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TITLE: PROJECTED DISCRETE ORDINATES METHODS FOR NUMERICAL TRANSPORT PROBLEMS

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PROJECTED DISCRETE-ORDINATES METHODS FOR NUMERICAL TRANSPORT PROBLEMS

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ABSTRACT

A class of "Projected Discrete-Ordinates" (PDO) methods is described for obtaining iterative solutions of discrete-ordinates problems with convergence rates comparable to those observed using Diffusion Synthetic Acceleration (DSA). The spatially discretized PDO solutions are generally not equal to the DSA solutions, but unlike DSA, which requires great care in the use of spatial discretizations to preserve stability, the PDO solutions remain stable and rapidly convergent with essentially arbitrary spatial discretizations. Numerical results are presented which illustrate the rapid convergence and the accuracy of solutions obtained using PDO methods with commonplace differencing methods.

I. INTRODUCTION

It is well known that iterative solutions of discrete-ordinates problems, obtained using the standard Source-Iteration (SI) method, can converge extremely slowly for optically thick regions with scattering ratios c close to unity.[1,2] Acceleration of such SI solutions using rebalance often works satisfactorily for c not too close to one, but unfortunately can become unstable as c approaches one - which is precisely the regime where acceleration is most needed. Chebyschev acceleration has not generally attained the popularity of rebalance because when rebalance is stable, it usually outperforms Chebyschev, and when c approaches one, the Chebyschev method can still converge very slowly. Diffusion synthetic acceleration (DSA) methods do converge very rapidly for all $c \leq 1$, but great care must be taken to ensure that these methods remain stable. In particular, DSA schemes are characterized by having within each iteration a transport and a diffusion sweep, and the spatial differencing of the diffusion part of the algorithm must be consistent with that of the transport part to guarantee stability.[1,2] In general multi-dimensional geometries, the only transport differencing scheme for which this has been successfully accomplished and fully tested is the diamond-difference scheme, and for this the spatial mesh is required to be rectangular. Unfortunately, for reasons which are algebraic in nature, the DSA method has had little success to date in general-geometry problems with non-diamond differencing schemes.

In this paper we discuss a class of "Projected Discrete-Ordinates" (PDO) methods, which are closely related to DSA methods, and which have the following features:

(1) They generate numerical solutions of the discrete-ordinates equations by alternating transport sweeps and diffusion calculations, just as in DSA.

(2) The transport and diffusion solutions individually converge very rapidly, with convergence rates which are comparable to those obtained using DSA.

(3) These convergence rates are essentially independent of the differencing schemes used in the transport and diffusion parts of the algorithm and the size of the spatial mesh. Moreover, these properties seem to carry over to a non-rectangular spatial grid.

(4) Generally, upon convergence, the transport and diffusion solutions are not equal to each other, neither equals the converged SI (or DSA) solution, and neither satisfies the conventional balance equation.

(5) With commonplace differencing schemes, the PDO solutions are generally less accurate than the SI or DSA solutions. This defect is probably due in part to the loss of particle balance, but also to the discretized diffusion boundary conditions. Numerical results described below show that with suitable care taken in the formulation of the discretized diffusion boundary conditions, this loss of accuracy can largely, if not completely, be overcome.

Thus, PDO methods are not SI acceleration methods, such as DSA; they do not produce, on any given mesh, the unaccelerated SI (or accelerated DSA) solution. However, the PDO methods are legitimate numerical methods in the same sense as the SI (or DSA) methods; namely, as the spatial mesh becomes increasingly fine, the solutions obtained from both sets of methods converge to the exact discrete-ordinates solution. The main difference between the SI-DSA solutions and the PDO solutions is that for each spatial grid, they possess different spatial truncation errors. The primary advantage of the PDO methods over DSA is that they allow great flexibility in the choice of differencing schemes for the transport and diffusion parts of the algorithm, with little or no degradation in the convergence rates. Also, PDO methods appear to be applicable in non-rectangular grids.

