LA-6149-MS

Informal Report

UC-34b

Reporting Date: October 1975

Issued: November 1975

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ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
CONTRACT W-7405-ENG. 36

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Price: Printed Copy \$4.00 Microfiche \$2.25

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A GENERAL NUMERICAL FLUID DYNAMICS ALGORITHM FOR ASTROPHYSICAL APPLICATIONS

by

H. M. Ruppel and L. D. Cloutman

ABSTRACT

Finite difference simulation of fluid flows under astrophysical conditions is often complicated by factors such as complex gas physics, the occurrence of dynamics at widely differing length scales, and the necessity of using implicit difference equations. This report describes a simple, general, and efficient algorithm for solving one-dimensional, spherically symmetric problems using a variation of the ICED-ALE method. A computer code named VEGA has been written based on this algorithm, and the early stages of the collapse of a one-solar mass protostellar cloud are presented as a sample solution.

I. INTRODUCTION

The application of the equations of fluid dynamics to astrophysical problems opens the possibility of studying complex dynamical phases of stellar evolution in considerable detail. However, the numerical algorithms in the astronomical literature tend to have restrictive stability limits; rezoning, when done at all, is done in a primitive, ad hoc fashion. In an attempt to overcome these difficulties we have implemented a variation on the YAUJI code of Hirt, Amsden, and Cook.¹ We report here the basic outline of our method and the progress we have made in applying it to astrophysics.

In our code, VEGA, the conservation equations are solved in two steps: In Phase I the solution is obtained in the coordinate system moving with the fluid; this is called the Lagrangian phase. In Phase II, the rezone or convective phase, the convection terms are added. By rezoning we mean the movement of mesh vertices to maintain a reasonable grid spacing. This is accomplished by defining a grid velocity as some arbitrary fraction of the fluid velocity. This fraction can be a function of space and time. In the limit that the grid velocity

is zero the calculation is Eulerian. If the grid velocity is set equal to the fluid velocity, the calculation is Lagrangian. This technique removes the ad hoc nature and numerical difficulties of rezoning by procedures such as the insertion and deletion of grid points.

Attempts to obtain numerical solutions to problems in stellar evolution must cope with limits on the time step imposed by the wave speeds associated with the problem. In an explicit calculation one simply updates the flow variables for each cell in terms of quantities available at the beginning of the calculational cycle. This approach imposes stability requirements that no waves (sound waves, elastic waves, thermal waves, etc.) can travel more than one cell per cycle. This is the well-known Courant condition, which is usually expressed as $c \delta t / \delta x < 1$, where c is the wave speed. To remove this restriction, we employ an implicit scheme that includes in the solution of the equations as much advanced time information as possible. This requires either an iterative scheme to reach a consistent set of advanced time values or a direct solution technique applied to a linearized set of difference equations.

In the former approach information tends to travel only one cell per iteration, although schemes such as successive overrelaxation (SOR) do propagate signals more rapidly in one direction if they use updated information as it becomes available. Direct solution techniques couple all nodes simultaneously. In either case, information can travel over many cells in any one cycle, even over the entire mesh if the wave speed is sufficiently great. This allows for much larger time steps since the Courant condition no longer constrains it.

There is a certain amount of controversy associated with implicit schemes. This controversy originates in the belief that accuracy is lost in the large time steps an implicit approach permits. There is, of course, validity in such a view. However, in many calculations the solution is changing extremely slowly during a portion of the calculation and nothing is lost by a large time step. If the fluid motion is experiencing changes that are of short duration compared to the time step allowed, the time step must be limited. Otherwise important or interesting phenomena may be unresolved. As an example of the restriction that can be imposed by the wave speed, the largest time steps used in the protostar calculation are sixteen orders of magnitude larger than the explicit thermal diffusion stability limit. We have no reason to believe we have suppressed any short-lived transients that would affect the solution. There are other phenomena associated with the calculation of stellar evolution that pose similar, if less dramatic, problems when treated explicitly. With this in mind we elected to solve the equations describing stellar evolution with as much advanced time information as possible, while making the difference equations tractable. Since the number of cells and the number of variables is significantly smaller in one dimension than in two or three dimensions, it is feasible to consider a direct solution technique for one-dimensional codes. This requires linearizing the system of equations in the time advanced variables and leads to a banded matrix. The width of the band will depend on the number of dependent variables included implicitly. An important feature of this approach is the absence of iterations, such as one finds in the standard Henyey technique. The result is an efficient, stable algorithm

free from convergence difficulties.

One final consideration which entered into our choice of techniques was the desire to be able to extend the set of equations, increasing the amount of physics to the included, with minimal structural alteration to the code. That is, we wished to be able to add equations, add variables, or change the functional form of constitutive relations, all in a direct and straightforward fashion.

To summarize, three factors played major roles in motivating us to adopt the present approach: we wished to be able to vary the resolution of the calculational mesh and to include a continuous rezone; we wanted to include the gas physics as implicitly as possible to maximize the efficiency of the code; we needed to have the flexibility of altering or adding equations with minimum difficulty. These considerations led us to construct a code divided into two phases: an implicit Lagrangian phase in which we solve the complete linear system for the flow variables and a rezone phase in which the contributions from the convection terms are added to the Lagrangian components.

II. EQUATIONS

Astrophysical hydrodynamical algorithms frequently use transformations of the variables in an attempt to improve accuracy. The variable mesh, continuous rezone feature allows us to resolve the solution of most problems with a reasonable number of cells, obviating the need to transform the independent variable. When reasonable resolution is achieved, a transformation of dependent variables is not desirable. Our experience has shown that the use of the primitive variables will give accuracy comparable to any transformed variables, and transformed variables almost always lead to more complex, less efficient programs. For a general method such as ours, variable transformations are not worth the trouble.

