JOURNAL OF COMPUTATIONAL PHYSICS 8, 197–213 (1971)

A Numerical Fluid Dynamics Calculation Method for All Flow Speeds

FRANCIS H. HARLOW AND ANTHONY A. AMSDEN*

University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544

Received December 7, 1970

The ICE technique for numerical fluid dynamics has been revised considerably, and generalized in such a way as to extend the applicability to fluid flows with arbitrary equation of state and the full viscous stress tensor. The method is useful for the numerical solution of time-dependent fluid flow problems in several space dimensions, for all Mach numbers from zero (incompressible limit) to infinity (hypersonic limit). This new version is considerably less complicated than the original form. The present description does not assume a familiarity with the previous one.

INTRODUCTION

An Implicit Continuous-fluid Eulerian (ICE) technique has been proposed [1] for the solution of time-dependent problems in multidimensional fluid dynamics, in which the Mach number may vary from zero to infinity. Test calculations have shown that the method as originally proposed works well, even though its scope of applicability is fairly limited. The crucial features that enable this are the advanced-time (implicit) treatment of the density in the equation of state and of the density and velocity in the mass equation. Accordingly, the technique reduces essentially to the MAC method for incompressible flow [2] as the sound speed becomes infinite, and to an implicit variant of the usual Eulerian techniques [3] as the sound speed becomes small.

In this paper, a modified ICE method is described, in which the procedure is considerably simplified and the scope of applicability is greatly extended. In particular, the present modified form

1. is applicable to arbitrary equation of state,
2. introduces a more meaningful variable for the Poisson equation,
3. reduces the finite-difference Poisson equation to a five-point form, with considerably simplified coefficients,

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

4. incorporates the correct, full viscous stress tensor, instead of a simple artificial viscosity,

5. is time-centered in such a way as to eliminate some undesirable low-order truncation errors,

6. contains an optional mass-diffusion term, which can enhance the numerical accuracy or stability in some circumstances,

7. is applicable to free-surface flows, as well as to those that are confined,

8. can be used for both plane and cylindrically symmetric calculations.

The following discussion describes the modified technique in detail, shows some properties of this type of implicit solution procedure, and demonstrates the applicability by means of results from a typical calculation.

The essential features of the methodology can be summarized as follows. We start from conservative differential equations for the transport of mass, momentum, and energy. The flow region is subdivided into an Eulerian mesh of rectangular cells, and the equations are approximated by conservative finite-difference expressions relative to these cells. In addition, the time advancement progresses through a sequence of finite intervals, the results of each cycle being calculated from data remaining from the previous cycle, or supplied as initial conditions.

In the mass equation, the convective fluxes are expressed as functions of the unknown advanced-time densities and velocities. Likewise, the pressure in the momentum equations is expressed as a function of the unknown advanced-time density. From these equations, the undetermined velocities can be eliminated, giving a Poisson equation for the new densities. Conversion of this to an equation for the pressure produces the Poisson equation that actually is solved. From the results can then be found densities and velocities for the new cycle. Finally, the energy changes are computed.

The Differential Equations

This solution process is illustrated for calculations in cylindrical coordinates with axial symmetry. For problems in plane coordinates, the equations are easily modified by replacing $r \to 1.0$ throughout. In the computer program this transformation can be exploited to increase the versatility considerably. In conservative form, with gravity parallel to the axis, the equations can be written

$$\frac{\partial \rho}{\partial t} + \frac{1}{r}\frac{\partial \rho u r}{\partial r} + \frac{\partial \rho v}{\partial z} = \tau\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \rho}{\partial r}\right) + \frac{\partial^2 \rho}{\partial z^2}\right], \tag{1}$$

$$\frac{\partial \rho u}{\partial t} + \frac{1}{r}\frac{\partial \rho u^2 r}{\partial r} + \frac{\partial \rho u v}{\partial z} = -\frac{\partial}{\partial r}(p+q) + \mu\frac{\partial}{\partial z}\left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r}\right), \tag{2}$$

$$\frac{\partial \rho v}{\partial t} + \frac{1}{r}\frac{\partial \rho uvr}{\partial r} + \frac{\partial \rho v^2}{\partial z} = \rho g - \frac{\partial}{\partial z}(p+q) - \frac{\mu}{r}\frac{\partial}{\partial r}\left[r\left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r}\right)\right], \tag{3}$$

$$\frac{\partial \rho E}{\partial t} + \frac{1}{r}\frac{\partial \rho uEr}{\partial r} + \frac{\partial \rho vE}{\partial z} = \rho vg + \frac{1}{r}\frac{\partial}{\partial r}\left\{r\left[B\mu\frac{\partial I}{\partial r} - pu - \left(\frac{\lambda}{\lambda+2\mu}\right)qu + \frac{\mu}{2}\frac{\partial}{\partial r}(2u^2+v^2) + \mu v\frac{\partial u}{\partial z}\right]\right\} + \frac{\partial}{\partial z}\left\{B\mu\frac{\partial I}{\partial z} - pv - \left(\frac{\lambda}{\lambda+2\mu}\right)qv + \frac{\mu}{2}\frac{\partial}{\partial z}(u^2+2v^2) + \mu u\frac{\partial v}{\partial r}\right\}, \tag{4}$$

where

$$q \equiv -(\lambda+2\mu)\left(\frac{1}{r}\frac{\partial ur}{\partial r} + \frac{\partial v}{\partial z}\right), \tag{5}$$

and

$$E \equiv I + (u^2+v^2)/2. \tag{6}$$

The pressure p is a prescribed function of the density ρ, and of the specific internal energy I; u and v are the radial (r) and axial (z) velocity components, respectively. The temperature in the heat conduction term has been eliminated by means of the constant coefficient B. For simplicity, the viscosity coefficients λ and μ have been chosen to be constants; in general, the incorporation of variable viscosity coefficients has no conceptual effect on the methodology, being manifested simply by changes in form of the R and S functions, defined below, and of the energy equation, which is treated separately at the end of the cycle. An additional coefficient τ has been utilized to allow for a mass diffusion term in Eq. (1); in most cases, $\tau = 0$, but in a few circumstances a negative mass diffusion ($\tau < 0$) can assist in the removal of an undesirable low-order truncation-error term in the finite-difference expressions, while a positive mass diffusion ($\tau > 0$) may sometimes be necessary for numerical stability.

