

Algebraic Limitations on Two-Dimensional Hydrodynamics Simulations

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Algebraic limitations imposed by the use of connected straightline segments to define meshes for hydrodynamics simulations in two-dimensional cylindrical geometries are shown. It is shown that in the simplest smooth isentropic flow of the spherical expansion of a gas with point symmetry, commonly, and currently, used finite difference, finite volume, or finite element staggered grid hydrodynamics equations cannot simultaneously preserve energy, entropy, and sphericity on an equal-angle $R - \Theta$ mesh. It is further shown why finite difference codes tend to preserve sphericity and entropy, while finite element codes tend to preserve sphericity and energy. Exact difference representations of interface (cell face) pressures and work terms and of the elements of the strain rate tensor in a cell are shown. © 1996 Academic Press, Inc.

INTRODUCTION

Commonly used staggered grid hydrodynamic approximations of the two-dimensional Euler equations cannot simultaneously preserve energy, entropy, and sphericity in cylindrical coordinates for a problem of isentropic flow with point symmetry. This limitation applies to Lagrangian calculations and to the Lagrangian phase of Eulerian or ALE calculations. Historically, this class of methods used independently modeled momentum and internal energy equations and total energy was not readily defined, much less conserved. The reasons for this will be elaborated below, but briefly there were two. For reasons of speed, calculations were done on a staggered time grid where internal energy was updated at one time level and kinetic energy at another time level. This made it difficult to define total energy. The other reason had to do with the desire to maintain sphericity in a problem with spherical symmetry. In cylindrical geometry, the mass of a cylindrical shell of material of constant density and constant thickness varies with the distance of the shell from the axis. This makes it difficult to construct a momentum equation which will preserve spherical flow. The solution historically adopted was to effectively solve the momentum equation in Cartesian geometry where the mass did not depend on the distance from the axis. But this leads to a quandary of how to define both total kinetic energy and total internal energy in cylindrical geometry. These problems have been resolved in

several ways and sets of compatible formulas for staggered grid hydrodynamics [1–3] which are derived to inherently conserve total energy are displayed. Compatible formulas have the property that different arrangements of pressure, mass, area, and velocity terms in the total energy conservation equation represent the momentum equation at cell vertices, the internal and total energy equations in the cell, and the interface work done by (or on) the faces of the cells. The interface pressure on the cell faces is a compatible derived quantity. Any particular equation can be used as a starting point and the others follow. But even with these formulas, algebraic limitations in cylindrical geometry do not allow the simultaneous conservation of energy and entropy and preservation of sphericity in a calculation of the expansion of an ideal gas with point symmetry.

STAGGERED GRID HYDRODYNAMICS

In staggered grid hydrodynamics, velocity, \mathbf{u}_n or $\dot{\mathbf{R}}_n$, and position vectors, \mathbf{R}_n , are associated with the nodes (vertices) of cells; volume, density, specific internal energy, and entropy, V_c, ρ_c, e_c, s_c , are associated with the interior of cells and interface work and cell face pressure terms are associated with the faces of the cells. The overdot indicates the Lagrangian derivative. The formulas presented, in general, apply to cells with an arbitrary number of nodes and faces. All hydrodynamic variables are assumed to be defined at time t and advanced in lockstep to time $t + \delta t$. This is an even time grid rather than a staggered time grid. The symbol δ is used to indicate time-level differencing. In the difference form of the formulas, use will be made of the relation

$$\left[\frac{(\mathbf{u} \cdot \mathbf{u})^{t+\delta t}}{2} - \frac{(\mathbf{u} \cdot \mathbf{u})^t}{2} \right] = \left(\frac{\mathbf{u}^{t+\delta t} + \mathbf{u}^t}{2} \right) \cdot (\mathbf{u}^{t+\delta t} - \mathbf{u}^t) = \mathbf{u} \cdot \delta \mathbf{u}$$

to express the change in specific kinetic energy over a time step in terms of the change in velocity at a node $\delta \mathbf{u}_n$ and define the velocity \mathbf{u}_n in the time step to be the mean velocity over the time step. The specific kinetic energy at time t on node n is $0.5 \mathbf{u}_n^t \cdot \mathbf{u}_n^t$. This is the scheme advocated by Trulio and Trigger

in their 1961 paper [4] describing the construction of a conservative set of equations in one-dimensional geometries. On a staggered time grid, Trulio and Trigger showed that in one-dimensional geometries, algebraically conservative equations could be constructed by defining the specific kinetic energy at time t on node n as $0.5 \mathbf{u}_n^{t+\delta t/2} \cdot \mathbf{u}_n^{t-\delta t/2}$ which is not necessarily a positive quantity. They also pointed out that total energy conservation on a staggered time grid could only be achieved if the time step were constant throughout the calculation; that is, the Courant condition must be known a priori.

