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Note

A Simple Rezoning Technique for Use with the Flux-Corrected Transport Algorithm

1. INTRODUCTION

In the last few years flux-corrected transport (FCT) algorithms for Eulerian hydrodynamics have attracted attention because they are more accurate and exhibit less numerical diffusion than several alternative Eulerian methods [1–3]. Successful two- and three-dimensional hydrocodes have been written using FCT [4, 5]. Because many physical problems of interest require rezoning, it is fortunate that the basic one-dimensional routines, developed by Boris [6] and used in our code SAGE [7], allow for the possibility of a general rezoning, in which the grid lines are moved with whatever velocity the user specifies.

One application of this rezoning facility, in which the $\mathbf{E} \times \mathbf{B}$ drift velocity is used to follow magnetic flux surfaces, has been described by Anderson [8]. In our work we are interested in following the fluid mass, and we shall describe a method of obtaining an appropriate grid velocity. This velocity is approximately but not identically equal to the fluid velocity and is obtained from an algorithm which integrates mass along grid lines. We shall show how the FCT treatment of a one-dimensional test problem, first reported (without rezoning) by Colombant and Gardner [9], may be greatly improved using our rezoning prescription; we shall also show how our technique may be adapted to two dimensions.

2. THE DYNAMIC MASS REZONING TECHNIQUE

The FCT routines published by Boris [6] accept as input the old "densities" ρ_i^n (which may represent momentum and energy as well), velocities u_i^n, source terms S_i^n and grid points r_i^n, defined at time t for $1 \leqslant i \leqslant N$, and new grid points r_i^{n+1} defined at time $t + \Delta t$. The routines return the new densities ρ_i^{n+1} at time $t + \Delta t$ defined at the new grid points. Built into these routines is therefore a rezoning facility; the question to be addressed is how to select the r_i^{n+1}. Expressed alternatively, we must determine the grid velocity U_g^n where

$$U_{gi}^n = (r_i^{n+1} - r_i^n)/\Delta t. \tag{1}$$

In the examples of Refs. [1–3, 6], U_g is set to zero. To make the grid behave in a

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Lagrangian manner the obvious choice is to set U_g equal to the fluid velocity u, but the straightforward application of such a prescription leads to difficulties.

The basic stability requirement for the FCT routines is that grid points and cell boundaries should not cross; this is ensured by selecting a Δt satisfying, for all i, the Courant–Friedrichs–Lewy (CFL) condition [10]

$$\Delta t < 0.5\lambda(\Delta r_i/|\, u_i\,|), \tag{2}$$

where

$$\Delta r_i = \min\{r_{i+1} - r_i\,,\, r_i - r_{i-1}\} \tag{3}$$

and λ is a parameter less than unity to which the results of calculations are generally insensitive. A similar restriction to (2) arises from the sound speed [1]. If the grid points are free to move and for some reason one of the Δr_i tends to zero, Eq. (2) will cause the time step to tend to zero and the calculation will fail unless there is some restoring mechanism. This is most likely to occur at a discontinuity in pressure.

We use Fig. 1, which illustrates possible FCT configurations at time steps 0 and n,

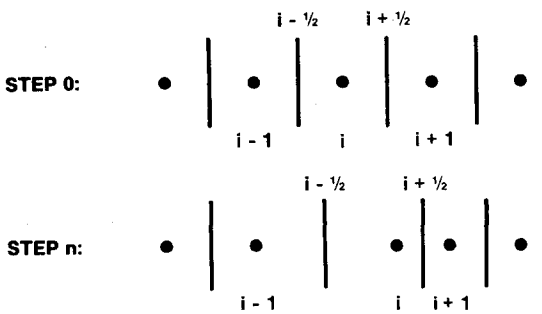

FIG. 1. FCT grid configuration initially and at step n.

