um + p + q_2, \tag{20}$$

$$F_e = u(e + p) + q_3. \tag{21}$$

Through combined neighbor-search and interpolation procedures, it is possible to determine the values of m, u, e, and, therefore, ρ and p at the position of every kind of f-tron. The value of q is less direct; it usually requires a knowledge of a field-variable gradient. With these quantities determined at every f-tron position, the fluxes there can be calculated by means of Eqs. (19)–(21).

Combining Eqs. (8), (16) and (17), we see that the f-tron velocities must be calculated by the equation

$$u_f = 2\frac{(F_f)_{j\to j+1} - (F_f)_{j-1\to j}}{f_{j+1} - f_{j-1}}. \tag{22}$$

Thus, it is not the flux at each f-tron position that is required, but rather the inter-f-tron fluxes. These can be found in any symmetric fashion; that is, by any procedure such that, when $k = j + 1$, $(F_f)_{j\to j+1} \equiv (F_f)_{k-1\to k}$. For example, the algebraic average of the two f-tron fluxes could be used:

$$(F_\rho)_{j\to j+1} = \tfrac{1}{2}(m_j + m_{j+1}) + (q_1)_{j\to j+1}, \tag{23}$$

$$(F_m)_{j\to j+1} = \tfrac{1}{2}(u_j m_j + u_{j+1}m_{j+1} + p_j + p_{j+1}) + (q_2)_{j\to j+1}, \tag{24}$$

$$(F_e)_{j\to j+1} = \tfrac{1}{2}[u_j(e_j + p_j) + u_{j+1}(e_{j+1} + p_{j+1})] + (q_3)_{j\to j+1}. \tag{25}$$

Alternatively, there may be some advantages to the use of ZIP-type fluxes [2], with which we would write

$$(F_\rho)_{j\to j+1} = \tfrac{1}{2}(m_j + m_{j+1}) + (q_1)_{j\to j+1}, \tag{23a}$$

$$(F_m)_{j\to j+1} = \tfrac{1}{2}(u_j m_{j+1} + u_{j+1}m_j + p_j + p_{j+1}) + (q_2)_{j\to j+1}, \tag{24a}$$

$$(F_e)_{j\to j+1} = \tfrac{1}{2}[u_j(e_{j+1} + p_{j+1}) + u_{j+1}(e_j + p_j)] + (q_3)_{j\to j+1}. \tag{25a}$$

It must be emphasized that the necessary quantities entering into each flux must be calculated from interpolations at the particular f-tron for which F_f is being evaluated. The forms of the interparticle q terms are not yet specified, various alternatives being discussed below.

The formation of interparticle fluxes by simple algebraic averages has one valuable property not obtained from the ZIP-type fluxes. For such a procedure, in the absence of the q terms, Eq. (22) could be written

$$u_f = \frac{(F_f)_{j+1} - (F_f)_{j-1}}{f_{j+1} - f_{j-1}}. \tag{26}$$

For f equal, successively, to ρ, m, and e, Eq. (26) becomes the set of three Rankine-Hugoniot equations, with u_f in every case being the shock velocity. In this case, the DOC method treats every finite-difference step as a shock, and propagates its

properties with the usual conservative shock relationships. Numerical calculations with both flux types, however, show very little difference in results for both shock and rarefaction propagation, as long as the structure is otherwise sufficiently resolved for accuracy.

The basic set of equations for the dynamics has now been specified. To completely define the methodology, we need add only the discussion of q terms, the specification of initial and boundary conditions, and appropriate procedures for the creation and destruction of f-trons.

The Q Terms

Artificial terms for numerical stability are required only for the calculation of shocks, in which there would otherwise be a tendency for f-trons to cross over one another. Analytical and calculational results show that no such terms are required for rarefactions or contact surfaces. Accordingly, it is important that the forms of the q terms be chosen in such a way as to avoid the introduction of excessive diffusive (or other) effects where they are not needed.

The usual concept of an "artificial viscosity" is illustrated by choosing $q_1 = 0$, $q_2 = -(V)(\partial u/\partial x)$, and $q_3 = uq_2$, in which V is a constant. A test of this, however, shows that it does not prevent ρ-tron crossover in shocks.

