

3

CIC-14 REPORT COLLECTION
REPRODUCTION
COPY

Radiation Transport
January 1, 1987 - March 31, 1987

LOS ALAMOS NATIONAL LABORATORY

3 9338 00323 2047

Los Alamos

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36.

Prepared by Connie Mazas Singleton, Group P-15

*This work was supported by the US Department of Energy,
Office of International Security Affairs.*

An Affirmative Action/Equal Opportunity Employer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Improvements to SOIL
(An Eulerian Hydrodynamics Code)

Cecil G. Davis



TABLE OF CONTENTS

I.	INTRODUCTION	1
II.	PRESENT SOIL ALGORITHMS	2
III.	ADVECTION SCHEMES	4
IV.	STRONG SHOCK TREATMENTS	10
V.	ADAPTIVE MESHES	13
VI.	MIXED CELL TREATMENTS	14
VII.	VISCOSITY	15
VIII.	SUMMARY AND RECOMMENDATIONS	16
IX.	REFERENCES	17

IMPROVEMENTS TO SOIL (AN EULERIAN HYDRODYNAMICS CODE)

By

Cecil G. Davis

ABSTRACT

Possible improvements to SOIL, an Eulerian hydrodynamics code* that can do coupled radiation diffusion and strength of materials, are presented in this report. Our research is based on the inspection of other Eulerian codes and theoretical reports on hydrodynamics. Several conclusions from the present study suggest that some improvements are in order, such as second-order advection, adaptive meshes, and speedup of the code by vectorization and/or multitasking.

I. INTRODUCTION

SOIL is an Eulerian hydrodynamics code with provisions to do coupled radiation diffusion and strength of materials. In this report we discuss possible improvements to SOIL based on the inspection of a variety of other Eulerian codes and theoretical reports on hydrodynamics. Discussions of improvements in the other areas of computational need, such as the radiation transport and material strength, will be reserved for future reports. Our general conclusions from this study are that improvements such as second-order advection, adaptive meshes and speed up of the code by vectorization and/or multitasking are in order. To add the more sophisticated aspects of turbulent diffusion and Gudonov shock treatments for instance would be unnecessary in our present application of the code.

In Section II we discuss the present algorithms in SOIL and their limitations. In Sections III to VII, we describe new advection schemes, strong shock treatments, adaptive meshes, mixed cell treatments, and viscosity consecutively. Section VIII contains a summary and our recommendations for improvements in the hydrodynamic portion of SOIL.

*SOIL, "Splitting in Eulerian Coordinates" property of C3 (Computer Code Consultants) Los Alamos, NM

II. PRESENT SOIL ALGORITHMS

SOIL (Johnson 1971a)¹ uses a splitting technique in order to solve the two-dimensional set of Eulerian hydrodynamic equations. The solution is also obtained in two phases, a Lagrangian phase followed by a REMAP to the Eulerian mesh. The Lagrangian phase is fairly standard as in the early one-dimensional codes FFF². In the advection phase an extrapolation on velocity is used which makes the code approach second-order accuracy. Shocks can be treated using a combination of quadratic and linear pseudo-viscosity terms; the added viscosity can be used in the expansion phase as well as in compression. The zoning is strictly rectangular but with variable size zones in the r and z directions. The code can also be used in x, y geometry. The differential equations approximated by finite differences forms and solved in (PH1) the Lagrangian phase and (PH2) the Eulerian Phase (from Ref. 3), are

$$\left. \begin{aligned} \rho \frac{\partial u}{\partial t} &= -\nabla P \quad , \\ \frac{\partial}{\partial t} (a\phi + E) &= -P\nabla \cdot \bar{u} \quad . \end{aligned} \right\} \text{PH1} \quad (1)$$

The equations solved in the Eulerian Phase (PH2) are

$$\left. \begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \bar{u}) &= 0 \quad , \\ \rho \frac{\partial \bar{u}}{\partial t} + \rho (\bar{u} \cdot \nabla) \bar{u} &= 0 \quad . \end{aligned} \right\} \text{PH2} \quad (2)$$

The advection, or phase 2 (PH2) differencing scheme can be derived from the following considerations (see Fig. 1).

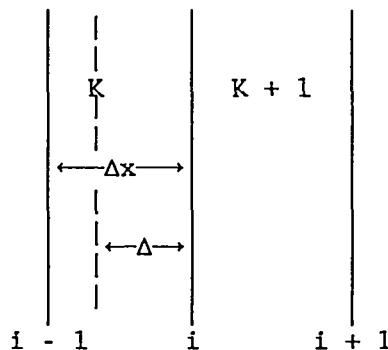


Fig. 1. Advection scheme for SOIL.

