EFFICIENT CONSTRUCTION AND UTILISATION OF APPROXIMATE RIEMANN SOLUTIONS

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Flux-difference-splitting (FDS) methods for the unsteady Euler equations are reviewed, and it is shown that any of the proposed methods can be regarded as a prescription for finding the entries in a "Riemann table", which records the effect on each flow quantity of the wave system generated by the differences between neighbouring pairs of states. For an associated finite-difference scheme to be efficient, it is first of all necessary that the table is constructed economically, and then that the information contained in it should be fully used. We describe a scheme which is efficient in both respects.

INTRODUCTION

There is at present a lot of interest in the development of numerical schemes for hyperbolic systems of partial differential equations; particularly in schemes whose numerical processes attempt to model fairly closely the physical events taking place in the flow. For a long time the equal importance of conservation laws and wave phenomena have been realised, but until quite recently it had not been apparent how to devise efficient numerical methods which give the same degree of emphasis to both. The pioneering work of Godunov [1] remained of largely academic interest, since it led to an algorithm which was only first order accurate, and was distinctly expensive to use. Certain aspects of Godunov's method, however, have very strongly influenced much of the more recent research; this is especially true of the use to which he puts exact solutions of the Riemann problem. To make our meaning clear we must recapitulate the basic Godunov scheme for a set of one-dimensional conservation laws

$$\underline{u}_t + \underline{F(u)}_x = 0 \qquad (1.1)$$

We assume that at time t^n data $\underline{u}^n(x)$ is available, where $\underline{u}$ is a vector-valued function of the continuous real variable x. The first step is to replace this data by a piecewise constant approximation $\underline{v}^n(x)$, such that within a given interval $(x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$ $\underline{v}^n(x)$ assumes the constant state

$$\underline{v}_i^n = \frac{1}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}} \int_{x_{i-\frac{1}{2}}}^{x+\frac{1}{2}} \underline{u}^n(x)dx \qquad (1.2)$$

In the language of finite elements, this stage would be called a projection. In this way we obtain an approximate problem which can be solved exactly, because in a portion of x, t space $(x_{i+\frac{1}{2}} - h, x_{i+\frac{1}{2}} + h)$ and $(t^n, t^n + \Delta t)$ defined by sufficiently small values of h and Δt, we can make use of the known algebraic solution to the Riemann problem [2]. The Riemann problem is, by definition, the interaction between two adjacent, and initially uniform, states. When this exact solution U(x, t) to the approximate problem has been worked out, we take

$$\underline{u}^{n+1}(x) = U(x, t^{n+1})$$

and repeat the process of alternating projections and solutions.

The theoretical foundations of Godunov's method are very sound. The projection step (1.2), and the subsequent set of Riemann solutions, all respect the conservation laws. The Riemann solutions serve to propagate information in the correct directions, and to maintain a proper distinction between compression and expansion waves. This latter feature ensures that Godunov's scheme obeys an appropriate entropy law [3]. Despite these virtues, however, the two halves of Godunov's scheme are, from the viewpoint of computational efficiency, ill-matched. Solving the Riemann problem exactly is an iterative process, which in the case of gasdynamics involves at each iteration the taking of logical decisions and the evaluation of fractional powers. It is a computational extravagence to employ this expensive machinery in the presence of the large truncation errors induced by (1.2).

In recognition of this fact, several authors [4-8] have devised approximate Riemann solvers, which provide, with varying degrees of accuracy, some or all of the information regarding wave speeds and intensities which could have been got from the exact solution. When these approximate solvers are substituted into the Godunov scheme, there is usually very little deterioration in the numerical results (see [5] and [9] for examples). At the same time, in order to remove the incompatibility from the other half of the partnership, there have been devised more elaborate numerical schemes within which the Riemann solvers play a role. Common to most of these, however, is the adoption of some assumed form for $\underline{u}^n(x)$, the continuously defined data whose projection is represented by $\underline{u}_i^n$. Harten, in the first-order version of his high resolution scheme [9, 10], and also in his collaborative work with Hyman on moving grids [11], assumes piecewise constant data within each interval, whereas van Leer [12] assumes piecewise linear data. In each case, the data is assumed to be discontinuous at almost all the interval edges. Woodward and Colella [13] assume piecewise parabolic data, which may be continuous if the average values within the cells vary sufficiently slowly. If the data varies rapidly, however, discontinuities at the edges of intervals are again allowed.

In all these methods [9-13], it is assumed that the purpose of the Riemann solver is to resolve the discontinuous parts of the data. The other parts of the algorithms then have to be carefully matched to the assumed behaviour of the smooth parts of the data. In contrast, we wish to adopt a point of view which is, intentionally, less clear cut in its interpretation. We still regard the numerical data as representing the average state inside a cell (eqn (1.2)), partly because this provides a natural way to deal with irregular grids [14], but we do not attempt to be precise about the distribution of states within the cell. Instead, we argue loosely that if most of cell i is occupied by fluid more-or-less in state $\underline{u}_i$, and most of cell (i+1) by fluid more-or-less in state $\underline{u}_{i+1}$, then whatever is happening within these cells, it will be a set of wave interactions closely resembling the wave interactions which take place in the Riemann problem defined by $(\underline{u}_i, \underline{u}_{i+1})$. To solve the Riemann problem approximately is then a perfectly natural procedure, because the error in the solution does no more than reflect our ignorance about what is really happening. We admit, however, one exception to this line of argument. If the two states are such that they can be connected by a shock transition, then it is in the nature of hyperbolic systems that either they are so connected or that they will be soon. We therefore attach especial importance to Riemann solvers which are able to recognise shock transitions.

We will use the word 'explanation' to denote whatever items of information about wave speeds, amplitudes, etc, will prove most helpful to incorporate into a numerical scheme. The best matching between a numerical scheme and an approximate Riemann solver will occur when the kind of explanation we wish for is generated as economically as possible.

In Section 2 we set out with some supporting arguments, the particular form of explanation that will in our judgement be the most generally useful. We show, for the particular case of the unsteady Euler equations in one space dimension, that it can be completely generated from a knowledge of three scalar quantities. The non-linear algebraic problem of finding these quantities turns out to have a unique solution, which is precisely the 'square-root-averaging' procedure of Ref [5]. The present paper therefore supplements and continues the analysis of [5] in the following ways.

(a) It puts forward in more detail the computational motives which underlay the somewhat abstract presentation given in [5].

(b) Certain properties of the averaging procedure which were not apparent from [5] are easily demonstrated in the course of its present derivation.

(c) We then demonstrate how we can generate, along the lines suggested in [15] and [16], a very simple numerical scheme which advances the solution in time, using almost no information, apart from that contained in the 'explanations'. This scheme can be third-order accurate in the case of linear advection, second-order accurate in smooth regions of non-linear flows, and free from spurious oscillations around discontinuities.

(d) To demonstrate the robustness and practicality of the method, we apply it to a rather severe test problem proposed by Woodward and Colella, [17], involving the collision, in a non-uniform environment, between two blast waves having pressure ratios of 10^4 and 10^5.