A better form is

$$\left.\begin{aligned} q_1 &= -V\frac{\partial \rho}{\partial x}, \\ q_2 &= -V\frac{\partial m}{\partial x}, \\ q_3 &= -V\frac{\partial e}{\partial x}, \end{aligned}\right\} \tag{27}$$

in which again V is a constant. With this, the smeared thickness of a shock can be estimated as

$$\text{thickness} \approx \frac{4V}{\delta U},$$

in which δU is the velocity jump across the shock.

With Eq. (27) it is not sufficient to simply set the q terms to zero for every f-tron pair that is moving apart. This could still allow for a spreading effect of any drift perturbation that would occur, for example, at the bounding f-trons of a contact discontinuity. In addition to vanishing q terms for spreading f-trons, it is useful to require that V be proportional to the magnitude of the gradient of some quantity (velocity, for example) that should be constant across the contact discontinuity.

Other forms of the q terms can also be envisioned. For example,

$$q_1 = -V\rho \frac{\partial u}{\partial x},$$

$$q_2 = -Vm \frac{\partial u}{\partial x},$$

$$q_3 = -Ve \frac{\partial u}{\partial x}.$$

This, too, has been tested in numerical calculations, but has not proved very successful in preventing f-tron crossovers.

Initial and Boundary Conditions

Initial conditions for a calculation program that does not allow for f-tron creation or destruction must contain f-trons of all those magnitudes that will be required. Relatively few interesting problems can be investigated with such a limited program. In general, with the incorporation of all required capabilities, the computer program can commence a calculation with nearly arbitrary initial conditions. In some cases, however, it is likely that the use of very small f-tron intervals adjacent to larger ones will result in numerical difficulties.

In many cases of interest, the boundary conditions of the problem can be described uniquely in terms of fluxes at some position (perhaps moveable) in space. At a rigid wall, for example, there is no flux of mass or energy, and the pressure gradient is flat.

One way to achieve the prescription of fluxes is by means of image f-trons. A rigid wall at $x = 0$, for example, would have image ρ-tron, m-tron and e-tron at coordinates that are always the negative of the first real corresponding f-tron within the true fluid region. The image m and u values would be the negatives of the corresponding interior values; while the image values of p and e would be the same as the interior values.

For prescribed inflow conditions at a wall, the image and interior values would average to the prescribed wall values. Prescribed inflow can also be accomplished by simply placing f-trons with the inflow properties at the wall position.

Free-surface boundary conditions would also be described by null fluxes of mass and energy; in addition, the flux of momentum would have to vanish.

In testing or applying the methodology, the general prescription for deriving boundary conditions is, therefore, much like those that are used in most other types of numerical solution techniques. It is necessary to assure the proper flux and gradient values, for which purpose the introduction of image f-trons or prescribed position f-trons will usually be convenient.

Two Examples

The DOC method as described so far is illustrated by the calculations of a propagating shock and a propagating rarefaction. Neither requires the creation or destruction of *f*-trons.

Figure 1 shows the *f*-tron positions and theoretical solution for a rarefaction fan moving to the right from an initial position very close to the left wall. The center of self-similarity is located at the left side of the figure. The *f*-tron values were chosen to have nonequal intervals; agreement with the analytical solution is nevertheless good.

In Fig. 2 are plotted the *f*-tron positions for a shock traveling to the right. In this case the *f*-tron intervals are uniform. The numerical shock position lies slightly to the right of the analytical prediction, an error that resulted from an effect occurring just after the calculation began, but getting no worse thereafter. The *e*-trons are not shown because they lie almost exactly in the same positions as the *m*-trons. The *q* terms are as shown in Eq. (27), with V equal to a constant value. Comparison runs with several V values show only the expected changes in shock width. In each case there was the same initial adjustment that puts the shock