GEOMETRY

The notation used is shown in Fig. 1. Nodes defining a cell are numbered in counterclockwise sequence around the cell. Cells surrounding a node are numbered in counterclockwise sequence around the node. One of a set of node area vectors $\mathbf{A}_{j,c}^n$ is shown. The node area vectors are outward directed vectors associated with the cell faces at each node n of cell c . The j index identifies various weightings of the node area vectors. The cell volume and node area vectors are specified per unit thickness in X - Y coordinates, and per radian in R - Z coordinates. Formulas will be written in terms of the nodal coordinates R_n , Z_n and $X_n = R_n^\nu$ with $\nu = 0$ for Cartesian (X , Y) coordinates and $\nu = 1$ for cylindrical (R , Z) coordinates. Let \hat{k} be the unit vector normal to the X - Y or R - Z plane, \hat{R} and \hat{Z} unit vectors in the R and Z directions, and

$$[(\hat{R} \times \hat{Z}) \cdot \hat{k}] = [\hat{R} \cdot (\hat{Z} \times \hat{k})] = 1.$$

With the node position vectors, \mathbf{R}_n , taken in cyclic fashion ($\mathbf{R}_{n-1} = \mathbf{R}_4$ when $n = 1$ and $\mathbf{R}_{n+1} = \mathbf{R}_1$ when $n = 4$ in a quadrilateral), explicit representations of the first few of an infinite series of formulas for the cell volume in terms of node

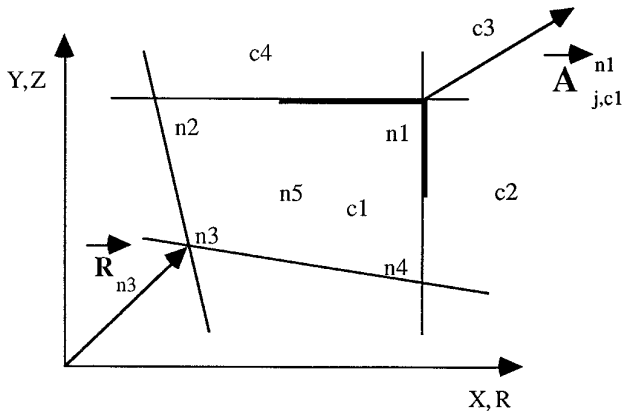


FIG. 1. Notation about cell showing nodes and the outward directed node area vector for cell $c1$ at node $n1$.

area vectors with different X_n weightings are derived in the Appendix;

$$(\nu + 2)V_c = \sum_n^c \mathbf{R}_n \cdot \mathbf{A}_{1,c}^n = \sum_n^c \mathbf{R}_n \cdot \left\{ \frac{[X_n(\mathbf{R}_{n+1} - \mathbf{R}_n) + X_n(\mathbf{R}_n - \mathbf{R}_{n-1})] \times \hat{k}}{1 \cdot 2} \right\}$$

$$(\nu + 2)V_c = \sum_n^c \mathbf{R}_n \cdot \mathbf{A}_{2,c}^n = \sum_n^c \mathbf{R}_n \cdot \left\{ \frac{[(X_{n+1} + X_n)(\mathbf{R}_{n+1} - \mathbf{R}_n) + (X_n + X_{n-1})(\mathbf{R}_n - \mathbf{R}_{n-1})] \times \hat{k}}{2 \cdot 2} \right\}$$

$$(\nu + 2)V_c = \sum_n^c \mathbf{R}_n \cdot \mathbf{A}_{3,c}^n = \sum_n^c \mathbf{R}_n \cdot \left\{ \frac{[(X_{n+1} + 2X_n)(\mathbf{R}_{n+1} - \mathbf{R}_n) + (2X_n + X_{n-1})(\mathbf{R}_n - \mathbf{R}_{n-1})] \times \hat{k}}{3 \cdot 2} \right\},$$

where the sum \sum_n^c is over the nodes n surrounding cell c . The sum \sum_c^n is over the cells c surrounding node n . This sequence can be extended indefinitely by forming linear combinations of the terms above corresponding to different weightings of the (scalar) $X_n = R_n^\nu$ coordinate values of the nodes. In $X - Y$ coordinates, the representations all reduce to a single formula as the $X_n = R_n^\nu$ are all equal 1.

In contrast to the many representations of the cell volume, there is only one representation, $j = 3$, for the rate of change of the cell volume

$$\dot{V}_c = \sum_n^c \dot{\mathbf{R}}_n \cdot \mathbf{A}_{3,c}^n = \sum_n^c \dot{\mathbf{R}}_n \cdot \left\{ \frac{[(X_{n+1} + 2X_n)(\mathbf{R}_{n+1} - \mathbf{R}_n) + (2X_n + X_{n-1})(\mathbf{R}_n - \mathbf{R}_{n-1})] \times \hat{k}}{3 \cdot 2} \right\}.$$

This algebraic difference between the single representation of the rate of change of the volume, and the infinite number of representations of the volume is the cause of the difficulty in simultaneously preserving energy, entropy, and sphericity in a problem with point symmetry in cylindrical coordinates.

The significance of the $j = 3$ node area vectors can be identified by considering the time differential of the cell volume. The total time derivative of a scalar function $f = f(\mathbf{R}, t)$ is given by

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{d\mathbf{R}}{dt} \cdot \nabla f.$$

The cell volume is a function only of the vectors defining the cell nodes $V_c = V_c(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_n)$. The rate of change of the cell volume can be written

$$\frac{dV_c}{dt} = \sum_n^c \frac{d\mathbf{R}_n}{dt} \cdot \frac{\partial V_c}{\partial \mathbf{R}_n} = \sum_n^c \dot{\mathbf{R}}_n \cdot \mathbf{A}_{3,c}^n.$$

