Lawrence Livermore Laboratory

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David Kershaw

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DIFFERENCING OF THE DIFFUSION EQUATION IN LASNEX*

David S. Kershaw

University of California, Lawrence Livermore Laboratory
Livermore, California

ABSTRACT

The general problem of finite differencing the diffusion equation on a two dimensional Lagrangian hydrodynamic mesh is discussed and a detailed description is given of the manner in which the diffusion equation is differenced in the Laser Fusion Code LASNEX.

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DIFFERENCING OF THE DIFFUSION EQUATION

IN LASNEX*

DAVID S. KERSHAW

LAWRENCE LIVERMORE LABORATORY, UNIVERSITY OF CALIFORNIA
LIVERMORE, CALIFORNIA 94550

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

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

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 τ , the characteristic relaxation time ($\tau = \ell^2/D$ where ℓ is the distance between mesh points), we must difference (1) fully implicitly.

That is

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

where f^n is f after the n 'th time step. Fully implicit differencing has the virtue that when $(\Delta t) \gg \tau$ the left side of (2) becomes negligible and we get

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

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

The next step is to difference the diffusion operator

$$\vec{\nabla} \cdot (D \vec{\nabla} f) .$$

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LASNEX assumes 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

$$K = 1, 2, \dots, KMAX$$

and

$$L = 1, 2, \dots, LMAX$$

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 LASNEX f and D are zone centered quantities.

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

$$Af \approx \vec{\nabla} \cdot (D \vec{\nabla}) f$$

Then equation (2) becomes

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

or

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

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 $f_{K,L} = f(R_{K,L}, Z_{K,L})$ and expand $f_{K',L'}$ in a Taylor series about a given point $R_{K,L}, Z_{K,L}$. If we neglect 3rd and higher order terms in the Taylor series, then we require to 2nd order in the Taylor series, that

$$\sum_{K',L'} A_{(K,L), (K',L')} f_{K',L'} - \vec{\nabla} \cdot (D \vec{\nabla} f) \Big|_{(R_{K,L}, Z_{K,L})} = 0 .$$

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

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

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

where $(x, y) = \left(\sum V_{K,L} x_{K,L} y_{K,L} \right)^{1/2} ,$

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,

$$\begin{aligned} & \int R dR dZ f \vec{\nabla} \cdot (D \vec{\nabla} f) \\ &= \int R dR dZ \vec{\nabla} \cdot (f D \vec{\nabla} f) - \int R dR dZ D (\vec{\nabla} f)^2 \\ &= - \int R dR dZ D (\vec{\nabla} f)^2 \leq 0 . \end{aligned}$$

We put

$$\int R dR dZ \vec{\nabla} \cdot (f D \vec{\nabla} f) = 0$$

because we assume $f = 0$ or $\vec{\nabla} S \cdot \vec{\nabla} f = 0$ on the boundary of the problem.

In LASNEX, 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 $(\Delta t) = \lambda^{-1} > 0$. So unless A is non-positive definite, there will always be a time step $(\Delta t) > 0$ for which the whole scheme blows up and so for numerical stability we require A to be non-positive definite and therefore for any $(\Delta t) > 0$, $M = (I - (\Delta t)A)$ is positive definite, and in fact $(x, Mx) \geq (x, x)$ for any x .

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

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

The diffusion operator has this property, for

$$\begin{aligned} & \int_{RdRdZ} g \vec{\nabla} \cdot (D \vec{\nabla} f) \\ &= - \int_{RdRdZ} D (\vec{\nabla} f) \cdot (\vec{\nabla} g) \\ &= \int_{RdRdZ} f \vec{\nabla} \cdot (D \vec{\nabla} g) \end{aligned}$$

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

$$\begin{aligned} \int \frac{\partial f}{\partial t} R dR dZ &= \frac{dE_{\text{total}}}{dt} = \int R dR dZ \vec{g} \cdot (D \vec{\nabla} f) \\ &= \int R dR dZ f \vec{\nabla} \cdot (D \vec{\nabla} g) = 0, \text{ since } \vec{\nabla} g = 0. \end{aligned}$$

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,

$$\begin{aligned} E_{\text{total}}^{(n+1)} - E_{\text{total}}^n &= (\Delta t) \sum_{(K,L)} \left(\frac{f_{K,L}^{(n+1)} - f_{K,L}^n}{(\Delta t)} \right) \\ &= (\Delta t) \sum_{K,L} A f_{K,L}^{(n+1)} = (\Delta t) (g, A f^{(n+1)}) = (\Delta t) (A g, f^{(n+1)}) = 0, \end{aligned}$$

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

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

- 4) We require a locality condition that A be a 9 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 5 point

scheme which was previously used in LASNEX². In this standard 5 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 5 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 5 point scheme on an orthogonal mesh satisfies all of requirements 1) through 5).