All quantities in SOIL are cell centered so,

$$u_i = \frac{U_K + U_{K+1}}{2} ,$$

and a quantity Δ is the transmitted flux defined as

$$\Delta = \tilde{u} \Delta t ,$$

then,

$$\tilde{u} = u_i + (-\Delta) \frac{(u_{k+1} - u_k)}{\Delta x} ,$$

and

$$\tilde{u} = \frac{u_i}{\left[1 + \frac{(u_{k+1} - u_k) \Delta t}{\Delta x} \right]} . \quad (3)$$

This is the algorithm used in SOIL for advecting the velocity. The method is approximately second-order accurate. Other considerations for improvements to SOIL are in the methods used in treating shocks, mixed cells and the question of vectorizing and/or multitasking the code. At present we believe that the Tillotson approach to the EOS is reasonable for geological materials, though the EONESS routine currently in CHARTD may eventually be preferable.

The pseudo-viscosity treatment used in SOIL, to treat shocks, is standard. The Q_s are formed in subroutine, PTWO in the following manner,

$$q = q_L \rho c |Au| + q_Q \rho (\Delta u)^2 , \quad (4)$$

where the sound speed c can either be constant or stored in an array as determined in the equation-of-state routine. The sound speed is determined from

$$c = (\gamma P / \rho)^{1/2} \quad \text{or} \quad (\partial P / \partial \rho)^{1/2} .$$

The use of pseudo-viscosity in SOIL differs somewhat from conventional wisdom. Generally the q is set to zero on expansion but in SOIL it can be used both in expansion and compression. The value for the linear contribution of ($q_L = 0.1$) produces fairly smooth profiles behind the shock front.

The mixed cell treatment of SOIL is also quite basic and relates to the Simple Line Interface Calculation (SLIC) method described by B. Noh (1975).⁴ First a NUMF (see Johnson 1971b) array is carried that identifies the materials in the cell. A mixed cell has a negative number for NUMF. The volume fractions (f) are calculated from pressure iterations in the mixed cell. Consider two materials in the cell with masses M_1 and M_2 . Using a simple iteration technique (secant) the volume fractions (f) and internal energies (I) are changed until, through the EOS of each material, pressure equilibration is attained.

In the transport of material from cell K to cell KA , the cell above, to or from a pure cell a simple decision of flow direction and adjacent like material is used. If both cells are mixed, the decisions are more complex as seen in Fig. 1, where cells K and KA are mixed and the flow is in the direction of KA . To remove preferential treatment of the mass transport, a look ahead feature is used based on the mass flows across boundaries of cells $KA+1$. The material that is moved first is the same material as that in the acceptor cell.

At present, SOIL is neither vectorized nor multitasked, but because of the splitting technique used in solving the hydrodynamic equations, the ability to improve SOIL in this regard is fairly straightforward.

III. ADVECTION SCHEMES

Generally, the problem of advection does not come up in the discussion of Lagrangian codes except in the process of rezoning the mesh when obtuse triangles or bow ties occur. We will not discuss this aspect of advection in terms of the Lagrangian section of SOIL. In an Eulerian mesh, material can be advected from cell to cell by a simple first-order upwind scheme. In the Lax-Wendroff scheme for instance material from cell i is advected with the velocity from cell $i + 1$ in the combination

$$u^{n+1} = u_i^n - (\Delta t / \Delta x) \left[F_{i+1/2}^{n+1/2} - F_i^{n+1/2} \right] ,$$

where

$$u_{i+1/2}^{n+1/2} = 1/2 \left(u_{i+1}^n + u_i^n \right) - (\Delta t / 2 \Delta x) \left[F_{i+1}^n - F_i^n \right] .$$

This is a two-step process that is stable but produces a lot of artificial diffusion. Other first-order schemes such as those due to MacCormick (1971)⁵ and Rusanov (1962)⁶ have been applied with various degrees of success. SOIL uses the upwind scheme described in Section II which is marginally second order.

In this discussion of advection schemes, we will assume an ideal gas equation of state, i.e.

$$e = P / (\gamma - 1) ,$$

in order to simplify the equations. The first order schemes we will consider are

1. Lax-Wendroff (two-step),
2. General upwind methods, and
3. FCT.⁷

In the Lax-Wendroff scheme, the first step is a provisional one with U^n based on the $U^{n+1/2}$ from the first step. The step $l+1/2, i-1/2$ is called a leapfrog step. There is some built in numerical viscosity but additional viscosity may be needed to smooth out ripples behind the shock front. Further discussions of Lax-Wendroff schemes can be found in the literature (Richmyer and Morton for instance).⁸