Let us now examine the set of equations currently in the code, their significance and the details of the solution algorithm. The full mass equation, including a term for turbulent diffusion^{2,3} is written as

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\sigma r^2 \frac{\partial \rho}{\partial r} \right). \quad (1)$$

Because we are including the nuclear burning of hydrogen, we need a species equation that will allow for hydrogen to be depleted by conversion to helium.

$$\frac{\partial \rho_H}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_H u) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\sigma r^2 \frac{\partial \rho_H}{\partial r} \right) + \left(\frac{\delta \rho_H}{\delta t} \right)_{\text{nuc}}, \quad (2)$$

where $(\delta \rho_H / \delta t)_{\text{nuc}}$ is the nuclear creation rate. The momentum equation contains both a gravitational acceleration, g , and a viscous term, Λ ,

$$\frac{\partial \rho u}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u^2) = -\rho g - \frac{\partial p}{\partial r} + \Lambda, \quad (3)$$

where

$$\Lambda = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 (2\mu + \lambda) \frac{\partial u}{\partial r} \right) - \frac{2u(2\mu + \lambda)}{r^2} + \frac{2u}{r} \frac{\partial \lambda}{\partial r}, \quad (4)$$

and

$$g = \frac{G}{r^2} \int_0^r 4\pi \rho x^2 dx. \quad (5)$$

For the specific internal energy, I , we write

$$\begin{aligned} \frac{\partial \rho I}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u I) = & -p \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u) + \rho \epsilon \\ & + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 K \frac{\partial T}{\partial r} \right) + 2\mu \left[\left(\frac{\partial u}{\partial r} \right)^2 + \frac{2u^2}{r^2} \right] \\ & + \lambda \left[\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u) \right]^2 \end{aligned} \quad (6)$$

In this equation ϵ is the rate of energy release from nuclear burning and K is the thermal conductivity. The temperature is obtained from the specific internal energy through the relation $T = I/c_v$, where c_v is the specific heat at constant volume. The nuclear energy production rate ϵ is discussed more fully in Sec. III. In addition to the conservation equations we include an equation of state of the form

$$P = \Gamma(\rho, \rho_i, I) \rho I + \frac{1}{3} a T^4, \quad (7)$$

where Γ is a function which includes the real gas effects such as variable mean molecular weight and electron degeneracy. For a simple gamma-law ideal gas neglecting radiation pressure, Γ is merely $(\gamma - 1)$. More complicated cases are discussed in the Appendix.

As an example of our solution technique, consider the equation for the internal energy in the form

$$\frac{\partial \rho I}{\partial t} + \nabla \cdot (\rho I \vec{u}) = R, \quad (8)$$

where R includes the work, diffusion, and source terms. Paralleling the approach of Hirt et al., we integrate this equation over a control volume V , which for a cell-centered quantity, like ρI , is simply a calculational cell. We obtain in this way

$$\iiint_V \frac{\partial}{\partial t} (\rho I) d^3V + \iint_V \nabla \cdot (\rho I \vec{u}) d^3V = \iiint_V R d^3V. \quad (9)$$

We also make use of the well-known relation⁴

$$\frac{d}{dt} \iiint_V \rho I d^3V = \iiint_V \frac{\partial}{\partial t} (\rho I) d^3V + \iint_S \rho I \vec{u}_g \cdot \hat{n} d^2S. \quad (10)$$

This relation states that the total change of a quantity in a control volume is made up of two parts: the change with time within the volume and the amount taken into the volume as the surface, S , of the control volume moves with velocity $\vec{u}_g$. We will refer to this velocity as the grid velocity. For a Lagrangian calculation, $\vec{u}_g = \vec{u}$. For an Eulerian calculation, $\vec{u}_g = 0$.

Combining Eqs. (9) and (10) and using the divergence theorem yields

$$\frac{d}{dt} \iiint_V \rho I d^3V - \iint_S \rho I (\vec{u}_g - \vec{u}) \cdot \hat{n} d^2S = \iiint_V R d^3V. \quad (11)$$

Although we have examined only the equation for ρI in detail, each of the conservation equations will contain an integral of the form

$$\iint_S \rho Q (\vec{u}_g - \vec{u}) \cdot \vec{n} dS.$$

As we mentioned above, in a Lagrangian calculation $\vec{u}_g = \vec{u}$, and this term vanishes. It is this structure that leads one to solve the equations without this term first and then to add its contribution as a separate step in the rezone or convective phase. We should comment that convection in this context has nothing to do with turbulent convection, but refers only to the flow of mass, momentum, and energy past a point in space as a result of the fluid motion. Performing the integrations over the cell volumes symbolically, we difference Eq. (11) for the internal energy in Lagrangian form as

$$M_{c,j}^{n+1} I_j^{n+1} - M_{c,j}^n I_j^n = \delta t R_j^{n+1} V_{c,j}^n$$

or equivalently

$$I_j^{n+1} = \frac{M_{c,j}^n}{M_{c,j}^{n+1}} \left(I_j^n + \frac{\delta t R_j^{n+1} V_{c,j}^n}{M_{c,j}^n} \right). \quad (12)$$

If there is no diffusion in the mass equation, i.e., if $\sigma = 0$, $M_{c,j}^{n+1} = M_{c,j}^n$ for a Lagrangian calculation. However, this is not true in general, and care must be taken to include the mass factor properly. Our procedure is to include it in the rezone phase so that $M_{c,j}^{n+1}$ contains contributions from both the turbulent diffusion and the convection. This means that the effect of σ on ρ is not included fully implicitly in the I equation, although it may be partially done through the dependence of R on ρ . Unless the effect of turbulent mass diffusion in one time step is large this should not lead to stability problems.

The calculational mesh is labeled with half-integral indices at the vertices as indicated in Fig. 1. The quantities ρ , ρ_H , I , p and M_c are cell-centered quantities, labeled with integral values; coordinates, velocities and vertex masses are assigned at vertices. The time level is indicated with a

Cell centered quantities: $\rho, \rho_H, I, p, M_c, \dots$

Vertex quantities: $u, K, M_v, \dots$

Fig. 1. A segment of the VEGA computing mesh that illustrates the subscript convention.

superscript.

In order to set up a system which is linear in the time advanced quantities, it is necessary to expand the nonlinear terms about the old time level, as for example

$$(\rho I)^{n+1} = \rho^{n,n+1} I^{n+1} + \rho^{n+1} I^n - \rho^n I^n. \quad (13)$$

This ignores the quadratic terms in the changes of the variables; in Eq. (13) we have dropped the term $(\rho^{n+1} - \rho^n)(I^{n+1} - I^n)$. Consequently, the equations are not fully time advanced and, should the quadratic term be appreciable compared to $\rho^n I^n$, numerical difficulties can occur.

As far as R_j^{n+1} is concerned, this can be a nonlinear function of the variables. Nonetheless, we attempt to include as much time-advanced information as possible in its evaluation. Consider that part of R_j that arises from the energy released in nuclear reactions. This is, in a single calculational cycle,

$$\delta(\rho I) \sim \rho \epsilon \delta t. \quad (14)$$

Because ϵ is, in general, a complicated function of ρ , ρ_H , and I , one might most simply include it explicitly. This could seriously limit the time step. In fact ϵ increases more rapidly than linearly with temperature which allows us to include some advanced time information by factoring out the internal energy I . Rates for the carbon cycle and for the proton chain are proportional to the first and second powers of ρ_H , respectively. For this reason we factor out ρ_H also and write

$$\epsilon(\rho, \rho_H, I) = \epsilon_0(\rho, \rho_H, I) \rho_H I, \quad (15)$$

then linearizing the product, $\rho_H I$, in the advanced time quantities. Although this term cannot be made fully implicit in the direct solution approach, the present treatment greatly improves stability over the explicit method.

