International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

NEGATIVE FLUX FIXUPS IN DISCONTINOUS FINITE ELEMENT SN TRANSPORT

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ABSTRACT

We introduce a conservative fixup strategy to remedy negative fluxes within a linear discontinuous spatially discretized radiation transport solver. The strategy is similar in principle to the classical set-to-zero fixup used with diamond difference schemes. We also discuss difficulties in creating an effective solver for such an approach and propose a hybrid source iteration/Krylov solver. Numerical results are presented for 2-D test cases.

Key Words: SN Transport, Flux Fixups

1. INTRODUCTION

The appearance of negative fluxes in a solution to the radiation transport equation can be extremely undesirable. When the transport equation is coupled to other equations (e.g. material energy equations), the appearance of negative fluxes can result in the computation of non-physical quantities (negative temperatures) which can cause numerical algorithms to become unstable. Additionally, negative fluxes may interact poorly with commonly used linear acceleration schemes, making their use difficult. Generally some compromise must be worked out between the positivity, accuracy, and linearity of a solution approach. This has been an open issue for a number of years [1] but a suitable compromise has yet to be identified. Schemes have been devised which have a high order of accuracy and are strictly non-negative [2, 3], but such methods are typically highly nonlinear, presenting significant difficulties in the solution process.

There seems to be a general belief in transport literature that negative flux fixups should be avoided because it is supposed that their use will result in a degradation of the accuracy of the underlying scheme (e.g. [4]). We feel that this is a generally unfounded fear because the concept of order of accuracy is only valid in an asymptotic limit as the mesh size is refined. The appearance of negative solutions is an indication that the asymptotic regime has not been reached and so it is quite possible that a method with a lower order of accuracy will yield results closer to the fully resolved solution than will a method with a higher order of accuracy. In this study, we propose a flux fixup for the linear discontinuous finite element method (LDFEM) which is similar to the classical fixup for the diamond difference method. This fixup is intended to counteract negative fluxes which occur due to the inability of the spatial discretization to yield physically meaningful (positive) solutions for a positive source. We do not address issues of negative fluxes which occur due to negative sources arising from truncated anisotropic source expansions. The strategy is conservative in that it preserves particle balance locally and retains the third order accuracy of the standard LDFEM. We feel that this strategy may be very powerful for situations where it is impractical or impossible to fully resolve the spatial domain.

2. TRANSPORT METHODOLOGY

We are interested in solutions to the steady-state one-group discrete ordinates radiation transport equation with isotropic scattering. For a quadrature set denoted by $[\hat{\Omega}_n, w_n]$ with $1 \le n \le N$, total cross-section σ, scattering cross-section σ_s, and known external source q^{ext}, this can be written as

$$\hat{\Omega}_n \cdot \nabla\psi_n + \sigma\psi_n = \sigma_s\phi + q_n^{ext} \tag{1}$$

The subscript n denotes the quantity evaluated at the corresponding quadrature node (e.g. $\psi_n = \psi(\hat{\Omega}_n)$) and will be suppressed where no confusion arises. The scalar flux is given by

$$\phi = \sum_{n=1}^{N} w_n\psi_n \tag{2}$$

For most iterative strategies we will be interested in solving subproblems for which the right hand side of (1) is constant

$$\hat{\Omega} \cdot \nabla\psi + \sigma\psi = q \tag{3}$$

For the spatial discretization in *d* dimensions we consider the linear discontinuous finite element method (LDFEM) in which the angular flux and source term are approximated as linear functions defined on a *d*-simplex (segment, triangle, or tetrahedron for *d*=1,2,3 respectively) denoted by T_i

$$\psi^i(\vec{x}) = \textstyle\sum_{k=0}^{d} \psi_k^i B_k^i(\vec{x}) \tag{4}$$

$$q^i(\vec{x}) = \textstyle\sum_{k=0}^{d} q_k^i B_k^i(\vec{x}) \tag{5}$$

The basis functions are the standard d-dimensional Lagrange polynomials given by

$$B_k^i(\vec{x}) = \begin{cases} \prod_{j\neq k} \frac{(\vec{x}-\vec{x}_j)}{(\vec{x}_k-\vec{x}_j)} & \vec{x} \in T_i \\ 0 & otherwise \end{cases} \tag{6}$$