In addition to the advantage of simplicity for the present demonstration, the use of constant viscosity coefficients yields terms that demonstrate quite close similarity to the "artificial viscosity" terms that ordinarily are used in both low-speed [2] and high-speed [3] flow calculations. Indeed, the relationship to usual forms of the artificial viscosity is considerably enhanced by replacing $\lambda \to \rho\lambda$ and $\mu \to \rho\mu$. For some types of problems, we have found this to be very useful for the purpose of enabling the viscosity stability condition to remain unchanged through a calculation.

The Difference Equations

A fragment of the Eulerian finite-difference mesh is shown in Fig. 1, which illustrates the centering of the field variables relative to a typical cell. The index i counts cell centers from left to right, while j counts them from bottom to top. Accordingly, quantities defined at cell edges are labeled with indices $i \pm \frac{1}{2}$ or $j \pm \frac{1}{2}$. Thus, for example, Eq. (5) becomes

$$q_{i,j} = -(\lambda + 2\mu)\left[\frac{1}{r_i\,\delta r}\left(r_{i+1/2}u_{i+1/2,j} - r_{i-1/2}u_{i-1/2,j}\right) + \frac{1}{\delta z}\left(v_{i,j+1/2} - v_{i,j-1/2}\right)\right], \tag{7}$$

in which δr and δz are the dimensions of a cell.

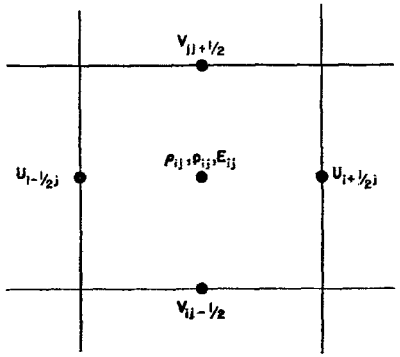

FIG. 1. Layout of variables and indices in the mesh.

For the finite-difference forms of the momentum equations, it is convenient to separate those parts that will contain no advanced-time factors. For such terms no additional index is required. Thus, we define

$$\begin{aligned} R_{i+1/2,j} \equiv{}& \frac{1}{r_{i+1/2}\,\delta r}\left[u_{i+1/2,j}(\rho_{i,j}r_i u_{i-1/2,j} - \rho_{i+1,j}r_{i+1}u_{i+3/2,j})\right] \\ &+ \frac{1}{\delta z}\left[(\rho uv)_{i+1/2,j-1/2} - (\rho uv)_{i+1/2,j+1/2}\right] + \frac{1}{\delta r}\left(q_{i,j} - q_{i+1,j}\right) \\ &+ \frac{\mu}{\delta z}\left[\frac{u_{i+1/2,j+1} - u_{j+1/2,j}}{\delta z} - \frac{v_{i+1,j+1/2} - v_{i,j+1/2}}{\delta r}\right. \\ &\left. - \frac{u_{i+1/2,j} - u_{i+1/2,j-1}}{\delta z} + \frac{v_{i+1,j-1/2} - v_{i,j-1/2}}{\delta r}\right], \end{aligned} \tag{8}$$

and

$$S_{i,j+1/2} \equiv \frac{1}{r_i\,\delta r}\left[(\rho uvr)_{i-1/2,j+1/2} - (\rho uvr)_{i+1/2,j+1/2}\right]$$

$$+ \frac{1}{\delta z}\left[v_{i,j+1/2}(\rho_{i,j}v_{i\,j-1/2} - \rho_{i,j+1}v_{i,j+3/2})\right] + \frac{1}{\delta z}(q_{i,j} - q_{i,j+1}) + g\rho_{i,j+1/2}$$

$$- \frac{\mu}{r_i\,\delta r}\left[r_{i+1/2}\left(\frac{u_{i+1/2,j+1} - u_{i+1/2,j}}{\delta z} - \frac{v_{i+1,j+1/2} - v_{i,j+1/2}}{\delta r}\right)\right.$$

$$\left. - r_{i-1/2}\left(\frac{u_{i-1/2,j+1} - u_{i-1/2,j}}{\delta z} - \frac{v_{i,j+1/2} - v_{i-1,j+1/2}}{\delta r}\right)\right]. \tag{9}$$

The cell-centered convection terms in Eqs. (8) and (9) have been put into ZIP form, according to which, for example,

$$(u_{i,j})^2 \rightarrow u_{i-1/2,j}u_{i+1/2,j}\,.$$

This accomplishes the useful purpose of removing one of the low-order truncation-error terms [4]. A donor-cell form [4] for the convection fluxes may also occasionally be useful, especially for problems that start from violently discontinuous initial conditions; see discussion below for the one-dimensional analog.