Note that instead of using an equation for the total energy, we elect to calculate the specific internal energy. Experience has shown that the use of this equation is more accurate than the use of the total energy equation because errors in the kinetic energy are not then buried in the internal energy. Since the pressure depends on the temperature, as do some of the more crucial physical parameters, it is important to obtain the internal energy as accurately as possible. What we sacrifice is total energy conservation.

The primary stability limit of our method is

$$u \frac{\delta t}{\delta x} < 1 \quad (16)$$

In practice we limit $u \delta t / \delta x$ to somewhat less than 0.5 over the entire mesh. If a quadratic term in the change of any two variables is large with such a time step, we cannot expect unconditional stability. For this reason we include an additional limit on the time step such that if any variable changes fractionally by more than a fixed amount in any cell, the time step is decreased. This prevents instabilities that might occur because of the partially explicit nature of the solution. With this test the quadratic term in the variable changes is effectively limited. The optimum value for the fractional change will clearly be problem dependent.

We now illustrate the differencing of the equation for a vertex quantity with the Lagrangian form of the momentum equation:

$$\frac{d}{dt} \iiint_V \rho u d^3V = \iiint_V \left(-\rho g - \frac{\partial p}{\partial r} + \Lambda \right) d^3V \quad (17)$$

Since the velocity is defined at vertices, the control volume over which the integration is performed runs from cell center to cell center, that is from r_j to r_{j+1} . Defining a vertex mass as the average mass of the adjacent cells,

$$\iiint_V \rho d^3V = M_{v,j+\frac{1}{2}} = \frac{1}{2} (M_{c,j} + M_{c,j+1}) \quad (18)$$

we difference Eq. (17) in a straightforward fashion to arrive at Eq. (A-28) in the Appendix. For completeness the Appendix contains the difference equations for the remaining variables and includes a discussion of some of the considerations which entered into decisions concerning the manner of differencing.

It must be remembered that it is necessary to couch the equation of state in such a fashion that it too can be linearized. Otherwise, point relaxation techniques would have to be employed.

III. GAS PHYSICS

Because in this initial development our emphasis has been on the solution algorithm for the basic fluid equations rather than on the details of the gas physics, we have limited the constitutive relations to fairly simple form. At the same time, we have included sufficient generality to solve a broad class of problems.

We assume the gas consists of three nuclear species: hydrogen, helium, and metals (atomic number > 2) with a fixed mass fraction Z . The equation of state allows for hydrogen to be converted to helium, allows for partial ionization and for H_2 dissociation, and includes radiation pressure and nonrelativistic electron degeneracy.

A. Equation of State

Under the assumptions listed above, the total pressure is

$$P = \frac{1}{3} a T^4 + \frac{kT}{H} \left[\nu_H \left\{ \frac{1}{\mu_H} - \frac{1}{\mu_{He}} + \psi \left[\frac{n_H}{\mu_H} - \frac{n_{He}}{\mu_{He}} \right] \right\} + \rho \left\{ \frac{(1-Z)}{\mu_{He}} + \frac{Z}{\mu_Z} + \psi \left[\frac{(1-Z)n_{He}}{\mu_{He}} + \frac{Z n_Z}{\mu_Z} \right] \right\} \right] \quad (19)$$

In the above, a is the Stefan-Boltzmann constant, k is the Boltzmann constant, H is the mass of one atomic mass unit, μ_i is the average molecular weight of the nuclei of species i , n_i is the average number of free electrons per nucleus of species i .

The degeneracy is included through the ratio

$$\epsilon = \frac{2}{3} \frac{F_{3/2}(\eta)}{F_{1/2}(\eta)}, \quad (20)$$

where $F_n(\eta)$ is the Fermi-Dirac integral of order n ,

$$F_n(\eta) = \int_0^\infty \frac{x^n dx}{1 + \exp(x - \eta)} \quad (21)$$

and η is the degeneracy parameter. We have made use of the relation

$$x_{\text{He}} = (1 - Z) x - x_{\text{H}} \quad (22)$$

to eliminate x_{He} . The degeneracy factor η is evaluated from the expressions given by Larson and Demarque,⁵ and n_i and x_i are evaluated using the ionization-dissociation equation of state from the stellar envelope program of Paczynski.⁶

B. Specific Heat

The internal energy per gram is

$$I = c_v T = \frac{aT^4}{4} + I_{\text{ex}} + \frac{1.5kT}{H} \left\{ \frac{\rho_{\text{H}}}{\rho} \left[\frac{1}{\mu_{\text{H}}} - \frac{1}{\mu_{\text{He}}} + \epsilon \left(\frac{n_{\text{H}}}{\mu_{\text{H}}} - \frac{n_{\text{He}}}{\mu_{\text{He}}} \right) \right] + \left[\frac{(1-Z)}{\mu_{\text{He}}} + \frac{Z}{\mu_{\text{Z}}} + \epsilon \left(\frac{(1-Z)n_{\text{He}}}{\mu_{\text{He}}} + \frac{Zn_{\text{Z}}}{\mu_{\text{Z}}} \right) \right] \right\}, \quad (23)$$

where I_{ex} includes the specific ionization energy, the H_2 dissociation energy and the H_2 vibrational, rotational, and excitation energies. We define I_{ex} so that it vanishes at zero temperature. With this definition of I_{ex} , c_v is the temperature averaged value of the thermodynamic derivative $(\partial I / \partial T)$ with density and composition fixed.

C. Nuclear Reaction Rate

We use the nuclear reaction rates of Larson and Demarque for the proton chain and carbon cycle. These rates assume equilibrium abundances, but the three branches of the proton chain are followed separately. The nuclear energy production rate ϵ is a complicated nonlinear function of ρ , T , and composi-

tion, and it will not be reproduced here.

D. Viscosity

Two regimes are of interest in estimating the viscosity of the stellar gas. At low temperatures the dominant source of viscosity is collisions between atoms. As a crude estimate for this regime, we can fit Edmonds⁷ viscosity table with the form

$$\mu = 7.15 \times 10^{-6} T^{1/2}. \quad (24)$$

Interactions between atoms and photons dominate the viscosity at higher temperatures,⁸ so that

$$\mu = \frac{4a}{15c} \frac{T^3}{\kappa \rho}, \quad (25)$$

where κ is the Rosseland mean opacity.

