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Diffusion-Accelerated Solution of the 2-D S_n Equations with Bilinear-Discontinuous Differencing

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ABSTRACT

A new diffusion-synthetic acceleration scheme is developed for solving the 2-D S_n equations in X-Y geometry with bilinear-discontinuous finite-element spatial discretization. This method differs from previous methods in that it is unconditionally efficient for problems with isotropic or weakly anisotropic scattering. Computational results are given which demonstate this property.

INTRODUCTION

The purpose of this work is to introduce a new diffusion-synthetic acceleration (DSA) scheme for solving the 2-D S_N equations in X-Y geometry with bilinear-discontinuous (BLD) finite-element spatial discretization. Our method is the first DSA method for the BLD S_N equations to be unconditionally efficient for problems with isotropic or weakly anisotropic scattering. For instance, Adams and Martin[1] have developed a DSA scheme based upon a BLD mixed finite-element discretization of the diffusion equation. This diffusion equation has a non-standard asymmetric form and is not ameanable to standard diffusion solution techniques. Adams and Martin were unable to define an unconditionally efficient solution technique for this equation. Although the spectral radius associated with their DSA method is always significantly less than one, their method nonetheless becomes inefficient in problems with high scattering ratios because their BLD diffusion equation becomes difficult to solve. Wareing, Larsen, and Adams[2] attempted to circumvent this difficulty by developing a DSA method based upon a diffusion discretization asymptotically derived from the BLD S_n equations. This asymptotic diffusion equation is much simpler than the BLD diffusion equation of Adams and Martin, and has a standard symmetric positive-definite form. Consequently, it can be efficiently solved under all conditions using Dendy's black-box multigrid method.[3] Unfortunately, the DSA method of Wareing-Larsen-Adams gives a spectral radius which

approaches unity in problems with both high scattering ratios and high aspect-ratio spatial zoning.

BACKGROUND

Before describing our method in detail, it is appropriate to review the basic concept of synthetic acceleration. Suppose that we wish to solve the following linear system of equations:

$$A\vec{x} = \vec{y} \quad , \tag{1}$$

where A is a matrix, $\vec{x}$ is the solution vector, and $\vec{y}$ is the source vector. If the matrix A is too large to solve directly, a basic iteration scheme is defined by splitting A into the difference of two matrices:

$$A = B - C \quad , \tag{2}$$

where the matrix B can be easily inverted. The corresponding iteration scheme can be represented as follows:

$$x^{\ell+1} = B^{-1}Cx^{\ell} + B^{-1}\vec{y} \quad , \tag{3}$$

where ℓ is the iteration index. Let us define the error associated with the $\ell + 1$'th solution as follows:

$$\vec{\epsilon}^{\,\ell+1} = \vec{x} - \vec{x}^{\,\ell+1} \quad , \tag{4}$$

where $\vec{x}$ denotes the solution to Eq. (1). It is not difficult to demonstrate that this error satisfies the following equation:

$$A\vec{\epsilon}^{\,\ell+1} = \vec{R}^{\,\ell+1} \quad , \tag{5}$$

where the residual is given by

$$\vec{R}^{\,\ell+1} = \vec{y} - A\vec{x}^{\,\ell+1} \quad . \tag{6}$$

In principle, one can obtain the error by solving Eq. (5), but this equation is just as difficult to solve as Eq. (1). Consequently, an exact solution of this error equation is not practical. However, it is conceivable that obtaining an approximate solution to the error equation could yield an error estimate that would significantly improve the accuracy of $\overrightarrow{x}^{\ell}$, and thereby accelerate the convergence of the iterative process. This is the basic theme of synthetic acceleration methods. For example, in the simplest synthetic acceleration scheme, one would approximate A in Eq. (5) with a *low-rank* operator:

$$< A > < \overrightarrow{\epsilon} >^{\ell+1} = < \overrightarrow{R} >^{\ell+1} \quad , \tag{7}$$

where "<>" denotes a low-rank approximation. The low-rank residual appearing in Eq. (7) would be obtained from the full-rank residual be means of a projection:

$$< \overrightarrow{R} >^{\ell+1} = P \overrightarrow{R}^{\ell+1} \quad , \tag{8}$$

where P is an operator which projects from the full-rank space to the low-rank space. The low-rank error equation would be solved to obtain the low-rank error estimate:

$$< \overrightarrow{\epsilon} >^{\ell+1} = < A >^{-1} < \overrightarrow{R} >^{\ell+1} \quad . \tag{9}$$

A full-rank error estimate would be obtained from the low-rank error-estimate by interpolation:

$$\overrightarrow{\epsilon}^{\ell+1} = T < \overrightarrow{\epsilon} >^{\ell+1} \quad , \tag{10}$$

where T is an interpolation operator. The error estimate would then be added to the iterate at step $\ell + 1$ to obtain an improved or accelerated iterate.

