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Differencing of the Diffusion Equation in Lagrangian Hydrodynamic Codes*

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The general problem of finite differencing the diffusion equation on a two-dimensional Lagrangian hydrodynamic mesh is discussed and a set of general criteria is developed. A detailed description is given of a particular difference scheme satisfying these criteria. A numerical test case is presented.

To model radiation transport and electron and ion thermal conduction, we want to difference an equation of the form

$$\frac{\partial f}{\partial t} = \nabla \cdot (D \nabla f) \tag{1}$$

on a Lagrangian hydrodynamic mesh. D (the diffusion coefficient) is a given *positive* function of space and time. f is the energy density and is also positive. Because our smallest practical time step is often much longer than the characteristic relaxation time ($\tau = l^2/D$ where l is the distance between mesh points), we must difference (1) fully implicitly.

In general one can use the partially implicit scheme

$$\frac{f^{n+1} - f^n}{\Delta t} = \nabla(D\nabla(\alpha f^{n+1} + (1-\alpha) f^n)),$$

where $0 \leqslant \alpha \leqslant 1$. If λ is the largest (positive) eigenvalue of the linear operator, $-\nabla D \nabla$, then $\tau \approx 1/\lambda$ and if f^n is the corresponding eigenvector, then

$$\frac{f^{n+1} - f^n}{\Delta t} = -\lambda(\alpha f^{n+1} + (1-\alpha) f^n) + Y_B,$$

where Y_B contains the boundary conditions. Thus

$$f^n = \rho^n f^0 + (1 - \rho^n)\, Y_B/\lambda,$$

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where

$$\rho = \frac{1 - (\Delta t)(1-\alpha)\lambda}{1 + (\Delta t)\,\alpha\lambda}.$$

This is to be compared with the exact solution

$$f(n\,\Delta t) = \sigma^n f^0 + (1 - \sigma^n)\, Y_B/\lambda,$$

where $\sigma = e^{-\lambda(\Delta t)}$.

If $\frac{1}{2} \leqslant \alpha \leqslant 1$, then $|\rho| < 1$ for all $\Delta t > 0$ and so stability is assured. However, the best choice of α is that which makes $\rho = \sigma$,

$$\alpha = \frac{1 - \lambda(\Delta t) - e^{-\lambda(\Delta t)}}{\lambda(\Delta t)(e^{-\lambda(\Delta t)} - 1)}.$$

For $(\Delta t)\lambda \to 0$, $\alpha \to \frac{1}{2}$, and for $(\Delta t)\lambda \to \infty$, $\alpha \to 1$. So for $(\Delta t) \gg \tau$ we choose $\alpha = 1$. Note that unless we choose $\alpha > 1 - [(\Delta t)\lambda]^{-1}$, we will have $\rho < 0$ and the numerical solution will oscillate instead of the f^0 component decreasing monotonically as the exact solution does. Furthermore if $(\Delta t)\lambda \gg 1$ and α is close to $\frac{1}{2}$ instead of being close to 1, then the f^0 component will decrease very slowly (as $[(1-\alpha)/\alpha]^n$ instead of dying out almost completely in one time step as it should.

Therefore we have,

$$\frac{f^{(n+1)} - f^n}{(\Delta t)} = \nabla \cdot (D\,\nabla f^{(n+1)}), \tag{2}$$

where f^n is f after the nth time step. Fully implicit differencing has the virtue that when $(\Delta t) \gg \tau$ the left side of (2) becomes negligible and we get

$$\nabla \cdot (D\,\nabla f^{(n+1)}) = 0,$$

i.e., we get the correct steady-state solution.

The next step is to difference the diffusion operator

$$\nabla \cdot (D\,\nabla f).$$

We assume cylindrical symmetry so the basic coordinates are R and Z and the mesh consists of a set of points

$$(R_{K,L}, Z_{K,L}),$$

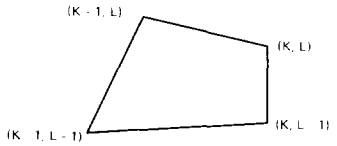
where

$$K = 1, 2, \ldots, K\,MAX$$

and

$$L = 1, 2, \ldots, L\,MAX$$

Each quadrilateral zone is labeled by the largest (K, L) pair of its four corners. Thus, a typical zone whose indices are (K, L) looks like



In most of our applications f and D are zone centered quantities.

The zone centers are given by

$$(\tilde{R}_{K,L}, \tilde{Z}_{K,L}),$$

where $\tilde{R}$ and $\tilde{Z}$ are chosen so that if the energy density f varies linearly through the zone, then $f(\tilde{R}, \tilde{Z})\, V_{K,L}$ is the energy in the zone. Thus

$$\int_{V_{K,L}} [f_0 + f_Z(Z - \tilde{Z}_{K,L}) + f_R(R - \tilde{R}_{K,L})] R\, dR\, dZ = f_0 V_{K,L},$$

where $V_{K,L} = \int_{V_{K,L}} R\, dR\, dZ$. So we have

$$\int_{V_{K,L}} (Z - \tilde{Z}_{K,L}) R\, dR\, dZ = 0,$$

and

$$\int_{V_{K,L}} (R - \tilde{R}_{K,L}) R\, dR\, dZ = 0.$$

Our zone centered energy density is given by

$$f_{K,L} = f(R, Z)\,|_{(\tilde{R}_{K,L}, \tilde{Z}_{K,L})}.$$

We want a finite-difference operator (a matrix A) which will approximate the diffusion operator, i.e.,

$$Af \approx \nabla \cdot (D\nabla) f.$$

Then Eq. (2) becomes

$$\frac{f_{K,L}^{(n+1)} - f_{K,L}^{n}}{(\Delta t)} = \sum_{K'L'} A_{(K,L),(K',L')} f_{K',L'}^{(n+1)}$$

or

$$(I-(\Delta t)A)f^{(n+1)}=f^n. \tag{3}$$

What properties do we wish the matrix operator A to have?

(1) Let $(R_{K,L}, Z_{K,L})$ be a given mesh and $f(R,Z)$ some energy density distribution. Then let $f_{K,L}=f(\tilde{R}_{K,L}, \tilde{Z}_{K,L})$ and expand $f_{K',L'}$ in a Taylor series about a given point $\tilde{R}_{K,L}, \tilde{Z}_{K,L}$. If we neglect third- and higher-order terms in the Taylor series, then we require to second order in the Taylor series that

$$\sum_{K',L'} A_{(K,L),(K',L')}f_{K',L'}-\nabla\cdot(D\nabla)f|_{(\tilde{R}_{K,L},\tilde{Z}_{K,L})}=0.$$

This is what we mean when we say Af approximates $\nabla\cdot(D\,\nabla f)$.