E. Conductivity

In radiative zones, we use

$$K_{\text{rad}} = \frac{4ac}{3} \frac{T^3}{\kappa \rho}. \quad (26)$$

The opacity tables used for $T > 2000^\circ\text{K}$ were taken from Paczynski's stellar envelope program. These tables are Cox-Stewart tables⁹ with an approximate correction for water vapor opacity. At temperatures below 1500°K , grains dominate the opacity, and the constant value, $\epsilon = 0.15$, used by Larson¹⁰ was chosen. Recent work by Alexander¹¹ indicates that this value is perhaps a factor of six too low. Between 1500°K and 2000°K , a linear interpolation between the two regimes is used.

F. Turbulence Modeling

At this point in the development, we have not incorporated a complete turbulence model. However, we have included turbulent diffusion of mass and heat. The Schwarzschild criterion is used to detect regions of turbulent convection. If we define

$$\frac{\Gamma_2}{\Gamma_2 - 1} \equiv \frac{12\beta(1-\beta)(\gamma_g - 1) + \beta^2 + (4-3\beta)^2(\gamma_g - 1)}{(4-3\beta)(\gamma_g - 1)}, \quad (27)$$

where γ_g is the ratio of specific heats for the gas alone, and ϵ is the ratio of gas pressure to total pressure, then in unstable zones the effective thermal diffusion coefficient for adiabatic convection is

$$K_{con} = \frac{2}{2-\epsilon} \frac{F}{g} \quad (28)$$

F is the energy flux and g is the local gravitational acceleration. Analogous expressions can easily be derived for other theories of turbulent convection, but this expression is adequate for our preliminary calculations.

The turbulent diffusion of mass is discussed by Cloutman² and by Rivard, Butler, and Farmer.³ We use equal values for the turbulent diffusivities of mass and internal energy (i.e., the turbulent Schmidt and turbulent Prandtl numbers are assumed to be equal). Thus, in convection zones,

$$\alpha = \frac{K_{con}}{\rho c_v} ; \quad (29)$$

α vanishes in radiative zones.

A more reliable approach to the treatment of convection zones would be a turbulence transport model along the lines of Daly and Harlow,¹² or Rivard, et al. Another usable, but less reliable, model could be based on the mixing length theory.

Further investigation of turbulence modeling for astrophysical applications is in progress.

IV. SOLVING THE LINEAR SYSTEM

One time step is accomplished in two distinct phases. In Phase I, we do an implicit Lagrangian time step; in Phase II, we do the rezoning. After rezoning we do any necessary bookkeeping and output. In this section, we discuss some computational details for carrying out these phases.

In Phase I, the linear difference equations we want to solve are Eqs. (A-3), (A-18), (A-24), (A-26), (A-27) and a species equation similar to (A-18) that includes nuclear burning. Thus we have $6N$ equations if there are N real cells. However, the matrix is sparse and block diagonal, with one 6 by 18 block for each cell as shown schematically in Fig. 2. This structure is similar to the structure of the matrix which occurs in the Henyey method. However, we solve our linear system only once per time step. One would expect, then, that our code uses about as much time for one time step as the Henyey method needs for one iteration. Comparison with Henyey method programs by Paczynski and by Larson and Demarque verify this observation.

The order of the six equations within each block and the order of the variables in the solution vector is very important for efficient matrix inversion.

Fig. 2. A representative portion of the banded matrix that is inverted to solve the fluid equations for cell i . Nonzero matrix elements are marked with x's. The symbols at the top show the order of the variables in each equation; the symbols at the left indicate which equation is associated with a given row.

Rather than use a block diagonal routine, we used a banded system solver that uses LU decomposition with partial pivoting.¹³ The diagonal is inside the solid lines, and the nonzero matrix elements are confined to the band indicated in Fig. 2 by dashed lines. Since the running time of this routine is proportional to the cube of the bandwidth, and most of our running time is spent in the matrix routines, it is crucial to minimize the bandwidth. The layout shown in Fig. 2 is optimum, with a bandwidth of 13. If a bandwidth of 14 were used, the code would run about 25% slower. A layout with nonzero elements in the upper right and lower left corners of each block would have a bandwidth of 23 and lead to a code that would be about 5.5 times slower. The narrow bandwidth also minimizes memory requirements and rounding errors. Running time and storage requirements would be prohibitive if one attempted to store and operate on the full matrix. The solution vector is given by the variables in the order shown across the top of the block in Fig. 2.

Boundary conditions are imposed by writing special difference equations for the innermost and outermost real cells. The inner boundary conditions at the origin are

$$u(0, t) = \tilde{r}(0, t) = 0,$$

where F is the heat flux, and

$$\left. \frac{\partial \tilde{r}}{\partial r} \right|_{r=0} = 0, \quad (30)$$

$$\left. \frac{\partial I}{\partial r} \right|_{r=0} = 0.$$

It is not necessary to specify the pressure in the inner fictitious cell.

The outer boundary conditions present a challenging problem that does not have a unique solution. For the protostar problem, we use a rigid wall:

$$u_{N-\frac{1}{2}} = 0,$$

$$\left. \frac{\partial D}{\partial r} \right|_{r=R_0} = 0,$$

$$\left. \frac{\partial H}{\partial r} \right|_{r=R_0} = 0. \quad (31)$$

The temperature is a fixed constant on the boundary, $r = R_0$. In the above, $N-\frac{1}{2}$ is the index of the outer boundary. The boundary temperature for the protostar problem is 10^4 K. The normal equations for p and F are used on the outer boundary.

The detailed equations used in Phase I are given in the Appendix but the philosophy of Phase II will be described here. We assume we have completed the Lagrangian time step of Phase I and that we have specified the velocity $u_{q,j+1}$ with which we want to move each grid point. In our scheme, the grid points cannot move more than a cell width or instability results. We compute the fluxes of mass, momentum, and energy through the moving vertices and cell centers, and use these fluxes to compute the amount of each conserved quantity that passes through each moving surface as it moves from its original position to its final position. Then this amount is transferred from one side of the surface to the other, thereby conserving mass, momentum, and energy to within computer rounding errors. From the original amount of mass, momentum, and energy in each cell and the changes due to rezoning, we can then recover the densities, velocities, and internal energies in each cell after rezoning. Finally we do bookkeeping, compute p_j^{n+1} from the equation of state, generate output (if any) and begin the next time step.