In the last decade, an interesting scheme was developed by Boris and Book at NRL called flux corrected transport (FCT). A quick look at the explicit version will help to understand this method. First, a highly diffusive step is taken:

$$\begin{aligned} \tilde{\rho}(t + \delta t) = & \rho_j(t) + \delta t \dot{\rho}_j(t + \delta t/2) , \\ & + \left[\nu_{j+1/2} \left(\rho_{i+1}(t) - \rho_i(t) \right) - \nu_{j-1/2} \left(\rho_j(t) - \rho_{j-1}(t) \right) \right] , \end{aligned}$$

the adjusted fluxes are

$$\tilde{\phi}_{j+1/2} = \nu_{j+1/2} \left[\tilde{\rho}_{j+1/2}(t + \delta t) - \rho_j(t + \delta t) \right],$$

where $\nu_{j+1/2}$ is the diffusion coefficient. The heart of the FCT method is in the limits on the fluxes that are corrected from overshooting by

$$\phi_{j+1/2} = \text{sgn} \tilde{\delta}_{j+1/2} \text{MAX} \left\{ 0, \text{MIN} \left[\tilde{\delta}_{j+1/2} \text{sgn} \tilde{\Delta}_{j+1/2}, \right. \right. \\ \left. \left. |\phi_{j+1/2}|, \tilde{\delta}_{j+3/2} \text{sgn} \tilde{\Delta}_{j+1/2} \right] \right\},$$

where

$$\tilde{\Delta}_{j+1/2} = \tilde{\rho}_{j+1/2}(t + \delta t) - \tilde{\rho}_j(t + \delta t).$$

In the anti-diffusion step, the mass fluxes are then

$$\dot{\rho}_j(t + \delta t) = \rho_j(t + \delta t) - \phi_{j+1/2} + \phi_{j-1/2}.$$

This same scheme is then used to advect the momentum as well as the energy.

We have also looked into the following 2nd-order schemes, in the advection phase, for possible improvements to SOIL:

- 1) Gudonov⁹,
- 2) Accelerated Compression Method (ACM)¹⁰ or Filtering Remedy and Methodology (FRAM)¹¹ postprocessors, and
- 3) Monotonic, (Van Leer).¹²

The Gudonov scheme has been found to be difficult to implement in two-dimensions and also has had energy conservation problems in its application in some two-dimensional codes. In the application of Gudonov's scheme, a fast Riemann solver is needed. In the last couple of years, new approaches to solving the Riemann equations for real equations-of-state have been developed.

Collela (1982)¹³ has found a way of simplifying the equations and by utilizing a fast iteration method can solve them efficiently using tables or fits to real equations-of-state. Duckowitz (1985)¹⁴, on the other hand, finds that a formulation based on the McQueen form of the EOS, i.e.

$$u = u_s + S \cdot U_p \quad ,$$

admits a solution where no iterations are necessary. More will be said about Gudonov in Section IV. It may be possible to use the Gudonov scheme in only one direction, in the two-dimensional mesh, and obtain energy conservation at the expense of flexibility. Before we would want to adopt this approach for SOIL, more work will be needed.

The ACM method was developed by Harten in 1977. The method adds a flux term to the equations in the form

$$u_t + f(U)_x = 0 \rightarrow U_t + (f(U) + g(U,t))_x = 0 \quad ,$$

where $g(u,t)$ is an artificial compression flux. In the FRAM method, Chapman (1981), a diffusion term is added to the equations to dampen the oscillations produced by higher-order schemes. The change to the advection equation looks like

$$\partial \frac{\partial \phi}{\partial t} + \nabla \cdot \phi u = 0 \rightarrow \frac{\partial \phi}{\partial t} + \nabla \cdot u = \nabla F \quad ,$$

where

$$F = \xi \frac{\partial \phi}{\partial x} \quad .$$

Take, for instance, the usual leapfrog scheme

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \frac{u}{2} \left[\frac{\phi_{j+1}^n - \phi_{j-1}^n}{\Delta x} \right] = \phi \quad ,$$

then add a second-order $\nabla \cdot F$ term such as Crowley's

$$\frac{u^2}{2} \Delta t \left[\frac{\phi_{j+1}^n - \phi_j^n + \phi_{j+1}^n}{\Delta x^2} \right] \quad .$$

The diffusion coefficient would be

$$\xi = \frac{\xi \Delta x}{2} - u \frac{\Delta t}{2} .$$

This addition results in a strong nonlinear damping. One could envision using an unstable scheme for advection and then adding the diffusion term for stability. Gudonov effectively reversed the emphasis; instead of building solutions from smooth small-amplitude results, he builds his solutions by piecing together discontinuous solutions. For shocks, his method is exact but problems do result in the smooth flow region of the solution (more will be said about this in the discussion of hybrid methods). As mentioned, the Riemann solver computes the nonlinear interaction of two constant states of the fluid. The narrow shock structure produced can reside in the larger, more uniform zoning structure of SOIL. We will discuss a second-order version of Gudonov's method in the next section. Barton and Norman's schemes are basically ways of improving on the Gudonov method, but at the added expense of more computer time. Barton selects a variety of slopes so as to locally maintain the "highest order" of approximation, which is consistent with the requirement of monotonicity. Norman, on the other hand, insures local conservation of specific energy and angular momentum, and his method can be applied to any advection scheme.

