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# Diffusion Synthetic Acceleration Methods for the Diamond-Differenced Discrete-Ordinates Equations

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*We investigate a class of acceleration schemes that resemble the conventional synthetic method in that they utilize the diffusion operator in the transport iteration schemes. These schemes are not dependent on diffusion theory as being a good approximation to transport theory; they only make use of the diffusion equation form. The accelerated iteration involves alternate diffusion and transport solutions where coupling between the equations is achieved using a correction term applied to either (a) the diffusion coefficient, (b) the removal cross section, or (c) the source of the diffusion equation. The methods involving the modification of the diffusion coefficient and of the removal term yield nonlinear acceleration schemes and are used in $k_{eff}$ calculations, while the source term modification approach is linear at least before discretization and is used for inhomogeneous source problems. A careful analysis shows that there is a preferred differencing method that eliminates the previously observed instability of the conventional synthetic method. Using this preferred difference scheme results in an acceleration method that is at the same time stable and efficient. This preferred difference approach renders the source correction scheme, which is linear in its continuous form and nonlinear in its differenced form. An additional feature of these approaches is that they can be used as schemes for obtaining improved diffusion solutions for approximately twice the cost of a diffusion calculation.*

*Numerical experimentation on a wide range of problems in one and two dimensions indicates that improvement from a factor of from 2 to 10 over rebalance or Chebyshev acceleration is obtained. The improvement is most pronounced in problems with large regions of scattering material where the unaccelerated transport solutions converge very slowly.*

## I. INTRODUCTION

The most widely used methods for accelerating the iterative schemes used in discrete-ordinates neutron transport computer codes[1-4] are the rebalance method[2] and the Chebyshev acceleration method.[1] The rebalance method, often applied to a mesh that is more coarse than the problem mesh, is very effective in reducing the number of iterations. However, for that class of problems where the spatial mesh length is large compared to a mean-free-path and where the scattering ratio is close to unity, the coarse-mesh rebalance method may yield an unstable algorithm.[5] The Chebyshev method has not proven to be as effective as the rebalance approach in multidimensional transport codes, and hence, has not gained wide acceptance, at least in acceleration of the within-group scattering source.

[1]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 Scientific Laboratory (1975).

[2]K. D. LATHROP and F. W. BRINKLEY, "TWOTRAN-II: An Interfaced, Exportable Version of the TWOTRAN Code for Two-Dimensional Transport," LA-4848-MS, Los Alamos Scientific Laboratory (1973).

[3]W. W. ENGLE, Jr., "A User's Manual for ANISN," K-1693, Oak Ridge Gaseous Diffusion Plant (1967).

[4]W. A. RHOADES and F. R. MYNATT, "The DOT III Two-Dimensional Discrete Ordinates Transport Code," ORNL-TM-4280, Oak Ridge National Laboratory (1973).

[5]W. H. REED, *Nucl. Sci. Eng.*, **45**, 245 (1973).

Several authors have investigated another approach to accelerating transport iterations referred to as the diffusion synthetic method.[5-11] This method makes use of the diffusion equation form, but its effectiveness is not dependent upon diffusion theory being a good approximation to transport theory. However, previous results have indicated that this scheme also suffers from instability problems, although when stable the algorithm is generally more effective than the rebalance approach.[5] In this paper, we develop a class of diffusion synthetic acceleration schemes that are stable and effective when applied to discrete-ordinates iterations. We show that the key to stability lies in the scheme used to spatially difference the equations.

In Sec. II, we develop three variants of the diffusion synthetic acceleration method and apply them to the iterative process used in transport codes. We introduce spatial and angular discretization and develop a stable iteration algorithm. We give an explanation as to why earlier approaches to differencing the equations led to unstable algorithms. In Sec. III we provide numerical results, while Sec. IV is devoted to conclusions and recommendations.

## II. THEORY

In this section, we develop three diffusion synthetic acceleration approaches using both analytic and discretized expressions and assuming a multigroup energy formulation throughout. We emphasize spatial differencing, since convergence of the methods depends upon the selected differencing scheme. Most of our detailed explanations are given in slab geometry for ease in understanding. All results apply equally well to all other generally used coordinate systems. We do not dwell on boundary conditions used with the transport and diffusion equations since they are the standard vacuum, reflective, and periodic conditions.

### *II.A. Diffusion Synthetic Acceleration Methods*

Discrete-ordinates neutron transport codes use a dual strategy for solving the transport equation.[12,13] The two nested iterations are referred to as outer and inner iterations. The outer iteration represents a sweep through all the energy groups, while the inner iteration is performed within each energy group. In this section, we present in their continuous form three different forms of the diffusion synthetic acceleration method as approaches to accelerating these iteration processes. One of the acceleration schemes, the source correction scheme, is linear in its continuous form and is used for inhomogeneous source problems. The other two are nonlinear and are used for eigenvalue problems.

#### *II.A.1. Source Correction Scheme*

To display the diffusion synthetic method used for inhomogeneous source problems, we first consider the inner iteration,

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\tilde{\psi}_g^l(\boldsymbol{r},\boldsymbol{\Omega}) + \sigma_g(\boldsymbol{r})\tilde{\psi}_g^l(\boldsymbol{r},\boldsymbol{\Omega}) = \sigma_{sg\to g}(r)\phi_g^{l-1}(\boldsymbol{r}) + QQ_g(\boldsymbol{r}) \quad . \tag{1}$$

In Eq. (1), $\tilde{\psi}_g^l$ is the angular flux for group $g$ at the $l$'th inner iteration calculated using a scalar flux, $\phi_g^{l-1}$, assumed to be known at each step of the iteration. The group source, $QQ_g$, contains scattering and fission contributions to the group as well as the inhomogeneous source. This source is computed from the multigroup flux of the previous outer iteration and is assumed to be known. We have assumed isotropic scattering and sources for simplicity. This scheme, as well as the related approaches discussed below, also apply to the more general anisotropic problem. In the diffusion synthetic method, we employ a corrected diffusion equation using $\tilde{\psi}_g$ to determine the scalar flux, $\phi_g$, needed for the next iteration. For the source correction scheme, this equation is

$$-\boldsymbol{\nabla}\cdot D_g(\boldsymbol{r})\boldsymbol{\nabla}\phi_g^l(\boldsymbol{r}) + \sigma_{Rg}(\boldsymbol{r})\phi_g^l(\boldsymbol{r}) = QQ_g(\boldsymbol{r}) - R_g^l(\boldsymbol{r}) \quad , \tag{2}$$

where

$$D_g(\boldsymbol{r}) = 1/3\sigma_{tr}(\boldsymbol{r}) \quad ,$$

$$\sigma_{Rg}(\boldsymbol{r}) = \sigma_g(\boldsymbol{r}) - \sigma_{sg\to g}(\boldsymbol{r}) \quad ,$$

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[6]E. M. GELBARD and L. A. HAGEMAN, *Nucl. Sci. Eng.*, **37**, 288 (1969).

[7]R. E. ALCOUFFE and E. E. LEWIS, "Synthetic Acceleration Methods for the Neutron Transport Equation," IAEA Specialist Mtg. Methods of Neutron Transport Theory in Reactor Calculations, Bologna, Italy, CONF-751152, International Atomic Energy Agency (Nov. 1975) (Unpublished).

[8]R. E. ALCOUFFE, *Trans. Am. Nucl. Soc.*, **23**, 203 (1976).

[9]E. E. LEWIS and W. F. MILLER, Jr., *Trans. Am. Nucl. Soc.*, **23**, 201 (1976).