To summarize, an accelerated iteration is carried out as follows.

1. A basic iteration is performed:

$$x^{\ell+\frac{1}{2}} = B^{-1} C x^{\ell} + B^{-1} \overrightarrow{y} \quad , \tag{11}$$

   where the index $\ell + \frac{1}{2}$ is used in anticipation of the acceleration step.

2. The residual associated with the basic iterate is calculated:

$$\overrightarrow{R}^{\ell+\frac{1}{2}} = \overrightarrow{y} - A \overrightarrow{x}^{\ell+\frac{1}{2}} \quad . \tag{12}$$

3. The low-rank residual is calculated from the high-rank residual via projection:

$$< \overline{R} >^{\ell+\frac{1}{2}} = P \overline{R}^{\ell+\frac{1}{2}} \quad . \tag{13}$$

4. The low-rank error equation is solved:

$$< \overline{\epsilon} >^{\ell+\frac{1}{2}} = < A >^{-1} < \overline{R} >^{\ell+\frac{1}{2}} \quad . \tag{14}$$

5. The high-rank error estimate is calculated from the low-rank estimate via interpolation:

$$\overline{\epsilon}^{\ell+\frac{1}{2}} = T < \overline{\epsilon} >^{\ell+\frac{1}{2}} \quad , \tag{15}$$

6. The high-rank error estimate is added to the unaccelerated iterate to obtain the accelerated iterate:

$$x^{\ell+1} = x^{\ell+\frac{1}{2}} + \overline{\epsilon}^{\ell+\frac{1}{2}} \quad . \tag{16}$$

A synthetic acceleration scheme will be effective if two conditions are met. First, the low-rank equation must accurately estimate the errors which are poorly attenuated by the basic iteration scheme. Second, the low-rank operator must not significantly overestimate the errors which are strongly attenuated by the basic iteration scheme.

For the specific case of diffusion-synthetic acceleration, A is the transport operator, B is the sum of the streaming and removal operators, C is the scattering operator, and $< A >$ is the diffusion operator. The scattering may be anisotropic, but only the isotropic component of the angular flux is accelerated. The projection operator, P, maps an angular flux function to its isotropic or P_0 moment, and the interpolation operator, T, maps a P_0 moment to the P_0 angular flux expansion. DSA is effective in terms of the error reduction per iteration with isotropic or weakly anisotropic scattering for two reasons. First, the errors which are poorly attenuated by the transport sweep are diffusive and thus accurately calculated with the diffusion operator. Second, the non-diffusive errors which are strongly attenuated by the transport sweep are underestimated by the diffusion equation.

More complicated synthetic acceleration methods have multiple levels of acceleration. For instance, the low-rank operator used in the Eq. (14) may still be too large or complicated to be solved efficiently using a direct or unaccelerated iterative method. Attempts to further simplify the low-rank operator may be fruitless because an operator which is simple enough to solve easily may be too simple to provide an effective approximation to the high-rank operator. One possible solution is to develop an accelerated iteration scheme for inverting the low-rank operator. This leads to a scheme with two acceleration levels. Any number of levels is possible. The low-rank operator on each level approximates the higher-rank operator on the level above it. Such schemes are also referred to as multigrid schemes. In multigrid terminology, the high-rank and low-rank operators are called the "fine-grid" and "coarse-grid" operators. In general, optimum efficiency in a multilevel scheme is obtained by fully solving the error equation only on the lowest level. The error equations on the intermediate levels are solved approximately.

THE NEW DSA METHOD

The DSA method which we have developed can be thought of as a multi-level synthesis of the Adams-Martin and Wareing-Larsen-Adams methods. In particular, at the first level, the BLD S_N iterations are accelerated with a slightly modified version of the Adams-Martin BLD diffusion equation. At the second level, the BLD diffusion iterations are accelerated with a bi-linear continuous (BLC) diffusion equation which is equivalent to the Wareing-Larsen-Adams asymptotic diffusion equation. Finally, at the third level, the BLC diffusion iterations are accelerated with Dendy's black-box multigrid algorithm. The overall DSA algorithm resulting from this multi-level approach is unconditionally efficient. In particular, a homogeneous infinite-medium Fourier analysis performed by Adams and Martin for the first iteration level gives a worst-case spectral radius of about 0.5. We have performed a similar Fourier analysis for the second iteration level which also gives a worst-case spectral radius of about 0.5. Dendy's algorithm, which is used on the third level of acceleration, has previously been shown to have a worst-case spectral radius of about 0.1. Unconditional efficiency for the overall DSA scheme follows directly from the unconditional efficiency achieved on each level.