(e) We present a simple modification of the method which ensures that it meets an evolutionary form of the entropy condition.

THE CHOICE OF A DESCRIPTION

We consider two adjacent states, which we shall refer to as $\underline{u}_L$, $\underline{u}_R$, and propose these as left-hand and right-hand input states for the Riemann problem. In general we expect the solution to consist of m waves (which may be shocks, contacts or expansions) separating a total of (m+1) piecewise constant states, including the two given input states (Fig 1). Here m is the number of independent conservation laws contained in (1.1). There are many possible ways to describe the solution once it has been obtained. We could give the constant states between the waves, or we could give the jumps across the waves. In either event we could use the primitive variables (usually thought of as ρ, u, p for Eulerian gasdynamics) or the conserved variables (more correctly described perhaps as densities or concentrations of conserved variables, ρ, $m = \rho u$, $e = p/(\gamma-1) + \frac{1}{2}\rho u^2$). We could also use the fluxes of the conserved quantities (ρu, $p+\rho u^2$, $u(e+p)$), or any set of derived quantities, like temperature, entropy, or kinetic energy. For conservation laws such that the characteristic equations can be integrated to produce Riemann invariants, we could use those.

It hardly seems possible to point to any set of variables as being for all purposes inherently superior to any other; indeed, an intelligent human calculator would change variables many times in the course of building up a picture of some complex flow. Lombard and his co-workers make some interesting observations on this topic [8, 18, 19], and in the present formulation of our work we have found these very stimulating. Of course a solution in one form can always be translated into another form, but the effort of translation may not be negligible, and information which is immediately apparent from one form may not be obvious in another. Our own views concerning the best presentation of a solution, although based on long reflection and debate, are still cautious and provisional. We are inclined to suppose that the best policy for the Euler equations

is to work primarily with the conserved variables, since we have found no other way of ensuring that the conservation laws are obeyed. However, as we shall show shortly, it turns out to be both possible and simple to enforce those laws by making use, not of the flux variables, but of the primitive variables. At least for one-dimensional problems, therefore, we propose to carry the primitive variables as auxiliary data. In multi-dimensional problems, we would save storage by computing the primitive variables as they are needed.

The foregoing may help to explain our choice of a format for solutions to the Riemann problem. It comprises a table with m columns, corresponding to the m waves, and (m+2) rows. The first m rows make up a square matrix of which the entry in the j^{th} row and k^{th} column is

$$\Delta u_j^{(k)} = (\text{change in } u_j \text{ across the } k^{th} \text{ wave}) \qquad (2.1)$$

The entries in the $(m+1)^{th}$ row are

$$a^{(k)} = (\text{average velocity of the } k^{th} \text{ wave}) \qquad (2.2)$$

The entries in the $(m+2)^{th}$ row are

$$\delta^{(k)} = (\text{spreading rate of the } k^{th} \text{ wave}) \qquad (2.3)$$

The quantities $\delta^{(k)}$ are needed to ensure a proper distinction between shocks and rarefaction fans. We define $\delta^{(k)}$ as the positive difference between the speeds of the fastest and slowest characteristics of the k^{th} family. This is a positive quantity for expansion waves, but zero for contacts and shocks.

We could fill in this table using any of the Riemann solvers referenced above, and we could exploit other methods also. The wave path analysis of Osher and Solomon [20] can be regarded in this way, as discussed by Roe [21]. We shall, however, attach particular significance to tables having the following conservation property; for j=1,..., m we require

$$(F_j)_R - (F_j)_L = \sum_k a^{(k)} \Delta u_j^{(k)} \qquad (2.4)$$

Note that we could use this formula in many different ways. Harten, Lax, and van Leer [4] begin by estimating the $a^{(k)}$ and then arrive at a set of jumps $\Delta u_j^{(k)}$ consistent with (2.4) by integrating around various control volumes. Colella [6] estimates the $\Delta u_j^{(k)}$ and then, in effect, solves the m simultaneous equations comprising (2.4) to find the $a^{(k)}$. Colella's process could also be used to define average wave speeds, if the $\Delta u^{(k)}$ were taken from the exact Riemann solution or from Osher and Solomon's analysis.

A further possibility is to define the $a^{(k)}$ and the $\Delta u_j^{(k)}$ in such a way that (2.4) is an algebraic identity. This is the approach we take here. For the special case of ideal compressible flow it leads to rather simple algebra, and generates a first-order algorithm equivalent to that given in [5]. That algorithm has the property that if $\underline{u}_i$, $\underline{u}_{i+1}$ are states which can be connected by a single shockwave or contact discontinuity, then no other wave system is activated. Colella's method shares that property, and has the advantage of being applicable to gases with non-ideal equations of state. Osher and Solomon's method does not have the "shock-recognising" property, but other advantages are claimed for it. Regardless of the actual method used to obtain the approximate (or, indeed, exact) solution to the Riemann problem, we will refer to the information specified in (2.1)-(2.3) as a Riemann table. In this way we impose some unity on the various first-order methods. More importantly, however, we

will show that once the information has been assembled as a Riemann table, it can be processed without regard to its origin so as to yield higher-order "monotone" solutions. We observe that the second-order method of Harten [9] could be formulated in much the same way.

CONSTRUCTING THE RIEMANN TABLE

In this section we are concerned with algebraic detail, and restrict attention to the unsteady Euler equations for ideal compressible gasdynamics in one dimension. The Eulerian conservation form is

$$\frac{\partial}{\partial t}\underline{u} + \frac{\partial}{\partial x}\underline{F} = 0 \tag{3.1}$$

where

$$\underline{u} = \begin{vmatrix} \rho \\ \rho u \\ e \end{vmatrix}, \quad \underline{F} = \begin{vmatrix} \rho u \\ p + \rho u^2 \\ u(e+p) \end{vmatrix} \tag{3.2}$$

The presure p and total energy e are related by

$$e = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u^2 \tag{3.3}$$

We also use the notations

$$a = (\gamma p/\rho)^{\frac{1}{2}} \tag{3.4}$$

for the sound speed, and

$$H = (e+p)/\rho \tag{3.5}$$

for the enthalpy.

Now consider the Riemann problem with initial data (ρ_L, u_L, p_L), (ρ_R, u_R, p_R). If both these states are close to some reference state $(\hat{\rho}, \hat{u}, \hat{p})$, the problem can be linearised about these reference conditions, and then tabulated in the form proposed above, with $\hat{a}$ having its natural meaning.

