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Unconditionally Stable Diffusion-Synthetic Acceleration Methods for the Slab Geometry Discrete Ordinates Equations. Part II: Numerical Results

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Diffusion-synthetic acceleration methods that have been proven analytically to be stable for model discrete ordinates problems (for infinite media, with isotropic scattering, constant cross sections, and a uniform spatial mesh) are shown to be experimentally stable for realistic problems (for finite media, with anisotropic scattering, variable cross sections, and a nonuniform spatial mesh). Also, the effect of negative flux fixups on the acceleration methods is discussed.

I. INTRODUCTION

In a companion paper[1] (hereafter referred to as Part I, all equations of which are prefaced by I), we derived acceleration methods for spatial differencing schemes appropriate to the slab geometry discrete ordinates equations. These acceleration methods are applicable to problems with anisotropic scattering, variable cross sections, general boundary conditions, and a nonuniform spatial mesh. The stability analyses for these methods, however, apply only to infinite medium problems with isotropic scattering, constant cross sections, and a uniform spatial mesh. In this paper we test these acceleration methods on one-group problems of the former type and demonstrate that the model problem stability results remain qualitatively correct: The spectral radius (which measures the asymptotic error reduction between iterations) for each method satisfies

$$\mathrm{spr} \leqslant cK_N \ , \tag{1a}$$

where c is the scattering ratio, N is the (even) order of the Gauss-Legendre quadrature set, and

$$K_2 = 0 \tag{1b}$$

and

$$K_N < \frac{1}{3} \quad \text{for} \quad N \geqslant 4 \ . \tag{1c}$$

The equation $K_2 = 0$ translates into the observation that, as they were designed to do, the acceleration methods for the S_2 quadrature set produce the solution in one iteration. In other words, the starting calculations themselves yield the exact transport cell-average and cell-edge fluxes. The results described in the remainder of this paper thus pertain to even-order S_N quadrature sets with $N \geqslant 4$.

The inequality $K_N < c/3$ for $N \geqslant 4$ translates into the observation that errors reduce by at worst one order of magnitude for every two iterations, for any spatial mesh. Although this is documented in Sec. II, we present in Table I, as an illustration, results pertaining to a $c = 0.98$ homogeneous slab problem, which is described in detail in Sec. II. This problem is solved by the weighted diamond (WD) method with weights

$$\alpha_m = a \frac{\mu_m}{|\mu_m|}$$

[1]E. W. LARSEN, *Nucl. Sci. Eng.*, **82**, 47 (1982).

TABLE I

Number of Iterations Required for Convergence of the $c = 0.98$ Homogeneous Slab Problem for the WD Scheme with Diffusion Synthetic Acceleration

σ_T	a = 0.0	0.1	0.5	1.0
1.0	4	4	4	4
2.0	4	4	3	4
4.0	5	5	4	4
6.0	7	5	4	4
10.0	5	6	5	4
20.0	4	5	6	5

[see Eq. I(10b)] and with various values of a and σ_T. Table I results are fully indicative of all our other results for acceleration methods without a negative flux fixup; convergence [with a pointwise 10^{-4} error, starting with an 0(1) error] occurs in a maximum of about eight iterations (which corresponds to an error reduction of an order of magnitude for every two iterations) for any size of spatial mesh. [For this problem, the width of a cell in mean-free-paths is numerically equal to σ_T.]

In Table II we give results for the same transport problem, but accelerated by the "diamond-synthetic" method, which consists of the WD transport equations [Eqs. I(10)] with the $\alpha_m = 0$ diamond difference (DD) diffusion equations [Eqs. I(27), I(28), and I(34) through I(37) with $\rho_i = 0$]. We include these results to illustrate the consequence of attempting to accelerate a transport differencing scheme with an acceleration method that is not fully compatible with it.[2] The Table II results, however, are also

TABLE II

Number of Iterations Required for Convergence of the $c = 0.98$ Homogeneous Slab Problem for the WD Scheme with Diamond-Synthetic Acceleration