The basis functions have the property that $\sum_{k=0}^{d} B_k(\vec{x}) = 1$ within any cell. Discrete equations are obtained by multiplying equation (3) by each of the (*d*+*1*) basis functions for a given spatial cell T_i and integrating over the volume

$$\int_{T_i} B_k(\vec{x})[\hat{\Omega} \cdot \nabla\psi + \sigma\psi = q]dV \quad 0 \le k \le d \tag{7}$$

The values of the angular flux are allowed to be discontinuous at cell boundaries and coupling between cells is achieved by integrating the first (streaming) term by parts (applying Green's theorem in higher dimensions) and evaluating the resulting boundary term according to its upwind value. Due to the fact that each basis function is non-zero in only a single cell, each equation defined by equation (7) contains as unknowns only the (*d+1*) fluxes which are non-zero in the cell of interest plus a small number of fluxes from neighboring cells which contribute via the boundary term. This guarantees that when the resulting system is written in matrix form the corresponding matrices will be sparsely populated. We write this matrix equation as

$$(L - MSD)\psi = q^{ext} \tag{8}$$

Here q is again the external source, L represents the discrete streaming plus collision operator, S is the scattering matrix, D and M are angular restriction and prolongation operators, respectively. The scalar flux is related to the angular flux via $\phi = D\psi$, simply the operator notation for equation (2). Multiplying equation (8) by DL^{-1} yields the integral form of the transport equation which has only the scalar fluxes as unknowns

$$(I - DL^{-1}MS)\phi = DL^{-1}q \tag{9}$$

A commonly used solution strategy is performing a Richardson iteration on equation (9). For an iteration index k, this iteration can be written as

$$\phi^{k+1} = DL^{-1}(MS\phi^{k} + q) \tag{10}$$

and is commonly referred to as source iteration [8]. It can be shown that source iteration is guaranteed to converge provided that the scattering ratio $c \equiv \frac{\sigma_s}{\sigma}$ is strictly less than unity. However, for scattering ratios very close to 1, convergence may be unacceptably slow and alternative methods must be used. One possibility is to use diffusion-synthetic acceleration (DSA) as a preconditioner to source iteration [9]. Another option is to apply Krylov subspace methods such as GMRES [10] to equation (9). The use of Krylov subspace methods require only the action of the matrix on the left hand side of (9) multiplying a given vector at each iteration. Because the computational effort of either one source iteration or one matrix-vector multiply is dominated by the cost of applying L^{-1} the cost of one iteration of a Krylov method is essentially identical to that of a single source iteration.

3. REMEDIES FOR NEGATIVE FLUXES

One commonly used approach to mitigating the occurrence of negative fluxes is to resort to lumping procedures. Finite element lumping amounts to moving selected off-diagonal matrix entries onto the diagonal, resulting in an increase in the positivity of the resulting solution at a cost of a reduction in the order of accuracy. Standard techniques involve lumping only the finite element mass matrix which impacts the collisional and source terms. More recent generalized lumping procedures also allow for the lumping of surface gradient terms [6]. Lumping procedures can be effective for some problems, but still do not guarantee a non-negative solution. Furthermore, the use of lumping reduces the order of accuracy of the method across the entire problem domain, negatively impacting the solution in regions of the domain where the solution is sufficiently well-behaved.

As an alternative to lumping procedures, we propose a technique to eliminate negative fluxes which is similar in spirit to the classical fixup for the diamond difference discretization (see p.

134 of [4]). In the course of a transport sweep, the solution for a given spatial cell is first calculated using the standard LDFEM. When a negative flux is encountered it is immediately set to zero and the remaining flux(es) within the cell are recalculated from a balance equation:

$$\int_{T_i} [\hat{\Omega} \cdot \nabla \psi + \sigma \psi = q] dV \tag{11}$$

Because the sum of the basis functions is identically equal to 1, this balance equation is automatically satisfied for the standard LDFEM. However, when one flux is set to zero it becomes necessary to explicity enforce a balance condition. In 1-D, enforcing equation 11 is sufficient to uniquely determine the solution within a cell. In 2-D, however, an additional degree of freedom remains and an additional condition is therefore required. One possibility for this condition is to preserve the ratio of the non-negative fluxes from the LDFEM solution. To clarify, let the angular fluxes computed by the LDFEM be denoted by $\tilde{\psi}_{i,j,k}$ and the angular fluxes computed by the fixup by $\psi_{i,j,k}$ and assume that $\tilde{\psi}_i < 0$ and $\tilde{\psi}_{j,k} > 0$. Then in addition to condition (11), the following condition is also enforced:

$$\psi_j / \psi_k = \tilde{\psi}_j / \tilde{\psi}_k \tag{12}$$

Because both quantities on the right are assumed to be positive, the fixed-up quantities will also be positive. This condition seeks to retain some information from the LDFEM solution with the hopes that more accuracy will be attained. Specifically, it guarantees the continuity of the discretization, that is at the threshold where the fixup is first activated (i.e. when $\psi_i \equiv 0$), standard LDFEM and the fixup produce the same solution. We note that as the spatial mesh is refined, the negative fluxes will eventually disappear and the discretization therefore becomes identical to LDFEM. Thus, the discretization suggested here has the same asymptotic accuracy as LDFEM. This method is guaranteed to produce non-negative fluxes in 1-D and 2-D provided that the incident flux and source terms are non-negative. In 2-D, if two angular fluxes become negative in a cell then they should each be set to zero and the remaining flux determined by equation (11).

4. SOLUTION STRATEGIES

We can write the discretized transport equation with flux fixups in a form analogous to equation (9):

$$(I - D\tilde{L}^{-1}MS)\phi = D\tilde{L}^{-1}q \tag{13}$$

Here, $\tilde{L}$ is not a single matrix (thought at each iteration it can be represented by a matrix), but rather the result of applying the fixup strategy to a given vector. One possible solution approach for this nonlinear equation is to define an iteration equivalent to source iteration. We write this iteration as

$$\phi^{k+1} = D\tilde{L}^{-1}(MS\phi^k + q) \tag{14}$$

This iteration is simply a nonlinear fixed point iteration, commonly called a Picard iteration [7]. In the absence of negative fluxes, iteration (14) reduces to the standard source iteration and we therefore expect the convergence behavior to be similar. In particular, it is expected that convergence will be quite slow for problems which contain materials with scattering ratios approaching unity.

Due to the nonlinearity of the fixups, a Krylov subspace method cannot be directly applied to equation (13). With the aim of achieving some of the benefit of a Krylov method, we propose a hybrid source iteration/Krylov approach. This approach consists of alternating between a few iterations of source iteration and a few iterations of a Krylov method (applied to a linearized system). If we let k and p be the number of source and Krylov iterations, respectively, per outer iteration and ϵ be the stopping tolerance, we can write the hybrid algorithm as follows.

```
for iter = 1 : maxiter do
    φ̂^0 = φ^iter
    for i = 1 : k do
        φ̂^i = D L̃^{-1}(M S φ̂^{i-1} + q)
    end
    if ||φ̂^k − φ̂^{k-1}|| < ε then
        φ = φ̂^k
    end
    φ^{iter+1} = GMRES((I − D[L̃(φ̂^k)]^{-1} M S), D[L̃(φ̂^k)]^{-1} q, p)
end
```

Algorithm 1: Hybrid SI/Krylov Method

In this algorithm, $[\tilde{L}(\hat{\phi}^k)]$ indicates that the transport operator used in the Krylov method (GMRES here) is a linearized version which is fixed based on the value produced by the source iterations. Because the nonlinear function defined by equation 13 is actually piecewise linear, this linearized version is obtained quite easily. It consists of storing the locations where flux fixups are applied during the source iteration and applying the exact same fixups during the Krylov solve. During early iterations, it is necessary to solve linearized systems which may differ considerably from the system near the solution. Therefore, it makes little sense to solve these systems to a high level of accuracy. An adaptive inner tolerance which is proportional to the current (nonlinear) residual seems to be an appropriate choice.

5. RESULTS

Figure (1) shows the effect of applying the flux fixup for a uniform medium with an isotropic source on the left boundary and vacuum boundaries on all other sides. The resolved solution contains 3858 triangles whereas the three unresolved solutions are on the same 150 triangle mesh. All solutions utilize an S_4 LQ_n angular quadrature. The behavior of the standard LDFEM is quite erratic and oscillatory for this problem. The lumped LDFEM manages to eliminate the oscillations and the negative fluxes, but the rate of attenuation across the domain is not consistent with the resolved solution. The solution with a fixup, however, is positive, non-oscillatory, and exhibits an attenuation rate which very nearly matches that of the resolved solution.