TABLE I

	Wave number (k)		
	1	2	3
$\Delta u_1^{(k)}$	$\alpha^{(1)}$	$\alpha^{(2)}$	$\alpha^{(3)}$
$\Delta u_2^{(k)}$	$\alpha^{(1)}(\hat{u} - \hat{a})$	$\alpha^{(2)}\hat{u}$	$\alpha^{(3)}(\hat{u} + \hat{a})$
$\Delta u_3^{(k)}$	$\alpha^{(1)}(\frac{\hat{a}^2}{\gamma-1} - \hat{u}\hat{a} + \frac{\hat{u}^2}{2})$	$\alpha^{(2)}\frac{\hat{u}^2}{2}$	$\alpha^{(3)}(\frac{\hat{a}^2}{\gamma-1} + \hat{u}\hat{a} + \frac{\hat{u}^2}{2})$
$a^{(k)}$	$\hat{u} - \hat{a}$	$\hat{u}$	$\hat{u} + \hat{a}$

where

$$\left.\begin{aligned} \alpha^{(1)} &= \frac{1}{2\hat{a}^2}\,(\Delta p - \hat{\rho}\hat{a}\Delta u) \\ \alpha^{(2)} &= \frac{1}{\hat{a}^2}\,(\hat{a}^2\Delta\rho - \Delta p) \\ \alpha^{(3)} &= \frac{1}{2\hat{a}^2}\,(\Delta p + \hat{\rho}\hat{a}\Delta u) \end{aligned}\right\} \qquad (3.6)$$

and $$\Delta(\bullet) = (\bullet)_R - (\bullet)_L$$

For the moment we omit mention of the spreading rate, since all characteristic slopes are constant in the linearised problem. It is easily checked that

$$\sum_k \Delta u_j^{(k)} = \Delta u_j \qquad (3.7)$$

and that

$$\sum_k a^{(k)}\Delta u_j^{(k)} = \Delta F_j \qquad (3.8)$$

with error terms which are $O(\Delta^2)$.

If the left and right states are widely different, we propose the following algebraic problem. Find some average state $(\tilde{\rho}, \tilde{u}, \tilde{p})$ such that (3.7), (3.8) are identically satisfied, when this average state is used to construct Table I, including the computation of the coefficients (3.6). At first sight, the proposal is unpromising; six simultaneous non-linear equations are to be satisfied by three scalar quantities $(\tilde{\rho}, \tilde{u}, \tilde{a})$. However, it can quickly be seen that the first equation of (3.7) is satisfied by any average state, and that the second equation of (3.7) is the same as the first of (3.8). It also turns out that the third of (3.7) is implied by the first and second of (3.8), so that (3.8) are the only equations we need to solve.

By substituting the coefficients $\alpha^{(k)}$ from (3.6),and also the contents of Table I,into the first two of (3.8), we find

$$\Delta(\rho u) = \tilde{\rho}\Delta u + \tilde{u}\Delta\rho \qquad (3.9)$$

and

$$\Delta(\rho u^2) = 2\tilde{\rho}\tilde{u}\Delta u + \tilde{u}^2\Delta\rho \qquad (3.10)$$

If we then eliminate $\tilde{\rho}$ from these equations we obtain for $\tilde{u}$ the quadratic equation

$$\tilde{u}^2\,\Delta\rho - 2\tilde{u}\,\Delta(\rho u) + \Delta(\rho u^2) = 0 \qquad (3.11)$$

whose solutions are

$$\tilde{u} = \frac{\Delta(\rho u) \pm \left[\{\Delta(\rho u)\}^2 - \Delta\rho\Delta(\rho u^2)\right]^{\frac{1}{2}}}{\Delta\rho}$$

$$= \frac{\rho_R u_R - \rho_L u_L \pm (\rho_L\rho_R)^{\frac{1}{2}}(u_R - u_L)}{\rho_R - \rho_L}$$

$$= \frac{[\rho_R \pm (\rho_L\rho_R)^{\frac{1}{2}}]u_R - [\rho_L \pm (\rho_L\rho_R)^{\frac{1}{2}}]u_L}{\rho_R - \rho_L}$$

If we take the positive roots, we do not arrive at a useful answer, but the

negative roots lead to

$$\tilde{u} = \frac{\rho_L^{\frac{1}{2}} u_L + \rho_R^{\frac{1}{2}} u_R}{\rho_L^{\frac{1}{2}} + \rho_R^{\frac{1}{2}}} \tag{3.12}$$

This is the 'square root averaging' which was derived from apparently very different considerations in [5]. Substituting this value of u back into (3.9) leads quickly to

$$\tilde{\rho} = (\rho_L \rho_R)^{\frac{1}{2}} \tag{3.13}$$

The third equation of (3.11) is now, in effect, a direct expression for $\tilde{a}$. Again we substitute the trial solution, and this time we find

$$\tilde{\rho}\tilde{a}^2 \Delta u = \gamma[\Delta(up) - \tilde{u}\Delta p] + \frac{\gamma-1}{2}[\Delta(\rho u^3) - \tilde{u}^3 \Delta\rho - 3\tilde{\rho}\tilde{u}^2 \Delta u] \tag{3.14}$$

After this equation has been expanded on the right-hand side, a factor Δu cancels throughout, leaving

$$r_L r_R \tilde{a}^2 = \gamma \frac{r_L p_R + r_R p_L}{r_L + r_R} + \frac{\gamma-1}{2} \frac{r_L^2 r_R^2 (u_R - u_L)^2}{(r_L + r_R)^2} \tag{3.15}$$

where for typographical clarity we have introduced

$$r_L = (\rho_L)^{\frac{1}{2}} \ , \ r_R = (\rho_R)^{\frac{1}{2}} \tag{3.16}$$

The expression (3.15) is not quite as simple as (3.12) and (3.13), but it does demonstrate two nice properties. First, that if we have physically realistic data, the square of $\tilde{a}$ must come out positive, and secondly, that our solution is invariant with respect to all uniformly moving observers because only velocity differences appear in (3.6) or (3.15). Actually, we have not quite finished with (3.15). Define a mean enthalpy

$$\tilde{H} = \frac{\tilde{a}^2}{\gamma-1} + \frac{\tilde{u}^2}{2} \tag{3.17}$$

Substituting (3.15) into this gives

$$\tilde{H} = \frac{r_L H_L + r_R H_R}{r_L + r_R} \tag{3.18}$$

which is, again, the same result as in [5]. In practice, $\tilde{a}$ can be found more quickly from (3.17), (3.18) than from (3.15). Finally, it may be checked that the coefficients (or wave strengths) given by (3.6) are identically equal to those derived from the matrix analysis in [5]; in particular, they share the property that whenever $\underline{u}_L$, $\underline{u}_R$ can be connected by a single shock or contact discontinuity, then every other wave is assigned zero strength.

From a mathematical point of view, it is quite striking to find such simple results emerging; one would like to know whether similar results hold for some special class of conservation laws. We were intrigued to learn that a very closely related result has been found by M. Brio of the University of California at Los Angeles. He sought the average state $\underline{u}^*(u_L, u_R)$, such that

$$\underline{\Delta F} = A(\underline{u^*})\underline{\Delta u} \qquad (3.19)$$

This is a weaker condition than (3.8), but its solution is $u^* = \tilde{u}$, $a^* = \tilde{a}$, ρ^* arbitrary.