σ_T	a = 0.0	0.1	0.5	1.0
1.0	4	4	6	8
2.0	4	4	9	17
4.0	5	6	18	91
6.0	7	8	43	*
10.0	5	13	*	*
20.0	4	22	*	*

*Denotes divergence.

indicative of our observations on acceleration methods with a negative flux fixup: As a increases from zero, the transport scheme increasingly departs from the differencing scheme on which the diffusion calculation is based (which roughly corresponds to the use of an increasing number of fixups), and the performance of the acceleration method declines to the point where, for coarse meshes, it causes divergence. In fact, for any nonzero value of a, no matter how small, we find experimentally that the diamond-synthetic iteration scheme becomes unstable for sufficiently large meshes.

An outline of the remainder of this paper follows. Our experimental verifications of Eqs. (1) are given in Sec. II, where we consider a finite homogeneous slab with isotropic scattering and a shielding problem with linearly anisotropic scattering, variable cross sections, and a nonuniform spatial mesh. Also, we vary the level of anisotropicity in certain regions of the shielding problem to demonstrate that the number of iterations required to obtain the converged solution remains essentially constant. (Morel has already shown this for the DD scheme.[3])

In Sec. III we reconsider the problems of Sec. II with negative flux fixup schemes introduced into the iteration methods. We find, as expected, that for large spatial meshes the performances of all the acceleration methods are severely degraded by the increasingly frequent implementation of the fixup schemes. The size of the spatial mesh at which difficulties begin to occur is very much problem and difference-scheme dependent. We conclude with a brief discussion in Sec. IV.

II. ACCELERATION METHODS WITHOUT NEGATIVE FLUX FIXUP

In this section we discuss the results observed by applying the acceleration methods in Part I to one-group transport problems in finite slabs. First, we consider an 8-cm-thick simple isotropically scattering slab with a reflecting boundary at the left edge, a vacuum boundary at the right edge, and a constant source in the left half of the slab. We consider eight spatial cells of equal (1-cm) thickness, σ_T to have the values 1.0, 2.0, 4.0, 6.0, 10.0, and 20.0 cm^{-1}, σ_S to have the values $\sigma_S = c\sigma_T$ with $c = 0.98$ and 0.8, and we employ the standard S_4 quadrature set. The number of iterations required to achieve a pointwise 10^{-4} error are given in Table III for the DD, linear characteristic (LC), linear discontinuous (LD), and linear moments (LM) methods. Results for the WD methods are given in Table I for $c = 0.98$.

The results are essentially as described in Sec. I.

[2]W. H. REED, *Nucl. Sci. Eng.*, **45**, 245 (1971).
[3]J. E. MOREL, *Nucl. Sci. Eng.*, **82**, 34 (1982).

TABLE III

Number of Iterations Required for Convergence of the Homogeneous Slab Problem

σ_T	$c = 0.98$				$c = 0.8$			
	DD[a]	LC	LD	LM	DD	LC	LD	LM
1.0	4	4	4	4	5	5	5	5
2.0	4	4	4	4	7	5	5	5
4.0	5	4	4	4	5	7	8	8
6.0	7	5	5	5	4	6	7	7
10.0	5	7	10	8	4	5	6	6
20.0	4	5	7	7	4	5	5	5

[a]DD ≡ diamond difference, LC ≡ linear characteristic, LD ≡ linear discontinuous, and LM ≡ linear moments.

For the $c = 0.8$ ($c = 0.98$) problems, the unaccelerated DD scheme requires more than 40 (200 to 300) iterations to converge.

Next we consider a model shielding problem described in Fig. 1. The cross sections are chosen to model those of water in the (from left to right) first, second, and fourth regions, and those of iron in the third region. A uniform source S is placed in the first region. Scattering is linearly anisotropic; we employ the S_4 quadrature set; and we seek a 10^{-4} pointwise error.