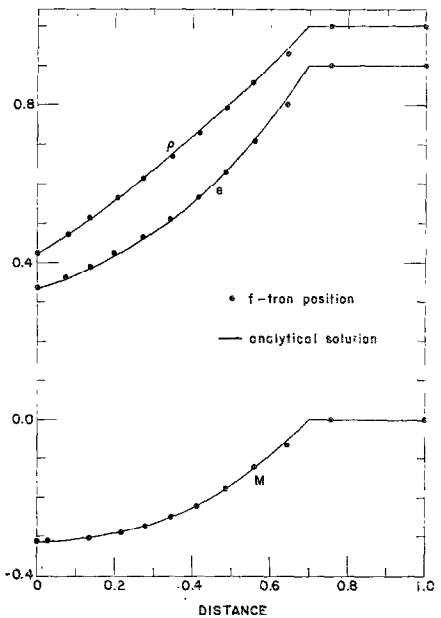

FIG. 1. Comparison of numerical and analytical solutions for a rarefaction moving towards the right.

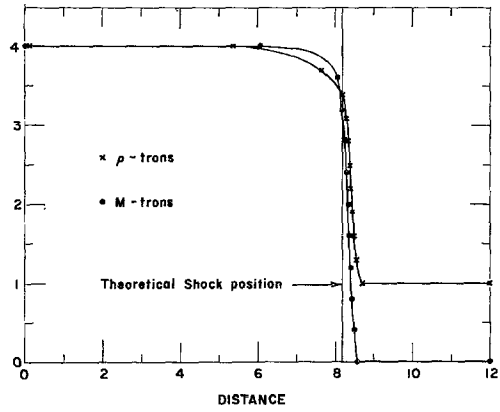

FIG. 2. Numerical solution for the example of a shock moving towards the right. Initially the shock was at the left of the figure.

ahead of its proper position, with correct shock speed thereafter. Comparison runs were also made to show the effects of the two types of flux expressions, Eqs. (23)–(25) and Eqs. (23a)–(25a). The results are so nearly the same that they would not be visible on the scale of Fig. 2.

The initial conditions for these calculations are specified by supplying the appropriate *f*-tron coordinates for the problem in a short spatial interval near the left boundary. For the shock, for example, the *f*-trons were located in such a way as to represent a linear variation of each profile across the spatial interval from 1.0 to 2.0. For the various values of V, this spacing would then either increase or decrease as the shock subsequently propagated to the right. For the rarefaction, the initial spacing extended from 0.0 to 0.2. In both cases, the *f*-trons at the wall supplied the required boundary conditions.

CREATION AND DESTRUCTION OF *f*-TRONS

It often occurs in fluid flow that the value of some field variables increases locally to values that exceed those of the adjacent fluid elements. To resolve such a situation, the creation of *f*-trons will be required. Conversely, the smoothing of an extremal in some field variable value will require the destruction of *f*-trons. Both of these processes, creation and destruction in the vicinity of an extremal, proceed in pairwise steps.

A related process can also be found, which requires *f*-tron splitting or coalescense. Where the spatial variation of some field variable had been monotonic, there may arise an inflection. The simultaneous or subsequent vanishing of the field-variable

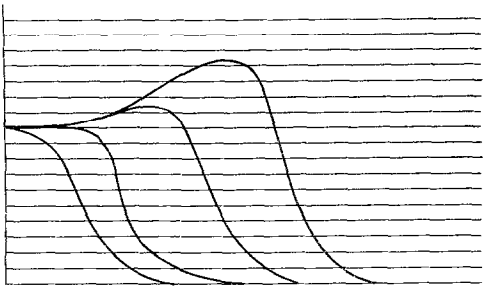

FIG. 3. Qualitative illustration of pairwise f-tron creation for an increasing extremal in a profile propagating to the right.

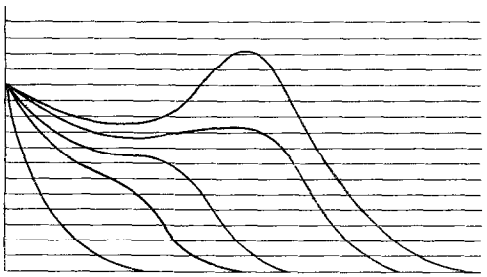

FIG. 4. Qualitative illustration of triplet slitting at a horizontal inflection, and subsequent pair creation and destruction in extremals. The profile is propagating to the right.

gradient will then require the splitting of one f-tron into three, the new lateral ones having the same f value as that of the central one.