From a philosophical point of view, it is interesting to see that the conservation condition (3.8) is met without any direct mention of the flux variables appearing in Table I or in equations (3.6). This also has practical consequences. Let us consider three-dimensional finite-volume methods in which the state of the flow is described by the average values of conserved variables within each cell. To balance the fluxes around the cell boundaries we might construct flux differences from combinations of the seven quantities (p, ρu^2, ρv^2, ρw^2, ρuv, ρvw, ρuw). Our formulae are constructed from differences of the five quantities (ρ, p, u, v, w). Of course, this apparent saving is more than offset by having to construct the five special averages ($\tilde{p}$, $\tilde{u}$, $\tilde{v}$, $\tilde{w}$, $\tilde{a}$). However, using these averages not only restores the conservation properties but also provides a full description of the flux difference splitting.

We will conclude this section by stating, in algorithmic form, a one-dimensional first order, conservative, FDS scheme algebraically identical to that in [5]. Data consisting of ρ, ρu, e is supposed to be given in cells of a uniform length Δx.

(a) Compute $R_{i+\frac{1}{2}} = (\rho_{i+1}/\rho_i)^{\frac{1}{2}}$

(b) Compute, in this order,

$$\tilde{\rho}_{i+\frac{1}{2}} = R_{i+\frac{1}{2}}\,\rho_i$$

$$\tilde{u}_{i+\frac{1}{2}} = (R_{i+\frac{1}{2}}\,u_{i+1} + u_i)/(R_{i+\frac{1}{2}}+1)$$

$$\tilde{H}_{i+\frac{1}{2}} = (R_{i+\frac{1}{2}}\,H_{i+1} + H_i)/(R_{i+\frac{1}{2}}+1)$$

$$\tilde{a}_{i+\frac{1}{2}} = \left[(\gamma-1)(\tilde{H}-\tfrac{1}{2}\tilde{u}^2)\right]^{\frac{1}{2}}$$

(c) Compute

$$p_i = (\gamma-1)\left[e_i - \tfrac{1}{2}\,\rho_i u_i^{\,2}\right]$$

$$u_i = (\rho u)_i/\rho_i$$

(d) Compute

$$\Delta p_{i+\frac{1}{2}} = p_{i+1} - p_i$$

$$\Delta u_{i+\frac{1}{2}} = u_{i+1} - u_i$$

$$\Delta \rho_{i+\frac{1}{2}} = \rho_{i+1} - \rho_i$$

(e) Compute $\alpha^{(1)}$, $\alpha^{(2)}$, $\alpha^{(3}$ from (3.6) and hence fill in Table I.

Note that all these stages, although they aim at providing the information needed to create an upwind scheme, do not yet involve any logic, and are therefore suitable for parallel or vector processing. Note also that the only abnormal expense is the computation of an additional square root at stage (a). For flows involving relatively small density fluctuations this can be evaluated cheaply by means of simple approximations, valid if x is close to unity, such as

$$x^{\frac{1}{2}} \doteq \frac{1}{4.5}\left[6 + x - 5/(1+x)\right] \tag{3.20}$$

The final stage (f) is the only one to involve logic.

(f) Subtract $(\Delta t/\Delta x)a^{(k)}\Delta u_j^{(k)}$ from $(u_j)_{i+1}$ if $a^{(k)} > 0$, or from $(u_j)_i$ if $a^{(k)} < 0$

ADMISSIBILITY CONDITIONS

The algorithm (a)-(f) above is identically equivalent to the first-order algorithm described in [5]. It therefore repeats the defects of that method; in particular the defect of admitting non-physical solutions. Let us recall how these come about. Consider systems of conservation laws such that the mapping $\underline{u} \to \underline{F}$ is many-one; for exmple, in the Euler equations, if $\underline{F}$ is given, a quadratic equation must be solved to find $\underline{u}$ giving two mappings of $\underline{u}$ onto $\underline{F}$. Let $\underline{u}_A$, $\underline{u}_B$ be two states which map to the same flux vector $\underline{F}_{AB}$, and consider two alternative sets of data, D_1, D_2, whose elements are

$$D_1 = \{\underline{u}_A, \underline{u}_A, \cdots, \underline{u}_A, \underline{u}_B, \cdots, \underline{u}_B\} \tag{4.1a}$$

$$D_2 = \{\underline{u}_B, \underline{u}_B, \cdots, \underline{u}_B, \underline{u}_A, \cdots, \underline{u}_A\} \tag{4.1b}$$

In general, one of D_1, D_2 will represent a physically admissible shockwave (in the case of the Euler equations, one such that pressure and density increase in the flow direction) and the other of D_1, D_2 will be inadmissible [2, 3, 4, 9]. However, either set of data will give rise to $\underline{F} \equiv \underline{F}_{AB}$, and the FDS algorithm accepts either set as a stable solution which need not be altered. To construct an algorithm which accepts only the admissible data it is necessary to break the symmetry of the scheme with respect to D_1, D_2. This is the purpose of the final entry in the Riemann table; that is, the spreading rate associated with each wave.

Note that there are several ways of attempting to ensure physical correctness, and that we make use of geometrical ideas rather then ideas based upon the concept of entropy, even though these latter are quite feasible for the Euler equations [3, 4,9]. One of our reasons is that there are important physical systems for which the concept of entropy is not available, but where the geometry of characteristics does reliably discriminate between admissible and inadmissible solutions. One such system involves the flow of a combustible mixture [22]. A second reason, deriving from our theme of numerical efficiency, is that the information needed to implement the geometrical arguments has already been generated (in hidden form) in the previous section.

The geometrical condition is, of course, that an admissible discontinuity must be associated with a wave family whose characteristics are non-divergent. That is, if the shock speed is S, and if it associated with waves of the k^{th} family whose speeds are $a_L^{(k)}$, $a_R^{(k)}$ in the states to the left and right of the shock, then

$$a_L^{(k)} \geq S \geq a_R^{(k)} \tag{4.2}$$

Normally in gasdynamics either both inequalities are strict inequalities (shocks), or else both are in fact equalities (contacts), but in other systems equality on just one side of (4.2) is possible. Clearly, if one of (4.1a, b) satisfies (4.2) the other does not. [See Jeffrey [23] for a proof that if (4.2) is not satisfied in a continuum solution, the discontinuity is unstable].

The task is to introduce a similar instability into the numerical scheme. Suppose we encounter $\underline{u}_A$, $\underline{u}_B$ as consecutive states i, i+1. If we meet them in their admissible order we need take no action, but if the order is reversed the

algorithm must respond. Conservation still requires the total change to be zero, so the only appropriate response is to make equal and opposite changes to the cells i, i+1. We now modify the algorithm described in the previous section so as to achieve this property whilst retaining continuous dependence on the data.