The results for the DD, LC, LD, and LM methods are given in Table IV. (The WD results are not given. However, for any value of a in Table I, the WD method converges in the same number or fewer iterations than that required by the DD method for the same mesh.) Again, the results are essentially as described in Sec. I. We remark that the LD method with coarse-mesh rebalance, as encoded[4] in ONETRAN, requires 440 iterations to converge for this problem.

[4]T. R. HILL, "ONETRAN, A Discrete Ordinates Finite Element Code for the Solution of the One-Dimensional Multigroup Transport Equation," LA-5990-MS, Los Alamos National Laboratory (1973).

TABLE IV

Number of Iterations Required for Convergence of the Shielding Problem

Number of Mesh Intervals per Region	$\sigma_T h$ per Region	DD	LC	LD	LM
(40,10,8,30)	(1,1,1,1)	5	5	5	5
(20,5,4,15)	(2,2,2,2)	6	5	5	5
(12,3,2,9)	(3.3,3.3,4,3.3)	7	7	7	6
(4,1,2,3)	(10,10,4,10)	5	7	7	6
(1,1,2,1)	(40,10,4,30)	5	6	7	5

Finally, to test the effect of the level of anisotropicity on the acceleration methods, we modified the above shielding problem by redefining σ_{S1} in the water regions as

$$\sigma_{S1} = \beta\sigma_{S0} ,$$

with $\beta = 0.5$, 0.8, 0.9, and 0.99. The results are listed in Table V for the "P_1" acceleration methods described in Part I (the cell-averaged scalar fluxes and currents are both accelerated), and the "P_0" acceleration method (only the cell-averaged scalar fluxes are accelerated), for the finest and coarsest meshes described in Table IV.

The P_1 acceleration results are, again, as described in Sec. I. We present the P_0 acceleration results to illustrate that for highly anisotropic materials, it is essential to accelerate both the scalar fluxes and currents via the P_1 methods described in Part I. (We discuss this point further in Sec. IV.) Morel[3] has already shown this to be true for the DD method, and our results verify this also for the LC, LD, and LM methods.

III. ACCELERATION METHODS WITH NEGATIVE FLUX FIXUP

In this section we discuss the results of applying acceleration methods with a negative flux fixup to

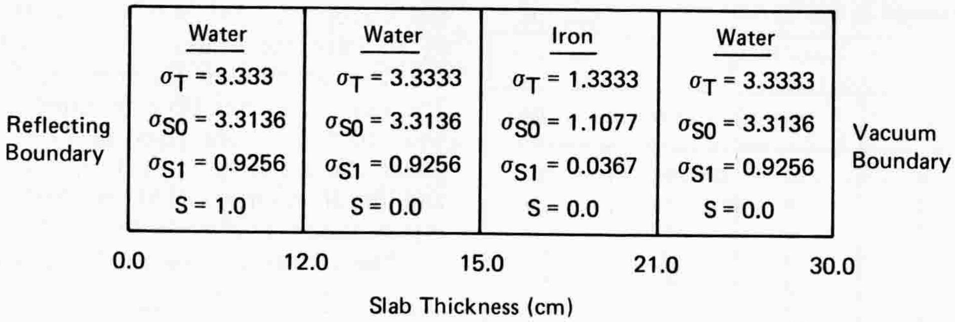

Fig. 1. The model shielding problem. The cross sections are in cm^{-1}.

TABLE V

Number of Iterations Required for Convergence of the Modified Shielding Problem

β	0.5				0.8				0.9				0.99			
	DD	LC	LD	LM	DD	LC	LD	LM	DD	LC	LD	LM	DD	LC	LD	LM
P_1 Fine mesh	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
P_1 Coarse mesh	5	6	5	6	5	6	6	6	5	6	7	6	5	6	6	7
P_0 Fine mesh	9	9	9	9	19	18	18	18	29	28	28	28	64	64	65	64
P_0 Coarse mesh	7	9	9	7	8	20	17	12	8	31	23	16	35	73	47	22

the transport problems of Sec. II and to a model problem described in an earlier paper.