To be fully consistent with the Fourier analyses which we have performed, the BLD and BLC diffusion solutions used in our acceleration scheme should be iterated to convergence. However, it is much more efficient to accept the solutions to these low-rank

equations after a fixed number of iterations. In particular, the BLD solution is accepted after three iterations, and the BLC solution is accepted after one iteration.

In order to facilitate a more detailed description of our acceleration technique, we now describe certain basic aspects of the spatial differencing schemes used on each level. Both the BLD S_n differencing scheme and the BLD diffusion differencing scheme have unknowns at the corners of each spatial cell. These locations are shown in Fig. 1. The BLD S_n scheme has an angular flux unknown at each location while the BLD diffusion scheme has a scalar flux unknown at each location. The BLC diffusion differencing scheme has a scalar flux unknown at each corner of the mesh. This is illustrated in Fig. 2.

The BLD S_n differencing scheme which we use is identical (after a similarity transformation) to that used by Adams and Martin,[1] and the BLC diffusion differencing scheme which we use is identical to that used by Wareing, Larsen, and Adams.[2] However, the BLD diffusion differencing scheme which we use is equivalent only on the interior of the mesh to the Adams-Martin scheme. Our scheme has additional scalar flux unknowns along the outer boundaries of the mesh, as illustrated in Fig. 3. These fluxes are referred to as "void" fluxes because they are associated with cells which are outside of the mesh. Although the void fluxes couple to the regular fluxes on the outer boundaries of the mesh, the solutions obtained for all of the regular fluxes are identical to those obtained with the Adams-Martin scheme. Since only the regular fluxes are explicitly used to estimate the BLD S_n iterate errors, our BLD diffusion scheme is completely equivalent (for acceleration purposes) to that of Adams and Martin. However, for reasons explained below, we can solve our BLD diffusion equations more efficiently than we can solve those of Adams and Martin.

Wareing, Larsen, and Adams asymptotically derived their BLC diffusion equations from the BLD S_n equations. However, they substituted standard Marshak boundary conditions for the asymptotic conditions because the later are not suitable for acceleration purposes. We found that the BLC diffusion equations can also be derived asymptotically from the Adams-Martin BLD diffusion equations. It was this result which first suggested to us that the BLC diffusion equations might be an effective low-rank approximation to the Adams-Martin BLD diffusion equations. As expected, we found that the asymptotic boundary conditions for the BLC equations are not suitable for acceleration purposes, so we substituted standard Marshak conditions. Unexpected difficulties

Figure 1: Bi-Linear-Discontinuous Spatial Mesh

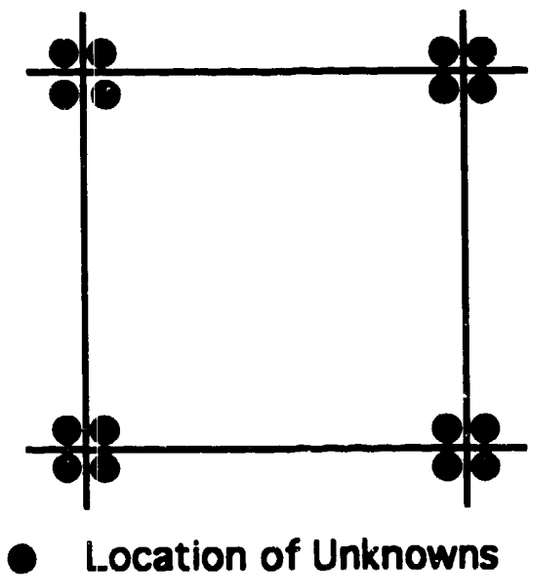
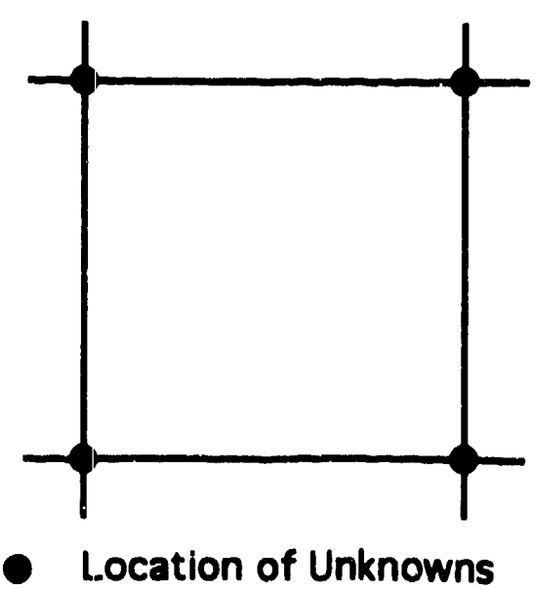


