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An Algorithm for the Discrete Rezoning of Lagrangian Meshes

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We describe a discrete method for rezoning Lagrangian hydrodynamics meshes. A test calculation of two hot interacting bubbles in air produced less mass diffusion than a comparable continuously rezoned Lagrangian.

I. INTRODUCTION

Hydrodynamics problems involving strong shock waves in two and three dimensions are notoriously difficult to solve by finite difference methods. This can be particularly true with those computer programs built for application to a range of problems; e.g., programs which satisfactorily handle problems analogous to flow driven by a piston or to shock tube flow may have difficulty with spherical blast waves. The spherical blast wave can be particularly difficult, because the peaked density profile can lead to mass diffusion away from the shock front both inward and outward. Asymmetries introduced by the interaction of a spherical blast wave with an obstacle, or with another shock, necessitate the rezoning of Lagrangian calculations, or result in accentuated diffusion of parameters in an Eulerian mesh.

Schemes to reduce numerical diffusion in Eulerian computations have been given by Boris and Book [1], who describe a "flux correction technique;" also Chevalier and Gardner [2], have described a two dimensional blast wave calculation using a continuously rezoned form of FCT to reduce diffusion.

Lagrangian calculations suffer little from diffusion, because no transport terms are necessary; viz., the mesh moves with the fluid, compressing zones automatically where it is most advantageous to have smaller cells. However, there is the tendency in two dimensions for cell boundaries to become concave, or for vertices to cross over boundaries and form bowties. Also as the cells compress, it is necessary to shorten the timestep when using the explicit mode of calculation. These effects are alleviated to some degree in coupled-Eulerian-Lagrangian schemes, such as the YAQUI [3, 4] code at Los Alamos Scientific Laboratory, since the mesh moves sufficiently to allow compression, but with enough "stiffness" to prevent zone concavity and crossover. Some fluxing of cell parameters is required, but not as much as for the pure Eulerian method. In the limit that the flux transport terms are small, the method is essentially a Lagrangian calculation with small Eulerian correction; but, when strong shocks occur, the method more closely resembles a continuously

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rezoned Eulerian calculation. In the latter case the mesh is prevented from overlapping and consequently the flux terms resemble Eulerian values in some regions.

Another method, described by W. Noh (5), has resulted in the CEL code used at the Lawrence Livermore Laboratory. It consists of the simultaneous use of an Eulerian mesh and a superposed Lagrangian mesh. Special mixed zone equations are used only in coupled zones. This code should be effective in minimizing diffusion, and preserving strong shocks.

The second disadvantage of the Lagrangian method, viz., timestep restriction, can be alleviated by employing an implicit procedure such as pressure iteration. The Lagrangian-Eulerian (ALE) scheme and the implicit difference formulation have been incorporated into the YAQUI [3, 4] code at the Los Alamos Scientific Laboratory. Problems involving strong shocks suffer from some numerical diffusion in the YAQUI code. This paper presents a discrete rezone technique that has proved very practical. It consists of running the program in pure Lagrangian mode until just before concavities and crossovers occur, at which time the entire mesh is mapped onto a new, rectangular mesh containing the same total number of cells. The Lagrangian hydrodynamics calculations proceed with very little numerical diffusion provided that the mapping (rezone) algorithm doesn't introduce more diffusion than would the alternative coupled-Eulerian-Lagrangian scheme. We have developed a simple automatic discrete-rezoning procedure for the YAQUI code. As an example of the method's application, we present a radiation-hydrodynamic calculation that was previously published [6] based on a solution with the older YAQUI scheme.

II. Method

At the end of each Lagrangian cycle mass density, ρ_{IJ}, and specific internal energy, I_{IJ}, are known at the center of each cell (IJ) and velocity components u_{IJ} and v_{IJ} are defined at vertex (IJ) (see Figure 1). Having determined that rezoning is necessary

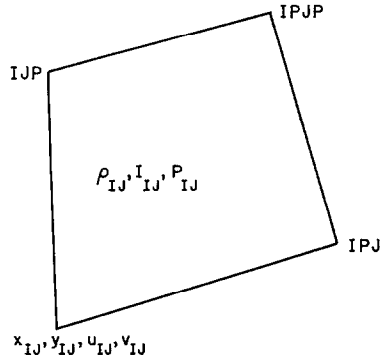

FIG. 1. The cross section of cell IJ is defined by vertices IJ, IPJ, $IPJP$, and IJP. Velocity components are defined at vertices while mass density, ρ, specific internal energy, I, pressure, p, and other state variables are defined at cell centers.