Finally, in the application of these first- and second-order schemes to advection, the idea of a hybrid scheme occurs. A first-order scheme gives the best reproduction of the shock jump conditions but the results usually oscillate behind the shock. A combination of first-order for the shock and higher-order schemes for the smooth flow is appropriate. Zalzek (1979)¹⁵ used this approach in his improvements of FCT (Boris and Book 1978).

A recent sequence of events in the improvement of advection treatments in Eulerian hydrodynamic of compressible flows follows from Gudonov through Van Leer and Woodward. Van Leer's second-order treatment of the Gudonov method is called Monotonic Upstream-Centered Scheme for Conservation Laws (MUSCL), while Woodward's improvements are called Piecewise Parabolic Method (PPM)¹⁶. We have already discussed the Gudonov method and in this section we will concentrate on the second-order methods of Van Leer and Woodward. These two methods have found wide use in recently developed codes of compressible hydrodynamics. There are actually two new methods applied in MUSCL, one, the usual Lagrangian

step with a REMAP to the Eulerian coordinate system and two, a method due to Collela (1986) that takes a direct Eulerian step. As indicated, MUSCL is a second-order improvement to Gudonov with the addition of gradient information from the local field. As in Gudonov, the Lagrangian step is carried out using a Riemann solver but in MUSCL the slopes used in the advection are not zero. To insure monotonicity, the slopes are limited appropriately in each slab. The limiting technique suppresses unwanted numerical oscillations to some degree. MUSCL and PPM use the time-splitting techniques that are so useful if one wants to use algorithms developed in one-dimensional models. The problem, as with SOIL, is that this approach begs the question of rotational conservation, and only experience supports this approximation. As a further improvement to MUSCL, Woodward developed PPM. The PPM has been carried to fourth order with subsequently improved modeling of turbulent flow as it occurs in convection cells and the formation of jets. At present, we do not believe we need this kind of capability in SOIL for our geologic modeling.

The most promising scheme, which we believe should be easily adapted to SOIL, is the monotonic method of Van Leer and subsequent investigators (Woodwards, Collela, Norman, etc.). By developing slope algorithms for the conservative quantities (ρ , u , e) that are properly limited, one can envision simple second- and higher-order methods of advection. The actual approach is called linear hybridization, where a low-order scheme is used to resolve the shock structure and higher-order scheme to resolve the smoothflows surrounding the shock structures. This hybridization method is the approach used by Zalesak (1979) in his improvements of Flux Corrected Transport (FCT). Fluxes of conserved quantities-mass, momentum and energy, are computed at zone interfaces using both a low-order and high-order difference schemes. Weight functions are then used which may be non-linear functions of the local conditions of flow. Normally, the mass flux for instance is advected during a time cycle as

$$MF_{j+1/2}^{n+1} = \rho_{j+1/2}^{n+1} \left[U_{j+1/2}^{n+1} \Delta t A \right],$$

where A is the area perpendicular to the assumed flow u , across which the flux is transferred. Usually ρ is assumed to be constant in the cell. Instead, we form $\partial\rho$ from a set of slope algorithms. To insure stability and reduce

oscillations, a minimum slope is set to zero, reducing the advection to first order. A simple such scheme would be

$$s_j = \bar{s}_j * (\text{sign} + 1.0)/2.0 \quad ,$$

where

$$\text{sign} = \text{sgn}(s(a)) * \text{sgn}(s(b)) \quad ,$$

$$s(a) = [\rho_j - \rho_{j-1}] * 2.0/\Delta x_j \quad ,$$

$$s(b) = [\rho_{j+1} - \rho_j] * 2.0/\Delta x_j \quad ,$$

and

$$\bar{s}_j = \text{sgn}[s_j(a)] * \min[|s_j(a)|, |s_j(b)|, |s_j(c)|] \quad .$$

Slopes depending on i and j as well as in the cross directions would be checked. If the slopes on one extensive quantity, say ρ , changed value, then all the conserved quantities would be treated as first order. Having slope values at the boundaries of the cells would also make it easier to apply proper boundary conditions to the mesh. The addition of the slope routine to SOIL with the addition of the logic for slope selection in the advection phases would be a recommendation for an improvement to SOIL.