The $j = 3$ node area vector is identified with the differential of the cell volume with respect to the node position vector. The divergence of the velocity over the cell is

$$(\nabla \cdot \dot{\mathbf{R}})_c = \frac{1}{V_c} \frac{dV_c}{dt} = \frac{1}{V_c} \sum_n^c \dot{\mathbf{R}}_n \cdot \mathbf{A}_{3,c}^n.$$

Integral definitions of the cell volume and rate of change of cell volume can also be written in terms of sums over the node area vectors. The integral and difference definitions of cell volume and rate of change of cell volume can be compared:

$$\begin{aligned} V_c &= \frac{1}{(\nu + 2)} \int_c \nabla \cdot \mathbf{R} dV & \dot{V}_c &= \int_c \nabla \cdot \dot{\mathbf{R}} dV \\ &= \frac{1}{(\nu + 2)} \oint_c \mathbf{R} \cdot d\mathbf{A} & &= \oint_c \dot{\mathbf{R}} \cdot d\mathbf{A} \\ &= \frac{1}{(\nu + 2)} \sum_n^c \mathbf{R}_n \cdot \mathbf{A}_{j,c}^n & &= \sum_n^c \dot{\mathbf{R}}_n \cdot \mathbf{A}_{3,c}^n. \end{aligned}$$

From Fig. 2 and the formulas for $\mathbf{A}_{j,c}^n$ above, it can be seen that in cylindrical geometry on an equal-angle $R - \Theta$ mesh, only the sum of $\mathbf{A}_{1,c}^n$ node area vectors of the cells adjoining node n with the common weighting X_n can produce a radial vector. The direction of this vector will determine the direction of the change of velocity at the node. This will be important later to the issue of preserving spherical symmetry in cylindrical coordinates for those problems with point symmetry. In [5],

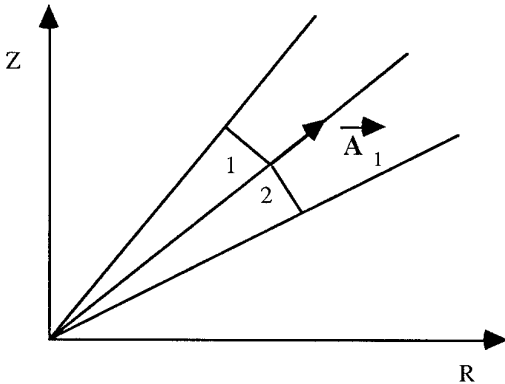


FIG. 2. Node area vectors in equal-angle mesh. Only the sum of $\mathbf{A}_{1,c}^n$ vectors for cells 1 and 2 with $j = 1$ will produce a radial vector in cylindrical coordinates.

Margolin and Nichols note that in a finite volume code, the acceleration calculated on a momentum control volume is correctly applied only to the center of mass of the body; not to the node.

COMPATIBLE EQUATIONS

Compatible difference equations provide a simple way to preserve the conservation properties of the differential equations being modeled. The construction of such equations is straightforward. Compatible formulas are formed by rearranging combinations of common terms (pressures, masses, areas, and velocities) in the total energy conservation equation to represent the change in momentum, internal energy, kinetic energy, and work done on a cell face. The technique will be illustrated for an ideal fluid. The conservation of energy equation in differential and difference forms is

$$\begin{aligned} \int_V \rho (\delta e + \delta \mathbf{u} \cdot \mathbf{u}) dV &= -\delta t \int_V \nabla \cdot (p\mathbf{u}) dV = -\delta t \oint_S (p\mathbf{u}) \cdot d\mathbf{A} \\ \sum_{\text{all } c} M_c \delta e_c + \sum_{\text{all } n} M_n \delta \mathbf{u}_n \cdot \mathbf{u}_n &= -\delta t \sum_b (p_b \mathbf{u}_b) \cdot \mathbf{A}_b^b, \end{aligned}$$

where the integrals and sums are over the domain of the problem. The cell and node masses, M_c, M_n , will be defined below. The subscript b indicates values on the domain boundary.

Over time, difference formulas for the momentum equation on a staggered space grid have been derived in many ways; from Taylor's series expansions of the pressure gradient terms in early finite difference equations [6, 7], through Green's transformations of the pressure gradients in finite volume equations [8], and the equations of virtual work [9] or solution of the Lagrange equation [10] to lumped-mass, uniform-strain finite element equations [11–13] and compatible finite volume equations [3, 14, 15]. Most of the difference formulas for the momentum equation have the generic form

$$\delta \mathbf{u}_n = \frac{\delta t}{X_n (\rho A)_n} \sum_c^n \mathbf{A}_{j,c}^n p_c = \frac{\delta t}{(\rho A)_n} \sum_c^n \left(\frac{\mathbf{A}_{j,c}^n}{X_n} \right) p_c,$$

where the sum is over the cells surrounding the node. The terms in the equation are variously defined. In finite difference [6, 7] and finite volume [8, 15] codes, the area node vector $\mathbf{A}_{1,c}^n$ with $j = 1$ is normally chosen (by experience or by default) to obtain spherical symmetry in a problem with point symmetry in cylindrical coordinates on the equal-angle mesh of Fig. 2. The X_n term in the denominator then cancels the X_n weighting in the definition of $\mathbf{A}_{1,c}^n$ and reduces the equation to the Cartesian form. The $(\rho A)_n$ term represents the product of the density and the area Jacobean at the node. In finite element codes, the effect of Petrov–Galerkin ($1/R$) weighting [11–13] is to choose $j = 1$ in $\mathbf{A}_{j,c}^n$ which also cancels the X_n in the denominator of the momentum equation. Direct solutions of the virtual work

[9], Lagrange equation [10], and finite-element equations derived without $1/R$ weighting introduce the vector direction of $\mathbf{A}_{3,c}^n$ in the momentum equation through the term $\partial V_c / \partial \mathbf{R}_n$. Some finite volume codes [3, 14] also introduce the vector direction of $\mathbf{A}_{3,c}^n$ in the momentum equation. Such codes cannot preserve spherical symmetry in a symmetric problem on the equal-angle mesh of Fig. 2.