V. SAMPLE CALCULATION

As an example of a calculation performed with VEGA, we present the early phases of collapse of a one-solar-mass protostar. We have tried to reproduce the results of Larson,¹⁰ and we find good agreement among the results from VEGA, Larson, and a special ICE method program. Larson used a variation of the so-called Henyey method^{5,14} and was limited to about 50 mesh cells in his calculations. The special ICE code is a one-dimensional, spherical coordinate variation of the basic ICE method.¹⁵ This variation includes a nonuniform mesh and an implicit internal energy equation.

The initial condition for our test problem is a one-solar-mass, uniform cloud of gas at 10^4 K.

The hydrogen is assumed to be in the form of H_2 and the radius of the cloud is

$$R_c = 0.41 \frac{GM}{RT} = 1.63 \times 10^{17} \text{ cm}, \quad (32)$$

where R is the universal gas constant divided by the mean molecular weight. This cloud is just unstable toward gravitational collapse according to the Jeans criterion. We assume the gas is a perfect gamma-law gas with $\gamma = 1.4$, and the specific heat, c_v , and mean molecular weight are assumed to be constants. We neglect changes of excitation energy in the H_2 molecules and terminate the calculation before dissociation becomes important. We neglect all anisotropic phenomena such as magnetic fields and rotation.

The code was run in an Eulerian mode with 150 cells. The radius of the central cell was 5×10^{12} cm, the cell width grows as a function of radius by a constant factor to cover the entire radius with 150 cells. The outer boundary condition is a fixed, rigid wall ($u = 0$) at 10 K.

Figure 3 shows the density and velocity profiles at several phases of collapse. The left-hand panel covers the entire radius of the cloud, while the right-hand panel covers only the innermost 0.1 of the radius. The curve labeled $\rho(0)$ is the initial density, and the initial velocity is zero.

The curves labeled $\rho(300)$ and $u(300)$ are the density and velocity, respectively, after 300 cycles. At this stage, the fluid is still isothermal at 10^4 K.

Fig. 3. The density and velocity profiles of a one-solar mass protostar at several different times. The numbers in parentheses denote the cycle numbers.

A rarefaction wave is moving inward at the local sound speed relative to the collapsing fluid. The velocity is linear and subsonic on both sides of the rarefaction, which is near $r = 1.0 \times 10^{17}$ cm. Inside the rarefaction, the density is spatially constant but increases with time. Outside the rarefaction, the density drops as $1/r^2$. This behavior is expected theoretically.

At 1250 cycles the entire character of the solution has changed. The rarefaction has hit the center and a nearly static core with a radius of 5×10^{13} cm has formed. Larson reports a core radius of 6×10^{13} cm. In the outer half of the cloud, the velocity has hardly changed since cycle 300. However, the infalling material goes supersonic outside the core. The velocity minimum at 5×10^{13} is about Mach 7. An accretion shock surrounding the core rapidly drops the velocity to Mach 1 at the surface of the core, and the velocity drops roughly linearly to zero at the origin. The core is now optically thick, and the center temperature is about 270 K.

The velocity profile just outside the accretion shock shows an appreciable oscillation. This is a numerical effect due to dispersive truncation errors. The true shock Mach number is probably closer to five than to seven. This problem was run with no viscosity. We could help smooth our solution by increasing the donor cell parameter λ , which has the same effect as artificial viscosity because it increases the diffusional truncation errors. In fact, it is the combination of an Eulerian calculation with large donor cell that allows us to run the strong shock stably without explicitly adding an artificial viscosity.

Figure 4 shows the central density as a function of time as computed by three different methods. The agreement among the three methods is impressive until shortly after 5×10^{12} secs, which is shortly before the rarefaction hits the origin. What happens next is a complicated series of radial pulsations. The details of these pulsations are sensitive to the numerical technique used to integrate the equations. Larson¹⁶ reports that the pulsations occurred with his Lagrangian calculations, but not with his Eulerian calculations. Because Eulerian methods tend to be more diffusive than Lagrangian methods, it appears that the pulsations

Fig. 4. Central density of a one-solar-mass protostar as computed by three different programs.

are weakly driven at first and then easily damped. These pulsations temporarily halt the collapse in the core. The longer the core pulsates, the longer

the rapid density rise is delayed. We feel that the differences in the time of onset of the collapse are due to the numerical differences in the various techniques during the pulsation phase. It is difficult to assess the numerical effects of Larson's methods. The ICE code employs a special truncation error cancellation scheme¹⁷ to reduce numerical diffusion appreciably compared to the standard ICE method. The density bump at 6×10^{12} secs is due to the first expansion after the rarefaction reaches the origin. Several oscillations follow, but their effect is too small to show on the figure except at 8.5×10^{12} sec. The VEGA calculation is more diffusive, resulting in lower amplitude and faster damping in the pulsations. While the flow velocity in the core actually changes sign in the ICE calculation, it does not in the VEGA calculation. The VEGA collapse merely goes in spurts.

APPENDIX

THE DIFFERENCE EQUATIONS

I. EQUATION OF STATE

We include in the code the general equation of state

$$P = \Gamma \rho I + \frac{1}{3} a T^4, \quad (A-1)$$

where Γ is a function that can represent all real gas effects. The special case,

$$P = (\gamma - 1) \rho I + \frac{1}{3} a \left(\frac{I}{c_v} \right)^4, \quad (A-2)$$

which often suffices, is approximated by

$$\begin{aligned} \rho_j^{n+1} &= \left[(\gamma - 1) I_j^n \right] \rho_j^{n+1} \\ &- \left[(\gamma - 1) \rho_j^n + \frac{4a}{3c_{v,j}^n} (T_j^n)^3 \right] I_j^{n+1} \end{aligned}$$

$$= - \rho_j^n - \frac{2a}{3} (T_j^n)^4. \quad (A-3)$$

Empirically, we find this form to be unconditionally stable with respect to the usual Courant condition. Equation (A-3) was used without radiation pressure in the protostar calculation.

The best treatment of equations of state with variable Γ is unknown; we are continuing our effort to clarify this point. A natural extension of Eq. (A-3) is to replace $(\gamma - 1)$ by Γ_j^n . It is not clear at this point if this procedure is unconditionally stable. There is some indication that it may be necessary to use a more implicit scheme such as

$$\begin{aligned} \rho_j^{n+1} &= \left[\rho_j^n \left(\Gamma_j^n + I_j^n \left(\frac{\partial \Gamma}{\partial I} \right)_j^n \right) + \frac{4a}{3c_{v,j}^n} (T_j^n)^3 \right] I_j^{n+1} \\ &- \left[I_j^n \left(\Gamma_j^n + \rho_j^n \left(\frac{\partial \Gamma}{\partial \rho} \right)_j^n \right) \right] \rho_j^{n+1} \end{aligned}$$

$$= -\rho_j^n - \frac{2a(T_j^n)^4}{3} - \rho_j^n I_j^n \left[\rho_j^n \left(\frac{\partial \Gamma}{\partial \rho} \right)_j^n + I_j^n \left(\frac{\partial \Gamma}{\partial I} \right)_j^n \right]. \quad (A-4)$$

This scheme has not been tested, but we expect it to have good stability properties; moreover, it provides a method for using equation of state tables that contain Γ and perhaps its derivatives.