IV. STRONG SHOCK TREATMENTS

The study of shocks forming in the hydrodynamical simulations has been studied since the advent of numerical methods and high-speed computers. We have looked into the use of improved schemes for the treatment of shocks in SOIL. A shock is described as a discontinuity even though there is some energy dissipation which results in a finite, though very small, shock front thickness. The basic jump conditions are well known,

$$\text{Mass:} \quad [u] = \pm [P]/W \quad ,$$

$$\text{Momentum:} \quad [P]/W^2 = - [\tau] \quad , \quad \text{and}$$

$$\text{Energy:} \quad [e] = - \bar{p}[\tau] \quad ,$$

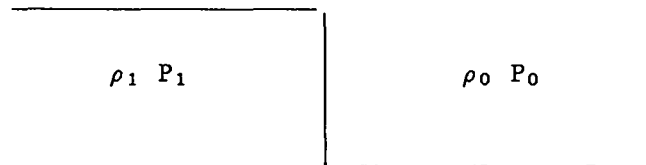
where, $[q] = q^* - q^S$, jump in q across the shock. The exact shock structure cannot be completely determined by the jump conditions alone; an entropy condition must also be applied.

In effect we have two gammas, $\Gamma(\tau, e) = c^2/P\rho$,

and

$$\gamma(\tau, e) = P\tau/e + \underline{1} .$$

For a polytropic gas, gamma is the ratio of specific heats and $\gamma=\Gamma$. W above is the Lagrangian wave speed across the front (a slope in the P - u plane). In the very early treatment of shocks, in finite difference codes, there were two basic approaches used: one, the characteristic method and two, the pseudo-viscosity method. These are well described in the literature (Courant and Fredricks¹⁷, or Richtmyer and Morton). It is difficult to apply the characteristic method in complex flows and the pseudo-viscosity method is approximate at best. For possible applications to SOIL, we want to look into the Gudonov and similar methods. The heart of the Gudonov method is in the use of a simple Riemann solver. To solve the Riemann shock tube problem, for every zone boundary, is expensive. The one-dimensional shock tube problem can be described as a discontinuity in ρ , i.e.,



where we want the velocity (u^*) and pressure (p^*) at the interface. For an ideal gas, the solution is analytic. First we define the variables as; $W_r = n \cdot u_r$, the normal velocity, $\rho_k = E_k = 1/2 u_k \cdot u_k$, the total energy, the density and $P_k = P(\rho_k, \rho_k)$ the pressure at k . From the Rankine-Hugoniot (R-H) conditions,

$$\Delta W_s = \pm \left[- \Delta P_s / \Delta V_s \right]^{1/2} \Delta V_s ,$$

$$\Delta e_s = - 1/2 \left[P_s + P^* \right] \Delta V_s ,$$

where

$$\Delta W_s = W^* - W_s \quad ,$$

and

$$\Delta V_s = V_s^* - V_s \quad .$$

The Hugoniot curves are $\Delta P_s = \pm |W_s| \Delta W_s$. Assume a rightward wave as a shock and a leftward wave a rarefaction; then,

$$P^* - P_L = - |V_L| \Delta W_L \quad ,$$

$$P^* - P_R = |W_R| \Delta W_R \quad ;$$

eliminate P^* and then $|W_R| \Delta W_R + |V_L| \Delta W_L + P_R - P_L = 0$ must be consistent with $P^* \leq P_L$ and $P^* \geq P_R$. As per Duckowitz (1987) we suppose that

$$|W_s| = \rho_s (a_s + A_s |\Delta W_s|) \quad ,$$

the McQueen approximation, and,

$$\Delta P_s = \rho_s (a_s + A_s |\Delta W_s|) \Delta W_s \quad ,$$

then one can solve the values for W^* and P^* at the interface. The terms in the equation above come from

$$U_s = a_s + A_s U_p \quad ,$$

where

$$a_s = \left[\left[\frac{\partial P}{\partial \rho} \right]_s + \frac{P_s}{\rho_s^2} \frac{\partial P}{\partial e} \right]_s^{1/2}$$

and

$$A_s = \text{Lim}/|\Delta W_s|/a_s \rightarrow \infty = \left[\rho^*/\rho_s / (\rho^*/\rho_s - 1) \right] .$$

For SOIL, a_s and A_s are available in the Tillotson formulation of the EOS.