to demonstrate why FCT lacks such a mechanism. All quantities of importance are defined at the grid points which are indexed by the integer i; interfaces and subsidiary quantities are defined at half-integer points $i + \frac{1}{2}$. At step n the points i and $i + 1$ have come close together. The pressure gradient at the point i is given by [6]

$$\nabla P_i = (P_{i+\frac{1}{2}} - P_{i-\frac{1}{2}})/(r_{i+\frac{1}{2}} - r_{i-\frac{1}{2}}) \tag{4}$$

$$= (P_{i+1} - P_{i-1})/(r_{i+1} - r_{i-1}) \tag{5}$$

because $P_{i+\frac{1}{2}}$ and $r_{i+\frac{1}{2}}$ are defined as

$$P_{i+\frac{1}{2}} = \tfrac{1}{2}(P_i + P_{i+1}), \tag{6}$$

$$r_{i+\frac{1}{2}} = \tfrac{1}{2}(r_i + r_{i+1}). \tag{7}$$

We use a predictor step to calculate all variables at the half-time $n + \frac{1}{2}$. In the corrector step all quantities in (4)–(7) have the superscript $n + \frac{1}{2}$.

From (5) we see that there is no direct coupling between ∇P_i and quantities defined at the point i; nor is there a direct dependence of any physical quantity on the crucial distance $r_{i+1} - r_i$: the density, for example, is sensitive instead to the distance between two interfaces. Because FCT defines interfaces as being midway between grid points, two grid points may come infinitesimally close without generating a zero volume.

Another point to note is that the mass actually enclosed between two adjacent interfaces does not necessarily remain constant, even if the fluid moves with zero velocity relative to the interfaces. This is a consequence of the nonlinear antidiffusion stage of FCT during which maxima may be "clipped" [2].

Our new technique is designed to ensure that the grid velocities U_{gi} are chosen as far as possible in an exactly Lagrangian sense. To effect this we introduce new interface positions $y_{i+\frac{1}{2}}$ $(0 \leqslant i \leqslant N)$, which from (8) are equal to the $r_{i+\frac{1}{2}}$ only if the grid is uniform. $y_{\frac{1}{2}}$ and $y_{N+\frac{1}{2}}$ always coincide with the physical boundaries, whether free or fixed.

Initially the grid is set as

$$r_i^0 = \tfrac{1}{2}(y_{i-1/2}^0 + y_{i+1/2}^0), \qquad 1 \leqslant i \leqslant N, \tag{8}$$

where the initial interface positions $y_{i+\frac{1}{2}}^0$ may be arbitrarily spaced, and the masses summed up to the $(i + \frac{1}{2})$th interfaces

$$M_{i+1/2}^0 = \sum_{k=1}^{i} \rho_k{}^0 \Delta V_k{}^0 \tag{9}$$

are calculated and stored. (Equivalently, the products $\rho_k{}^0 \Delta V_k{}^0$ may be stored.) $\Delta V_k{}^0$ is the volume bounded by the interfaces $y_{k-\frac{1}{2}}^0$ and $y_{k+\frac{1}{2}}^0$.

On each subsequent time step, after the fluid variables have been integrated to step n, we calculate new volumes $\Delta V_i{}^n$ from

$$M_{i+1/2}^0 = \sum_{k=1}^{i} \rho_k{}^n \Delta V_k{}^n, \tag{10}$$

and hence new interface positions $y_{i+\frac{1}{2}}^n$. On the next step new grid positions

$$r_i^{n+1} = \tfrac{1}{2}(y_{i+1/2}^n + y_{i-1/2}^n), \qquad 1 \leqslant i \leqslant N, \tag{11}$$

are input to the FCT routines. (The summations in (9) and (10) start with $k = 1$, but it is equally possible to scan backwards from $k = N$.)

From the definitions of the $y_{i+\frac{1}{2}}^n$ it is impossible for the grid points $r_i{}^n$ to cross: for example, for shock problems with density discontinuities of order $(\gamma + 1)/(\gamma - 1)$, where γ is the specific-heat ratio, the spacing between two interfaces never falls below a fraction $(\gamma - 1)/(\gamma + 1)$ of its initial value.

It may be noted that the interface positions always lag the density by one time step, because the r_i^{n+1} are calculated before the fluid quantities are advanced from

step n to step $n + 1$. We have tried using a predicted ρ^{n+1} in (10) to counter this, but have obtained almost identical results which do not warrant the additional computational complexity.

3. Application to a Shock Wave Test Problem

To illustrate the need for and the application of our new technique, we consider the same problem as was treated by Colombant and Gardner [9]. It is the self-similar solution of a shock wave propagating in a background of exponentially increasing density [11], described by the standard one-temperature fluid equations.