(2) A must be non-positive definite, i.e., for any vector x,

$$(x, Ax)\leqslant 0$$

where

$$(x,y)=\sum V_{K,L}x_{K,L}y_{K,L},$$

and $V_{K,L}$ is the volume of zone (K,L). Clearly the diffusion operator has this property for if f is any function of space,

$$\int R\,dR\,dZ\,f\nabla\cdot(D\,\nabla f)=\int R\,dR\,dZ\,\nabla\cdot(fD\,\nabla f)-\int R\,dR\,dZ\,D(\nabla f)^2$$

$$=-\int R\,dR\,dZ\,D(\nabla f)^2\leqslant 0.$$

We put

$$\int R\,dR\,dZ\,\nabla\cdot(fD\,\nabla f)=0$$

because we assume $f=0$ or $\mathbf{dS}\cdot\nabla f=0$ on the boundary of the problem. We sometimes have the condition $f=f_B\neq 0$ on the boundary of the problem. However, when Eq. (3) is finite differenced, the terms in $(Af)_{K,L}$ that involve f_B get put on the right-hand side of the equation (since f_B is known) and so the remaining matrix A on the left-hand side of Eq. (3) which operates only on the vector of unknowns is the same as if $f=0$ on the boundary. Boundary conditions will be discussed in detail later. We require that A be non-positive definite because if it were not, it would have some positive eigenvalues. Let V be an eigenvector with positive eigenvalue λ. Then if $f^n=V$ we have (from Eq. (3))

$$(I-(\Delta t)A)f^{n+1}=f^n$$

or

$$f^{(n+1)} = (1 - (\Delta t)\lambda)^{-1} f^n$$

which blows up if $\Delta t = \lambda^{-1} > 0$. Unless A is non-positive definite, there will always be a time step $\Delta t > 0$ for which the whole scheme blows up. Therefore numerical stability requires A to be non-positive definite, which implies for any $\Delta t > 0$, $M = I - (\Delta t)A$ is positive definite, and $(x, Mx) \geqslant (x, x)$ for any x.

(3) We require A to be symmetric, i.e.,

$$(x, Ay) = (Ax, y).$$

The diffusion operator has this property, for

$$\int R\, dR\, dZ\, g\nabla \cdot (D\, \nabla f) = -\int R\, dR\, dZ\, D(\nabla f) \cdot (\nabla g)$$

$$= \int R\, dR\, dZ\, f\nabla \cdot (D\, \nabla g).$$

For the diffusion equation this property gives us energy conservation for if $g = 1$ everywhere, then

$$\int \frac{\partial f}{\partial t} R\, dR\, dZ = \frac{dE_{\text{total}}}{dt} = \int R\, dR\, dZ\, g\nabla \cdot (D\, \nabla f)$$

$$= \int R\, dR\, dZ\, f\nabla \cdot (D\, \nabla g) = 0, \qquad \text{since} \quad \nabla g = 0.$$

Similarly if we choose A to be symmetric, our finite-difference scheme will conserve energy exactly for if $g_{K,L} = 1$, for all (K, L), then

$$E_{\text{total}}^{(n+1)} - E_{\text{total}}^{n} = (\Delta t) \sum_{(K,L)} \left(\frac{f_{K,L}^{(n+1)} - f_{K,L}^{n}}{(\Delta t)} \right) V_{K,L}$$

$$= (\Delta t) \sum_{K,L} V_{K,L} A f_{K,L}^{(n+1)} = (\Delta t)(g, Af^{(n+1)})$$

$$= (\Delta t)(Ag, f^{(n+1)}) = 0,$$

since $Ag = 0$. It is shown below (see Eq. (6a)) that property (1) implies $Ag = 0$ if g is constant.

In deriving $dE_{\text{total}}/dt = 0$, we assumed that $\nabla f = 0$ on the boundary. If this is not the case, then we obtain $dE_{\text{total}}/dt = \int \mathbf{dS} \cdot D\, \nabla f =$ rate at which energy is escaping from the problem. Analogously, in the finite-difference case, if we allow energy to escape, then Ag will be $\neq 0$ on the boundary of the problem and $(\Delta t)(Ag, f^{(n+1)})$ will give the energy that has escaped during the current time step.

We have shown that the symmetry of A is sufficient but not necessary for global energy conservation. Let us now look at local energy conservation. Using the property $Ag = 0$ if g is a constant, we can rewrite $(Af)_{K,L}$ as

$$V_{K,L}(Af)_{K,L} = \sum_{K',L'} V_{K,L}A_{K,L;K',L'}(f_{K',L'} - f_{K,L}),$$

where the sum is over the eight nearest neighbors of (K, L). $V_{K,L}A_{K,L;K',L'}(f_{K',L'} - f_{K,L})$ has a simple physical interpretation as the energy flux from zone (K', L') into zone (K, L). The symmetry of the matrix A assures us that the energy flux from zone (K', L') into zone (K, L) is equal to minus the energy flux from zone (K, L) into zone (K', L'). Combining this with Eq. (3) we have

$$V_{K,L}(f^{(n+1)}_{(K,L)} - f^n_{K,L}) = (\Delta t) \sum_{K',L'} V_{K,L}A_{K,L;K',L'}(f_{K',L'} - f_{K,L}).$$

Thus the change in the energy in zone (K, L) during the nth time step is just equal to the sum of the energy fluxes coming into the zone from each of its eight neighbors and energy is locally conserved.

(4) We require a locality condition that A be a nine-point difference operator (we shall show that this is the smallest number of points to which one can couple and still satisfy property 1). In the special case where the K and L lines of the mesh are orthogonal we require that A reduce to the standard five-point scheme which is widely quoted in the literature. In this standard five-point scheme $A = A_K + A_L$ and A_K (A_L) is just the one-dimensional three-point diffusion operator along a K (L) line. This five-point scheme has been extensively tested and we thus tie ourselves to a successful tradition in the special case of an orthogonal mesh. We note in passing that the standard five-point scheme on an orthogonal mesh satisfies all of requirements 1 through 5.

(5) We would like A to satisfy $i \neq j$ implies $A_{ij} \geqslant 0$. Then $M = (I - (\Delta t)A)$ is a positive definite, symmetric "M matrix" or Stieltjes matrix, i.e.,

$$M_{ii} > 0 \qquad \text{and} \qquad M_{ij} \leqslant 0, \qquad i \neq j.$$

This is desirable because $f^{(n)}$ is an energy density and so $f^{(n)}_{K,L} \geqslant 0$. From Eq. (3),

$$Mf^{(n+1)} = f^n,$$

and it is shown in Ref. [1] that $(f^n \geqslant 0) \Rightarrow (f^{(n+1)} \geqslant 0)$ if and only if M is an "M matrix." Thus unless A is an "M matrix" we will be plagued with occasional negative energy densities in certain zones.

To sum up, our basic requirements are:

(1) $Af \rightarrow \nabla \cdot (D \nabla f)$ as the mesh size goes to zero, i.e., A approximates $\nabla \cdot D\nabla$.

(2) A is non-positive definite. This gives us numerical stability.

(3) A is symmetric. This gives us energy conservation.

(4) When the mesh is orthogonal, A becomes the standard five-point scheme. This assures us that in the special case of an orthogonal mesh we have an extensively tried and tested tradition working for us. A is a nine-point coupling scheme. This makes $M = I - (\Delta t)A$ as sparse as possible (and therefore $Mf^{(n+1)} = f^{(n)}$ as easy to solve as possible) while still satisfying condition 1.

(5) A is an "M matrix." This assures us that energy densities stay positive.

We now show that on a general Lagrangian mesh a nine-point coupling scheme is the smallest possible, and that conditions 1 and 5 are incompatible.

