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The Construction of Compatible Hydrodynamics Algorithms Utilizing Conservation of Total Energy

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The principal goal of all numerical algorithms is to represent as faithfully and accurately as possible the underlying continuum equations to which a numerical solution is sought. However, in the transformation of the equations of fluid dynamics into discretized form important physical properties are either lost, or obeyed only to an approximation that often becomes worse with time. This is because the numerical methods used to form the discrete analog of these equations may only represent them to some order of local truncation error without explicit regard to global properties of the continuum system. Although a finite truncation error is inherent to all discretization methods, it is possible to satisfy certain global properties, such as conservation of mass, momentum, and total energy, to numerical roundoff error. The purpose of this work is to show how these equations can be differenced compatibly so that they obey the aforementioned properties. In particular, it is shown how conservation of total energy can be utilized as an intermediate device to achieve this goal for the equations of fluid dynamics written in Lagrangian form, and with a staggered spatial placement of variables for any number of dimensions and in any coordinate system. For staggered spatial variables it is shown how the momentum equation and the specific internal energy equation can be derived from each other in a simple and generic manner by use of the conservation of total energy. This allows for the specification of forces that can be of an arbitrary complexity, such as those derived from an artificial viscosity or subzonal pressures. These forces originate only in discrete form; nonetheless, the change in internal energy caused by them is still completely determined. The procedure given here is compared to the "method of support operators," to which it is closely related. Difficulties with conservation of momentum, volume, and entropy are also discussed. The proper treatment of boundary conditions and differencing with respect to time are detailed. © 1998 Academic Press

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1. INTRODUCTION

In discretizing the equations of fluid dynamics one should attempt to mirror into the numerical formulation of the equations as many of the mathematical properties of the continuum system as possible. The most important of such properties are expressed as conservation laws. In this work it is shown how this can be achieved to a substantial extent; limitations that are of a fundamental character are also indicated. This is accomplished utilizing the conservation of total energy associated with any physical model. The numerical error in this quantity results from inconsistencies among the various terms that compose the system of equations in discrete form. This is because in order to derive the discrete form of the conservation of total energy the same mathematical relations must hold between the discrete terms as do for the undiscretized, continuum model. Thus, by removing these inconsistencies one recovers exact conservation of energy in discrete form. The mathematical relations that must be obeyed to achieve this are the discrete analogs of the vector identities that involve the dependent variables of the physical system. Numerical algorithms constructed in this manner are said to be compatible, in that the forms of the discrete terms that compose them are not specified independently. They therefore mimic to the degree possible the properties of the continuum system.

The physical model that is our main concern is the equations of fluid dynamics written in Lagrangian form. The main part of our theoretical development is given in Section 2 where we begin with the statement of our model, and some preliminary definitions and ideas that set the framework for the rest of this paper. Next, we present the fundamental piece of this work, where the consequences of requiring that conservation of total energy be obeyed to roundoff error for the discrete equations are developed in detail. This is done for a staggered spatial placement of variables wherein the position and velocity are defined at grid points, and density, internal energy, and the pressure are defined at zone centers. The important concepts of a corner mass and a corner force that are common to both a given zone and one of its defining points are introduced. It is then shown how these quantities can be used to construct both the zone and grid point masses as well as the total force that acts on a point, and the rate of work done with respect to a zone. The momentum and specific internal energy equations are then related via the expression for the conservation of total energy in a simple and totally generic manner; it is shown how one can easily transform from one to the other using this conservation law. The relationship of this development to the method of support operators [2,3] is then given. In this method one specifies a discrete form for one of the vector operators (divergence, gradient, or curl) and then uses the vector identities in discrete form to obtain the others in a compatible manner. This is shown to be virtually identical to the conservation of energy procedure that utilizes common corner force objects in the case of a staggered grid placement of variables. The important difference is that the conservation of energy method allows a straightforward generalization to the case where the forces in question are specified directly in discrete form, and where there exist no continuum differential operators that define them [4,5]. Nonetheless, the work performed by these forces is unambiguously determined. This is because the results that we derive relating force to work utilizing the conservation of total energy are true in a purely algebraic sense that is independent of the actual functional form of the force; this fact can be viewed as an extension of the support operators method. Next, the staggered grid formulation is contrasted to that where all variables are defined at the same spatial locations (point-centered).

Here compatible vector operators can be constructed using the support operators method and conservation of total energy can thus be guaranteed to roundoff error; however, the conservation of total energy cannot be used to connect force and work algebraically as is the case for a staggered grid scheme. This leads to important limitations associated with point-centered discretizations. Finally, possible errors in entropy production and momentum conservation are discussed. The former can arise because two kinds of zone volumes are defined in the differencing of the fluid equations in Lagrangian form: one overtly to obtain the zone density, and one implicitly in constructing the work performed by the scalar pressure. These may not always be equal, resulting in errors in the accounting of entropy. Both linear and angular momentum conservation is also analyzed in terms of volume topology. Although both are exactly conserved, an important additional property, which is that the force density due to the scalar pressure have zero curl in discrete form, is not obeyed in general by control volume, or other, discretizations. This has important consequences that are briefly detailed.

The basic theoretical ideas developed in this work can be viewed as an extension to discrete form of the principle of virtual work and the principle of least action as they are known in classical mechanics [6]. The principle of virtual work has been used in the finite element context to connect the discrete equations for a force and the work that it produces [7]. The method of support operators gives results that can be shown to be directly obtainable from the discrete form of the principle of least action [8]. The essential idea is that a force and the work that it produces should be conjugate quantities in discrete form just as they are in the usual Lagrangian or Hamiltonian formulation of the continuum laws of classical mechanics [9].

In Section 3 an example is presented that illustrates the above ideas. Here is presented an analysis of the so-called "area-weighted" schemes in two-dimensional, cylindrical geometry [10–12,7,13,14]. These schemes have been used extensively for problems where it is desired that perfect one-dimensional spherical symmetry be preserved as a possible limiting case in two-dimensional cylindrical geometry. They have arisen in various forms over a period of 40 years, and have generated some confusion as to their real meaning and domain of validity, and possess a number of novel properties. Among these are conditional conservation of volume, momentum, and entropy. They are analyzed in a succinct and transparent manner using the ideas developed in Section 2. Comparison to the various older versions of these methods are detailed briefly.

Some issues that are necessary for a successful implementation of the ideas presented here into a working code are discussed in Section 4. Principal among these are the proper implementation of various types of boundary conditions in the compatible framework for the staggered grid formulation of Section 2. Discretization with respect to time by means of a predictor-corrector method is also discussed. A numerical example is given that illustrates difficulties that can be encountered with the implementation of boundary conditions.

A brief summary and final conclusions are detailed. It is emphasized that various extensions and amplifications of the ideas developed here are presented in other related papers [13,4,5]. It is this paper that forms the theoretical basis for this other work. Finally, an appendix is included that illustrates the derivation of difference formulas in vector, operator form in two-dimensional, Cartesian geometry. These formulas are utilized in the development and analysis performed in Section 3.

2. FUNDAMENTAL IDEAS AND BASIC EQUATIONS

The basic assumption of all Lagrangian algorithms is that there exists a discrete volume element, V_i, that may deform in shape but through whose boundary no mass flows. Thus the original mass present in the volume at some starting time, M_i, is constant. At any later time, t, the density, ρ, inside the given element is simply found from $\rho_i(t) = M_i / V_i(t)$. Substituting this expression into the usual equation for continuity of mass results in the statement that

$$\frac{1}{V_i}\frac{dV_i}{dt} = (\nabla \cdot \vec{v})_i, \tag{1}$$

where d/dt is the total time derivative following the fluid element.

Next, consider the equation of motion with the force given as the gradient of a scalar pressure P, and also, the associated equation for the evolution of the specific internal energy e. Written in Lagrangian form these are

$$\rho\frac{d\vec{v}}{dt} = -\nabla P, \tag{2}$$

$$\rho\frac{de}{dt} = -P\nabla \cdot \vec{v}. \tag{3}$$

To complete this system an equation of state of the form $P = P(\rho, e)$ is assumed to have been specified.

An energy equation can be formulated from the above simply by multiplying Eq.(2) by the velocity $\vec{v}$, adding the result to Eq.(3), and integrating over some domain D in which these equations are defined. This gives the result

$$\int_D \left(\frac{\rho}{2}\frac{d\vec{v}^2}{dt} + \rho\frac{de}{dt}\right) dV = -\int_D (\vec{v} \cdot \nabla P + P\nabla \cdot \vec{v})\, dV = -\oint_{\partial D} P\vec{v} \cdot d\vec{S}, \tag{4}$$

where the last term arises from the vector identity $\nabla \cdot (P\vec{v}) = \vec{v} \cdot \nabla P + P\nabla \cdot \vec{v}$. From this equation the total energy density per unit volume can be defined as $\epsilon \equiv \rho e + \rho\vec{v}^2/2$. If the force on the RHS of Eq.(2) is given in the more complicated form as $\vec{f} \equiv \nabla \cdot \overline{\overline{Q}}$, where $\overline{\overline{Q}}$ is the total stress tensor, then the energy source term on the RHS of Eq.(3) is $\overline{\overline{Q}}: \nabla\vec{v}$. The same procedure results in an equation for total energy that is completely analogous to Eq.(4) by means of the similar vector identity $\nabla \cdot (\overline{\overline{Q}} \cdot \vec{v}) = \vec{v} \cdot (\nabla \cdot \overline{\overline{Q}}) + \overline{\overline{Q}}: \nabla\vec{v}$.

The fundamental equation describing the Lagrangian representation of fluid flow is given by Eq.(1). It can be utilized in two different ways. First, given a set of velocities $\vec{v}_j$ that determine the time evolution of the points "j" that define the ith volume element, and its initial value $V_i(0)$ at time $t = 0$, Eq.(1) determines the evolution of this volume, $V_i(t)$, with time. On the other hand, given a prescription for the ith volume element as a function of some specified defining coordinates $\vec{R}_j$, $V_i(t) = V_i(\vec{R}_1(t), \vec{R}_2(t) \cdots)$, then by differentiating $V_i(t)$ with respect to time, and using the fact that for any Lagrangian point j, $d\vec{R}_j/dt = \vec{v}_j$, Eq.(1) determines $(\nabla \cdot \vec{v})_i$, the divergence of the velocity field in discretized form defined in the ith zone.

Although we have not yet made any direct statements about the discretization of the equations for the evolution of momentum and specific internal energy, one can see already from the above remarks that inconsistencies may arise if one is not careful how the terms that enter the RHS of these equations are chosen. Since we have given a prescription for the calculation of density and have shown that this is equivalent to the specification

of $\nabla \cdot \vec{v}$, which enters into the RHS of Eq.(3), this latter equation cannot be discretized arbitrarily. That is, from our definition of density the consistency of Eqs.(1),(3) states that $M_i de_i = -P_i dV_i$, and thus implies the form of de_i associated with the volume change dV_i. Analogously, in Eq.(4), which gives the equation for the evolution of total energy, we have used a vector identity to obtain a surface term; this will not hold in discrete form unless the discrete representations of the terms that enter into the discrete analogs of Eqs.(2),(3) obey the same integral relations, written in summation form, as do the terms in the original continuum equations.

In the next two subsections we investigate the consequences of the conservation of total energy to the development of discrete difference equations that are useful for the numerical integration of the equations of hydrodynamics. This is performed for a staggered spatial placement of variables, which is the main concern of this work; our results are then interpreted using the framework of the method of support operators. The point-centered formulation is also investigated. The important considerations of entropy, volume, and momentum conservation are explored in this context. The control volume method is used as the underlying basis for all of our discretization formulas, although this is not necessary to establish the validity of our results. All dependent variables are considered to be piecewise constant functions of space on the respective meshes on which they are defined. For simplicity, most of our arguments in Section 2 are given with respect to two Cartesian spatial dimensions, although extension to three dimensions is readily apparent.

2.1. *Staggered Spatial Grid Formulation*

2.1.1. Staggered grid geometry/masses. We begin the staggered grid formulation by introducing some basic concepts and notation that set the framework for the rest of this work. For purposes of illustration we consider a quadrilateral grid in two-dimensional, Cartesian geometry as in Fig.1. There is shown a quadrilateral z that is defined by points labeled as

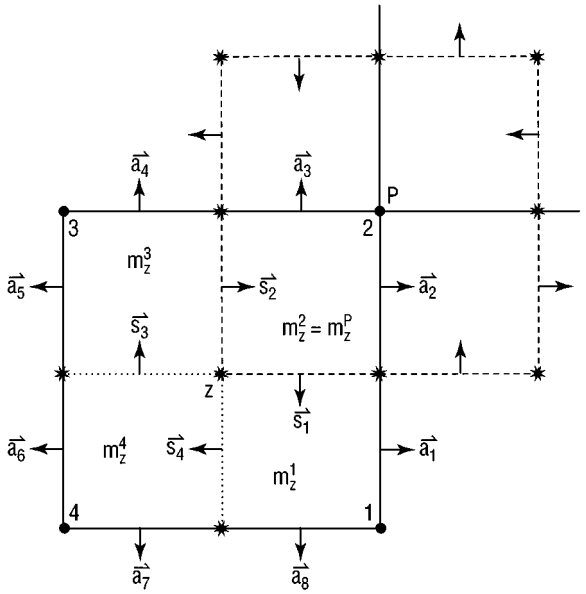


FIG. 1. Grid with respect to zone z and point p showing coordinate-line (solid lines) and median (dashed and dotted lines) mesh with associated half-edge vectors ($\vec{a}_i$ with coordinate-line mesh, and $\vec{S}_i$ with median mesh). Corner masses, m_z^p, are also indicated.

solid dots $1 \cdots 4$ that are connected by straight lines. Points labeled by asterisks denote the midpoints of these lines. The point in the center of the quadrilateral, also labeled by an asterisk, is defined by coordinates that are the simple average of those of the quadrilateral grid points. (For a quadrilateral this is the same as the point defined by the intersection of the lines connecting the midpoints of the opposite quadrilateral sides.) The solid lines connecting the grid points define the "coordinate-line" mesh, while the dotted and dashed lines that connect the points given by asterisks make up the "median" mesh. These are our primary and dual grids, respectively. Position and velocity are defined at the grid points; these quantities are "slaved" at points that form the median mesh as a simple average of respective grid point quantities. The density, specific internal energy, and thus the pressure are defined as functions that are constant inside the quadrilateral zone. The dependent variables are thus staggered with respect to their spatial locations. There are eight vectors, $\vec{a}_i$, that are the outward normals to the coordinate lines of a given quadrilateral zone. As shown in Fig.1, these have a magnitude of one-half of the distance between grid points, and thus $\vec{a}_1 = \vec{a}_2$, etc. However, in general these pairs have neither the same magnitude nor the same direction once the straight line condition used to join grid points is relaxed. The four vectors, $\vec{S}_i$, that are the normals to the median mesh segments interior to a zone are also shown. These have magnitudes of the distance between the points that define these line segments. Also shown is a point labeled p (the same point as 2 of quadrilateral z) about which is drawn a dashed line that is its associated median mesh. The variables p and z are always used as subscripts or superscripts with integer values that range over all of the grid points and zones, respectively.