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

$$M_{ii} \geq 0 \text{ and}$$

$$M_{ij} \leq 0, i \neq j.$$

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

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

and it is shown in reference 1, that $(f^n \geq 0) \Rightarrow (f^{(n+1)} \geq 0)$ 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) $Af \rightarrow \vec{\nabla} \cdot (D \vec{\nabla} f)$ as the mesh size goes to zero, i.e. A approximates $\vec{\nabla} \cdot D \vec{\nabla}$.

- 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 5 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 9 point coupling scheme is the smallest possible, and that conditions 1) and 5) are incompatible.

Let our 9 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

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

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

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

This gives 6 equations for the α 's and β 's. Namely:

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

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

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

$$D = 1/2 \sum_{(K',L')} \beta_{K',L'} (R_{K',L'} - R_{K,L})^2 \quad (6d)$$

$$0 = \sum_{(K',L')} \beta_{K',L'} (R_{K',L'} - R_{K,L}) (Z_{K',L'} - Z_{K,L}) \quad (6e)$$

$$D = 1/2 \sum_{(K',L')} \beta_{K',L'} (Z_{K',L'} - Z_{K,L})^2, \quad (6f)$$

where the sum is over the eight neighbors of (K,L).

Clearly, in general we cannot satisfy six equations with five unknowns (i.e. with a 5 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 9 point scheme to difference the diffusion operator on an arbitrary quadrilateral mesh. Condition 5) requires that

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

and

$$\beta_{K',L'} \geq 0 \quad (7)$$

for all eight neighbors (K',L') of (K,L). However, there are many meshes

such that $(R_{K',L'} - R_{K,L})(Z_{K',L'} - Z_{K,L}) > 0$ for all eight neighbors (K',L') . But this, together with (6e) and (7), implies $\beta_{(K',L')} = 0$ for all 8 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 $(R_{K',L'} - R_{K,L})(Z_{K',L'} - Z_{K,L}) > 0$ for all 8 neighbors (K',L') is

Thus for a general Lagrangian hydrodynamic mesh we must use at least a 9 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:

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

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

$$\vec{R}_K = \begin{pmatrix} \frac{\partial R}{\partial K} \\ \frac{\partial Z}{\partial K} \end{pmatrix} \text{ and } \vec{R}_L = \begin{pmatrix} \frac{\partial R}{\partial L} \\ \frac{\partial Z}{\partial L} \end{pmatrix} . \quad (8)$$

To difference eq. 8 we use the variational method.³ For our problem from eq. 8 it follows that

$$\begin{aligned} \int R dR dZ f \vec{\nabla} \cdot (D \vec{\nabla} f) &= - \int R dR dZ D(\vec{\nabla} f)^2 \\ &= - \int dK dL \left[\sqrt{\frac{DR}{j}} \left(\vec{R}_L \frac{\partial}{\partial K} - \vec{R}_K \frac{\partial}{\partial L} \right) f \right]^2 . \end{aligned} \quad (9)$$

The finite difference analogue of (9) is

$$- \sum_{(K,L)} \left[\vec{B} f \right]_{K,L}^2 \quad (10)$$

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

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

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

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, $\vec{\nabla} \cdot (D\vec{\nabla}f)$, 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 $(\vec{B}f)$ in equation (11).