Let our nine-point scheme be

$$\begin{aligned}(Af)_{K,L} = &- \alpha_{K,L} f_{K,L} + \beta_{K+1,L} f_{K+1,L} + \beta_{K-1,L} f_{K-1,L} \\ &+ \beta_{K,L+1} f_{K,L+1} + \beta_{K,L-1} f_{K,L-1} \\ &+ \beta_{K+1,L+1} f_{K+1,L+1} + \beta_{K-1,L-1} f_{K-1,L-1} \\ &+ \beta_{K+1,L-1} f_{K+1,L-1} + \beta_{K-1,L+1} f_{K-1,L+1}. \end{aligned} \tag{4}$$

A superscript K, L on the α's and β's has been suppressed.

In the limit as the zone size goes to zero we have

$$\begin{aligned} f_{K+1,L} = f_{K,L} &+ (\tilde{R}_{K+1,L} - \tilde{R}_{K,L}) \frac{\partial f}{\partial R}\bigg|_{K,L} \\ &+ (\tilde{Z}_{K+1,L} - \tilde{Z}_{K,L}) \frac{\partial f}{\partial Z}\bigg|_{K,L} \\ &+ 1/2(\tilde{R}_{K+1,L} - \tilde{R}_{K,L})^2 \frac{\partial^2 f}{\partial R^2}\bigg|_{K,L} \\ &+ (\tilde{R}_{K+1,L} - \tilde{R}_{K,L})(\tilde{Z}_{K+1,L} - \tilde{Z}_{K,L}) \frac{\partial^2 f}{\partial R\, \partial Z}\bigg|_{K,L} \\ &+ 1/2(\tilde{Z}_{K+1,L} - \tilde{Z}_{K,L})^2 \frac{\partial^2 f}{\partial Z^2}\bigg|_{K,L}, \end{aligned} \tag{5}$$

and similar equations for $f_{K-1,L}, \ldots, f_{K-1,L+1}$. Condition 1 requires that substituting Eq. (5) into Eq. (4) should give

$$\begin{aligned}(Af)_{K,L} &= \frac{1}{R}\frac{\partial}{\partial R} DR \frac{\partial f}{\partial R}\bigg|_{K,L} + \frac{\partial}{\partial Z} D \frac{\partial f}{\partial Z}\bigg|_{K,L} \\ &= \left(\left(\frac{\partial D}{\partial R}\right) + \frac{D}{R}\right)\frac{\partial f}{\partial R}\bigg|_{K,L} + D \frac{\partial^2 f}{\partial R^2}\bigg|_{K,L} + D \frac{\partial^2 f}{\partial Z^2}\bigg|_{K,L} + \frac{\partial D}{\partial Z}\frac{\partial f}{\partial Z}\bigg|_{K,L}. \end{aligned}$$

This gives six equations for the α's and β's. Namely,

$$\alpha_{(K,L)} = \sum_{(K',L')} \beta_{K',L'}, \tag{6a}$$

$$\left(\frac{\partial D}{\partial R} + \frac{D}{R}\right)\Bigg|_{K,L} = \sum_{(K',L')} \beta_{K',L'}(\tilde{R}_{K',L'} - \tilde{R}_{K,L}), \tag{6b}$$

$$\left(\frac{\partial D}{\partial Z}\right) = \sum_{(K',L')} \beta_{K',L'}(\tilde{Z}_{K',L'} - \tilde{Z}_{K,L}), \tag{6c}$$

$$D = 1/2 \sum_{(K',L')} \beta_{K',L'}(\tilde{R}_{K',L'} - \tilde{R}_{K,L})^2, \tag{6d}$$

$$0 = \sum_{(K',L')} \beta_{K',L'}(\tilde{R}_{K',L'} - \tilde{R}_{K,L})(\tilde{Z}_{K',L'} - \tilde{Z}_{K,L}), \tag{6e}$$

$$D = 1/2 \sum_{(K',L')} \beta_{K',L'}(\tilde{Z}_{K',L'} - \tilde{Z}_{K,L})^2, \tag{6f}$$

where the sum in (6a) through (6f) is over the eight neighbors of (K, L).

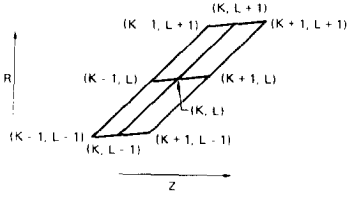
Clearly, in general we cannot satisfy six equations with five unknowns (i.e., with a five-point scheme where $\beta_{K+1,L+1} = \beta_{K-1,L-1} = \beta_{K+1,L-1} = \beta_{K-1,L+1} = 0$) so in order to preserve symmetry we must go to a nine-point scheme to difference the diffusion operator on an arbitrary quadrilateral mesh. Condition 5 requires that

$$\alpha_{K,L} \leqslant 0$$

and

$$\beta_{K'L'} \geqslant 0 \tag{7}$$

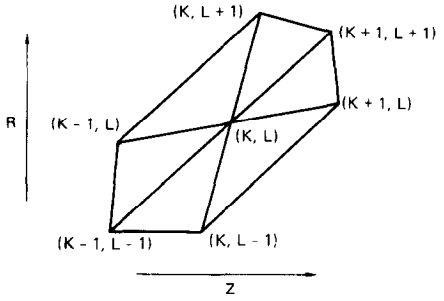
for all eight neighbors (K', L') of (K, L). However, there are many meshes such that $(\tilde{R}_{K',L'} - \tilde{R}_{K,L})(\tilde{Z}_{K',L'} - \tilde{Z}_{K,L}) > 0$ for all eight neighbors (K', L'). But this, together with (6e) and (7), implies $\beta_{(K',L')} = 0$ for all eight neighbors and clearly then (6b), (6c), (6d), and (6f) cannot be satisfied. Therefore on a general quadrilateral mesh conditions 1 and 5 are incompatible. A simple example of a mesh which gives $(\tilde{R}_{K',L'} - \tilde{R}_{K,L})(\tilde{Z}_{K',L'} - \tilde{Z}_{K,L}) > 0$ for all eight neighbors (K', L') is



Thus for a general Lagrangian hydrodynamic mesh we must use at least a nine-point difference scheme and we cannot help violating condition 5. Occasional negative values for the energy density are unavoidable but the numerical stability condition 2 assures us that they will be transient and small which is indeed found to be the case in practice. Note also that the above argument applies equally well to triangular meshes. If we regard (K, L) as labelling points in a triangular mesh, and $\sum_{(K',L')}$ as a sum over the six neighbors of (K, L) in this mesh, then it is again easy to find meshes for which

$$(R_{K',L'} - R_{K,L})(Z_{K',L'} - Z_{K,L}) > 0$$

for all neighbors. A simple example is the grid:



To difference the diffusion operator so as to satisfy 1 through 4 we imagine R and Z to be functions of continuous variables K and L. Then a simple exercise in partial derivatives shows that

$$\begin{aligned}\nabla \cdot (D \nabla f) = \frac{1}{jR} \Bigg\{ & \frac{\partial}{\partial K} \left[\left(\frac{DR(\mathbf{R}_L)^2}{j} \right) \frac{\partial f}{\partial K} \right] \\ & + \frac{\partial}{\partial L} \left[\left(\frac{DR(\mathbf{R}_K)^2}{j} \right) \frac{\partial f}{\partial L} \right] \\ & - \frac{\partial}{\partial K} \left[\left(\frac{DR(\mathbf{R}_K \cdot \mathbf{R}_L)}{j} \right) \right] \frac{\partial f}{\partial L} - \frac{\partial}{\partial L} \left[\left(\frac{DR(\mathbf{R}_K \cdot \boldsymbol{R}_L)}{j} \right) \frac{\partial f}{\partial K} \right] \Bigg\},\end{aligned}$$

where

$$j = \det \begin{pmatrix} \dfrac{\partial R}{\partial K} & \dfrac{\partial R}{\partial L} \\ \dfrac{\partial Z}{\partial K} & \dfrac{\partial Z}{\partial L} \end{pmatrix},$$

$$\mathbf{R}_K = \begin{pmatrix} \dfrac{\partial R}{\partial K} \\ \dfrac{\partial Z}{\partial K} \end{pmatrix} \quad \text{and} \quad \mathbf{R}_L = \begin{pmatrix} \dfrac{\partial R}{\partial L} \\ \dfrac{\partial Z}{\partial L} \end{pmatrix}. \tag{8}$$

j is the Jacobian of the transformation from (R, Z) to (K, L) and is just the area of the Lagrangian cell.

