A NEW TRANSPORT DISCRETIZATION SCHEME FOR ARBITRARY SPATIAL MESHES IN XY GEOMETRY

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Received by OSTI

FEB 1 9 1991

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ABSTRACT

We introduce a new spatial discretization scheme for transport on arbitrary spatial grids in XY geometry. Our "arbitrary" spatial grid is composed of arbitrarily-connected polygons, each of which may have an arbitrary number of sides. We begin our derivation by imposing particle balance on every "corner" of each cell. (Consequently, we call our scheme the corner-balance (CB) method.) We complete the derivation by introducing simple closure formulas that relate volume-averaged unknowns to surface-averaged unknowns in each corner. We discuss the relationship of the new scheme to discontinuous finite-element methods and to multiple-balance methods. We demonstrate that on simple grids, the method reduces to very robust schemes that have been studied previously. We discuss the theoretical performance of the method in the thick diffusion limit, and provide numerical results for that limit. We present additional numerical results from simple problems that test the new scheme in other limits. Finally, we offer some concluding remarks about the method.

INTRODUCTION

We introduce a new spatial discretization scheme for the XY-geometry transport equation. The method is designed to be applicable to arbitrily-connected grids with arbitrary polygonal cells. It resembles discontinuous finite-element methods[1-4] in some ways, and multiple-balance methods[5] in others. Its derivation is simple and intuitively appealing, even on arbitrary polygonal cells. We find that the method is more robust than standard discontinuous finite-element methods, especially for problems with optically thick cells.

The basis of the new scheme is particle conservation over sub-cell volumes that we call *corners*. We therefore call the scheme the corner-balance (CB) method. There is one conservation equation in each corner; it contains volume-averaged as well as surface-averaged unknowns. We close our system of equations with simple approximations that relate these different kinds of unknowns. We note that this concept of cell *corners* as the fundamental volume of discretization is not our creation; Burton[6] has used it extensively in computational hydrodynamics on arbitrary grids.

In this paper we derive the CB scheme in full generality, assuming arbitrary polygonal cells. We then examine the scheme in some simple limits. We find that in slab geometry the method reduces to a very robust modified linear discontinuous (MLD) finite-element scheme that has been studied previously.[7] We find that on rectangles in XY geometry, the method reduces to a modified bilinear discontinuous (MBLD) finite-element scheme that has been introduced and studied very recently.[4,8] This MBLD scheme performs very well in the thick diffusion limit, even in the presence of unresolved boundary layers, but it exists only for rectangular grids.[4] We note that the CB derivation of these methods is much simpler than their original derivations and modifications, and that furthermore it applies to arbitrary polygonal cells. We find, however, that given non-

rectangular cells the CB method does not perform as robustly in the thick diffusion limit as it does on rectangular cells. We present numerical results from several test problems, comparing the CB scheme against a discontinuous finite-element method. We close with some concluding remarks.

DERIVATION OF THE CB SCHEME

We begin with the definition of a *corner*, which is the volume of a polygonal cell that we associate with a given vertex of the cell. This concept, taken from Burton[6], is defined graphically in Fig. 1 below. The corners in a cell are defined by line segments that connect the midpoint of every edge to a common point in the interior. (The coordinates of the interior point are averages of the cell's vertex coordinates.) Each corner is a quadrilateral; two of its sides are formed by halves of cell edges, and two are formed by the aforementioned line segments. Within each cell, we number corners in a counter-clockwise direction. That is, corner $c+1$ is counter-clockwise of corner c. We assign the index $c+1/2$ to the edge that connects corners c and $c+1$.