It is useful to have a mass associated with a cell corner just as the node area vector is associated with the cell corner [15]. Schulz in his 1964 paper [7] defined cell and nodal masses in terms of masses associated with cell corners M_n^c such that

$$M_n = \sum_c^n M_n^c, \quad M_c = \sum_n^c M_n^c.$$

The Schulz corner masses were defined in a way easy to compute with 1960's equipment

$$M_n^c = X_n \frac{(\rho A)_c}{4},$$

where ρ and A are the density and planar area of cell c . The mass of cell c is then

$$M_c = \sum_n^c M_n^c = \sum_n^c \frac{X_n (\rho A)_c}{4} = (\rho A)_c \sum_n^c \frac{X_n}{4}$$

which is obviously not the true mass of the cell in cylindrical geometry. The node mass is

$$M_n = \sum_c^n M_n^c = \sum_c^n \frac{X_n (\rho A)_c}{4} = X_n \sum_c^n \frac{(\rho A)_c}{4} = X_n (\rho A)_n$$

which defines $(\rho A)_n$. This definition sets the term appearing in the compatibility equations

$$\frac{M_n}{X_n (\rho A)_n} = 1.$$

These definitions have the properties that the sum of cell masses equals the sum of node masses,

$$\sum_{\text{all } c} M_c = \sum_{\text{all } c} \sum_n^c M_n^c = \sum_{\text{all } n} \sum_c^n M_n^c = \sum_{\text{all } n} M_n$$

and the total kinetic energy

$$KE = \sum_{\text{all } c} \sum_n^c M_n^c (.5 \mathbf{u}_n \cdot \mathbf{u}_n) = \sum_{\text{all } n} \sum_c^n M_n^c (.5 \mathbf{u}_n \cdot \mathbf{u}_n)$$

can be summed over either cells or nodes. Note that M_n is zero on the z axis in cylindrical coordinates. As the hydro equations calculate the change in specific quantities, $\delta \mathbf{u}_n$, δe_c , ρ_c , the Schulz mass definition works just fine (but care must be taken to introduce sources and sinks as specific quantities).

A corner mass can be based on the $\mathbf{A}_{1,c}^n$ definition of cell volume by considering a path around the quadrilateral q in Fig. 3 defined by nodes $(5, n-1, n+1; n=1, \dots, 4)$, where \mathbf{R}_5 is the mean of the node position vectors $\mathbf{R}_1, \dots, \mathbf{R}_4$ defining the cell. Then

$$M_n^c = \rho_c \sum_n^q \frac{X_n}{2(\nu+2)} \left\{ \mathbf{R}_n \cdot \left[\frac{(\mathbf{R}_{n+1} - \mathbf{R}_{n-1})}{2} \times \hat{k} \right] \right\}_c$$

is basically half the mass of the triangle with sides $n-1, n$ and $n, n+1$ except in cells with extreme distortion. The sum of the corner masses about the node n is

$$M_n = \sum_n^c M_n^c = X_n \sum_n^c \frac{\rho_c}{2(\nu+2)} \sum_n^q \left\{ \mathbf{R}_n \cdot \left[\frac{(\mathbf{R}_{n+1} - \mathbf{R}_{n-1})}{2} \times \hat{k} \right] \right\}_c$$

which defines $M_n = X_n (\rho A)_n$. $M_c = \sum_n^c M_n^c = \rho_c V_c$ is the Lagrangian cell mass. This definition of corner mass has all of the properties of the Schulz corner mass and, in addition, represents the true mass of the cell. Many other definitions of corner, cell, and node masses and the area Jacobian, generally based on concepts of momentum control volume, have been used. The equations which follow are general and do not assume specific relations among the mass variables.

The steps to produce a compatible internal energy equation, while conserving total energy are to substitute the difference form of the momentum equation for $\delta \mathbf{u}_n$ into the difference

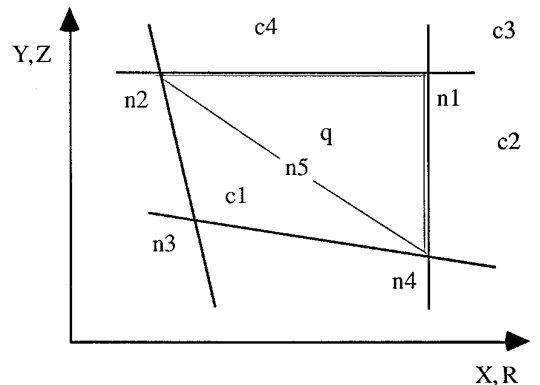


FIG. 3. Notation for defining cell corner mass M_n^c as half the mass in quadrilateral q .