The first important subzonal concept that we introduce is that of a "corner." The corner volume associated with a grid point p and a zone z in two-dimensions, as indicated in Fig.1, is the volume inside the surface defined through the point p, the two midpoints of the lines through point p of zone z, and the center point of zone z (vectors $\vec{a}_2$, $\vec{a}_3$, $\vec{S}_1$, and $-\vec{S}_2$ of Fig.1). There are four corner volumes to each quadrilateral zone. In two dimensions the corner volume, as just defined, is always a quadrilateral regardless of the type of zones that compose the underlying grid. Next we define the corner mass associated with the point p and zone z, m_p^z, as the mass inside the associated corner volume at time $t = 0$. We use z or p as a superscript or a subscript interchangeably so that $m_p^z = m_z^p$, but we always perform summations with respect to the lower index. The corner mass is now used as the primitive quantity from which we can construct both the zone and nodal, or grid point, masses. To construct the total mass of zone z one simply forms the sum of all corner masses with fixed label z; likewise, to find the nodal mass of a point p one sums all corner masses with the fixed label p. This is given simply as

$$M_z = \sum_p m_p^z, \qquad M_p = \sum_z m_z^p. \tag{5}$$

Since the zone and nodal masses are composed of the same objects that are simply added in a different order it follows that

$$\sum_p M_p = \sum_z M_z. \tag{6}$$

The above equation simply states that the total zonal and nodal mass in a problem are equal, and is the statement of consistency of the zonal and nodal grids. When computing the nodal

mass at points that lie on the boundary of a physical region it is always assumed that the corner masses exterior to that region are zero.

It is usual to declare M_z a constant by the Lagrangian assumption. However, often M_p is allowed to vary with time. We consider both M_z and M_p on a totally equal footing. Thus, in the rest of our development we assume that both M_z and M_p are constant, Lagrangian objects [4].

2.1.2. Compatibility—semi-discrete form. The first important characteristic of a staggered placement of variables is that the evolutionary equations are defined with respect to different, but overlapping, spaces: Eq.(2) that evolves momentum in time is defined at the nodes, while Eq.(3) that evolves internal energy is defined in the zones. The equation for conservation of total energy, Eq.(4), is thus composed of a mix of variable definitions. Although this may at first appear to be an added complexity over defining all variables at the same spatial locations, it actually turns out to be superior to a point-centered placement of variables. This is because it allows one to extend the Lagrangian assumption in a natural manner that eliminates underconstrained modes of distortion [4], and to specify forces in discrete form without the need to make additional assumptions about the manner in which the work performed at interfaces between cells is to be divided between kinetic and internal energies, as is necessary for point-centered formulations when operator prescriptions for these forces are not available. However, care must be taken with staggered grid formulations so that logical inconsistencies between quantities defined at nodes and zones do not occur.

The momentum equation is utilized next to introduce the important concept of a corner force, using pressure forces as an example. After this the total energy is defined on a single zone basis. It is then shown how this definition can be extended across the entire domain of integration, and how by this extension the internal energy equation can be derived in a generic form that is identical to that obtained by a direct discretization of Eq.(3) for the special case of forces that arise from a pressure that is piecewise constant in a zone.

Consider the momentum equation, Eq.(2), and integrate it over a volume element V_p defined about point p in Fig.1 by the dashed lines that form the median mesh. Since the nodal mass M_p is Lagrangian this yields the result

$$M_p \frac{d\vec{v}_p}{dt} = -\int_{V_p} \vec{\nabla} P \, dV = -\oint_b P d\vec{S} = \sum_z \vec{f}_z^{\,p} \equiv \vec{F}_p. \tag{7}$$

At this point we define the corner force, $\vec{f}_z^{\,p}$, using the same notation as was used for the corner mass. The corner force acting on point p due to the pressure P_z in zone z is defined as $\vec{f}_z^{\,p} \equiv P_z(\vec{S}_2 - \vec{S}_1) = P_z(\vec{a}_2 + \vec{a}_3)$, where the last equality follows simply from vector addition, as can be seen from Fig.1. Thus we see that the boundary integral through zone z depends only on the side midpoints, and is thus path independent. To obtain the total force, F_p, that is exerted on point p one simply sums the corner forces about all zones associated with this point, as indicated in Eq.(7). For the case of the full stress tensor, $\underline{\underline{Q}}_z$, given as piecewise constant in a zone, the corner force is determined by $\vec{f}_z^{\,p} = \underline{\underline{Q}}_z \cdot (\vec{a}_2 + \vec{a}_3)$, where we have favored the coordinate-line mesh over the median mesh for defining this quantity.

At this point a generalization is made. The corner forces from here on are thought of as emerging from completely general origins, and not just due to a scalar pressure or a tensor that is constant throughout a given zone. In certain instances one can have forces that arise from scalars or tensors that are constant only in a part of a zone [4,5]. In this case subzonal forces can be calculated along the various pieces of the coordinate-line mesh, the median

mesh, or both. These forces can be specified in an almost arbitrary manner and added to the corner forces that are already present due to pressures and tensors that are constant in a zone. The only restriction is that total zone momentum, as discussed later, must be conserved. In this instance the total force acting on a point p is still just the sum of the corner forces about that point, as given by Eq.(7).

It is next shown how to construct conservation of total energy in semi-discrete form. We begin by defining the total energy of a zone. Since the internal energy is zone centered, its definition is automatic. The kinetic energy is defined at the nodes; however, it can be interpolated to the zones by means of the overlap of the zonal and nodal masses. This is given by the corner mass m_p^z that is common to both a zone and a point. Thus we define the total energy, E_z, in a single zone z as

$$E_z = M_z e_z + \sum_p m_p^z \vec{v}_p^2/2. \tag{8}$$

Next, we take the total derivative with respect to time of this quantity and substitute from Eq.(7) for momentum to obtain

$$\frac{dE_z}{dt} = M_z \frac{de_z}{dt} + \sum_p \frac{m_p^z \vec{v}_p}{M_p} \cdot \sum_{z'} \vec{f}_{z'}^{\,p}, \tag{9}$$

where the corner mass has been assumed to be constant in time—a point to which we later return. This equation can be summed over all zones to yield

$$\frac{d}{dt}\left(\sum_z E_z\right) = \sum_z M_z \frac{de_z}{dt} + \sum_z \sum_p \frac{m_p^z \vec{v}_p}{M_p} \cdot \sum_{z'}^{p} \vec{f}_{z'}^{\,p}. \tag{10}$$

At this point we note from the definition of the nodal mass given by Eq.(5) that $\sum_z \sum_p m_p^z \vec{v}_p^2/2 = \sum_p M_p \vec{v}_p^2/2$. Using this fact in Eqs.(8),(10) gives the result for conservation of total energy for the entire region as

$$\begin{aligned}\frac{d}{dt}\left(\sum_z M_z e_z + \sum_p M_p \vec{v}_p^2/2\right) &= \sum_z M_z \frac{de_z}{dt} + \sum_p \sum_z \vec{f}_z^{\,p} \cdot \vec{v}_p \\ &= \sum_z \left(M_z \frac{de_z}{dt} + \sum_p \vec{f}_p^{\,z} \cdot \vec{v}_p\right) + \sum_i \vec{f}_{bd,i} \cdot \vec{v}_{bd,i}, \end{aligned} \tag{11}$$

where in our notation $z' \to z$ in obtaining the first form of the RHS of this equation. The first form of the RHS of this equation can be regrouped to obtain the second wherein the order of the double sum has been interchanged: and also, divided into the parts that are due to corner forces that act from the interior zones of the domain onto points, and those that act from the exterior boundary onto boundary points through the momentum equation. (Note that $\vec{f}_z^{\,p} \to \vec{f}_p^{\,z}$ in the above, since the lower index is always summed.) Now if the sum over zones in the second form of the RHS of Eq.(11) is set to zero for each zone z there results

$$M_z \frac{de_z}{dt} = -\sum_p \vec{f}_p^{\,z} \cdot \vec{v}_p. \tag{12}$$

This is the form of the internal energy equation in terms of arbitrary corner forces $\vec{f}_p^z$ that are common to both it and the momentum equation. These forces are simply manipulated in a different manner. That is, to obtain the total force acting on a grid point the corner forces associated with that point are simply summed; while to obtain the heating rate of a zone the corner forces of that zone are dotted into their associated grid point velocity, and then summed. It is important to note that no boundary average quantities appear on the RHS of Eq.(12). What one has are common corner forces that exchange zone internal energy for nodal kinetic energy, or vice versa.

To verify that this makes physical sense, Eq.(12) is written out explicitly for corner forces that originate from a pressure P_z that is constant in zone z, as previously defined by means of Fig.1, to obtain

$$M_z \frac{de_z}{dt} = -\sum_p \vec{v}_p \cdot \vec{f}_p^z = -P_z[(\vec{a}_8 + \vec{a}_1) \cdot \vec{v}_1 + (\vec{a}_2 + \vec{a}_3) \cdot \vec{v}_2 + (\vec{a}_4 + \vec{a}_5) \cdot \vec{v}_3 + (\vec{a}_6 + \vec{a}_7) \cdot \vec{v}_4] \equiv -\int_{V_z} P \nabla \cdot \vec{v}\, dV. \tag{13}$$

Here it is noted that the discrete expression that results is equal to the exact discretization of Eq.(3) that is obtained by directly integrating it over the zone z in Cartesian geometry. Thus, compatibility is naturally obtained for control volume differencing in Cartesian geometry in any number of dimensions.

From the LHS of Eq.(11) it is natural to define the total energy over the entire domain at time t as

$$E_T(t) \equiv \sum_z M_z e_z + \sum_p M_p \vec{v}_p^2/2. \tag{14}$$

This equation can be integrated in time to obtain

$$E_T(t) = E_T(0) + \sum_{m=1}^{n} \Delta t_m \sum_i \vec{f}_{bd,i}^{\sigma} \cdot \vec{v}_{bd,i}^{m+1/2}, \tag{15}$$

where Δt_m is the magnitude of the timestep on the mth cycle. This is the discrete analog of Eq.(4). If one subtracts the left and right sides of Eq.(15) and divides the result by the sum of these two quantities there results a nondimensional measure of energy conservation that should always be equal to zero to within numerical roundoff error.

2.1.3. Compatibility—fully discrete form. Although the basic ideas of a compatible discretization have been illustrated by the semi-discrete derivation just given, it is useful to consider compatibility starting from Eq.(14) for total energy, and the momentum equation, Eq.(7), where these equations are both discretized with respect to time. Denoting the discrete time variation of any quantity as Δ applied to that object, the time variation of the total energy equation, Eq.(15), yields the result

$$\sum_z M_z \Delta e_z + \sum_p M_p \vec{v}_p^{n+1/2} \cdot \Delta \vec{v}_p = \Delta t \sum_i \vec{f}_{bd,i}^{\sigma} \cdot \vec{v}_{bd,i}^{n+1/2}. \tag{16}$$

The time centered velocity $\vec{v}_p^{n+1/2} \equiv (\vec{v}_p^{n+1} + \vec{v}_p^n)/2$ follows directly from the time variation of the kinetic energy defined at the points since $\vec{v}_p^{n+1/2} \cdot \Delta \vec{v}_p = [(\vec{v}_p^2)^{n+1} - (\vec{v}_p^2)^n]/2$, where

$\Delta\vec{v}_p \equiv \vec{v}_p^{n+1} - \vec{v}_p^{n}$, $\Delta e_z \equiv e_z^{n+1} - e_z^{n}$, and the superscript n indicates time level. The discrete time form of the momentum equation, Eq.(7), is given as

$$M_p \Delta\vec{v}_p = \sum_z \vec{f}_z^{\,p,\sigma}\,\Delta t. \tag{17}$$

The time centering of the corner forces exterior to the boundary in Eq.(16) and in the above momentum equation is given at some intermediate value, denoted by σ, between time level n and $n+1$.

Because both the internal energy and the kinetic energy must be defined at the same time level so that the total energy, $E_T(t)$, is at a single time level, it follows that we must use an even time integration scheme [15]. Schemes that have the definitions of variables staggered in time are not appropriate when total energy is exactly conserved, since both the internal energy and the kinetic energy must be at the same time level if they are to be exchanged by common corner forces (these may still have arbitrary time centering.).