With these defined quantities, the momentum equations can be written

$$\frac{(\rho u)^{n+1}_{i+1/2,j} - (\rho u)^{n}_{i+1/2,j}}{\delta t} = \frac{\phi}{\delta r}(\bar{p}_{i,j} - \bar{p}_{i+1,j}) + \frac{(1-\phi)}{\delta r}(p^{n}_{i,j} - p^{n}_{i+1,j}) + R_{i+1/2,j}\,, \tag{10}$$

$$\frac{(\rho v)^{n+1}_{i,j+1/2} - (\rho v)^{n}_{i,j+1/2}}{\delta t} = \frac{\phi}{\delta z}(\bar{p}_{i,j} - \bar{p}_{i,j+1}) + \frac{(1-\phi)}{\delta z}(p^{n}_{i,j} - p^{n}_{i,j+1}) + S_{i,j+1/2}\,, \tag{11}$$

in which the index, $n+1$, indicates an advanced-time value, while the bar over p denotes a hybrid function, defined below. The weighting constant ϕ, with magnitude between 0.0 and 1.0, denotes the relative level of time centering of the pressure term. For $\phi = 1.0$, that term is at the advanced time, as in the original version of ICE, whereas for $\phi = 0.5$ the term is exactly time-centered, insofar as certain crucial truncation-error terms are concerned. For $\phi = 0.0$, the method is purely explicit, closely resembling previous Eulerian techniques [3]. It is the flexibility of variable ϕ that enables a comparison to be made between the potentially more accurate time-centered version and the completely advanced-time form, which had previously been tested.

The hybrid function $\bar{p}$ is formed from the equation-of-state pressure function

$p(\rho, I)$ in a manner similar to that used by Janenko and Neuvazaev [5] for a somewhat different purpose.

$$\bar{p}_{i,j} \equiv p^n_{i,j} + c^n_{i,j}(\rho^{n+1}_{i,j} - \rho^n_{i,j}), \tag{12}$$

where $c^n_{i,j} \equiv (\partial p/\partial \rho)^n_{i,j}$ is closely related to the speed of sound. (With a constant specific heat, $c_{i,j}$ is the square of the isothermal sound speed.) Thus $\bar{p}_{i,j}$ singles out from the equation of state its principal dependence upon the density and for it uses the advanced-time density, while the rest remains at the beginning-of-cycle values. This should not be interpreted as neglecting the effects of internal energy variations on the pressure. It simply means that those variations must be treated implicitly for the density, but can remain purely explicit for the internal energy. The usual purely explicit techniques for high-speed Eulerian calculations treat *both* variations explicitly in the equation of state, which can be accomplished in the present method simply by setting $\theta = \phi = 0$, in which case the calculational results are independent of the value of $c^n_{i,j}$.

In a similar fashion, the right side of the finite-difference mass equation can be weighted between a purely explicit form and an advanced time form, utilizing a constant θ such that $0.0 \leqslant \theta \leqslant 1.0$.

$$\begin{aligned}
\frac{\rho^{n+1}_{i,j} - \rho^n_{i,j}}{\delta t} = {} & \frac{\theta}{r_i\,\delta r}\left[(\rho u)^{n+1}_{i-1/2,j} r_{i-1/2} - (\rho u)^{n+1}_{i+1/2,j} r_{i+1/2}\right] \\
& + \frac{(1-\theta)}{r_i\,\delta r}\left[(\rho u)^{n}_{i-1/2,j} r_{i-1/2} - (\rho u)^{n}_{i+1/2,j} r_{i+1/2}\right] \\
& + \frac{\theta}{\delta z}\left[(\rho v)^{n+1}_{i,j-1/2} - (\rho v)^{n+1}_{i,j+1/2}\right] + \frac{1-\theta}{\delta z}\left[(\rho v)^{n}_{i,j-1/2} - (\rho v)^{n}_{i,j+1/2}\right] \\
& + \frac{\tau}{r_i\,\delta r^2}\left[r_{i+1/2}(\rho^n_{i+1,j} - \rho^n_{i,j}) - r_{i-1/2}(\rho^n_{i,j} - \rho^n_{i-1,j})\right] \\
& + \frac{\tau}{\delta z^2}\left[\rho^n_{i,j+1} + \rho^n_{i,j-1} - 2\rho^n_{i,j}\right].
\end{aligned} \tag{13}$$

In Eqs. (10), (11), and (13) there occur the quantities $(\rho u)^{n+1}_{i\pm 1/2,j}$ and $(\rho v)^{n+1}_{i,j\pm 1/2}$, which must be eliminated by algebraic substitution. The process of doing so introduces the quantity $G_{i,j}$ which is formed entirely of data available at the

beginning of the cycle. Also, the occurrence of $\rho_{i,j}^{n+1}$ is eliminated by means of Eq. (12). Thus, with

$$G_{i,j} \equiv \frac{p_{i,j}^n}{c_{i,j}^n} + \frac{\theta \delta t^2}{r_i \delta r}\left[\frac{r_{i-1/2}(1-\phi)}{\delta r}(p_{i-1,j}^n - p_{i,j}^n)\right.$$

$$\left. - \frac{r_{i+1/2}(1-\phi)}{\delta r}(p_{i,j}^n - p_{i+1,j}^n) + r_{i-1/2}R_{i-1/2,j} - r_{i+1/2}R_{i+1/2,j}\right]$$

$$+ \frac{\theta \delta t^2}{\delta z}\left[\frac{1-\phi}{\delta z}(p_{i,j-1}^n + p_{i,j+1}^n - 2p_{i,j}^n) + S_{i,j-1/2} - S_{i,j+1/2}\right]$$