Figure 1. A *corner*, whose index is c, of a polygonal cell.
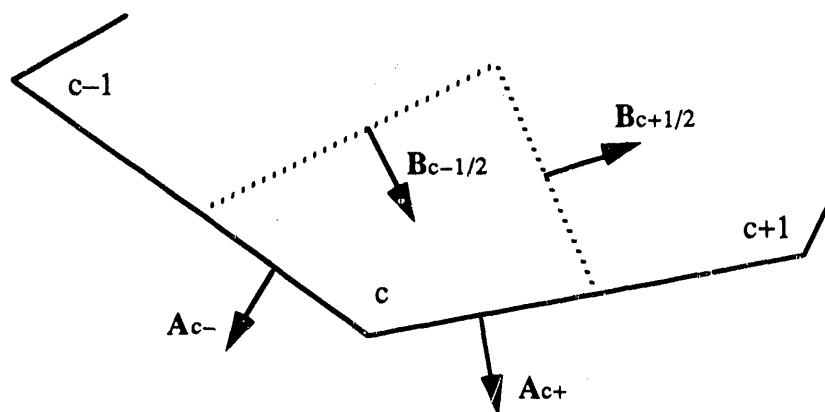
We note that each corner has four bounding surfaces. For each of these bounding surfaces, we shall need the product of the surface area and the unit normal. For corner c, these are $A_{c\pm}$ and $B_{c\pm1/2}$, as depicted in Fig. 1. We note that the $A_{c\pm}$ vectors are outward, $B_{c-1/2}$ is inward for corner c (but outward for $c-1$), and $B_{c+1/2}$ is outward for corner c (but inward for $c+1$).

We write the transport equation for a given energy group as follows:

$$\mathbf{\Omega \cdot \nabla} \psi + \sigma_t \psi(r, \mathbf{\Omega}) = Q(r, \mathbf{\Omega}) , \quad r \in D , \tag{1a}$$

$$\psi(r, \mathbf{\Omega}) = F(r, \mathbf{\Omega}) , \qquad r \in \partial D , \; \mathbf{n \cdot \Omega} < 0 , \tag{1b}$$

where ψ is the angular flux, F is the incident angular flux, σ_t is the total cross section, and Q is *total* source (including fission, within-group scattering, scattering in from other groups, etc.). We integrate the transport equation over corner c, obtaining a balance equation for the corner. After we use the divergence theorem to convert the first term to a surface integral, we obtain:

$$\int_{\partial c} d^2r\,\mathbf{\Omega}\cdot\mathbf{n}\,\psi + \int_c d^3r\,\sigma_t\psi = \int_c d^3r\,\sigma_t Q\ , \qquad \text{or}$$

$$\mathbf{\Omega}\cdot\left[\mathbf{A}_{c+}\psi_{c+} + \mathbf{A}_{c-}\psi_{c-} + \mathbf{B}_{c+1/2}\psi_{c+1/2} - \mathbf{B}_{c-1/2}\psi_{c-1/2}\right] + \sigma_{tc}V_c\psi_c = V_c Q_c\ . \tag{2}$$

Here $\psi_{c\pm}$ and $\psi_{c\pm1/2}$ are surface-averaged angular fluxes, while ψ_c and Q_c are volume-averaged. These quantities are located as shown in Fig. 2 below.

Figure 2. Location of unknowns in a corner.
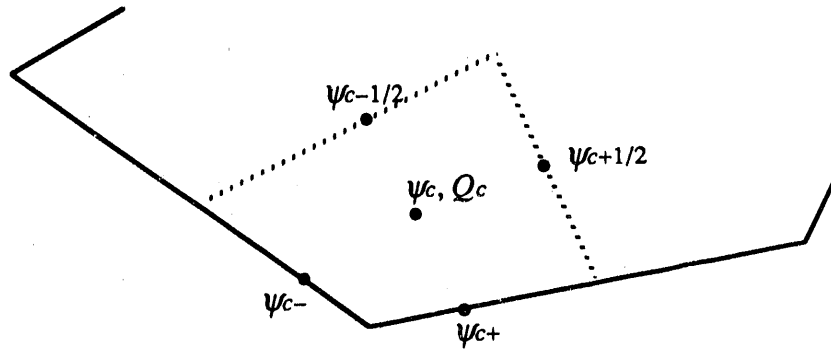
At this point, we have one Eq. (2) per corner but more than one unknown per corner. We now introduce simple approximations to close our system of equations. These relations define each surface-averaged unknown in terms of the volume-averaged unknowns on either side of the surface. On surfaces *between cells*, we define each surface-averaged quantity to be the *upstream* volume-averaged quantity. On surfaces between corners in the *same cell*, we define the surface-averaged quantity to be the half the sum of the two corner-averaged quantities. Introducing these approximations into Eq. (2), we obtain our CB scheme:

$$\mathbf{\Omega}\cdot\left[\mathbf{A}_{c+}\psi_{c+} + \mathbf{A}_{c-}\psi_{c-} + \mathbf{B}_{c+1/2}\frac{\psi_c + \psi_{c+1}}{2} - \mathbf{B}_{c-1/2}\frac{\psi_c + \psi_{c-1}}{2}\right] + \sigma_{tc}V_c\psi_c = V_c Q_c\ , \tag{3}$$

$$\psi_{c+} \equiv \begin{cases} \psi_c\ , & \mathbf{A}_{c+}\cdot\mathbf{\Omega} > 0\ , \\ \psi_{inc}\ , & \mathbf{A}_{c+}\cdot\mathbf{\Omega} < 0\ , \end{cases} \tag{4a}$$

$$\psi_{c-} \equiv \begin{cases} \psi_c\ , & \mathbf{A}_{c-}\cdot\mathbf{\Omega} > 0\ , \\ \psi_{inc}\ , & \mathbf{A}_{c-}\cdot\mathbf{\Omega} < 0\ . \end{cases} \tag{4b}$$

We note that in Eqs. (4), ψ_{inc} refers to the angular flux impinging on the cell edge. For interior cells, this is the angular flux from the neighboring cell. For cell edges on the problem boundary ∂D, it is the incident angular flux, F, of the boundary condition (1b).

Equations (3) and (4) define our CB scheme for transport on arbitrary spatial grids in XY geometry. We remark that the equations are very simple, both conceptually and algebraically.

$$\frac{\eta \Delta x}{2}\psi_{4-} - \frac{\mu \Delta y}{2}\psi_{4+} - \frac{\eta \Delta x}{2}\frac{\psi_4 + \psi_1}{2} + \frac{\mu \Delta y}{2}\frac{\psi_4 + \psi_3}{2} + \frac{\Delta x \Delta y}{4}\sigma_t \psi_4 = \frac{\Delta x \Delta y}{4}Q_4 \quad , \qquad (6)$$

where c=1 refers to the lower left corner of the rectangle, and the other corners are numbered in the counter-clockwise direction (c=4 is the top left corner). This scheme is algebraically equivalent to the "heavily modified" BLD scheme that is analyzed in reference [4]. This scheme has excellent properties in the thick diffusion limit. It appears to be a robust method; once again, we are encouraged that our CB scheme is equivalent to it in the rectangle limit.

The "heavily modified" BLD scheme was obtain via several approximations to the standard BLD scheme.[4] One of these is mass-matrix lumping, the physical content of which is to make certain terms *local*. It is interesting that the other modifications are also *localizing* in some sense. We remark that the CB scheme is automatically localizing, in that balance is imposed over *sub-cell* volumes.

CB in the Thick Diffusion Limit

We have seen that the CB scheme performs exceptionally well in the thick diffusion limit, provided spatial cells are slabs or rectangles. Here we briefly discuss its performance in the more general case. We have performed an asymptotic analysis[4] of the CB scheme in the thick diffusion limit, allowing the spatial grid to be arbitrary. We find that for all grids, the leading-order CB solution inside coarsely-zoned diffusive regions is isotropic and continuous. We find further that this leading-order interior solution satisfies a discretization of the diffusion equation, again regardless of the grid. These are highly desirable properties, for the correct leading-order solution in the interior of such regions is isotropic and satisfies a diffusion equation. However, we find that as cells become distorted, the performance of the scheme degrades. This occurs in two ways. First, the diffusion discretization satisfied by the leading-order solution becomes less robust, in the sense that it may permit oscillations and/or negative solutions. Second, the boundary condition satisfied by the leading-order solution inside diffusive regions can become inaccurate. These are the predictions of our asymptotic analysis; at present we have numerically tested only the rectangle limit.

We are not completely satisfied with this behavior, and we are attempting to improve it. However, we reiterate that the diffusion-limit performance of CB on rectangular cells is exceptionally good. Thus, given arbitrary cells that are not too distorted, we expect the CB scheme to perform reasonably well in this limit.