Figure (2) displays the impact of the flux fixup on problem with difficulties of a different nature. A unit source is placed on the lower boundary in only a single direction (a direction of 45 degrees in the first quadrant) and the entire domain is a void. The analytic solution to this problem is a constant value of 1 in the lower right portion of the domain and a constant value of 0 in the upper left. As shown in the figure, the unlumped LDFEM solution displays oscillations which propagate perpendicular to the direction of streaming. The lumped LDFEM displays significantly damped oscillations, though they are still quite evident and significant negative fluxes still appear. For the solution with the fixup, no oscillations are present. A significant flux still permeates into the

Table I. Error Norms for Solution Strategies

	Unlumped DFEM	Lumped DFEM	Fixup
Problem 1	0.1339	0.1021	0.0902
Problem 2	0.0983	0.0890	0.0929

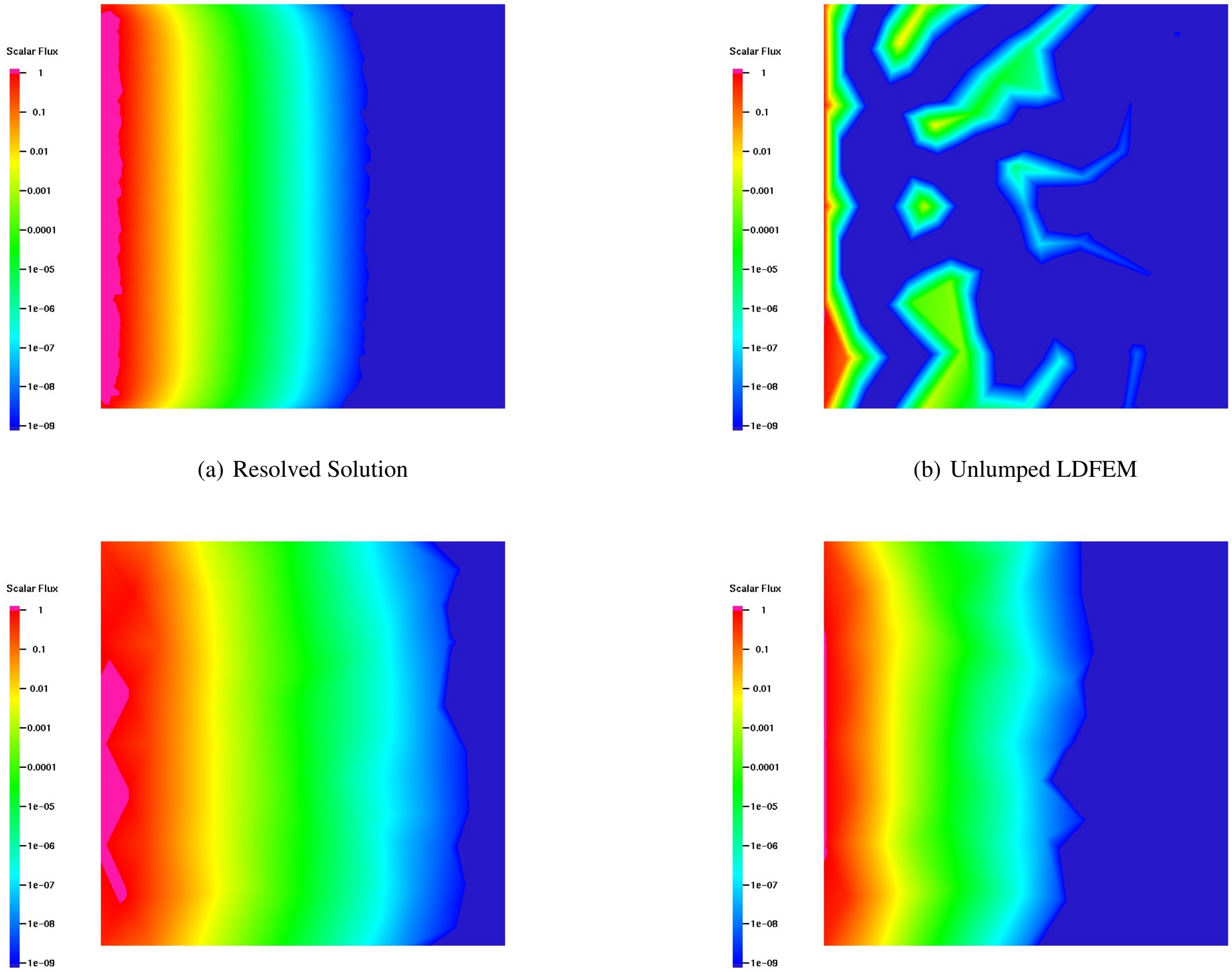
upper left portion of the domain, but this occurs in a smooth, monotonic manner rather than the erratic behavior seen in the other solutions.