In short, there is a trade-off: On any given spatial grid, the PDO solutions will generally not be equal to the SI-DSA solutions, but they will be obtained very rapidly, and with great freedom in the choice of transport and diffusion differencing schemes. Therefore, PDO methods may be attractive for multi-dimensional problems in which either the mesh is not rectangular, or the diamond-difference method is not deemed adequate.

In their basic form, PDO methods are not new and have existed in the literature for several years.[3-9] However, their stability and convergence properties have not been discussed and appear to be largely unrecognized. The purpose of this paper is to show that these PDO methods exist, discuss their

properties, and introduce modifications which improve some of their properties. In so doing, we hope to demonstrate that one can, in a practical fashion, obtain numerical solutions of discrete-ordinates problems as rapidly as one can with DSA, but under very general conditions pertaining to the geometry, the spatial mesh, and the choice of differencing schemes.

An outline of the remainder of this paper follows. In Sec. II we define the various PDO methods in terms of analytic transport and diffusion operators, for a general three-dimensional geometry. In Sec. III we present slab geometry numerical results which demonstrate the rapid PDO convergence rates and which compare the accuracies of the PDO and DSA solutions for commonplace differencing schemes. For these particular results, the PDO solutions are, as stated above, generally less accurate than the DSA solutions. This and other topics are discussed briefly in Sec. IV.

II. DERIVATIONS

To describe PDO methods, we consider the one-group transport equation in a three-dimensional convex region D:

$$\underline{\Omega}\cdot\underline{\nabla}\psi + \sigma_T\psi = \sigma_S\phi_0 + Q \quad , \quad \underline{r}\in D, \ |\underline{\Omega}| = 1 \quad . \tag{2.1}$$

Here $\psi(\underline{r},\underline{\Omega})$ is the angular flux, $Q(\underline{r},\underline{\Omega})$ is the source, and ϕ_0 is the scalar flux,

$$\phi_0(\underline{r}) = \frac{1}{4\pi}\int \psi(\underline{r},\underline{\Omega})d\Omega \quad . \tag{2.2}$$

Letting $\underline{n}$ be the unit outer normal at a point $\underline{r}$ on the boundary ∂D of D, we prescribe as a boundary condition the incident angular flux f on ∂D:

$$\psi(\underline{r},\underline{\Omega}) = f(\underline{r},\underline{\Omega}) \quad , \quad \underline{r}\in\partial D \quad , \quad \underline{\Omega}\cdot\underline{n} < 0 \quad . \tag{2.3}$$

Other boundary conditions (e.g. derived by making use of symmetries in the problem) are possible but are not considered here. We define

$$\underline{\phi}_1(\underline{r}) = \frac{1}{4\pi}\int \underline{\Omega}\psi d\Omega \quad , \tag{2.4}$$

$$\underline{\underline{\Phi}}_2(\underline{r}) = \frac{1}{4\pi} \int \frac{1}{2} (3\underline{\Omega}\underline{\Omega} - \underline{\underline{I}}) \psi d\Omega \quad , \tag{2.5}$$

and

$$\underline{\underline{D}} = \frac{\int \underline{\Omega}\underline{\Omega}\psi d\Omega}{\int \psi d\Omega} = \frac{1}{3} \underline{\underline{I}} + \frac{2}{3} \underline{\underline{\Phi}}_2 \phi_0^{-1} \quad . \tag{2.6}$$

Then ϕ_0 is a scalar, consisting of the zero-th order spherical-harmonic moment of ψ, $\underline{\Phi}_1$ is a vector whose components contain only first-order spherical-harmonic moments of ψ, and $\underline{\underline{\Phi}}_2$ is a tensor, whose components contain only second-order spherical harmonic moments of ψ. Likewise, we define

$$Q_0(\underline{r}) = \frac{1}{4\pi} \int Q d\Omega \quad , \tag{2.7}$$

$$\underline{Q}_1(\underline{r}) = \frac{1}{4\pi} \int \underline{\Omega} Q d\Omega \quad . \tag{2.8}$$