[10]J. W. PAINTER, "A Nonlinear Synthetic Iteration Method for Discrete Ordinates Neutron Transport Calculations," PhD Dissertation, Department of Nuclear Engineering, University of Virginia (Aug. 1976).

[11]WM. H. REED, Los Alamos Scientific Laboratory, Personal Communication (Dec. 1976).

[12]WM. H. REED, T. R. HILL, F. W. BRINKLEY, Jr., and K. D. LATHROP, "TRIPLET: A Two-Dimensional, Multigroup Triangular Mesh, Planar Geometry, Explicit Transport Code," LA-5428-MS, Los Alamos Scientific Laboratory (1973).

[13]T. J. SEED, W. F. MILLER, Jr., and F. W. BRINKLEY, Jr., "TRIDENT: A Two-Dimensional, Multigroup Triangular Mesh Discrete Ordinates, Explicit Neutron Transport Code," LA-6735-MS, Los Alamos Scientific Laboratory (1977).

and the correction term is

$$R_g^l(\boldsymbol{r}) = \nabla \cdot \tilde{\boldsymbol{J}}_g^l(\boldsymbol{r}) + \nabla \cdot D_g(\boldsymbol{r}) \nabla \tilde{\phi}_g^l(\boldsymbol{r}) \quad . \tag{3}$$

In Eq. (3),

$$\tilde{\phi}_g^l(\boldsymbol{r}) = \int d\Omega \tilde{\psi}_g^l(\boldsymbol{r}, \boldsymbol{\Omega}) \tag{4a}$$

and

$$\tilde{\boldsymbol{J}}_g^l(\boldsymbol{r}) = \int d\Omega \, \boldsymbol{\Omega} \tilde{\psi}_g^l(\boldsymbol{r}, \boldsymbol{\Omega}) \quad . \tag{4b}$$

Note that we use a tilda to indicate quantities calculated using the angular flux, $\tilde{\psi}_g^l$, while the scalar flux calculated from the corrected diffusion equation is without the tilda.

The source correction scheme for the inner iteration proceeds as follows: Using $\phi_g^{l-1}$, known from the previous iteration, we solve Eq. (1) for $\tilde{\psi}_g^l$. In present-day discrete-ordinates codes, this involves one sweep through the space-angle mesh. The correction term, $R_g^l$, is then calculated using Eqs. (3) and (4) and, in turn, is used in Eq. (2) to calculate $\phi_g^l$, completing one cycle of the iteration. The steps are repeated until some convergence criterion is satisfied. Note that for $l = 0$, a logical first guess is obtained by setting $R_g^0$ to zero and solving the diffusion equation for $\phi_g^0$.

It is easy to show that if the iteration converges, it converges to the transport equation solution, namely, drop all $l$ superscripts and set the transport scalar flux equal to the corrected diffusion flux, $\phi_g = \tilde{\phi}_g$. Then, substituting Eq. (3) into Eq. (2) yields

$$\nabla \cdot \tilde{\boldsymbol{J}}_g(\boldsymbol{r}) + \sigma_{Rg}(\boldsymbol{r}) \tilde{\phi}_g(\boldsymbol{r}) = QQ_g \quad ,$$

which is the converged transport balance equation, also obtained by integrating Eq. (1) over all $\boldsymbol{\Omega}$. The question of convergence of the method is discussed in Secs. II.B.3 and III.

We now discuss an outer iteration procedure, which is consistent with the above outlined inner iteration. The outer iteration consists of one pass through each of the groups using Eqs. (1), (2), and (3) to obtain the group-converged correction terms $R_g^k(\boldsymbol{r})$, and then to solve the multigroup corrected diffusion equation. A new multigroup source for the inner iterations is then obtained from the corrected diffusion solution. That is, we solve the following multigroup diffusion equation:

$$\begin{aligned} -\nabla \cdot D_g(r) \nabla \phi_g^{k+1}(\boldsymbol{r}) + \sigma_{Rg}(\boldsymbol{r}) \phi_g^{k+1}(\boldsymbol{r}) \\ = Q_g(\boldsymbol{r}) - R_g^k(\boldsymbol{r}) + \chi_g \sum_{g'=1}^{G} \nu\sigma_{fg'}(\boldsymbol{r}) \phi_{g'}^{k+1}(\boldsymbol{r}) \\ + \sum_{g' \neq g} \sigma_{sg' \to g}(\boldsymbol{r}) \phi_{g'}^{k+1}(r) \quad . \end{aligned} \tag{5}$$

Hence, the solution procedure for the multigroup transport equation is to first solve Eq. (5) with $R_g(\boldsymbol{r}) = 0$ for all groups obtaining the diffusion equation solution as the initial flux guess. We then evaluate $QQ_g$ for $k = 1$ and cycle through the inner iteration [Eqs. (1), (2), and (3)], obtaining an estimate of $R_g^k$. We use this in the multigroup diffusion equation to obtain a new value of $\phi_g^{k+1}$, from which we start the procedure over. We continue this iteration cycle until all convergence criteria have been satisfied. We have found that for all problems requiring outer iterations that we have solved, we need take only one inner iteration per group until the multigroup source is converged, $|QQ_g^{k+1} - QQ_g^k| \leq \epsilon$, and then we converge the group flux as required by increasing the inner iteration count. This usually requires only one additional outer iteration. The procedure outlined here with one inner per outer can be viewed as using the diffusion equation to perform the outer iteration of the transport equation and only invoking the transport equation to obtain the necessary corrections.

As is discussed in detail in Secs. II.B.3 and III, this outer and inner iteration process does converge, and in fact, is more efficient than existing methods in one- and two-dimensional problems if one is careful in the spatial differencing process. The general idea of a source correction scheme for the inner iteration is a result of simultaneous, and at times, joint work of Alcouffe, Lewis, and Miller (see Refs. 7, 8, and 9). The latter two authors have shown that in the analytic form, at least in slab geometry, this approach is equivalent to the traditional synthetic method.[5,6]

The above method of inner and outer iteration acceleration depends on the problem being one with an extraneous source, i.e., subcritical system. To be able to extend the method to handle eigenvalue problems, we have to recast the acceleration equations as discussed in the following.

### *II.A.2. Diffusion Coefficient Correction Scheme*

To implement the iteration acceleration procedure outlined in Sec. II.A.1, above, for eigenvalue problems we require that Eq. (5) be homogeneous. In our definition of $R_g(r)$ of Eq. (3), we see that if we redefine the diffusion coefficient such that

$$D_g(\boldsymbol{r}) \to \{D_g(\boldsymbol{r})\}_{ii} = -\frac{\tilde{J}_{gi}(\boldsymbol{r})}{\nabla_i \tilde{\phi}_g(\boldsymbol{r})} \quad , \quad i = 1, 2, 3 \quad , \tag{6}$$

where $i$ designates one of the orthogonal coordinate directions and $\{D_g\}_{ii}$ designates diagonal tensor of rank 2, then $R_g(\boldsymbol{r}) = 0$ for all $\boldsymbol{r}$ and $g$. Therefore, when $Q_g(\boldsymbol{r}) = 0$, Eq. (5) has the required homogeneous form. With this expression for the diffusion coefficient, we then transform the inner iteration

diffusion equation into

$$-\nabla \cdot \mathbf{D}_g^{l-1}(\boldsymbol{r}) \cdot \nabla \phi_g^l(\boldsymbol{r}) + \sigma_{Rg}(\boldsymbol{r})\phi_g^l(\boldsymbol{r}) = QQ_g(\boldsymbol{r}) \quad , \quad (7)$$

and the multigroup diffusion Eq. (5) becomes

$$-\nabla \cdot \mathbf{D}_g^k(\boldsymbol{r}) \cdot \nabla \phi_g^{k+1}(\boldsymbol{r}) + \sigma_{Rg}(\boldsymbol{r})\phi_g^{k+1}(\boldsymbol{r})$$

$$= \frac{\chi_g}{k_{\text{eff}}} \sum_{g'=1}^{G} \nu\sigma_{fg}(\boldsymbol{r})\phi_{g'}^{k+1}(\boldsymbol{r})$$

$$+ \sum_{g' \neq g} \sigma_{sg' \to g}(\boldsymbol{r})\phi_{g'}^{k+1}(\boldsymbol{r}) \quad , \quad (8)$$

where $k_{\text{eff}}$ is the multiplication factor for the system. We then follow precisely the same iterations procedure outlined for the source method using Eqs. (1), (6), (7), and (8) instead. The initial solution for the scalar flux is found from Eq. (8) by setting $\{D_g(\boldsymbol{r})\}_{ii} = D_g(\boldsymbol{r})$ for $i = 1, 2, 3$. Equations (1), (6), and (7) then define the inner iterations, with the final resultant diffusion coefficient $\mathbf{D}_g^k(\boldsymbol{r})$ used in Eq. (8).