Substituting Eq.(17) into Eq.(16) yields

$$\sum_z M_z \Delta e_z + \sum_p \vec{v}_p^{n+1/2} \cdot \sum_z \vec{f}_z^{\,p,\sigma}\,\Delta t = \Delta t \sum_i \vec{f}_{bd,i}^{\,\sigma} \cdot \vec{v}_{bd,i}^{n+1/2}, \tag{18}$$

where the nodal mass M_p no longer enters. The crucial step is the interchange in the order of the double discrete summation on the LHS of this equation. This is equivalent to a discrete integration by parts. Regrouping all terms in Eq.(18) with the same integer index z there results

$$\sum_z \left[M_z \Delta e_z + \sum_p \vec{v}_p^{n+1/2} \cdot \vec{f}_p^{\,z,\sigma}\,\Delta t \right] = \Delta t \sum_i \vec{f}_{bd,i}^{\,\sigma} \cdot \vec{v}_{bd,i}^{n+1/2}. \tag{19}$$

The final step is to satisfy Eq.(19) in the strong form by setting the quantity in brackets equal to zero for every value of z (or for every zone). This yields the same equation as that given by Eq.(12), but with the additional conclusion that $\vec{v}_p = \vec{v}_p^{n+1/2}$, an important result. Thus the equation for the evolution of specific internal energy becomes

$$\Delta e_z = -\sum_p \vec{f}_p^{\,z,\sigma} \cdot \vec{v}_p^{n+1/2} \Delta t / M_z. \tag{20}$$

The time centering of the forces, given by σ, is still left undetermined.

The strong solution is not the only solution to Eq.(19), but it is the only one that has any physical significance for forces that originate from pressures or tensors that are constant throughout a given zone. This important fact is shown in the next section. For the subzonal forces mentioned earlier, other possible solutions have not been found useful in practice. The solution of Eq.(19) in strong form has a simple physical interpretation. This is that a corner force $\vec{f}_p^{\,z}$, whatever its origin, produces a momentum change by acting on its associated point p, and does work at the rate $-\vec{f}_p^{\,z} \cdot \vec{v}_p$ with respect to its associated zone z. Finally, we could just as well have specified the discrete form for Δe_z from Eq.(20) and inserted this into Eq.(16). Then an analogous interchange of the order of a double summation results in an outer sum over index p, which when satisfied for every value of this index yields the discrete momentum equation.

Next, we show how interface pressures that act between zones, and perform total work on a zone, can be derived. These pressures produce changes in both the internal and kinetic

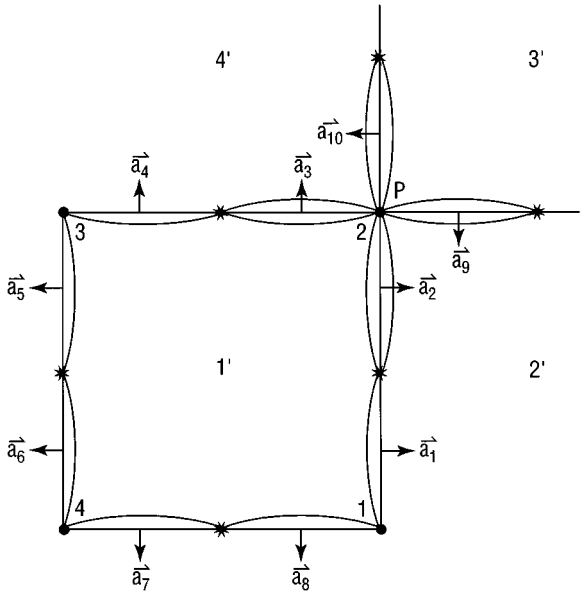


FIG. 2. Coordinate-line mesh with half-edge vectors and force "contours" (curved lines) with respect to zone $1'$ and point p. Zones about point p are indicated by numbers $1' \cdots 4'$.

energy of a single zone. We denote them as $\mathcal{P}_i$, where $i = 1 \cdots 8$ for each quadrilateral zone, and formally rewrite Eq.(19) as

$$\sum_z [(\mathcal{P}_1\vec{a}_1 + \mathcal{P}_8\vec{a}_8) \cdot \vec{v}_1) + (\mathcal{P}_2\vec{a}_2 + \mathcal{P}_3\vec{a}_3) \cdot \vec{v}_2) + (\mathcal{P}_4\vec{a}_4 + \mathcal{P}_5\vec{a}_5) \cdot \vec{v}_3 + (\mathcal{P}_6\vec{a}_6 + \mathcal{P}_7\vec{a}_7) \cdot \vec{v}_4]_z = \sum_i P_{bd,i}\vec{S}_{bd,i} \cdot \vec{v}_{bd,i}. \tag{21}$$

Then for pressure forces the terms on the LHS of Eq.(19) can be written as the sum of the interface work terms and regrouped as coefficients of the eight half-edge vectors $\vec{a}_i$ to give explicit forms for the $\mathcal{P}_i$. These are the interface pressures on the half-edges of the zones; they do equal and opposite work with respect to each of their two adjacent zones. All internal work sums to just the boundary term, as indicated. Choosing the corner defined by point p and zone $1'$ of Fig.2, we can use Eq.(17) and Eq.(20) to rewrite the coefficients of vectors $\vec{a}_2$ and $\vec{a}_3$ in Eq.(19) as

$$\vec{a}_2 \cdot \vec{v}_2 \left[P_{1'} - (P_{1'} - P_{2'}) \frac{\left(m_{z=1'}^{p=2} + m_{z=4'}^{p=2}\right)}{M_{p=2}} \right],$$

$$\vec{a}_3 \cdot \vec{v}_2 \left[P_{1'} - (P_{1'} - P_{4'}) \frac{\left(m_{z=1'}^{p=2} + m_{z=2'}^{p=2}\right)}{M_{p=2}} \right].$$

By comparing these terms to those in Eq.(21), and recalling that $M_{p=2} = \sum_{z=1'}^{4'} m_z^p$, it follows that the interface pressures $\mathcal{P}_2$ and $\mathcal{P}_3$ are given by

$$\mathcal{P}_2 = \left[\left(m_{z=2'}^{p=2} + m_{z=3'}^{p=2}\right) P_{1'} + \left(m_{z=1'}^{p=2} + m_{z=4'}^{p=2}\right) P_{2'}\right] / M_{p=2}, \tag{22}$$

$$\mathcal{P}_3 = \left[\left(m_{z=3'}^{p=2} + m_{z=4'}^{p=2}\right) P_{1'} + \left(m_{z=1'}^{p=2} + m_{z=2'}^{p=2}\right) P_{4'}\right] / M_{p=2}. \tag{23}$$

These pressures give the total work done on a given zone in terms of the grid point velocities; interface velocities need not be defined! If we subtract the change of internal energy in a zone, as given by Eq.(20), from this total work, we exactly obtain the change of kinetic energy with respect to that zone. The change in kinetic energy is given from Eq.(17), with Eq.(8) used to define the kinetic energy in a zone via the corner mass. This argument can be reversed to compute the change of zone internal energy given the change in zone kinetic energy. This situation is what we call "local conservation" form; that is, these quantities are all internally consistent with each other and total energy conservation is valid on a single zone basis. Lastly, note that we must define eight interface pressures for each quadrilateral and not just four, as is often assumed with Riemann solutions [15].

2.1.4. Additional considerations. An important part of the derivations just completed is that the nodal mass as well as the usual zonal mass is considered constant. Often in Lagrangian algorithms only the zonal mass is constant, and the nodal mass is recomputed on each timestep as a different number. This leads to a flux of momentum and kinetic energy from the nodes and results in an extra term $\vec{v}_p(dM_p/dt)$ that should appear on the LHS of the momentum equation, but which is often neglected in practice. By keeping M_p constant in time we have employed a stronger form of the Lagrangian assumption than usually given. This has additional far-reaching consequences as now discussed.

Because M_z is a constant no mass flows through the boundary of zone z in Fig.1. Also, since M_p is a constant no mass flows through the median mesh boundary about point p as shown in Fig.1. However, the intersection of these two boundaries, through which no mass flows, defines a new volume in which the mass is constant, and thus defines a new Lagrangian subzonal mass. From Fig.1 this is the corner mass m_z^p. Thus we have that because both M_z and M_p are constant, it follows that their intersection m_z^p must also be a constant [4]. Therefore there exist auxiliary subzonal pressures in addition to the mean zone pressure P_z. These subzonal pressures arise from the subzonal corner densities ρ_z^p computed as $\rho_z^p = m_z^p / V_z^p(t)$, where the $V_z^p(t)$ are the corner volumes associated with the median and coordinate-line meshes, as shown in Fig.1. The contributions to the corner forces $\vec{f}_z^p$ from these subzonal pressures result in the elimination of spurious grid distortion and the resultant grid tangling that has plagued these methods. This type of integration, whereby four pressures per quadrilateral zone are utilized, is a common practice in finite element formulations [7]. However, we stress that these pressures arise only from subzonal densities and not from subzonal internal energies. Although this does, by intent and necessity, increase grid stiffness, this is not found to present difficulties in the wide range of problems investigated. Also, artificial grid stiffness is mitigated by the fact that we employ subzonal quadrilaterals and not subzonal triangles, as has often been used previously. Rayleigh–Taylor instability problems have been run far into the nonlinear regime successfully, and long after traditional Lagrangian algorithms would terminate due to excessive grid tangling. The full development of this subject considered in the framework given here is pursued in depth elsewhere [4].

It is sometimes useful to define the forces in a zone solely with respect to the individual pieces of the median mesh within that zone. For example, the pressure forces can be defined as $\vec{f}_i^z = P_z \vec{S}_i$ in zone z, where $i = 1 \cdots 4$, as shown in Fig.1. Then the pressure force $\vec{f}_{i=1}^z$ acts with a plus sign in the momentum equation on point 1, and with a minus sign in the momentum equation on point 2, of Fig.1. The rate of change of internal energy due to this force with respect to zone z is thus $-\vec{f}_i^z \cdot (\vec{v}_1 - \vec{v}_2)$. From this rearrangement of terms,

Eq.(20) can be rewritten equivalently as

$$\Delta e_z = -\sum_{i=1}^{4} \vec{f}_i^{\,z} \cdot \delta\vec{v}_i^{\,n+1/2} \Delta t / M_z, \tag{24}$$

where $\delta\vec{v}_i^{\,n+1/2} \equiv \vec{v}_i^{\,n+1/2} - \vec{v}_{i+1}^{\,n+1/2}$ and the cyclic index i is as denoted in Fig.1. This form explicitly displays the Galilean invariance of the internal energy equation. It is most useful in the development of an edge-centered artificial viscosity where the tensor term for the force that is computed from each $\vec{S}_i$ of a given zone is different, and where each term of Eq.(24) is required to be positive definite [5].

A nondynamical, but still useful, way to construct an equation for the change in specific internal energy is just to substitute the definition of M_p from Eq.(5) into Eq.(16) with boundary forces neglected. One then changes the order of the double summation, as before, to arrive at the kinematical expression

$$\Delta e_z = -\sum_{p} m_p^z \vec{v}_p \cdot \Delta\vec{v}_p / M_z, \tag{25}$$

valid in each zone. This equation involves only the corner masses of a zone and the velocities of its associated points. It is useful when one wishes to make kinematical adjustments to the velocity field without specifying any forces and still conserve total energy. It just gives a way of distributing a prescribed change of kinetic energy at a node among its associated zones.

To simulate problems involving instability it is useful to incorporate a constant gravitational force into our preceding formulation. To do this one must add the potential energy term $\sum_p M_p g y_p$ defined with respect to the nodes into Eq.(14) for the total energy E_T. Here g is the strength of the constant gravitational field that acts in the negative y direction, denoted as $\hat{y}$. Then the force term $-(M_p g \Delta t)\hat{y}$ is entered into the RHS of the momentum equation as given by Eq.(17). If one then follows the algebra leading to Eq.(19) it is seen that this equation is unchanged (recall that $\Delta y/\Delta t = v_y$). Thus the internal energy equation, Eq.(20), is unchanged, as it should be for nodal masses moving in a gravitational field, since only the potential and kinetic energy are interchanged. With this modification total energy is still exactly conserved.

2.2. *Relation to Method of Support Operators*

2.2.1. Staggered grid formulation. The method of support operators utilizes the vector identities of differential calculus to derive compatible sets of the fundamental vector differential operators: gradient, divergence, and curl (**GRAD**, **DIV**, and **CURL**) in discrete form. This is done by first specifying one of these operators and then using the vector identities written in discrete summation form to consistently determine the others. In the case of a staggered grid the gradient can act to produce a vector function defined at the points, as in Eq.(17) with zone centered pressures, but it can also act on scalar functions defined at the points to produce a vector function centered in the zones. We will denote the first of these operators as $\mathbf{GRAD}_{z\to p}$, and the latter as $\mathbf{GRAD}_{p\to z}$. Since this also holds for the divergence and the curl, there are six discrete operators to determine for the staggered grid case considered here. This leads to two forms of the discrete Laplacian, one defined on the

points via the zones, and vice versa. For the point-centered case there are only the usual three operators. In the case where variables are defined with respect to points, zones, and sides of zones, more complicated possibilities result [16].

The principal idea of the method of support operators is that because the equations of mathematical physics are given in terms of differential vector operators it is enough to determine these operators in discrete form in order to spatially discretize all such equations. In addition, the proper relations between various dependent variables are automatically built into the discrete equations, at least in integral form. It is next shown that the procedure just given for connecting the momentum and internal energy equations through the conservation of total energy on a staggered spatial grid includes, as a subset for this application, the method of support operators. Conservation of energy is more general in that it allows one to specify forces that arise from subzonal pressures and tensors and still calculate the work performed by them in an automatic manner. These latter forces originate as discrete objects and are not a priori written as a function of the vector operators in continuum form.