Table I displays a measure of the error for the different solution approaches for the two problems previously described. For problem 1, this measure is the 2-norm of the difference between the given solution and the refined solution evaluated at the same points. We see that the fixup approach is the most accurate according to this error measure. In fact, the fixed-up solution was more accurate than the standard LDFEM at 79 of the 88 nodes in the problem and more accurate than the lumped LDFEM at 85 of the 88 nodes. For problem 2, the error measure is the 2-norm of the difference between the given solution and the analytic solution. The fixup strategy is again more accurate than the standard LDFEM, although in this case the lumped approach slightly outperforms the fixup in this error measure. However, we still find that the fixup approach yields a better solution at a larger number of nodes, beating out the standard LDFEM at 3114 of the 3938 nodes and besting the lumped LDFEM at 3260 nodes.

Table II shows the computational effort required by various solution strategies for a variety of problems. Problem 3 is a 1-D slab consisting of uniform elements of width 8 cm with total cross section 1 and scattering ratio 0.7. Problem 4 is the same as problem 1 except the mesh width is 64 cm and the scattering ratio is 0.99. Problem 5 is the same scenario as shown in figure 1. Problem 6 is identical to problem 3 with the scattering ratio changed to 0.99. The results for methods without a flux fixup are provided to illustrate the amount of improvement that can be obtained through the use of Krylov methods, but in all cases these solutions contain negative fluxes and would be deemed unsatisfactory for our purposes. Just as the use of Krylov methods on a standard linear discretization provides a great improvement in computational effort for highly scattering problems, the hybrid approach which we have proposed also seems to show a fairly dramatic reduction in computational cost for highly scattering problems. The effect is not quite so dramatic as that seen with a Krylov on the original linear system, but nonetheless a significant gain is experienced.

6. SUMMARY

We have proposed a negative flux fixup strategy for a linear discontinuous finite element solver. The fixup preserves particle balance and reverts to the standard discretization in the absence of



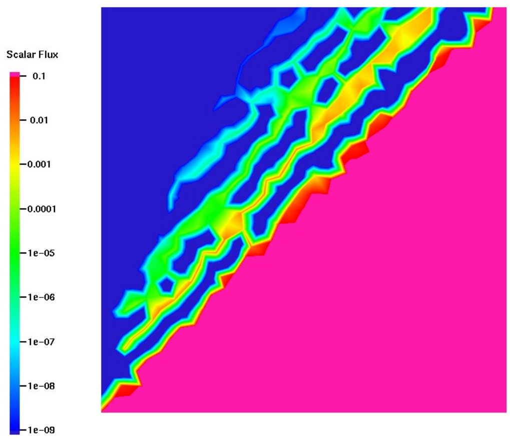
(a) Resolved Solution (b) Unlumped LDFEM

(c) Lumped LDFEM (d) Unlumped w/Fixup

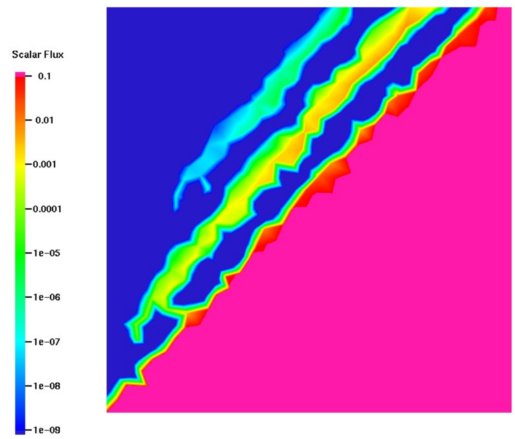
Figure 1. Solutions for Boundary Source Problem on $[0,1]^2$. $\sigma = 40,\ c = 0.7$