Let $a^{(k)}_{i+\frac{1}{2}}$ be the average wavespeed, and $\delta^{(k)}_{i+\frac{1}{2}}$ the spreading rate (whose estimation we have yet to describe) for the k^{th} wave across the $i+\frac{1}{2}$ interface. We will ensure that $\delta^{(k)}_{i+\frac{1}{2}}$ is zero for compression waves or contacts. For rarefaction waves there will be respectively least and greatest wavespeeds equal to $a - \frac{1}{2}\delta$, $a + \frac{1}{2}\delta$. We test to see if both of these are of the same sign; if so it will still be appropriate to use the unmodified algorithm. Therefore, almost the whole cost of the modification comes from making this simple test for each wave system and each pair of consecutive cells. If the least and greatest speeds are of different sign, we will send to the i^{th} cell a signal

$$\frac{\Delta t}{2\Delta x}(a - \tfrac{1}{2}\delta)\Delta u \qquad (4.3a)$$

and to the $(i+1)^{th}$ cell a signal

$$\frac{\Delta t}{2\Delta x}(a + \tfrac{1}{2}\delta)\Delta u \qquad (4.3b)$$

the indices $i+\frac{1}{2}$ and k being understood. The total signal is, as before, $\nu\Delta u$, where $\nu = a\,\Delta t/\Delta x$ is the Courant number, and this ensures conservation. If the test is only just met, one of the signals is zero.

It remains to give an inexpensive prescription for evaluating δ in the case of the Euler equations. Across simple waves, with k=1 or 3, there is no change of the generalised Riemann invariants [23]

$$J^{(1)} = u + \frac{2}{\gamma-1}\,a \qquad (4.4a)$$

$$J^{(3)} = u - \frac{2}{\gamma-1}\,a \qquad (4.4b)$$

Hence, the change in u-a across a wave of the first family, or u+a across a wave of the third family is, in either case

$$\delta^{(k)} = \frac{\gamma+1}{2}\,\Delta u^{(k)}_{+} \qquad (4.5)$$

where $\Delta u^{(k)}$ is the change in fluid velocity across the k^{th} wave and the notation x_+ denotes the positive part $x_+ = \frac{1}{2}(x + |x|)$. Later we employ the analogous notation $x_- = \frac{1}{2}(x - |x|)$.

The expression (4.5) is exact; it is more in the spirit of approximate Riemann solvers to replace it by an approximation which uses information already available. From the facts that for an ideal gas $a^2 = \gamma p/\rho = \partial p/\partial \rho$ we readily obtain across either the first or third wave

$$\Delta a \approx \frac{\gamma-1}{2\rho a}\,\Delta p \qquad (4.6)$$

From this approximate equation, and the constancy of $J^{(1)}$ across the first wave, we obtain

$$\delta^{(1)} \simeq -\frac{(\gamma+1)\tilde{a}}{2\tilde{\rho}}\,\alpha_-^{(1)} \tag{4.7a}$$

and, by a similar argument

$$\delta^{(3)} = \frac{(\gamma+1)\tilde{a}}{2\tilde{\rho}}\,\alpha_+^{(3)} \tag{4.7b}$$

For the Euler equations, of course

$$\delta^{(2)} = 0 \tag{4.7c}$$

For other systems of equations, alternatives to (4.7) would have to be sought. It might be necessary to take into account any distinctive type of non-linearity associated with a particular system.

HIGHER-ORDER ALGORITHMS

In the previous sections we described, in effect, a first-order FDS algorithm for solving initial-value-problems. The required information was assembled as a set of Riemann tables; in computing terms this set defines an array having dimensions m x (m+2) x (n-1), where m is the number of unknowns (or, equivalently, the number of independent wave systems) and n is the number of cells in the computing domain. We now employ this information to obtain higher-order solutions which give clear resolution of any discontinuities which may appear in the flow. Our procedure is independent of the method used to construct the Riemann tables. Indeed, it is independent of the particular system of conservation laws for which the Riemann problems have been solved.

The technique relies on the still somewhat heuristic concept that by calculating separately the changes in each flow variable due to each wave system we are effectively computing the solution to m^2 independent scalar problems. It is therefore sufficient to describe the scalar case, with the understanding that u can be interpreted as u_j, a as $a^{(k)}$, ν as $\nu^{(k)}$, and Δu as $\Delta u_j^{(k)}$. Frequently the subscript $i+\frac{1}{2}$ is also to be understood. Any other spatial index is always explicitly stated. We introduce $\sigma^{(k)} = \text{sgn}\ \nu^{(k)}$ and note that the first-order algorithm involves sending a <u>signal</u> of strength $\nu_{i+\frac{1}{2}}\,\Delta u_{i+\frac{1}{2}}$ to be <u>subtracted</u> from u at $i+\frac{1}{2}+\frac{1}{2}\sigma$. An algorithm equivalent to the Lax-Wendroff scheme results from sending $\frac{1}{2}\nu(1-\nu)\Delta u$ to i, and $\frac{1}{2}\nu(1+\nu)\Delta u$ to i+1. Let the weaker of these two signals, that is $\frac{1}{2}\nu(1-|\nu|)\Delta u$, be written as Δu^*. Then a reformulation of Lax-Wendroff is that after completing the first-order algorithm we subtract Δu^* from the physically unrealistic target $i+\frac{1}{2}-\frac{1}{2}\sigma$, but maintain conservation by adding Δu^* at $i+\frac{1}{2}+\frac{1}{2}\sigma$. This transfer can be regarded as analogous in its purpose to the antidiffusion stage of Flux-Corrected Transport [24, 25]. In the scheme being described here, the low-order component of an FCT method is represented by the first-order FDS algorithm, and the higher-order component will be either Lax-Wendroff, or a small perturbation of it. As with FCT, the key element which allows us to avoid the 'wiggles' associated with classical high-order methods is to limit the magnitude of the antidiffusive term. The particular recipe which we adopt for this limiting process has been described elsewhere [16, 26] but for completeness we repeat it, with some discussion, below.

Define

$$b_1 = \Delta u^*_{i+\frac{1}{2}} \tag{5.1}$$

$$b_2 = \Delta u^*_{i+\frac{1}{2}-\sigma} \tag{5.2}$$

In the Lax-Wendroff scheme, transferring the effect of b_1 from the physically realistic target $i+\frac{1}{2}+\frac{1}{2}\sigma$ to the unrealistic target $i+\frac{1}{2}-\frac{1}{2}\sigma$ is something which contravenes the proper direction for information flow, but is justifiable on formal mathematical grounds whenever the flow is sufficiently smooth. In fact, for smooth flows this non-physical transfer term could be estimated with sufficient accuracy by examining the interaction between any other nearby pair of adjacent cells. Thus, b_2, the estimate taken from the upwind cell, is equally valid from the viewpoint of accuracy. If we do decide to use b_2, then the scalar version of the algorithm is "wholly upwinded", and the systems version is wholly upwinded with respect to each wave system.

Experience shows that wholly upwinded algorithms are very effective indeed at capturing shockwaves which are strong and either stationary or nearly so, but are much less effective if the shocks are weak or rapidly moving. The practical criterion seems to be whether the shockwave is sufficiently strong to reverse the sign of $a^{(k)}$. When this is not the case, the wholly upwinded schemes cannot claim to be any more physically realistic than Lax-Wendroff. Information, although sent in the right direction, is being propagated too fast, and wiggles build up ahead of the shockwave rather than behind it [26, 27]. A recipe which deals equally well with both strong and weak shockwaves is to transfer neither b_1 nor b_2, but some "average" value of the two. The essential features of the averaging process are that if b_1, b_2 are close to each other in value, then the average $B(b_1, b_2)$ shall be close to both of them, and if b_1, b_2 are very different then the average shall be close to the smaller of the two. The first of these properties ensures that second-order accuracy is retained for smooth flows; the second property reduces the disruptive effect of the anti-diffusion in non-smooth flows. Note that the averaging function B must have the homogeneous property $B(kb_1, kb_2) = kB(b_1, b_2)$; otherwise the result will depend on the units of measurement.