Actually we shall use

$$\begin{aligned} \int R dR dZ \vec{\nabla} \cdot (D\vec{\nabla}f) &\approx -\frac{1}{4} \sum_{(K,L)} \sum_{i=1}^4 \left[\vec{B}^i f \right]_{K,L}^2 \\ &= + \sum_{(K,L)} f_{K,L} (Af)_{K,L} V_{K,L}. \end{aligned} \quad (12)$$

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

$$(\vec{B}f)_{K,L} \approx \sqrt{\frac{DR}{J}} \left(\vec{r}_L \frac{\partial f}{\partial k} - \vec{r}_K \frac{\partial f}{\partial L} \right). \quad (13)$$

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

$$(\vec{B}f)_{K,L} = K_{K,L} \vec{R}_L - L_{K,L} \vec{R}_K$$

where

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

and

$$L_{K,L} \approx \sqrt{\frac{DR}{j}} \frac{\partial f}{\partial L} \quad (14)$$

Clearly K and L are face centered quantities and we difference (14) as:

$$K_{K,L} = \Sigma_{K,L} (f_{K+1,L} - f_{K,L}) \quad , \quad (15a)$$

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

Currently LASNEX has been using $\Sigma_{K,L}^2 = (R_{K,L} + R_{K,L-1}) / ((j_{K,L}/D_{K,L}) + (j_{K+1,L}/D_{K+1,L}))$ but any method of averaging can be used without upsetting our conditions 1) through 4).

$$L_{K,L} = \Lambda_{K,L} (f_{K,L+1} - f_{K,L}) \quad , \quad (15b)$$

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

In diagrams:

$K_{K,L}$

$L_{K,L}$

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

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

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

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

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

will hold.

The difference of these two terms we call $\vec{B}^1$

$$(\vec{B}^1_f)_{K,L} = K_{K,L}(\vec{R}_L)_{K,L} - L_{K,L}(\vec{R}_K)_{K,L} \quad (16a)$$

and in diagram form

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

$$(\vec{B}^2_f)_{K,L} = K_{K-1,L}(\vec{R}_L)_{K,L} - L_{K,L}(\vec{R}_K)_{K,L} \quad (16b)$$

$$(\vec{B}^3_f)_{K,L} = K_{K-1,L}(\vec{R}_L)_{K,L} - L_{K,L-1}(\vec{R}_K)_{K,L} \quad (16c)$$

$$(\vec{B}^4_f)_{K,L} = K_{K,L} (\vec{R}_L)_{K,L} - L_{K,L-1} (\vec{R}_K)_{K,L} \quad (16d)$$

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

$$\begin{aligned} \int R dR dZ f \vec{\nabla} \cdot (D \cdot \vec{\nabla} f) &\approx -\frac{1}{4} \sum_{(K,L)} \sum_{i=1}^4 (\vec{B}^i_f)^2_{K,L} \\ &= + \sum_{(K,L)} f_{K,L} (Af)_{K,L} V_{K,L} \end{aligned} \quad (12)$$

This defines the matrix A and substituting equations (16) into (12) and shifting indices one finds:

$$\begin{aligned} V_{K,L} \Lambda_{(K,L),(K,L)} &= \sigma_{(K,L)} - \sigma_{(K-1,L)} - \lambda_{(K,L)} - \lambda_{(K,L-1)} \\ &+ \frac{1}{2} \left(\rho^1_{(K,L)} + \rho^2_{(K,L)} - \rho^3_{(K,L)} - \rho^4_{(K,L)} \right), \end{aligned} \quad (17a)$$

$$V_{K,L} A_{(K,L),(K+1,L)} = \sigma_{(K,L)} - \frac{1}{4} \left(\rho_{(K,L)}^1 + \rho_{(K+1,L)}^2 - \rho_{(K+1,L)}^3 - \rho_{(K,L)}^4 \right), \quad (17b)$$

$$V_{K,L} A_{(K,L),(K,L+1)} = \lambda_{(K,L)} - \frac{1}{4} \left(\rho_{(K,L)}^1 + \rho_{(K,L+1)}^2 - \rho_{(K,L)}^3 - \rho_{(K,L+1)}^4 \right), \quad (17c)$$

$$V_{K,L} A_{(K,L)(K+1,L+1)} = -\frac{1}{4} \left(\rho_{(K+1,L)}^3 + \rho_{(K,L+1)}^4 \right), \quad (17d)$$

$$V_{K,L} A_{(K,L),(K-1,L+1)} = \frac{1}{4} \left(\rho_{(K-1,L)}^1 + \rho_{(K,L+1)}^2 \right), \quad (17e)$$