For certain special equations of state, it may be possible to use explicit mean molecular weights and write the linearized equation of state in terms of ρ_j , $\rho_{H,j}$, and I_j . For example, Eq. (19) may be approximated by

$$\begin{aligned} \rho_j^{n+1} - \frac{I_j^{n+1}}{c_{v,j}^n} \left\{ \frac{4a(T_j^n)^3}{3} + \frac{k}{H} \left[\rho_{H,j}^n \beta_{H,j} + \rho_j^n \beta_{He,j} \right] \right\} \\ - \rho_{H,j}^{n+1} \left\{ \frac{kT_j^n}{H} \beta_{H,j} \right\} - \rho_j^{n+1} \left\{ \frac{kT_j^n}{H} \beta_{He,j} \right\} \\ = -\rho_j^n - \frac{2a}{3} (T_j^n)^4 \end{aligned} \quad (A-5)$$

where

$$\beta_{H,j} = \left[\frac{1}{\mu_H} - \frac{1}{\mu_{He}} + \psi \left(\frac{n_H}{\mu_H} - \frac{n_{He}}{\mu_{He}} \right) \right] \quad (A-6)$$

and

$$\beta_{He,j} = \left[\frac{(1-Z)}{\mu_{He}} + \frac{Z}{\mu_Z} + \psi \left(\frac{(1-Z)n_{He}}{\mu_{He}} + \frac{Zn_Z}{\mu_Z} \right) \right]. \quad (A-7)$$

We have used Larson and Demarque's⁵ approximation to ψ :

$$\psi = (1 + 0.1938 F_{\frac{1}{2}}(\eta))^{5/3} / (1 + 0.12398 F_{\frac{1}{2}}(\eta)), \quad (A-8)$$

where

$$F_{\frac{1}{2}}(\eta) = \left[\frac{h^3}{4\pi H(2m_e k)^{3/2}} \right] \frac{\rho}{\mu_e T^{3/2}}, \quad (A-9)$$

and μ_e is the mean molecular weight per free electron; h is Planck's constant. The stability properties of this form are not clear; it may be necessary to make the function ψ partially implicit with an approximation such as

$$\begin{aligned} \psi_j^{n+1} \approx \psi_j^n + \left(\frac{\partial \psi}{\partial \rho} \right)_j^n (\rho_j^{n+1} - \rho_j^n) \\ + \left(\frac{\partial \psi}{\partial I} \right)_j^n (I_j^{n+1} - I_j^n) \end{aligned} \quad (A-10)$$

II. CONTINUITY EQUATION

Let us write the continuity equation as

$$\frac{d\rho}{dt} + \rho D = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \sigma \frac{\partial \rho}{\partial r} \right), \quad (A-11)$$

where

$$D = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u). \quad (A-12)$$

Define the quantity

$$d_j^n = - \frac{\delta t}{1 + \delta t D_j^n}. \quad (A-13)$$

In spherical coordinates,

$$D_j^n = \frac{u_{j+\frac{1}{2}}^n - u_{j-\frac{1}{2}}^n}{r_{j+\frac{1}{2}} - r_{j-\frac{1}{2}}} + 2 \frac{u_{j+\frac{1}{2}}^n + u_{j-\frac{1}{2}}^n}{r_{j+\frac{1}{2}} + r_{j-\frac{1}{2}}}. \quad (A-14)$$

Then Eq. (A-11) is approximated by

$$\begin{aligned} \rho_j^{n+1} - d_j^n \rho_j^n D_j^{n+1} + d_j^n \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \sigma^n \frac{\partial \rho}{\partial r} \right)^{n+1} \right]_j \\ = \rho_j^n. \end{aligned} \quad (A-15)$$

Defining normalized cell volumes

$$V_{c,j} \equiv r_{j+\frac{1}{2}}^3 - r_{j-\frac{1}{2}}^3, \quad (A-16)$$

and normalized vertex areas

$$A_{j-\frac{1}{2}} = 3r_{j-\frac{1}{2}}^2, \quad (A-17)$$

we approximate Eq. (A-11) by

$$\begin{aligned} \rho_j^{n+1} & \left\{ 1 - \frac{2d_j^n}{V_{c,j}} \left[\frac{\sigma_{j+\frac{1}{2}}^n A_{j+\frac{1}{2}}}{r_{j+3/2} - r_{j-\frac{1}{2}}} + \frac{\sigma_{j-\frac{1}{2}}^n A_{j-\frac{1}{2}}}{r_{j+\frac{1}{2}} - r_{j-3/2}} \right] \right\} \\ & + \rho_{j+1}^{n+1} \left\{ \frac{2d_j^n}{V_{c,j}} \frac{\sigma_{j+\frac{1}{2}}^n A_{j+\frac{1}{2}}}{(r_{j+3/2} - r_{j-\frac{1}{2}})} \right\} \\ & + \rho_{j-1}^{n+1} \left\{ \frac{2d_j^n}{V_{c,j}} \frac{\sigma_{j-\frac{1}{2}}^n A_{j-\frac{1}{2}}}{(r_{j+\frac{1}{2}} - r_{j-3/2})} \right\} \\ & + u_{j+\frac{1}{2}}^{n+1} \left[-d_j^n \left(\frac{2}{r_{j+\frac{1}{2}} + r_{j-\frac{1}{2}}} + \frac{1}{r_{j+\frac{1}{2}} - r_{j-\frac{1}{2}}} \right) \right] \\ & + u_{j-\frac{1}{2}}^{n+1} \left[-d_j^n \left(\frac{2}{r_{j+\frac{1}{2}} + r_{j-\frac{1}{2}}} - \frac{1}{r_{j+\frac{1}{2}} - r_{j-\frac{1}{2}}} \right) \right] \\ & = \rho_j^n. \end{aligned} \quad (A-18)$$

As with all our difference equations, the geometric quantities, r , A , and V are always the old-time values. The left-hand side of Eq. (A-11) is differenced directly because the integration procedure would provide no immediate information on the new densities. It would merely give us the trivial fact that the mass in a cell does not change in the absence of turbulence. The advanced time-cell volume, necessary to compute the advanced time density from the cell mass, is not directly available. Only the diffusion term is differenced as if we followed the integration procedure described in Sec. II for the momentum and energy equations.