(see below), we define a new mesh where the coordinates of vertex $(\alpha\beta)$ are $x_{\alpha\beta}$, $y_{\alpha\beta}$. The number of cells does not change. For the new mesh, we establish arrays for accumulation of cell centered mass, $m_{\alpha\beta}$, and energy, $e_{\alpha\beta}$, as well as vertex mass $M_{\alpha\beta}$ and momenta, $(Mu)_{\alpha\beta}$ and $(Mv)_{\alpha\beta}$. Each array is initially empty.

We map each old cell onto the new mesh separately. The cross section of old cell (IJ) is divided by the diagonal between vertices IJP and IPJ into two triangles (Figure 2). In each triangle, we distribute K particles which serve to redistribute the mass, energy, and momenta associated with the triangle. Each triangle is subdivided into K similar, equal-area subtriangles. Subtriangle (k) has particle (k) at its centroid. A situation with $K = 16$ is shown in Figure 2; we usually use $K = 576$ in a mesh containing 7000 cells.

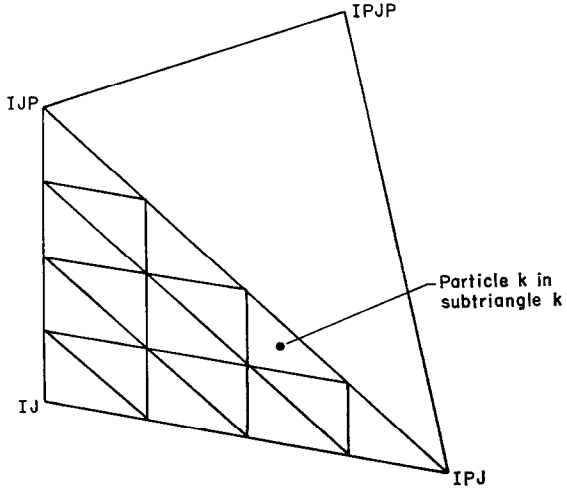

FIG. 2. During the rezoning procedure each old cell is divided by the diagonal $IJP - IPJ$ into two triangles. Each triangle is divided into K similar subtriangles with a particle at the centroid of each subtriangle. Here $K = 16$.

It is not necessary to have intermediate storage for the quantities associated with each particle; the temporary arrays defined above suffice. For rezoning in cylindrical geometry we assign particle mass

$$m_k^p = \rho_{IJ} A x_k^p,$$

where A is the subtriangle area and x_k^p is the distance from the axis to its centroid. The internal energy of a particle is

$$e_k^p = I_{IJ} m_k^p.$$

To assign momenta to the particle, we determine which of the three old vertices

defining the triangle is nearest to the particle. Denoting this vertex as $(\tilde{I}\tilde{J})$, we define

$$(Mu)_k^p = m_k{}^p u_{\tilde{I}\tilde{J}} .$$

and

$$(Mv)_k^p = m_k{}^p v_{\tilde{I}\tilde{J}}$$

Next, we determine which new cell $(\alpha\beta)$ contains the particle and which is the nearest new vertex $(\tilde{\alpha}\tilde{\beta})$. The nearest new vertex must be one of the three vertices of the new triangle containing the particle.

We use the nearest vertex method because it is conservative, simple, and preserves the flow field in an identity mapping.

For particles equidistant from vertices an arbitrary choice of nearest vertex is made; a random choice could be programmed, if desired. We find that rezoning cell centered quantities proceeds very rapidly on the computer, but vertex defined quantities take considerably more time, since distances to vertices are involved; indeed area mapping appears to be a good alternative.

The particle quantities are now stored in the approrpiate "new-mesh" array

$$\begin{aligned}
m_{\alpha\beta} &= m_{\alpha\beta} + m_k{}^p, \\
e_{\alpha\beta} &= e_{\alpha\beta} + e_k{}^p, \\
M_{\tilde{\alpha}\tilde{\beta}} &= M_{\tilde{\alpha}\tilde{\beta}} + m_k{}^p, \\
(Mu)_{\tilde{\alpha}\tilde{\beta}} &= (Mu)_{\tilde{\alpha}\tilde{\beta}} + (Mu)_k^p , \\
(Mv)_{\tilde{\alpha}\tilde{\beta}} &= (Mv)_{\tilde{\alpha}\tilde{\beta}} + (Mv)_k^p .
\end{aligned}$$

Having completed this procedure for each subtriangle of both triangles in each old cell, the "new-mesh" quantities become

$$\begin{aligned}
\rho_{\alpha\beta} &= m_{\alpha\beta}/V_{\alpha\beta} \\
I_{\alpha\beta} &= e_{\alpha\beta}/m_{\alpha\beta} \\
u_{\alpha\beta} &= (Mu)_{\alpha\beta}/M_{\alpha\beta} \\
v_{\alpha\beta} &= (Mv)_{\alpha\beta}/M_{\alpha\beta} .
\end{aligned}$$

$V_{\alpha\beta}$ is the volume of the new cell.