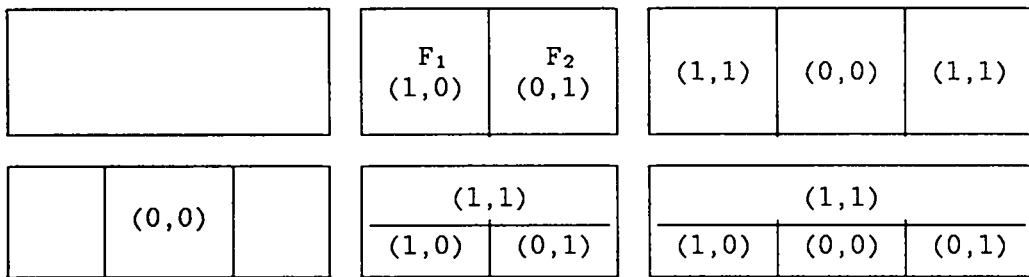
V. ADAPTIVE MESHES

There have been many recent improvements in the resolution of Lagrangian codes using the methods of adaptive meshes, Davis and Davison (1978)¹⁸, Winkler (1976)¹⁹, and Lund (1978)²⁰, to name a few. The methods are designed to resolve regions where important physics is going on such as the ionization shock front or chemical reaction fronts as in the case of Lund's HCT code. In two-dimensional mesh codes, the problem is much more difficult. Moving Finite Element (MFE) methods have been discussed by Miller and Miller (1981)²¹ and particle tracking methods by Glimm (1965)²². For SOIL, we are considering some recent ideas by Rodrique and Hedstrom (1984)²³, Brackbill and Saltzman (1982)²⁴ and Berger and Oliger (1984)²⁵. The methods are usually considered as REMAP or continuous rezones. Another possible second-order scheme is that due to Duckowitz and Kodis (1987)²⁶.

The idea, as mentioned, for adaptive meshes is to put the zonal resolution where the action is; in our case, this is usually at the shock front. Generally, in the use of high resolution meshes it is necessary to solve the equations implicitly to avoid the CFL limit. Consider Winkler's approach in 1D, and his use of compression and expansion algorithms. He indicates that he can resolve jumps the order of 10^{10} or so in an active mesh. This is a great deal more resolution than we will need in our applications of SOIL. If we could say get even 10 times more zones in the moving shock front, we would expect the jump conditions to be more nearly correct and eliminate pseudo-viscosity. Certainly, we would not need a Gudonov method if we had an adaptive mesh scheme. In the ALE (Arbitrary Eulerian-Lagrangian) methods, it is possible to prescribe a motion to the mesh that from previous experience follows the important flows.

VI. MIXED CELL TREATMENT

When using Eulerian codes, we have a problem in treating the materials in mixed cells. In a Lagrangian code, there is no problem since the material remains in the zone boundaries. Utilizing PIC, the particle in cell treatment, the interface is followed by the location of the particles in the cell. In a pure Eulerian code, usually a volume fraction treatment is used, as in SOIL where the NUMF array describes the materials in the cell and the function F the fraction of that material in the cell. To transfer material from cell to cell a description is needed as to what material moves first, the filling of the cell, and possibly the location of the interface in the cell. SOIL utilizes the so called SLIC method which is based on the movement of squares. Observe Fig. 2, a typical Eulerian mesh with an inferred material interface. An improvement to SOIL may be to use boxes on configuration of materials as shown below.



Possible Configurations

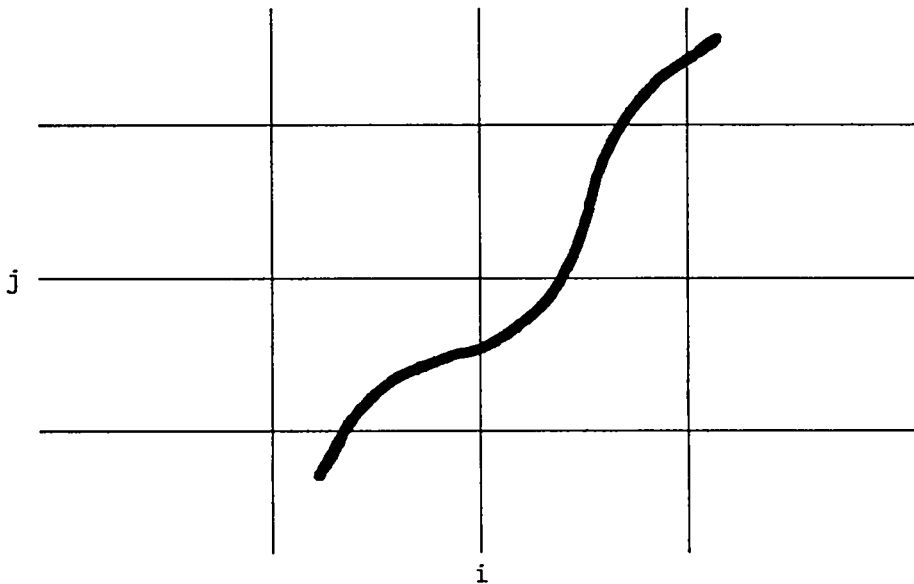


Fig. 2. Eulerian Mesh with inferred material interface.