III. NUMERICAL RESULTS

Our first test problem is a transparent square, the left side of which is subjected to a mono-directional beam of particles. The particles are directed downward and rightward ($\mu = 1/\sqrt{3}$, $\eta = -1/\sqrt{3}$). Physically, the particles simply stream through the lower left half of the square; the solution in the upper right half is zero. We use the S_2 level-symmetric discrete-ordinates quadrature set for this problem; it has an ordinate in exactly the beam direction. When we place a grid of square spatial cells on the problem, we find that the discontinuity in the exact solution occurs along the diagonals of certain spatial cells. This will cause trouble with most spatial discretization schemes, and CB is no exception. We place a 20 by 20 grid of cells on the problem, and solve it with CB and with the mass-matrix-lumped bilinear discontinuous finite-element method (LBLD). In Figure 3, we display the exact, the LBLD, and CB solutions. Both the LBLD and CB solutions suffer from numerical diffusion (spreading of the discontinuity) as well as undershoot and overshoot. The two methods over- and under-shoot by approximately the same amount. We see that the CB method introduces somewhat more numerical diffusion than does LBLD, but not a great deal more.

We display our second test problem in Fig. 4. It problem contains 5 regions: a source region, two thick absorbing regions, a very thin absorbing region, and a very thick diffusive region. Physically, most particles are born in the source region either mostly leak out or are absorbed in one of the thick absorbing regions. The more interesting particles are born in the lower part of the source region, stream through the thin region, and impinge on the diffusive region. We have solved this problem numerically using the standard bilinear discontinuous finite-element method (BLD), the mas-matrix-lumped lumped BLD method, and our CB method. The spatial grid is indicated by dotted lines in Fig. 4. We display a crude shaded-contour depiction of the results in Fig. 5. The BLD scheme generates negative scalar fluxes in several regions; we depict negative values as solid white in the figure. The LBLD scheme is better, but it too generates negative scalar fluxes, mainly near the edges of the diffusive region. The CB scheme generates *no negative scalar fluxes* in this problem. To demonstrate the diffusion-limit performance of the method, we have extracted the LBLD and CB solutions in the diffusive region. We present an enlarged contour plot of both solutions in Fig. 6. In crude features, the two are similar. In detail, however, the CB solution is a better representation of the correct diffusion solution, in several ways. For example, it is positive, whereas the LBLD solution is not. Further, the LBLD solution shows evidence of "remembering" that incident particles were directed to the right; the CB solution does not. We know from asymptotic analyses[9] that the exact solution, to leading order, does not "remember" such information.

CONCLUSIONS

We have introduced a new spatial discretization scheme for the transport equation in XY geometry. The scheme, which is based on sub-cell balance equations, is applicable to arbitrarily-connected spatial grids composed of arbitrary polygons. We have shown that our scheme, which we call the corner-balance (CB) method, shares some features of multiple-balance methods[5] and discontinuous finite-element methods. We have shown that given slab or rectangular cells, the method reduces to recently-proposed schemes that are based on discontinuous finite elements. These schemes are quite robust and perform very well in thick, diffusive regions.

We have mentioned that a heavily-modified discontinuous finite-element method (DFEM) for spatial discretization performs very well given rectangular spatial cells in XY geometry. The present work began as an attempt to create a (heavily-modified, if necessary) DFEM that would perform well on arbitrary spatial grids. We have not been successful in this attempt. Instead, we have been led by our analyses to something new, namely the corner-balance approach. Our new method is quite simple, both conceptually and algebraically. We remark that the aforementioned modified DFEMs require quite a bit of algebraic effort to derive, and then quite a bit of analysis and modification before they actually perform well. We reiterate, moreover, that the modified DFEM approach does not appear to generalize to arbitrary grids in a straightforward manner.

We have presented numerical results from two test problems, comparing our CB scheme against the standard bilinear DFEM and a mass-matrix-lumped version of the bilinear DFEM. Our scheme appears produce slightly more numerical diffusion than the DFEMs do. However, given a difficult problem with coarse spatial zoning, CB clearly outperforms the DFEMs. All of our tests to date have employed rectangular grids.