form of the total energy equation and rearrange (assemble) terms by cell quantities,

$$\sum_{\text{all } c} M_c \delta e_c + \sum_{\text{all } n} M_n \delta \mathbf{u}_n \cdot \mathbf{u}_n = -\delta t \sum_b (p_b \mathbf{u}_b) \cdot \mathbf{A}_b^b$$

$$\sum_{\text{all } c} M_c \left[\delta e_c + \frac{\delta t p_c}{M_c} \sum_n \frac{M_n}{X_n(\rho A)_n} \mathbf{A}_{j,c}^n \cdot \mathbf{u}_n \right] = -\delta t \sum_b (p_b \mathbf{u}_b) \cdot \mathbf{A}_b^b$$

$$\delta e_c = \frac{-\delta t p_c}{M_c} \sum_n \frac{M_n}{X_n(\rho A)_n} \mathbf{A}_{j,c}^n \cdot \mathbf{u}_n.$$

The result is the compatible equation for the change in specific internal energy. For compatibility and total energy conservation in cylindrical coordinates, the choice of j in the $\mathbf{A}_{j,c}^n$ area vector terms must be the same in the momentum and in the internal energy equations. To preserve sphericity on an equal-angle mesh in cylindrical coordinates for a problem with point symmetry, the $j = 1$ node area vector must be chosen.

The differential and difference equations for the conservation of total energy can now be put in the form

$$\sum_{\text{all } c} M_c \delta e_c + \sum_{\text{all } n} M_n \delta \mathbf{u}_n \cdot \mathbf{u}_n = -\delta t \sum_b (p_b \mathbf{u}_b) \cdot \mathbf{A}_b^b$$

$$\delta t \int_V (-p \nabla \cdot \mathbf{u} - \mathbf{u} \cdot \nabla p) dV = -\delta t \oint_S (p \mathbf{u}) \cdot d\mathbf{A}$$

$$\delta t \left[\sum_{\text{all } c} -p_c \sum_n \frac{M_n}{X_n(\rho A)_n} \mathbf{A}_{j,c}^n \cdot \mathbf{u}_n + \sum_{\text{all } n} \frac{M_n}{X_n(\rho A)_n} \mathbf{u}_n \cdot \sum_c \mathbf{A}_{j,c}^n p_c \right]$$

$$= -\delta t \sum_b (p_b \mathbf{u}_b) \cdot \mathbf{A}_b^b,$$

where the first term is the change in internal energy and the second term is the change in kinetic energy. If $M_n = X_n(\rho A)_n$ the total energy equation is

$$\delta t \left[\sum_{\text{all } c} -p_c \sum_n \mathbf{A}_{j,c}^n \cdot \mathbf{u}_n + \sum_{\text{all } n} \mathbf{u}_n \cdot \sum_c \mathbf{A}_{j,c}^n p_c \right] =$$

$$-\delta t \sum_b (p_b \mathbf{u}_b) \cdot \mathbf{A}_b^b.$$

Solving the momentum equation allows the node coordinates to be moved and the cell volume and density at the advanced time to be calculated. Solving the compatible internal energy equation defined above determines the internal energy at the advanced time. With the density and internal energy defined in each cell, the cell entropy can be determined from the equation-of-state. (Consider evaluating $p_c V_c^\gamma$ at successive times for an ideal gas.) The change of entropy in the cell will be the same as if it were calculated from the equation

$$T_c \delta s_c = \delta e_c + \frac{\delta t p_c}{M_c} \sum_n \frac{M_n}{X_n(\rho A)_n} \mathbf{A}_{j,c}^n \cdot \mathbf{u}_n,$$

where T is the temperature and s is the entropy of the cell. The cell entropy in smooth isentropic flow can only be preserved, $\delta s_c = 0$, if the internal energy equation were calculated with $j = 3$ $\mathbf{A}_{j,c}^n$ area node vectors. For compatibility and total energy conservation, $j = 3$ area node vectors would then be used in the momentum equation. But $j = 3$ node area vectors do not combine to radial vectors in an equal-angle mesh and will not preserve a spherical flow.

The usual choice in finite difference and finite volume hydrodynamic codes [6–8] is to use $j = 1$ area node vectors in the momentum equation and $j = 3$ area node vectors in the internal energy equation. This choice preserves spherical symmetry on an equal-angle mesh and keeps a smooth flow on the starting isentrope. Total energy conservation is abandoned. In contrast, by the very nature of their construction, finite element codes are inherently compatible and energy conserving. The typical Petrov–Galerkin weighting [11–13] introduces the $j = 1$ area node vectors which preserve spherical symmetry and these are automatically used in both the momentum and internal energy equations as written above. The change in entropy, of course, is based on the *change* in volume, $d(\text{volume})$ is given by $j = 3$, not $j = 1$ area node vectors, and is not preserved.

As a result of these observations, Burton in 1994 modified a cylindrical geometry code [15] to use the $j = 1$ area node vectors in the momentum and internal energy equations and to simultaneously preserve entropy by an interesting device. Except at the initial time, the cell volume is not calculated from the coordinates of the cell but is carried as an internal variable and updated by calculating the change in cell volume using the $j = 1$ vector in the expression for the divergence of velocity.