One straightforward improvement to this scheme is to simply assign priorities to material motion at the start of the problem. This idea will retain some memory of the initial layering but it will be problem-dependent. SOIL does not attempt to recognize the initial layering but does take into account preferential treatment of like materials moving first. If cell 6, for instance, contains only material 1, then material 1 will be moved preferentially from cell 5 to 6 assuming the flow (u) is in that direction. More complicated schemes that tend to track the interfaces through the cell, such as that in HELP for instance, act again as Lagrangian cells and mesh tangling can occur (or particle chain tangling). It is possible to determine slope interfaces in each cell, from the volume fractions and flow directions, but it is nearly impossible to connect up these interfaces from cell to cell. The SLIC method works quite well for four materials and with a process called "gluing" can be extended to say ten materials in a cell. "Gluing" attempts to combine like materials in a combination again of four final masses that are moved across the cell boundaries and then redistributed into the ten materials. Usually, conservation of pressure is attained in the reconstructed cell.

VII. VISCOSITY

Naturally, an Eulerian hydrodynamics code does not need added viscosity in the mesh to handle shocks. The artificial viscosity due to the material diffusion is normally adequate. In SOIL though, viscosity is added in order to improve on the description of the shock front in terms of its location and strength. The form of the pseudo-viscosity is a combination of quadratic and linear terms as shown in Section II.

The linear term helps to remove oscillations formed behind the shock front. To treat the viscosity correctly, it is also necessary to carry the zone-dependent speed of sound. A basic improvement to the viscosity in SOIL would be to use a more nearly TENSOR form. A simple description of the use of viscosity in hydrocodes will now be given.

In the merging of compression waves, a steep front develops that then turns into a shock front at an undetermined location. If the location is known beforehand, a characteristic ray treatment could follow the shock movement exactly. Instead, we generally do not know where the shock will develop and the idea of pseudo-viscosity was developed by Richtmyer and Von

Neumann in 1943. This formulation treats the conversion of kinetic energy to internal dissipation through a quadratic term conserving the jump conditions. Usually, the process smooths the shock over 3-5 zones. The Gudonov method described in Section IV would allow the jump to occur in one or two zones. A linear form of pseudo-viscosity was developed by R. Landshof (1955)²⁷, which corrects for the oscillations that occurred behind the shock when the quadratic form is used. A combination of quadratic and linear is then useful in tailoring conditions developed in following shocks.

Recently a considerable amount of study on the use of pseudo-viscosity in the 1D Lagrangian form of the equations by B. Noh and others has occurred. The result is that one should use a, the tensor equation viscosity, that may be coupled with a form of heat flow term, such as,

$$\phi^r = \rho a^2 \Delta U \left(\frac{\partial u}{\partial r} - \frac{\nabla \cdot U}{3} \right) \frac{3}{2} \Delta r \quad .$$

These results are confirmed in a simple test problem where a shock converges in the center of a sphere with a density ratio of $\rho/\rho_0 = 64$ and energy and pressure jumps, as determined analytically, are obtained (see summary by Noh 1985)²⁸. In the same context, for a two-dimensional code, the TENSOR formulation of Shultz (1956)²⁹ should be implemented correctly, but for Eulerian codes this is more difficult. Splitting is generally used in the Eulerian phase and a one-dimensional description of viscosity is used, as in SOIL. To add the TENSOR character in SOIL implies a cross term that conserves rotation as well as total energy. The question of the correct form for the TENSOR viscosity is fairly mute since it was found to make little difference in the 1D Lagrangian codes tests made in real applications. Even so, the viscosity should be formulated correctly in the codes if at all possible. Generally, viscosity is turned off on expansion with the feeling that it will affect the results unnecessarily.

VIII. SUMMARY AND RECOMMENDATIONS

Eulerian codes are very useful in many areas of hydrodynamic flow simulations. Since the material flows through the mesh there is no problem of mesh entanglement as occurs in Lagrangian codes. Eulerian codes do suffer though from the artificial diffusion of the mass, which makes the tracking of

interfaces and the treatment of shocks more difficult. The low-order treatment of advection in SOIL tends to smear out features of interest. SOIL is a very robust code and has been applied successfully to problems in containment, hypervelocity impact, and ground coupling. We have approached this study in the anticipation of making some possible improvements to the SOIL code, based on recent theoretical and experimental studies and comparisons with other Eulerian codes.