$$+ \frac{\delta t}{r_i \delta r}[r_{i-1/2}(\rho u)_{i-1/2,j}^n - r_{i+1/2}(\rho u)_{i+1/2,j}^n] + \frac{\delta t}{\delta z}[(\rho v)_{i,j-1/2}^n - (\rho v)_{i,j+1/2}^n]$$

$$+ \frac{\tau \delta t}{r_i \delta r^2}[r_{i+1/2}(\rho_{i+1,j}^n - \rho_{i,j}^n) - r_{i-1/2}(\rho_{i,j}^n - \rho_{i-1,j}^n)]$$

$$+ \frac{\tau \delta t}{\delta z^2}(\rho_{i,j+1}^n + \rho_{i,j-1}^n - 2\rho_{i,j}^n), \tag{14}$$

the equation to be solved for $\bar{p}_{i,j}$ is

$$\bar{p}_{i,j}\left[\frac{1}{c_{i,j}^n} + 2\theta\phi\,\delta t^2\left(\frac{1}{\delta r^2} + \frac{1}{\delta z^2}\right)\right]$$

$$= G_{i,j} + \theta\phi\,\delta t^2\left[\frac{r_{i-1/2}\bar{p}_{i-1,j} + r_{i+1/2}\bar{p}_{i+1,j}}{r_i \delta r^2} + \frac{\bar{p}_{i,j-1} + \bar{p}_{i,j+1}}{\delta z^2}\right]. \tag{15}$$

If an iterative procedure is to be used for the solution of Eq. (15), there is a transformation that is useful for calculations with large spatial variations in density. Let $\sigma_{i,j} \equiv \bar{p}_{i,j}/\rho_{i,j}^n$; find the iterative solution for $\sigma_{i,j}$; and then convert this back to the required $\bar{p}_{i,j}$.

This completes the basic derivation of those equations that especially characterize the features of our revised ICE procedure. In summary, the procedure for a calculation cycle is as follows:

1. Calculate the required beginning-of-cycle terms, $R_{i+1/2,j}$, $S_{i,j+1/2}$, $G_{i,j}$,
2. Solve for $\bar{p}_{i,j}$ for every cell, using Eq. (15). For some circumstances, a direct solution method can be used; for others it may be necessary to employ a relaxation technique,
3. Solve for $\rho_{i,j}^{n+1}$, using Eq. (12),
4. Solve for the new values of the velocities, using Eqs. (10) and (11),

5. Calculate the new energy for every cell, using the following finite-difference approximation to Eq. (4):

$$
\begin{aligned}
(\rho E)^{n+1}_{i,j} = (\rho E)^{n}_{i,j} + \delta t \Big\{ & \frac{1}{r_i\,\delta r}\left[(\rho u E r)_{i-1/2,j} - (\rho u E r)_{i+1/2,j}\right] \\
& + \frac{1}{\delta z}\left[(\rho v E)_{i,j-1/2} - (\rho v E)_{i,j+1/2}\right] + \rho_{i,j} v_{i,j} g \\
& + \frac{1}{r_i\,\delta r}\Big[r_{i+1/2}\Big[\frac{B\mu}{\delta r}(I_{i+1,j} - I_{i,j}) - \bar{p}_{i+1/2,j} u_{i+1/2,j} \\
& - \frac{\lambda}{\lambda + 2\mu} u_{i+1/2,j} q_{i+1/2,j} + \frac{\mu}{2\delta r}(2u^2_{i+1,j} + v^2_{i+1,j} - 2u^2_{i,j} - v^2_{i,j}) \\
& + \frac{\mu v_{i+1/2,j}}{\delta z}(u_{i+1/2,j+1/2} - u_{i+1/2,j-1/2})\Big] - r_{i-1/2}\Big[\frac{B\mu}{\delta r}(I_{i,j} - I_{i-1,j}) \\
& - \bar{p}_{i-1/2,j} u_{i-1/2,j} - \frac{\lambda}{\lambda + 2\mu} u_{i-1/2,j} q_{i-1/2,j} \\
& + \frac{\mu}{2\delta r}(2u^2_{i,j} + v^2_{i,j} - 2u^2_{i-1,j} - v^2_{i-1,j}) \\
& + \frac{\mu v_{i-1/2,j}}{\delta z}(u_{i-1/2,j+1/2} - u_{i-1/2,j-1/2})\Big]\Big] + \frac{1}{\delta z}\Big[\Big[\frac{B\mu}{\delta z}(I_{i,j+1} - I_{i,j}) \\
& - \bar{p}_{i,j+1/2} v_{i,j+1/2} - \frac{\lambda}{\lambda + 2\mu} v_{i,j+1/2} q_{i,j+1/2} + \frac{\mu}{2\delta z}(u^2_{i,j+1} + 2v^2_{i,j+1} \\
& - u^2_{i,j} - 2v^2_{i,j}) + \frac{\mu u_{i,j+1/2}}{\delta r}(v_{i+1/2,j+1/2} - v_{i-1/2,j+1/2})\Big] \\
& - \Big[\frac{B\mu}{\delta z}(I_{i,j} - I_{i,j-1}) - \bar{p}_{i,j-1/2} v_{i,j-1/2} - \frac{\lambda}{\lambda + 2\mu} v_{i,j-1/2} q_{i,j-1/2} \\
& + \frac{\mu}{2\delta z}(u^2_{i,j} + 2v^2_{i,j} - u^2_{i,j-1} - 2v^2_{i,j-1}) \\
& + \frac{\mu u_{i,j-1/2}}{\delta r}(v_{i+1/2,j-1/2} - v_{i-1/2,j-1/2})\Big]\Big]\Big\},
\end{aligned}
\tag{16}
$$

together with an equation for the specific internal energy,

$$
I_{i,j} = E_{i,j} - \tfrac{1}{8}[(u_{i+1/2,j} + u_{i-1/2,j})^2 + (v_{i,j+1/2} + v_{i,j-1/2})^2]. \tag{17}
$$

Time indices have been omitted from most of Eq. (16); we ordinarily use the advanced-time densities and velocities, but there may be circumstances in which the previous-cycle values should be used.