Although this is a nonlinear iteration procedure [due to Eq. (6)], we have observed numerically that it converges as readily as does the source correction scheme if properly spatially differenced. This scheme is due to Alcouffe[8] extending his earlier work on diffusion correction schemes.[14] Painter[10] and Reed[11] have also done work, taking a different approach, in extension of the Alcouffe method.[14]

The diffusion coefficient correction scheme has the disadvantage that it is possible to compute infinite and negative diffusion coefficients [see Eq. (6)], rending Eq. (7) impossible to solve numerically using current techniques. To overcome this difficulty, we introduce another method, used in conjunction with the diffusion correction scheme, for eigenvalue problems.

### *II.A.3. Removal Correction Scheme*

An alternative way of making Eq. (5) homogeneous is to move the correction term into the removal terms, defining a new removal term as[8,15]

$$\tilde{\sigma}_{Rg}^k(\boldsymbol{r}) = \sigma_{Rg}(\boldsymbol{r}) + R_g^k(\boldsymbol{r})/\tilde{\phi}_g^k(\boldsymbol{r}) \quad . \quad (9)$$

Thus, the diffusion synthetic acceleration method is altered, and Eq. (2) becomes

$$-\nabla \cdot D_g(\boldsymbol{r})\nabla\phi_g^l(\boldsymbol{r}) + \tilde{\sigma}_{Rg}^{l-1}(\boldsymbol{r})\phi_g^l(\boldsymbol{r}) = QQ_g(\boldsymbol{r}) \quad , \quad (10)$$

while Eq. (5) becomes

$$-\nabla \cdot D_g(\boldsymbol{r})\nabla\phi_g^{k+1}(\boldsymbol{r}) + \tilde{\sigma}_{Rg}^k(\boldsymbol{r})\phi_g^{k+1}(\boldsymbol{r})$$

$$= \frac{\chi_g}{k_{\text{eff}}} \sum_{g'=1}^{G} \nu\sigma_{fg'}(\boldsymbol{r})\phi_{g'}^{k+1}(\boldsymbol{r})$$

$$+ \sum_{g' \neq g} \sigma_{sg' \to g}(\boldsymbol{r})\phi_{g'}^{k+1}(\boldsymbol{r}) \quad . \quad (11)$$

This iteration procedure is now entirely analogous to the diffusion coefficient method using Eqs. (1), (9), (10), and (11) instead, and again, if it converges, it converges to the transport balance equation solution. Although nonlinear, we have numerically observed that this method too is as convergent as the source correction scheme. The basic idea of the removal scheme is due to Cahalan[15] and Alcouffe[8] working independently.

In practice, for eigenvalue problems we use the diffusion coefficient method in conjunction with the removal term method when negative diffusion coefficients are computed.

## *II.B. The Discretized Transport Equation for One-Dimensional Cases*

### *II.B.1. General*

Now that we have presented, analyzed, and compared the three forms of the diffusion synthetic method, it is important that we consider the angularly and spatially discretized equations. This is necessary to show that a convergent diffusion accelerated iteration depends on the selected difference method. We show that Reed[5] obtained divergent results for some problems using the source correction scheme because of his selected difference procedure. We present a difference scheme yielding a stable, efficient iteration algorithm. The procedure can be completely described with the inner iteration, and, hence, we restrict ourselves to the one-group problem. We consider in this section only the one-dimensional case, leaving considerations of importance in two dimensions to Sec. II.C. The angular derivative term appearing in the neutron transport equation also adds interesting complications to the procedure presented below. The steps taken in resolution of these difficulties, however, are somewhat tedious. Accordingly, we refer the reader to Ref. 16 for a detailed presentation of the implementation of the diffusion synthetic acceleration method in curvilinear geometry. The important points can be made in slab geometry with isotropic scattering and sources and, therefore, we restrict ourselves to this simple case.

We begin by applying the discrete-ordinates approximation to the directional variables and the diamond-difference approximation to the spatial

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[14]R. E. ALCOUFFE, *Nucl. Sci. Eng.*, **56**, 321 (1975).

[15]J. E. CAHALAN, K. O. OTT, and D. R. FERGUSON, *Trans. Am. Nucl. Soc.*, **23**, 203 (1976).

[16]R. E. ALCOUFFE and G. E. BOSLER, "ONETRAN-DA: A Discrete Ordinates Diamond Difference Code for the Solution of the One-Dimensional Transport Equation Using Diffusion Acceleration," Los Alamos Scientific Laboratory (to be published).

variables of the transport equation to obtain from Eq. (1),

$$\mu_m(\tilde{\psi}^l_{mi+1/2} - \tilde{\psi}^l_{mi-1/2}) + \sigma_i h_i \tilde{\psi}_{mi} = \sigma_{si} h_i \phi^{l-1}_{0i} + QQ_i h_i \quad ,$$
$$m = 1, 2, \ldots, M \quad , \quad i = i, 2, \ldots, I \quad . \quad (12)$$

The $m$ is the directional subscript, $i$ is the spatial subscript, and we define the angular moments by

$$\phi_{ni} \simeq \sum_{m=1}^{M} w_m P_n(\mu_m)\psi_{mi} \quad ,$$
$$n = 1, 2, \ldots, N \quad , \quad i = 1, 2, \ldots, I \quad , \quad (13)$$

with the set $\{w_m\}$ as the weights of a selected quadrature set normalized so that

$$\sum_{m=1}^{M} w_m = 1 \quad .$$

To derive Eq. (12), we have imposed a spatial mesh in which the mesh centers are given by the whole number indices (e.g., $i - 1$, $i$, $i + 1$), the mesh boundaries are given by half integral indices ($i + \frac{1}{2}$, $i + \frac{3}{2}$, . . . ), and

$$h_i = x_{i+1/2} - x_{i-1/2} \quad .$$

In addition to Eq. (12), we assume the diamond scheme[17]

$$\tilde{\psi}^l_{mi} = \tfrac{1}{2}(\tilde{\psi}^l_{mi+1/2} + \tilde{\psi}^l_{mi-1/2}) \quad ,$$
$$m = 1, 2, \ldots, M \quad , \quad i = 1, 2, \ldots, I \quad . \quad (14)$$