Our negative flux fixups are implemented in three places. First, it is possible that the source for the first transport calculation, determined by combining the results of the starting calculation with the fixed inhomogeneous source, is negative due to a negative solution from the starting calculation. [This possibility exists because of the three-point removal term in the discretized diffusion equations. See, for example, Eq. I(30).] For the LC, LD, and LM methods, if the computed average source in a cell [right side of Eq. I(70a)] is positive but the source slope [right side of Eq. I(70b)] is such that the source representation is negative, we alter the value of the slope in that cell by the minimum amount so that the representation becomes nonnegative. For all of the methods, if the computed average source is negative in a cell, we simply set the average source (and slope) to zero in that cell. This procedure guarantees that the source for the first transport calculation is nonnegative.

Second, it is possible that even with a nonnegative transport source, the results of the transport calculation can be negative, due to the nonpositivity of the transport differencing schemes. Thus the transport calculations must also be fixed up. In the DD scheme, we use the standard set-to-zero fixup, and for the LC, LD, and LM methods, we use the LC fixup described in Ref. 5. This fixup scheme is as follows: For each of the three methods in any given cell, the computed cell-averaged flux must be nonnegative but the flux slope can be large enough that the linear representation for the angular flux [Eq. I(42)] becomes negative in part of the cell. In this case we modify the flux slope by the minimum amount so that this linear representation is nonnegative. The LD scheme has the property that if this fixup is employed, the exiting flux is altered. This defect, which is not shared by the LC and LM methods, causes the LD method to be more severely affected by transport fixups.

Finally, it is possible that even for positive transport calculation results, the solution of the succeeding diffusion calculation can be negative, and this can generate a negative source for the next transport calculation. For the LC, LD, and LM schemes, if all of the cell-averaged transport sources are nonnegative but the linear representations for the source become negative in certain cells, then we alter the source slopes in these cells by the minimum amount so that the representations become nonnegative. However, for all of the methods, if any cell-averaged transport source is negative, then we discard the results of the diffusion calculation and compute the transport source directly from the previous fixed-up transport calculation. (This corresponds to turning off the acceleration process for this iteration.)

Our results for the $c = 0.98$ and $c = 0.8$ homogeneous slab problems and the model shielding problem are given in Tables VI, VII, and VIII. We include the DD ONEDANT results[6] because they differ somewhat from ours; this is because ONEDANT employs a nonlinear source-correction method.

In Tables VI and VII, all of the methods are eventually affected by the implementation of negative flux fixups as σ_T increases, and the point at which serious problems arise corresponds closely to

[5] R. E. ALCOUFFE, E. W. LARSEN, W. F. MILLER, Jr., and B. R. WIENKE, *Nucl. Sci. Eng.*, **71**, 111 (1979).

[6] R. D. O'DELL, F. W. BRINKLEY, Jr., and D. MARR, "User's Manual for ONEDANT: A Code Package for One-Dimensional, Diffusion-Accelerated, Neutral Particle Transport," LA-9184-M, Los Alamos National Laboratory (1982).

TABLE VI

Number of Iterations Required for Convergence of the Methods with Fixup for the $c = 0.98$ Homogeneous Slab Problem

σ_T	DD	DD (ONEDANT)	LC	LD	LM
1.0	4	4	4	4	4
2.0	4	4	4	4	4
4.0	5	7	4	4	4
6.0	10	14	5	5	5
8.0	40[a]	39[a]	7	7	7
9.0	a,b	a,b	a,b	8	7
10.0	a,b	a,b	269[a]	b	8
11.0	a,b	a,b	233[a]	206[a]	b
12.0	a,b	a,b	305[a]	124[a]	166[a]
20.0	a,b	a,b	452[a]	442[a]	358[a]

[a]Denotes the occurrence of a negative cell-averaged scalar flux for the methods without fixup.
[b]Denotes divergence.