In simplest terms, PDO methods are iteration schemes for solving the problem (2.1), (2.3) such that within each iteration, there is a transport sweep and a particular type of diffusion calculation. For the ℓ-th iteration, the transport sweep is always described by the problem

$$\underline{\Omega}\cdot\underline{\nabla}\psi^{\ell+1/2} + \sigma_T\psi^{\ell+1/2} = \sigma_S\phi_0^{\ell} + Q \quad , \tag{2.9a}$$

$$\psi^{\ell+1/2}(\underline{r},\underline{\Omega}) = f(\underline{r},\underline{\Omega}) \quad , \quad \underline{r}\in\partial D \quad , \quad \underline{\Omega}\cdot\underline{n} < 0 \quad , \tag{2.9b}$$

which uniquely determines $\psi^{\ell+1/2}$, and then the diffusion calculations use $\psi^{\ell+1/2}$ in various ways to compute $\phi_0^{\ell+1}$. These diffusion problems are based on the following equations, which are obtained by multiplying Eq. (2.9a) by 1 and $\underline{\Omega}$ and integrating over $\underline{\Omega}$:

$$\underline{\nabla}\cdot\underline{\Phi}_1^{\ell+1/2} + \sigma_T\phi_0^{\ell+1/2} = \sigma_S\phi_0^{\ell} + Q_0 \quad , \tag{2.10}$$

$$\underline{\nabla}\cdot\left[\frac{1}{4\pi} \int \underline{\Omega}\underline{\Omega}\psi^{\ell+1/2} d\Omega\right] + \sigma_T\underline{\Phi}_1^{\ell+1/2} = \underline{Q}_1 \quad . \tag{2.11}$$

Chronologically, the first PDO method was proposed by Gol'din.[3] The transport part of this method consists of Eq. (2.9), while the diffusion part, based on Eqs. (2.2), (2.6), (2.10), and (2.11), is defined by

$$\underline{\nabla}\cdot\underline{\phi}_1^{\ell+1} + (\sigma_T - \sigma_S)\phi_0^{\ell+1} = Q_0, \tag{2.12a}$$

$$\underline{\nabla}\cdot\underline{\underline{D}}^{\ell+1/2}\phi_0^{\ell+1} + \sigma_T\underline{\phi}_1^{\ell+1} = \underline{Q}_1 \quad , \tag{2.12b}$$

$$\underline{n}\cdot\underline{\phi}_1^{\ell+1} = C^{\ell+1/2}\phi_0^{\ell+1} - B \quad , \tag{2.12c}$$

where

$$C^{\ell+1/2} = \frac{\int_{\underline{\Omega}\cdot\underline{n}>0}\underline{\Omega}\cdot\underline{n}\psi^{\ell+1/2}d\Omega}{\int\psi^{\ell+1/2}d\Omega} \quad , \tag{2.13a}$$

$$B = -\frac{1}{4\pi}\int_{\underline{\Omega}\cdot\underline{n}<0}\underline{\Omega}\cdot\underline{n}f\,d\Omega \quad . \tag{2.13b}$$

Using Eqs. (2.12b) to eliminate $\phi_1^{\ell+1/2}$ from Eqs. (2.12a,c), we obtain the following diffusion problem:

$$-\underline{\nabla}\cdot\frac{1}{\sigma_T}\underline{\nabla}\cdot\underline{\underline{D}}^{\ell+1/2}\phi_0^{\ell+1} + (\sigma_T-\sigma_S)\phi_0^{\ell+1} = Q_0 - \underline{\nabla}\cdot\frac{1}{\sigma_T}\underline{Q}_1 \quad , \tag{2.14a}$$

$$\frac{1}{\sigma_T}\underline{n}\cdot\underline{\nabla}\cdot\underline{\underline{D}}^{\ell+1/2}\phi_0^{\ell+1} + C^{\ell+1/2}\phi_0^{\ell+1} = B + \frac{1}{\sigma_T}\underline{n}\cdot\underline{Q}_1 \quad . \tag{2.14b}$$

Thus, Gol'din's method consists of Eqs. (2.9), followed either by Eqs. (2.12) or (2.14).

We emphasize that Gol'din's derivation of this method (which he termed the "quasi-diffusion" method) is specifically for spherical geometry, with the incident flux f set equal to zero. Nevertheless, his ideas apply quite generally in other geometries and for other boundary conditions.