A first recommendation is the use of the second-order schemes of Van Leer and others based on monotonic slope selection, in possibly a hybrid mode. The Gudonov, or strong shock methods, appear to be more difficult to apply to an existing code. Improvements in the viscosity and mixed cell treatment in SOIL are also possible but with much less to gain than in the other areas mentioned above. We have also looked into the question of adaptive meshes in 1D and find their application to the 2D mesh of SOIL to be somewhat imposing. The idea, as in the ALE codes, to prescribe a continuous motion to the mesh, may be more easily attainable. Finally, the vectorization and/or multitasking should be pursued especially if a production version of the code has been reached.

IX. REFERENCES

1. (SOIL) Johnson, W., 1971a, "Radoil and Ram," DASA 2649.
2. (FFF) Cox, A., Brownlee, R., and Eilers, D. 1966, Ap. J. 144, p. 1024.
3. (SOIL) Johnson, W., 1971b, "Code Correlation Study," AFWL-TR-70-144.
4. (SLIC) Noh, B., 1975, "Simple Interface Calculation," Lawrence Livermore Laboratory Rept. UCRL-77651.
5. MacCormick, R., 1971, Lecture Notes in Physics #8., Springer Verlag, New York/Berlin.
6. Rusanov, V. V., 1962, J. Comp. Math. Phys. USSR #2.
7. (FCT) Boris, J. P. and Book, D. L., 1978, J. Comput. Phys. 40, p. 202.
8. Richtmyer, R. and Morton, K., 1962 Difference Methods For Initial Value Problems, New York: Interscience.
9. Gudonov, S. K., 1959, Nat. Sb 47, p. 271.
10. (ACM) Harten A., 1977, Comm. Pure Appl. Math. 30. p. 611.

11. (FRAM) Chapman, M., 1981, J. Comput. Phys. 43, p. 84.
12. Van Leer, B., 1977, J. Comp. Phys. 23, p. 276.
13. Collela, P., 1982, SIAM. J. Sci. Stat. Comp. 3, p. 76.
14. Duckowitz, J. K., 1985, J. Comput. Phys. 61, p. 119.
15. Zalzek, S. T., 1979, J. Comput. Phys. 31, p. 335.
16. (PPM) Woodward and P. Collella, P., 1983, J. Comput. Phys., 54, p. 11.
17. Courant, R. J. and Fredricks, K. O., 1948, Supersonic Flow and Shock Waves, New York: Interscience.
18. Davis, C. and Davison, D., 1978, Ap. J. 221, p. 929.
19. Winkler, K-H, 1976, Tech. Rep. MPI-PAE/Astro 90, Max Planck Inst. Phys. Astrophys, Garching, W. Germany.
20. (HCT) Lund, C., 1978, "HCT", Lawrence Livermore Report UCRL-52504.
21. (MFE) Miller, K. J. and Miller, R., 1981, SIAM J. Numer. Anal. 18, #6, p. 1019.
22. Glim, J., 1965, Comm. Pure Appl. Math. 18, p. 697.
23. Rodrique, G. J. and Hedstrom, G., 1984 "Adaptive Mesh Refinement", to be published in Lecture Notes in Computer Science, Springer Verlag.
24. Brackbill, J. and Saltzman, J., 1982, Numerical Grid Generation, ed. J. F. Thompson, North Holland, NY, p. 865.
25. Berger, A. and Oliger, B., 1984, J. Comput. Phys. #53, p. 484.
26. Duckowitz, J. K. and Kodis, J. W., 1987, SIAM J. Sci. Statist. Comput. Vol 8, #3, p. 305.
27. Landshof, R., 1955, "A Numerical Method for Treating Fluid Flow in the Presence of Shocks," LA1930.
28. Noh, W. E., 1987, J. Comput. Phys. Vol 72, #1, p. 78.
29. Shultz, W., 1964, Methods in Computational Physics, Vol. III, New York/London: Academic Press.

Printed in the United States of America
Available from
National Technical Information Service
US Department of Commerce
5285 Port Royal Road
Springfield, VA 22161

Microfiche (A01)

NTIS		NTIS		NTIS		NTIS	
Page Range	Price Code	Page Range	Price Code	Page Range	Price Code	Page Range	Price Code
001-025	A02	151-175	A08	301-325	A14	451-475	A20
026-050	A03	176-200	A09	326-350	A15	476-500	A21
051-075	A04	201-225	A10	351-375	A16	501-525	A22
076-100	A05	226-250	A11	376-400	A17	526-550	A23
101-125	A06	251-275	A12	401-425	A18	551-575	A24
126-150	A07	276-300	A13	426-450	A19	576-600	A25
						601-up*	A99

*Contact NTIS for a price quote.

Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545