The configuration is shown schematically in Fig. 2. For a specific heat ratio γ of 2, the position of the shock is given by

$$X_F = x_0 + \tfrac{3}{2}\Delta \log_e(t/t_0) \tag{12}$$

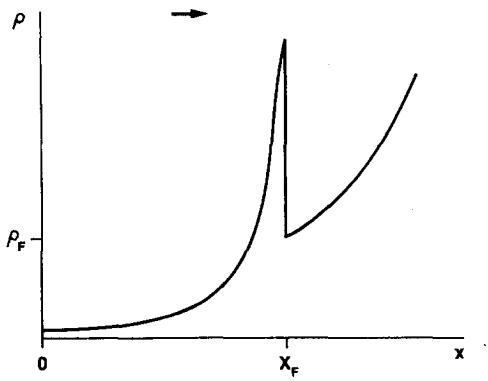

FIG. 2. Schematic representation of the density profile in the exponential atmosphere shock problem.

and the density is given by

$$\rho(x) = \rho_0 \exp\left[\frac{x - x_0}{\Delta}\right], \quad x \geqslant X_F\,; \qquad 3\rho(X_F)(1 + 2\xi)^{-5/2}, \quad x < X_F\,, \tag{13}$$

where

$$\xi = (X_F - x)/\Delta. \tag{14}$$

At time $t = t_0$ the shock is at $x = x_0$ and the fluid is cold for $x > x_0$; ρ_0 is the undisturbed density at $x = x_0$ and Δ is the scale length.

The result of using a uniform grid for this problem is shown in Fig. 3. The grid has 25 points per scale length Δ and 130 points in total. Calculated and analytic curves

are superimposed for four successive times. Referring to the initial profile (a), the extent to which the initial shock deviates from the vertical provides a direct indication of the resolution of this grid. A result very similar to Fig. 3 was obtained by Colombant and Gardner [9]. Generally the agreement between calculated and analytic solutions is good, except at the very sharp peak where there are insufficient grid points for adequate resolution: the analytic solution drops to 82% of the peak value just one

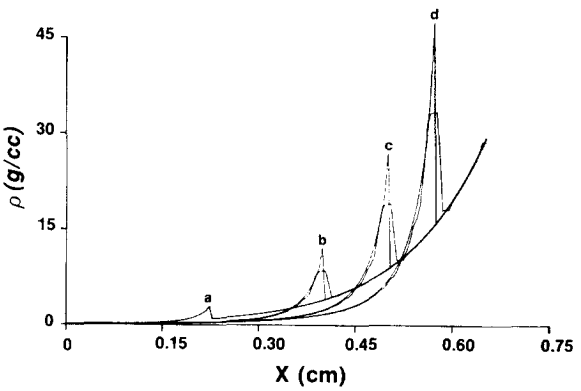

FIG. 3. Analytic and calculated density profiles at four successive times, on a uniform grid.

grid point to the left of the peak and to 69% two points away. This almost singular feature makes this particular problem a severe test for any code.

Using the rezoning technique, up to three times the resolution may be obtained at the peak (because for $\gamma = 2$ the density jump is 3), and the result for the same problem is shown in Fig. 4. The improvement is dramatic.

A similar result could have been achieved without rezoning by taking three times as many grid points. This would have required nine times the computer time, and extra storage as well. In contrast, the run with rezoning took just 55% extra computer

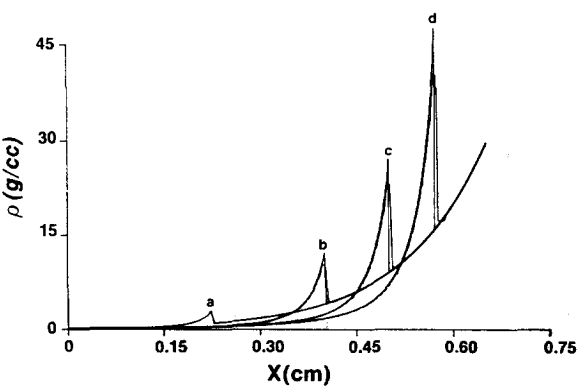

FIG. 4. Analytic and calculated density profiles at four successive times, with rezoning.

time, partly due to the overhead imposed by the zoning routines (13%), but mostly because smaller time steps were required (37%). The time step, chosen from the CFL condition (2) modified to include the sound speed, did not decrease by a factor of 3 because it was not determined at the shock front.