The logic behind this iterative method is as follows. The terms in the diffusion part of the iteration [Eqs. (2.12) or (2.14)] which depend on $\psi^{\ell+1/2}$ are $\underline{\underline{D}}^{\ell+1/2}$ and $C^{\ell+1/2}$, and these depend only on the angular shape of $\psi^{\ell+1/2}$,

not on its amplitude. Thus, if at any iteration, $\psi^{\ell+1/2}$ has the exact angular shape but the incorrect amplitude, then $\phi^{\ell+1}$ will be exact and any further iterations will merely reproduce the converged solutions. In other words, the scheme is based upon the premise that the transport sweep [Eq. (2.9)] generates an accurate angular shape for ψ (but not necessarily an accurate amplitude), while the diffusion calculation with the transport corrections [Eqs. (2.12) or (2.14)], given an accurate shape, generates a much more accurate amplitude.

Variations on Gol'din's method have appeared elsewhere in the Soviet literature;[4,6] all this work makes use of the basic ideas stated above.

The second basic PDO method was proposed by Lewis and Miller.[7] To describe the boundary condition for the diffusion part of this method, we note that at any point $\underline{r}\in\partial D$ with $\underline{\Omega}\cdot\underline{n}<0$, we have for every ℓ,

$$f(\underline{r},\underline{\Omega}) = \psi^{\ell+1/2}(\underline{r},\underline{\Omega}) = \phi_o{}^{\ell+1/2}(\underline{r}) + 3\underline{\Omega}\cdot\underline{\phi}_1{}^{\ell+1/2}(\underline{r}) + R^{\ell+1/2}(\underline{r},\underline{\Omega}) \quad , \tag{2.15}$$

where $R^{\ell+1/2}$ is a remainder, expressible as a sum of spherical harmonics of order greater than or equal to two. Multiplying Eq. (2.15) by $\underline{\Omega}\cdot\underline{n}$, integrating over $\underline{\Omega}\cdot\underline{n}<0$, and rearranging, we obtain the relation

$$\phi_o{}^{\ell+1/2}(\underline{r}) - 2\underline{n}\cdot\underline{\phi}_1{}^{\ell+1/2}(\underline{r}) = \frac{1}{\pi}\int_{\underline{\Omega}\cdot\underline{n}<0} \underline{\Omega}\cdot\underline{n}(R^{\ell+1/2} - f)d\Omega \quad . \tag{2.16}$$

As before, the transport part of the Lewis-Miller method consists of Eq. (2.9), while the diffusion part, based on Eqs. (2.2), (2.6), (2.10), (2.11), and (2.16), is defined by

$$\underline{\nabla}\cdot\underline{\phi}_1{}^{\ell+1} + (\sigma_T - \sigma_S)\,\phi_o{}^{\ell+1} = Q_o \tag{2.17a}$$

$$\frac{1}{3}\underline{\nabla}\phi_o{}^{\ell+1} + \frac{2}{3}\underline{\nabla}\cdot\underline{\Phi}_2{}^{\ell+1/2} + \sigma_T\underline{\phi}_1{}^{\ell+1} = \underline{Q}_1 \quad , \tag{2.17b}$$

$$\phi_o{}^{\ell+1}(\underline{r}) - 2\underline{n}\cdot\underline{\phi}_1{}^{\ell+1}(\underline{r}) = \frac{1}{\pi}\int_{\underline{\Omega}\cdot\underline{n}<0} \underline{\Omega}\cdot\underline{n}(R^{\ell+1/2} - f)d\Omega \quad . \tag{2.17c}$$