Consider the time derivative of total energy as given by Eq.(11), where Eq.(12) has been utilized to replace the term $M_z \frac{de_z}{dt}$ to obtain

$$-\sum_z \sum_p \vec{f}_p^{\,z} \cdot \vec{v}_p + \sum_p \sum_z \vec{f}_z^{\,p} \cdot \vec{v}_p = \sum_i \vec{f}_{bd,i} \cdot \vec{v}_{bd,i}. \tag{26}$$

Let us focus on the LHS of this expression, recalling that the term on the RHS is due to forces, $\vec{f}_{bd,i}$, exterior to the boundary, that act on the system through the momentum equation. We now examine what this statement amounts to for forces determined by piecewise constant zonal pressures.

Consider the staggered grid of Fig.2 where zones labeled $1' \cdots 4'$ and the associated coordinate-line mesh associated with zone $z = 1'$ and point p is shown. Half-edge vectors are indicated by the arrows labeled $\vec{a}_i$, that are sufficient to describe the divergence of the velocity with respect to zone $1'$, and the pressure gradient with respect to point p. The curved lines indicate "force lobes" that connect the side midpoints with the coordinate points. They are straight lines that are shown as curved only so they can be distinctly seen apart from the coordinate lines. They indicate that there are distinct discontinuous forces on either side of these lines. Define the corner vector $\vec{C}^{\,p}_{z=1'} \equiv (\vec{a}_2 + \vec{a}_3)$, that is associated with zone $1'$ and point p; then the piece of the corner force that acts from zone $1'$ to form part of minus the pressure gradient at point p in Fig.2 is $\vec{f}^{\,p}_{z=1'} = P_{z=1'} \vec{C}^{\,p}_{z=1'}$, while the part of the divergence of the velocity field associated with this same corner is given by $\vec{C}^{\,p}_{z=1'} \cdot \vec{v}_p$.

The control volume differencing of the divergence of the velocity in zone $1'$ is given by

$$\begin{aligned}(\nabla \cdot \vec{v})_{z=1'} &= \frac{1}{V_{1'}}[(\vec{a}_1 + \vec{a}_8) \cdot \vec{v}_1 + (\vec{a}_2 + \vec{a}_3) \cdot \vec{v}_2 + (\vec{a}_4 + \vec{a}_5) \cdot \vec{v}_3 + (\vec{a}_6 + \vec{a}_7) \cdot \vec{v}_4] \\ &\equiv \frac{1}{V_{1'}} \sum_p \vec{C}_p^{\,z=1'} \cdot \vec{v}_p. \end{aligned} \tag{27}$$

Next, the discrete form of the vector identity that expresses the divergence of pressure times velocity can be written in summation form as

$$\sum_z V_z P_z \nabla \cdot \vec{v} + \sum_p V_p \vec{v}_p \cdot \nabla P = \sum_i P_{bd,i} \vec{S}_{bd,i} \cdot \vec{v}_{bd,i}, \tag{28}$$

where V_z and V_p are the zone and point volumes, respectively. The explicit functional forms of $\nabla \cdot \vec{v}$ and ∇P are left unspecified. Now if we insert the result given in Eq.(27) for the divergence into the first term on the LHS of Eq.(28), for all zones z, and interchange the order of the double summation in that term, then, by setting the resulting equation to zero for each value of the index p one obtains for the interior points

$$(\nabla P)_p = \frac{1}{V_p}[-P_{1'}(\vec{a}_2 + \vec{a}_3) + P_{2'}(\vec{a}_2 + \vec{a}_9) - P_{3'}(\vec{a}_9 + \vec{a}_{10}) + P_{4'}(\vec{a}_3 + \vec{a}_{10})]$$
$$\equiv -\sum_z P_z \vec{C}_z^p / V_p, \tag{29}$$

which is the compatible discrete form of the gradient operator defined with respect to the grid points, written here for the point labeled p in Fig.2. We could just as well have specified ∇P as Eq.(29) and derived the divergence as given by Eq.(27) by a completely analogous set of steps.

The above arguments can all be translated directly into the language involving corner forces that was employed earlier. To see this note that in the zone $z = 1'$, $(V P \nabla \cdot \vec{v})_{z=1'} = \sum_p \vec{f}_p^{z=1'} \cdot \vec{v}_p$; and likewise for point p, $(V \nabla P)_p = -\sum_z \vec{f}_z^p$. Using these expressions in Eq.(26) results in the vector identity, Eq.(28). Thus, an explicit specification of the corner force can be viewed as specifying ∇P. Then the work done can be found by the series of steps starting from conservation of total energy and leading to Eq.(19). Thus the previously stated procedure using conservation of total energy encompasses the method of support operators; however, because the former can be derived in a very generic form that involves only the corner forces it is more general for the staggered grid case. However, it is important to note that the compatibility of the gradient and divergence operators, as given by Eqs.(27)–(29), justifies the solution given for Eq.(19) that yields the equation for specific internal energy. This is seen to be the only solution that leads to compatible, discrete forms for the vector operators. Thus, a proper determination of the corner forces becomes the central issue. This involves the specification of the corner vectors of the coordinate-line mesh, or alternatively, the associated vectors of the median mesh.

The corner vector, $\vec{C}_z^p$, is not necessarily a simple object. It is composed of two "half-edges" in two dimensions and many analogous "edges" in three dimensions. These half-edges may depend on some or all of the dynamical grid point coordinates and not on just those of two points connected by a straight line, as indicated in Fig.2. The definition of these edges depends on the definition of the zone volume which is of arbitrary complexity and, as will be seen for the "area-weighted schemes" investigated in the next section, can be non-integrable. In the language of the method of support operators one defines one operator, say $\mathbf{DIV}_{p\to z}$ acting from points to zones (this can always be found from a specification of the zone volume), and then by an interchange of the order of discrete double sums one derives $\mathbf{GRAD}_{z\to p}$ acting from zones to points. Note that what is important here is not the entire edge between two points, but the corners or half-edge vectors that are common to both the gradient and divergence operators. (The procedure for obtaining the corner vectors $\vec{C}_z^p$ is given in Appendix A for a simple case where the functional form of the zone volume is specified.)

The support operators method can be viewed in the following intuitive terms for piecewise constant functions, and for the staggered grid placement of variables given here. Consider a set of specified corner vectors $\vec{C}_z^p$, and a set of scalars and vectors Q_p, P_z, $\vec{A}_p$,

$\vec{B}_z$, where those with the subscript p are defined at points and those with subscript z are defined in zones. Then the corner pieces of the operators for gradient, divergence, and curl that take data defined at points and produce data defined in zones are given by $\mathbf{grad}_{p\to z} = Q_p \vec{C}_p^z$, $\mathbf{div}_{p\to z} = \vec{A}_p \cdot \vec{C}_p^z$, and $\mathbf{curl}_{p\to z} = \vec{A}_p \times \vec{C}_p^z$. The full operators $\mathbf{GRAD}_{p\to z}$, $\mathbf{DIV}_{p\to z}$, and $\mathbf{CURL}_{p\to z}$ are then given as sums of these corner pieces with respect to index p, and divided by the zone volume V_z. To obtain the operators going from zones to points we may consider the vector identities to be effectively defined collectively by conservation of total energy, or individually as in Eq.(28). For the control volume differencing used here this will result in $\mathbf{grad}_{z\to p} = P_z \vec{C}_z^p$, $\mathbf{div}_{z\to p} = \vec{B}_z \cdot \vec{C}_z^p$, and $\mathbf{curl}_{z\to p} = -\vec{B}_z \times \vec{C}_z^p$ (recall that $\vec{C}_z^p = \vec{C}_p^z$), where the full operators $\mathbf{GRAD}_{z\to p}$, $\mathbf{DIV}_{z\to p}$, and $\mathbf{CURL}_{z\to p}$ are then given as sums over the index z, and divided by the volume, V_p, associated with the point p. For our particular staggered grid formulation it is this latter set of operators that make up the corner forces $\vec{f}_z^p$, whereas the former set compose the equation for internal energy.

The other important operator expressions that can be obtained from gradient, divergence, and curl [$\nabla \times \nabla p = 0$ and $\nabla \cdot (\vec{\nabla} \times \vec{A}) = 0$, for arbitrary p and $\vec{A}$] are not generally satisfied locally in discrete form. This is not surprising since we utilized the vector identities only in integral form. Spurious numerical errors arising from the fact that these relations are not valid do occur. This is a more general problem associated with all discretization methods. It has important implications that are discussed after momentum conservation is considered.

2.2.2. Point-centered formulation. It is interesting to compare the staggered grid formulation just given with that obtained with a point-centered placement of variables. Consider the grid shown in Fig.3 with all variables placed at the zone center points indicated by solid dots. Zone boundaries are indicated by solid lines labeled as the vectors, $\vec{S}_{j,i}$ where $j = 1 \cdots 4$, that connect auxiliary points given as asterisks. The position of these auxiliary points is specified in terms of the zone points in some manner. The mass, M_i, associated with the zone points is a constant, Lagrangian quantity. The momentum equation for the ith zone point is given by

$$M_i \frac{d\vec{v}_i}{dt} = \sum_j \vec{f}_{j,i}, \tag{30}$$

where the forces $\vec{f}_{j,i}$ are calculated as functions that are piecewise constant on the zone boundaries, $\vec{S}_{j,i}$, of the ith zone. For forces that originate from a scalar pressure, $\vec{f}_{j,i} = -P_{j,i}\vec{S}_{j,i}$, where the pressure on the jth boundary segment, $P_{j,i}$, must be determined in

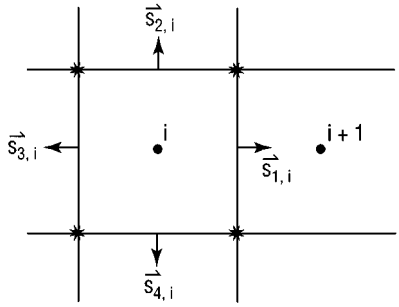


FIG. 3. Zone surrounding point i with grid lines for point-centered grid. Asterisks are nondynamical points used to define zone i with edge vectors, $\vec{S}_{j,i}$, for $j = 1 \cdots 4$.

some manner. This is usually done as an interpolation from the zone pressures, or from the solution of a local Riemann problem across this edge. (Note that with respect to the zone adjacent to the ith zone, $i+1$, on the opposite side of the jth edge, $\vec{S}_{j,i+1} = -\vec{S}_{j,i}$.)

Multiplying Eq.(30) by the zone velocity $\vec{v}_i$ gives the time evolution of the kinetic energy as

$$\frac{d}{dt}\left(\frac{M_i \vec{v}_i^2}{2}\right) = \vec{v}_i \cdot \sum_j \vec{f}_{j,i} = -\vec{v}_i \cdot \sum_j P_{j,i}\vec{S}_{j,i}. \tag{31}$$

Next we find the equation for the evolution of the internal energy by integrating Eq.(3) over the ith zone. This yields

$$M_i \frac{de_i}{dt} = -P_i \int_{V_i} \nabla \cdot \vec{v}\, dV = -P_i \sum_j \vec{S}_{j,i} \cdot \vec{v}_{j,i}, \tag{32}$$

where now we must also define the velocity along the jth edge, $\vec{v}_{j,i}$. This can be given by the same procedure used for determining the edge pressures. Summing the internal and kinetic energies we can write an equation for the total energy change inside the ith zone as

$$\frac{d}{dt}\left(\frac{M_i \vec{v}_i^2}{2} + M_i e_i\right) = -\vec{v}_i \sum_j P_{j,i}\vec{S}_{j,i} - P_i \sum_j \vec{S}_{j,i} \cdot \vec{v}_{j,i}. \tag{33}$$

In the staggered grid case both the momentum and internal energy equations involved the same entities, the corner forces. This is seen not to be true for the point-centered case. The equation for kinetic energy evolution involves forces, but these forces must be broken apart to obtain the internal energy equation. If we specify both $P_{j,i}$ and $\vec{v}_{j,i}$ independently, then the sum of Eqs.(31),(32), as given by Eq.(33), will not in general be a quantity that can be written in divergence form, and thus reducible to a boundary integral. Unless this is the case, conservation of total energy will be violated.

A crude way around this difficulty is to specify both $\vec{v}_{j,i}$ and $P_{j,i}$ at the cell interfaces and redefine the RHS of Eq.(33) to be given as $-\sum_j P_{j,i}\vec{S}_{j,i} \cdot \vec{v}_{j,i}$. One then uses this equation directly to evolve the total energy as a function of time. This equation along with the momentum equation is advanced in time, after which the kinetic energy computed from the advanced velocity is subtracted from the total energy to obtain the internal energy that is needed to compute the pressure using the equation of state. This completely eliminates Eq.(32) and guarantees exact conservation of total energy. However, this can result in large errors if the kinetic energy is large, since quantities sometimes nearly equal in size are subtracted to obtain a small difference. Compatibility is never an issue since the errors are simply hidden and subsumed by the total energy equation.

In the support operators prescription no interface work is defined; instead it is required that the RHS of Eq.(33) be expressed as

$$\sum_i \left(\vec{v}_i \cdot \sum_j \vec{S}_{j,i} P_{j,i} + P_i \sum_j \vec{v}_{j,i} \cdot \vec{S}_{j,i}\right) = \sum_{bd} P_{bd}\vec{S}_{bd} \cdot \vec{v}_{bd}, \tag{34}$$

where the RHS of Eq.(34) is evaluated at the boundary. Given a specification for $P_{j,i}$ in the above equation is equivalent to specifying the form of the gradient operator, and specifying

$\vec{v}_{j,i}$ is the same as specifying the form for the divergence operator. This equation is thus the vector identity for $\nabla \cdot (P\vec{v})$ in summation form. By specifying one or the other of these quantities, Eq.(34) is used to determine the coefficients of the unknown operator. However, this equation is satisfied only globally, and never in the strong sense of setting each term with respect to an outer summation index equal to zero, as was true for the staggered grid case in Eq.(19). Therefore, unlike in the staggered grid case, the particular functional form of the undiscretized terms that enter into both the momentum and internal energy equations must be known for this procedure to be carried out. Many examples of this method have been given [17,18,14,19].