It is probable that even greater resolution could be obtained by an adaptive gridding procedure to overcompress the zones in the shock. We have not attempted this as our technique is easy to implement and performs more than adequately.

It is interesting that the FCT routines, optimized for a uniform grid [6], should perform so well on a nonuniform grid. In order for this to occur it would intuitively appear to be necessary that the grid spacing vary smoothly [6], which is indeed the case to the left of the shock. The point may also be made that, since the grid and fluid velocities are almost equal, the diffusion and antidiffusion terms almost cancel [6].

We have also obtained very similar results [7] for the spherical blast wave similarity solution described by Zel'dovich and Raizer [11]; this confirms that our technique is not dependent on a particular choice of coordinate system.

It is interesting to note that FCT does not need an explicit artificial viscosity to treat shocks, in contrast to several other numerical schemes. The reason for this is that the nonlinear flux-correction stage of the FCT algorithm, in requiring that no new maxima are generated, damps the numerical oscillations in velocity that would otherwise grow, thereby ensuring the necessary conversion of kinetic energy into thermal energy. Use of the total energy equation ensures that energy conservation is not violated. Colombant and Gardner [9] found that FCT schemes not based on the total energy equation performed poorly in comparison, even with the addition of an artificial viscosity.

4. Extension to two Dimensions

Our technique is also applicable to two dimensions, although the grid cannot move in a truly Lagrangian manner: it is impossible to apply the method to every row and column and maintain an orthogonal mesh. Our code SAGE [7] supports Cartesian, cylindrical, and spherical geometries, and uses the basic hydrodynamic routines of Boris [6]. Typical zoning schemes of interest are shown in Fig. 5; the orthogonality requirement imposes upon us a maximum of two grid velocities, one for each direction.

In two dimensions the interfaces $y_{i+\frac{1}{2}}$ are generalized to two sets of interfaces, $R_{i+\frac{1}{2}}$ and $Z_{j+\frac{1}{2}}$ ($1 \leqslant i \leqslant M$, $1 \leqslant j \leqslant N$), one along each orthogonal direction, as illustrated in Fig. 5. The notation is applicable to cylindrical geometry, but the method is general. The masses $M^0_{i+\frac{1}{2}}$ of Eqs. (9) and (10) are replaced by two sets of masses $M^{(r)}_{i+\frac{1}{2}}$ and $M^{(z)}_{j+\frac{1}{2}}$; $M^{(r)}_{i+\frac{1}{2}}$ is the initial mass between interfaces $r = R_{\frac{1}{2}}$ and $r = R_{i+\frac{1}{2}}$, accumulated from a subset of grid lines parallel to the r axis, i.e.,

$$M^{(r)}_{i+1/2} = \sum_{j=j_1}^{j_2} \sum_{k=1}^{i} \rho_{kj} \, \Delta V_{kj} \, . \tag{15}$$

$M^{(z)}_{j+\frac{1}{2}}$ is defined similarly. In general we could choose any weighted combination of these grid lines, but in practice it is probably sufficient to consider just two possibilities:

(a) one grid line only in each direction ($j_1 = j_2$);

(b) a sum over all grid lines in each direction ($j_1 = 1, j_2 = N$)

Note that the zoning will be affected if there is significant perpendicular mass flow into the selected lines, because the mesh will not then move with the average velocity parallel to these lines. In the example presented below this does not arise.

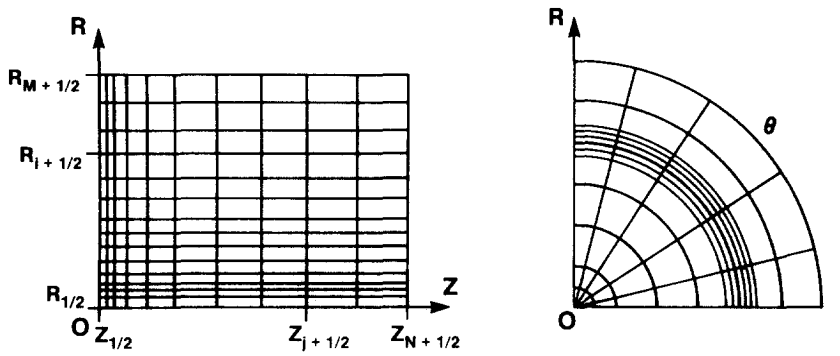

FIG. 5. Interfaces for (a) cylindrical and (b) spherical geometries as used in SAGE.