Using the second of these equations to eliminate $\underline{\phi}_1^{\ell+1}$ from the first and third, we obtain the following diffusion problem:

$$-\underline{\nabla}\cdot\frac{1}{3\sigma_T}\underline{\nabla}\phi_0^{\ell+1}+(\sigma_T-\sigma_S)\phi_0^{\ell+1}=Q_0-\underline{\nabla}\cdot\frac{1}{\sigma_T}\underline{Q}_1$$

$$+\underline{\nabla}\cdot\frac{2}{3\sigma_T}\underline{\nabla}\cdot\underline{\underline{\phi}}_2^{\ell+1/2}\quad,\quad \underline{r}\in D\quad, \tag{2.18a}$$

$$\phi_0^{\ell+1}+\frac{2}{3\sigma_T}\underline{n}\cdot\underline{\nabla}\phi_0^{\ell+1}=\frac{1}{\pi}\int_{\underline{\Omega}\cdot\underline{n}<0}\underline{\Omega}\cdot\underline{n}(R^{\ell+1/2}-f)d\Omega$$

$$+\frac{2}{\sigma_T}\left(\underline{n}\cdot\underline{Q}_1-\frac{2}{3}\underline{n}\cdot\underline{\nabla}\cdot\underline{\underline{\phi}}_2^{\ell+1/2}\right)\quad,\quad \underline{r}\in\partial D\quad. \tag{2.18b}$$

Thus, the Lewis-Miller method consists of Eq. (2.9), followed either by Eqs. (2.17) or (2.18).

The logic behind this iterative method is as follows. The terms in the diffusion part of the iteration [Eqs. (2.17) or (2.18)] which depend on $\psi^{\ell+1/2}$ are $\underline{\underline{\phi}}_2^{\ell+1/2}$ and $R^{\ell+1/2}$, and these terms vanish if $\psi^{\ell+1/2}$ is a linear function of $\underline{\Omega}$, i.e, if $\psi^{\ell+1/2}$ has the form

$$\psi^{\ell+1/2}(\underline{r},\underline{\Omega})=\phi_0^{\ell+1/2}(\underline{r})+3\underline{\Omega}\cdot\underline{\phi}_1^{\ell+1/2}(\underline{r})\quad. \tag{2.19}$$

Thus, if the converged angular flux has this form (which implies that diffusion theory is exact) it will be computed in one iteration provided the starting guess itself is the diffusion solution. In other words, this scheme is based upon the premise that the transport sweep [Eqs. (2.9)] generates a more accurate result in non-diffusive regions than in diffusive regions, while the diffusion calculation with the transport corrections [Eqs. (2.17) or (2.18)] generates a much better result in the diffusive regions. This logic is the same as that which motivates the DSA method.

We add that Lewis and Miller's published derivation of this method,[7] which they term the "second-moment" method, is specifically of Eq. (2.18a) for slab geometry, and they give no details on the derivation of boundary conditions. However, the boundary condition used in the Ref. 7 numerical calculations does possess the property stated above, namely, the solution is computed in one iteration if ψ is linear in angle.[7,10]

At this point, we discuss some features of the two methods presented above.

(1) If for the spatially discretized discrete-ordinates equations one is able to follow precisely the same algebraic steps as given above to derive a discretized Lewis-Miller method, one will obtain a set of equations which is algebraically equivalent to the DSA result. For these equations, the scalar flux arising from the transport and diffusion parts of the algorithm will agree, upon convergence. However, if one chooses another discretization for the PDO Eqs. (2.18), one will retain the rapid convergence but the converged transport and diffusion scalar fluxes will no longer precisely agree with each other or the DSA result. If one chooses another discretization for the DSA diffusion equation, the transport and scalar fluxes will still converge to the SI result for small enough meshes, but for larger meshes, the scheme will generally become unstable. We refer the reader to Ref. 2 for a full discussion on the stability issues pertaining to DSA.

(2) If ψ is linear in angle, i.e, if it has the form of Eq. (2.19), then $\underline{D} = 1/3\ \underline{I}$, and Eq. (2.14a) becomes independent of $\ell+1/2$. [However, this is not true of Eq. (2.14b).] Therefore, use of Eq. (2.14a) with the boundary condition (2.18b) will produce a method which generates the converged solution in one iteration if the solution is linear in angle. This method has been termed the "Variable Eddington Factor" (VEF) method,[5,8] and 1-D numerical results in Ref. 8 have shown that it converges very rapidly.