Direct specification of a force that acts between two points lies outside of the domain of the method of support operators. For the case of a staggered spatial grid scheme conservation of total energy can be used to compute work given force, or vice versa, in a way that is not possible for a point-centered placement of variables. When forces are specified in a heuristic manner, as is the case for an artificial viscosity, the conservation of energy approach enables one to construct the work equation in a simple, unique, and generic manner when the functional form of this equation would not at all be obvious otherwise. In the case of a point-centered scheme, if one simply specifies a discrete form for a force acting between two points, additional information must be provided in order to decide how the work performed by that force on a given zone is to be partitioned between the kinetic and the internal energy of that zone. In the staggered grid case this information is already given by the assumption that a corner force $\vec{f}_z^{\,p}$, whatever its origin, acts on a point p and does work with respect to zone z. This was seen to be a consequence of satisfying Eq.(19) in the strong form for every zone label z. There is no arbitrariness in this arrangement that is also necessary for the discrete vector operators to be compatible with one another. Thus, for a staggered placement of variables the conservation of total energy procedure, as developed here, includes the method of support operators and allows for an important extension in an automatic manner.

2.3. *Entropy Errors and Volume Consistency*

In both point-centered and staggered spatial grid formulations two definitions of volume have been introduced. The first is through the definition of a cell volume, $V_1(t)$, used to compute the cell density, given the initial cell mass. The second volume, $V_2(t)$, is implicitly defined through the change of internal energy caused by the pressure as $-P_z\, dV_2$. This latter volume is not necessarily the same as the first. In particular, when work is done compatibly, for instance by Eq. (20), the change of the second volume has been constructed by the use of mesh vectors and point velocities, and not by subtracting volumes defined by coordinate positions at different time levels. For a staggered spatial grid scheme implemented with total energy conserved to roundoff error these two definitions of volume will agree (to within truncation error with respect to time) only if we choose the divergence of the velocity field defined from Eq.(1) as the determining operator from which the others are derived from the requirement of compatibly. In the case of two-dimensional cylindrical geometry, for example, the median and coordinate-line meshes describe different volume elements and are not equivalent within a single zone, as is the case for Cartesian geometry. Thus for the compatible change of internal energy caused by the zone pressure to be consistent with dV_1 of the coordinate volume, the gradient operator that determines the pressure forces acting on the points should be defined with respect to the same mesh as the divergence operator.

The divergence operator is naturally defined with respect to the coordinate-line mesh in order to correspond to the time derivative of the zone volume. In other instances, as will be seen in Section 3, the zone volume and the volume compatible with the gradient operator may be guaranteed to agree only for certain kinds of velocity flow fields.

The error that results from an inconsistency in these two volumes appears as an entropy error. To see this consider the second law of thermodynamics written for an isentropic flow as

$$T\Delta S = -P_z(V_1, e_z)[\Delta V_2 - \Delta V_1]. \tag{35}$$

$T\Delta S$ is the entropy production term, which for an isentropic flow should vanish; P_z is given as a function of V_1 through its dependence on density. ΔV_2 is the volume change used in the internal energy equation and ΔV_1 is the actual volume change calculated from the zone coordinates. For $\Delta V_1 \neq \Delta V_2$ the error in the internal energy term shows itself as an addition to the entropy; it can obviously have either sign.

Point-centered schemes can also have this same kind of entropy error. In fact, for some such schemes, where interpolation functions are used to smear the cell mass over some characteristic length, the computation of density and work are not related in a manner that even makes the assessment of this error simple to estimate [20]. Where one has easy estimates of these two volumes, for instance, by integrating Eq.(1) in time and comparing the result to that obtained from computing the volume directly as a function of the point coordinates, it is possible to construct a nondimensional estimate of this error term.

2.4. *Momentum Conservation*

Unlike the total energy, one does not usually care what the value of the total momentum is. However, momentum must be conserved. In general, this is the statement of Newton's third law in discrete form and says that the action and reaction of a given force should be equal in magnitude and opposite in direction. For the case of forces that are computed with respect to the median mesh of a staggered spatial grid discretization this is automatic. This is seen from the arguments that led to the form for the specific internal energy equation given as Eq.(24). There it was seen that each piece of force along a part of the median mesh acts with equal magnitude and opposite sign with respect to the two dynamical points with which it is associated. Likewise, for point-centered schemes momentum will be conserved for the same reason.

For the case where there are no boundary forces the statement of conservation of momentum is given simply as

$$\sum_p \vec{F}_p = \sum_p \sum_z \vec{f}_z^{\,p} = 0. \tag{36}$$

Now consider the case when the forces are due to piecewise constant zone-centered pressures, and interchange the order of the double sum in the above equation. Then for these forces calculated along the coordinate-line mesh in Cartesian geometry we have the result

$$\sum_p \vec{f}_p^{\,z} = P_z \sum_{i=1}^{8} \vec{a}_i \equiv 0, \tag{37}$$

since the sum of the outward normal vectors of any closed volume is always zero. This result followed from the equivalence of the median and coordinate-line meshes in Cartesian

geometry, since momentum was seen to be trivially conserved in the former case. It expresses a simple topological property of the zones: namely, they consist of closed surfaces. This simply says that when we construct a zone from edge vectors, those lengths should join without gaps or overshoots.

In an exactly similar manner angular momentum is also perfectly conserved on a single zone basis. The change in angular momentum is computed by taking the cross product of the radius vector of each point $\vec{R}_p$ with the momentum equation and summing over all points p. Then decomposing this sum on a single quadrilateral zone basis yields

$$\sum_p \vec{R}_p \times \vec{f}_p^z = P_z \sum_p \vec{R}_p \times \vec{C}_p^z = 0, \tag{38}$$

where the sum that vanishes identically is again a purely geometrical property of any closed zone that is valid independently of P_z.

While the above may seem simple enough, there are schemes in cylindrical geometry that achieve important physical properties by allowing both linear and angular momentum to be violated at truncation error levels by modifying the zone normal vectors such that gaps and overshoots are present [13]. This is done in order to preserve certain symmetry properties that are broken by angular momentum, or spurious vorticity, errors that are present with control volume, as well as other, discretizations. This is in spite of the fact that angular momentum is exactly conserved on a zone basis, and thus appears rather paradoxical. The important criterion that must be satisfied to prevent the generation of spurious vorticity is that the force density due to the scalar pressure have zero curl, or $\nabla \times \nabla p = 0$ [21]. This is a property that, as previously noted, is not generally satisfied locally. For our staggered grid, control volume differencing, this criterion is operationally measurable in each zone as

$$\nabla \times \left(\frac{\vec{F}_p}{V_p} \right) = 0, \tag{39}$$

where $\vec{F}_p$ is the total force on a point p due to the scalar pressure, and V_p is the total volume associated with this point (the sum of the corner volumes with the index p). In calculating Eq.(39) one always uses the surface normals of a particular zone in unmodified form, although for the symmetry preserving procedure given in [13] these normals are modified when used to compute the pressure forces. To satisfy the above criterion in this instance it is necessary to violate at truncation error levels both linear and angular momentum conservation. In the special case of symmetry preservation investigated in [13], the procedure presented there results in Eq.(39) being satisfied to roundoff error for very particular kinds of flow conditions. (In these instances the total force density also has zero curl since the flow is one-dimensional, although $\nabla \times \nabla \cdot \overline{\overline{Q}} \neq 0$ for an arbitrary tensor $\overline{\overline{Q}}$.) However, making $\nabla \times \nabla p = 0$ in discrete form does not generally mean that all spurious vorticity generation has been eliminated. This is because given any analytical prescription for ∇p, which is then projected onto a grid with arbitrarily spaced points, one finds that $\nabla \times \nabla p \neq 0$ in discrete form. Thus, Eq.(39) is not a general, well-defined measure.

With the above said, it is still a central requirement that momentum be conserved, even if it might be violated at truncation error levels in some instances. In the case of forces that arise from subzonal pressures or tensors, and that are added to $\vec{f}_z^p$, this must be done so that Eq.(37) is obeyed. This places an important restriction on how these subzonal pieces of force may be distributed among the corner forces of a given zone [5].

Finally, we note that the concept of closure of a volume for proper momentum conservation is important in three dimensions. If one uses arbitrary interpolations between points to approximate curved surfaces, each described by a single normal vector, it is not clear that the sum of all such vectors about a closed figure will actually vanish. If this does not happen then, not only is momentum conservation violated, but there exists no median mesh that can be equivalent to the coordinate-line/surface mesh, since, as just argued, for forces calculated with respect to the median mesh momentum is always conserved for piecewise constant pressures. This restriction thus places some limitations on the definition of the normal direction used in these interpolations.

3. AN EXAMPLE: AREA-WEIGHTED DIFFERENCING

The most straightforward way to derive a scheme that is compatible in any geometry or number of dimensions is to use what we now define as "proper" control volume differencing. In this kind of scheme one uses a staggered placement of variables, as previously discussed, with piecewise constant functions. The main starting point is then to use Eq.(1) to define the operator $\mathbf{DIV}_{p\to z}$, given some specified form for the zone volume as a function of its defining coordinates, $V_z(\vec{R}_1, \vec{R}_2, \ldots)$. Then using Eq.(28) one can derive the compatible gradient operator $\mathbf{GRAD}_{z\to p}$. This essentially determines the form of the vectors $\vec{C}_z^p$ that mutually compose the coordinate-line and median meshes. Then the corner masses are defined, and thus the zone and nodal masses. Postulated forces, such as those arising from artificial viscosity, can also be specified; all change in internal energy is calculated using Eq.(20) since the complete corner forces can now be constructed. Except for numerical error associated with time integration, there is no entropy problem because the volume used to compute work is automatically the same as that used to compute the zone volume and density. Momentum is also conserved since this volume is closed, and total energy is conserved.

The problem is that in some instances the kind of scheme detailed above will not preserve other important properties. An example of this situation is two-dimensional, cylindrical (r, z) geometry in the case of spherical flow. Here one can specify one-dimensional, spherically symmetric initial and boundary conditions and the numerical solution, computed with the control volume scheme described above, will not remain spherical in time. Since it is important to investigate perturbations in two dimensions of this type of one-dimensional symmetry, other kinds of schemes were developed for solving this type of problem. These are the so-called "area-weighted" schemes [10–12,18]. They have been used extensively for almost 40 years and have arisen in several incarnations that sometimes look quite different but are the same in their principal features. They have a staggered spatial placement of variables that are piecewise constant functions. All have the useful property that they will preserve spherical symmetry in cylindrical geometry for an equal angle zoned initial grid. This subject, its extension to unequal angle zoning, and the rectification of this difficulty for a control volume scheme are given elsewhere [13]. However, a detailed analysis of the salient features of area-weighted schemes proves very useful for displaying the possible difficulties previously discussed. This is because for this type of scheme one essentially begins by postulating the form of the gradient operator $\mathbf{GRAD}_{z\to p}$, based on physical reasoning of what is necessary for symmetry preservation for a grid that is constructed with equal angle zoning. This implicitly determines the zone volume, and leads to an interesting set of problems that are amenable to analysis in the framework given here. These schemes violate strict momentum conservation; in compatible form they possess a non-integrable

volume element, and thus may give rise to entropy errors of the type previously mentioned. Nonetheless, they have been used extensively because of the above mentioned symmetry property.

The formalism introduced in Section 2 allows the area-weighted schemes to be derived and analyzed in a most economical manner. This is done starting from the momentum equation. To transform the momentum equation of the control volume scheme in two-dimensional (r, z) Cartesian geometry into two-dimensional (r, z) cylindrical geometry one must multiply the normal vector edge lengths of a quadrilateral zone, $\vec{a}_i$ or $\vec{S}_i$, from which the forces are computed, by a factor $\bar{r}$ that is defined as the average of the r coordinate values at the respective endpoints of the straight line segments. This gives "true" zone volume, or nodal volume, in cylindrical geometry depending on whether one calculates along a closed segment of the coordinate-line, or the median, mesh.

Spherical symmetry in cylindrical geometry is not preserved with the control volume scheme because the areas along the angular direction are not equal even when the angles between the radial lines are equal. Thus for pressures that are radially symmetric the force is not in the radial direction, leading to the aforementioned violation of symmetry. However, for an equal angle zoned grid cylindrical symmetry is preserved in Cartesian geometry. This is because the lengths along the angular direction are then equal, and thus the net force on a node perpendicular to the radial direction vanishes for a spherically symmetric distribution of pressures [13]. It is this fact that is used to construct the area-weighted schemes in cylindrical geometry that preserve spherical symmetry.

To obtain the area-weighted schemes one simply multiplies the vector lengths, as defined in Cartesian geometry, of the entire force contour defined with respect to a given grid point, p, by the value of the coordinate r_p at that point. This is done in place of multiplying the separate vector lengths that make up this contour by their respective values of $\bar{r}$ that would result in true volume for cylindrical geometry. Then the Lagrangian nodal mass is also defined at point p as an effective "areal inertia" times r_p so that the momentum equation in cylindrical geometry becomes

$$M_P \frac{d\vec{v}_p}{dt} \equiv r_p (\rho A)_p \frac{d\vec{v}_p}{dt} = r_p \sum_z \vec{f}^p_{C,z}, \tag{40}$$

where we indicate as $\vec{f}^p_{C,z}$ the force as computed in two-dimensional, Cartesian geometry. Now the common factor of r_p cancels in Eq.(40) and one is left with essentially the same momentum equation as was used in Cartesian geometry, hence the term "area-weighted." This modification to control volume differencing points the acceleration in the radial direction and can be shown to preserve spherical symmetry in cylindrical geometry for equal angle initial zoning if $(\rho A)_p$ is the same for all points on an arc of constant radius [13,7].