Other relationships needed in the ensuing analysis are obtained by operating on Eq. (12) with the operators

$$\sum_{m=1}^{M} w_m P_0(\mu_m)$$

and

$$\sum_{m=1}^{M} w_m P_1(\mu_m)$$

[i.e., taking the zero and first-order discrete moments of Eq. (12)] to obtain, respectively,

$$\tilde{\phi}^l_{1i+1/2} - \tilde{\phi}^l_{1i-1/2} + \sigma_i h_i \tilde{\phi}_{0i} = \sigma_{si} h_i \phi^{l-1}_{0i} + QQ_i h_i \quad , \quad (15)$$

and

$$\tfrac{1}{3}(\tilde{\phi}_{0i+1/2} - \tilde{\phi}^l_{0i-1/2}) + \tfrac{2}{3}(\tilde{\phi}^l_{2i+1/2} - \tilde{\phi}^l_{2i-1/2}) + \sigma_i h_i \tilde{\phi}_{1i} = 0 \quad , \quad i = 1, 2, \ldots, I \quad . \quad (16)$$

### *II.B.2. Difference Equations for the Source Correction Scheme*

To implement the source correction method, we must now select a differencing scheme for the diffusion equation and correction term [see Eqs. (17) and (18)]. The heretofore used method[5] is to difference $R$ as

$$R^l_i = -\tilde{\phi}^l_{1i+1/2} + \tilde{\phi}^l_{1i-1/2} - D_{i+1/2}\frac{(\tilde{\phi}^l_{0i+1} - \tilde{\phi}^l_{0i})}{\frac{1}{2}(h_i + h_{i+1})} + D_{i-1/2}\frac{(\tilde{\phi}^l_{0i} - \tilde{\phi}^l_{0i-1})}{\frac{1}{2}(h_{i-1} + h_i)} \quad ,$$
$$i = 1, 2, \ldots, I \quad , \quad (17)$$

where

$$D_{i+1/2} = \tfrac{1}{2}\frac{h_i D_i + h_{i+1} D_{i+1}}{h_{i+1}} \quad .$$

Equation (17) results from integrating $R(x)$ over a spatial mesh interval $(x_{i-1/2}, x_{i+1/2})$, the same procedure used to derive Eq. (12). Using this scheme to difference Eq. (2), we obtain

$$-D_{i+1/2}\frac{(\phi^l_{0i+1} - \phi^l_{0i})}{\frac{1}{2}(h_i + h_{i+1})} + D_{i-1/2}\frac{(\phi^l_{0i} - \phi^l_{0i-1})}{\frac{1}{2}(h_i + h_{i-1})} + \sigma_{Ri} h_i \phi^l_{0i} = QQ_i h_i - R^l_i \quad ,$$
$$i = 1, 2, \ldots, I \quad . \quad (18)$$

Equations (17) and (18) are compatible in that assuming convergence ($\tilde{\phi}^l_{0i} = \phi^l_{0i}$ and $\tilde{\phi}^l_{1i} = \phi_{1i}$), we obtain the discretized transport balance equation,

$$\tilde{\phi}_{1i+1/2} - \tilde{\phi}_{1i-1/2} + \sigma_{Ri} h_i \tilde{\phi}_{0i} = QQ_i h_i \quad ,$$
$$i = 1, 2, \ldots, I \quad . \quad (19)$$

The numerical form of the source correction method that has commonly been utilized[5] is that expressed by Eqs. (17) and (18); as shown in Ref. 5, this form does not yield a stable algorithm for all problems. The nonconvergent problems are those that have optically thick regions in which the scattering ratio, $c = \sigma_s/\sigma$, is close to one and the mesh spacing is greater than a mean-free-path. These same problems are, however, very well approximated by diffusion theory, and we expect that the converged $R_i$ of Eq. (17) would be small in these cases and in the limit (of a very large region) approach zero. However, in a homogeneous region where $D_{i+1/2} = D_{i-1/2} = 1/3\sigma_i$, $R_i$ does not go to zero using Eq. (17) unless the mesh spacing $h_i$ goes to zero. This is clear, since setting the second moment terms in Eq. (16) to zero (the diffusion limit), a relationship for the first moment at the cell centers results, while Eq. (17) utilizes the first moment at the cell boundaries. Thus, for diffusion-type problems,

[17] B. G. CARLSON and K. D. LATHROP, "Transport Theory–Method of Discrete Ordinates," in *Computation Methods in Reactor Physics*, Chap. III, p. 173, Gordon and Breach, Science Publishers, Inc., New York (1968).

the differencing scheme does not adequately account for the physical situation, and this is the likely source of the instability of the algorithm as the spatial mesh width increases.

We now use the fact that $R_i$ should go to zero in the diffusion limit to select another difference scheme. In formulating this scheme, we realize that for the solution of the accelerated equation to converge to the diamond-differenced transport solution, Eqs. (17) and (18) must reduce to a diamond-differenced transport balance equation upon convergence. To obtain a more appropriate balance equation, we add to the standard transport balance equation [Eq. (19)] for the $i$'th cell this same equation for the $i+1$ cell and use the relationship resulting from taking the first angular moment of Eq. (14) to obtain

$$\tilde{\phi}_{1i+1} - \tilde{\phi}_{1i} + \tfrac{1}{2}(\sigma_{Ri+1}h_{i+1}\tilde{\phi}_{0i+1} + \sigma_{Ri}h_i\tilde{\phi}_{0i}) = \tfrac{1}{2}(QQ_ih_i + QQ_{i+1}h_{i+1}) \quad , \quad i = 1, 2, \ldots, I \quad . \tag{20}$$

It is clear from its derivation that this is another form of the diamond-differenced balance equation. Solving the converged form of Eq. (16) for $\phi_{1i}$ and $\phi_{1i+1}$ and substituting the result in Eq. (20) yields

$$-D'_{i+1}\frac{\phi_{0i+3/2} - \phi_{0i+1/2}}{h_{i+1}} + D'_i\frac{\phi_{0i+1/2} - \phi_{0i-1/2}}{h_i} + \tfrac{1}{2}(\sigma_{Ri+1}h_{i+1}\phi_{0i+1} + \sigma_{Ri}h_i\phi_{0i}) = \tfrac{1}{2}(QQ_ih_i + QQ_{i+1}h_{i+1}) \quad , \quad i = 1, 2, \ldots, I-1 \quad , \tag{21}$$

where

$$D'_i = \frac{1}{3\sigma_i}\left(1 + 2\,\frac{\phi_{2i+1/2} - \phi_{2i-1/2}}{\phi_{0i+1/2} - \phi_{0i-1/2}}\right) \quad .$$

Equation (21) has the form of the diffusion equation with a general expression for the diffusion coefficients. For the case that $\phi_{2i} = 0$ (diffusion limit) for all $i$, Eq. (21) is in fact, the conventional diffusion equation differenced so that the fluxes are evaluated on the mesh boundaries. We conclude, then, that if, in lieu of Eq. (17), we use the following difference scheme for $R$,

$$R_i^l = \tilde{\phi}_{1i+1}^l - \tilde{\phi}_{1i}^l + D_{i+1}\frac{\tilde{\phi}_{0i+3/2}^l - \tilde{\phi}_{0i+1/2}^l}{h_{i+1}} - D_i\frac{\tilde{\phi}_{0i+1/2}^l - \tilde{\phi}_{0i-1/2}^l}{h_i} \quad , \quad i = 1, 2, \ldots, I \quad , \tag{22}$$

we then obtain the desired result that $R_i = 0$ in the diffusion theory limit. In conclusion, we find that we must difference the corrected diffusion equation as

$$-D_{i+1}\frac{(\phi_{0i+3/2}^l - \phi_{0i+1/2}^l)}{h_{i+1}} + D_i\frac{(\phi_{0i+1/2}^l - \phi_{0i-1/2}^l)}{h_i} + (\tilde{\sigma}_R h)_{0i+1/2}^l\phi_{0i+1/2}^l = (QQh)_{i+1/2} + R_i^l \quad , \quad i = 1, 2, \ldots, I \quad , \tag{23}$$