(3) The application of Gol'din's method in 1-D is relatively straightforward, because in this case $\underline{D}$ reduces to a positive scalar. However, the solutions must for each iterate remain positive so that $\underline{D}$ and C can be computed, and with a sufficiently anisotropic source Q, the $\underline{S}_1$ terms in Eqs. (2.14) could lead to a negative numerical solution. In 2- and 3-D, Eqs. (2.14) are more problematical because although $\underline{D}$ is a positive-definite, symmetric tensor, Eq. (2.14a) is not positive-definite because $\underline{D}$ is not suitably located between the two gradient operators. Also, the boundary conditions contain oblique (non-normal) derivatives. Thus, the issues of positivity and efficiency of computation in 2- and 3-D are of much greater concern than in 1-D.

(4) The Lewis-Miller method [Eqs. (2.18)] is straightforward in 1-, 2-, and 3-D problems, although upon discretization, one cannot guarantee a positive solution. However, the method is linear and should be unaffected by negative solutions, the diffusion operator is symmetric and positive-definite, and the boundary condition contains only outward normal derivatives. Also, Fourier analyses on model x,y-geometry problems for both the analytic and discretized methods (with general weighted-diamond S_N differencing) show that the method converges rapidly, with a spectral radius always less than one-third.

(5) Even though the converged analytic solutions of the Gol'din and Lewis-Miller methods are guaranteed to be positive, there appears to be no way to directly discretize these methods to guarantee a positive solution at the end of any iteration, or even a positive converged solution.

To circumvent some of the difficulties listed above, we propose the following modifications to the Lewis-Miller method.

Let us define the right sides of Eqs. (2.18a and b) as $\alpha^{\ell+1/2}$ and $\beta^{\ell+1/2}$, respectively:

$$\alpha^{\ell+1/2} = Q_o - \underline{\nabla}\cdot\frac{1}{\sigma_T}\underline{Q}_1 + \underline{\nabla}\cdot\frac{2}{3\sigma_T}\underline{\nabla}\cdot\underline{\underline{\Phi}}_2^{\ell+1/2} \quad , \tag{2.20a}$$

$$\beta^{\ell+1/2} = \frac{1}{\tau}\int_{\underline{\Omega}\cdot\underline{n}<0}\underline{\Omega}\cdot\underline{n}(R^{\ell+1/2}-f)d\Omega + \frac{2}{\sigma_T}\left(\underline{n}\cdot\underline{Q}_1 - \frac{2}{3}\underline{n}\cdot\underline{\nabla}\cdot\underline{\underline{\Phi}}_2^{\ell+1/2}\right) \quad . \tag{2.20b}$$

Then we modify Eq. (2.18) as follows:

$$-\underline{\nabla}\cdot\frac{1}{3\sigma_T}\underline{\nabla}\phi_o^{\ell+1} + \left(\sigma_T-\sigma_S + \frac{|\alpha^{\ell+1/2}|-\alpha^{\ell+1/2}}{2\phi_o^{\ell+1/2}}\right)\phi_o^{\ell+1}$$

$$= \frac{1}{2}\left(|\alpha^{\ell+1/2}| + \alpha^{\ell+1/2}\right) \quad , \quad \underline{r}\in D \quad , \tag{2.21a}$$

$$\left(1 + \frac{|\beta^{\ell+1/2}|-\beta^{\ell+1/2}}{2\phi_o^{\ell+1/2}}\right)\phi_o^{\ell+1} + \frac{2}{3\sigma_T}\underline{n}\cdot\underline{\nabla}\phi_o^{\ell+1}$$

$$= \frac{1}{2}\left(|\beta^{\ell+1/2}| + \beta^{\ell+1/2}\right) \quad , \quad \underline{r}\in\partial D \quad . \tag{2.21b}$$

These equations have non-negative right-hand sides and thus can be differenced positively, so that after each iteration and upon convergence, the solution is positive. A minor variation of this method was proposed originally by Larsen.[9] Other modifications of the basic Lewis-Miller and Gol'din methods are possible, but will not be considered here.

To conclude this section, we note that all of the iteration methods proposed above combine a transport (or discrete-ordinates) sweep with a P_1 or diffusion calculation, and that the latter calculation is derived by projecting the transport (discrete-ordinates) equation onto the space of functions which are linear in the angular variable. This is the origin of our term "Projected Discrete-Ordinates" method.