In most of the equations, there are ambiguities regarding quantities that are required at localities other than those for which they are stored. In every case, these are to be formed of appropriate averages of nearby values. For example,

$$u_{i+1/2,j+1/2} \equiv \tfrac{1}{2}(u_{i+1/2,j} + u_{i+1/2,j+1}),$$
$$u_{i,j+1/2} \equiv \tfrac{1}{4}(u_{i+1/2,j} + u_{i+1/2,j+1} + u_{i-1/2,j} + u_{i-1/2,j+1}).$$

Initial and Boundary Conditions

The original ICE technique [1] required pre-initial-time data as well as the usual array of initial conditions. This is not true for the present version. Accordingly, all that is required is a program setup for generating the distribution of variable values throughout the mesh and appropriate for representing the desired initial configuration of the fluid. The calculation carries on from there.

Boundary conditions are derived in such a way as to describe the various walls or surfaces that may occur. These are of several types:

1. No-slip rigid walls,
2. Free-slip rigid walls,
3. Prescribed-input walls,
4. Prescribed-output walls,
5. Continuative-output walls,
6. Moveable surface adjacent to a vacuum,
7. Moveable surface adjacent to an applied pressure,
8. Moveable surface adjacent to another fluid.

The first four are uniquely specified by the behavior of the normal and tangential velocity components, by the constraints these imply through the dynamical equations for their variations, and by the prescribed nature of the temperature or the heat flux. The fifth has no unique prescription, but must be derived in such a way as to have minimal effect on the flow in the region of interest.

For the moveable surfaces the guiding principle is that of stress continuity; for a free surface, for example, the normal and tangential stresses must both vanish. The prescriptions resemble those of the MAC and SMAC methods [2] for incompressible fluid flow calculations.

A One-Dimensional Analogy

A summary of the properties of the new ICE method has been given for a version of the program with allowance for a free surface [6]. Here, we illustrate some of the properties through an examination of a one-dimensional version. Analogous to Eqs. (1) and (2), the starting point is

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = \tau \frac{\partial^2 \rho}{\partial x^2},$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u^2}{\partial x} = -\frac{\partial (p + q)}{\partial x}.$$

For the viscosity function q, we choose for illustration

$$q = -\lambda \frac{\partial u}{\partial x}.$$

Again, it is convenient to define, in analogy to Eq. (8),

$$R_{i+1/2} \equiv \frac{1}{\delta x}\left[u_{i+1/2}(\rho_i u_{i-1/2} - \rho_{i+1} u_{i+3/2}) + q_i - q_{i+1}\right],$$

so that the difference equations become

$$\frac{\rho_i^{n+1} - \rho_i{}^n}{\delta t} = \frac{\theta}{\delta x}\left[(\rho u)_{i-1/2}^{n+1} - (\rho u)_{i+1/2}^{n+1}\right] + \frac{1-\theta}{\delta x}\left[(\rho u)_{i-1/2}^{n} - (\rho u)_{i+1/2}^{n}\right] + \tau(\rho_{i+1}^n + \rho_{i-1}^n - 2\rho_i{}^n), \tag{18}$$

and

$$\frac{(\rho u)_{i+1/2}^{n+1} - (\rho u)_{i+1/2}^{n}}{\delta t} = \frac{\phi}{\delta x}(\bar{p}_i - \bar{p}_{i+1}) + \frac{1-\phi}{\delta x}(p_i{}^n - p_{i+1}^n) + R_{i+1/2}^n. \tag{19}$$

As in Eq. (14), we define

$$G_i \equiv \frac{p_i{}^n}{c_i{}^n} + \frac{\delta t}{\delta x}\left[(\rho u)_{i-1/2}^n - (\rho u)_{i+1/2}^n\right] + \frac{\theta(1-\phi)\,\delta t^2}{\delta x^2}(p_{i-1}^n + p_{i+1}^n - 2p_i{}^n) + \frac{\theta \delta t^2}{\delta x}(R_{i-1/2}^n - R_{i+1/2}^n) + \frac{\tau \delta t}{\delta x^2}(\rho_{i+1}^n + \rho_{i-1}^n - 2\rho_i{}^n),$$

in terms of which the equation to be solved is

$$\frac{\bar{p}_i}{c_i^n} = \frac{\theta\phi\,\delta t^2}{\delta x^2}(\bar{p}_{i-1} + \bar{p}_{i+1} - 2\bar{p}_i) + G_i\,.$$

These expressions for the one-dimensional version form the basis for the discussion in the remainder of the paper, which illustrate restrictions and properties that are directly related to the full methodology.

The Convective Fluxes

There are various ways that the energy and momentum convective fluxes can be written, the precise form being irrelevant to the conceptual formulation of the ICE technique, but nevertheless crucial to the assurance of accuracy and numerical stability of the calculations. At least four types of flux expressions are appropriate for consideration, each having advantages and disadvantages. Consider, for example, the momentum flux term $(\rho u^2)_i$. While the density is already stored for the position at which the flux is to be evaluated (that is, at the center of cell i) the velocity positions are at $i \pm \frac{1}{2}$, so that some type of interpolation is needed.