INTERIOR INTERFACE (CELL FACE) WORK TERMS AND INTERFACE (CELL FACE) PRESSURES

Just as the assembly of terms in the conservation equation for total energy as coefficients of p_c and \mathbf{u}_c lead to representations of $p \text{ div } \mathbf{u}$ and $\mathbf{u} \cdot \text{grad } p$, another grouping of terms as coefficients of the cell face area vectors lead to difference representations of cell face work terms, $(p \mathbf{u}) \cdot d\mathbf{A}$, and cell face pressure terms. The cell face area vectors will be formed of the common vector parts of the two node area vectors defining the cell face $n, n + 1$,

$$\mathbf{A}^{n,n+1} = \frac{(X_{n+1} + X_n)}{2} (\mathbf{R}_{n+1} - \mathbf{R}_n) \times \hat{k},$$

where the notation used is illustrated in Fig. 4. (The j distinction drops out in the definition of the cell face area vector as the coefficients of X_n and X_{n+1} become equal in the sum.) The coefficients of this term for one cell face, $n, n + 1$, will be extracted from the difference form of the total energy conservation equation.

Collecting all coefficients of the cell face area vectors from the expressions for the change of internal and kinetic energy

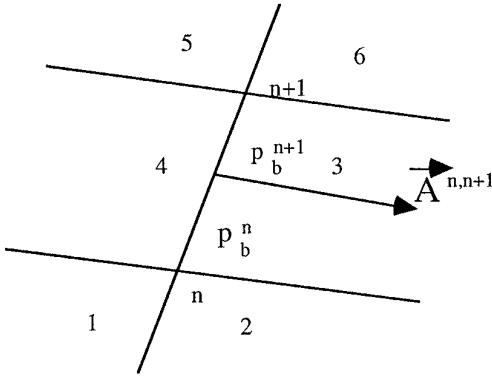


FIG. 4. Notation for describing interface work and pressure terms.

of a cell leads to the equation (in a quadrilateral mesh) for the work done on the cell face (interface) in time δt ,

$$\delta W^{n,n+1} = -\delta t \frac{\mathbf{A}^{n,n+1}}{2} \cdot \left\{ \begin{array}{l} \left[\mathbf{u}_{n+1} \left(\frac{p_3(M_{n+1}^4 + M_{n+1}^5) + p_4(M_{n+1}^3 + M_{n+1}^6)}{M_{n+1}^4 + M_{n+1}^6 + M_{n+1}^3 + M_{n+1}^5} \right) \right] \\ \left[+ \mathbf{u}_n \left(\frac{p_3(M_n^1 + M_n^4) + p_4(M_n^2 + M_n^3)}{M_n^2 + M_n^4 + M_n^1 + M_n^3} \right) \right] \end{array} \right\},$$

which corresponds to one cell face term of the interior boundary work in the conservation equation

$$\begin{aligned} \sum_{\text{int } c} M_c \delta e_c + \sum_n M_n \delta \mathbf{u}_n \cdot \mathbf{u}_n \\ = -\delta t \sum_{\text{int } b} \mathbf{A}_{b,b}^b \cdot (p_b \mathbf{u}_b) = \sum_{\text{int } n} \delta W^{n,n+1}, \end{aligned}$$

where the sum is over an interior region of cells with the associated nodes and cell face boundaries. With this definition of the work on a cell face, total energy conservation can be examined over any subregion of a mesh, including a single cell. The change in internal energy, for example, could be calculated by subtracting the change in cell kinetic energy from the work done on the cell. The result would be identical to that obtained from solving the internal energy equation (with the same j value used in the momentum equation).

For clarity in this illustration of the compatible definition of the interface work and pressure, the term $X_n(\rho A)_n$ has been identified with the sum of the cell corner components of the nodal mass, $M_n^1 + M_n^2 + M_n^3 + M_n^4$ in Fig. 4 which would be the case in a well-organized code. It will be noted that in the compatible definition of the interface work term, two values of the pressure are defined on each cell face. The two pressures

reduce to a single value only if cell masses across the interface are constant. The interface pressure nearest node n , Fig. 4, is

$$p_b^n = \frac{p_3(M_n^1 + M_n^4) + p_4(M_n^2 + M_n^3)}{(M_n^1 + M_n^2 + M_n^3 + M_n^4)}.$$

This formula reduces to the average of the two cell pressures if the cell components of the nodal masses on either side of the interface are equal. As in compatible one-dimensional codes [16], if the interface is an exterior boundary, the cell face pressure reduces to the applied boundary pressure, p_3 (the exterior masses, M_n^2 and M_n^3 , are zero). The two values of interface pressure on each face of a cell are in contrast to the single value of interface pressure associated with Godunov solutions on the face of a cell. This is related to the difference between solving for vertex and face velocities. (The eight velocity components on the vertices of a quadrilateral allow the representation of the four fundamental modes of motion of the cell: translation, dilation/compression, shear/rotation, and hour glassing. The four (normal) velocity components on the faces of a cell allow the representation of the translation and dilation/compression modes. The two velocity components of a cell centered velocity code allow only the representation of the translation mode.)