We have analyzed the thick-diffusion-limit behavior of the CB scheme under the assumption of an arbitrary spatial grid. (We have yet to test the method on such a grid.) Our analysis predicts that the performance of the scheme will degrade, in thick diffusive regions, as the spatial grid distorts. We are not satisfied with this behavior, and we are investigating ways to improve the scheme. We intend to retain the balance equation for each corner; our efforts are focused on obtaining "closure relations" that are more accurate for distorted cells.

ACKNOWLEDGEMENTS

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9. F. Malgavi and G.C. Pomraning, "Initial and Boundary Conditions for Diffusive Linear Transport Problems," to appear in *J. Math. Physics* (1990).

Figure 3. Streaming problem (inset) and solutions. LB = lumped bilinear, CB = corner balance.
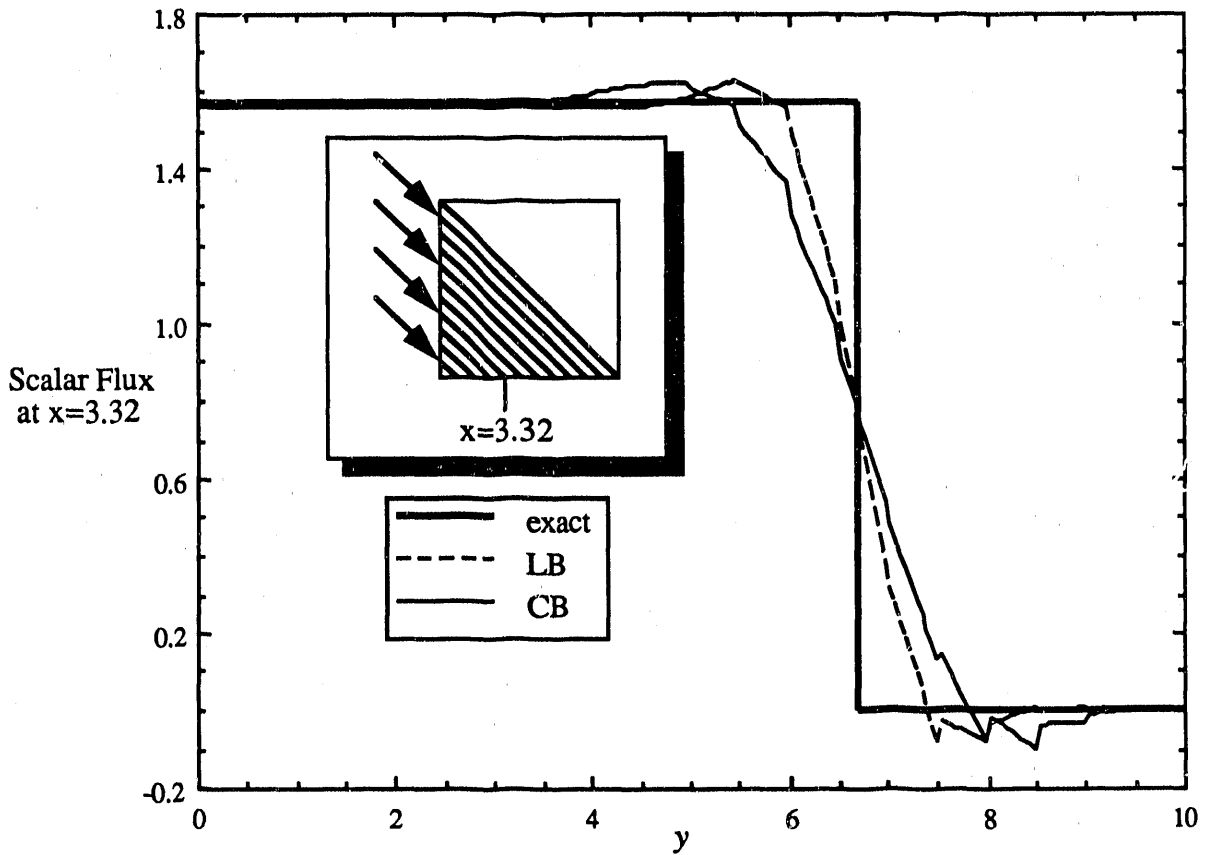

Scalar Flux
at x=3.32

x=3.32

exact
LB
CB

Figure 4. Test Problem 2. Dotted lines indicate cell boundaries. Boundaries are vacuum.