To difference Eq. (8) we use the variational method [2]. For our problem from Eq. (8) it follows that

$$\int R\, dR\, dZ f \nabla \cdot (D \nabla f) = -\int R\, dR\, dZ\, D(\nabla f)^2$$

$$= -\int dK\, dL \left[\sqrt{\frac{DR}{j}} \left(\mathbf{R}_L \frac{\partial}{\partial K} - \mathbf{R}_K \frac{\partial}{\partial L}\right) f\right]^2. \tag{9}$$

The finite difference analogue of (9) is

$$-\sum_{(K,L)} [\mathbf{B}f]^2_{K,L}, \tag{10}$$

where the two matrices B_R and B_Z will be specified shortly. Then if we take (10) and perform the finite-difference analogue of integration by parts (i.e., shift the indices appropriately), then (10) can be written in the form

$$-\sum_{(K,L)} [\mathbf{B}f]^2_{K,L} = +\sum_{K,L} f_{K,L}(Af)_{K,L} V_{K,L}, \tag{11}$$

$$V_{K,L} = Rj|_{K,L} = \text{zone volume}/(2\pi),$$

where A is the matrix we seek. Equation (11) assures us that Gauss' theorem will apply to our finite-difference analogue just as it does to the exact diffusion operator and therefore the proofs we gave to show that conditions 2 and 3 were satisfied by the exact operator, $\nabla \cdot (D \nabla f)$, will apply equally well to our finite-difference operator (Af). Therefore we are assured that A will be non-positive definite and symmetric.

It remains only to decide on the form of $(\mathbf{B}f)$ in Eq. (11). Actually we shall use

$$\int R\, dR\, dZ f \nabla \cdot (D \nabla f) \approx -\tfrac{1}{4} \sum_{(K,L)} \sum_{i=1}^{4} [\mathbf{B}^i f]^2_{K,L}$$

$$= +\sum_{(K,L)} f_{K,L}(Af)_{K,L} V_{K,L}. \tag{12}$$

The above remarks apply equally well to this slightly generalized form. Condition 1 will be satisfied if

$$(\mathbf{B}f)_{K,L} \approx \sqrt{\frac{DR}{j}} \left(\mathbf{R}_L \frac{\partial f}{\partial k} - \mathbf{R}_K \frac{\partial f}{\partial L}\right), \tag{13}$$

and $\mathbf{R}_L, \mathbf{R}_K$ become continuous functions of K, L as the mesh size goes to zero.[1]

[1] The use of coordinate transformations from physical to logical space as an aid in constructing difference equations in Lagrangian meshes has been discussed by W. D. Schulz ("Methods in

We break $(\mathbf{B}f)$ into two parts

$$(\mathbf{B}f)_{K,L} = \mathscr{K}_{K,L}\mathbf{R}_L - \mathscr{L}_{K,L}\mathbf{R}_K,$$

where

$$\mathscr{K}_{K,L} \approx \sqrt{\frac{DR}{j}}\frac{\partial f}{\partial K}$$

and

$$\mathscr{L}_{K,L} \approx \sqrt{\frac{DR}{j}}\frac{\partial f}{\partial L}. \tag{14}$$

Clearly $\mathscr{K}$ and $\mathscr{L}$ are face centered quantities and we difference (14) as

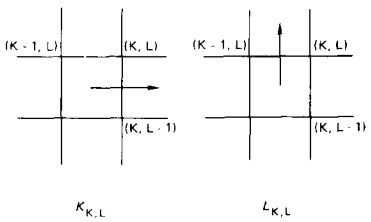
$$\mathscr{K}_{K,L} = \Sigma_{K,L}(f_{K+1,L} - f_{K,L}), \tag{15a}$$

where $\Sigma_{K,L} = (DR/j)^{1/2}$ suitably averaged between zones K, L and $K+1, L$. We prefer to use $\Sigma^2_{K,L} = (R_{K,L} + R_{K,L-1})/((j_{K,L}/D_{K,L}) + (j_{K+1,L}/D_{K+1,L}))$ but any method of averaging can be used without upsetting our conditions 1 through 4.

$$\mathscr{L}_{K,L} = \Lambda_{K,L}(f_{K,L+1} - f_{K,L}), \tag{15b}$$

where $\Lambda_{K,L}$ is $(DR/j)^{1/2}$ suitably averaged between zones K, L and $K, L+1$.

In diagrams:



$\mathbf{R}_K$ and $\mathbf{R}_L$ we differenced as

$$(\mathbf{R}_K)_{K,L} = (\mathbf{R}_{K,L} + \mathbf{R}_{K,L-1} - \mathbf{R}_{K-1,L} - \mathbf{R}_{K-1,L-1})/2, \tag{15c}$$

$$(\mathbf{R}_L)_{K,L} = (\mathbf{R}_{K,L} + \mathbf{R}_{K-1,L} - \mathbf{R}_{K,L-1} - \mathbf{R}_{K-1,L-1})/2, \tag{15d}$$

Computation Physics," Vol. 3, pps. 1–45, Academic Press, New York, 1964) and Stein *et al.* (*Comput. Methods Appl. Mech. Eng.* **11** (1977), 57). Note that by writing $(\mathbf{B}f)_{K,L}$ in terms of partial derivatives with respect to K and L and then differencing this expression, we tacitly assume that $\mathbf{R}(K, L)$ and it derivatives $\mathbf{R}_K$ and $\mathbf{R}_L$ are continuous functions of K and L. In order for $Af \to \nabla(D\nabla f)$ as the mesh size goes to zero, $\mathbf{R}_K$ and $\mathbf{R}_L$ must become continuous functions of $(K/KMAX)$ and $(L/LMAX)$. For a finite mesh, $\mathbf{R}_K$ and $\mathbf{R}_L$ must be smoothly varying with K and L in order for A to be a good approximation to $\nabla \cdot D\nabla f$. This restriction may be removed by simply writing $(\mathbf{B}f)_{K,L} = \sqrt{DV_{K,L}}\,\nabla f$ and then obtaining a finite-difference expression for $\mathbf{B}^1$ by fitting $f = Rf_R + Zf_Z + f_0$ to the three zonal values $f_{K,L}$, $f_{K+1,L}$, $f_{K,L+1}$, and proceeding similarly for $\mathbf{B}^2$, $\mathbf{B}^3$, and $\mathbf{B}^4$. This fitting could be done, e.g., by requiring that $\int R\,dR\,dZ\,(Rf_R + Zf_Z + f_0) = V_{K,L}f_{K,L}V_{K,L}$ for each of the three zones.