The first difficulty encountered with the above is the proper definition of the nodal mass M_p. (The definition of the zonal mass and the areal inertia is the place where differences in the various forms of the area-weighted schemes arise.) We require that the total values of the zone and nodal mass be the same over the entire grid and that the zone mass be the "true" initial mass in the cylindrical quadrilateral volume. That is, the relations given by Eqs.(5),(6) must be satisfied. The areal inertia used in this equation can be obtained by $(\rho A)_p = M_p / r_p$, as seen from Eq.(40). Consider the center point c of the quadrilateral zone defined in Fig.4. There we indicate four triangular subzones labeled as numbers $1 \cdots 4$ inside circles, each corresponding to an edge of the zone. We denote the areas of these

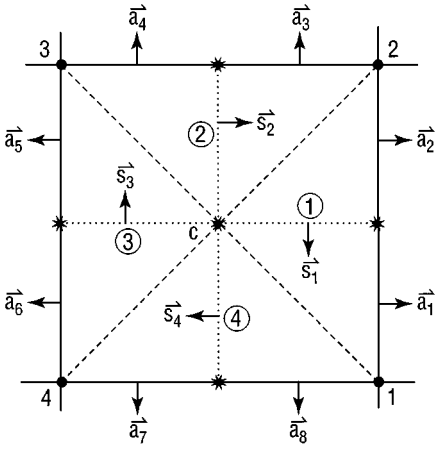


FIG. 4. Quadrilateral zone with center point c and coordinate-line mesh (solid) vectors $\vec{a}_i$, and median mesh (dotted) vectors $\vec{S}_i$. Triangular sub-division indicated by dashed lines and their associated solid coordinate lines.

respective triangles by the symbol A_i. Then from the fact that the true volume of the ith triangular subzone of the quadrilateral is $A_i(r_i + r_{i+1} + r_c)/3$ we have

$$M_z = \rho_z \sum_{i=1}^{4} A_i(r_i + r_{i+1} + r_c)/3. \tag{41}$$

Using the fact that the r coordinate of the center point r_c is given by $r_c = (r_1 + r_2 + r_3 + r_4)/4$ allows us to find the corner masses m_z^p by simply decomposing Eq.(41) with respect to the factors r_i. For instance, for point 1 of the zone shown in Fig.4 we have the result that $m_z^1 = \rho_z r_1(5A_1 + 5A_4 + A_2 + A_3)/12$. Now the relations given by Eq.(5) can be applied directly and Eq.(6) will be satisfied. This construction can obviously be used to find the corner masses in area-weighted form for a zone of any number of sides in two dimensions. It provides a solution to what has heretofore been a major difficulty in the formulation of these types of schemes.

The only problem with this definition of nodal mass is that along the z-axis where $r_p = 0$, the nodal mass $M_p = 0$, and the areal inertia is indeterminate. This defect can be remedied in more than one manner. One can simply extrapolate its value from nearby points or calculate the areal inertia from ρA taken with respect to the median mesh about these points. The first curious property of the area-weighted scheme just specified is that since $M_p = 0$ on the z-axis these points carry no momentum or kinetic energy. They just serve as marker points to determine the size of the zones (and thus their density) adjacent to the z-axis. Total energy will be conserved regardless of how these points move in time.

The last step in our derivation of the area-weighted scheme is the specification of the equation for the evolution of specific internal energy. This we do for forces defined with respect to the median mesh. Note that the force acting on a point p from a piece of the median mesh of a given zone is not $\vec{f}^z_{C,i}$, but $r_p \vec{f}^z_{C,i}$. Using this fact in Eq.(24) we have that the rate of change of internal energy due to forces applied from zone z is

$$M_z \frac{de_z}{dt} = -\sum_{i=1}^{4} \vec{f}^z_{C,i} \cdot \delta(r\vec{v})_i \stackrel{\text{def}}{=} -P_z \frac{dV_z}{dt}. \tag{42}$$

The forces $\vec{f}^{\,z}_{C,i}$ are evaluated with respect to the median mesh vectors $\vec{S}_i$ of zone z in Cartesian geometry. Since $\delta(r\vec{v})_i = (r\vec{v})_{i+1} - (r\vec{v})_i$, in this equation, unlike in the momentum equation, r_p enters; this is necessary to approximate a zone volume in cylindrical geometry. The last equality in Eq.(42), which is true only for pressure forces, is the real concern. Since for pressure forces $\vec{f}^{\,z}_{C,i} = P_z\vec{S}_i$, Eq.(42) defines a rate of change of the differential volume of zone z with time. What this volume is and how it is related to the true volume of a quadrilateral zone in cylindrical geometry is the important question. First, notice from Eq.(42) that momentum is not in general conserved by this scheme. This is because the force $\vec{f}^{\,z}_{C,i}$ acts with a factor r_i on point i, and with a different factor r_{i+1} on point $i+1$, of zone z. These forces have opposite signs but not equal magnitudes, and thus Eq.(36) is not exactly satisfied.

Substituting $\vec{f}^{\,z}_{C,i} = P_z\vec{S}_i$ into Eq.(42) yields the result for dV_z/dt given as the first equality in the equation

$$\frac{dV_z}{dt} = -\sum_{i=1}^{4} \vec{S}_i \delta(r\vec{v})_i = A_z\left(\frac{\partial r v_r}{\partial r} + \frac{\partial r v_z}{\partial z}\right)_c = \frac{V_z}{\langle r\rangle_z}\nabla_c \cdot r\vec{v}; \tag{43}$$

the second equality in this equation follows from the form for the discrete divergence in Cartesian geometry, as given by Eq.(62) of Appendix A with argument $r\vec{v}$ inserted in place of $\vec{v}$. The partial derivatives are understood to be the discrete form of these objects. The last equality in this equation follows from using the identity $A_z \equiv V_z/\langle r\rangle_z$, which defines an average r coordinate for zone z (A_z is zone area); by ∇_c we understand the Cartesian form of the divergence operator where there are no unit vector differentiation contributions. From this last term of Eq.(43), and using Eq.(1), the divergence of the velocity field in cylindrical geometry is given by

$$\nabla \cdot \vec{v} = \frac{1}{\langle r\rangle_z}\nabla_c \cdot r\vec{v} \approx \frac{1}{r}\frac{\partial r v_r}{\partial r} + \frac{1}{r}\frac{\partial r v_z}{\partial z}, \tag{44}$$

where we have let $\langle r\rangle_z \to r$. We thus see that we have obtained from Eq.(42) a consistent discrete representation of the divergence operator, and thus the discrete volume, in cylindrical geometry. One derivation of an area-weighted scheme starts with $\nabla \cdot \vec{v}$ written in continuum form as given above [12]. Then the full system of hydrodynamics equations is discretized using what amounts to formulas given by Eqs.(58),(59) of Appendix A. An area-weighted scheme is then derived, but by a much more involved path.

The time rate of change of the compatible zone volume given by Eq.(43) can be explicitly written in terms of the coordinates of the quadrilateral zone shown in Fig.4 as

$$\begin{aligned}\frac{dV_2}{dt} = \frac{1}{2}[&(r_2v_{r2} - r_4v_{r4})(z_3 - z_1) + (r_1v_{r1} - r_3v_{r3})(z_2 - z_4)\\ &+ (r_3v_{z3} - r_1v_{z1})(r_2 - r_4) + (r_2v_{z2} - r_4v_{z4})(r_1 - r_3)].\end{aligned} \tag{45}$$

(This is most easily seen by the use of Eqs.(58),(59) of Appendix A in Eq.(43) with $r v_r$ and $r v_z$ as arguments.) We label this volume as V_2 to denote that it is the second (and compatible) form of the zone volume. Given any function $V(\vec{R}_1(t), \vec{R}_2(t), \ldots)$ that depends on time only implicitly through its arguments, it is true in general that

$$\frac{dV}{dt} = \sum_i \vec{v}_i \cdot \nabla_i V, \tag{46}$$

where $\vec{v}_i = d\vec{R}_i/dt$, and by ∇_i is meant the generalized gradient with respect to all vector arguments of the volume V. By simply comparing the expressions given by Eq.(45) and Eq.(46) one can find the partial derivatives of V with respect to all zone coordinates. For point 2 of Fig. 4 this is

$$\frac{\partial V_2}{\partial r_2} = \frac{1}{2} r_2 (z_3 - z_1), \qquad \frac{\partial V_2}{\partial z_2} = \frac{1}{2} r_2 (r_1 - r_3), \tag{47}$$

as is seen from the coefficients of v_{r2} and v_{z2} in Eq.(45). Forming the second mixed derivatives of these quantities with respect to the index 2 leads to the interesting result

$$\frac{\partial}{\partial z_2}\frac{\partial V_2}{\partial r_2} = 0 \neq \frac{\partial}{\partial r_2}\frac{\partial V_2}{\partial z_2} = \frac{1}{2}(r_1 - r_3). \tag{48}$$

Thus, the compatible volume of the quadrilateral zones defined by area-weighted differencing in cylindrical coordinates is non-integrable; there exists no scalar function $V_2(\vec{R}_1(t), \vec{R}_2(t), \ldots)$ whose time derivative yields Eq.(45). Since Eq.(45) does not define the true volume of the zones, we show how this expression is related to this volume.

If we write Eq.(43) along the coordinate grid lines, then the rate at which volume is swept in time along any edge described by the outward normal $\vec{a}$ as calculated by area-weighted differencing is given by

$$\left.\frac{dV_{edge}}{dt}\right|_{area\_weight} = \frac{1}{2}(r_1 \vec{v}_1 + r_2 \vec{v}_2) \cdot \vec{a}, \tag{49}$$

where the labels 1 and 2 denote the endpoints of this edge. The rate at which volume is swept in time along this edge as calculated from true "control volume" differencing is given by

$$\left.\frac{dV_{edge}}{dt}\right|_{true} = \frac{1}{4}(r_1 + r_2)(\vec{v}_1 + \vec{v}_2) \cdot \vec{a}. \tag{50}$$

The difference between these two rates is due to the factor $\bar{r} = (r_1 + r_2)/2$ that appears in Eq.(50) versus r_p $(p = 1, 2)$ in Eq.(49). Subtracting these two equations, the difference in these two rates of change of volume can be written as

$$\left.\frac{dV_{edge}}{dt}\right|_{area\_weight} - \left.\frac{dV_{edge}}{dt}\right|_{true} = \frac{\Delta r}{4}(\Delta\vec{l} \times \Delta\vec{v}), \tag{51}$$

where $\Delta\vec{v} = \vec{v}_2 - \vec{v}_1$ and $\Delta\vec{l}$ is the vector along the given coordinate-line edge (perpendicular to $\vec{a}$ and with the same magnitude). Thus it is seen that *if the velocity difference along an edge is parallel to the direction of that edge, then there is no difference in the volume change calculated with area-weighted differencing relative to true control volume differencing.* Now consider a spherically symmetric velocity field as shown in Fig.5. For this type of flow field it is obvious that the above condition is satisfied along all edges of the quadrilateral zones. Thus the volume change calculated for this kind of flow field with the area-weighted scheme gives the same volume change as calculated from the control volume scheme. The latter is what is obtained from computing the difference of the quadrilateral volumes at two different time levels to obtain dV of a zone. So there is no volume consistency

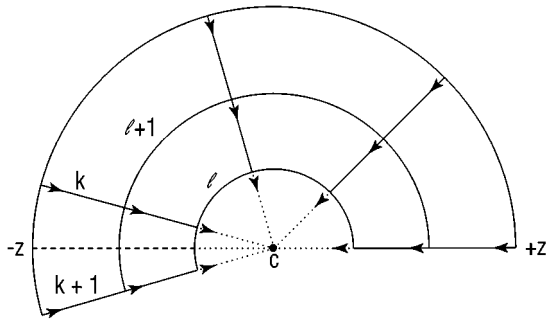


FIG. 5. Grid lines for a 180° symmetric flow (radially inward arrows) problem with point c as a center of convergence. $+z$ axis is a reflective boundary containing grid points; $-z$ axis is a reflecting boundary without grid points on this line (dashed and dotted). Dotted lines indicate degenerate quadrilateral zones that are common to the center of convergence.

problem or associated entropy error for spherically symmetric flow, although there is for an arbitrary velocity flow field. The reason that area-weighted differencing preserves spherical symmetry in cylindrical geometry for equal angle zoning is because the criterion given by Eq.(39) is unchanged in moving from Cartesian to cylindrical geometry for this type of differencing. This is because the terms $\vec{F}_p$ and V_p that are divided in that expression both acquire only a common factor of r_p in cylindrical geometry. Thus the force density that was curl free for equal angle zoning in Cartesian geometry remains so in cylindrical geometry.

Although the zone mass of this area-weighted scheme and the control volume scheme is equal, their nodal masses, M_p, and corner masses, m_z^p, are not. As shown earlier, the assumption of M_z and M_p as both constant, Lagrangian masses leads to the conclusion that the corner masses m_z^p are also constant. When this concept is used to derive subzonal pressures as described in [4] for use with an underlying area-weighted force differencing, these subzonal pressures are calculated from subzonal masses and volumes computed from the true volumes of the corners of the quadrilaterals. The corner masses used to construct M_p for an area-weighted scheme do not turn out to be useful Lagrangian objects because of their dependence on r_p.

Lastly, in the variant of the area-weighted scheme due to Schulz, the quadrilateral zone volume is defined as the zone area times r_c, the r coordinate of the center point of the zone. This never exactly matches the true zone volume so that this form of area-weight differencing can never be cast in a form that is compatible with total energy conservation. In this case the work done in a zone by pressure forces is calculated as $-P_z dV$, where dV is the change in zone volume computed from the "postulated" functional form.