Before specifying the averaging procedure more precisely, we note that many authors have by now published schemes which are akin to the above, and are often identical to it in the simple special case of linear advection. All the methods are supported by heuristic arguments. At first, these arguments seem different, but closer examination reveals strong similarities between the arguments used to support the methods, as well as between the methods themselves. Historical precedence goes to van Leer, whose work is mostly based on the idea of preprocessing data which is assumed to be piecewise linear within cells. No cell is allowed, however, to have a variation much stronger than that found in its neighbours. Instead, discontinuities are allowed to develop at cell interfaces, and this strengthens the first-order terms in the algorithm at the expense of certain second-order terms. The culmination of this approach is the somewhat complex MUSCL code described in [12], which has since been considerably simplified, see for example [28]. Harten [9] supports his scheme by arguments which associate certain second-order terms with a spurious wavespeed, which must be limited to avoid the spread of wiggles. Since the effect of a wave is proportional to the product of its speed and amplitude, it probably makes no real difference which of the two we choose to limit. Harten has shown [10] that his scheme is identical to MUSCL in the case of linear advection, and in fact both schemes are then also identical to the present scheme.

An averaging function which appears widely in these references is the function, christened by Sweby the "minmod" function, which is zero if b_1, b_2 have opposite sign, and otherwise equals whichever of b_1, b_2 is closer to zero. If this function is inserted into each scheme at the appropriate place, then the results are very similar indeed [29]. Something which has much more effect on the quality of the results is to change the averaging function, and van Leer [30] has recommended the harmonic mean, defined by

$$B(b_1, b_2) = \frac{2b_1 b_2}{b_1 + b_2} \qquad \text{if } b_1\, b_2 > 0$$
$$= 0 \qquad \text{if } b_1\, b_2 \leq 0 \qquad (5.3)$$

as well as other choices [31], all designed to produce a value biased toward the smaller input. Numerical experiments reveal that all such choices work well with moving shocks as well as with stationary shocks, but still find difficulty if the shocks are very weak, in the sense of producing only small changes in $a^{(k)}$. This will not be serious if the shocks are also weak in the sense of having small amplitude. The case which causes practical difficulty is the so-called linearly degenerate case [23, 26] which manifests itself in the Euler equations as the contact discontinuity, across which pressure is continuous, but density is not. The relevant "wavespeed" is the fluid velocity (or, in multidimensional flows, its normal component) and this is also a continuous quantity. Experiments on this case reveal [32] a slow spreading of discontinuous data, such that the transition regions will exceed any stated width within finite time.

Woodward and Colella have described [13] an elaborate MUSCL-type code, containing a mechanism which appears to treat contact discontinuities rather well, by actually augmenting the "anti-diffusive" terms under some circumstances. We can incorporate this effect very cleanly into the present scheme, by adopting an averaging function such that if b_1, b_2 are not very different, then the average is biassed toward the larger of the two. The following rule has been found remarkably effective.

If b_1, b_2 are of different sign choose
$B(b_1, b_2) = 0.$

If b_1, b_2 are of the same sign, and differ by a factor greater than 2.0, choose
$B(b_1, b_2) = 2\ \text{minmod}\ (b_1, b_2)$

If b_1, b_2 are of the same sign, and differ by a factor less than 2.0, choose
$B(b_1, b_2) = \text{maxmod}\ (b_1, b_2)$ (5.4)

where maxmod is the function which selects the argument furthest from zero. The rule (5.4) defines a continuous function of two variables, which has been christened "Superbee". It has the remarkable property, established by extensive numerical experiments [32] that when it is used as the averaging function in the present scheme, and the scheme is specialised to linear advection, then discontinuities in the initial data no longer diffuse without limit. By this we mean that a given fraction of the amplitude is contained within a zone of finite width for all time. Further information regarding this, and other, averaging functions is available in [32, 33, 34]. A note of caution is required by Sweby's observation [34] that the Superbee function can give rise to instability in non-linear problems, unless the CFL number is kept below $\frac{1}{2}$. He recommends that the use of Superbee should be reserved for the degenerate fields (ie contact discontinuities) and a more conventional average, such as (5.3), employed for the remaining waves.

We shall now set out the above scheme in a more explicitly algorithmic form; supposing that steps (a) - (f) as described in Section 3 have already been carried out.

(g) To ensure admissible solutions, test each pair of cells for sonic expansion waves. Flag any interface found with an integer indicating the wave number k involved. For each flagged interface where $a^{(k)}_{i+\frac{1}{2}} > 0$, transfer a signal

$$\frac{\Delta t}{2\Delta x}\left(a^{(k)}_{i+\frac{1}{2}} - \tfrac{1}{2}\,\delta^{(\kappa)}_{i+\frac{1}{2}}\right)\,\underline{\Delta u}^{(k)}_{i+\frac{1}{2}} \tag{5.5a}$$

from i+1 to i. For each flagged interface where $a^{(k)}_{i+\frac{1}{2}} < 0$, transfer a signal

$$\frac{\Delta t}{2\Delta x}\left(a^{(k)}_{i+\frac{1}{2}} + \tfrac{1}{2}\,\delta^{(k)}_{i+\frac{1}{2}}\right)\,\underline{\Delta u}^{(k)}_{i+\frac{1}{2}} \tag{5.5b}$$

from i to i+1.

(h) To compute a second-order correction, begin by finding the non-physical signals needed to implement the present version of Lax-Wendroff, ie

$$\underline{\Delta u}^{*(k)}_{i+\frac{1}{2}} = \tfrac{1}{2}\,\nu^{(k)}_{i+\frac{1}{2}}\left(1 - |\,\nu^{(k)}_{i+\frac{1}{2}}\,|\,\right)\underline{\Delta u}^{(k)}_{i+\frac{1}{2}} \tag{5.6}$$

For any flagged interface, it seems satisfactory to set $\underline{\Delta u}^{*(k)}_{i+\frac{1}{2}} = 0$.

(i) Let $b_1 = b^{(k)}_{i+\frac{1}{2}}$ be a scalar which acts as a norm for the vector $\underline{\Delta u}^{*(k)}_{i+\frac{1}{2}}$. In practice, we use merely the first component, ie the change in density.