where,

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

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

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

$$\rho_{(K,L)}^2 = \Sigma_{(K-1,L)} \Lambda_{(K,L-1)} C_{K,L},$$

$$\rho_{(K,L)}^3 = \sum_{(K-1,L)} \Lambda_{(K,L)} C_{K,L} ,$$

$$\rho_{(K,L)}^4 = \sum_{(K,L)} \Lambda_{(K,L-1)} C_{K,L} ,$$

and

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

Since VA is symmetric

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

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

In the case of an orthogonal mesh $\vec{R}_K \cdot \vec{R}_L = 0$, and so $\rho^1 = \rho^2 = \rho^3 = \rho^4 = 0$, and only the σ and λ terms remain, but equation (17) with just the σ and λ terms is nothing but the standard 5 point approximation previously used in LASNEX. 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 5 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.

In LASNEX there are two types of boundary conditions

$$d\vec{S} \cdot \vec{\nabla} f = 0 ,$$

or "no escape" boundaries, and

$$f = f_0 ,$$

or "escape" boundaries where a known vacuum energy density f_0 is given.

LASNEX has 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)

$$f_{(K,L)}^{(n+1)} - (\Delta t) \left(A f^{(n+1)} \right)_{(K,L)} = f_{(K,L)}^n$$

(3)

The basic building blocks of A are $\Sigma_{K,L}(\vec{R}_L)_{K,L}$, $\Sigma_{K,L}(\vec{R}_L)_{K+1,L}$, $\Lambda_{K,L}(\vec{R}_K)_{K,L}$ and $\Lambda_{K,L}(\vec{R}_K)_{K,L+1}$ (see eqs. (16) and (17)). $\Sigma_{K,L}$ connects zone (K,L) with zone $(K+1,L)$, and $\Lambda_{K,L}$ 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 $\Sigma_{K,L}(\vec{R}_L)_{K,L}$ and $\Sigma_{K,L}(\vec{R}_L)_{K+1,L}$ 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, or vice versa, and the face separating the two zones has "no escape" ($\hat{n} \cdot \vec{\nabla} f = 0$) boundary conditions across it, use $\Sigma_{K,L} = 0$.
- 4) 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 $\Sigma_{K,L}(\vec{R}_L)_{K,L}$ and $\Sigma_{K,L}(\vec{R}_L)_{K+1,L}$ as described above except that $\Sigma_{K,L}$ is now $(DR/j)^{1/2}$ suitably averaged between zone K,L and the vacuum and $(\vec{R}_L)_{K+1,L}$ is now given by $(\vec{R}_L)_{K+1,L} = \vec{R}_{K,L} - \vec{R}_{K,L-1}$ instead of (15d), since $\vec{R}_{K+1,L}$ and $\vec{R}_{K+1,L-1}$ may not exist. Then whenever a term with $f_B = f_{(K+1,L)}$ (e.g. $-(\Delta t)A_{(K,L),(K+1,L)}f_B$) turns up on the left hand side of eq. (3), just move it to the right hand side since f_B is known.
- 5) If (K,L) is a vacuum zone and (K+1,L) is a physical zone and the interface has "escape" boundary conditions, use $\Sigma_{K,L}(\vec{R}_L)_{K,L}$ and $\Sigma_{K,L}(\vec{R}_L)_{K+1,L}$ as described above, except that $\Sigma_{K,L}$ is now averaged between zone K+1,L and the vacuum and $(\vec{R}_L)_{K,L} = \vec{R}_{K,L} - \vec{R}_{K,L-1}$ instead of (15d). Then whenever a term with $f_B = f_{(K,L)}$ (e.g. $-(\Delta t)A_{(K+1,L)(K,L)}f_B$) 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 $\Lambda_{K,L}$.

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 $\vec{B}^i$'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.

This difference scheme is now being used in LASNEX to determine A, and the ICGG method² is used to solve the linear system,

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

at each time step.

References

- 1) R. S. Varga, Matrix Iterative Analysis, Prentice Hall, N.J. 1962, Sec. 3.5, Exercise 6.
- 2) D. S. Kershaw, "The Incomplete Cholesky - Conjugate Gradient Method", Lawrence Livermore Laboratory pub., UCLR 78333, Revision 1, 1977.
- 3) Ibid. Reference 1), section 6.1.

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