We consider a problem, for which we are unaware of any analytic solution, where two strong shocks collide with each other in a cylindrical configuration; this is set up by supposing that the density is initially uniform everywhere ($\rho_0 = 0.213$ g/cm^3), while in the cylindrical region $\{0 \leqslant r \leqslant r_0, 0 \leqslant z \leqslant z_0\}$ the temperature ($T_0 =$ 1 eV) is much lower than everywhere else ($T_1 = 973$ eV). This cylinder will be imploded by the high surrounding pressure. The simulation region is taken as $\{0 \leqslant r \leqslant r_1, 0 \leqslant z \leqslant z_1\}$, with $r_1 = z_1 = 1200\,\mu$m and $r_0 = z_0 = 800\,\mu$m, and the zoning is

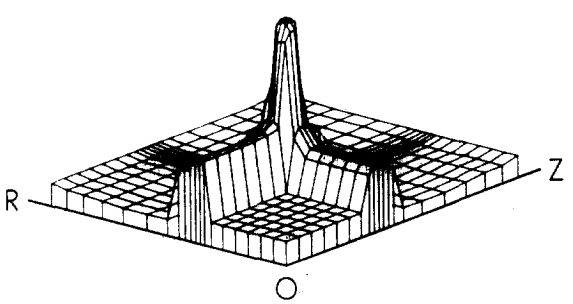

FIG. 6. Density as a function of r and z for the colliding shocks problem on a 20 × 20 grid.

initially uniform. The ion mass is 2.5 times the hydrogen mass and $\gamma = 5/3$. This problem was suggested by Morse and Verdon [12].

Figure 6 shows a plot of ρ as a function of r and z after 1.55 nsec (55 time steps). Along the lines $r = 0$ and $z = 0$ we find one-dimensional shock solutions, with density jumps of 2.7 for the plane shock moving in the $-z$ direction and 3.5 for the converging cylindrical shock moving in the $-r$ direction. Choice (a) above was used, with the axes as the selected lines ($j_1 = j_2 = 1$), and it may be seen from Fig. 6 how the resolution is improved in the regions of interest by the rezoning. Even so, 20 points in each direction is clearly insufficient. Nonetheless, the qualitative result that a small region of high density is formed where the two shocks collide is apparent from the figure. The peak is 7.6 times the initial density.

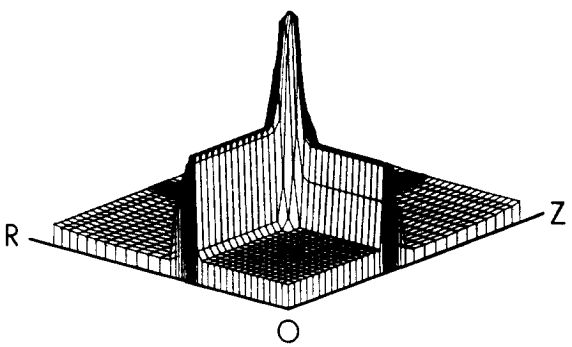

FIG. 7. Density as a function of r and z for the colliding shocks problem on a 40 × 40 grid.

The problem was repeated using a 40 × 40 grid. Figure 7 is the equivalent of Fig. 6, and is drawn with the same vertical scale; the improvement due to the finer zoning is apparent. Here the jump ratios are 4.2 for the plane shock (slightly overshooting the analytic value of 4.0), 4.8 for the cylindrical shock, and 10.3 for the central peak.

The extension of our technique to two dimensions is of limited applicability because we presuppose that we may use an orthogonal coordinate system which in some general sense matches the contours of the physical problem; it is difficult, for example, to conceive of an Eulerian rezoning method that will treat an imploding spherical shell on an orthogonal (r, z) grid.

5. CONCLUSION

We have shown that by a simple modification of the published FCT routines it is possible to significantly improve the treatment of a one-dimensional blast wave test problem with a minimum increase in computational effort. We have also shown that our new technique may be applied in two dimensions to a class of problems where the coordinate system is reasonably suited to the geometry of the physical problem being solved.

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