These two processes are illustrated in Figs. 3 and 4. The horizontal lines in the figures show the equal-interval f-tron levels, while the curves show a hypothetical sequence of field-variable profiles at a succession of times. (For both figures, the profile propagates to the right as time increases.)

For the creation or destruction of f-tron pairs, we note the following features:

1. Creation of a pair of equal-valued f-trons will always occur only between members of a pre-existing pair of equal-valued f-trons, and only if they are moving apart from each other.

2. Destruction of f-trons can only occur in pairs, involving two of equal value that are moving towards each other.

3. One member of a pair may be an image f-tron, across a boundary position and outside of the region of the true fluid.

4. Each f-tron pair requires data as to the extremal level for the region

between the pair members. Let the pair be numbers j and $j + 1$, and let $f_{j+1/2}$ be the extremal value for the interval. Then $f_{j+1/2}$ varies according to the equation

$$\frac{\partial f_{j+1/2}}{\partial t} = \frac{(F_f)_j - (F_f)_{j+1}}{x_{j+1} - x_j},$$

in which the fluxes are evaluated at the pair-member positions. Whenever $f_{j+1/2} - f_j$ changes sign, the pair should be destroyed, with $f_{j+1/2}$ becoming the in-between value for f-trons $j - 1$ and $j + 2$. (Note that f_{j-1} and f_{j+2} would be equal to each other, except in the case of triplet coalescence, for which see below.) Conversely, whenever $f_{j+1/2}$ lies outside the interval $f_j \pm \delta f$, where δf is the fixed f-tron interval, then a new pair would be required, with $f_{j+1/2}$ again becoming the in-between value for the new pair, and $f_j \pm \delta f$ being the f-tron value for the new pair members.

5. The coordinates of the newly created f-tron pair can be determined by passing a parabolic f profile among f_j, $f_{j+1/2}$, and f_{j+1}, assuming that $f_{j+1/2}$ is located at the midpoint between the preexisting pair, for which the coordinates are x_j and x_{j+1}. The resulting coordinates for the new pair are

$$\frac{1}{2}(x_{j+1} + x_j) \pm (x_{j+1} - x_j)\left[1 - \frac{\delta f}{f_{j+1/2} - f_j}\right]^{1/2}.$$

This equation is also valid if $\delta f < 0$ and $f_{j+1/2} < f_j$.

For the coalescence of an f-tron triplit, or the splitting into a triplet, there also are some guiding ideas that can be described.

1. Coalescence must always occur in triplets. Thus, whenever the criterion for pair destruction is satisfied, a test should be made of the f values of the f-trons adjacent to the pair. If one or the other has the same value as that of the pair members, then triplet coalescence is indicated, the two lateral members of the triplet being destroyed with the central one remaining at its former coordinate and f value.

2. The criterion for triplet creation would seem most appropriately to be based upon the distance to nearest adjacent neighbors. In general, it should be based on the reversal in sign of $\partial f/\partial x$, but this cannot be sensed in the method as here proposed. Instead, the occurrence of isolation for any particular f-tron should be taken as indicative of the tendency to a reversal of the sign of $\partial f/\partial x$, so that a trial splitting should be made whenever the nearest distance to a neighboring f-tron exceeds some specified or calculated value, D. All members of the newly created triplet will have the same f values. What must be determined are the coordinates of the lateral members, and the in-between f values for each of the pairs, of which the central one is the original f-tron with unchanged coordinate,

and is a common member for each pair. Note, however, that Eq. (22) will give trouble for an f-tron triplet, indicating that in this special case, the value of u_f for the central member should probably be calculated as an average of the values for the two lateral members.

3. The coordinates of the lateral members formed on each side of the central f-tron, which is number j, should be $x_j - \xi D$ and $x_j + \xi D$, where D is the criterion distance and ξ is a numerical constant less than about 0.5.