Problems of present interest to the authors contain ambient medium at rest at two of the three problem boundaries (top and outer cylindrical radius). The new mesh is always chosen such that no signals propagate to these boundaries, and we must therefore consider new cells that may be partially or entirely outside the old mesh. For these cells the new masses $m_{\alpha\beta}$ and the other arrays are either empty or partly filled. Such cells are identified and given values appropriate to the ambient medium. Conservation of total energy for an isothermal atmosphere is unaffected by this procedure since the YAQUI code tallies internal and potential energy and momentum

in excess of the ambient values to compute the conserved sums. This expedient is necessary because total problem energies are often small (less than 1 part in 10^5) compared to the energy of the ambient medium. If the problem expands into vacuo, the new cells have null content and obviously play no part in the conservation calculation.

III. Rezone Trigger Mechanisms

The rezoning procedure described above requires only the definition of a new mesh which may or may not resemble the old mesh. The decision to rezone is made in our problems by one of three automatic procedures. First we test all angles made by adjacent cell sides. We trigger a rezone if any angle exceeds a given critical angle $\Theta_c < 180°$. We use $\Theta_c = 150°$. This avoids concavities. Also a rezone is triggered if the length of any cell side becomes smaller than a preassigned length; the latter is either $0.1\ \Delta x$ or $0.1\ \Delta z$ (whichever is least), where Δx or Δz are average cell dimensions in the radial and vertical directions.

Our program incorporates reflective boundary conditions on all three sides (top, bottom, and cylindrical outer radius). We use a signal sensor to prevent shock waves from reaching the boundaries. If the fluid speed at any vertex in regions "near" any boundary exceeds, say, five percent of the maximum speed anywhere in the mesh, we perform a rezone. The critical region is usually chosen to be five cells away from each boundary. An exception is made in cases where one of the boundaries represents an actual reflective surface, such as the ground. In these cases, we do not trigger a rezone because signals are at or near the reflective surface, but the reflection process may compress cells sufficiently to activate a rezone.

IV. The New Mesh

For the moment let us assume that Rayleigh-Taylor, and Kelvin-Helmholtz instabilities are not important; nor are material interfaces, since we consider only a single fluid. For simplicity, we choose a rectangular, uniform new mesh. The new mesh contains all "active" regions of the old mesh and a cushion of 10 ambient cells on all sides, except not adjacent to the cylindrical symmetry axis, and possibly the bottom boundary, if the latter is to be a true reflection surface. In the case described below rezones occur every time the shock wave sufficiently distorts the mesh, about once every 30 hydrodynamic cycles.

For some problems instabilities are important, and we suggest the following untested procedure. Suppose a few vertices have one or more angles exceeding Θ_c. Assign a vertex flag IFLAG $= 0$ to all other vertices and IFLAG $= 1$ to the critical vertices. Move any vertex with IFLAG $= 1$ toward the centroid of its four vertices. The move *to* the centroid is not completed because this could create concave cells. These new vertex locations define the new mesh. The remapping of mass and internal

energy is performed only for those cells having one or more vertices with IFLAG = 1. Momenta need only be reassigned at those vertices with IFLAG = 1.

Rectangular rezones consume about 15 percent of our total computing time; more efficient programming may cut this in half. We expect that adoption of selective rezoning will cut this fraction substantially more. Although more rezones may be required, each rezone would involve far fewer than $2K$ times N particles where N is the total number of cells.