Let $b_2 = b^{(k)}_{i+\frac{1}{2}-\sigma}$, where $\sigma = \operatorname{sgn} a^{(k)}_{i+\frac{1}{2}}$, be the norm associated with the same wave family in the upwind cell. Let us define a limiting factor

$$\beta = B(b_1,\, b_2)/b_1 \tag{5.7}$$

where B is one of the averaging functions discussed above. Because B must be homogeneous, this may be written

$$\beta = B(1,\, b_2/b_1) \tag{5.8}$$

(j) Transfer $\beta\Delta u^{*(k)}_{i+\frac{1}{2}}$ from $i+\frac{1}{2}+\frac{1}{2}\sigma$ to $i+\frac{1}{2}-\frac{1}{2}\sigma$.

Steps (g) to (j) complete a second-order, "monotone", FDS algorithm for one-dimensional initial-value problems. These steps are difficult to vectorise, and their efficient implementation depends on the machine being used. On a CRAY 1, it has proved possible to update about 60,000 data points in each second of CPU time.

Boundary procedures for one-dimensional flow are usually very simple. Closed ends are dealt with by using image cells. Open ends merely require a statement that there are no incoming waves. Again, image cells can be used, with a Riemann table describing the interaction between the image cells and the last real cell. The only time this table is ever consulted is for information about the strength

of waves which may be entering the domain. Therefore, this table is filled with zeroes for all the waves, including the unused outgoing waves. Boundary procedures which model more complex events usually need to be supplied from ad hoc arguments.

NUMERICAL RESULTS

To illustrate the robust nature of our scheme, we have applied it to a test problem proposed by Colella and Woodward [17]. Since this problem involves very strong wave interactions, we feel that it gives convincing support to our strategy of splitting the flux differences into "scalar" components. We also take satisfaction that the code used to produce these results contains no "adjustable constants" or "problem-specific" features. The most empirical aspect of the code is the choice of an averaging function, and even this is closely based on the scalar analysis [32, 33, 34]. In fact, we also choose this test problem because it allows us to display the improvements brought about by a more sophisticated averaging function.

The problem involves flow in a parallel pipe extending over $0 \leq x \leq 1$ and closed at each end. At t=0, the tube contains an ideal gas ($\gamma = 1.4$), of unit density everywhere, and at rest. However, two diaphragms at $x = 0.1$ and $x = 0.9$ separate the gas into three regions with different pressures. In the central region $p = 10^{-2}$, and at the left and right $p = 10^{3}$ and $p = 10^{2}$ respectively. The diaphragms burst simultaneously and strong shockwaves rush into the central region, followed by contact discontinuities, whilst expansion fans move out to each end and are then reflected. When the shockwaves meet, a brief spike of very high pressure and density is created, and a third contact discontinuity is created. A more detailed description is to be found in [17].

Our graphs (see Fig 3) show density distributions at t = 0.010, 0.016, 0.026, 0.028, 0.030, 0.032, 0.034 and 0.038. The left-hand member of each pair shows results computed using the "minmod" averaging function, and the right-hand member shows results from the Superbee function. The computing grid comprises 1200 equal intervals. In every plot we can identify two shockwaves, each usually marked by two points occupying the transition region. The other regions of strong variation are the contact discontinuities, which are not so cleanly represented. In fact, they extend, in the left-hand plots, over 25 to 30 mesh intervals, but in the right-hand plots the extent is typically 6 or 7 intervals. This fourfold increase in resolution implies an order of magnitude reduction in the computing times required to achieve results of similar quality at the same elapsed times.

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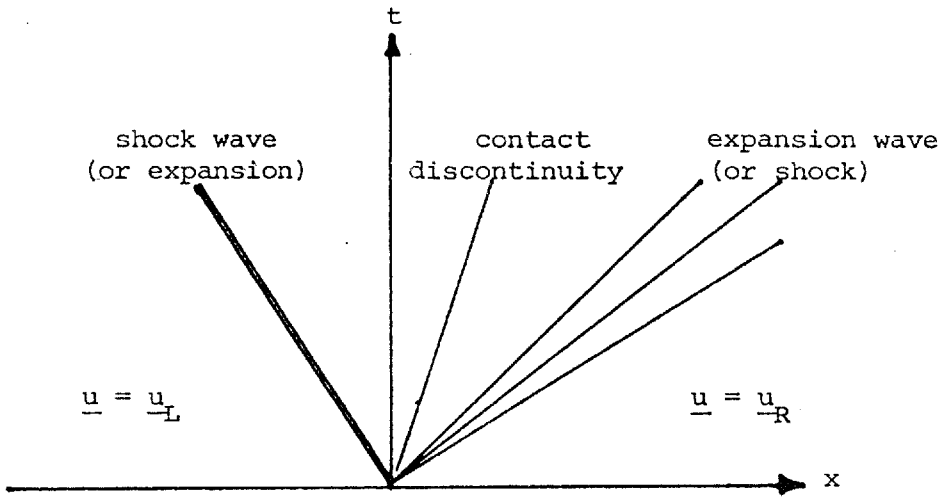

Fig 1 - General solution to the Riemann problem for the Euler equations.

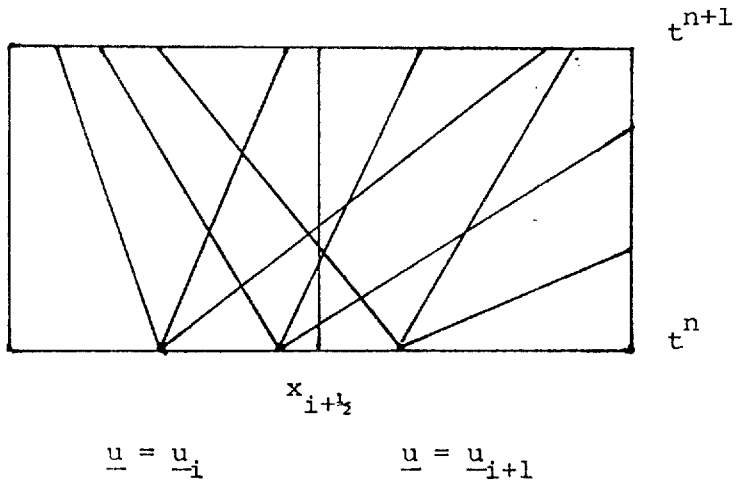

Fig 2 - Interaction of fluid in adjacent cells.