where

$$(\tilde{\sigma}_R h)_i^l \equiv \tfrac{1}{2}(\sigma_{Ri+1}h_{i+1}\tilde{\phi}_{0i+1} + \sigma_{Ri}h_i\tilde{\phi}_{0i}^l)/\tilde{\phi}_{0i+1/2}^l \tag{23a}$$

and

$$(QQh)_{i+1/2} = \tfrac{1}{2}(QQ_ih_i + QQ_{i+1}h_{i+1}) \quad . \tag{23b}$$

From Eqs. (22) and (23), we see that the balance Eq. (20) is attained upon convergence. Note that to achieve this objective without assuming that the diamond-difference relationship holds, we have introduced a nonlinearity into the iteration scheme [Eq. (23a)]. Because Eq. (20) is a valid neutron balance equation for the transport scalar flux, the solution to the accelerated differenced equation will be the solution to the differenced transport equation itself. Since we have formulated this differencing method to be compatible with the diffusion limit, we expect the instability problems of the synthetic acceleration method to be mitigated, and this is shown to be the case for a wide class of numerical examples in Sec. III.

### *II.B.3. Demonstration of Unconditional Convergence for the Source Correction Scheme*

As previously mentioned in his work on diffusion synthetic acceleration, Reed[5] used a difference scheme that resulted in an iteration algorithm that does not behave properly in the diffusion limit. Using a model problem, Reed demonstrates that convergence with his scheme depends upon the spatial mesh spacing. In the following, we follow Reed's development and show that with the difference scheme developed above, convergence is unconditional for that model problem. In slab geometry with isotropic scattering, constant mesh spacing $h$, and constant cross sections, we express the differenced source correction scheme [Eqs. (12), (22), and (23)] as

$$\mu_m\frac{\tilde{\psi}_{mi+1/2}^l - \tilde{\psi}_{mi-1/2}^l}{h} + \sigma\tilde{\psi}_{mi}^l = c\sigma\phi_{0i}^{l-1} + QQ_i \quad , \quad m = 1, 2, \ldots, M \quad , \tag{24}$$

$$-\frac{D}{h^2}(\phi_{0i+3/2}^l - 2\phi_{0i+1/2}^l + \phi_{0i-1/2}^l) + \tfrac{1}{4}\sigma_R(\phi_{0i+3/2} + 2\phi_{0i+1/2} + \phi_{0i-1/2}) = QQ_i - R_i^l \quad , \tag{25}$$

and

$$R_i^l = \frac{\tilde{\phi}_{1i+1}^l - \tilde{\phi}_{1i}^l}{h} + \frac{D}{h^2}\left(\tilde{\phi}_{0i+3/2}^l - 2\tilde{\phi}_{0i+1/2}^l + \tilde{\phi}_{0i-1/2}^l\right) ,$$

$$i = 1, 2, \ldots, I \quad , \qquad (26)$$

where we have assumed the diamond-difference relationship in Eq. (25).

Taking the first Legendre moment of Eq. (24) and using the results in Eq. (26) yields

$$R_i^l = -\frac{2D}{h^2}\left(\tilde{\phi}_{2i+3/2}^l - 2\tilde{\phi}_{2i+1/2}^l + \tilde{\phi}_{2i-1/2}^l\right) \quad . \qquad (27)$$

Using Eq. (27), we can write Eq. (25) in matrix form as

$$[\mathbf{D} + (1 - c)\boldsymbol{\sigma}]\tilde{\boldsymbol{\phi}}_0^l = -2\mathbf{D}\tilde{\boldsymbol{\phi}}_2^l \qquad (28)$$

where $\mathbf{D}$ is the diffusion operator and $\tilde{\boldsymbol{\phi}}_2^l$ is the second Legendre flux moment vector, and we have set the source to zero. We show that for an infinite medium,

$$\tilde{\boldsymbol{\phi}}_2^l = -\mathbf{N}\phi_0^{l-1} \quad , \qquad (29)$$

where $\mathbf{N}$ is a matrix to be determined.

We first combine Eqs. (28) and (29), yielding the iteration procedure,

$$\boldsymbol{\phi}_0^l = 2[\mathbf{D} + (1 - c)\boldsymbol{\sigma}]^{-1}\mathbf{D}\mathbf{N}\boldsymbol{\phi}_0^{l-1} \quad .$$

Thus, the diffusion synthetic iteration matrix is

$$\mathbf{M}_s = 2[\mathbf{D} + (1 - c)\boldsymbol{\sigma}]^{-1}\mathbf{D}\mathbf{N} \quad . \qquad (30)$$

The matrix elements of $\mathbf{N}$ are found in a manner completely analogous to that developed by Reed.[5] We quote the result here as

$$\tilde{\phi}_{2i+1/2}^{l+1} = \left\{\frac{cP_2(\mu_m)r_m}{1 + r_m}\right\}\phi_{0i+1/2}^l + \left\{\frac{cP_2(\mu_m)r_m}{(1 + r_m)^2}\right\} \times \left(\phi_{0i-1/2}^l + \phi_{0i+3/2}^l\right) + \left\{\frac{cP_2(\mu_m)r_m(1 - r_m)}{(1 + r_m)^3}\right\} \times \left(\phi_{0i-3/2}^l + \phi_{0i+5/2}^l\right) + \ldots ,$$

$$i = 1, 2, \ldots, I \quad ,$$

where

$$\{f_m\} = \sum_{m=1}^{M} w_m f_m \quad , \quad r_m = \frac{\sigma h}{2|\mu_m|} \quad ,$$

and $P_2$ is the Legendre polynomial of order 2. This is in the form of Eq. (29). Now, to find the spectral radius of $\mathbf{M}_s$, we must determine the eigenvalues of the matrices $\mathbf{N}$ and $\mathbf{D}$. Reed[5] has shown that the appropriate eigenfunctions for each operator are

$$\phi_k = \frac{\cos(i + \frac{1}{2})\pi}{k} \quad , \quad k = 1, 2, \ldots \quad .$$

We find that the eigenvalues for $\mathbf{N}$ are

$$\lambda_k = c\left\{\frac{r_m^2 P_2(\mu_m)}{r_m^2 + \tau_k}\right\} \quad , \qquad (31)$$

where

$$\tau_k = \frac{1 - \cos\pi/k}{1 + \cos\pi/k} \quad , \qquad (32)$$

and for $\mathbf{D}$ are

$$\eta_k = \frac{2D}{h^2}(1 - \cos\pi/k) \quad . \qquad (33)$$

From Eqs. (31), (32), and (33), we write the eigenvalues of $\mathbf{M}_s$ as

$$\theta_k = \frac{2\eta_k\lambda_k}{\eta_k + \frac{1}{2}(1 - c)\sigma(1 + \cos\pi/k)} \quad .$$

From Eq. (31) it is clear that

$$\lambda_k = \frac{c}{2}\left\{\frac{3r_m^2\mu_m^2}{r_m^2 + \tau_k}\right\} - \frac{c}{2}\left\{\frac{r_m^2}{r_m^2 + \tau_k}\right\} < \frac{3c}{2}\left\{\frac{r_m^2\mu_m^2}{r_m^2 + \tau_k}\right\}$$

for $\lambda_k \neq 0$, since

$$\left\{\frac{r_m^2}{r_m^2 + \tau_k}\right\} > 0 \text{ for } \tau_k \neq \infty \quad .$$

From its definition, the minimum $\tau_k$ is zero for $k = \infty$. Thus,

$$\lambda_k < \frac{3c}{2}\left\{\frac{r_m^2\mu_m^2}{r_m^2 + \tau_\infty}\right\} = \frac{c}{2} \quad .$$

Thus,

$$\theta_k < \frac{c}{1 + (1 - c)\dfrac{\sigma h^2}{4D}\cot^2\pi/2k} < C \quad . \qquad (34)$$

Since Eq. (34) is a strict inequality, it is seen that the spectral radius is always less than unity, independent of the value of $\sigma h^2/4D$, since $0 \leq c \leq 1$. Thus, the method is unconditionally convergent for this model problem.