STRAIN RATE TENSOR

The difference forms of the elements of the strain rate tensor in cylindrical geometry are not generally reported. Using the form for \dot{V}_c derived in the Appendix, it is easy to write the exact difference forms of the terms in the strain rate tensor for either plane or cylindrical geometry for a cell with any number (>2) of nodes:

$$\|\varepsilon(R, Z)\| = \begin{pmatrix} \frac{\partial \dot{R}}{\partial R} & \frac{1}{2} \left(\frac{\partial \dot{R}}{\partial Z} + \frac{\partial \dot{Z}}{\partial R} \right) & 0 \\ \frac{1}{2} \left(\frac{\partial \dot{R}}{\partial Z} + \frac{\partial \dot{Z}}{\partial R} \right) & \frac{\partial \dot{Z}}{\partial Z} & 0 \\ 0 & 0 & \frac{\dot{R}}{R} \end{pmatrix},$$

where

$$\begin{aligned} \frac{\partial \dot{R}}{\partial R} &= \frac{1}{2(\nu + 2)V_c} \sum_n \dot{R}_n [(X_n + X_{n+1})Z_{n+1} - (X_{n-1} + X_n)Z_{n-1}] \\ \frac{\partial \dot{R}}{\partial Z} &= \frac{1}{2(\nu + 2)V_c} \sum_n \dot{R}_n [(X_n + X_{n+1})R_{n+1} - (X_{n-1} + X_n)R_{n-1}] \\ \frac{\partial \dot{Z}}{\partial R} &= \frac{1}{2(\nu + 2)V_c} \sum_n \dot{Z}_n [(X_n + X_{n+1})Z_{n+1} - (X_{n-1} + X_n)Z_{n-1}] \end{aligned}$$

$$\frac{\partial \dot{Z}}{\partial Z} = \frac{1}{2(\nu + 2)V_c} \sum_n^c -\dot{Z}_n[(X_n + X_{n+1})R_{n+1} - (X_{n-1} + X_n)R_{n-1}]$$

$$\frac{\dot{R}}{R} = \frac{1}{2(\nu + 2)V_c} \sum_n^c \dot{R}_n[(X_n Z_{n+1} - X_{n+1} Z_n + X_{n-1} Z_n - X_n Z_{n-1})].$$

As usual, the sums are to be taken in cyclic order over the nodes around the cell and $X_n = R_n^\nu$ with $\nu = 1$ in R - Z geometry and $\nu = 0$ in X - Y geometry. It can be noticed that the derivative terms limit to the Cartesian values (the cell volume is numerically equal to the cell area) and the \dot{R}/R term goes to 0 in X - Y geometry. As the terms are derived from the exact expression for the time rate of change of the cell volume, the trace of the strain rate tensor is automatically preserved.

CONCLUSIONS

This note has attempted to set forth the algebraic causes of effects familiar to most people working with solutions of the Euler equations in cylindrical coordinate systems. That is, the difficulty of simultaneously conserving total energy and preserving entropy and sphericity in the simple problem of the expansion of a gas with point symmetry. The note has addressed only typical staggered grid difference schemes, where the momentum equation can be forced into the generic form chosen. No attempt is made to discuss Godunov type schemes which calculate cell edge velocities and pressures, or schemes where all information is carried on nodes or mass points. It is hoped that the discussion presented alerts the reader to the consequences of certain choices of differencing techniques.

Because they are rarely, if ever, shown for staggered grid hydrodynamics, formulas are presented for cell face pressures and work terms. For the same reason, exact difference formulas for the elements of the strain rate tensor in cylindrical geometry are shown.

APPENDIX: DERIVATION OF VOLUME FORMULAS

The notation used is illustrated in Fig. 5. By Pappus' rule, in cylindrical coordinates the volume per radian of each of the triangles emanating from the origin is

$$V_{n+n+1} = \frac{(X_n + X_{n+1} + 0)}{(\nu + 2)} \frac{(\mathbf{R}_n \times \mathbf{R}_{n+1})}{2} \cdot \hat{k},$$

where \hat{k} is the unit vector normal to the R - Z plane and $X_n = R_n^\nu$ with $\nu = 1$ in R - Z geometry and $\nu = 0$ in X - Y geometry. In the example shown, triangles 012, 023, 034, and 045 contribute positive values to the total volume of the polygon; triangle 051 subtracts out the excess volume. Thus the volume

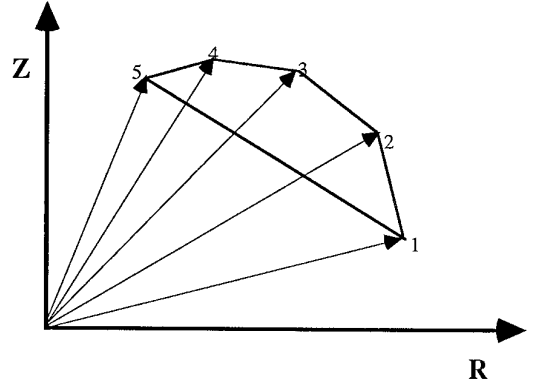


FIG. 5. Geometry to define volume formulas for cell c defined by nodes 1 to 5.

of the cell, c , formed by a polygon rotated one radian about the z axis is

$$\begin{aligned} (\nu + 2)V_c &= \frac{1}{2} \sum_n^c (X_n + X_{n+1})(\mathbf{R}_n + \mathbf{R}_{n+1}) \cdot \hat{k} \\ &= \frac{1}{2} \sum_n^c (X_n \mathbf{R}_n \times \mathbf{R}_{n+1} - X_{n+1} \mathbf{R}_{n+1} \times \mathbf{R}_n) \cdot \hat{k} \\ &= \frac{1}{2} \sum_n^c X_n \mathbf{R}_n \times (\mathbf{R}_{n+1} - \mathbf{R}_{n-1}) \cdot \hat{k} \\ &= \frac{1}{2} \sum_n^c \mathbf{R}_n \cdot [X_n (\mathbf{R}_{n+1} - \mathbf{R}_{n-1}) \times \hat{k}] \\ &= \sum_n^c \mathbf{R}_n \cdot \frac{\{[X_n (\mathbf{R}_{n+1} - \mathbf{R}_n) + X_n (\mathbf{R}_n - \mathbf{R}_{n-1})] \times \hat{k}\}}{1 \cdot 2} \\ &= \sum_n^c R_n \cdot \mathbf{A}_{1,c}^n, \end{aligned}$$

where the sums are to be taken in cyclic fashion.