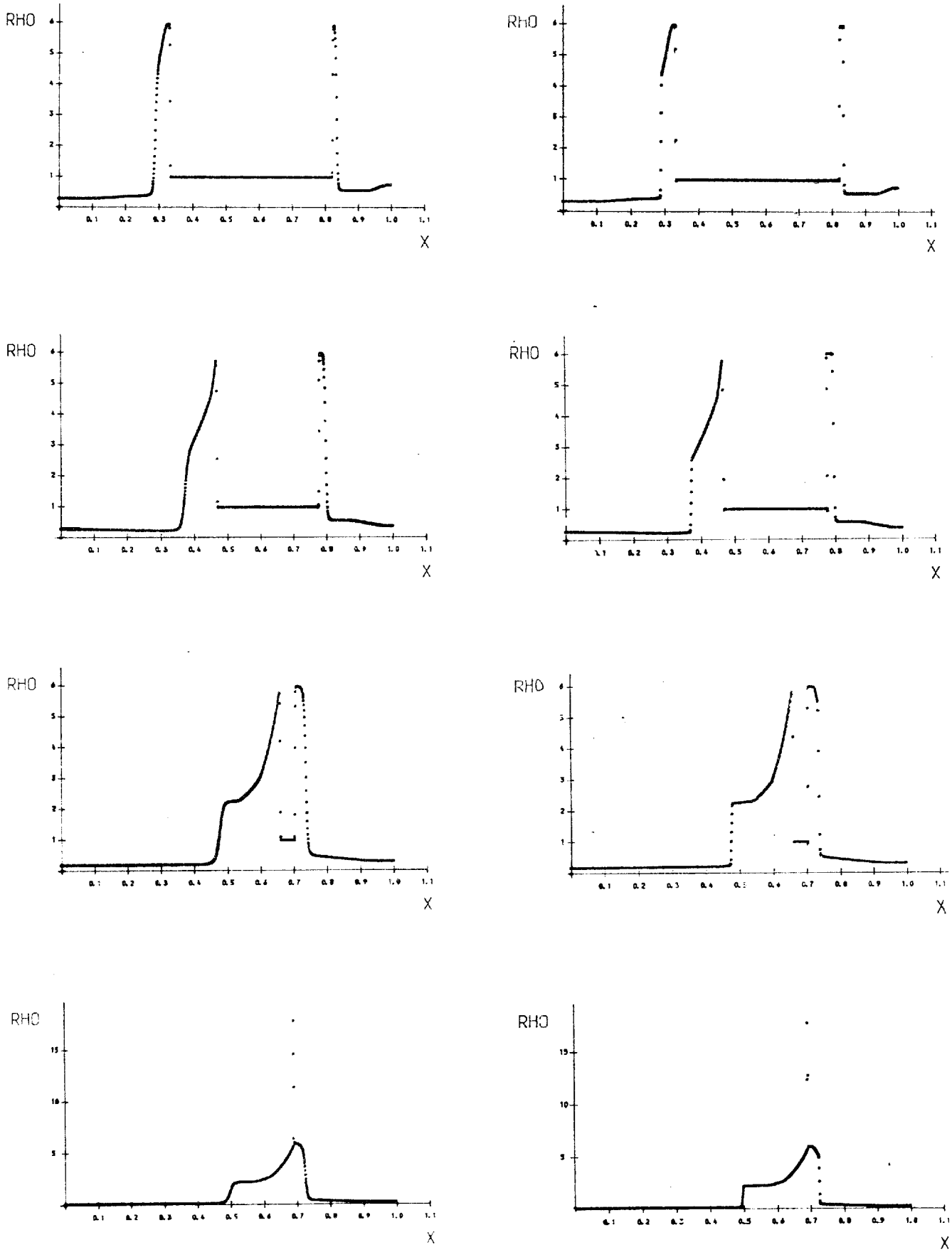

Fig 3 - Distributions of density for the interacting blast wave problem at times t = 0.010 (at top), 0.016, 0.026, and 0.028 (at bottom). Results on left employ minmod, on right Superbee. Note the changes of vertical scale.

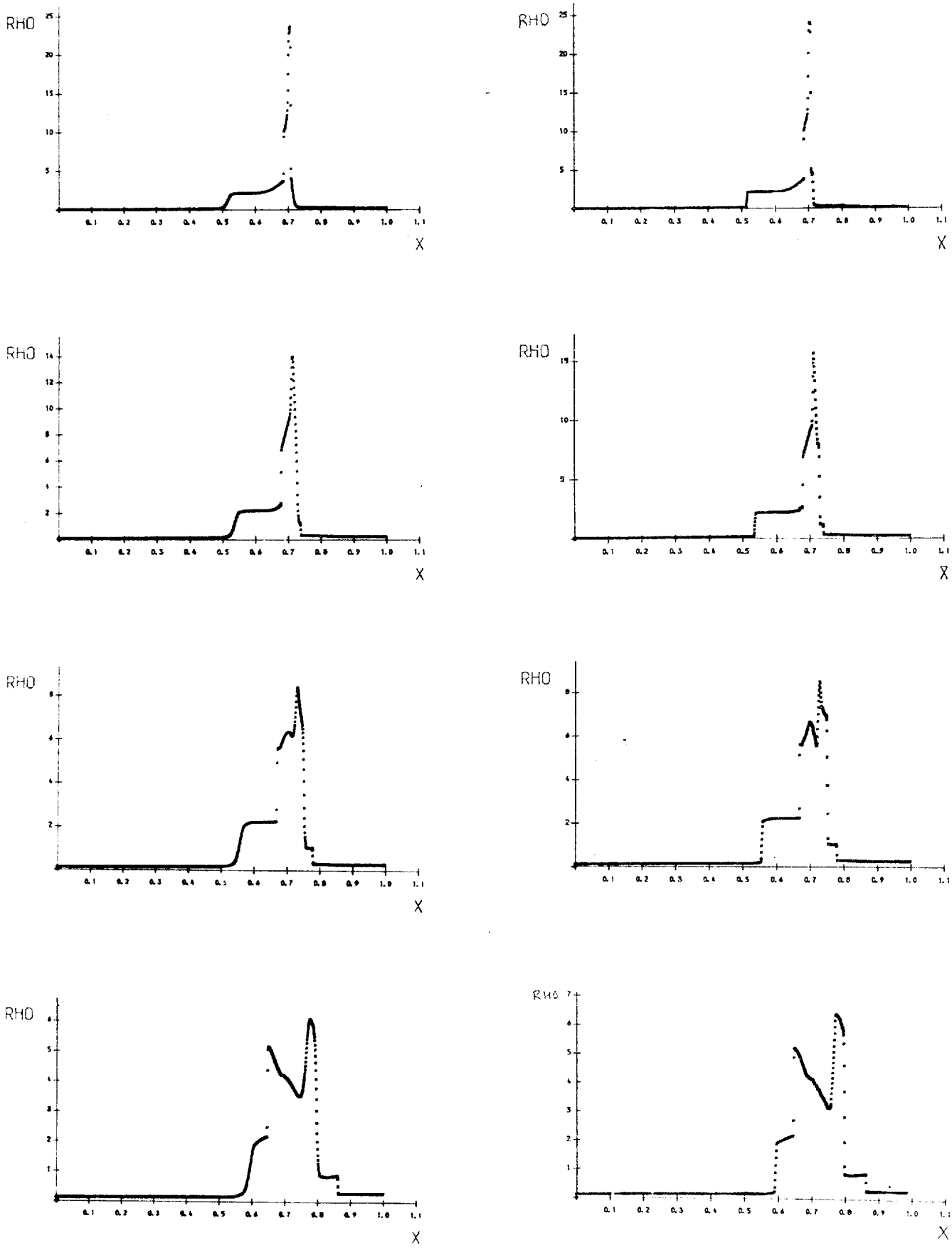

Fig 3 (Contd) - Results at times t = 0.030 (at top), 0.032, 0.034, and 0.038 (at bottom).