### *II.B.4. Difference Equations for the Diffusion Coefficient and Removal Correction Schemes*

The diffusion coefficient and removal correction schemes are both nonlinear schemes even for this model problem and, hence analyses such as that in the preceding section are much more complicated. Numerical experimentation has verified, however, that with these nonlinear schemes,

spatial differencing analogous to Eqs. (22) and (23) is required for stability. Namely, the two differenced acceleration equations for the diffusion coefficient correction scheme are

$$-\tilde{D}_{i+1}\frac{(\phi^l_{0i+3/2}-\phi^l_{0i+1/2})}{h_{i+1}}+\tilde{D}_i\frac{(\phi^l_{0i+1/2}-\phi^l_{0i-1/2})}{h_i}+(\tilde{\sigma}_R h)^l_{i+1/2}\phi^l_{0i+1/2}=(QQh)_{i+1/2}\quad,\quad i=1,2,\ldots,I-1\quad, \tag{31}$$

and

$$\tilde{D}^l_i=-h_i\tilde{\phi}^l_{1i}/(\tilde{\phi}^l_{0i+1/2}-\tilde{\phi}^l_{0i-1/2})\quad. \tag{32}$$

For the removal correction scheme, the corresponding equations are

$$-D_{i+1}\frac{(\phi^l_{0i+3/2}-\phi^l_{0i+1/2})}{h_{i+1}}+D_i\frac{(\phi^l_{0i+1/2}-\phi^l_{0i-1/2})}{h_i}+(\sigma_R h)^l_{i+1/2}\phi^l_{0i+1/2}=(QQh)_{i+1/2}\quad,\quad i=1,2,\ldots,I-1\quad, \tag{33}$$

and

$$(\sigma_R h)^l_{i+1/2}=(\tilde{\sigma}_R h)^l_i+(1/\tilde{\phi}^l_{0i+1/2})\times\left[(\tilde{\phi}^l_{1i+1}-\tilde{\phi}^l_{1i})+D_{i+1}\frac{(\tilde{\phi}^l_{0i+3/2}-\tilde{\phi}^l_{0i+1/2})}{h_{i+1}}-D_i\frac{(\tilde{\phi}^l_{0i+1/2}-\tilde{\phi}^l_{0i-1/2})}{h_i}\right]\quad. \tag{34}$$

With these selections, both methods behave correctly in the diffusion limit and converge to the balance equation, Eq. (20).

### *II.B.5. Implementation in the Production Computer Code, ONETRAN-DA*

The diffusion synthetic acceleration method has been implemented in a computer code derived from ONETRAN (Ref. 1), entitled ONETRAN-DA (Ref. 16). This latter code uses diamond-differencing in the spatial variables and operates in all three one-dimensional geometries—slab, spherical, and cylindrical. The source correction scheme is used to accelerate the inner and outer iterations for inhomogeneous source problems, while the diffusion coefficient correction scheme is used for eigenvalue programs, again for both inner and outer iterations. The removal correction scheme is used if either negative or inordinately large diffusion coefficients are calculated. Thus, the diffusion coefficient or removal correction schemes may be alternatively selected on a mesh-cell-by-mesh-cell basis. We also use the coupled, inner-outer iteration scheme described in Sec. II.A.1.

It should be pointed out that one can use the diffusion synthetic method as a diffusion improvement scheme in lieu of an approach to accelerating transport iterations. For example, with the source correction scheme of Sec. II.A.1 after one transport sweep and associated calculation of the correction term, $R$, a corrected diffusion flux can be calculated. The solution procedure can stop at that point and the results used as an improved diffusion solution. The cost of this result is approximately twice the cost of one diffusion calculation, and our experience indicates that the results are normally significantly more accurate than diffusion results. ONETRAN-DA has an improved diffusion solution option and can also be used simply as a diffusion theory code.

## *II.C. Two-Dimensional Diffusion Synthetic Acceleration Method*

To develop the two-dimensional diffusion synthetic acceleration method in a finite differenced form, we follow the same procedure as used in Sec. II.B. The essential features of the development can be displayed using the $x$-$y$ geometry case with isotropic scattering and sources. For that case, the diamond-differenced discrete-ordinates equations are

$$\mu_m h_j(\psi_{mi+1/2j}-\psi_{mi-1/2j})+\eta_m h_i(\psi_{mij+1/2}-\psi_{mij-1/2})+\sigma_{ij}V_{ij}\psi_{mij}=\sigma_{sij}V_{ij}\phi^0_{0ij}+QQ_{mij}V_{ij}\quad,\quad m=1,2,\ldots,M\quad,\quad i=1,2,\ldots,I\quad,\quad j=1,2,\ldots,J\quad, \tag{35}$$

with

$$h_i=x_{i+1/2}-x_{i-1/2}\quad,\qquad h_j=y_{j+1/2}-y_{j-1/2}\quad,\qquad V_{ij}=h_ih_j\quad,$$

and the diamond equations

$$\psi_{mij}=\tfrac{1}{2}(\psi_{mi+1/2j}+\psi_{mi-1/2j})=\tfrac{1}{2}(\psi_{mij+1/2}+\psi_{mij-1/2})\quad. \tag{36}$$

We now seek the form of the differenced two-dimensional source corrected diffusion equation such that, in the diffusion limit, the correction term $R_{ij}\rightarrow 0$ is independent of the mesh opening and at the same time is compatible with the transport balance equation (see Sec. II.B).

We define the flux moments

$$\phi^q_{pij}\simeq\sum_{m=1}^{M}w_mY^q_p(\mu_m,\eta_m)\psi_{mij}\quad,$$

with the spherical harmonics polynomials defined by

$$Y^q_p(\mu,\eta)=\frac{(2-\delta_{q0})\,(p-q)!}{(p+q)!}P^q_p(\mu)\cos q$$

$$\int_{-1}^{1} d\mu \int_0 d\phi\, Y_p^q(\mu,\eta) Y_s^r(\mu,\eta) = \frac{2\pi}{2q+1}\,\delta_{qr}\delta_{ps} \quad ,$$

$$q = -p_0, \ldots, p \quad , \quad p = 0, 1, \ldots, N \quad ,$$

and

$$\eta = (1 - \mu^2)\cos\phi \quad .$$

The $P_p^q$ are associated Legendre polynomials, related to the Legendre polynomials by

$$P_p^q(\mu) = (1 - \mu^2)^{q/2} \frac{d^q P_p}{du^q}(\mu) \quad .$$

As a prelude to deriving a diffusion equation from the $S_N$ equation, we take three discrete moments of Eq. (35), namely,

$$\sum_{m=1}^{M} w_m Y_0^0(\mu_m,\eta_m) \quad ,$$

$$\sum_{m=1}^{M} w_m Y_1^0(\mu_m,\eta_m) \quad ,$$

and

$$\sum_{m=1}^{M} w_m Y_1^1(\mu_m,\eta_m) \quad ,$$

to obtain, respectively,

$$h_j(\phi^0_{1i+1/2j} - \phi^0_{1i-1/2j}) + h_i(\phi^1_{1ij+1/2} - \phi^1_{1ij-1/2}) + \sigma_{ij}V_{ij}\phi^0_{0ij} = \sigma_{sij}V_{ij}\phi^0_{0ij} + QQ_{ij}V_{ij} \quad , \tag{37}$$