III. SPECIES EQUATION

The species equation is identical to the continuity equation except for the nuclear term. The nuclear term is written as

$$\begin{aligned} -d_j^n \left(\frac{\delta \rho_H}{\delta t} \right)_j &= -d_j^n \rho_j^n \left(\frac{m_H n}{Q} \right) \epsilon_{0j} \left(\rho_{H,j}^{n+1} I_j^n \right. \\ & \left. + \rho_{H,j}^n I_j^{n+1} - \rho_{H,j}^n I_j^n \right), \end{aligned} \quad (A-19)$$

where m_H is the mass of one atom of species H , n is the number of H atoms destroyed per reaction that releases energy Q , and

$$\epsilon_{0j} = \frac{\epsilon_j^n}{\rho_{H,j}^n I_j^n}. \quad (A-20)$$

The term (A-19) is added to the right-hand side of Eq. (A-18), and, of course, ρ_H replaces ρ .

IV. ENERGY EQUATION

The equation for the specific internal energy may be written as

$$\frac{\partial \rho I}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \rho u I \right) = -pD + \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 K \frac{\partial T}{\partial r} \right) + \rho \epsilon + \phi. \quad (A-21)$$

For numerical reasons we have found it expedient to define the flux

$$F = K \frac{\partial T}{\partial r} = K \frac{\partial}{\partial r} \left(\frac{I}{c_V} \right), \quad (A-22)$$

and carry along this extra equation. In both the above $K = \text{Max}(K_{\text{rad}}, K_{\text{con}})$. The diffusion term in Eq. (A-21) is then calculated as

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 F \right).$$

This is necessary whenever $\chi \equiv \log_{10}(K \delta t / \rho c_V \delta r^2)$ approaches or exceeds the number of digits carried in the calculation, because the coefficient matrix

has a term like $1 + 2 \times 10^X$. The one gets lost in round off if X is too large, and the matrix package cannot successfully recover the one in the course of solving the linear system.

In Eq. (A-21) we define the variable, ϕ , for the viscous work, that is,

$$\phi \equiv \mu \left[\left(\frac{\partial u}{\partial r} \right)^2 + \frac{2u^2}{r^2} \right] + \lambda \left[\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u) \right]^2. \quad (A-23)$$

The difference approximation to Eq. (A-21) is derived by integrating over the spherical shell between $r = r_{j-1/2}$ and $r = r_{j+1/2}$, using the procedure described in Sec. II. The compressional work term is time centered to conserve energy; everything else is made as implicit as possible consistent with our constraint of linear equations.

$$\begin{aligned} I_j^{n+1} = I_j^n + \delta t \left\{ \epsilon_{0j} \left[\rho_{H,j}^{n+1} I_j^n + \rho_{H,j}^n I_j^{n+1} \right. \right. \\ \left. \left. - \rho_{H,j}^n I_j^n \right] + \frac{V_{C,j}}{M_{C,j}} \phi_j + \frac{1}{M_{C,j}} \left[A_{j+1/2} F_{j+1/2}^{n+1} \right. \right. \\ \left. \left. - A_{j-1/2} F_{j-1/2}^{n+1} \right] - \frac{1}{2M_{C,j}} \left[p_j^{n+1} \left(A_{j+1/2} u_{j+1/2}^n \right. \right. \right. \\ \left. \left. - A_{j-1/2} u_{j-1/2}^n \right) + p_j^n \left(A_{j+1/2} u_{j+1/2}^{n+1} \right. \right. \\ \left. \left. - A_{j-1/2} u_{j-1/2}^{n+1} \right) \right] \right\}, \quad (A-24) \end{aligned}$$

where

$$M_{C,j}^n = \rho_j^n V_{C,j},$$

and

$$\begin{aligned} \phi_j = \mu_j^n \left\{ \left[2 \left(u_{j+1/2}^{n+1} - u_{j-1/2}^{n+1} \right) \left(u_{j+1/2}^n - u_{j-1/2}^n \right) \right. \right. \\ \left. \left. - \left(u_{j+1/2}^n - u_{j-1/2}^n \right)^2 \right] \left(r_{j+1/2} - r_{j-1/2} \right)^{-2} \right. \\ \left. + \left[4 \left(u_{j+1/2}^{n+1} + u_{j-1/2}^{n+1} \right) \left(u_{j+1/2}^n + u_{j-1/2}^n \right) \right. \right. \end{aligned}$$

$$\begin{aligned} \left. \left. - 2 \left(u_{j+1/2}^n + u_{j-1/2}^n \right)^2 \right] \left(r_{j+1/2} + r_{j-1/2} \right)^{-2} \right. \\ \left. - \frac{2}{3(V_{C,j})^2} \left[2 \left(A_{j+1/2} u_{j+1/2}^{n+1} - A_{j-1/2} u_{j-1/2}^{n+1} \right) \right. \right. \\ \left. \left. \left(A_{j+1/2} u_{j+1/2}^n - A_{j-1/2} u_{j-1/2}^n \right) \right. \right. \\ \left. \left. - \left(A_{j+1/2} u_{j+1/2}^n - A_{j-1/2} u_{j-1/2}^n \right)^2 \right] \right\}. \quad (A-25) \end{aligned}$$

Here we have assumed $\lambda = -\frac{2}{3}\mu$. The viscous dissipation term is positive-definite if all velocities are at the same time level, but we lose this physical characteristic by using velocities from a mixture of time levels. This is probably not serious, but it should be kept in mind.

The flux equation is

$$F_{j+1/2}^{n+1} = \frac{2K_{j+1/2}^n}{r_{j+3/2} - r_{j-1/2}} \left(\frac{I_{j+1}^{n+1}}{c_{v,j+1}^n} - \frac{I_j^{n+1}}{c_{v,j}^n} \right). \quad (A-26)$$

V. MOMENTUM EQUATION

The momentum equation is given by

$$\begin{aligned} \frac{\partial \rho u}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u^2) = -\rho g - \frac{\partial p}{\partial r} \\ + \frac{1}{r^2} \frac{\partial}{\partial r} \left[r^2 (2\mu + \lambda) \frac{\partial u}{\partial r} \right] - \frac{2u(2\mu + \lambda)}{r^2} + \frac{2u}{r} \frac{\partial \lambda}{\partial r}. \quad (A-27) \end{aligned}$$

The Lagrangian form of (A-27) is differenced by integrating over a spherical shell (momentum control volume) between $r_{j-1} = \frac{1}{2} (r_{j-3/2} + r_{j-1/2})$ and $r_j = \frac{1}{2} (r_{j+1/2} + r_{j-1/2})$, using the procedure outlined in Sec. II.