The four flux expressions to be considered are:

Centered: $$(\rho u)^2{}_i \rightarrow \rho_i(u_{i-1/2} + u_{i+1/2})^2/4,$$

ZIP: $$(\rho u^2)_i \rightarrow \rho_i u_{i-1/2} u_{i+1/2}\,,$$

Partial Donor: $$(\rho u^2)_i \rightarrow \begin{cases} \rho_i u_{i-1/2}(u_{i-1/2} + u_{i+1/2})/2 & \text{for } (u_{i-1/2} + u_{i+1/2}) > 0 \\ \rho_i u_{i+1/2}(u_{i-1/2} + u_{i+1/2})/2 & \text{for } (u_{i-1/2} + u_{i+1/2}) < 0, \end{cases}$$

Complete Donor: $$(\rho u^2)_i \rightarrow \begin{cases} \rho_i u_{i-1/2}^2 & \text{for } (u_{i-1/2} + u_{i+1/2}) > 0 \\ \rho_i u_{i+1/2}^2 & \text{for } (u_{i-1/2} + u_{i+1/2}) < 0. \end{cases}$$

In addition, there is an interpolated donor form, not considered here. For the energy-equation convection terms there are analogous flux expressions for two of these forms:

Centered: $$(\rho u E)_{i+1/2} \rightarrow (\rho_i + \rho_{i+1})\, u_{i+1/2}(E_i + E_{i+1})/4,$$

Donor: $$(\rho u E)_{i+1/2} \rightarrow \begin{cases} \rho_i u_{i+1/2} E_i & \text{for } u_{i+1/2} > 0 \\ \rho_{i+1} u_{i+1/2} E_{i+1} & \text{for } u_{i+1/2} < 0. \end{cases}$$

Some properties of each of these are the following:

1. *Centered.* This form eliminates one order of truncation error in δx, compared with the donor cell flux, but this advantage is overshadowed by the

tendency to numerical instability that is produced by not *time* centering the convective flux. This tendency to instability is usually mitigated by the addition of a counterbalancing diffusive flux (either real or artificial) and can also be tolerated in circumstances in which the growth of the instability is bounded by nonlinear dissipative effects.

2. *ZIP.* This form is also one order more "accurate" in δx than the donor cell flux, but, in addition, has the advantages of eliminating a nonlinear contribution to instability [4]. For these reasons, the ZIP flux is often preferred for the momentum convection. The ZIP flux also needs a counterbalancing diffusive flux when it is not centered in time.

3. *Donor.* Neither the partial nor the complete donor cell flux is space centered, and, accordingly, both have low order (in δx) truncation errors. These contribute a positive diffusive effect and accordingly tend to automatically stabilize the numerical calculations. The magnitude, however, can be excessive, thereby masking the true diffusive effects and leading to erroneous interpretations (for example, for flows at high Reynolds numbers). Accordingly, the once-popular donor-cell flux representation is being abandoned by most investigators except for very spcial circumstances.

Our recommendation for ICE calculations is to use ZIP fluxes or centered fluxes, the instability of these mitigated by the controlled use of artificial diffusion with a coefficient that just slightly exceeds the effective value predicted by truncation error analysis. The only circumstance in which a donor-cell flux appears desirable is in the early stages of problems with especially violent initiation (for example, in high-speed projectile impact), the later stages of the calculation automatically shifting to the centered or ZIP flux.

Truncation Errors

Analogous to the derivations in Refs. [1] and [4], we may expand the difference equations in a form that reveals the lowest order diffusional truncation effects. With ZIP differencing for the momentum convection terms, for example, the result is

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = \left[(2\theta - 1)(c^2 + u^2)\frac{\delta t}{2} - \left(\frac{\delta x^2}{4} - \frac{\tau \delta t}{2}\right)\frac{\partial u}{\partial x} + \tau\right]\frac{\partial^2 \rho}{\partial x^2}, \quad (20)$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x} = \left\{[(2\phi - 1)c^2 - 3u^2]\frac{\delta t}{2} - \frac{u\delta x^2}{8\rho}\frac{\partial \rho}{\partial x} + \frac{\lambda}{\rho}\right\}\frac{\partial^2 u}{\partial x^2}. \quad (21)$$

We have used c^2 to denote either of several partial derivatives of p with respect

to ρ; accordingly, the symbol as used in this section is only approximately related to the square of the sound speed, being progressively more accurately so in the limit as $c^2 \to \infty$.

Several classes of effects can be noted from these equations. For $c^2 \to \infty$ (the incompressible limit), the effective diffusion coefficient becomes large and negative if θ and/or ϕ is less than 0.5, corresponding to intolerable numerical instability. In contrast, for θ and ϕ both constants greater than 0.5, the diffusion is positive (hence stabilizing) but can become intolerably large for one-dimensional problems, and in some cases also for two-dimensional problems. Accordingly, an alternative formulation of the ICE method could have variable functions for θ and ϕ, with each varying as $0.5 + k/c^2$ as $c^2 \to \infty$, in which k is an appropriate constant, with θ and ϕ approaching some bound (perhaps zero) as $c^2 \to 0$. (If, indeed, θ and ϕ vanish as $c^2 \to 0$, then care will be necessary to assure the stability of the difference equations; for example, with centered flux differencing in the mass equation an added artificial mass diffusion, the τ term, is required.) In any case, with variable θ and ϕ, these functions will have to be incorporated somewhat differently into the equations from the manner shown in Eqs. (18) and (19). To assure conservation, Eq. (18), for example, would be written

$$\begin{aligned}\frac{\rho_i^{n+1} - \rho_i{}^n}{\delta t} = \frac{1}{\delta x}\,[&\theta^n_{i-1/2}(\rho u)^{n+1}_{i-1/2} - \theta^n_{i+1/2}(\rho u)^{n+1}_{i+1/2} \\ &+ (1 - \theta^n_{i-1/2})(\rho u)_{i-1/2} - (1 - \theta^n_{i+1/2})(\rho u)^n_{i+1/2}] \\ &+ \tau(\rho^n_{i+1} + \rho^n_{i-1} - 2\rho_i{}^n),\end{aligned}$$

in which the cell-edge θ values are appropriate functions of the interpolated sound speed (or some measure thereof) at that locality.