The $j = 2$ formula is

$$\begin{aligned} (\nu + 2)V_c &= \frac{1}{2} \sum_n^c (X_n + X_{n+1})(\mathbf{R}_n \times \mathbf{R}_{n+1}) \cdot \hat{k} \\ &= \frac{1}{2} \sum_n^c \left[\frac{(X_n + X_{n+1})}{2} (\mathbf{R}_n \times \mathbf{R}_{n+1}) \right. \\ &\quad \left. + \frac{(X_{n-1} + X_n)}{2} (\mathbf{R}_{n-1} \times \mathbf{R}_n) \right] \cdot \hat{k} \\ &= \frac{1}{2} \sum_n^c \mathbf{R}_n \times \left\{ \left[\frac{(X_n + X_{n+1})}{2} (\mathbf{R}_{n+1} - \mathbf{R}_n) \right. \right. \\ &\quad \left. \left. + \frac{(X_n + X_{n-1})}{2} (\mathbf{R}_n - \mathbf{R}_{n-1}) \right] \cdot \hat{k} \right\} \end{aligned}$$

$$= \sum_n^c \mathbf{R}_n \cdot \left\{ \frac{[(X_n + X_{n-1})(\mathbf{R}_{n+1} - \mathbf{R}_n) + (X_n + X_{n-1})(\mathbf{R}_n - \mathbf{R}_{n-1})] \times \hat{k}}{2 \cdot 2} \right\}$$

$$= \sum_n^c \mathbf{R}_n \cdot \mathbf{A}_{2,c}^n$$

A continuing sequence of relations can be formed by summing the formulas above.

The formula for the time derivative of the cell volume is

$$2(\nu + 2)V_c = \sum_n^c (X_n + X_{n+1})(\mathbf{R}_n \times \mathbf{R}_{n+1}) \cdot \hat{k}$$

$$2(\nu + 2)\dot{V}_c = \sum_n^c \left[(X_n + X_{n+1})(\mathbf{R}_n \times \dot{\mathbf{R}}_{n+1} + \dot{\mathbf{R}}_n \times \mathbf{R}_{n+1}) \right] \cdot \hat{k}$$

$$= \sum_n^c \left\{ (X_n + X_{n+1})(R_n \dot{Z}_{n+1} - \dot{R}_{n+1} Z_n + \dot{R}_n Z_{n+1} - R_{n+1} \dot{Z}_n) \right. \\ \left. + \nu(\dot{X}_n + \dot{X}_{n+1})(R_n Z_{n+1} - R_{n+1} Z_n) \right\}$$

$$= \sum_n^c \left\{ +\dot{R}_n \left[(X_n + X_{n+1})Z_{n+1} - (X_{n-1} + X_n)Z_{n-1} \right. \right. \\ \left. \left. + \nu(X_n Z_{n+1} - X_{n+1} Z_n + X_{n-1} Z_n - X_n Z_{n-1}) \right] \right. \\ \left. - \dot{Z}_n [(X_n + X_{n+1})R_{n+1} - (X_{n-1} + X_n)R_{n-1}] \right\}$$

$$\Rightarrow \sum_n^c \left\{ +\dot{R}_n [(2X_n + \nu X_{n+1})(Z_{n+1} - Z_n) + (2X_n + \nu X_{n-1})(Z_n - Z_{n-1})] \right. \\ \left. - \dot{Z}_n [(2X_n + \nu X_{n+1})(R_{n+1} - R_n) + (2X_n + \nu X_{n-1})(R_n - R_{n-1})] \right\}$$

$$\dot{V}_c = \sum_n^c \dot{\mathbf{R}}_n \cdot \left\{ \frac{[(2X_n + \nu X_{n+1})(\mathbf{R}_{n+1} - \mathbf{R}_n) + (2X_n + \nu X_{n-1})(\mathbf{R}_n - \mathbf{R}_{n-1})] \times \hat{k}}{2 \cdot (\nu + 2)} \right\}$$

$$\dot{V}_c = \sum_n^c \dot{\mathbf{R}}_n \cdot \mathbf{A}_{3,c}^n.$$

Strain Rate Tensor. The difference form of the elements of the strain rate tensor can be identified from the intermediate equation for \dot{V}_c above which defines the elements of the divergence operator integrated over the cell

$$2(\nu + 2)\dot{V}_c = \sum_n^c \left\{ +\dot{R}_n \left[(X_n + X_{n+1})Z_{n+1} - (X_{n-1} + X_n)Z_{n-1} \right. \right. \\ \left. \left. + \nu(X_n Z_{n+1} - X_{n+1} Z_n + X_{n-1} Z_n - X_n Z_{n-1}) \right] \right. \\ \left. - \dot{Z}_n [(X_n + X_{n+1})R_{n+1} - (X_{n-1} + X_n)R_{n-1}] \right\}.$$

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