$$\tfrac{1}{3}h_j(\phi^0_{0i+1/2j} - \phi^0_{0i-1/2j}) + \tfrac{2}{3}h_j(\phi^0_{2i+1/2j} - \phi^0_{2i-1/2j}) + \frac{1}{\sqrt{3}}h_i(\phi^1_{2ij+1/2} - \phi^1_{2ij-1/2}) + \sigma_{ij}V_{ij}\phi^0_{1ij} = 0 \quad , \tag{38}$$

and

$$\frac{1}{\sqrt{3}}h_j(\phi^1_{2i+1/2j} - \phi^1_{2i-1/2j}) + \tfrac{1}{3}h_i(\phi^0_{0ij+1/2} - \phi^0_{0ij-1/2}) + \tfrac{1}{3}h_i(\sqrt{3}\,\phi^2_{2ij+1/2} - \sqrt{3}\,\phi^2_{2ij-1/2} - \phi^0_{2ij+1/2} + \phi^0_{2ij-1/2})$$

$$+ \sigma_{ij}V_{ij}\phi^1_{1ij} = 0 \quad . \tag{39}$$

Rearranging Eqs. (38) and (39) results in the following expressions for the $i$ and $j$ direction currents:

$$\phi^0_{1ij} = -\frac{D_{ij}}{h_i}(\phi^0_{0i+1/2j} - \phi^0_{0i-1/2j}) + F(\phi^0_2, \phi^1_2)$$

and

$$\phi^1_{1ij} = -\frac{D_{ij}}{h_j}(\phi^0_{0ij+1/2} - \phi^0_{0ij-1/2}) + G(\phi^2_2, \phi^1_2) \quad , \tag{40}$$

where $D_{ij} = 1/3\sigma_{ij}$ and $F$ and $G$ are functions of the second-order moments whose forms are obtainable from Eqs. (38) and (39). In the diffusion theory limit (problem for which the diffusion equation provides the exact solution in the absence of truncation error), $F$ and $G$ go to zero.

We now seek a balance equation analogous to the one-dimensional case of Eq. (20), which the corrected diffusion equation will converge. This is obtained by adding to Eq. (35) the corresponding equations for the $(i+1, j)$, $(i, j+1)$, and $(i+1, j+1)$ mesh cells and using Eq. (36), yielding

$$\tfrac{1}{2}(h_j\phi^0_{1i+1j} + h_{j+1}\phi^0_{1i+1j+1}) - \tfrac{1}{2}(h_j\phi^0_{0ij} + h_{j+1}\phi^0_{1ij+1}) + \tfrac{1}{2}(h_i\phi^1_{1ij+1} + h_{i+1}\phi^1_{1i+1j+1}) - \tfrac{1}{2}(h_i\phi^1_{1ij} + h_{i+1}\phi^1_{1+1j})$$

$$+ \tfrac{1}{4}(\sigma_{Rij}V_{ij}\phi^0_{0ij} + \sigma_{Ri+1j}V_{i+1j}\phi^0_{0i+1j} + \sigma_{Rij+1}V_{ij+1}\phi^0_{0ij+1} + \sigma_{Ri+1j+1}V_{i+1j+1}\phi^0_{0i+1j+1})$$

$$= \tfrac{1}{4}(QQ_{ij}V_{ij} + QQ_{i+1j}V_{i+1j} + QQ_{ij+1}V_{ij+1} + QQ_{i+1j+1}V_{i+1j+1}) \quad , \tag{41}$$

where we have used the diamond-difference relationship to combine some of the terms. We now substitute Eq. (40) into Eq. (41) and derive the following diffusion equation:

$$-D'_{i+1j+1/2}(\phi^0_{0i+3/2j+1/2} - \phi^0_{0i+1/2j+1/2}) + D'_{ij+1/2}(\phi^0_{0i+1/2j+1/2} - \phi^0_{0i-1/2j+1/2}) - D'_{i+1/2j+1}(\phi^0_{0i+1/2j+3/2} - \phi^0_{0i+1/2j+1/2})$$

$$+ D'_{i+1/2j}(\phi^0_{0i+1/2j+1/2} - \phi^0_{0i+1/2j-1/2}) + (\sigma_R V)_{i+1/2j+1/2}\phi^0_{0i+1/2j+1/2} = (QQV)_{i+1/2j+1/2} - R_{ij} \quad , \tag{42}$$

with

$$D'_{ij+1/2} = (D_{ij}h_j + D_{ij+1}h_{j+1})/h_i \quad , \qquad D'_{i+1/2j} = (D_{ij}h_i + D_{i+ij}h_{i+1})/h_j \quad , \tag{42a}$$

$$(\sigma_R V)_{i+1/2\,j+1/2} = \tfrac{1}{4}(\sigma_{Rij}V_{ij}\phi^0_{0ij} + \sigma_{Ri+1j}V_{i+1j}\phi^0_{0i+1j} + \sigma_{Rij+1}V_{ij+1}\phi^0_{0ij+1} + \sigma_{Ri+1j+1}V_{i+1j+1}\phi^0_{0i+1j+1})/\phi^0_{0i+1/2j+1/2} \quad , \tag{42b}$$

$$(QQV)_{i+1/2\,j+1/2} = \tfrac{1}{4}(QQ_{ij}V_{ij} + QQ_{i+1j}V_{i+1j} + QQ_{ij+1}V_{ij+1} + QQ_{i+1j+1}V_{i+1j+1}) \quad , \tag{42c}$$

and

$$\begin{aligned} R_{ij} = {} & D'_{i+1j+1/2}(\phi^0_{0i+3/2j+1/2} - \phi^0_{0i+1/2j+1/2}) - D'_{ij+1/2}(\phi^0_{0i+1/2j+1/2} - \phi^0_{0i-1/2j+1/2}) \\ & + D'_{i+1/2j+1}(\phi^0_{0i+1/2j+3/2} - \phi^0_{0i+1/2j+1/2}) - D'_{i+1/2j}(\phi^0_{0i+1/2j+1/2} - \phi^0_{0i+1/2j-1/2}) \\ & + \tfrac{1}{2}(h_j\phi^0_{1i+1j} + h_{j+1}\phi^0_{1i+1j+1}) - \tfrac{1}{2}(h_j\phi^0_{1ij} + h_{j+1}\phi^0_{1ij+1}) \\ & + \tfrac{1}{2}(h_i\phi^1_{1ij+1} + h_{i+1}\phi^1_{1i+1j+1}) - \tfrac{1}{2}(h_i\phi^1_{1ij} + h_{i+1}\phi^1_{1i+1j}) \quad . \end{aligned} \tag{43}$$

In deriving Eq. (42) from Eqs. (40) and (41), we have used the fact that

$$h_jD_{i+1j}\phi^0_{0i+3/2,j} + h_{j+1}D_{i+1,j+1}\phi^0_{0i+3/2\,j+1} = (h_jD_{i+1,j} + h_{j+1}D_{i+1\,j+1})\phi^0_{0i+3/2\,j+1/2} + O(h_j^2) \quad .$$

The corresponding equations for the diffusion coefficient and removal correction schemes can be deduced from the above and the one-dimensional equations.

Note that to generate the correction term, the flux moments must be evaluated on the spatial mesh cell corners. To implement the scheme, we have altered the TWOTRAN-II (Ref. 2) code so that it determines the corner angular fluxes and calculates the required moments. This test version of TWOTRAN-II is operable in three two-dimensional geometries ($x$-$y$, $r$-$z$, and $r$-$\theta$) and follows the same outer/inner iteration procedure and the same scheme for selection of source, diffusion coefficient, or removal methods as described in Sec. II.A.