It should be emphasized that the excessive diffusion as $c^2 \to \infty$ is purely longitudinal, so that two-dimensional incompressible flow calculations with the ICE method ordinarily will not suffer from the effect, since longitudinal signal propagation is extremely rapid, anyway.

Stability

Part of the necessary conditions for stability can be surmised from Eqs. (20) and (21). Assuming that θ and ϕ are properly chosen, we note the additional necessary requirements

$$\frac{\tau}{\rho} > \frac{\delta x^2}{4}\left(\frac{\partial u}{\partial x}\right)_{\max},$$

$$\frac{\lambda}{\rho} > \frac{3}{2}u^2_{\max}\,\delta t + \frac{u_{\max}\,\delta x^2}{8\rho}\left(\frac{\partial \rho}{\partial x}\right)_{\max}.$$

Actually, the conditions for stability for the full two-dimensional case are even more stringent than implied by these statements. They are also more difficult to specify precisely. We have found from experience that it is necessary to have τ, λ and μ all large enough so that

$$\tau \gtrsim \rho_{\max} \delta x^2 \left(\frac{\partial u}{\partial x}\right)_{\max},$$

$$\lambda, \mu \gtrsim \frac{3}{2} \rho u_{\max}^2 \delta t + \rho_{\max} \left(\frac{\partial u}{\partial x}\right)_{\max} \delta x^2.$$

We also require $u_{\max} \delta t < \delta x$, in order that fluid move less than one cell per cycle. As an additional restriction, it is necessary that

$$\frac{(\lambda + 2\mu)\, \delta t}{\rho_{\min} \delta x^2} < \frac{1}{4},$$

which, however, is more than sufficient for exclusively very low speed flows. (It may be noted that these various restrictions are not completely independent; satisfaction of all but one nearly implies satisfaction of them all.) As mentioned previously, the replacement $\lambda \to \lambda\rho$, $\mu \to \mu\rho$ can be useful for artificial viscosity purposes, in that it removes $\rho_{\min}$ from the last of the above stability requirements, thereby avoiding the requirement of very small time steps in regions of severe rarefaction.

A Calculational Example

Figures 2 and 3 illustrate an application of the ICE method to a typical problem with both high and low speed flows. The initial configuration shows a large heated sphere of air imbedded in the Earth's atmosphere. Outside of the sphere the density variations are arranged to give exact pressure balance with gravity for a depth of 100 km (approximately thirteen e-foldings of density variation from the ground to the top). The frames in Fig. 2 show the development of the atmospheric dynamics at intervals of 50 sec., illustrated by marker-particle configurations. The corresponding velocity vectors are shown in Fig. 3.

In the early stages, the air is highly compressible, and the high-speed properties of the ICE method are principally utilized. Later stages show a variety of stagnation circumstances in which the low-speed capabilities are crucial to successful calculations.

The present computer program ordinarily rezones the region to add on more cells whenever a signal reaches the edge. To demonstrate the ICE technique properties for this paper, we turned off the rezone feature and allowed the shocks to reflect from the rigid walls of the computing region. Despite the severe stagnation in the reflection regions, there were no signs of instability such as would occur