TABLE VII

Number of Iterations Required for Convergence of the Methods with Fixup for the $c = 0.8$ Homogeneous Slab Problem

σ_T	DD	DD (ONEDANT)	LC	LD	LM
1.0	5	6	5	5	5
2.0	9[a]	11[a]	5	5	5
3.0	16[a]	25[a]	6	33	6
4.0	a,b	a,b	36[a]	37[a]	8
5.0	a,b	a,b	40[a]	41[a]	38[a]
6.0	a,b	a,b	49[a]	a,b	39[a]
10.0	a,b	a,b	68[a]	a,b	59[a]

[a]Denotes the occurrence of a negative cell-averaged scalar flux for the methods without fixup.
[b]Denotes divergence.

the optical cell width for which negative cell-averaged scalar fluxes would first occur if the fixup were not used. Interestingly, the DD solution always diverges for spatial meshes larger than a certain "critical" size, while the LC, LD, and LM methods exhibit a different behavior. For the $c = 0.98$ problem (Table VI), they all diverge for a certain mesh but converge again for larger meshes—although at a much slower convergence rate, comparable to that for the unaccelerated methods. For the $c = 0.8$ problem (Table VII), the LC, LD, and LM methods converge at about the unaccelerated rate immediately when the methods without fixup would yield negative cell-averaged scalar fluxes, and then for somewhat coarser meshes the LD method diverges. (We believe that this divergence is due to the relatively "hard" LD transport fixup discussed above.) For the model shielding problem (Table VIII), the DD method diverges on every mesh for which the method without fixup would yield negative cell-averaged scalar fluxes, and it performs satisfactorily on the other meshes. The LC, LD, and LM methods produce no negative cell-averaged scalar fluxes for any of the spatial meshes, and these methods all converge on every mesh. The LD convergence is slower on two of the meshes because the starting calculation yields negative cell-averaged scalar fluxes, while the final converged solution (without fixup) does not; the hard LD negative flux fixup apparently interferes with the convergence process until the transport iterates are close enough to the converged solution that negative cell-averaged fluxes do not occur.

As a final example, we consider the one-group model problem of Ref. 5, with three meshes, denoted in Ref. 5 as M6, M3, and M1. (The spatial cells for these meshes have widths of 0.5, 1.0, and 3.0 mpf,

TABLE VIII

Number of Iterations Required for Convergence of the Methods with Fixup for the Model Shielding Problem

Number of Mesh Intervals per Region	$\sigma_T h$ per Region	DD	DD (ONEDANT)	LC	LD	LM
(40,10,8,30)	(1,1,1,1)	5	5	5	5	5
(20,5,4,15)	(2,2,2,2)	7	10	5	5	5
(12,3,2,9)	(3.3,3.3,4,3.3)	a,b	a,b	6	27	6
(4,1,2,3)	(10,10,4,10)	a,b	a,b	7	8	6
(1,1,2,1)	(40,10,4,30)	a,b	a,b	6	22	7

[a]Denotes the occurrence of a negative cell-averaged scalar flux for the methods without fixup.
[b]Denotes divergence.

respectively. The quadrature set is S_8 and the pointwise convergence criterion is 10^{-5}. The LD method with coarse-mesh rebalance, as encoded[4] in ONETRAN, requires 50 iterations to converge for this problem on the M6 mesh.) As shown in Table IX, all of the methods perform satisfactorily except for the DD and LD methods on the coarsest mesh, for which, again, negative cell-averaged scalar fluxes would occur if the fixup were not used.

To summarize, our results indicate that the application of a negative flux fixup on a spatial mesh for which a method without fixup would yield (or would almost yield) negative cell-averaged fluxes is an anathema to all of the acceleration methods. The more accurate LC, LD, and LM methods generally require larger spatial cells to obtain negative cell-averaged scalar fluxes than the DD method, and thus they are first affected by negative flux fixups on meshes larger than that at which the DD method is first affected.