## III. CALCULATIONAL RESULTS

To demonstrate the effectiveness of the synthetic diffusion acceleration method, we present some one- and two-dimensional calculations of typical systems for which transport calculations are frequently used. Unless stated otherwise, all of the problems are converged to a pointwise criterion on the scalar flux of 0.0001 and are in cylindrical geometry. The one-dimensional problems are labeled as follows:

1. LMFBR. A configuration typical of current liquid-metal fast breeder reactor (LMFBR) designs with two core regions, a blanket region, and a structure or reflector region (28 groups, $S_4$).
2. HTGR. A configuration typical of current high-temperature gas-cooled reactor (HTGR) designs with a homogeneous core or graphite and $^{235}U$ fuel and a graphite reflector. This is an upscatter problem with nine groups, $S_4$.

3-4. TREAT 1 and 2. A fast, filtered experiment situated in the TREAT thermal reactor. Number 1 is a 20-group formulation with no upscatter groups, and 2 is a 44-group formulation with 20 upscatter groups ($S_4$, $P$-1).

5. CTR. A shield coupled neutronics-gamma transport problem for a representative fusion reactor configuration (46 groups, $S$-6, $P$-3).
6. SPHERE. A coupled neutron-gamma transport adjoint source problem in spherical geometry (42 groups) (converged to 0.001 for the point fluxes) ($S$-8, $P$-3).

Not all the possible iteration methods were employed with all of these problems because of the excessive computing time involved. Displayed in Table I are the total numbers of iterations required for flux convergence for each of the

TABLE I

One-Dimensional Diffusion Synthetic Acceleration Results Compared with Other Methods*

| Problem | NE | CY | CMR | FMR | DSA | Time Ratio |
|---|---|---|---|---|---|---|
| 1. LMFBR | 1114 | 2 382 | 3133 | [a] | 154 | 0.18 |
| 2. HTGR | --- | 12 000 | 6400 | [a] | 124 | 0.08 |
| 3. TREAT 1 | --- | 5 047 | [a] | [a] | 188 | 0.06 |
| 4. TREAT 2 | --- | --- | --- | --- | 663 | --- |
| 5. CTR | --- | 1 204 | --- | --- | 329 | 0.26 |
| 6. SPHERE | 1879 | --- | [a] | --- | 456 | 0.33 |

*FMR = fine-mesh rebalance
CMR = coarse-mesh rebalance
DSA = diffusion synthetic acceleration
CY = Chebyshev acceleration
NE = no acceleration.
[a] Divergence.

acceleration methods tested. Also displayed is the ratio of the iteration time calculated as the synthetic diffusion acceleration method time divided by the iteration time of the best performer of the other methods used. In running the problems, the preferred iteration strategy for the synthetic diffusion method was used in that one inner iteration was used until the fission and upscatter sources were converged and then the point flux was converged to its convergence criterion by increasing the allowed inner iterations. Because the same strategy does not work for the other methods, the inner iteration limit was chosen at 5 per outer until source convergence and then increased to 10 to 20, depending on the problem. The NON-DSA calculations were performed using a diamond-differenced form of ONETRAN (Ref. 1).

As outlined in Sec. II.A, the base formulation of the synthetic diffusion method for eigenvalue problems is the diffusion coefficient method. With a switch to the removal term method, negative diffusion coefficients are computed at a mesh interval. Very infrequently this switch also results in a removal term for that mesh point that may be sufficiently negative to lead to the calculation of negative diffusion fluxes. When this situation arises (as it does in problem 6), the synthetic acceleration is abandoned and no acceleration is employed for that group.

Examining the results in Table I, one sees that the synthetic diffusion method converges for all of the problems. We see a substantial reduction in the number of iterations needed for convergence particularly for the eigenvalue problems 1 through 4.

We stated in Sec. II that the diffusion synthetic acceleration method can be used as a diffusion improvement scheme. We illustrate this in Table II, where we display the $k_{\text{eff}}$ iteration sequence for the TREAT 1 problem. The first column labels the outer iteration, with the first entry being the conventional diffusion calculation. In the third column, we post the elapsed iteration time for this problem, and in the fourth column we give the percent error in the eigenvalue. In outer iterations 1 and 2, only 1 inner iteration per group was used, and in the third the flux was iterated to convergence. It is seen that the first outer iteration yields a very satisfactory improvement over diffusion theory, and we see this behavior in many of the eigenvalue problems we have performed.

We present some numerical results in Tables III and IV using the two-dimensional diffusion synthetic acceleration method. Table III depicts results for a homogeneous square comprised of a purely scattering material with a $5 \times 5$ mesh, reflective boundary conditions on the left and bottom boundaries, and a flat source. By altering the total cross section, one mesh interval is varied from 1 to 15 mean-free-paths. The results demonstrate the stability of DSA with increasing mesh size. In Table IV we solve a series

TABLE II

Eigenvalue Convergence as a Function of the Outer Iteration

| Outer | $k_{\text{eff}}$ | Time (s) | Error (%) |
|---|---|---|---|
| Diffusion | 1.234-6 | 4.3 | -0.83 |
| 1 | 1.245 1 | 6.5 | 0.01 |
| 2 | 1.244 9 | 8.5 | -0.005 |
| 3 | 1.245 0 | 13.0 | 0.0 |

TABLE III

Total Iterations Using Two-Dimensional Diffusion Synthetic Acceleration for Varying Mesh Size

| Mesh (mfp) | FMR | DSA |
|---|---|---|
| 1 | 12 | 5 |
| 5 | 112 | 6 |
| 15 | 293 | 6 |

TABLE IV

Total Iterations Using Two-Dimensional Diffusion Synthetic Acceleration for Eigenvalue Problems

| Problem | FMR | CMR | DSA |
|---|---|---|---|
| 1 | 48 | --- | 17 |
| 2 | 143 | --- | 24 |
| 3 | 149 | 369 | 80 |

of simple eigenvalue problems. The first two problems are for the homogeneous square problem of Table III with 1 and 2 energy groups. The nine-group problem is a cylindrical reactor with a plutonium core having a radius of 7.62 cm and a half-height of 1.966 cm surrounded by a 7.62-cm depleted uranium reflector. The cross sections are tabulated elsewhere.[18] In these small systems, the inner iteration acceleration is of very little value and the factors of two in iterations over FMR are due to the outer acceleration. We have not posted comparative running times for the two-dimensional problems because the diffusion equation solver in TWOTRAN is presently very inefficient. However, previous experience[14] has shown that the diffusion calculated time is $<10\%$ of the total time; therefore, we expect the iteration time to be proportional to the reduction in the number of iterations for large problems.

## IV. CONCLUSIONS AND RECOMMENDATIONS

In conclusion, we have presented the diffusion synthetic method and demonstrated its effectiveness. In two-dimensional geometries, however, some development is still necessary. In implementation of the diamond equations, negative fluxes can be calculated.[2] TWOTRAN uses a negative flux fixup scheme that violates the diamond equations by which negative fluxes are set to zero. For this case, the compatible diffusion and transport difference equations that we labored so carefully to construct are no longer compatible. We are testing various schemes to efficiently restore this compatibility. Upon correction of this deficiency, the diffusion synthetic acceleration will no doubt serve as a new generation in transport acceleration schemes.

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[18] W. F. MILLER, Jr., "Transport and Reactor Theory July 1-September 30, 1976," LA-6571-PR, Los Alamos Scientific Laboratory (1976).