Table II. Matrix-Vector Multiplies Required for Convergence

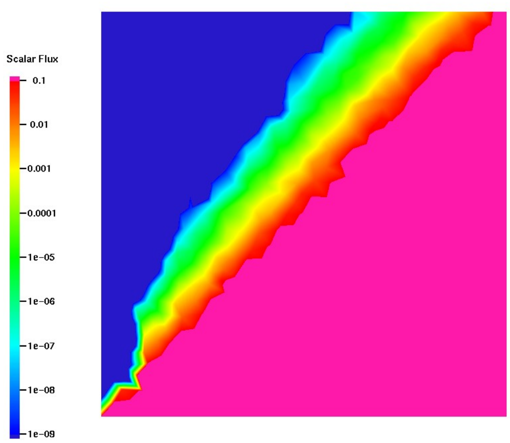
	No Fixup			With Fixup	
	SI w/o Fix	GMRES	GMRES(10)	SI w/Fix	Hybrid
Problem 3	55	16	19	49	25
Problem 4	1569	44	46	744	91
Problem 5	51	16	18	48	39
Problem 6	1218	51	76	1211	246



(a) Unlumped LDFEM



(b) Lumped LDFEM



(c) Unlumped w/Fixup

Figure 2. Solutions for Ray Streaming Problem on $[0, 1]^2$. Material is void everywhere.

negative solutions. Preliminary numerical tests suggest that the fixup introduces no appreciable degradation in the solution accuracy and may in fact improve the accuracy for certain problems. At a minimum it produces a solution which is physically meaningful (non-negative and conservative) and more qualitatively pleasing (free of non-physical oscillations) than a solution without the fixup.

Though an inherently nonlinear process, we have suggested an iterative process which allows for the use of Krylov methods to speed up the nonlinear iterations. Though rigorous proof of stability is not available currently, numerical experiments indicate that it is indeed stable. Further work is necessary to refine the method into a more practical strategy. Another issue which has not yet been addressed is the compatibility of the fixup strategy with common acceleration schemes such as diffusion synthetic acceleration. A reasonable compatibility with acceleration schemes could significantly reduce the computational effort required and make for a more viable solution approach.

ACKNOWLEDGEMENTS

The authors would like to thank Jim Morel of Texas A&M University for the beneficial conversations which aided in the development of this paper. The work of the primary author was supported by a Department of Energy Computational Science Graduate Fellowship.

REFERENCES

[1] K.D. Lathrop. *Spatial Differencing of the Transport Equation: Positivity vs. Accuracy.* Journal of Computational Physics 4, 475-498 (1969).

[2] Todd A. Wareing. *An Exponential Discontinuous Scheme for Discrete-Ordinate Calculations in Cartesian Geometries.* Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications, Saratoga Springs, NY, 6-10 Oct 1997.

[3] Wallace F. Walters and Todd A. Wareing. *A Nonlinear Positive Method for Solving the Transport Equation on Course Meshes.* 8th International Conference on Radiation Shielding, Austin, TX, 24-27 April 1994.

[4] E.E. Lewis and W.F. Miller, Jr. *Computational Methods of Neutron Transport.* American Nuclear Society, La Grange Park, 1993.

[5] W. H. Reed and T. R. Hill. *Triangular Mesh Methods for the Neutron Transport Equation.* Tech Report LA-UR-73-479, Los Alamos Scientific Laboratory (1973).

[6] James S. Warsa. *A Continuous Finite Element-Based, Discontinuous Finite Element Method for S_N Transport.* Nuclear Science and Engineering 160, 1-16 (2008).

[7] C. T. Kelley. *Iterative Methods for Linear and Nonlinear Equations*. Frontiers in Applied Mathematics Vol. 16. SIAM: Philadelphia (1995).

[8] Anne Greenbaum. *Iterative Methods for Solving Linear Systems.* Frontiers in Applied Mathematics Vol. 17. SIAM: Philadelphia (1997).

[9] E. W. Larsen. *Unconditionally Stable Diffusion-Synthetic Acceleration Methods for the Slab Geometry Discrete Ordinates Equations. Part I: Theory.* Nuclear Sci. Eng. 82, 47-63 (1982).

[10] Y. Saad and M. H. Schultz. *GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems.* SIAM J. Sci. Stat. Comput. 7, 856-869 (1986).