IV. DISCUSSION

Here, we briefly comment on certain practical aspects of our work described above. First, we have compared only the number of iterations required by the accelerated and unaccelerated methods to achieve convergence, not the central processing unit (CPU) time required. However, the results of a timing study on our test code show that the ratio of the CPU time spent doing diffusion calculations versus the CPU time spent doing transport calculations is <0.1 for the S_4 quadrature set and even smaller for the higher order quadrature sets. Therefore, from a practical viewpoint, the CPU time required to perform one accelerated iteration is essentially equal to the CPU time required to perform one unaccelerated iteration.

Our results have been derived only for one-group problems, and thus for multigroup problems they can be regarded as applicable only to the acceleration of inner iterations. We have not tested our methods on multigroup problems, partly because of time constraints, but mainly because the extension of our methods to the multigroup arena (with the ensuing strategy of accelerating the outer iterations) is conceptually straightforward. At least, this has been the experience with the DD acceleration method,[6,7] and we have observed no anomolous behavior in the LC, LD, and LM acceleration methods, which suggests that they would behave unpredictably in the performance of outer iterations.

The acceleration of very highly anisotropic transport problems has been examined thoroughly by Morel,[3] and we briefly summarize some of his findings. For problems in which $\sigma_{S0} \approx \sigma_{S1}$, it is also generally true that

$$\sigma_{S0} > \sigma_{S1} > \sigma_{S2} > \sigma_{S3} \ldots$$

and

$$\sigma_{S0} \approx \sigma_{S1} \approx \sigma_{S2} \approx \sigma_{S3} \ldots .$$

In this situation, the procedure of accelerating the scalar flux and current is more efficient than that of only accelerating the scalar flux, but the convergence properties become more severely affected as σ_{S2} approaches σ_{S0} in value. (This is very similar to the case of P_0 acceleration, whose convergence properties deteriorate as σ_{S1} approaches σ_{S0} in value.) Morel recommends the following procedure: Perform the diffusion calculation, and then multiply all the even transport angular flux moments by a certain factor and all the odd transport angular flux moments by another factor; these factors are such that the new scalar fluxes and currents are equal to those computed by the diffusion calculation. In any event, one should not expect that for all highly anisotropic scattering problems, our methods will perform as stated in the top half of Table V. As $\sigma_{S2} \to \sigma_{S0}$, one should expect, even with Morel's method, convergence behavior somewhat akin to that shown in the bottom half of Table V.

In Table II we displayed some results to illustrate that if the diffusion calculation is incompatible with the transport calculation, then one can expect deterioration of the convergence properties for a sufficiently large spatial mesh. The results of Table II were generated by coupling the WD transport calculation with the DD diffusion calculations; the resulting diffusion calculation is incompatible with the transport calculation both with regard to the diffusion equation and the diffusion boundary conditions. We wish to emphasize that, from our practical experience, it is essential that both the diffusion equation *and* its boundary conditions be compatible with the transport calculation to achieve convergence

TABLE IX

Number of Iterations Required for Convergence of the Methods with Fixup for the Model Problem of Ref. 5

Mesh Spacing	DD	DD (ONEDANT)	LC	LD	LM
M6	7	7	7	7	7
M3	7	7	7	7	7
M1	a,b	a,b	8	a,b	8

[a]Denotes the occurrence of a negative cell-averaged scalar flux for the methods without fixup.
[b]Denotes divergence.

[7]R. E. ALCOUFFE, *Nucl. Sci. Eng.*, **64**, 344 (1977).

properties that are essentially independent of the spatial mesh. This statement is particularly true for highly anisotropic scattering problems, which are very sensitive to any incompatibilities between the transport and diffusion calculations.

Finally, we comment on the serious decline of stability for all the acceleration methods with fixup as the spatial cell widths become optically thick. This behavior is not limited to acceleration methods; it is seen also for the unaccelerated methods. For source problems, the only remedy at present is to avoid the situation by refining the spatial mesh until convergence occurs. (For eigenvalue problems, the recommended procedure is to turn off the negative flux fixup algorithm altogether, and this also avoids the problem.) A preferable solution would be to design a transport differencing scheme and acceleration method that are either inherently positive or that are compatible with a negative flux fixup. We are currently investigating this difficult and long-standing problem.

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