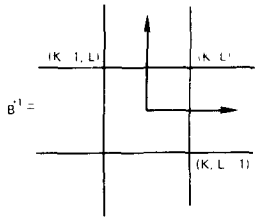
where $\mathbf{R}_{K,L} = (R_{K,L}, Z_{K,L})$. This choice for $\mathbf{R}_K$ and $\mathbf{R}_L$ ensures that if we zone up a sphere as concentric equilateral polygons, our diffusion routine will still consider it to be an orthogonal mesh, i.e.,

$$(\mathbf{R}_K)_{K,L} \cdot (\mathbf{R}_L)_{K,L} = 0$$

will hold. The difference of these two terms we call $\mathbf{B}^1$

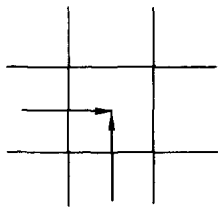
$$(\mathbf{B}^1 f)_{K,L} = \mathscr{K}_{K,L}(\mathbf{R}_L)_{K,L} - \mathscr{L}_{K,L}(\mathbf{R}_K)_{K,L} \tag{16a}$$

and in diagram form

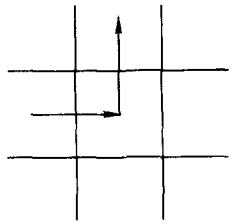


Clearly there are three other equally plausible choices for the zone centered quantity $(\mathbf{B}f)_{K,L}$, namely,

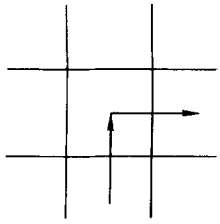
$$(\mathbf{B}^2 f)_{K,L} = \mathscr{K}_{K-1,L}(\mathbf{R}_L)_{K,L} - \mathscr{L}_{K,L-1}(\mathbf{R}_K)_{K,L}, \tag{16b}$$



$$(\mathbf{B}^3 f)_{K,L} = \mathscr{K}_{K-1,L}(\mathbf{R}_L)_{K,L} - \mathscr{L}_{K,L}(\mathbf{R}_K)_{K,L}, \tag{16c}$$



$$(\mathbf{B}^4 f)_{K,L} = \mathscr{K}_{K,L}(\mathbf{R}_L)_{K,L} - \mathscr{L}_{K,L-1}(\mathbf{R}_K)_{K,L}, \tag{16d}$$



By symmetry (under 90° rotations about zone (K, L)) all four $\mathbf{B}$'s are equally likely so we take

$$\int R\, dR\, dZ f \nabla \cdot (D \cdot \nabla f) \approx -\tfrac{1}{4} \sum_{(K,L)} \sum_{i=1}^{4} (\mathbf{B}^i f)^2_{K,L}$$

$$= + \sum_{(K,L)} f_{K,L}(Af)_{K,L} V_{K,L}. \tag{12}$$

If follows that

$$VA = -1/4 \sum_{i=1}^{4} (\mathbf{B}^i)^T \cdot (\mathbf{B}^i),$$

and in this form the symmetry and non-positive definiteness of the matrix VA is obvious. This defines the matrix A and substituting Eqs. (16) into (12) and equating coefficients of $f_{K,L} f_{K',L'}$, one finds

$$V_{K,L} A_{(K,L),(K,L)} = -\sigma_{(K,L)} - \sigma_{(K-1,L)} - \lambda_{(K,L)} - \lambda_{(K,L-1)} + \tfrac{1}{2}(\rho^1_{(K,L)} + \rho^2_{(K,L)} - \rho^3_{(K,L)} - \rho^4_{(K,L)}), \tag{17a}$$

$$V_{K,L} A_{(K,L),(K+1,L)} = \sigma_{(K,L)} - \tfrac{1}{4}(\rho^1_{(K,L)} + \rho^2_{(K+1,L)} - \rho^3_{(K+1,L)} - \rho^4_{(K,L)}), \tag{17b}$$

$$V_{K,L} A_{(K,L),(K,L+1)} = \lambda_{(K,L)} - \tfrac{1}{4}(\rho^1_{(K,L)} + \rho^2_{(K,L+1)} - \rho^3_{(K,L)} - \rho^4_{(K,L+1)}), \tag{17c}$$

$$V_{K,L} A_{(K,L)(K+1,L+1)} = -\tfrac{1}{4}(\rho^3_{(K+1,L)} + \rho^4_{(K,L+1)}), \tag{17d}$$

$$V_{K,L} A_{(K,L),(K-1,L+1)} = \tfrac{1}{4}(\rho^1_{(K-1,L)} + \rho^2_{(K,L+1)}), \tag{17e}$$

where

$$\sigma_{(K,L)} = (\Sigma_{(K,L)})^2 ((\mathbf{R}_L)^2_{K,L} + (\mathbf{R}_L)^2_{K+1,L})/2,$$

$$\lambda_{(K,L)} = (\Lambda_{(K,L)})^2 ((\mathbf{R}_K)^2_{K,L} + (\mathbf{R}_K)^2_{K,L+1})/2,$$

$$\rho^1_{(K,L)} = \Sigma_{(K,L)} \Lambda_{(K,L)} C_{K,L},$$

$$\rho^2_{(K,L)} = \Sigma_{(K-1,L)} A_{(K,L-1)} C_{K,L},$$
$$\rho^3_{(K,L)} = \Sigma_{(K-1,L)} A_{(K,L)} C_{K,L},$$
$$\rho^4_{(K,L)} = \Sigma_{(K,L)} A_{(K,L-1)} C_{K,L},$$

and

$$C_{K,L} = (\mathbf{R}_K)_{K,L} \cdot (\mathbf{R}_L)_{K,L}.$$

Since VA is symmetric

$$V_{K'L'} A_{(K',L'),(K,L)} = V_{K,L} A_{(K,L),(K',L')}, \tag{17f}$$

and all elements of A not defined by Eqs. (17a) through (17f) are zero.

In the case of an orthogonal mesh $\mathbf{R}_K \cdot \mathbf{R}_L = 0$, and so $\rho^1 = \rho^2 = \rho^3 = \rho^4 = 0$, and only the σ and λ terms remain, but Eq. (17) with just the σ and λ terms is nothing but the standard five-point approximation that is widely used. Note that only the ρ's involve square roots; σ and λ do not. Thus condition 4 is satisfied.

We note in passing that the square roots in (15a) and (15b) seem to be necessary if conditions 1 through 4 are to be satisfied. In particular, $\sigma_{K,L}$ depends only on $D_{K,L}$ and $D_{K+1,L}$ and $\lambda_{K,L}$ depends only on $D_{K,L}$ and $D_{K,L+1}$. This is a basic feature of the standard five-point scheme and is only achieved because we factored D into $D^{1/2} * D^{1/2}$ and differenced each square root separately. Any scheme which does not involve square roots of D in this way will inevitably produce a $\sigma_{K,L}$ which depends on $D_{K,L}$, $D_{K+1,L}$, $D_{K,L+1}$, $D_{K,L-1}$, $D_{K+1,L+1}$, and $D_{K+1,L-1}$, a highly non-local and therefore undesirable kind of differencing. For example, if we have a slot filled with large D material embedded in a slab of material with very small D and if the slot is two zones wide and many zones long and the zoning is orthogonal, then our scheme will give the proper diffusion rate along the slot, whereas any scheme where $\sigma_{K,L}$ was an average of the six neighboring D's would get too slow a diffusion rate along the slot.