$$\begin{aligned}
\frac{M_{v,j-\frac{1}{2}}}{\delta t} (u_{j-\frac{1}{2}}^{n+1} - u_{j-\frac{1}{2}}^n) = & -M_{v,j-\frac{1}{2}} g_{j-\frac{1}{2}} - 2V_{v,j-\frac{1}{2}} \frac{(p_j^{n+1} - p_{j-1}^{n+1})}{r_{j+\frac{1}{2}} - r_{j-3/2}} \\
& + \frac{4}{3} \left[A_j \mu_j^n \frac{u_{j+\frac{1}{2}}^{n+1} - u_{j-\frac{1}{2}}^{n+1}}{r_{j+\frac{1}{2}} - r_{j-\frac{1}{2}}} - A_{j-1} \mu_{j-1}^n \frac{u_{j-\frac{1}{2}}^{n+1} - u_{j-3/2}^{n+1}}{r_{j-\frac{1}{2}} - r_{j-3/2}} \right] \\
& - \frac{4}{3} V_{v,j-\frac{1}{2}} \left\{ \frac{u_{j-\frac{1}{2}}^{n+1}}{r_{j-\frac{1}{2}}} \left[2 \frac{\mu_j^n - \mu_{j-1}^n}{r_{j+\frac{1}{2}} - r_{j-3/2}} + \frac{(\mu_j^n + \mu_{j-1}^n)}{r_{j-\frac{1}{2}}} \right] \right\}, \quad (A-28)
\end{aligned}$$

where the vertex masses and vertex volumes are given by

$$M_{v,j-\frac{1}{2}} = \frac{1}{2} (M_{c,j} + M_{c,j-1}), \quad (A-29)$$

$$V_{v,j-\frac{1}{2}} = r_j^3 - r_{j-1}^3. \quad (A-30)$$

The shell areas, A_j , are defined at cell centers, as indicated by the integral subscripts. To obtain the gravitational acceleration, we perform the sum

$$g_{j-\frac{1}{2}} = \frac{4\pi G}{3r_{j-\frac{1}{2}}^2} \sum_{i=2}^{j-1} M_{c,i}. \quad (A-31)$$

This procedure is more accurate for computing the gravitational potential than is solving the Poisson equation. We assume $\lambda = -2\mu/3$ in Eq. (A-28).

VI. PHASE II

In Phase II we are modeling the convection term

$$\iint_S \rho Q (u_g - \tilde{u}) \cdot \hat{n} dS, \quad (A-32)$$

where u_g is the grid velocity and $\tilde{u}$ is the fluid velocity at the end of Phase I. We define the difference velocity for our one-dimensional problem, $w_{j-\frac{1}{2}} \equiv u_{g,j-\frac{1}{2}} - \tilde{u}_{j-\frac{1}{2}}$, which is the velocity of the mesh relative to the fluid. Then $w_{j-\frac{1}{2}} A_{j-\frac{1}{2}} \delta t$ is the volume relative to the fluid that is swept out by the moving grid point. One might be tempted to take

for, say the density, simply an average of the densities on either side of the moving mesh point. This is called centered differencing and is only conditionally stable.¹⁷ For this reason we use a mixture of centered differencing and donor cell differencing. The donor cell component adds a strong stabilizing diffusional truncation error.

Define the donor cell parameter, $\alpha_{j+\frac{1}{2}}$, by

$$\alpha_{j+\frac{1}{2}} = -\bar{\alpha} \operatorname{sgn} (w_{j+\frac{1}{2}}), \quad (A-33)$$

where the function sgn is the sign of the argument, and $\bar{\alpha}$ is a constant, $0 \leq \bar{\alpha} \leq 1$. As an example of the difference form of the convection term for a cell centered quantity,

$$\begin{aligned}
M_{c,j}^{n+1} = & M_{c,j}^n - \frac{\delta t}{2} \left\{ w_{j-\frac{1}{2}} A_{j-\frac{1}{2}} \left[(1 + \alpha_{j-\frac{1}{2}}) \tilde{\rho}_{j-1} \right. \right. \\
& \left. \left. + (1 - \alpha_{j-\frac{1}{2}}) \tilde{\rho}_j \right] \right. \\
& \left. - w_{j+\frac{1}{2}} A_{j+\frac{1}{2}} \left[(1 + \alpha_{j+\frac{1}{2}}) \tilde{\rho}_j \right. \right. \\
& \left. \left. + (1 - \alpha_{j+\frac{1}{2}}) \tilde{\rho}_{j+1} \right] \right\}. \quad (A-34)
\end{aligned}$$

The tildes denote results from Phase I. This is a straightforward approximation to Eq. (A-32), if Q is taken to be unity. The density is obtained by calculating volumes from the new mesh position

$$r_{j-\frac{1}{2}}^{n+1} = r_{j-\frac{1}{2}}^n + u_g \delta t. \quad (A-35)$$

Then

$$\rho_j^{n+1} = \frac{M_{c,j}^{n+1}}{V_{c,j}^{n+1}}, \quad (A-36)$$

which ensures mass conservation. The convection of internal energy or mass of any species is handled in exactly the same manner.

For momentum the control volume runs from cell center to cell center, and a slight modification is necessary. The difference velocity must be obtained by averaging the difference velocities of the neighboring vertices. This leads to

$$u_{j-1/2}^{n+1} = \frac{1}{M_{v,j-1/2}^{n+1}} \left\{ M_{v,j-1/2}^n u_{j-1/2}^n - \frac{\delta t}{4} \left[\tilde{\rho}_{j-1} (w_{j-1/2} + w_{j-3/2}) A_{j-1} ((1 + \alpha_{j-1}) \tilde{u}_{j-3/2} + (1 - \alpha_{j-1}) \tilde{u}_{j-1/2}) \right. \right. \\ \left. \left. - \tilde{\rho}_j (w_{j-1/2} + w_{j+1/2}) A_j ((1 + \alpha_j) \tilde{u}_{j-1/2} + (1 - \alpha_j) \tilde{u}_{j+1/2}) \right] \right\}, \quad (A-37)$$

where

$$\alpha_j = -\bar{\alpha} \operatorname{sgn}(w_{j-1/2} + w_{j+1/2}). \quad (A-38)$$

It is not necessary to use the same $\bar{\alpha}$ in the momentum equation as in the equation for the mass or energy. We have found empirically that we need more donor cell in the mass and energy equations to keep cells from emptying out in the neighborhood of steep gradients.

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