$\sigma_t = 1.$
$\sigma_a = 0.$
$Q = 1.$

$\sigma_t = 10.$
$\sigma_a = 10.$
$Q = 0.$

$\sigma_t = 1000.$
$\sigma_a = 0.$
$Q = 0.$

$\sigma_t = .001$
$\sigma_a = .001$
$Q = 0.$

$\sigma_t = 10.$
$\sigma_a = 10.$
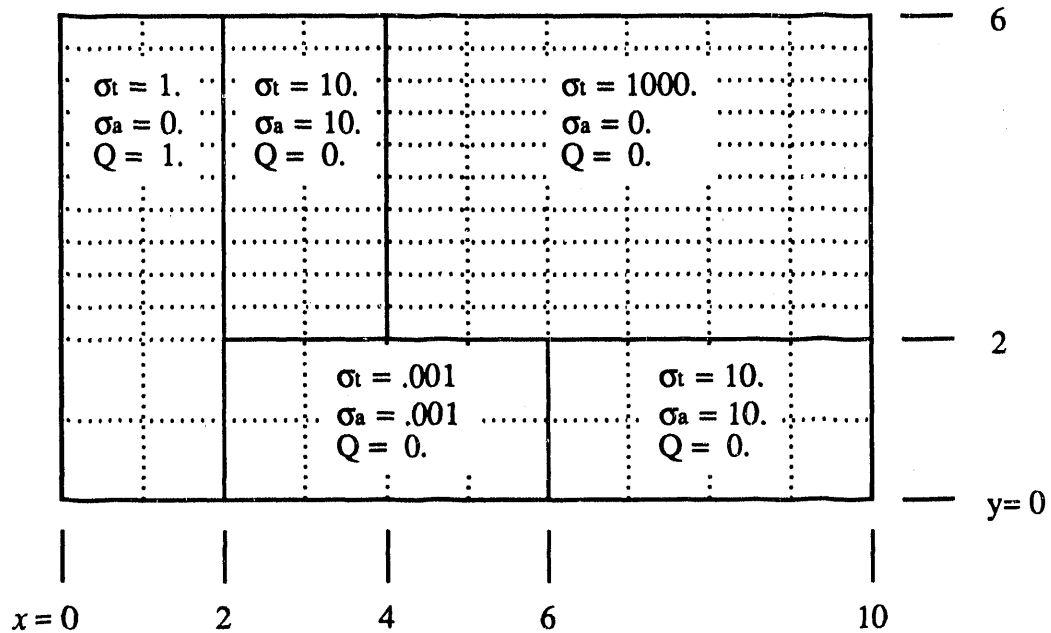$Q = 0.$