In our application the diffusion coefficient, D, may often jump by many orders of magnitude from one row of zones to the next due to changes in materials. This is particularly true in realistic problems where limitations of computer memory and speed often restrict one to rather coarse zoning. In this case if $\sigma_{K,L+1}$ depends on $D_{K,L}$ and $D_{K+1,L}$ and $D_{K,L} \gg D_{K,L+1}$, then flow along the $(L+1)$st line well be greatly (and incorrectly enhanced) by the much larger D on the Lth line.

Our diffusion problems have two types of boundary conditions

$$d\mathbf{S} \cdot \nabla f = 0$$

or "no escape" boundaries, and

$$f = f_B,$$

or "escape" boundaries where a known vacuum energy density f_B is given.

We manage to allow irregular-shaped material boundaries while still having a rectangular logical mesh by having two types of zones, physical zones that are part of the problem and vacuum zones. The physical zones are completely surrounded by vacuum zones.

Our basic equation is (3)

$$f^{(n+1)}_{(K,L)} - (\Delta t)(Af^{(n+1)})_{(K,L)} = f^{n}_{(K,L)}. \tag{3}$$

The basic building blocks of A are $\Sigma_{K,L}(\mathbf{R}_L)_{K,L}$, $\Sigma_{K,L}(\mathbf{R}_L)_{K+1,L}$, $A_{K,L}(\mathbf{R}_K)_{K,L}$, and $A_{K,L}(\mathbf{R}_K)_{K,L+1}$ (see Eqs. (16) and (17)). $\Sigma_{K,L}$ connects zone (K, L) with zone $(K+1, L)$, and $A_{K,L}$ connects zone (K, L) with zone $(K, L+1)$. The boundary conditions are incorporated by the following set of rules:

(1) If (K, L) and $(K+1, L)$ are both physical zones use $\Sigma_{K,L}(\mathbf{R}_L)_{K,L}$ and $\Sigma_{K,L}(\mathbf{R}_L)_{K+1,L}$ as described above.

(2) If (K, L) and $(K+1, L)$ are both vacuum zones, $\Sigma_{K,L} = 0$.

(3) If (K, L) is a physical zone and $(K+1, L)$ is a vacuum zone and the face separating the two zones has "no escape" ($\hat{n} \cdot \nabla f = 0$) boundary conditions across it, use $\Sigma_{K,L} = 0$. Also in Eqs. (16a) and (16d), $(\mathbf{R}_K)_{K,L}$ is replaced by

$$\hat{n}(\hat{n} \cdot (\mathbf{R}_K)_{K,L}),$$

where $\hat{n}$ is the unit normal to the vacuum surface.

(4) If (K, L) is a vacuum zone and $(K+1, L)$ is a physical zone and $\hat{n} \cdot \nabla f = 0$ across the boundary, use $\Sigma_{K,L} = 0$. Also in Eqs. (16b) and (16c), with $K \to (K+1)$, $(\mathbf{R}_K)_{K+1,L}$ is replaced by

$$\hat{n}(\hat{n} \cdot (\mathbf{R}_K)_{K+1,L}).$$

(5) If (K, L) is a physical zone and $(K+1, L)$ is a vacuum zone and the face separating them has an "escape" ($f = f_B$) boundary condition across it, use $\Sigma_{K,L}(\mathbf{R}_L)_{K,L}$ and $\Sigma_{K,L}(\mathbf{R}_L)_{K+1,L}$ as described above except that $\Sigma_{K,L}$ is now $(DR/j)^{1/2}$ suitably averaged between zone K, L and the vacuum and $(\boldsymbol{R}_L)_{K+1,L}$ is now given by $(\mathbf{R}_L)_{K+1,L} = \mathbf{R}_{K,L} - \mathbf{R}_{K,L-1}$ instead of (15d), since $\mathbf{R}_{K+1,L}$ and $\mathbf{R}_{K+1,L-1}$ may not exist. Also in Eqs. (16a) and (16d), $(\mathbf{R}_K)_{K,L}$ is replaced by

$$\hat{n}(\hat{n} \cdot (\mathbf{R}_K)_{K,L}),$$

where $\hat{n}$ is the unit normal to the vacuum surface. Then whenever a term with $f_B = f_{(K+1,L)}$ (i.e., $-(\Delta t) A_{K,L,(K+1,L)} f_B$) turns up on the left-hand side of Eq. (3), just move it to the right-hand side since f_B is known. In our application $\Sigma_{K,L}$ is averaged so that if $\hat{n} \cdot \nabla f$ is constant, f extrapolates to f_B at two-thirds of a mean free path outside the surface (Milne boundary condition).

(6) If (K, L) is a vacuum zone and $(K+1, L)$ is a physical zone and the interface has "escape" boundary conditions, use $\Sigma_{K,L}(\mathbf{R}_L)_{K,L}$ and $\Sigma_{K,L}(\mathbf{R}_L)_{K+1,L}$ as

described above, except that $\Sigma_{K,L}$ is now averaged between zone $K+1, L$ and the vacuum and $(\mathbf{R}_L)_{K,L} = \mathbf{R}_{K,L} - \mathbf{R}_{K,L-1}$ instead of (15d). Also in Eqs. (16b) and (16c), with $K \to (K+1)$, $(\mathbf{R}_K)_{K+1,L}$ is replaced by

$$\hat{n}(\hat{n} \cdot (\mathbf{R}_K)_{K+1,L}).$$

Then whenever a term with $f_B = f_{(K,L)}$ (i.e., $-(\Delta t) A_{(K+1,L)(K,L)} f_B$) turns up on the left-hand side of Eq. (3), just move it to the right-hand side.

A completely analogous set of rules applies to the $A_{K,L}$.

We leave it to the reader to convince himself that this prescription leaves conditions 1 through 4 satisfied. This is because we have introduced the boundary conditions as modifications of the $\mathbf{B}^{l}$'s in our variational equation (12) and therefore we know as before that since it is derived from a variational principle, our modified A matrix is still non-positive definite and symmetric.

In our applications we use this difference scheme to determine A, and the ICCG method [3] is used to solve the linear system,

$$(I - (\Delta t)A) f^{(n+1)} = f^n,$$

at each time step.

Numerical Test

This difference scheme was tested by simulating diffusion through a mesh with highly skewed zones. The mesh is shown in Fig. 1. K goes from 1 to 78 and L from 1 to 76. R goes from 0. at $L = 1$ to 1. at $L = 76$ and Z goes from 0. at $(K, L) = (2, 1)$ to 1. at (77, 1). We solve

$$\frac{\partial f}{\partial t} = \nabla(D \cdot \nabla f),$$

where D is constant over the whole mesh and does not change with time. The boundary conditions are $f = 0$ in the column of zones between $K = 1$ and $K = 2$, $f = 8$ in the column of zones between $K = 77$ and $K = 78$, and $\hat{n} \cdot \nabla f = 0$ along the $L = 1$ and $L = 76$ lines, where n is the direction normal to the boundary surface. Initially $f = 0$ everywhere between the source and sink and we watch the diffusion front move out of the source and spread toward the sink until the steady state,

$$f = 8Z,$$

is reached. This is just a one-dimensional problem and f should be a function of Z only at all times. Will the highly distorted mesh distort the isotherms away from vertical straight lines?