Figure 2: Bi-Linear-Continuous Spatial Mesh



arose on the outer boundaries of the mesh when we attempted to accelerate the iterative convergence of the Adams-Martin BLD diffusion scheme with the BLC diffusion scheme.

We were able to eliminate these difficulties after recognizing that a simple relationship exists between the Adams-Martin BLD equations and the BLC equations on the interior of the mesh. Specifically, the interior-mesh BLC diffusion equations can be derived from the interior-mesh Adams-Martin BLD diffusion equations in the following manner:

1. Assume that four BLD fluxes associated with each corner of the mesh are identical. This is equivalent to requiring continuity of the scalar flux solution, and leaves a single scalar flux unknown at each corner.

2. Obtain an equation for each "continuous" corner flux by summing the BLD equations for the four scalar fluxes associated with that corner.

Having recognized the existence of this relationship on the interior of the mesh, we postulated that it should also apply on the mesh boundaries. Our BLD diffusion scheme was obtained by modifying the Adams-Martin scheme to achieve this property. Specifically, if one follows the derivation procedure defined above using our BLD diffusion equations, and one carries out the procedure at all cell corners (including those on the outer mesh boundaries,) one obtains the BLC diffusion equations with Marshak boundary conditions. The difficulties which we encountered on the outer boundaries when trying to accelerate the Adams-Martin BLD diffusion scheme with the BLC diffusion scheme do not arise when our scheme is substituted for the Adams-Martin scheme.

The basic iteration scheme used for our BLD diffusion equations is a line-Jacobi scheme.[4] One complete line-Jacobi iteration consists of an x-line-Jacobi iteration followed by a y-line-Jacobi iteration. An x-line consists of all of the fluxes having the same y-coordinate, and a y-line consists of all of the fluxes having the same x-coordinate. An x-line is illustrated in Fig. 4. The iteration equations for each x-line iteration are constructed from the full equations by lagging the coupling to all other fluxes not in the x-line. The lagged fluxes are held at iterate values associated with the beginning of the x-line-Jacobi iteration, and the fluxes in all x-lines are calculated with the same lagged values. A y-line-Jacobi iteration is analogously defined. The lagged fluxes are updated between the x-line-Jacobi and y-line-Jacobi iterations.

The accelerated iteration scheme used for the BLC equations is Dendy's black-box multigrid scheme.[3] This is a true multigrid scheme which uses diffusion operators de-

Figure 3: Bi-Linear-Discontinuous Void Fluxes

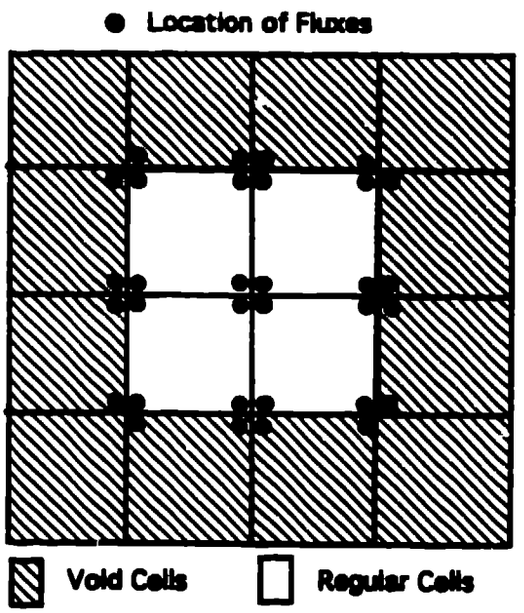
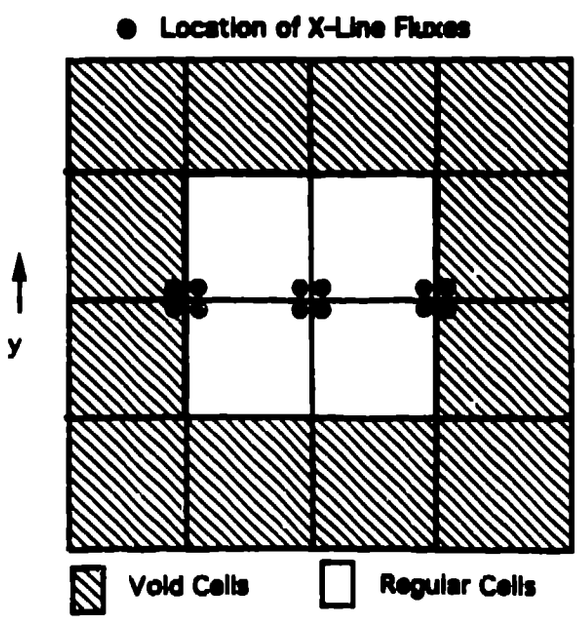