6

2

y= 0

x = 0   2   4   6   10

Figure 5. Shade-contour representation of logarithm of solutions to Test Problem 2.
Solid white regions indicate negative scalar fluxes.
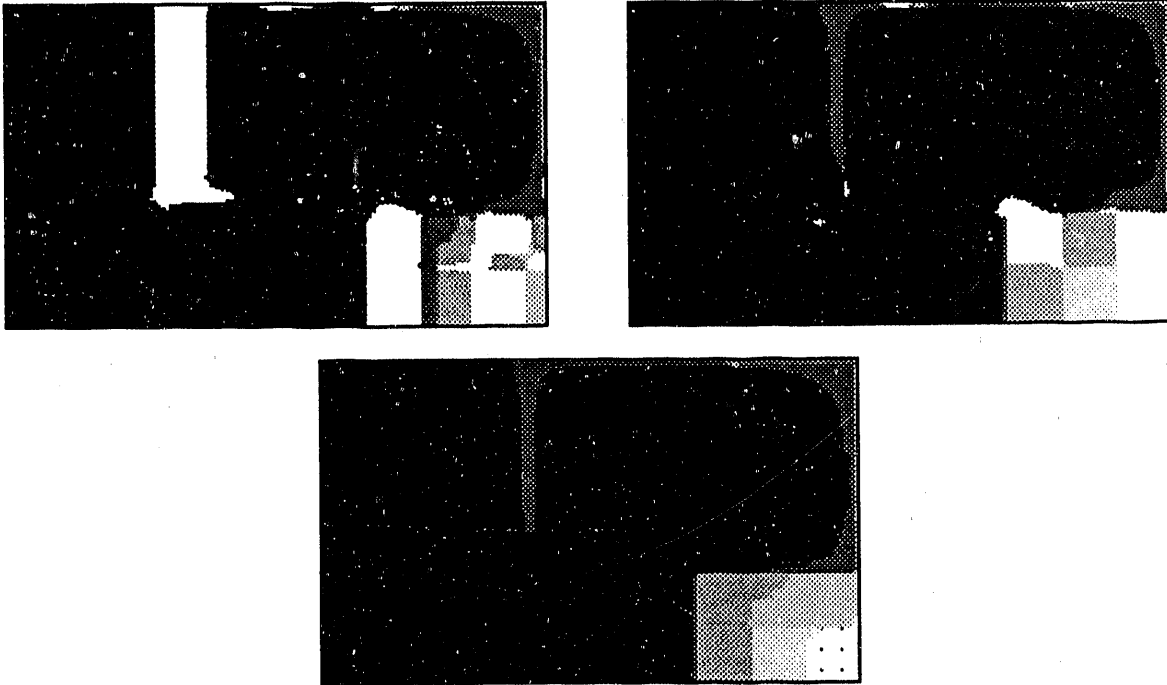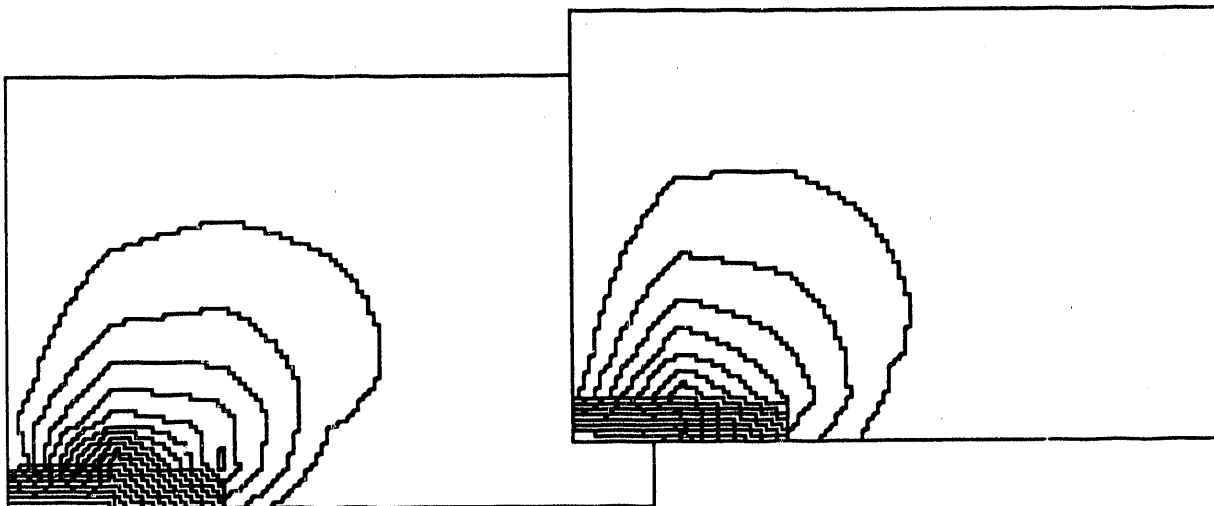BLD (top left), mass-lumped BLD (top right), and CB (bottom).

Figure 6. Solution contours from diffusive region of Test Problem 2 (enlarged by factor of 2).
Mass-lumped BLD is left; CB is right.

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