4. PRACTICAL CONSIDERATIONS

Here we briefly discuss other issues that are of importance for constructing a complete numerical implementation of the ideas developed in this paper. Principal among these are time integration and a proper implementation of appropriate boundary conditions. These subjects are treated here only to the extent that our specific numerical formalism impacts upon them. In particular, we describe how we have implemented time integration and boundary conditions in a working code, results from which are shown here only to clarify

very specific issues; however, numerical examples in a much larger context and with respect to a much broader range of problems, obtained from the same code, are given elsewhere [13,4,5].

4.1. *Time Integration*

It was already noted in Section 2 that an even time integration scheme must be used with this model since we wish to have all quantities that enter into the definition of total energy at the same time level. Given this fact there remain three issues to be addressed: numerical stability, time centering of the corner forces, and timestep control. Our time integration method is a predictor-corrector technique where on the predictor we always advance all variables a full timestep to the $n+1$ time level.

Our discretization that conserves total energy to numerical roundoff error implies a specific ordering to the solution of the equations: namely, that the momentum equation is first advanced to obtain $\vec{v}_p^{n+1}$, and only then is the internal energy equation advanced. When the latter is advanced information from the velocity field at the $(n+1)$ level is used, since in Eq.(20), $\vec{v}_p^{n+1/2} = (\vec{v}_p^{n+1} + \vec{v}_p^{n})/2$ is what enters. This sequence forms our initial predictor step, as well as following corrector steps.

If the momentum and internal energy equations, Eqs.(17),(20), are linearized for pressure forces in one spatial dimension it is readily found that this sequence of steps yields the usual CFL stability constraint with respect to the sound speed. Thus, this system is stable for just one predictor step. Therefore, the very structure of these equations, in which they obey discrete conservation of total energy, appears to imply linear stability.

Although a single predictor step is numerically stable, and we could simply advance all variables at this point, we always do at least one additional corrector step. The sequence of operations in performing either a predictor or a corrector step is advance velocity, then specific internal energy (using $\vec{v}^{n+1/2}$), and last coordinates, and therefore zone volume and density. To advance coordinates one always uses the average of the velocity at the old and new time levels; this is formally second order accurate. However, on the predictor step we have effectively calculated a volume change in computing the time advanced specific internal energy. This step uses forces centered at the old time level and is thus only first order accurate, and will result in an entropy error for the reasons previously mentioned. (This is measured since we also integrate Eq.(1) in time and compare this zone volume to that defined by the coordinates.) Thus, on the corrector step we always time center the grid lines, $\vec{a}_i$ and $\vec{S}_i$, at the $(n+1/2)$ time level by averaging the old and new values of the coordinates. Then the time advance of the compatible volume and work has the same order of accuracy as the coordinate advance. This still results in a residual numerical integration error between the compatible volume and the coordinate volume since the velocity at the $n+1$ time level that is used to time center the grid lines is not the same velocity that is used to advance the coordinates at the end of the corrector step. The pressure may also be centered at the $(n+1/2)$ level or used fully advanced; we observe little difference in these choices. However, the pressure used in the momentum and internal energy equations is always the same since the corner forces are common to both. In the case where we have an artificial viscosity, the subzonal tensors from which this force is computed are always kept at the unadvanced time level; this centering choice is found to produce less numerical noise than any others. More than one corrector step may be employed and the results from all preceding steps can be easily factored into the calculation of the time-centered corner

forces and grid lines [22]. Time is always advanced after some fixed, predetermined number of corrector steps; usually, only one corrector step is utilized.

A new value for the timestep is always chosen on the predictor step. This is done as follows for quadrilateral zones in two spatial dimensions: first we define a characteristic zone length, l_z, as the minimum distance of the two sides of the median mesh of a given zone. Next we compute a generalized sound speed, c_z^*, in every zone. This is defined by adding the maximum pressure in a zone to the maximum value of the scalar part of the artificial viscosity tensors in a zone to form a generalized pressure, p_z^*: then, $c_z^* = (\gamma p_z^*/\rho_z)^{1/2}$, where γ is the ratio of specific heats and ρ_z is the mean zone density. We then require that

$$\frac{c_z^* \Delta t}{l_z} \leq f_1 \approx 0.25, \tag{52}$$

be satisfied for every zone. In addition, we also require that a zone not change its volume by too large an amount in a timestep; namely,

$$\left|(\nabla \cdot \vec{v})_z^n\right| \Delta t \leq 0.8 f_1, \tag{53}$$

where $(\nabla \cdot \vec{v})_z^n$ is known at time level n. Although Eq.(52) almost always sets Δt, the criterion given by Eq.(53) is a useful supplement in certain, some what pathological, situations. The increase of a given value of the timestep over the previous one is limited to no greater than 10% to 20%, while the decrease is unrestricted in order to always maintain numerical stability. If there are characteristic speeds due to sources other than pressure and artificial viscosity, for example, shear wave speeds that result from material strength, then the maximum value of these characteristics speeds is used in Eq.(52).

4.2. *Boundary Conditions*

Initial and boundary conditions are crucial to the complete description of any physical problem. The latter must be treated carefully in any numerical model. Here we consider the following cases: externally applied force, specified velocity at a boundary, a reflective boundary, and a center of convergence that can move with time. As before, conservation of total energy is central to our development.

For an externally applied force one can compute the velocity with time of the boundary points in the same manner as for the interior points. Since there is assumed to be no mass outside the boundary, the nodal mass of the boundary points is due only to the interior zones adjacent to the boundary. The equation for total energy, Eq.(15), becomes

$$E_T(t) = E_T(0) + \sum_{m=1}^{n} \sum_i W_{bd,i}^m, \tag{54}$$

where the rate of boundary work performed at point i on the mth cycle is computed as $W_{bd,i}^m = \vec{f}_{bd,i}^{\,m} \cdot \vec{v}_{bd,i}^{\,m+1/2} \Delta t_m$. Since the external boundary forces, $\vec{f}_{bd,i}$, are specified, energy balance is complete.

Suppose the velocity at the boundary is specified. Then in order to compute total energy balance from Eq.(54) we must find the work, $W_{bd,i}^m$, that is effectively performed by the exterior boundary forces $\vec{f}_{bd,i}^{\,m}$. Since the velocity is known the momentum equation, given

as Eq.(17), can be used to find $\vec{f}_{bd,i}$; thus the boundary work is given by

$$W^m_{bd,i} = \vec{f}^{\,m}_{bd,i} \cdot \vec{v}^{\,m+1/2}_{bd,i} \Delta t_m = \vec{v}^{\,m+1/2}_{bd,i} \cdot \left(M_i \Delta \vec{v}_{bd,i} - \sum_z \vec{f}^{\,i,\sigma}_z \Delta t_m \right), \qquad (55)$$

where $\vec{f}^{\,i,\sigma}_z$ is an interior corner force that acts on the ith boundary point.

While the above is simple enough, a more complicated situation that can be viewed as a combination of the above two cases is that of a slide line between two different materials [10,7]. Since the equation of state is different for each material, the force and thus the velocity in the direction tangential to be interface can be discontinuous. In addition, one can have friction forces that act between the two sides of an interface; these must be specified by some prescription that is consistent with momentum conservation. Once this is done the corner forces are completely known on both sides of the sliding interface, but simply do not line up so that they can be summed about a point to obtain the complete momentum equation. What one does in this instance is to interpolate both the corner masses and forces from one side to the other to complete the momentum equation at all points on the interface. (In this way the construction of "ghost cells" to complete the force on either side of the interface is avoided.) Then this completed momentum equation is advanced in time with respect to the direction normal to the interface, while in the tangential direction only the uninterpolated forces (including friction) and masses are used to advance this component of the velocity. The internal energy equation, Eq.(20), is then advanced using the uninterpolated corner forces (including friction) dotted into the velocity of their associated points, just as before. This equation is unmodified by the interpolation of corner forces and masses.

By the above procedure one essentially specifies the advanced velocity at either side of the interface, wherein total energy is therefore exactly conserved for each region. In computing the boundary work for each region by means of Eq.(55) all nodal masses on either side of the interface consist of a single material with the corner masses of the opposite material set to zero, but with boundary velocity specified. Then the total interface work done by each material on the other should be equal in magnitude and opposite in sign so that there is no net interior energy source. This is not exact due to numerical truncation error in the interface treatment. However, how closely this is satisfied gives a goodness criterion for this type of interior boundary condition. Kinematical adjustments in the velocity of the interface points may be needed to prevent material interpenetration. In this case total energy can still be exactly conserved by using Eq.(25) to modify the internal energy of the zones associated with the affected interface points.

In principle, a center of convergence need not be treated in any special form since this is an arbitrary property of the solution of the equations that can occur at any spatial location. However, in practice one often constructs the initial grid knowing approximately where this point is likely to occur: for example, along a given axis or at a fixed, predetermined location. In this case this point can be allowed for in a special manner that increases code robustness. Such an instance is shown as point *c* of Fig.5. In this case we choose to treat this point as the center of a zone that has more nearest neighbors than other zones. As shown in Fig.5 this zone is composed of triangles, indicated by dotted lines, that are degenerate quadrilaterals adjacent to point *c*. These triangles all have the same values of density and specific internal energy since they are all part of the same zone. The position and velocity of point *c* is computed in the same manner as any other zone center; namely, by a simple arithmetic average

of the positions and velocities of the points that compose the zone. It is important to note that because this point is the center point of a zone there is no nodal mass associated with it.

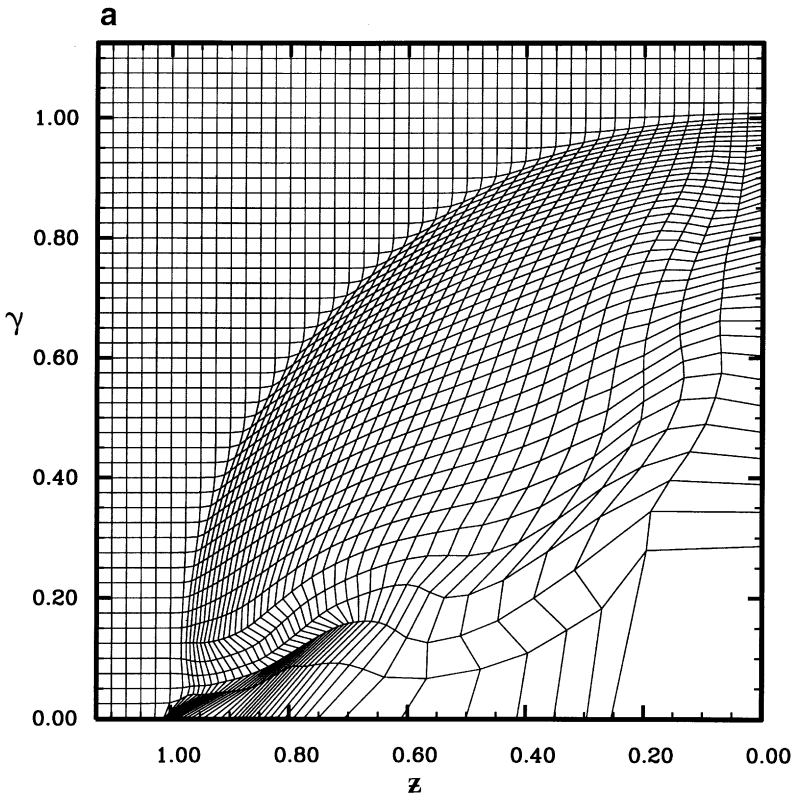
Reflective boundary conditions can be implemented in two forms, as shown with respect to the z-axis in Fig.5, where a spherically symmetric flow is indicated by the velocity field arrows that point radially inward. The more usual case, shown with respect to the line labeled $+z$ in Fig.5, is where points lie on the reflective boundary but are constrained to move parallel to some specified direction defined as $\hat{c}$. This is the z direction in Fig.5. Along this kind of reflective boundary one simply modifies the velocity at these points after the advance of the momentum equation to be equal to $(\vec{v}_{bd,i}^{n+1} \cdot \hat{c})\,\hat{c}$. Note that any motion of these points along the $\hat{c}$ direction is consistent with this boundary condition, and in this sense these points are unconstrained. If they carry little or no nodal mass, as in the case of two-dimensional cylindrical geometry, this can lead to spurious motion and grid distortion. A remedy for this difficulty when using area-weighted differencing is to enslave these points to their nearby neighbors since they carry no mass. One way to achieve this is to require that $\Delta\vec{l} \times \Delta\vec{v} = 0$, as suggested by Eq.(51), for these points relative to their nearest neighbor that is not on the z-axis. If $\vec{v}^k$ is the velocity of points on the z-axis, and $\vec{v}^{k-1}$ is the velocity of their associated nearest neighbors not on the z-axis, this yields $v_z^k = v_z^{k-1} - v_r^{k-1}\delta z/\delta r$, where δr and δz are the difference in the r and z coordinates of these points.

The reflective boundary condition as implemented in Fig.4 with respect to the $-$z-axis has no points on the actual boundary. Instead, points on the line labeled $k+1$ are reflected from the line labeled k about the z direction to obtain their velocity. In this case the velocity of points on the line $k+1$ is given in terms of the velocity on their associated points on line k by the relation $\vec{v}^{k+1} = 2(\vec{v}^k \cdot \hat{c})\,\hat{c} - \vec{v}^k$. This type of reflective boundary condition is better constrained than the previous one in that there is no extra freedom that can be associated with it. However, caution must be exercised with this implementation. For the case of an area-weighted scheme in cylindrical geometry, as discussed in Section 3, the compatible work computed with this kind of reflective boundary condition about the z-axis can be shown to result in a volume change that is different from that obtained from "true" coordinate volume in zeroth order. This results in zeroth order errors in the internal energy equation for all zones that lie next to the z-axis. It is therefore recommended only for use with a proper control volume differencing where compatibility is always obeyed.