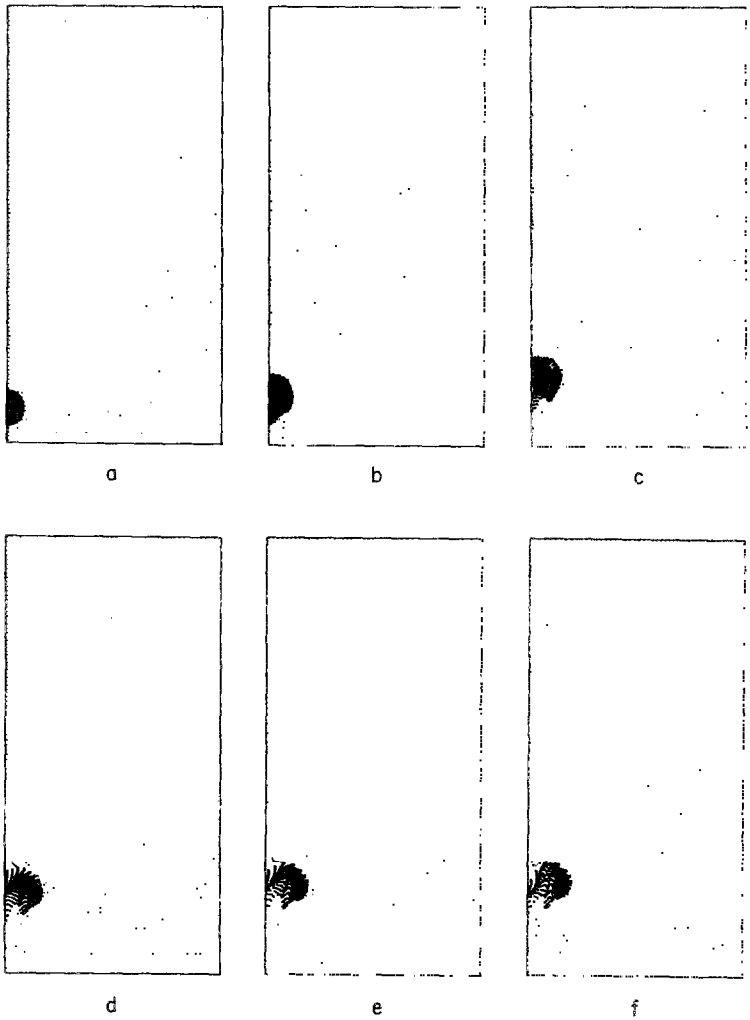

FIG. 2. Cylindrically-symmetric explosion, with axis at the left, of a large, heated sphere of the Earth's atmosphere. Marker particles trace the motion of the air. The times are (a) $t = 0$, (b) $t = 50$ sec, (c) $t = 100$ sec, (d) $t = 150$ sec, (e) $t = 200$ sec, (f) $t = 250$ sec.

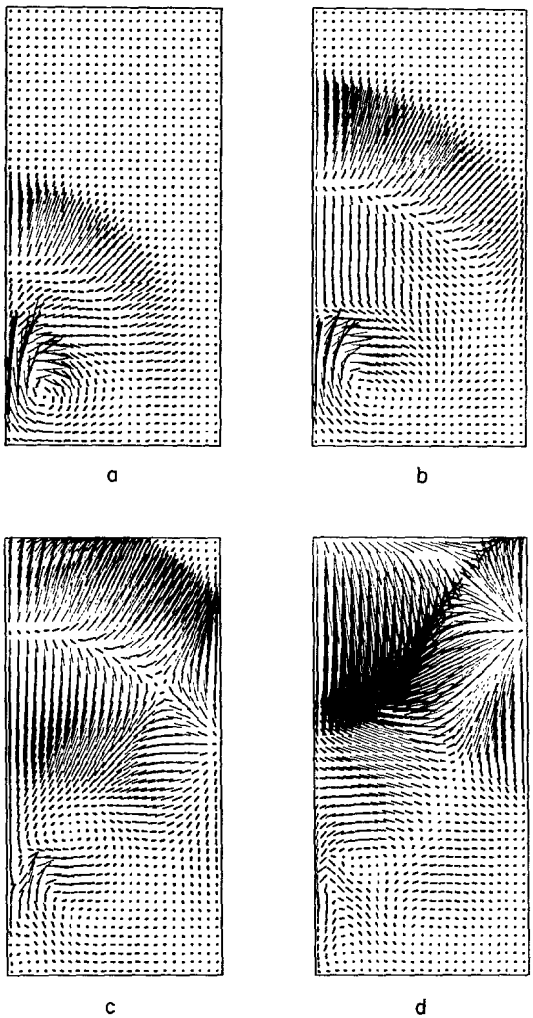

FIG. 3. Velocity vectors for the problem illustrated in Fig. 2. The times are (a) $t = 100$ sec, (b) $t = 150$ sec, (c) $t = 200$ sec, (d) $t = 250$ sec.

in the usual explicit formulations for high-speed flow, and there was no necessity for reducing the time step per cycle.

With the very great intensity of the explosion in this particular example, it is especially apparent that the upward propagating shock dynamics differ appreciably from those in a uniform material. While the shock strength increases, there simultaneously develops a stagnation behind the shock front, and indeed there is a reflection behind this stagnation in which the air velocity is actually downwards.

ACKNOWLEDGMENT

We are grateful to C. W. Hirt for valuable discussions and suggestions.

REFERENCES

1. F. H. HARLOW AND A. A. AMSDEN, Numerical calculation of almost incompressible flow, *J. Computational Phys.* **3** (1968), 80.
2. F. H. HARLOW AND J. E. WELCH, Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface, *Phys. Fluids* **8** (1965), 2182. See also J. E. WELCH, F. H. HARLOW, J. P. SHANNON, AND B. J. DALY, "The MAC Method," Los Alamos Scientific Laboratory Report LA-3425 (1966); C. W. HIRT AND J. P. SHANNON, Free surface stress conditions for incompressible-flow calculations, *J. Computational Phys.* **2** (1968), 403–411; A. A. AMSDEN AND F. H. HARLOW, "The SMAC Method," Los Alamos Scientific Laboratory Report No. LA-4370 (1970); F. H. HARLOW, "Numerical Methods for Fluid Dynamics, An Annotated Bibliography," Los Alamos Scientific Laboratory Report No. LA-4281 (1969).
3. R. A. GENTRY, R. E. MARTIN, AND B. J. DALY, An Eulerian differencing method for unsteady compressible flow problems, *J. Computational Phys.* **1** (1966), 87.
4. C. W. HIRT, Heuristic stability theory for finite difference equations, *J. Computational Physics* **2** (1968), 339.
5. N. N. Janenko and V. E. Neuvazaev, *Akad. Nauk SSSR, Mat. Inst. Trudy* (English Translation) **174** (1966), 150.
6. F. H. HARLOW, A. A. AMSDEN, AND C. W. HIRT, "Numerical Calculation of Fluid Flows at Arbitrary Mach Number," Proc. Second Int. Conf. Numerical Methods in Fluid Dynamics, University of California, Berkeley, California, Sept. 15-19, 1970.