III. NUMERICAL RESULTS

In this section, we discuss the following slab geometry transport problem: $\sigma_T = 1.0$, $\sigma_S = 0.97$, $Q = 0$, the right boundary ($x = 20$) has zero incident flux, and the left boundary ($x = 0$) has an isotropic incident flux with magnitude unity. A spatial mesh consisting of M equal cells, with

$$\Delta x = 20/M \tag{3.1}$$

is used, and the pointwise convergence criterion

$$\max_j \left| 1 - \frac{\phi_{o,j}^{\ell+1}}{\phi_{o,j}^{\ell}} \right| < 10^{-5} \quad , \tag{3.2}$$

is imposed, where j spans the spatial mesh.

We use the standard diamond difference scheme for each transport calculation[11] (with the starting guess $\phi_o^o = 0$ for the first iterate), and standard cell-center or cell-edge differencing (unless stated otherwise) for the various diffusion calculations. For the S_2 and S_8 Gauss-Legendre quadrature sets, the unaccelerated SI method requires approximately 300 iterations to achieve convergence for each spatial mesh, and for the S_2 set all the various PDO methods except for Gol'din's require two iterations to converge. (Only one iteration would have been required if the starting guess had been the diffusion solution.) For the S_8 quadrature set, we present detailed numerical results obtained using the following PDC methods:

DD-DSA : Standard diffusion synthetic acceleration.
G/C : Gol'din's method, with centrally-differenced diffusion.
LM/C : Lewis-Miller, with centrally-differenced diffusion.
LM/E : Lewis-Miller, with edge-differenced diffusion.
VEF/C : Variable Eddington Factor, with centrally differenced diffusion.
MLM/E : Eqs. (2.21), with edge-differenced diffusion.
MVEF/E* : Eqs. (2.21), with edge-differenced diffusion and discretized diffusion boundary conditions which are fully consistent with the diamond-differenced discrete-ordinates equations.

The numbers of iterations required for these methods to converge the given problem are listed in Table I. Essentially, convergence takes place for all but the G/C method in 7 to 11 iterations. The G/C method seems to deteriorate somewhat with coarser meshes; this happens with both the diamond and the (positive) step "transport differencing schemes, so the deterioration is not strictly due to the tendency of the diamond scheme to give negative solutions on coarse meshes.

TABLE I: NUMBER OF ITERATIONS VERSUS M

M	DD-DSA	G/C	LM/C	LM/E	VEF/C	MLM/E	MLM/E*
5	9	21	9	7	10	7	8
10	9	19	10	9	9	10	11
20	8	12	7	8	11	10	10
40	7	13	7	8	8	8	8
80	7	11	7	7	8	9	9
160	7	9	7	7	8	9	9
320	7	11	7	7	8	9	9
640	7	12	7	7	8	9	9

To discuss the accuracy of the various methods, we define A as the absorption rate on the interval $16 \leq x \leq 20$:

$$A = \int_{16}^{20} \phi_0(x)dx \quad . \tag{3.3}$$

The exact value of A, determined by a very fine-mesh calculation, is

$$A_{ex} = 0.01317920 \quad . \tag{3.4}$$

The relative error in a numerical approximation A_{num},

$$RE = 1 - \frac{A_{num}}{A_{ex}} \quad , \tag{3.5}$$

is given in Table II for the various methods and meshes treated in Table I. (Here the upper numbers correspond to the transport result, and the lower numbers to the diffusion result.)

In general, the DD-DSA and MLM/E* methods have errors which are second-order in Δx and are more accurate than the other methods, which are first-order. The reason for these orders of error can be explained by considering Eq. (2.18). In general, it is straightforward to construct a high-order differencing of Eq. (2.18a), but it is not straightforward to construct a differencing of Eq. (2.18b) which is compatible with the transport boundary conditions to $O(\Delta x^2)$. In particular, straightforward central or edge differencings of Eq. (2.18) lead to a second-order approximation in Eq. (2.18a) and a first-order approximation in Eq. (2.18b). Such differencings were used in all but the MLM/E* method, where we did construct discretized diffusion boundary conditions which were consistent with the transport calculation; this led to the much more accurate results indicated for this method in Table II.