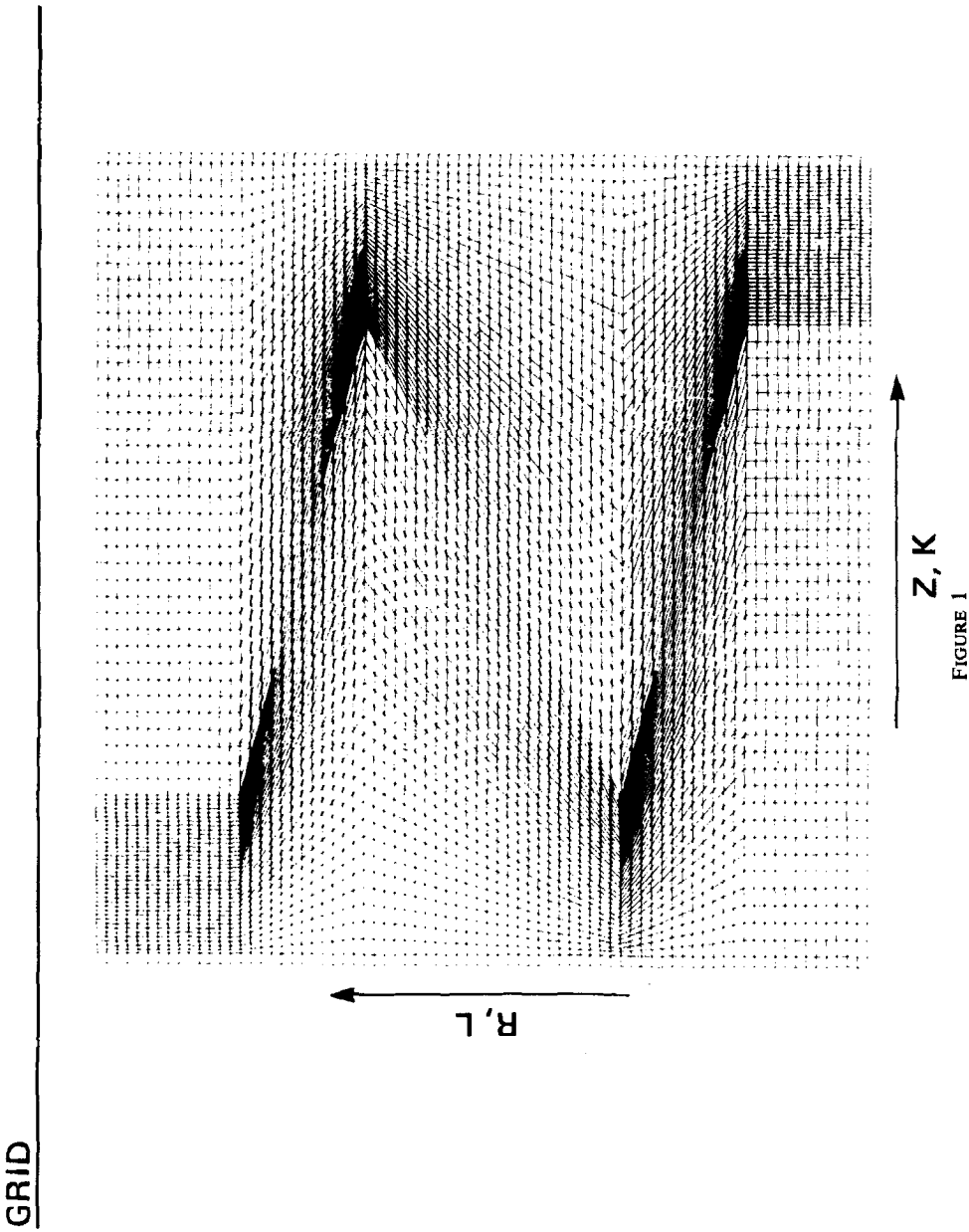


FIGURE 1

Figures 2 and 3 show isotherms of f at an intermediate time (Fig. 2) and after steady state is reached (Fig. 3). The isotherms are

$$A - f = 0.1,$$
$$B - f = 0.5,$$
$$C - f = 2,$$
$$D - f = 4,$$
$$E - f = 6,$$

and the background is the $K = 1$, 2, 39, 77, and 78 lines and the $L = 1$ and 76 lines.

In this problem the time step was constrained so that

$$\sum_{K,L} (f^{n+1}_{K,L} - f^{n}_{K,L})^2 \Big/ \sum (f^{n}_{K,L})^2 \leqslant 0.01$$

for all successive time steps n and $n+1$. Thus at the start of the problem $\Delta t \leqslant$ the explicit time step $= 1/\lambda_{\mathrm{MAX}}$, where λ_{MAX} is the largest eigenvalue of $(-\nabla D \nabla) \approx D/(\Delta Z)^2$, where ΔZ is the average zone width. As the problem proceeds, the diffusion front, which was initially one zone wide, gets less and less steep and as it does so the large λ components in f die out and Δt gets larger and larger until steady state is reached and $\Delta t \to \infty$.

The long wavelength noise (deviations from straight vertical lines) apparent in Fig. 2 in contours A and B and in Fig. 3 in contour D is due to the sharp bends in the K lines. As is pointed out in footnote 1 our difference scheme is most accurate when $\mathbf{R}_K$ and $\mathbf{R}_L$ vary smoothly with K and L. Since in this test problem $\mathbf{R}_K$ and $\mathbf{R}_L$ change abruptly when L goes from just above the angles in the K lines to just below them we can expect some distortion in the vicinity of these L values and that is indeed where the distortion occurs. Decreasing the time step further has no effect on the distortions.

The same problem was also run for the diffusion equation in f to the fourth power,

$$\frac{\partial f^4}{\partial t} = \nabla D \, \nabla f^4,$$

which was differenced in the form

$$4(f^n)^3 \frac{(f^{n+1} - f^n)}{(\Delta t)} = \nabla \, 4D(f^n)^3 \, \nabla f^{n+1},$$

with $f^4 = 0$ between $K = 1$ and 2 and $f^4 = 8$ between $K = 77$ and 78. Here the fact that $\sigma_{K,L}$ depends only on $(4D(f^n)^3)_{K,L}$ and $(4D(f^n)^3)\,K + 1, L$ and is not averaged over other more distant zones gives a better approximation to the analytic operator