4. The in-between f values, denoted by $f_{j-1/2}$ and $f_{j+1/2}$, should differ from f_j by equal magnitudes, one value exceeding f_j and the other being less. Let $j - 1$ and $j + 1$ still refer to the preexisting lateral neighbors of f-tron number j, before the triplet splitting. If $f_{j-1} < f_j$, then we expect $f_{j+1} > f_j$; otherwise, f-tron number j would have to be one member of an equal-valued pair. In this case, we expect $f_{j-1/2} > f_j$ and $f_{j+1/2} < f_j$, in order that a true inflection is represented. Conversely, if $f_{j-1} > f_j$, then $f_{j+1} < f_j$; and we expect $f_{j-1/2} < f_j$, $f_{j+1/2} > f_j$. To calculate $f_{j\pm1/2}$, we pass an antisymmetric cubic among f-trons at x_j, $x_j + \xi D$ and x_{j+1}, at which points the f values are, respectively, f_j, f_j, and $f_j + \delta f$. Then $f_{j+1/2}$ is evaluated at $x_j + \frac{1}{2}\xi D$, with the result

$$f_{j\pm1/2} = f_j \mp \left(\frac{3}{8}\right)\left(\frac{\xi^3\,\delta f}{1 - \xi^2}\right).$$

This formula would also be valid if $\delta f < 0$.

5. With these procedures for triplet creation completed, each pair can then continue in the pair-wise fashion described previously. As the extremals of the inflection increase in amplitude, additional pairs should be inserted whenever the creation criterion is satisfied. In addition, as in Fig. 4, pair-wise destruction may be appropriate, even resulting in the annihilation of the original f-tron which had split into the triplet. At a later stage, if both extremals of the inflection have decayed sufficiently in amplitude then a triplet coalescence will be the final stage of the smoothing process, the center of the coalescence usually being an entirely different f-tron from that which had originally split.

Cylindrical or Spherical Coordinates

For one-dimensional fluid dynamics investigations in cylindrical or spherical geometries, the basic DOC methodology remains the same. The flux equations must be properly modified to include the appropriate functions of radius; the examination of conservation requires a slightly different definition of volume; and the creation-destruction processes require slight modifications for the

in-between-value formulas. These generalizations are easily accomplished, so that the detailed formulas need not be written here.

Multi-Fluid Problems

If a problem involves several different types of material, then Lagrangian markers are useful for definition of the interface position. Some types of f-trons will pass easily over the interface; others (for example, ρ-trons) may tend to accumulate at an interface, just as they would at a contact discontinuity within a one-component fluid. This close-packing at an interface may lead to numerical instability, unless special procedures are used for those f-trons for which proximity to an interface marker is sensed. One technique that seems worth trying is to have the interface markers serve as source or sink positions for f-trons.

Several Space Dimensions

DOC methodology for fluid dynamics calculations in several space dimensions is complicated by one particular difficulty, namely, defining the volume of space about each f-tron. In two dimensions, an f-tron is a contour line; in three dimensions, it is a contour surface; in each case, the volume (per unit contour length or area) must be given by the sum of the distances half-way to the two adjacent f-trons. If the contours are not too strongly distorted, the volume definition becomes relatively unambiguous. For strongly distorted contours (for example, during the process of pair-wise mutual destruction of two adjacent f-trons) the definition may become extremely difficult to formulate.

Nevertheless, it seems entirely possible that a multidimensional version of the DOC method will be feasible, giving a powerful methodology with optimal distribution of resolution.

Conclusion

The DOC method has been described as a novel procedure for numerically solving problems in the dynamics of compressible fluids. Proof tests indicate that the technique will have several advantages over all others. The principal advantage is the automatic achievement of fine resolution wherever required.

While this report describes some of the necessary procedures for applying DOC methodology, it is clear that further developments will require considerable innovation in solving the difficulties that inevitably arise.

Interested investigators can find somewhat similar methodology applied to solving the Vlasov equation [3], and the heat conduction equation [4].

ACKNOWLEDGMENTS

I am very grateful to W. E. Pracht for helpful discussions during the formulation of these ideas. The computer program was written and applied to various test problems by B. E. Thompson and N. C Romero, to whom I am also grateful. References [3] and [4] were brought to my attention by a referee, and by Dr. J. Nachamkin

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