Figure 4: Fluxes In One X-Line



fined on coarse spatial grids as low-rank operators.

We now give a final and more detailed description of our DSA method. One accelerated S_n iteration proceeds in the following manner:

1. The BLD S_n scattering sources are calculated and the sweep equations are solved.
2. The isotropic moments of the S_n residuals are calculated for use in the BLD diffusion equation.
3. A line-Jacobi iteration is performed on the BLD diffusion equations.
4. The BLD diffusion residuals are calculated and projected onto the BLC diffusion mesh by suming the four BLD residuals associated with each corner to obtain a single corner residual.
5. One V-cycle of Dendy's black-box multigrid algorithm is performed on the BLC diffusion equations.
6. The BLC diffusion iterate is interpolated onto the BLD diffusion mesh by assuming continuity, i.e., the four BLD-mesh values needed for each corner are set equal to the single BLC corner value.
7. The interpolated BLC iterate is then added to the BLD iterate.
8. Steps 3 through 7 are repeated twice, resulting in three "acccelerated" BLD diffusion iterations.
9. The BLD diffusion iterate is added to the BLD S_n scalar flux iterate. This completes one accelerated S_n iteration.

COMPUTATIONAL RESULTS

In this section we give computational results which demonstrate that our DSA method remains efficient for problems that cause the Adams-Martin[1] and Wareing-Larsen-Adams[2] methods to become inefficient. We have performed a set of calculations corresponding to a homogeneous rectangular region with isotropic scattering, a scattering ratio of unity, and a uniform isotropic inhomogeneous source. There are 25 zones along

the x-axis and 25 zones along the y-axis. The zone widths are fixed in each calculation, but vary between calculations. The x and y widths are not necessarily identical in each calculation. The rectangle has reflective boundaries on two adjacent sides and vacuum boundaries on the other two sides. All of the calculations were performed on a CRAY-YMP computer using S_4 quadrature. The scalar flux in each calculation was subject to a pointwise relative convergence criterion of 10^{-4}. In Table 1 we give for each problem configuration, the number of iterations required to converge the S_n solution, the associated CPU time, and the CPU time spent doing the DSA. It can be seen from Table 1 that our method is efficient even with a scattering ratio of unity and extremely high aspect-ratio spatial zoning. The former condition causes difficulty for the Adams-Martin method, and the latter condition causes difficulty for the Wareing-Larsen-Adams method. The theoretical analyses and the computational testing which we have done indicate that our method is efficient for all problems with isotropic or weakly anisotropic scattering.

Table 1. Computational Results

$\Delta X\,(mfp)$	$\Delta Y\,(mfp)$	Total CPU (sec)	DSA CPU (sec)	Iterations
0.1	0.1	2.31	0.67	6
0.1	1.0	2.70	0.78	7
0.1	5.0	2.32	0.67	6
0.1	10.0	2.32	0.67	6
0.1	100.0	2.32	0.67	6
1.0	1.0	3.08	0.90	8
1.0	5.0	3.08	0.90	8
1.0	10.0	3.08	0.90	8
1.0	100.0	3.08	0.90	8
5.0	5.0	2.32	0.67	6
5.0	10.0	2.32	0.67	6
5.0	100.0	2.32	0.67	6
10.0	10.0	1.93	0.56	5
10.0	100.0	1.93	0.56	5
100.0	100.0	1.93	0.56	5

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