4.3. *A Numerical Example*

The Sedov blast wave problem [23] is used here to demonstrate the differences that can be encountered with the two types of reflective boundary conditions just discussed. This problem gives a diverging shock wave; it is run in two-dimensional cylindrical geometry. Our initial setup consists of a square grid with an edge of length 1.125 divided into 45×45 square zones. Two of these edges correspond to the r and z axes where reflective boundary conditions are specified. The initial density is unity and the initial velocity is zero. The specific internal energy is zero except in the first zone where it has a value of 5027.7. We use an artificial viscosity that is detailed in [5], and corner pressure forces with a fixed

FIG. 6. Sedov blast wave in cylindrical geometry: (a) grid at unit time for reflective boundary conditions with dynamical points on both the r and z axes. (b) grid at unit time for reflective boundary conditions with no dynamical points on the r or z axes. These axes are indicated by dashed lines through zone centers.


a
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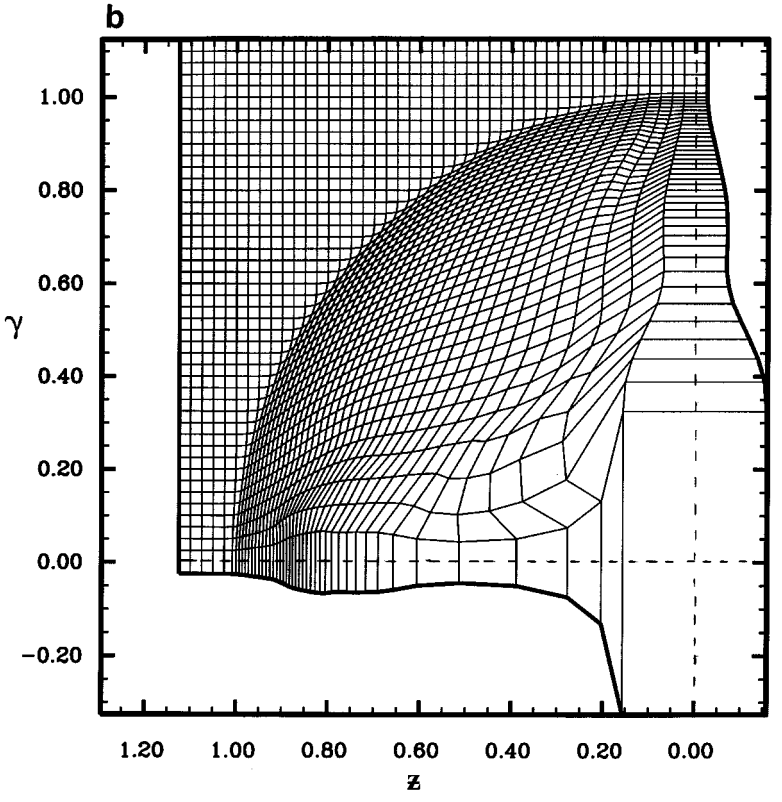
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z

strength factor of 0.25 as discussed in [4]. The hydrodynamics equations are discretized using a proper control volume differencing. For these parameters the analytic solution predicts that the expanding shock wave should be at a major radius of unity at a time of unity, with a peak density of four. In Fig.6a the grid is shown at this time, wherein we have used the first form for the reflective boundary conditions; points are present on both the r and z axes. Note that difficulties arise in the grid along the z-axis for this problem. These points carry less nodal mass than other points and are more sensitive to numerical error than the ones along the r axis. In Fig.6b is shown results with identical run parameters but with the reflecting boundary conditions implemented as a line reflected about each of the r and z axes. Note that the first zone, where all energy is initially deposited, is divided into quarters by the intersection of these two axes; they are shown in Fig.6b as dashed lines through the centers of the zones that contain them. No difficulties with spurious grid distortion occur along the z-axis with this type of boundary condition, as can be seen from this figure. In the case where this problem is run using area-weighted differencing (cf. [5, Fig.8]). we find that enslavement of the points on the z-axis using the first form of reflective boundary condition is the best solution to this difficulty. (Recall that the second form of the reflective boundary condition is not appropriate for the z-axis with area-weighted differencing.)

5. SUMMARY AND CONCLUSIONS

The central feature of this paper was to show how conservation of total energy could be used to construct difference equations for the system of hydrodynamics equations in such a way that the discrete equations that one numerically solves obey the relationships that occur in the equations that compose the original continuum system. A crucial part of this development was the staggered placement of variables in space. This allowed a set of useful definitions of corner objects, masses and forces, that are common to both a zone and a dynamical grid point to be made. Given these definitions it was shown how conservation of total energy could be utilized to link the momentum and specific internal energy equations in a completely generic manner that is true algebraically given any set of corner forces. This was true independent of the precise functional form of these terms. This allows for enormous generality and rests on a simple physical assumption; namely, the corner forces act on their associated nodal point to produce a change in momentum, and do work with respect to their associated zone at rate given by minus their dot product with the velocity of that point, independent of their functional form or origin. That this assumption was also mathematically necessary followed from comparing the results obtained from it to those of the support operators method. This showed that the assumption stated is required for the vector identities of differential calculus to be valid in discrete form for this kind of differencing. By satisfying these identities in discrete form one ensures that the algebraic manipulations that are performed on the continuum system of equations to prove properties such as conservation of energy all have discrete analogs. This then ensures that these properties are mirrored into the discrete equations. (The exception being that $\nabla \times \nabla p = 0$ is not locally satisfied.) The conservation of energy approach allows for an extension of the support operators method in the staggered grid case in that forces in discrete form may be specified, and their associated energy contributions calculated, regardless of their functional form. The specification of such forces is of extreme importance to the development of robust and advanced hydrodynamics algorithms [4,5].

An extension of the usual Lagrangian assumption of constant mass in a zone was also given. By noting that if the nodal mass is not constant there will be momentum flux from a node, it was concluded that this mass should also be constant. This is necessary for the momentum equation to appear in the form in which it is almost always used in Lagrangian calculations. Because these two masses were defined in terms of common corner masses it then follows that these latter masses must also be constant, Lagrangian objects. This conclusion leads to the important concept of subzonal corner pressures and forces that inhibits spurious grid distortion in these algorithms [4].

Other concerns with the numerical solutions of the equations of fluid dynamics, both fundamental and practical, were explored. Among these were difficulties with momentum, volume, and entropy conservation in the former context: and, the proper treatment of boundary conditions and time integration in the latter. The possible difficulties that can be encountered were illustrated by a first principles analysis of the so-called area-weighted schemes that have been used for many years in different forms, and have heretofore remained somewhat of an enigma.

Although numerical results were shown here only to explore practical concerns with the implementation of reflective boundary conditions, a much larger set of results is presented as part of the wider development of this work. This is contained in the related papers [13,4,5] that have been referenced extensively throughout this one. Finally, we wish to note that the ideas developed here in two spatial dimensions are directly applicable to any number of dimensions [24].

APPENDIX A

In this appendix we illustrate the derivation of difference operators given a prescription for the volume of a zone element. (Our development here somewhat parallels that in [25].) This is done for a quadrilateral zone in two-dimensional, Cartesian geometry specified by the coordinates (r, z). Necessary changes in going to two-dimensional, cylindrical geometry are indicated. The area, A, of a quadrilateral zone in terms of the coordinates of its defining points, as shown in Fig.4, is given by

$$A = \frac{1}{2}[(r_2 - r_4)(z_3 - z_1) + (r_1 - r_3)(z_2 - z_4)]. \tag{56}$$

From the Lagrangian assumption, as stated by Eq.(1), and the expression for the divergence in Cartesian geometry we have

$$\nabla \cdot \vec{v} = \frac{\partial v_r}{\partial r} + \frac{\partial v_z}{\partial z} = \frac{1}{A}\frac{dA}{dt}. \tag{57}$$

Using the fact that $\vec{v}_i = d\vec{R}_i/dt$, where $\vec{R}_i = (r_i, z_i)$, the above expression can be explicitly evaluated and the partial derivatives with respect to both coordinates can be obtained as

$$\frac{\partial v_r}{\partial r} = \frac{1}{2A}[(v_{r2} - v_{r4})(z_3 - z_1) + (v_{r1} - v_{r3})(z_2 - z_4)], \tag{58}$$

$$\frac{\partial v_z}{\partial z} = \frac{1}{2A}[(r_2 - r_4)(v_{z3} - v_{z1}) + (r_1 - r_3)(v_{z2} - v_{z4})]. \tag{59}$$

The important fact to note about the above formulas is that not only do they express the partial derivatives of v_r and v_z with respect to coordinates r and z, respectively, but they

also give the formulas for the partial derivatives of any function defined at the grid points of the quadrilateral with respect to these coordinates. For example, if one wants the expression for the cross derivatives inside zone z, $\partial v_z/\partial r$ and $\partial v_r/\partial z$, one simply substitutes v_z for v_r in Eq.(58), and v_r for v_z in Eq.(59), respectively. Thus, by the procedure outlined we have derived operator expressions that can act on any data that are given at the respective points to obtain a discrete form of the derivatives of that data inside the zone. Another feature of Eqs.(58),(59) as operator expressions is that they obey the results of simple calculus to lowest order. For example, inserting z in place of v_r in Eq.(58) and r in place of v_z in Eq.(59) gives $\frac{\partial z}{\partial r} = \frac{\partial r}{\partial z} = 0$. However, inserting z^2 for v_r in Eq.(58) does not yield zero for an arbitrary spacing of the quadrilateral grid points. This shows that these formulas are only first order accurate.

Our next goal is to write the derivative formulas given by Eqs.(58),(59) in vector form by the use of either set of vectors, $\vec{a}_i$ or $\vec{S}_i$, as shown in Fig.4. To this end, the representation that corresponds quantitatively to the notation in Fig.4 of the vectors $\vec{a}_i$ is defined by

$$\vec{a}_1 = \vec{a}_2 = \frac{(z_2 - z_1)}{2}\hat{r} - \frac{(r_2 - r_1)}{2}\hat{z}, \tag{60}$$

etc., which gives the outward normal prescription. Then the form for the divergence of velocity given by the usual control volume differencing in Cartesian geometry is

$$A(\nabla \cdot \vec{v}) = (\vec{a}_1 + \vec{a}_8) \cdot \vec{v}_1 + (\vec{a}_2 + \vec{a}_3) \cdot \vec{v}_2 + (\vec{a}_4 + \vec{a}_5) \cdot \vec{v}_3 + (\vec{a}_6 + \vec{a}_7) \cdot \vec{v}_4. \tag{61}$$

It is easy to verify by straightforward algebraic manipulation that this equation is identical to Eqs.(58),(59) obtained by time differentiation of A. By vector manipulation the above expression can be written in an equivalent form with respect to the median mesh. By use of the vector relations between the two sets, $(\vec{S}_1 - \vec{S}_4) = \vec{a}_1 + \vec{a}_8$, $(\vec{S}_2 - \vec{S}_1) = \vec{a}_2 + \vec{a}_3, \ldots,$ etc., there follows that

$$\begin{aligned} A(\nabla \cdot \vec{v}) &= \vec{S}_1 \cdot (\vec{v}_1 - \vec{v}_2) + \vec{S}_2 \cdot (\vec{v}_2 - \vec{v}_3) + \vec{S}_3 \cdot (\vec{v}_3 - \vec{v}_4) + \vec{S}_4 \cdot (\vec{v}_4 - \vec{v}_1) \\ &\equiv -\sum_{i=1}^{4} \vec{S}_i \cdot \delta\vec{v}_i, \end{aligned} \tag{62}$$

where $\delta\vec{v}_i = \vec{v}_{i+1} - \vec{v}_i$, and i is cyclic as before.

To complete this discussion we now have that the partial derivatives given by Eqs.(58), (59) can be written with respect to these sets of vectors. For example, the partial derivative with respect to the coordinate r using the vectors $\vec{a}_i$ for any grid point function $*$ is given by

$$\frac{\partial *}{\partial r} = \frac{1}{A}[(a_{1r} + a_{8r})* + (a_{2r} + a_{3r})* + (a_{4r} + a_{5r})* + (a_{6r} + a_{7r})*], \tag{63}$$

where a_{ir} is the r component of vector $\vec{a}_i$; a similar expression holds for the partial derivatives with respect to the coordinate z. These derivatives expressed in vector form can be used to define all vector operators (**GRAD**, **DIV**, and **CURL**) in Cartesian geometry with respect to functions defined on the grid points.

We wish to note that the procedure carried out here for Cartesian geometry can be done for two-dimensional (r, z) cylindrical geometry with minor modifications. For this case the

volume element given by Eq.(56) becomes more complicated but the net result obtained for the divergence, as given by either Eq.(61) or Eq.(62), is modified simply by multiplying each vector length by a factor $\overline{r}$, This factor is given as the average of the value of the coordinate r at the endpoints that define each vector length. So, for instance, $\vec{a}_1 \to \vec{a}_1(3r_1 + r_2)/4$ and $\vec{a}_2 \to \vec{a}_2(3r_2 + r_1)/4$, etc., as seen from Fig.4; for the vectors $\vec{S}_i$ the endpoints are defined by the midpoints of the associated side and the common center point of the zone.

Finally, in the case of curvilinear coordinates it is not possible to uniquely distinguish single derivatives since, for example, in cylindrical coordinates the term $\frac{\partial P}{\partial r} = \frac{1}{r}\frac{\partial r P}{\partial r} - \frac{P}{r}$ can have different discrete representations. However, if one is given the vector set $\vec{a}_i$ or $\vec{S}_i$ as functions of the coordinate points, then the discrete form of the differential vector operators can still be completely specified directly in vector form. The specification of the half-edge vectors that compose these operators is what is important. This can often be a very complicated step since the half-edge vectors can be given as arbitrary functions of the grid point coordinates.

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