TABLE II: RELATIVE ERRORS IN THE TRANSPORT (UPPER) AND DIFFUSION (LOWER) VALUES OF A VERSUS M

M	DD-DSA	G/C	LM/C	LM/E	VEF/C	MLM/E	MLM/E*
5	-3.73E-1	-2.46	-2.80	-6.41E-1	-2.77	-9.30E-1	-1.66
	-3.73E-1	-3.53	-5.68	-6.91E-1	-5.61	-9.50E-1	-1.31
10	1.18E-1	-3.31E-1	-1.23E-1	-1.60E-1	-1.20E-1	-2.41E-1	-2.48E-1
	1.18E-1	-3.49E-1	-7.73E-2	-1.65E-1	-7.43E-2	-2.76E-1	-2.55E-1
20	2.87E-2	-9.14E-2	-1.17E-1	-5.25E-2	-1.14E-1	-5.72E-2	-3.00E-2
	2.87E-2	-9.46E-2	-1.02E-1	-5.39E-2	-9.93E-2	-5.87E-2	-3.10E-2
40	7.717E-3	-3.15E-2	-6.02E-2	-1.98E-2	-5.79E-2	-2.08E-2	-7.35E-3
	7.717E-3	-3.22E-2	-5.35E-2	-2.02E-2	-5.10E-2	-2.12E-2	-7.60E-3
80	1.79E-3	-1.23E-2	-3.10E-2	-8.34E-3	-2.99E-2	-8.58E-3	-1.94E-3
	1.79E-3	-1.26E-2	-2.83E-2	-8.50E-3	-2.46E-2	-8.73E-3	-2.00E-3
160	4.46E-4	-5.40E-3	-1.65E-2	-3.78E-3	-1.55E-2	-3.80E-3	-5.13E-4
	4.46E-4	-5.48E-3	-1.48E-2	-3.85E-3	-1.36E-2	-3.87E-3	-5.28E-4
320	1.09E-4	-2.49E-3	-8.56E-3	-1.80E-3	-7.92E-3	-1.77E-3	-1.34E-4
	1.09E-4	-2.53E-3	-7.67E-3	-1.82E-3	-6.97E-3	-1.80E-3	-1.37E-4
640	2.73E-5	-1.21E-3	-4.37E-3	-8.74E-4	-4.02E-3	-8.50E-4	-3.33E-5
	2.73E-5	-1.21E-3	-3.92E-3	-8.89E-4	-3.53E-3	-8.65E-4	-3.64E-5

IV. DISCUSSION

The numerical results presented in Sec. III show that PDO methods converge with rates comparable to that of DSA, but that in general, the PDO methods are less accurate. However, we emphasize that we have not, in this paper, attempted to discretize the various PDO methods in ways which provide optimal accuracy; our primary aim has been to demonstrate that with well-known transport transport and diffusion discretizations, PDO methods provide rapidly convergent numerical solutions of discrete-ordinates problems.

The dual questions of accuracy and efficiency for more general problems cannot be addressed in detail here. However, we have seen that the proper discretization of the PDO boundary conditions are essential for good accuracy, and it is clear that the use of a positive differencing scheme can be important for the nonlinear PDO methods, where division by zero or a negative number could be fatal.

The present situation can be summarized as follows. For years, the SI method has been regarded as a legitimate procedure for obtaining discrete-ordinates solutions iteratively, and much work has gone into the development of spatial discretizations for it. Due to the frequent slow convergence of the SI method, the DSA method was developed and grafted onto SI, but it now appears that DSA is probably too algebraically complex to be of wide use for non-diamond differencing schemes in multi-dimensional geometries. The PDO

methods proposed here provide a different way to obtain rapidly convergent solutions, but these methods are at too early a stage of development to know whether discretizations exist which are accurate enough for problems of general interest. Thus, only future work can determine whether the capabilities of PDO methods are sufficient to solve problems of interest for which SI or DSA methods are deemed to be inadequate.

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