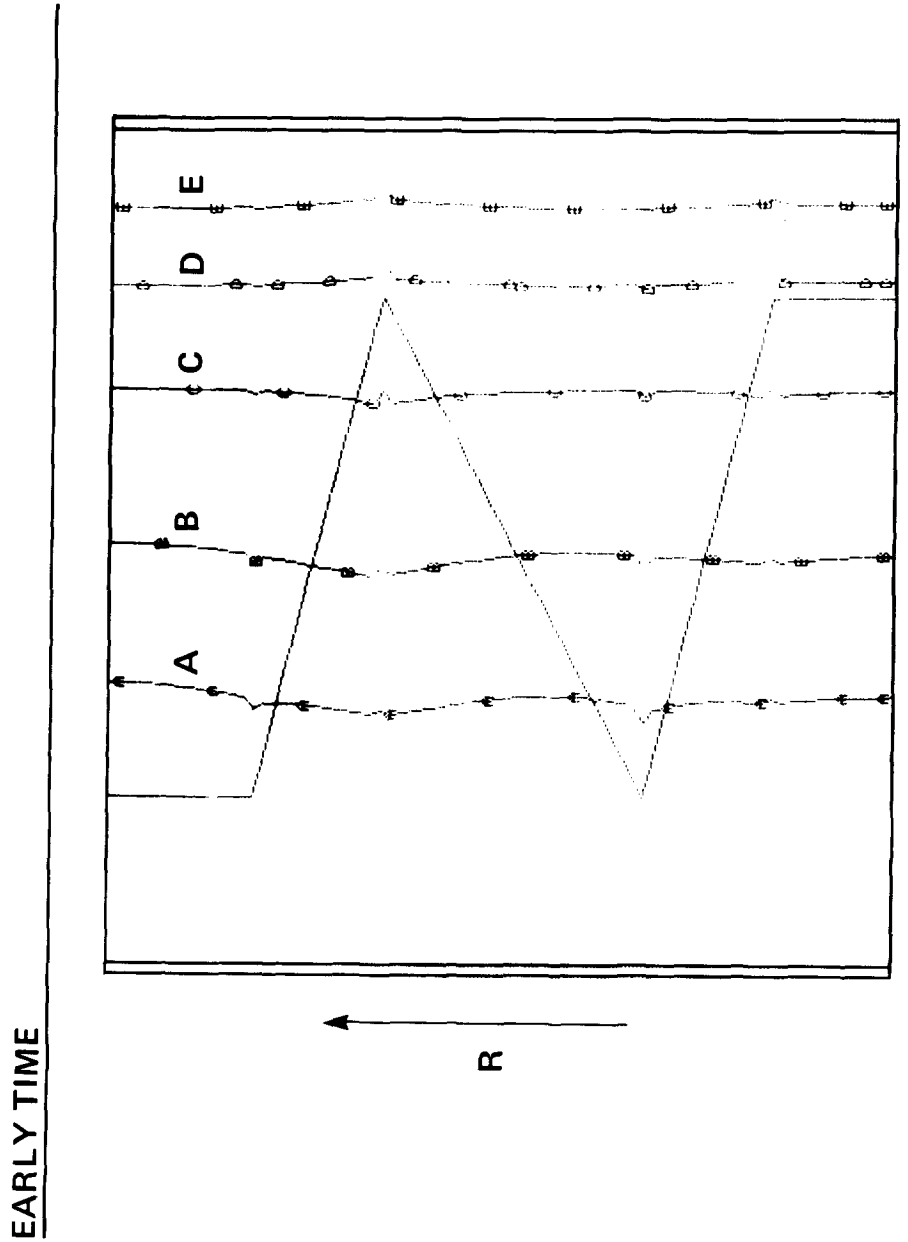


FIGURE 2

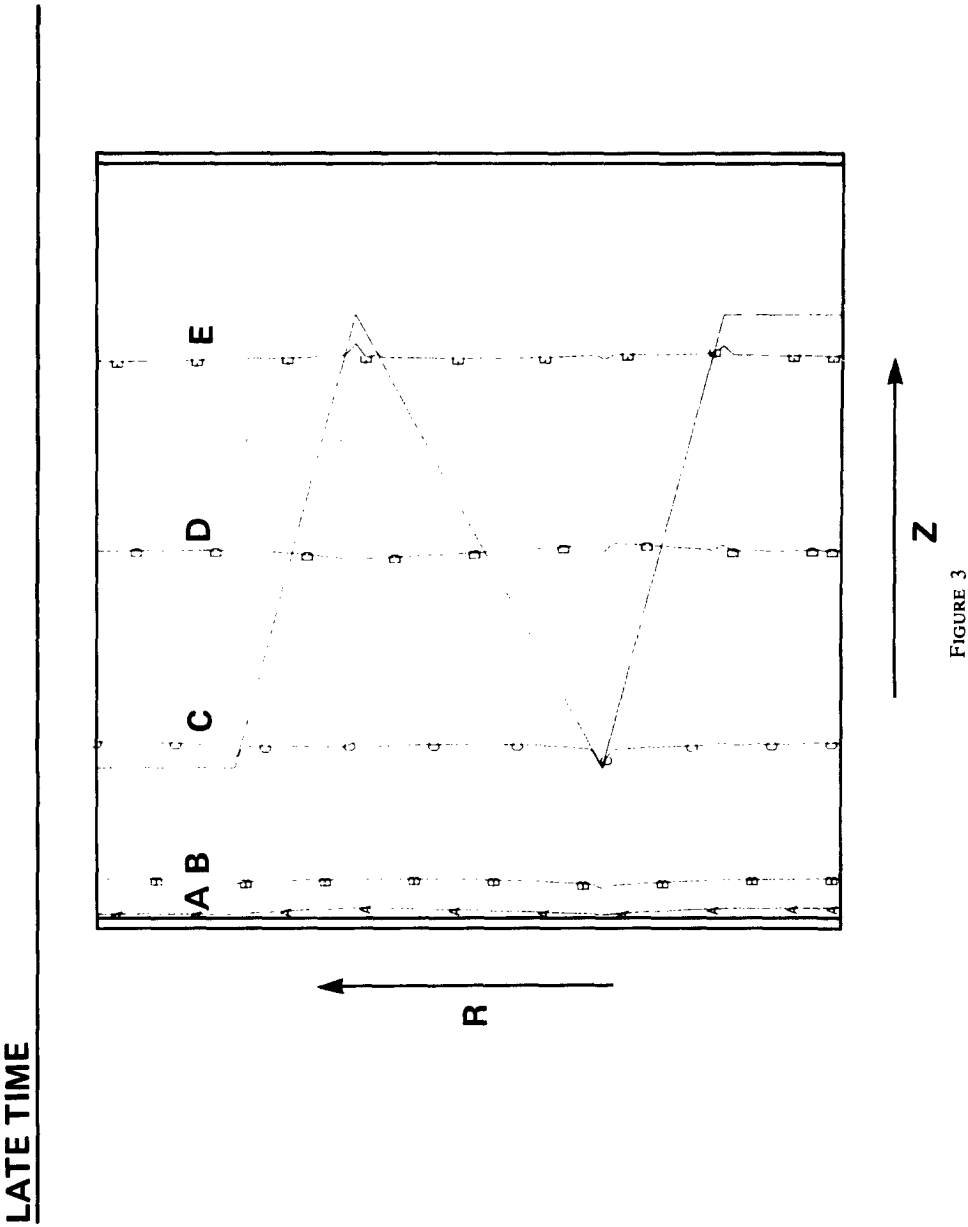


FIGURE 3

since f^3 is falling steeply through the diffusion front. Isocontours for $f^4 = 0.1$, 0.5, 2., 4., and 6. at the same times were indistinguishable in Figs. 2 and 3.

Our difference scheme is able to simulate diffusion through a highly distorted mesh without the diffusion front taking on the shape of the mesh distortions.

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