V. Test Case

To display the application of the method we use the two-bubble test problem previously published [6]. Figure 3 shows the velocity field in the problem at 90 ms calculated in Lagrangian fashion using the new particle rezone method, and displays considerable improvement over the older results in resolving the main and reflected shocks. Figure 4 shows the peak pressure between the bubbles *vs* time. The older, fluxing method produces 0.875 MPa at 0.55 s. The new method produces a higher

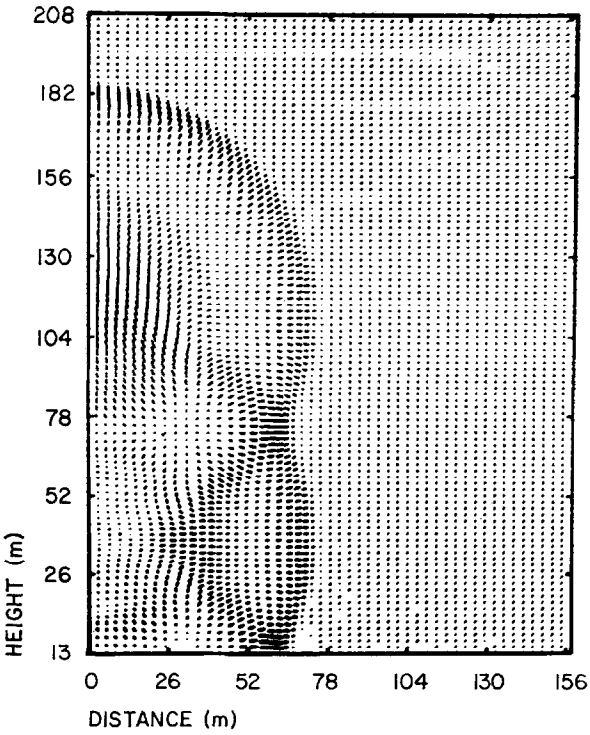

Fig. 3. Velocity vectors at 90 ms in the two-bubble test problem calculated with the rezoned-Lagrangian method.

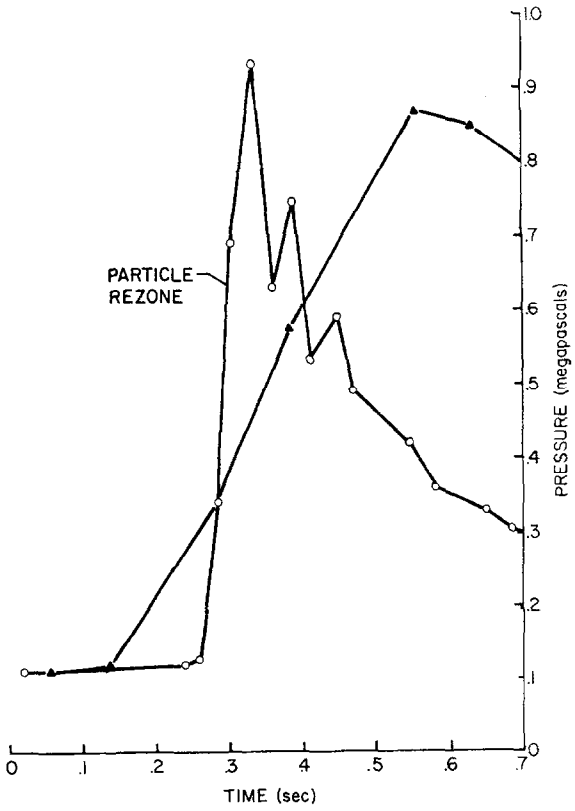

FIG. 4. Peak pressure between the bubbles calculated with the rezoned-Lagrangian (open circles) and Lagrangian-Eulerian (solid triangles) method.

pressure 0.94 MPa at 0.34 s, but displays spikes after the maximum; these occur because the maximum pressure is confined to a single cell, and is unavoidably divided by rezoning. The computations for this problem required about 10^3 hydrodynamic cycles which include some 30 applications of the rezone scheme.

VI. DISCUSSION

We wish to emphasize that one of the main advantages of the particle rezoning procedure is its simplicity. Excellent results are obtained without invoking intricate and subtle lines or reasoning. In contrast we have found the continuously rezoning method to be considerably more difficult to implement.

The method presented is successful in preserving resolution because rezones are done infrequently; furthermore fewer cells are required to achieve a given resolution. In the limit of one rezone following each computing cycle the method is equivalent

to a pure "donor-cell" transport, and would be more diffusive than a procedure using some form of centered differencing.

Our procedure has also been very useful in coupling the discrete ordinates radiative transfer method (SN), which requires rectangular cells, to Lagrangian hydrodynamics with its quadrilateral cells. Temporary particle rezoning of specific internal energy and density is carried out from the Lagrangian to an appropriate rectangular mesh; the SN calculation then gives the change in internal energy in each rectangular cell, and finally the resulting energy change is rezoned back to the original Lagrangian mesh. Conservation of energy to a very high degree is readily obtained by this procedure; also the radiant power, so computed, agrees well with the characteristic ray method applied to the original Lagrangian mesh and, when the geometry is not too extreme, with one-dimensional results.

ACKNOWLEDGMENT

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